



Full wwPDB EM Validation Report ⓘ

Sep 8, 2025 – 12:55 PM EDT

PDB ID : 9NGU / pdb_00009ngu
EMDB ID : EMD-49393
Title : In situ cryo-EM structure of outer membrane cap (OMC) of the Legionella Dot/Icm T4SS machine
Authors : Yue, J.; Jun, L.
Deposited on : 2025-02-22
Resolution : 2.96 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

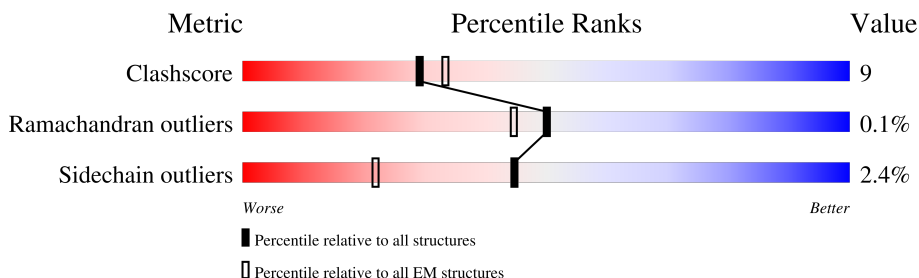
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Aa	163	
1	Ae	163	
1	Ak	163	
1	Ao	163	
1	Au	163	
1	Ay	163	
1	Be	163	
1	Bi	163	







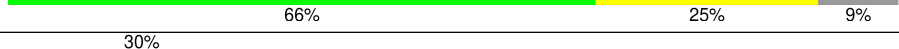
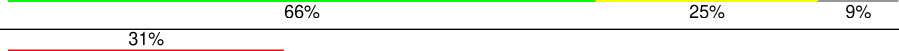
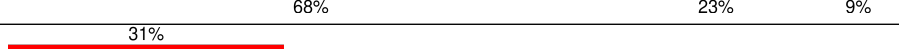
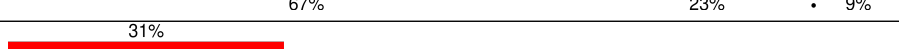
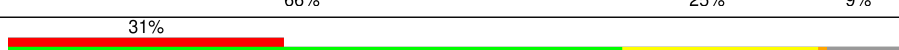

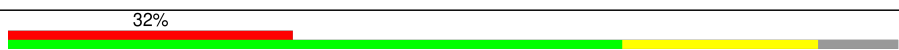

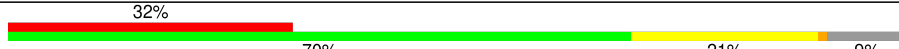





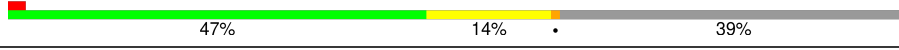




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Mol	Chain	Length	Quality of chain
1	Bo	163	
1	Bs	163	
1	By	163	
1	Cc	163	
1	Ci	163	
1	Cm	163	
1	Cs	163	
1	Cw	163	
1	Dc	163	
1	Dg	163	
1	Dm	163	
1	Dq	163	
1	Dw	163	
1	Ea	163	
1	Eg	163	
1	Ek	163	
1	Eq	163	
1	Eu	163	
2	Ab	189	
2	Al	189	
2	Av	189	
2	Bf	189	
2	Bp	189	
2	Bz	189	
2	Cj	189	




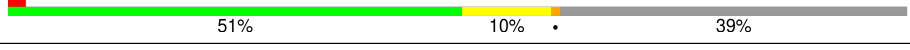
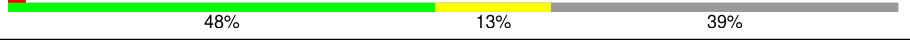

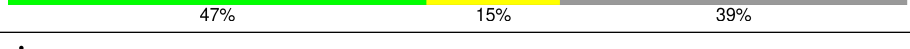
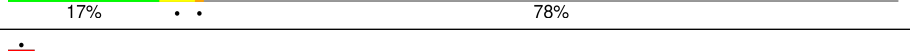
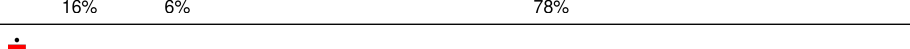
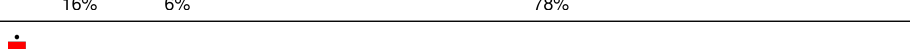















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Mol	Chain	Length	Quality of chain
2	Ct	189	
2	Dd	189	
2	Dn	189	
2	Dx	189	
2	Eh	189	
2	Er	189	
3	Ac	320	
3	Am	320	
3	Aw	320	
3	Bg	320	
3	Bq	320	
3	Ca	320	
3	Ck	320	
3	Cu	320	
3	De	320	
3	Do	320	
3	Dy	320	
3	Ei	320	
3	Es	320	
4	Ad	124	
4	An	124	
4	Ax	124	
4	Bh	124	
4	Br	124	
4	Cb	124	


























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Mol	Chain	Length	Quality of chain
4	Cl	124	
4	Cv	124	
4	Df	124	
4	Dp	124	
4	Dz	124	
4	Ej	124	
4	Et	124	
5	Af	269	
5	Ap	269	
5	Az	269	
5	Bj	269	
5	Bt	269	
5	Cd	269	
5	Cn	269	
5	Cx	269	
5	Dh	269	
5	Dr	269	
5	Eb	269	
5	El	269	
5	Ev	269	
6	Ag	361	
6	Aq	361	
6	Ba	361	
6	Bk	361	
6	Bu	361	

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Mol	Chain	Length	Quality of chain
6	Ce	361	
6	Co	361	
6	Cy	361	
6	Di	361	
6	Ds	361	
6	Ec	361	
6	Em	361	
6	Ew	361	
7	Ah	249	
7	Ar	249	
7	Bb	249	
7	Bl	249	
7	Bv	249	
7	Cf	249	
7	Cp	249	
7	Cz	249	
7	Dj	249	
7	Dt	249	
7	Ed	249	
7	En	249	
7	Ex	249	
8	Ai	303	
8	As	303	
8	Bc	303	
8	Bm	303	

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Mol	Chain	Length	Quality of chain
8	Bw	303	
8	Cg	303	
8	Cq	303	
8	Da	303	
8	Dk	303	
8	Du	303	
8	Ee	303	
8	Eo	303	
8	Ey	303	
9	Aj	93	
9	At	93	
9	Bd	93	
9	Bn	93	
9	Bx	93	
9	Ch	93	
9	Cr	93	
9	Db	93	
9	Dl	93	
9	Dv	93	
9	Ef	93	
9	Ep	93	
9	Ez	93	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 147498 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DotD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Ae	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Ak	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Ao	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Au	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Ay	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Be	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Bi	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Bo	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Bs	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	By	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Cc	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Ci	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Cm	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Cs	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Cw	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Dc	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Dg	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Dm	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Dq	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Dw	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Ea	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Eg	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Ek	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Eq	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Eu	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		

- Molecule 2 is a protein called LphA (DotK).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Al	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Av	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Bf	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Bp	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Bz	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Cj	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Ct	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Dd	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Dn	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Dx	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Eh	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Er	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		

- Molecule 3 is a protein called Putative auto-transporter adhesin head GIN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ac	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Am	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Aw	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Bg	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Bq	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Ca	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Ck	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Cu	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	De	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Do	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Dy	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Ei	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Es	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		

- Molecule 4 is a protein called Neurogenic locus notch protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ad	76	Total	C	N	O	S	0	0
			565	347	96	109	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	An	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Ax	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Bh	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Br	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Cb	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Cl	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Cv	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Df	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Dp	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Dz	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Ej	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Et	76	Total 565	C 347	N 96	O 109	S 13	0	0

- Molecule 5 is a protein called IcmG (DotF).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Af	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Ap	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Az	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Bj	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Bt	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Cd	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Cn	59	Total 449	C 290	N 77	O 81	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Cx	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
5	Dh	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
5	Dr	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
5	Eb	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
5	El	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
5	Ev	59	Total	C	N	O	S	0	0
			449	290	77	81	1		

- Molecule 6 is a protein called IcmK (DotH).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Ag	91	Total	C	N	O	S	0	0
			691	440	121	126	4		
6	Aq	91	Total	C	N	O	S	0	0
			691	440	121	126	4		
6	Ba	91	Total	C	N	O	S	0	0
			691	440	121	126	4		
6	Bk	91	Total	C	N	O	S	0	0
			691	440	121	126	4		
6	Bu	91	Total	C	N	O	S	0	0
			691	440	121	126	4		
6	Ce	91	Total	C	N	O	S	0	0
			691	440	121	126	4		
6	Co	91	Total	C	N	O	S	0	0
			691	440	121	126	4		
6	Cy	91	Total	C	N	O	S	0	0
			691	440	121	126	4		
6	Di	91	Total	C	N	O	S	0	0
			691	440	121	126	4		
6	Ds	91	Total	C	N	O	S	0	0
			691	440	121	126	4		
6	Ec	91	Total	C	N	O	S	0	0
			691	440	121	126	4		
6	Em	91	Total	C	N	O	S	0	0
			691	440	121	126	4		
6	Ew	91	Total	C	N	O	S	0	0
			691	440	121	126	4		

- Molecule 7 is a protein called Outer membrane protein, OmpA family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ah	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Ar	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Bb	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Bl	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Bv	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Cf	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Cp	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Cz	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Dj	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Dt	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Ed	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	En	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Ex	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		

- Molecule 8 is a protein called DotC.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ai	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	As	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Bc	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Bm	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Bw	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Cg	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	Cq	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Da	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Dk	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Du	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Ee	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Eo	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Ey	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		

- Molecule 9 is a protein called Secreted protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Aj	71	Total	C	N	O	S	0	0
			562	355	93	109	5		
9	At	71	Total	C	N	O	S	0	0
			562	355	93	109	5		
9	Bd	71	Total	C	N	O	S	0	0
			562	355	93	109	5		
9	Bn	71	Total	C	N	O	S	0	0
			562	355	93	109	5		
9	Bx	71	Total	C	N	O	S	0	0
			562	355	93	109	5		
9	Ch	71	Total	C	N	O	S	0	0
			562	355	93	109	5		
9	Cr	71	Total	C	N	O	S	0	0
			562	355	93	109	5		
9	Db	71	Total	C	N	O	S	0	0
			562	355	93	109	5		
9	Dl	71	Total	C	N	O	S	0	0
			562	355	93	109	5		
9	Dv	71	Total	C	N	O	S	0	0
			562	355	93	109	5		
9	Ef	71	Total	C	N	O	S	0	0
			562	355	93	109	5		
9	Ep	71	Total	C	N	O	S	0	0
			562	355	93	109	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ez	71	Total	C	N	O	S	0	0
			562	355	93	109	5		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aj	43	ALA	GLY	conflict	UNP A0AAN5PM39
Aj	44	SER	ALA	conflict	UNP A0AAN5PM39
Aj	46	LEU	SER	conflict	UNP A0AAN5PM39
At	43	ALA	GLY	conflict	UNP A0AAN5PM39
At	44	SER	ALA	conflict	UNP A0AAN5PM39
At	46	LEU	SER	conflict	UNP A0AAN5PM39
Bd	43	ALA	GLY	conflict	UNP A0AAN5PM39
Bd	44	SER	ALA	conflict	UNP A0AAN5PM39
Bd	46	LEU	SER	conflict	UNP A0AAN5PM39
Bn	43	ALA	GLY	conflict	UNP A0AAN5PM39
Bn	44	SER	ALA	conflict	UNP A0AAN5PM39
Bn	46	LEU	SER	conflict	UNP A0AAN5PM39
Bx	43	ALA	GLY	conflict	UNP A0AAN5PM39
Bx	44	SER	ALA	conflict	UNP A0AAN5PM39
Bx	46	LEU	SER	conflict	UNP A0AAN5PM39
Ch	43	ALA	GLY	conflict	UNP A0AAN5PM39
Ch	44	SER	ALA	conflict	UNP A0AAN5PM39
Ch	46	LEU	SER	conflict	UNP A0AAN5PM39
Cr	43	ALA	GLY	conflict	UNP A0AAN5PM39
Cr	44	SER	ALA	conflict	UNP A0AAN5PM39
Cr	46	LEU	SER	conflict	UNP A0AAN5PM39
Db	43	ALA	GLY	conflict	UNP A0AAN5PM39
Db	44	SER	ALA	conflict	UNP A0AAN5PM39
Db	46	LEU	SER	conflict	UNP A0AAN5PM39
Dl	43	ALA	GLY	conflict	UNP A0AAN5PM39
Dl	44	SER	ALA	conflict	UNP A0AAN5PM39
Dl	46	LEU	SER	conflict	UNP A0AAN5PM39
Dv	43	ALA	GLY	conflict	UNP A0AAN5PM39
Dv	44	SER	ALA	conflict	UNP A0AAN5PM39
Dv	46	LEU	SER	conflict	UNP A0AAN5PM39
Ef	43	ALA	GLY	conflict	UNP A0AAN5PM39
Ef	44	SER	ALA	conflict	UNP A0AAN5PM39
Ef	46	LEU	SER	conflict	UNP A0AAN5PM39
Ep	43	ALA	GLY	conflict	UNP A0AAN5PM39
Ep	44	SER	ALA	conflict	UNP A0AAN5PM39
Ep	46	LEU	SER	conflict	UNP A0AAN5PM39

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Chain	Residue	Modelled	Actual	Comment	Reference
Ez	43	ALA	GLY	conflict	UNP A0AAN5PM39
Ez	44	SER	ALA	conflict	UNP A0AAN5PM39
Ez	46	LEU	SER	conflict	UNP A0AAN5PM39

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

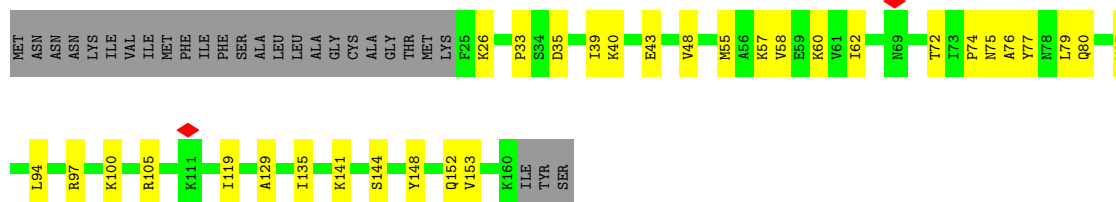
• Molecule 1: DotD

Chain Aa: 



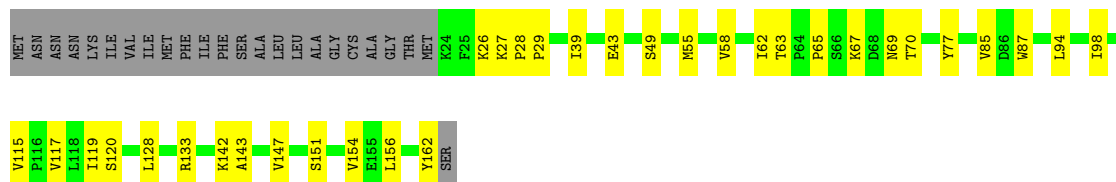
• Molecule 1: DotD

Chain Ae: 



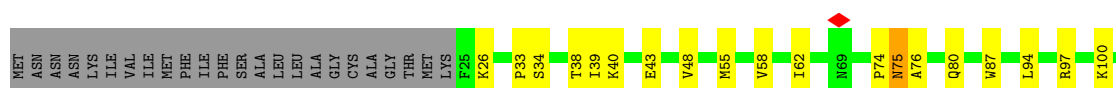
• Molecule 1: DotD

Chain Ak: 



• Molecule 1: DotD

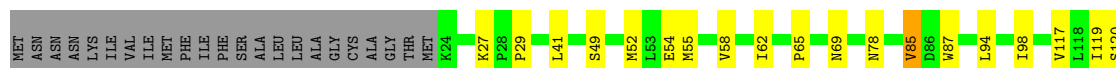
Chain Ao: 





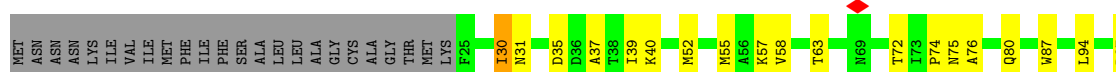
- Molecule 1: DotD

Chain Au: 69% 16% 15%



- Molecule 1: DotD

Chain Ay: 63% 20% 17%



- Molecule 1: DotD

Chain Be: 64% 20% 15%



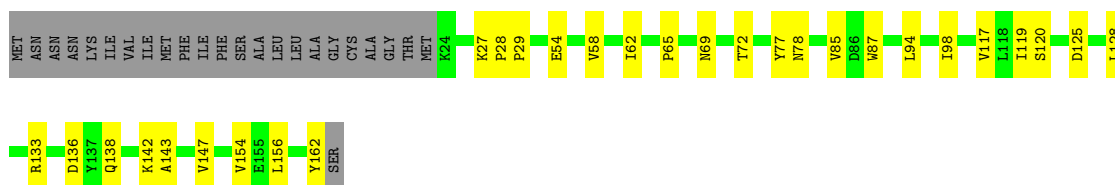
- Molecule 1: DotD

Chain Bi: 63% 19% 17%

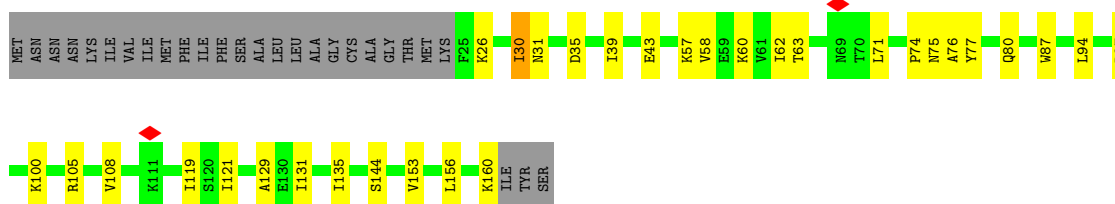


- Molecule 1: DotD

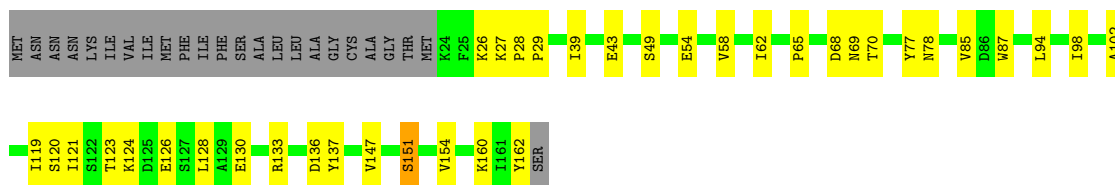
Chain Bo: 67% 18% 15%



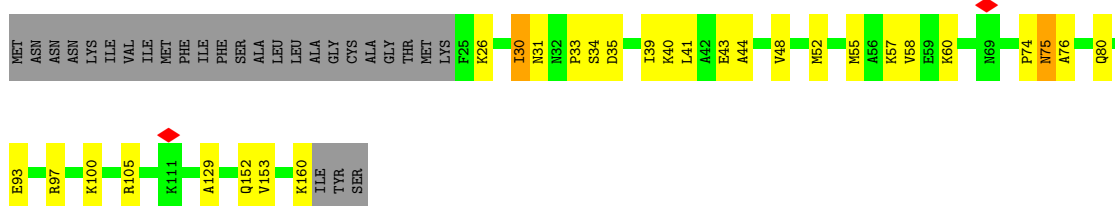
• Molecule 1: DotD



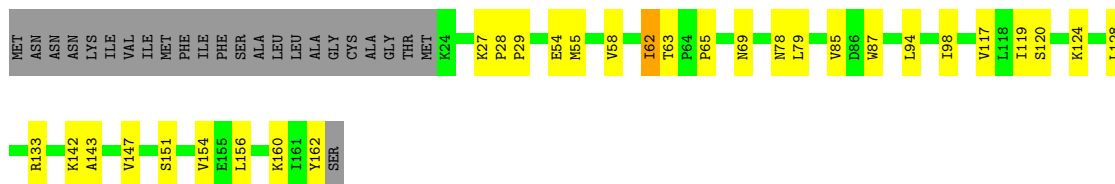
• Molecule 1: DotD



• Molecule 1: DotD

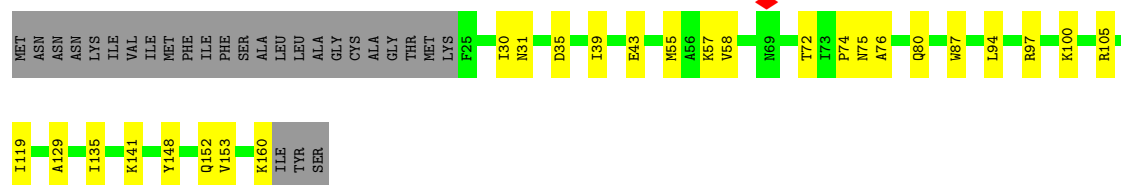


• Molecule 1: DotD



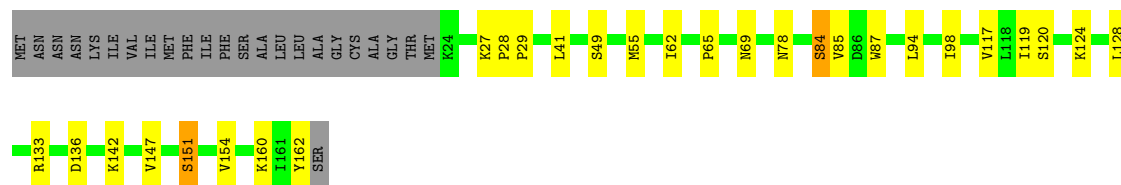
• Molecule 1: DotD

Chain Cm: 



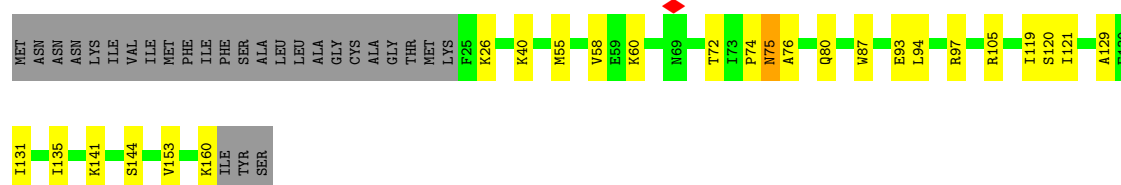
• Molecule 1: DotD

Chain Cs: 



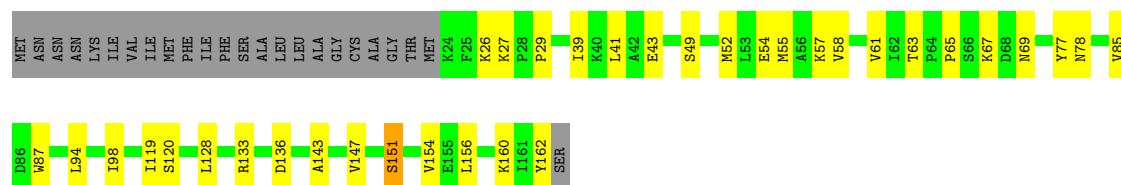
• Molecule 1: DotD

Chain Cw: 



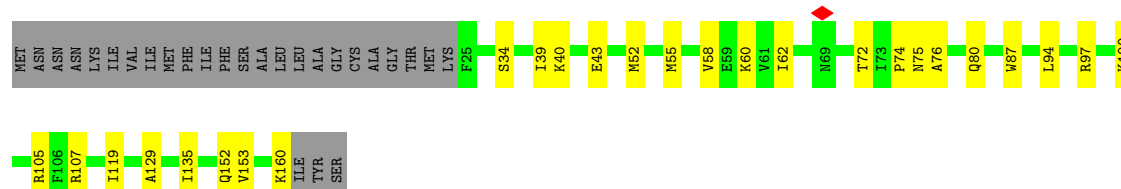
• Molecule 1: DotD

Chain Dc: 



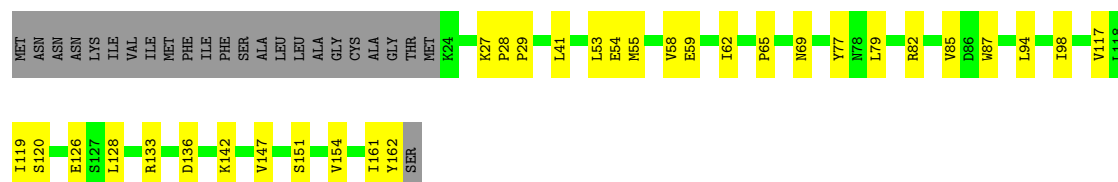
• Molecule 1: DotD

Chain Dg: 



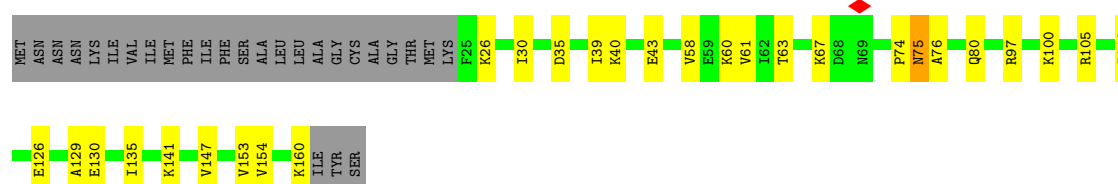
- Molecule 1: DotD

Chain Dm:  66% 20% 15%



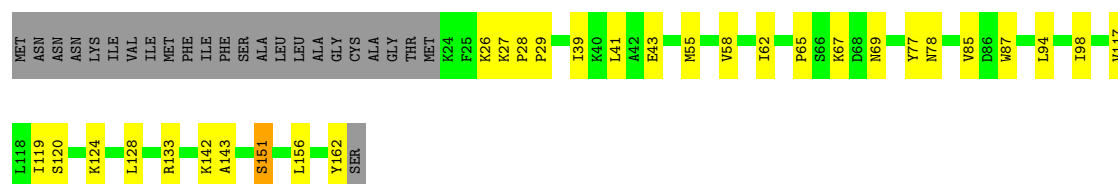
- Molecule 1: DotD

Chain Dq:  66% 17% 17%



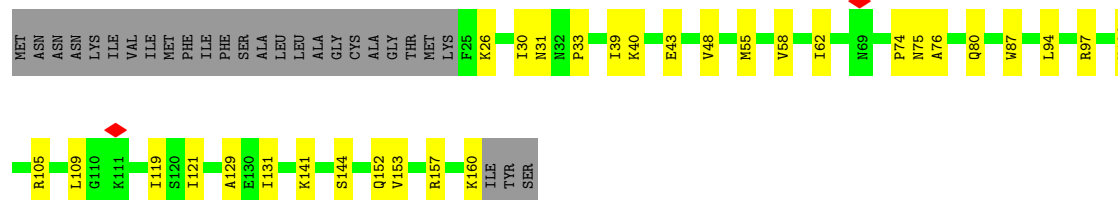
- Molecule 1: DotD

Chain Dw:  67% 18% 15%



- Molecule 1: DotD

Chain Ea:  64% 19% 17%



- Molecule 1: DotD

Chain Eg:  63% 22% 15%





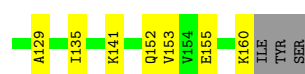
- Molecule 1: DotD



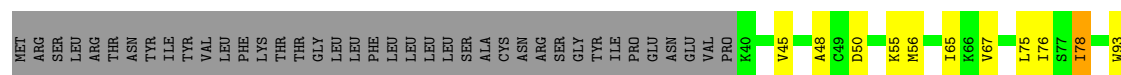
- Molecule 1: DotD



- Molecule 1: DotD

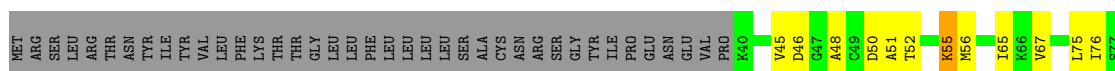


- Molecule 2: LphA (DotK)

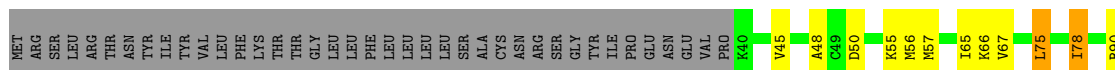


- Molecule 2: LphA (DotK)

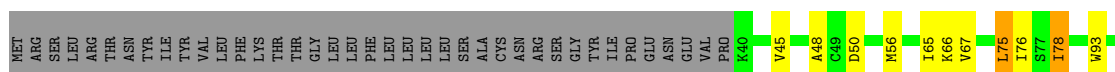




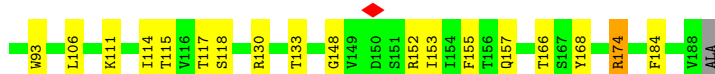
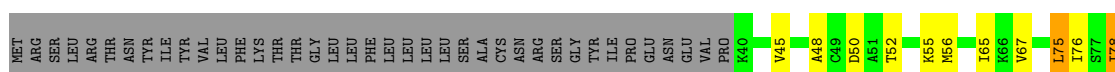
• Molecule 2: LphA (DotK)



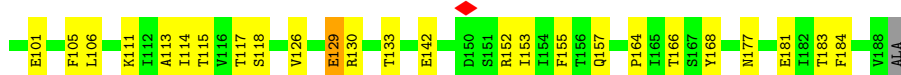
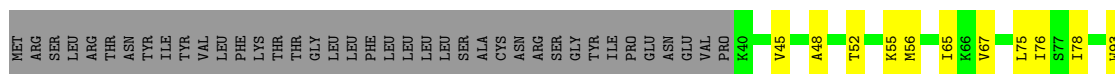
• Molecule 2: LphA (DotK)



• Molecule 2: LphA (DotK)

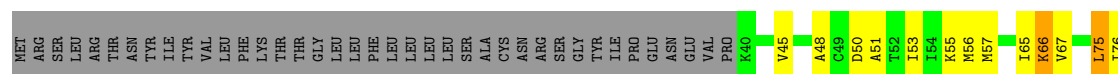


• Molecule 2: LphA (DotK)



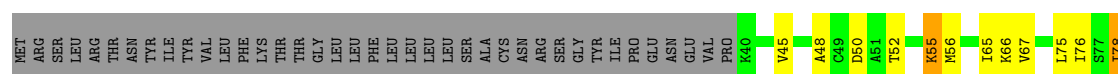
- Molecule 2: LphA (DotK)

Chain Cj: 



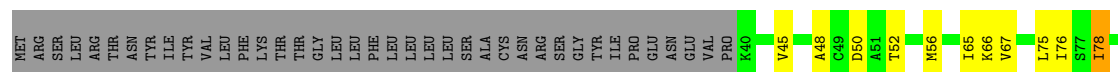
- Molecule 2: LphA (DotK)

Chain Ct: 



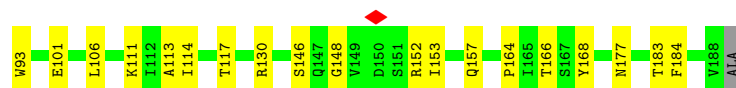
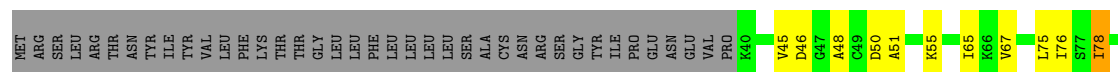
- Molecule 2: LphA (DotK)

Chain Dd: 



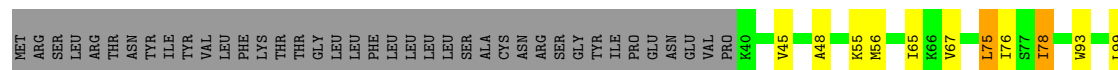
- Molecule 2: LphA (DotK)

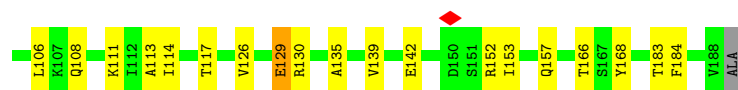
Chain Dn: 



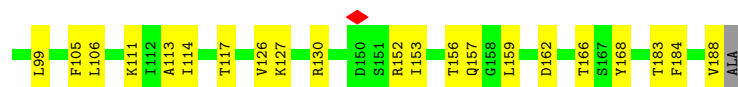
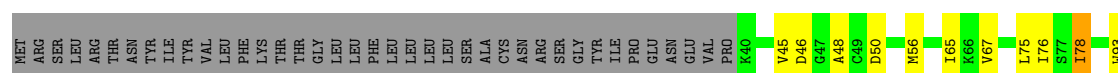
- Molecule 2: LphA (DotK)

Chain Dx: 

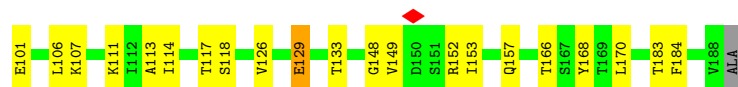
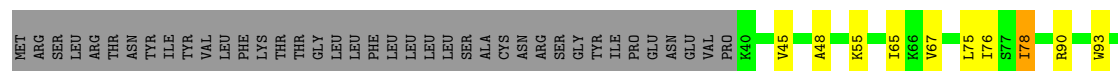




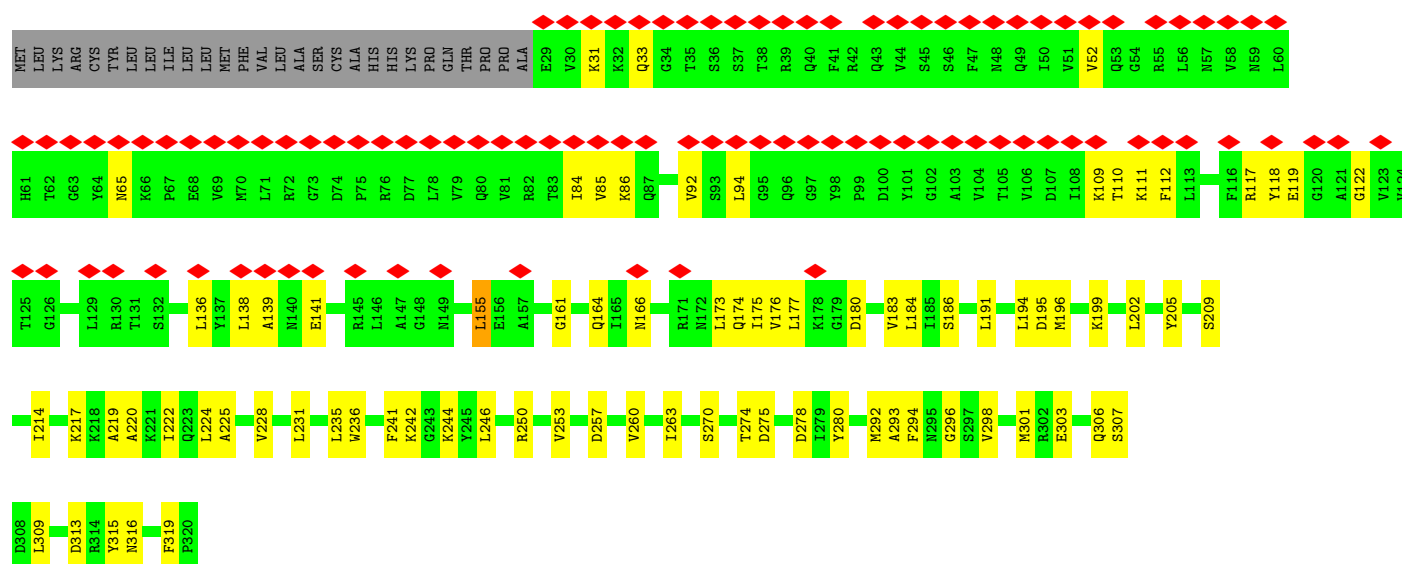
• Molecule 2: LphA (DotK)



• Molecule 2: LphA (DotK)

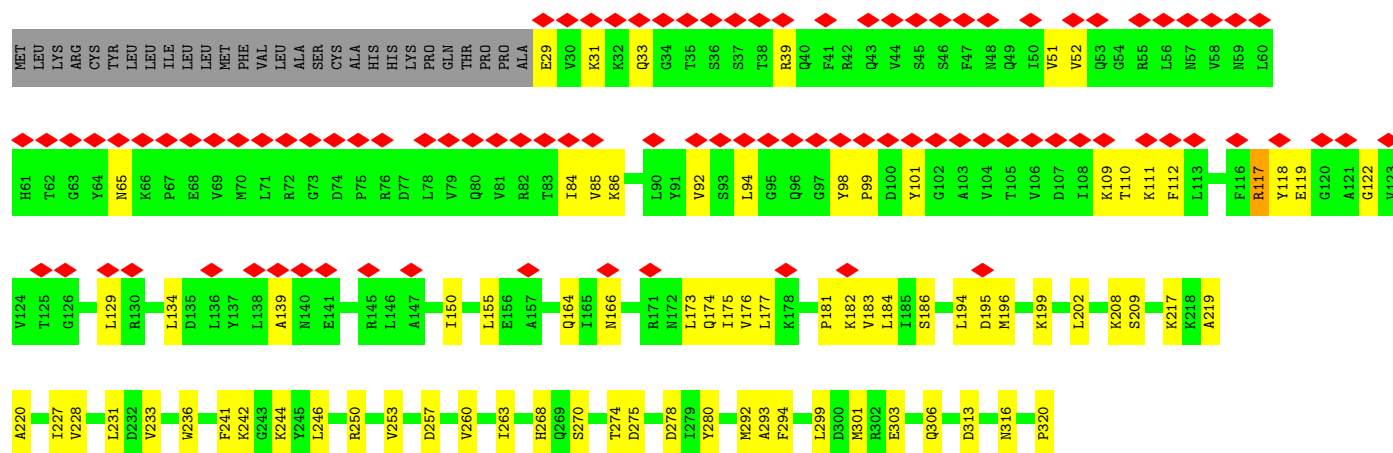


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

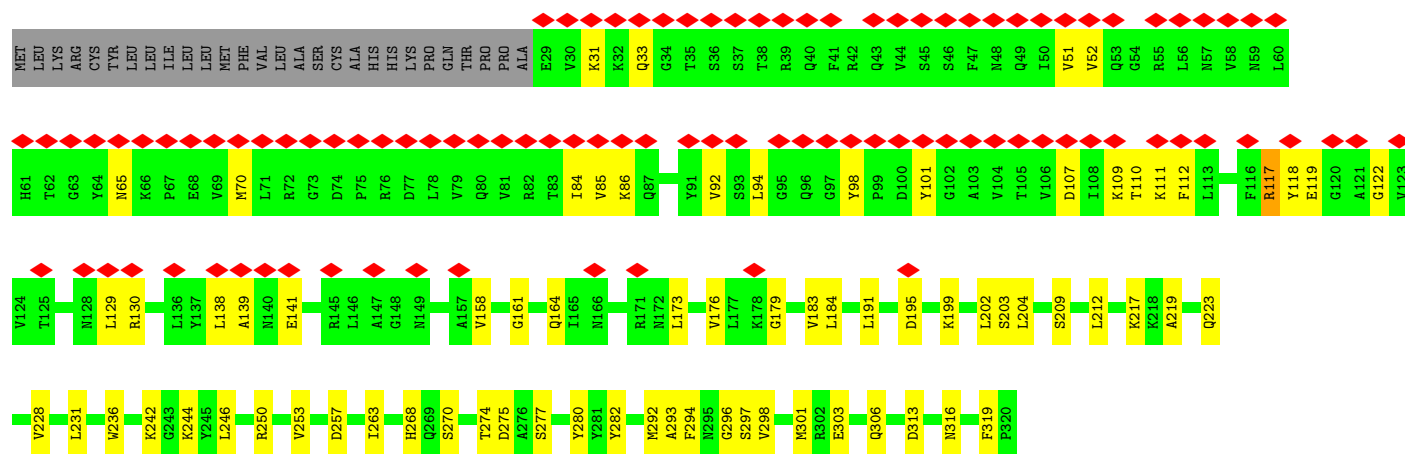


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

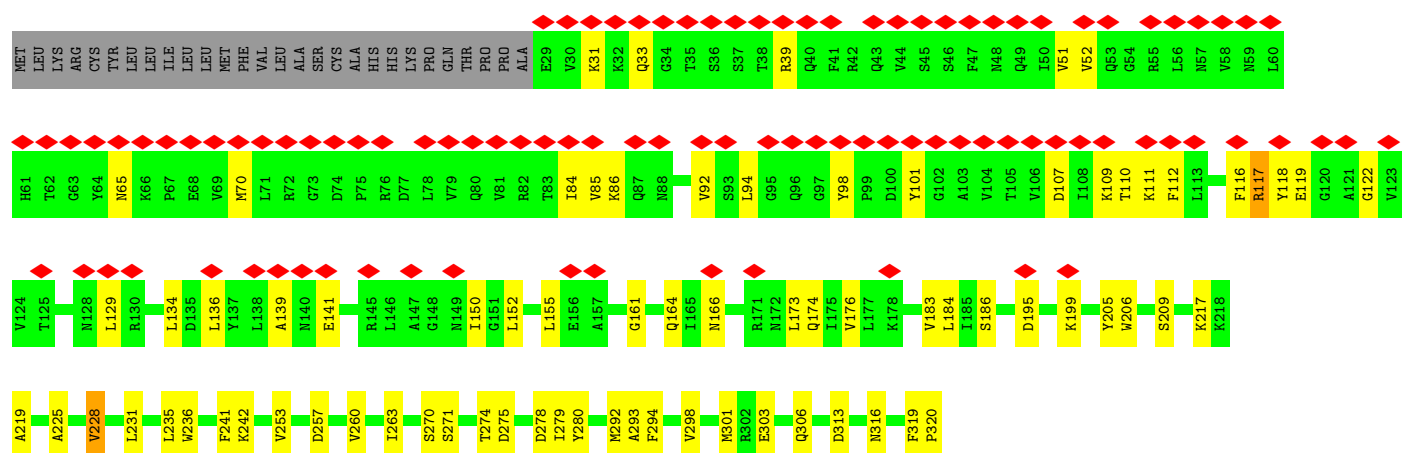




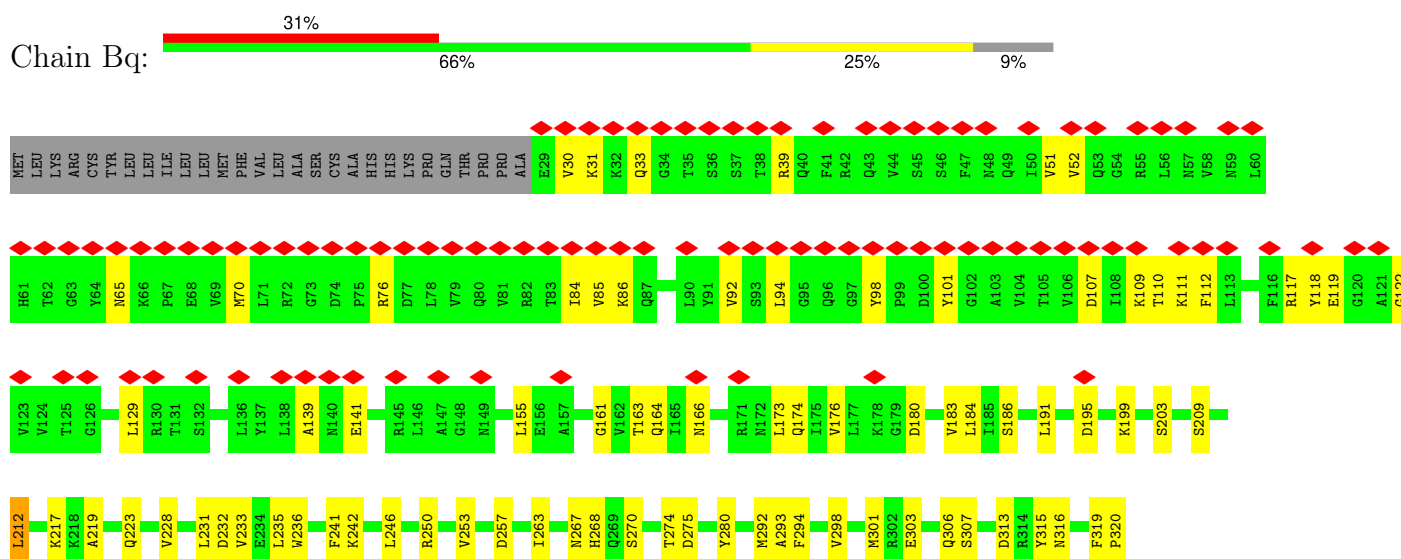
• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein



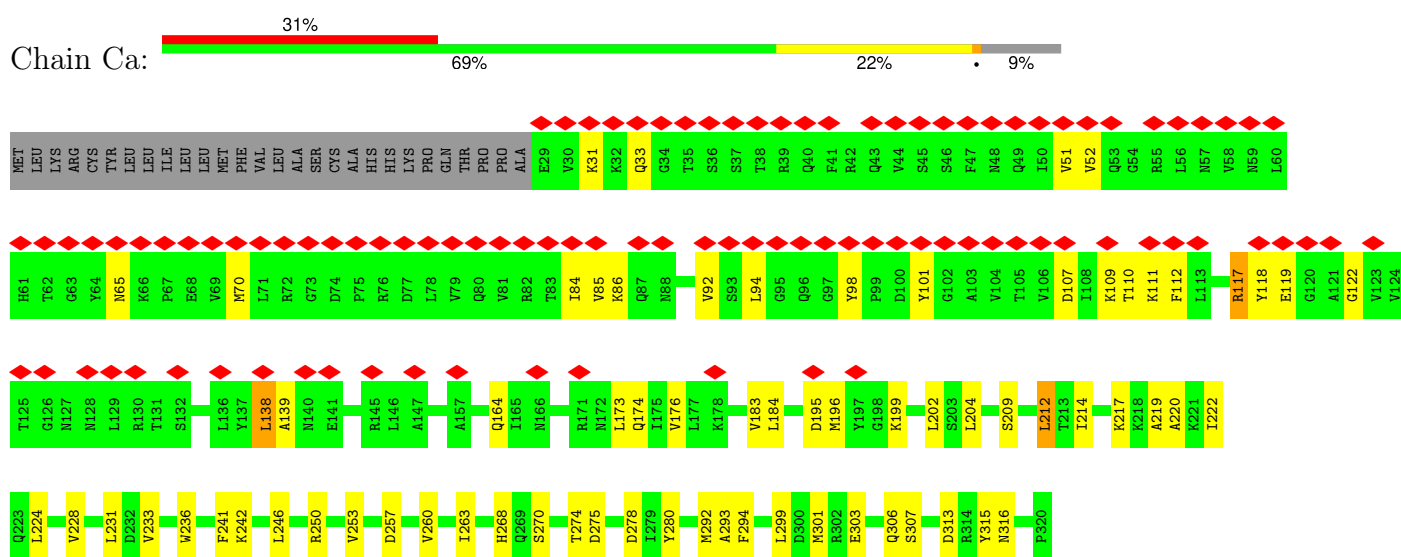
• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein



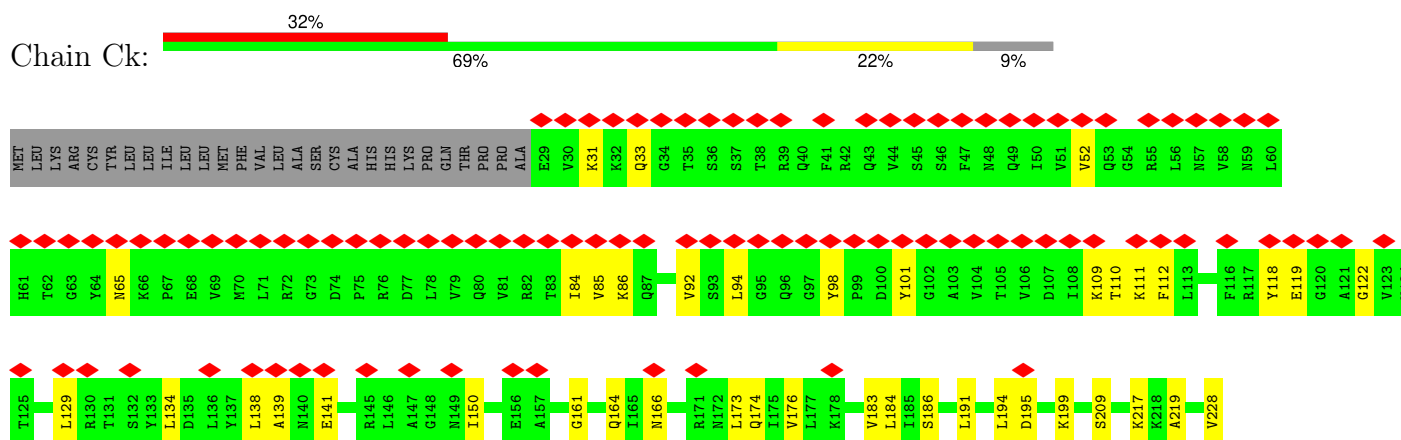
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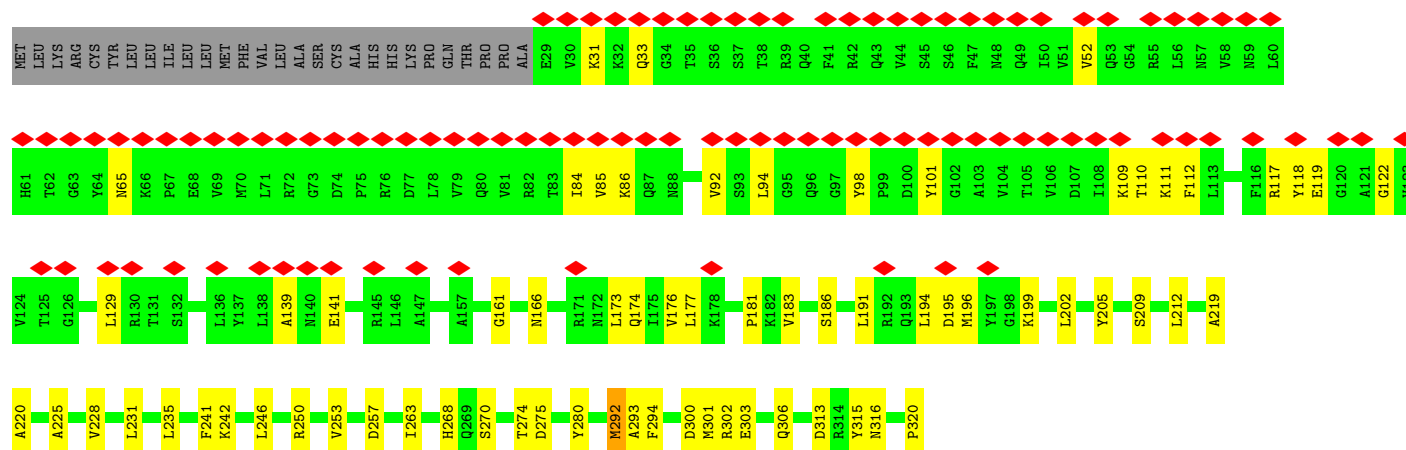


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

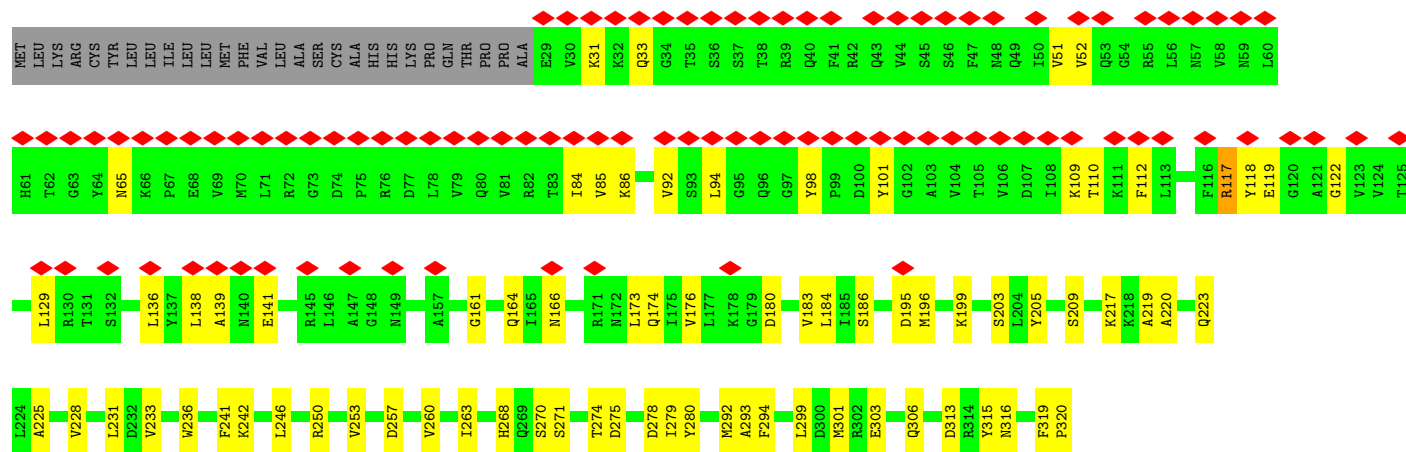




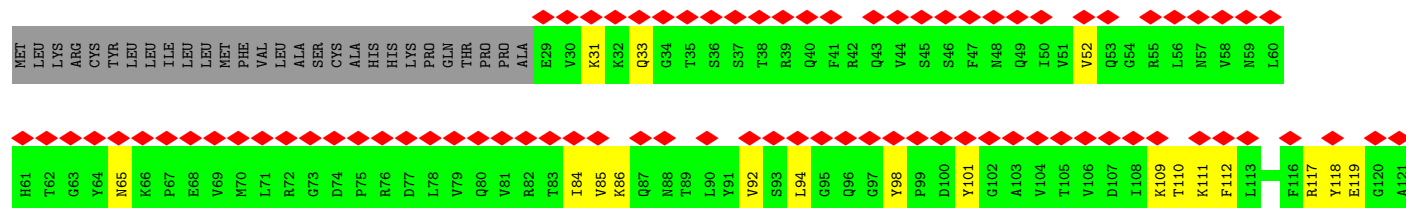
• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

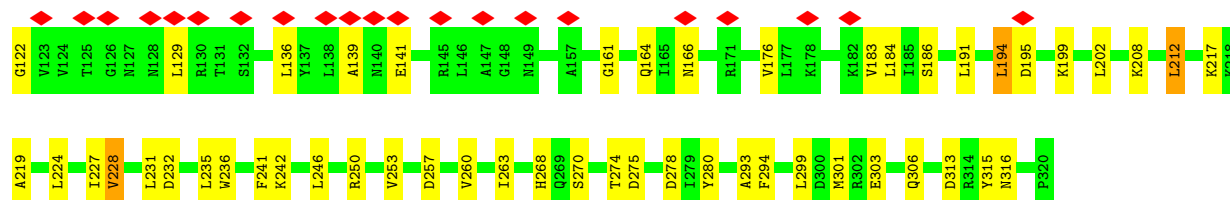


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

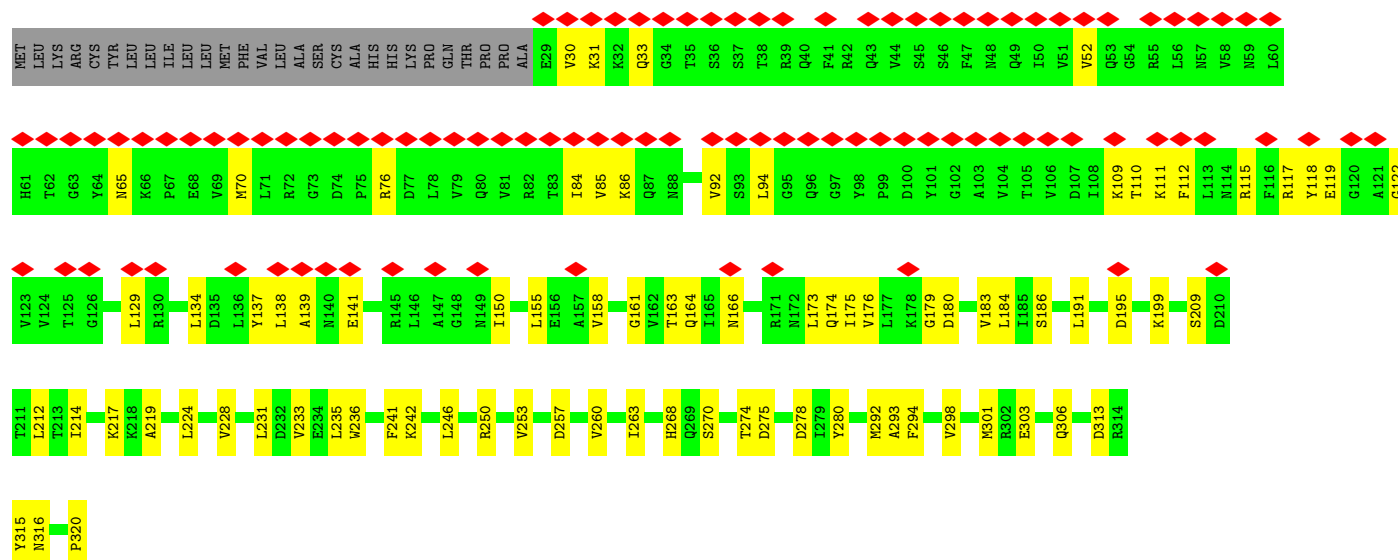


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

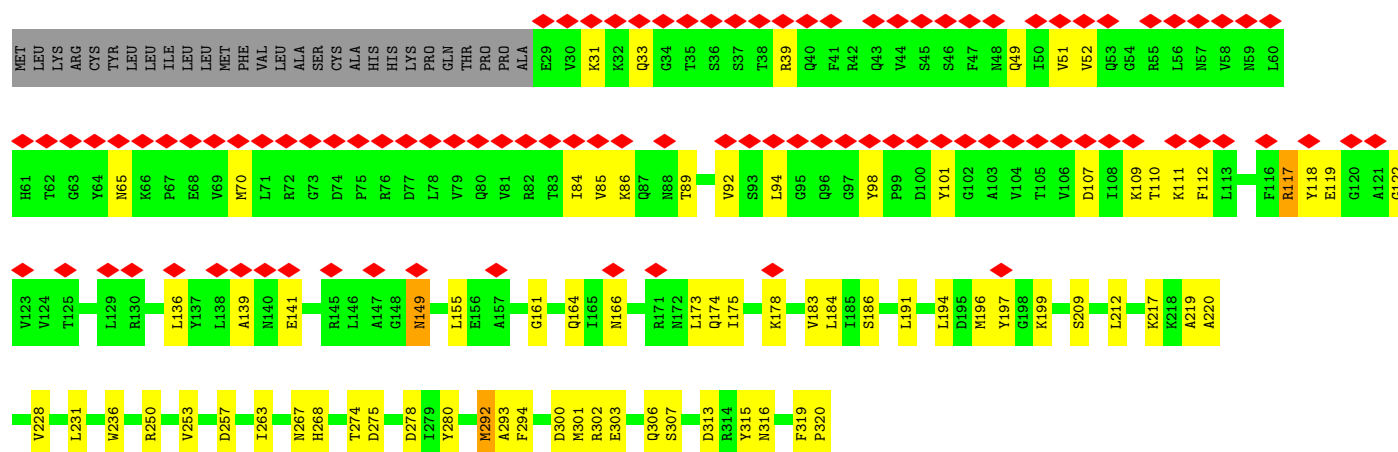




• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

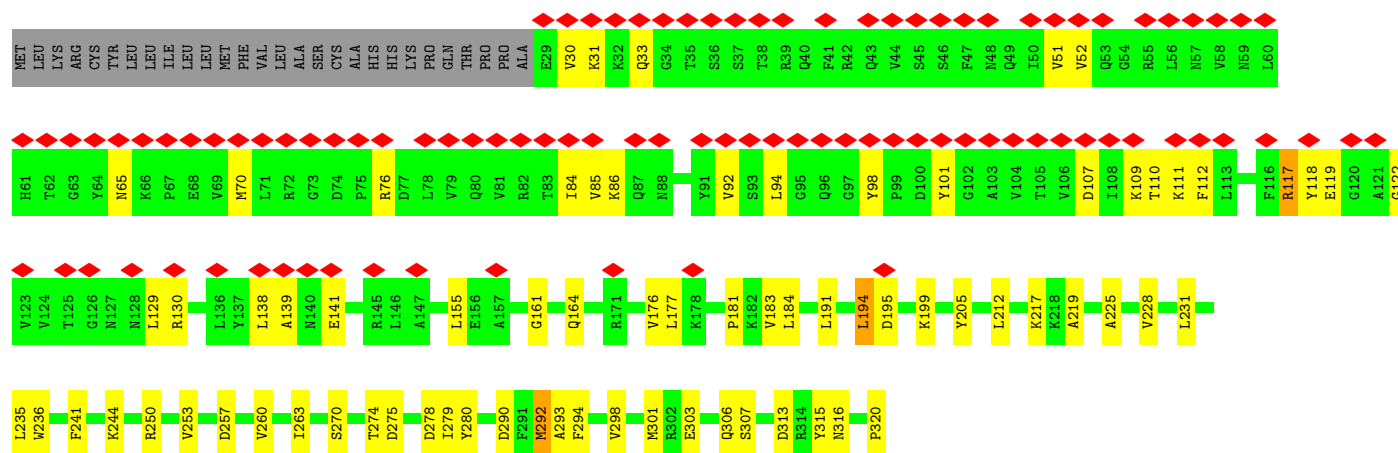


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

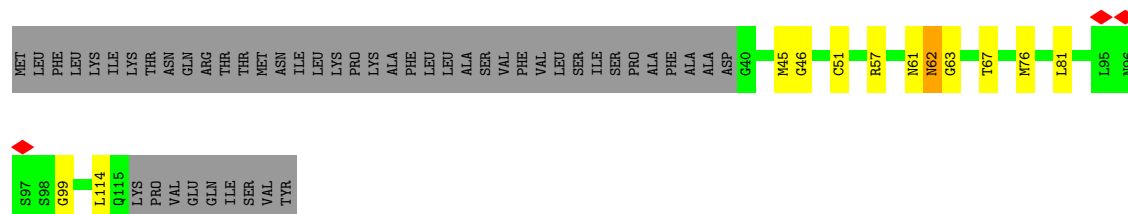


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

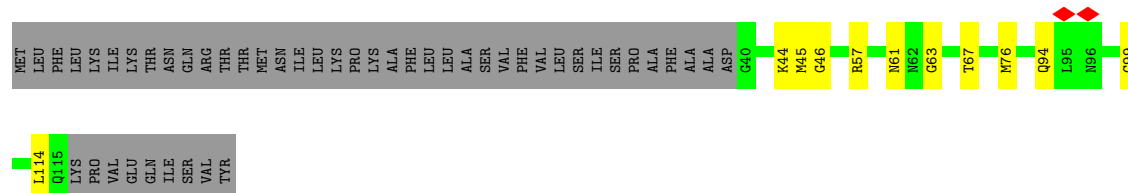




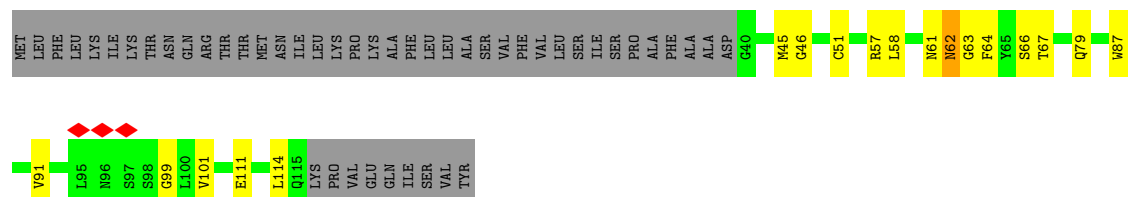
• Molecule 4: Neurogenic locus notch protein homolog



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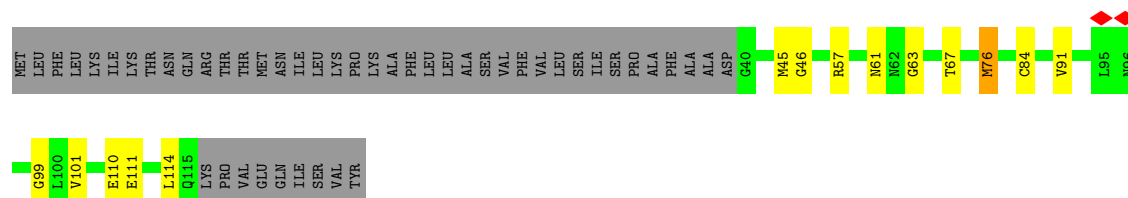


• Molecule 4: Neurogenic locus notch protein homolog

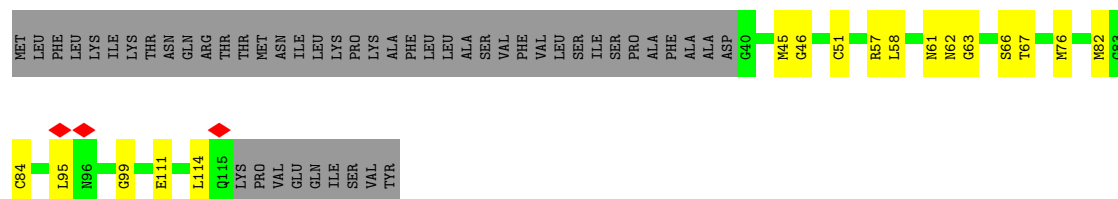


• Molecule 4: Neurogenic locus notch protein homolog

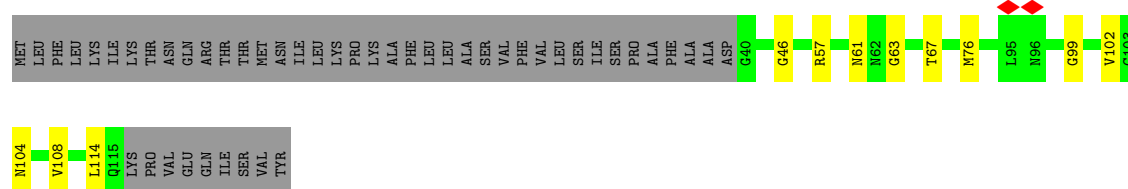




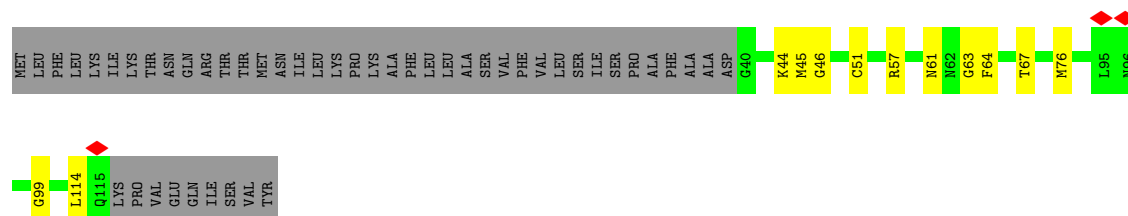
- Molecule 4: Neurogenic locus notch protein homolog



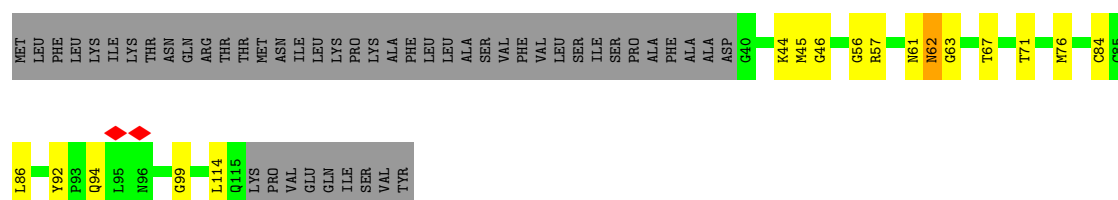
- Molecule 4: Neurogenic locus notch protein homolog



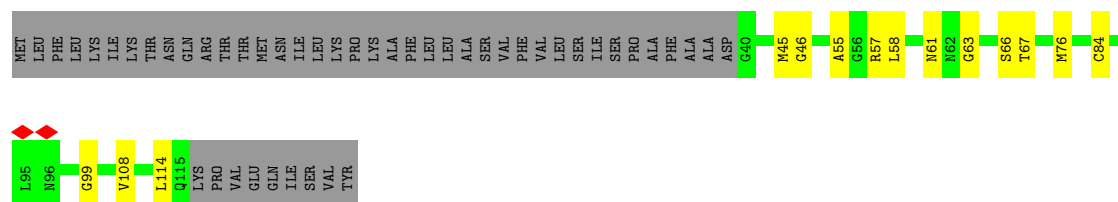
- Molecule 4: Neurogenic locus notch protein homolog



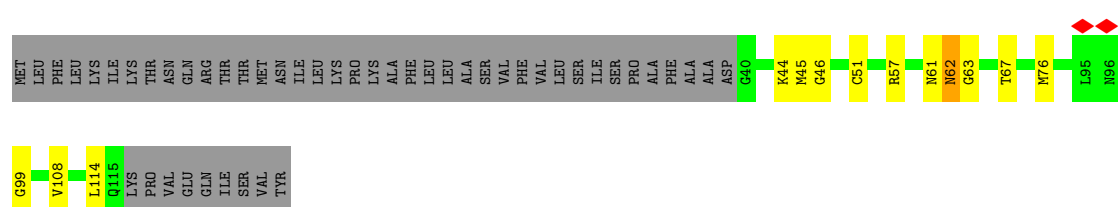
- Molecule 4: Neurogenic locus notch protein homolog



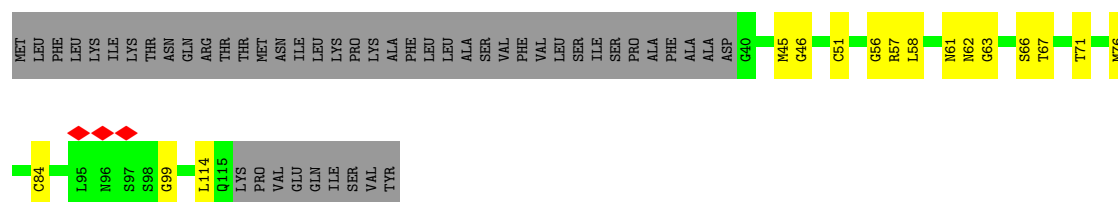
● Molecule 4: Neurogenic locus notch protein homolog



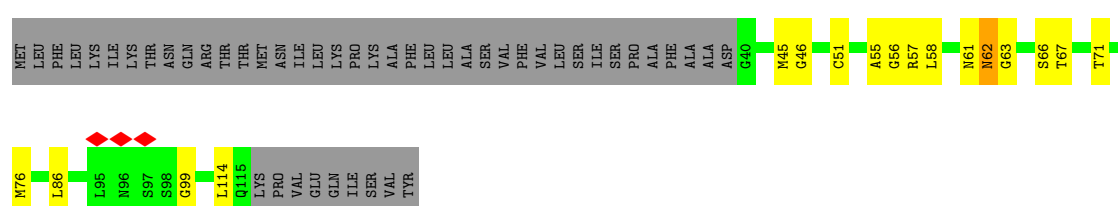
● Molecule 4: Neurogenic locus notch protein homolog



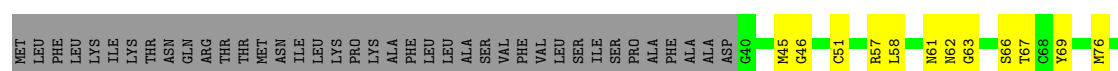
● Molecule 4: Neurogenic locus notch protein homolog

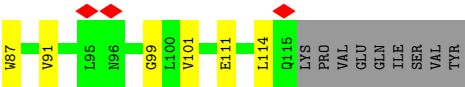


● Molecule 4: Neurogenic locus notch protein homolog

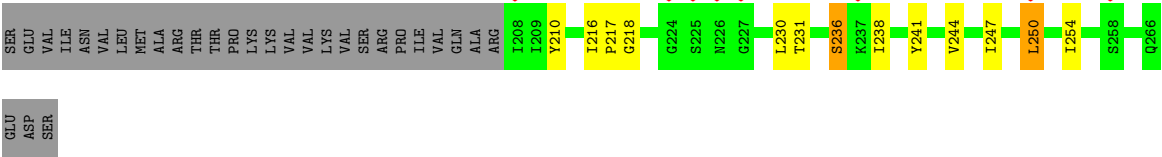
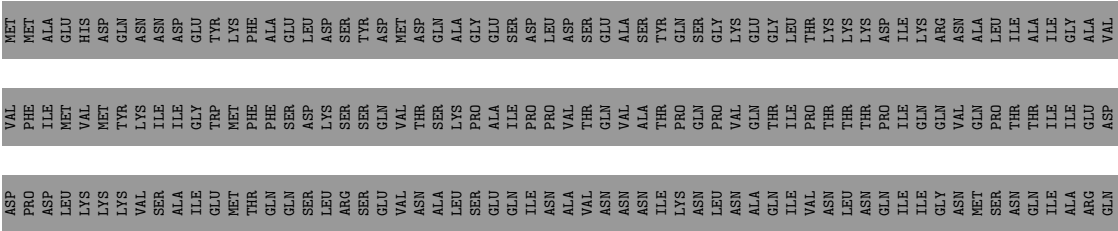


● Molecule 4: Neurogenic locus notch protein homolog

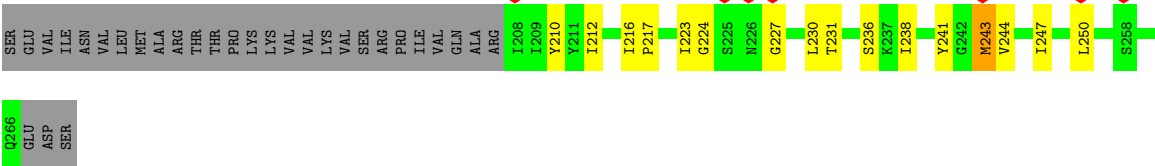
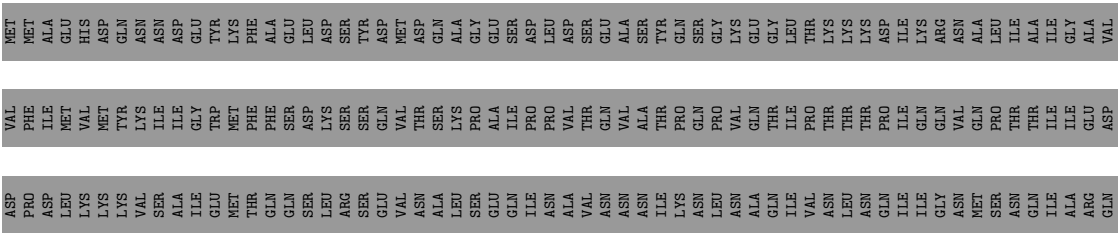




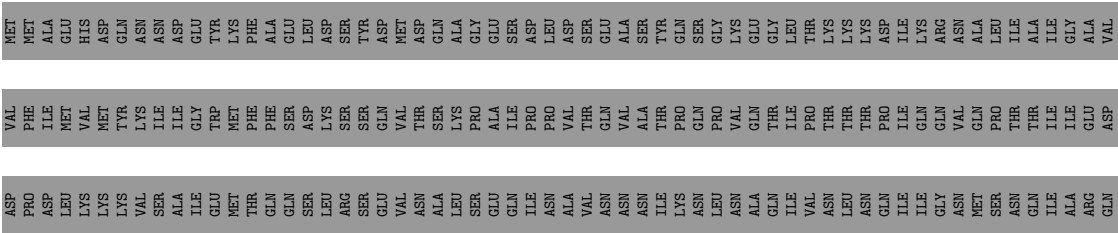
• Molecule 5: IcmG (DotF)



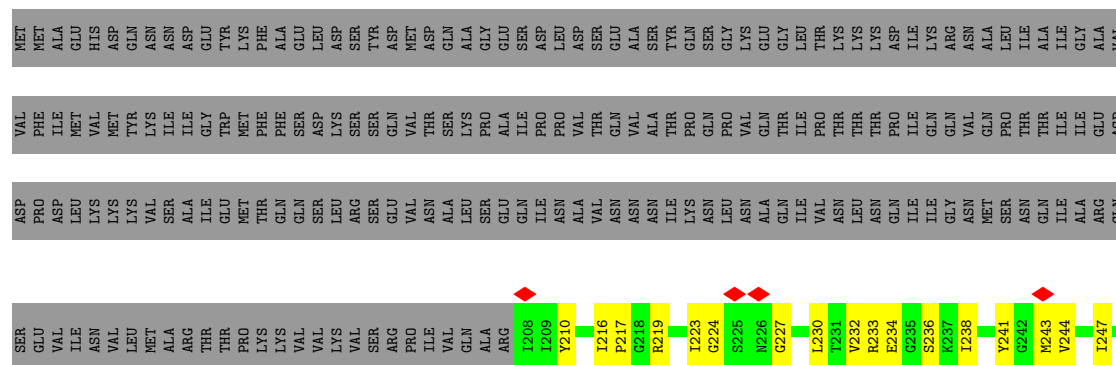
• Molecule 5: IcmG (DotF)



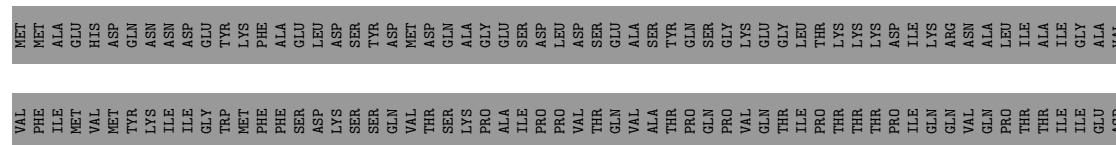
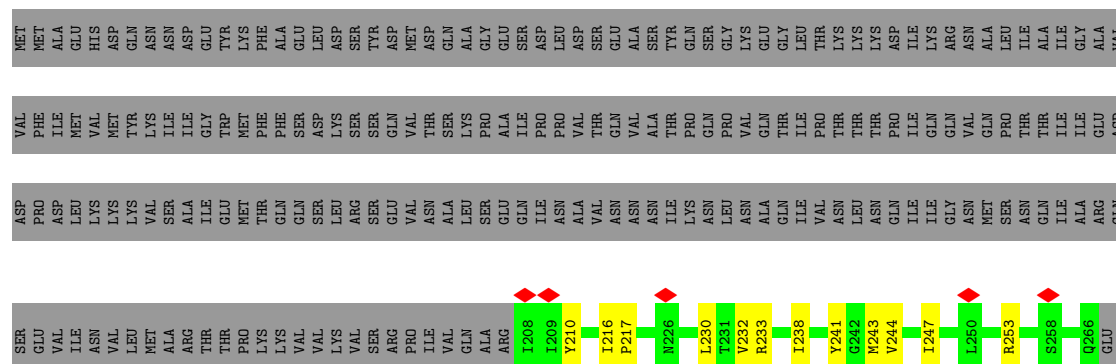
• Molecule 5: IcmG (DotF)

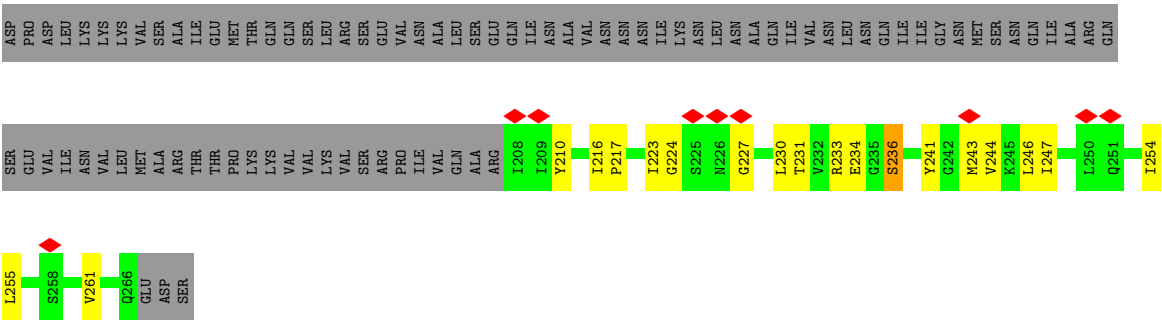


- Molecule 5: IcmG (DotF)

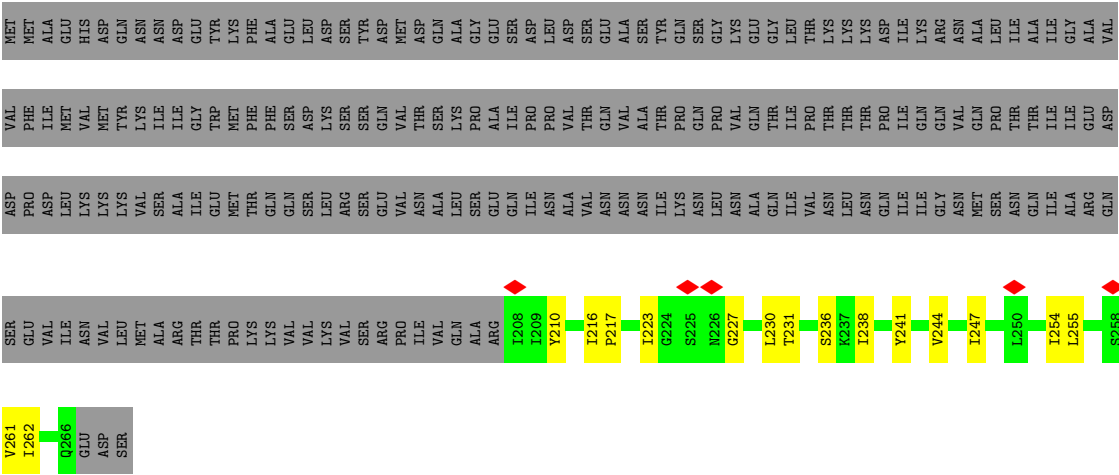


- Molecule 5: IcmG (DotF)

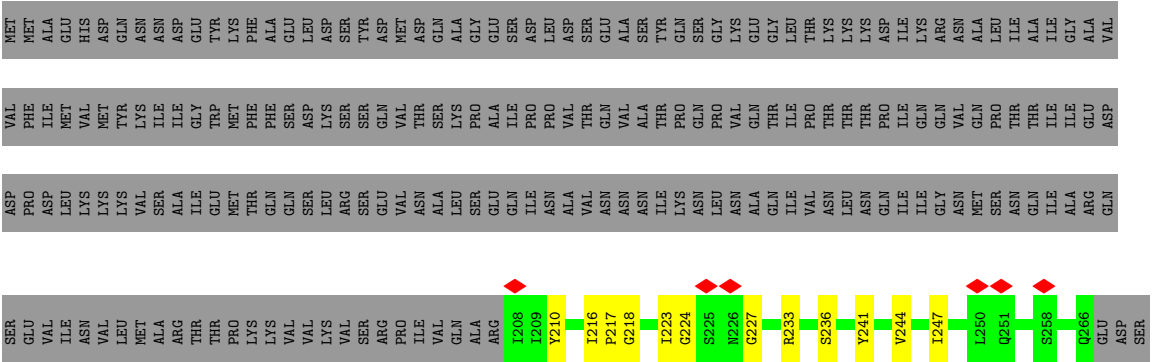




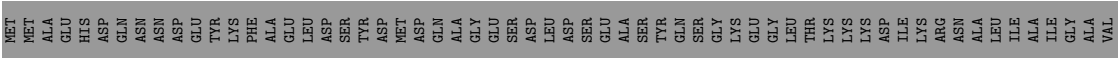
● Molecule 5: IcmG (DotF)



● Molecule 5: IcmG (DotF)



● Molecule 5: IcmG (DotF)



[illegible]

- Molecule 5: IcmG (DotF)

[illegible]

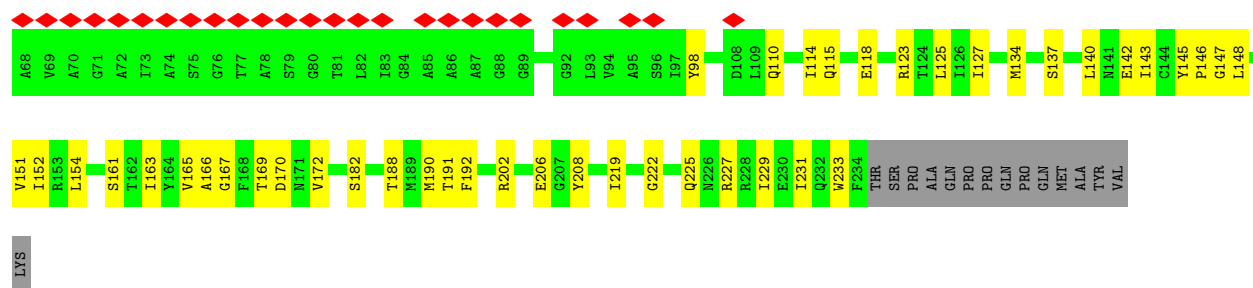
- Molecule 6: IcmK (DotH)



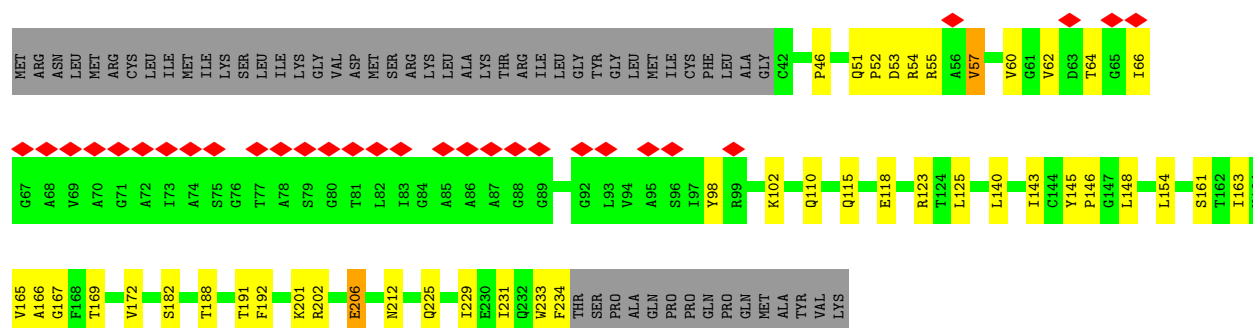
LEU	LEU	PHE	PRO	GLY	MET
ILE	LEU	LEU	ASN	ASP	MET
PRO	PRO	ASP	ASN	GLY	GLY
GLY	GLY	SER	PRO	GLY	LYS
GLN	GLN	THR	GLU	ASP	TYR
LYS	LYS	GLY	GLN	ASN	ASP
ALA	ALA	ALA	VAL	ALA	GLN
VAL	VAL	PRO	VAL	ALA	LEU
ASP	ASP	TRP	LYS	SER	CYS
TYR	TYR	PRO	LEU	ASP	CYS
ARG	ARG	ILE	LYS	SER	TYR
VAL	VAL	ALA	GLN	THR	CYS
ASP	ASP	ALA	ILE	GLN	LEU
LEU	LEU	TYR	TYR	GLN	VAL
ARG	ARG	ASP	GLU	PRO	ILE
VAL	VAL	LEU	THR	ASN	GLY
GLN	GLN	GLY	SER	GLN	LEU
GLY	GLY	ASP	GLU	SER	THR
TYR	TYR	PRO	TYR	GLY	THR
GLY	GLY	SER	ALA	GLN	PHE
PRO	PRO	SER	LYS	ALA	SER
ASN	ASN	PHE	ALA	ASN	MET
ALA	ALA	ALA	ALA	ALA	CYS
LYS	LYS	ILE	THR	PRO	CYS
SER	SER	GLN	PRO	ALA	ILE
MET	MET	TRP	GLY	ALA	TYR
PRO	PRO	ASP	THR	ASN	ALA
GLY	GLY	LYS	PRO	THR	ALA
GLU	GLU	THR	PRO	THR	ASP
GLY	GLY	SER	LYS	ALA	GLN
C271	C271	ASN	PRO	THR	SER
C275	C275	THR	THR	ALA	ASP
V283	V283	LEU	ALA	GLY	ASP
L284	L284	ILE	THR	GLY	ALA
E285	E285	GLN	SER	ASP	GLN
C294	C294	ALA	PHE	GLY	GLN
R294	R294	THR	VAL	GLN	ALA
V297	V297	LYS	VAL	ILE	LEU
S298	S298	LYS	ASN	ILE	LEU
C299	C299	LEU	LEU	GLN	GLN
A302	A302	TYR	SER	GLN	ARG
M311	M311	ASN	PRO	ASP	MET
Y312	Y312	GLY	GLY	ASP	LEU
L320	L320	ASN	SER	ALA	GLN
M328	M328	THR	THR	GLU	GLN
T329	T329	LEU	PRO	VAL	GLN
S330	S330	GLY	PRO	ILE	LYS
L346	L346	ASN	VAL	ASP	SER
K352	K352	THR	ILE	LYS	THR
V353	V353	VAL	ARG	ASP	ALA
M354	M354	MET	SER	MET	ALA
		THR	SER	THR	ASN
		THR	LEU	LEU	SER
			VAL	TYR	GLY
					ALA



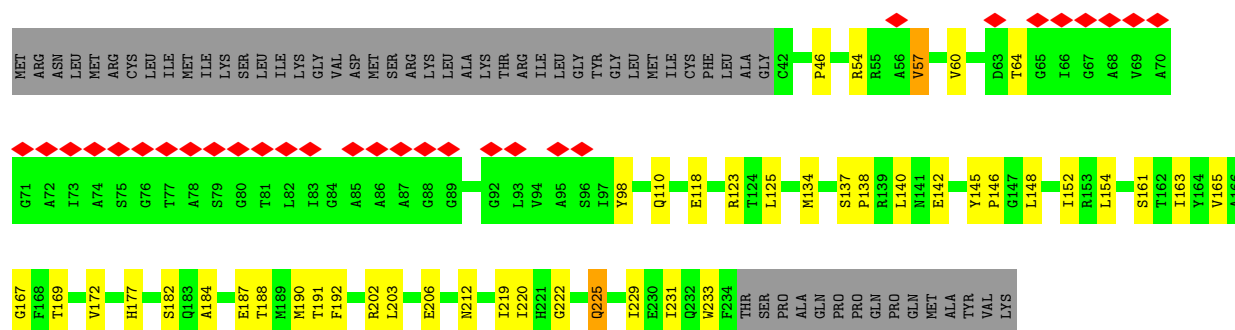




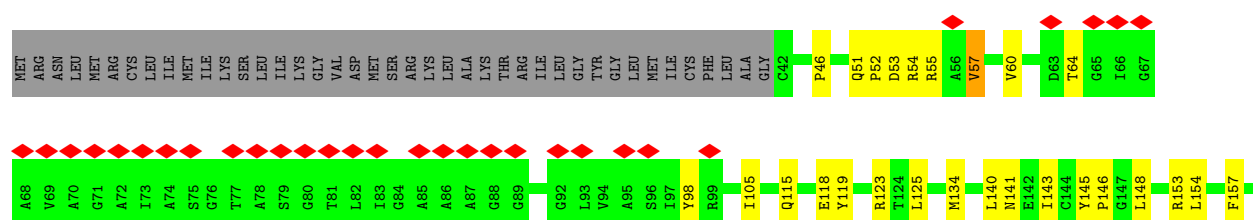
- Molecule 7: Outer membrane protein, OmpA family protein



- Molecule 7: Outer membrane protein, OmpA family protein

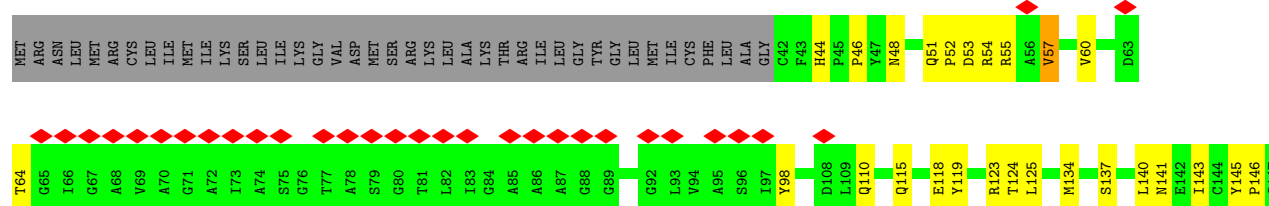


- Molecule 7: Outer membrane protein, OmpA family protein

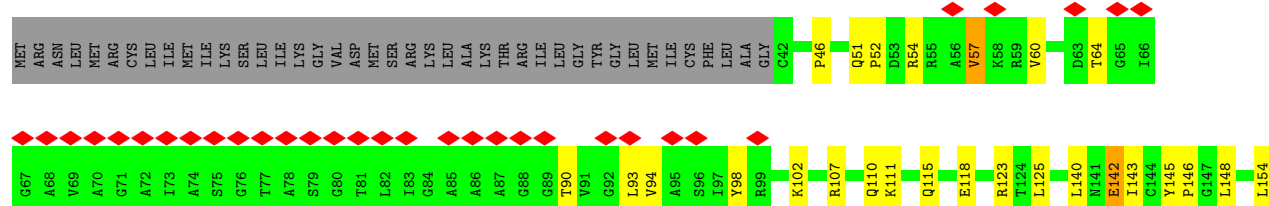




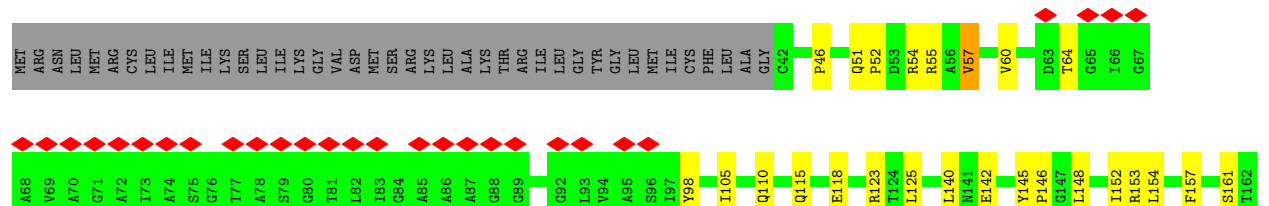
• Molecule 7: Outer membrane protein, OmpA family protein



• Molecule 7: Outer membrane protein, OmpA family protein

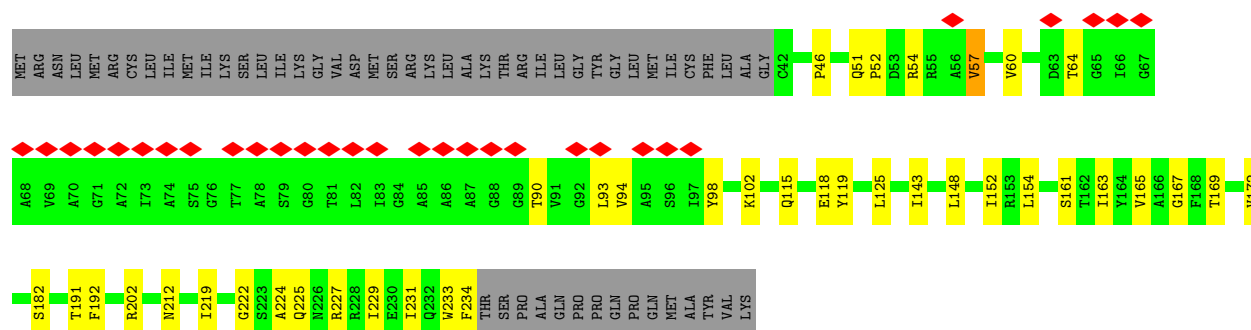


• Molecule 7: Outer membrane protein, OmpA family protein

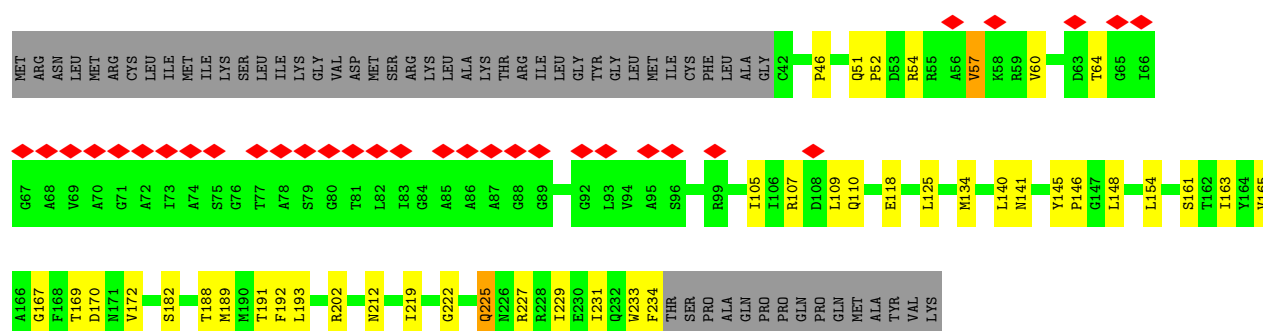


• Molecule 7: Outer membrane protein, OmpA family protein

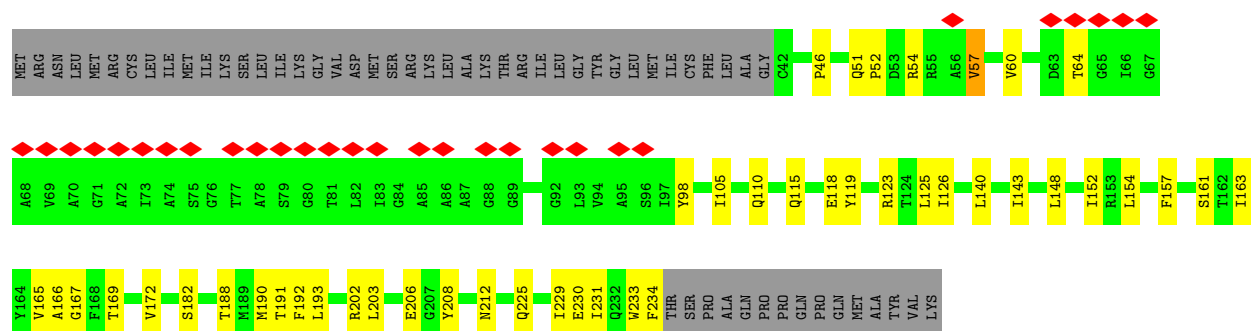




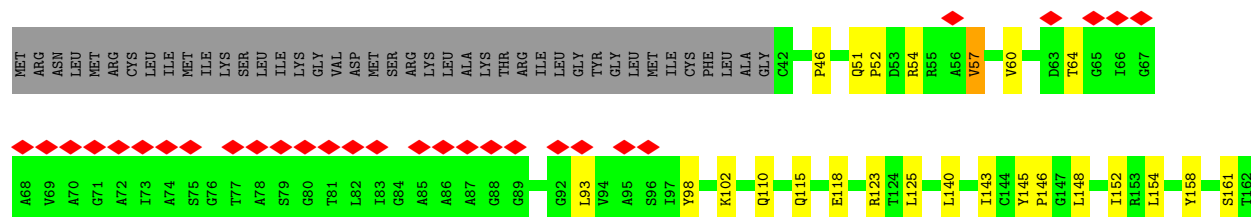
• Molecule 7: Outer membrane protein, OmpA family protein



• Molecule 7: Outer membrane protein, OmpA family protein

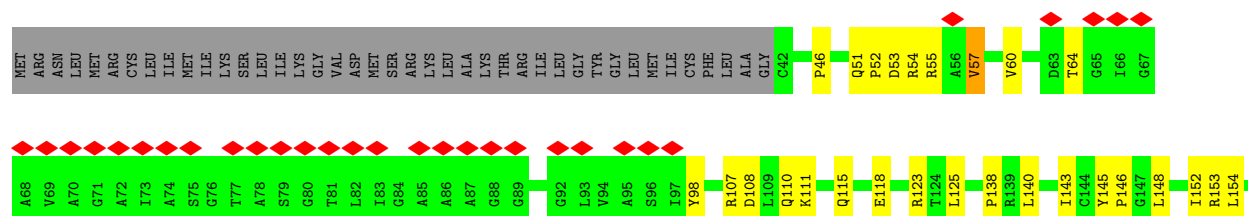


• Molecule 7: Outer membrane protein, OmpA family protein

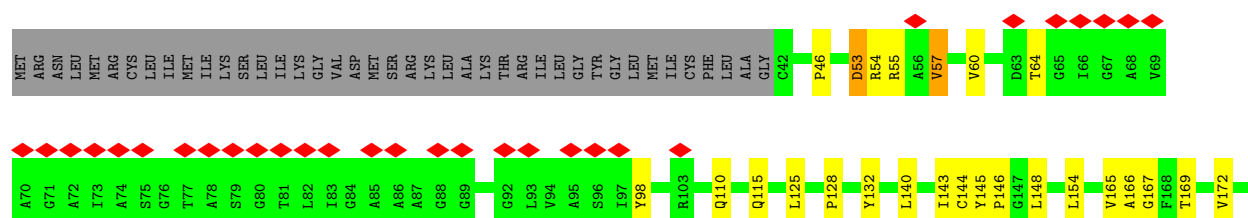




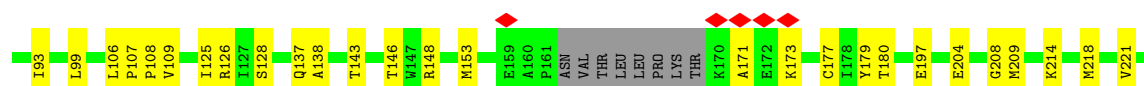
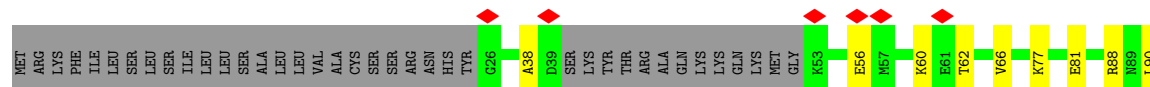
• Molecule 7: Outer membrane protein, OmpA family protein



• Molecule 7: Outer membrane protein, OmpA family protein

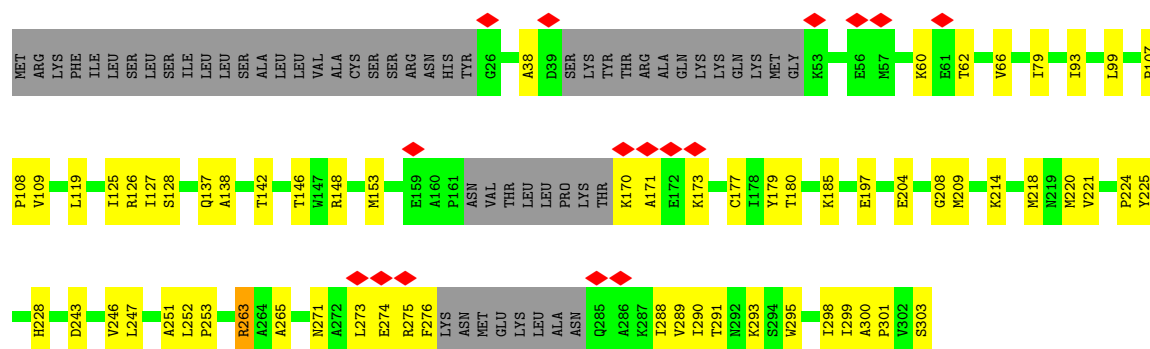


• Molecule 8: DotC

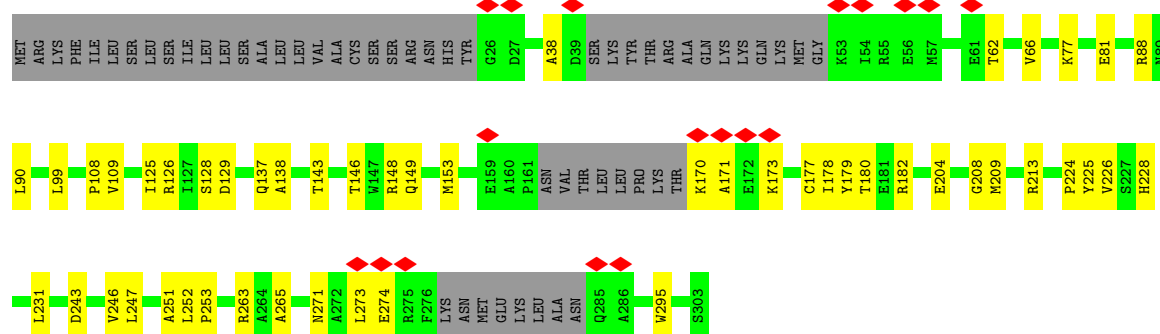


• Molecule 8: DotC

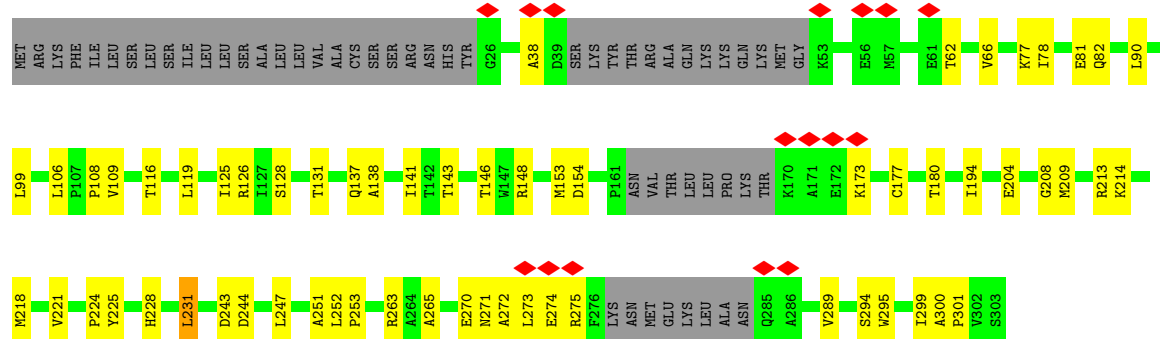




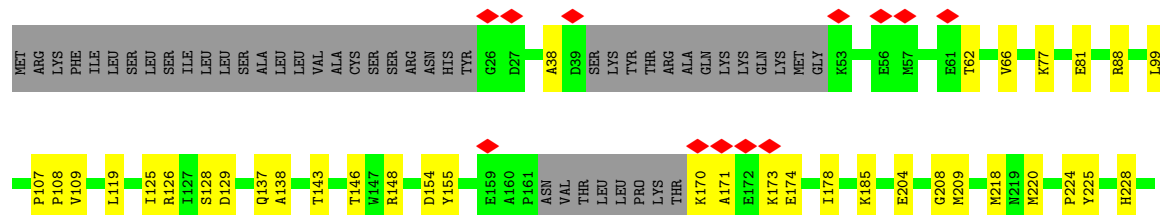
• Molecule 8: DotC



• Molecule 8: DotC

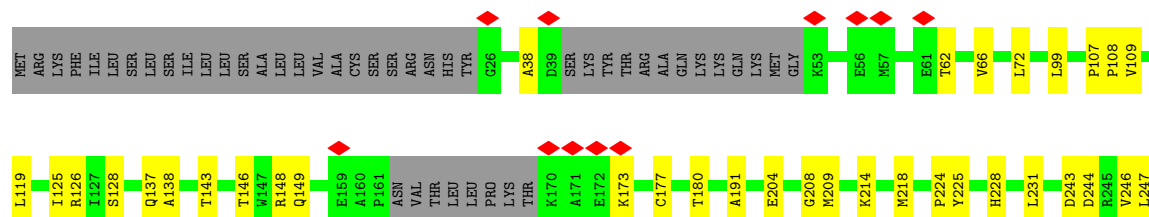


• Molecule 8: DotC

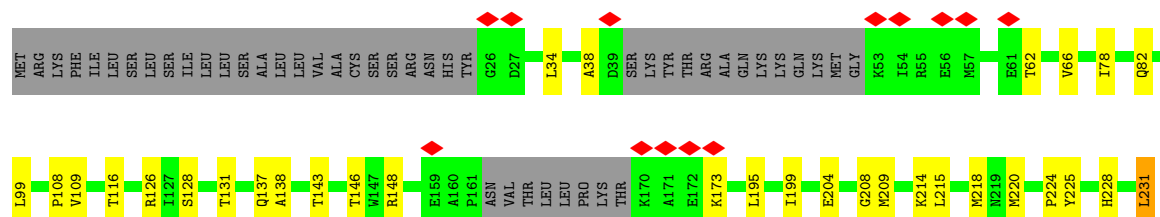




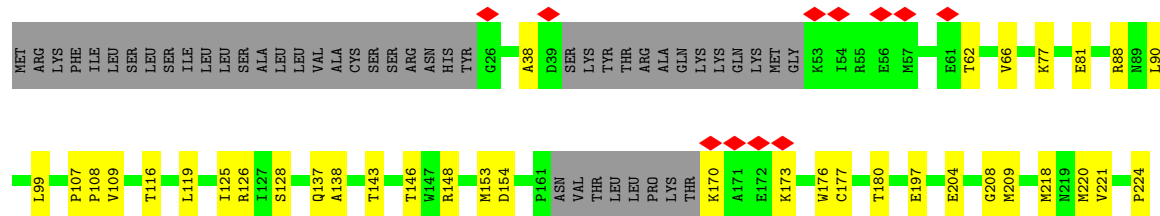
- Molecule 8: DotC



- Molecule 8: DotC

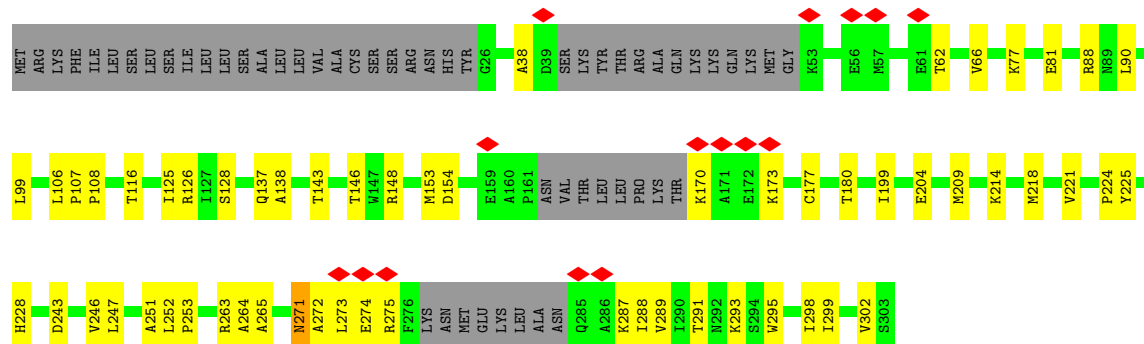


- Molecule 8: DotC

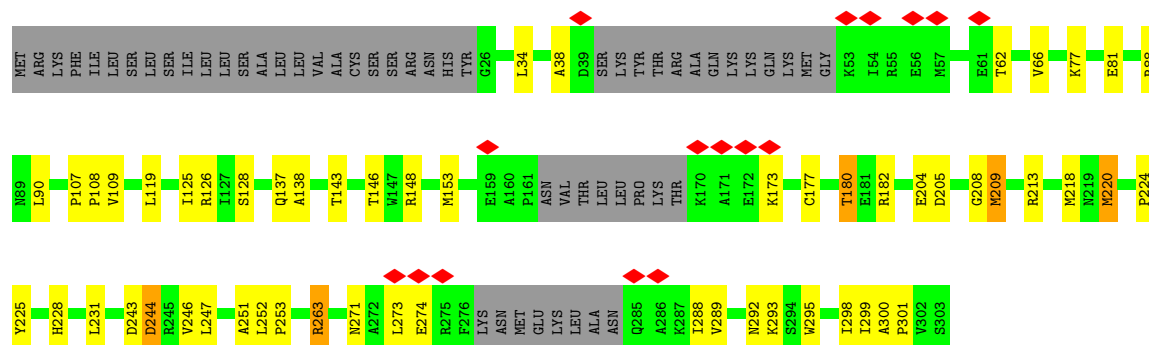


- Molecule 8: DotC

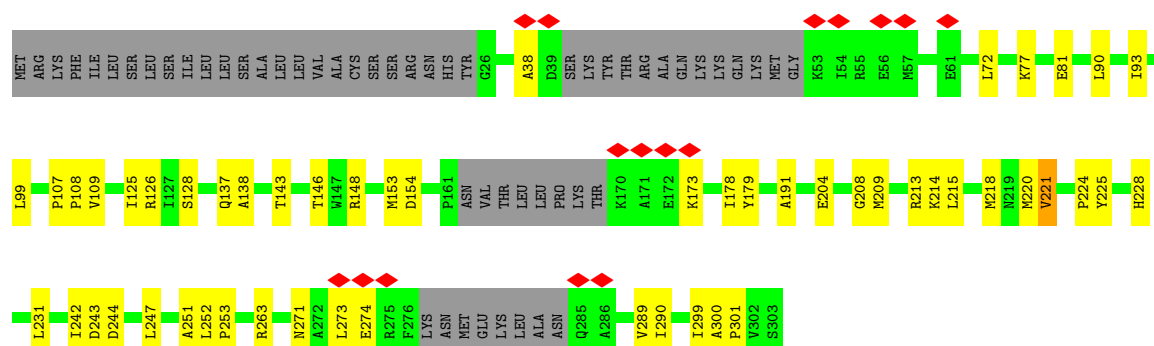




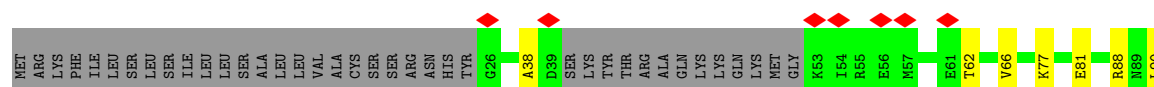
• Molecule 8: DotC

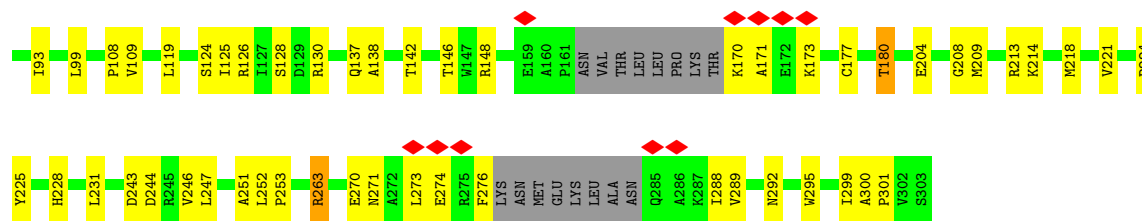


• Molecule 8: DotC

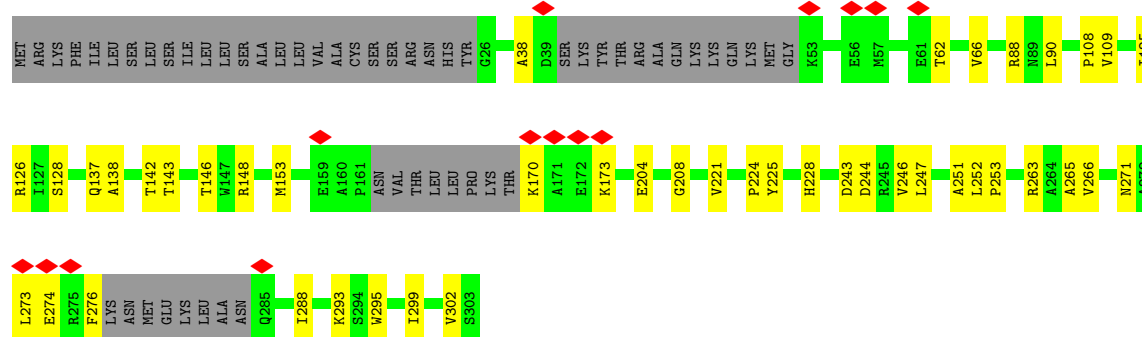


• Molecule 8: DotC

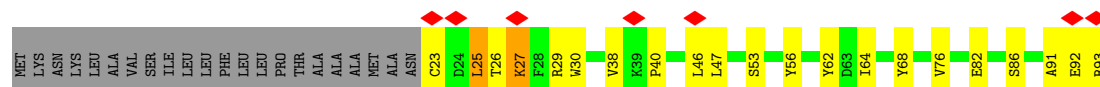




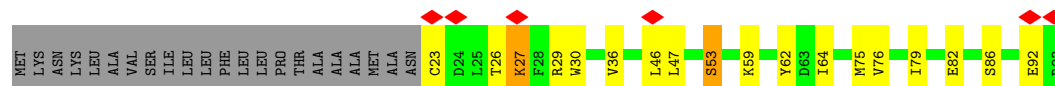
- Molecule 8: DotC



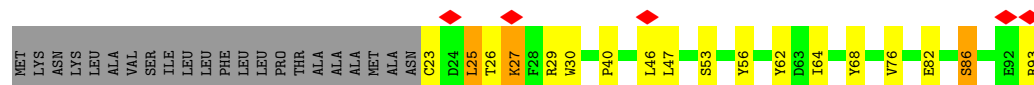
- Molecule 9: Secreted protein



- Molecule 9: Secreted protein

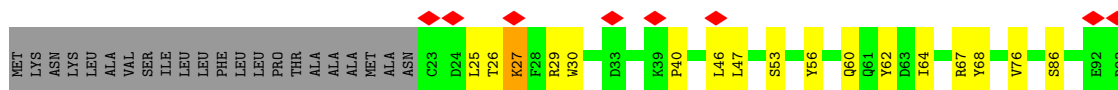


- Molecule 9: Secreted protein



- Molecule 9: Secreted protein





- Molecule 9: Secreted protein



- Molecule 9: Secreted protein



- Molecule 9: Secreted protein



- Molecule 9: Secreted protein

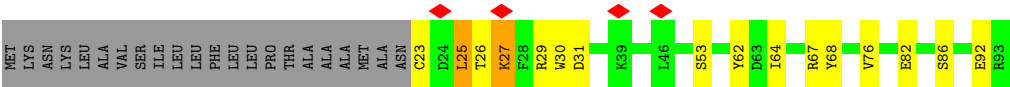


- Molecule 9: Secreted protein

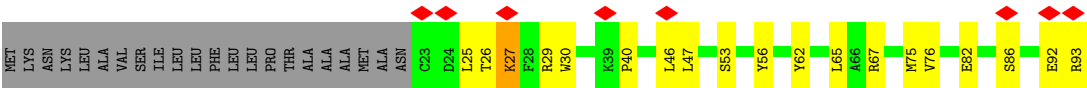


- Molecule 9: Secreted protein

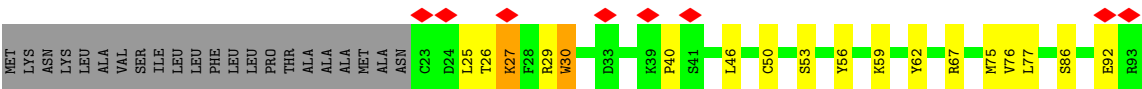




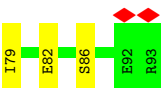
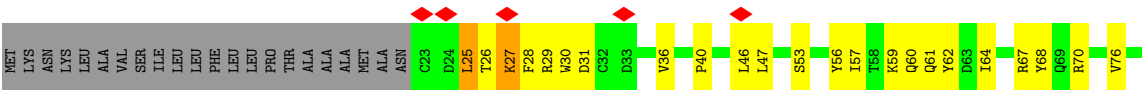
• Molecule 9: Secreted protein



• Molecule 9: Secreted protein



• Molecule 9: Secreted protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76409	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	73	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.656	Depositor
Minimum map value	-0.995	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	598.08, 598.08, 598.08	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.335, 1.335, 1.335	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	Aa	0.22	0/1099	0.36	0/1492
1	Ae	0.20	0/1069	0.37	0/1452
1	Ak	0.21	0/1099	0.37	0/1492
1	Ao	0.19	0/1069	0.33	0/1452
1	Au	0.21	0/1099	0.35	0/1492
1	Ay	0.19	0/1069	0.32	0/1452
1	Be	0.25	0/1099	0.38	0/1492
1	Bi	0.20	0/1069	0.38	0/1452
1	Bo	0.21	0/1099	0.36	0/1492
1	Bs	0.19	0/1069	0.32	0/1452
1	By	0.22	0/1099	0.36	0/1492
1	Cc	0.19	0/1069	0.35	0/1452
1	Ci	0.21	0/1099	0.37	0/1492
1	Cm	0.21	0/1069	0.39	0/1452
1	Cs	0.21	0/1099	0.36	0/1492
1	Cw	0.18	0/1069	0.31	0/1452
1	Dc	0.22	0/1099	0.35	0/1492
1	Dg	0.19	0/1069	0.34	0/1452
1	Dm	0.21	0/1099	0.35	0/1492
1	Dq	0.19	0/1069	0.33	0/1452
1	Dw	0.21	0/1099	0.34	0/1492
1	Ea	0.19	0/1069	0.33	0/1452
1	Eg	0.21	0/1099	0.37	0/1492
1	Ek	0.19	0/1069	0.32	0/1452
1	Eq	0.21	0/1099	0.35	0/1492
1	Eu	0.19	0/1069	0.33	0/1452
2	Ab	0.21	0/1180	0.32	0/1594
2	Al	0.21	0/1180	0.35	0/1594
2	Av	0.22	0/1180	0.35	0/1594
2	Bf	0.21	0/1180	0.34	0/1594
2	Bp	0.20	0/1180	0.31	0/1594
2	Bz	0.21	0/1180	0.34	0/1594
2	Cj	0.22	0/1180	0.37	0/1594
2	Ct	0.21	0/1180	0.32	0/1594

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Dd	0.21	0/1180	0.32	0/1594
2	Dn	0.21	0/1180	0.34	0/1594
2	Dx	0.21	0/1180	0.35	0/1594
2	Eh	0.21	0/1180	0.35	0/1594
2	Er	0.22	0/1180	0.36	0/1594
3	Ac	0.15	0/2360	0.35	0/3183
3	Am	0.15	0/2360	0.35	0/3183
3	Aw	0.14	0/2360	0.35	0/3183
3	Bg	0.15	0/2360	0.35	0/3183
3	Bq	0.15	0/2360	0.35	0/3183
3	Ca	0.14	0/2360	0.35	0/3183
3	Ck	0.14	0/2360	0.34	0/3183
3	Cu	0.15	0/2360	0.34	0/3183
3	De	0.14	0/2360	0.35	0/3183
3	Do	0.14	0/2360	0.36	0/3183
3	Dy	0.16	0/2360	0.35	0/3183
3	Ei	0.16	0/2360	0.38	0/3183
3	Es	0.15	0/2360	0.35	0/3183
4	Ad	0.21	0/576	0.33	0/777
4	An	0.22	0/576	0.35	0/777
4	Ax	0.22	0/576	0.34	0/777
4	Bh	0.22	0/576	0.40	0/777
4	Br	0.23	0/576	0.38	0/777
4	Cb	0.22	0/576	0.34	0/777
4	Cl	0.22	0/576	0.34	0/777
4	Cv	0.23	0/576	0.40	0/777
4	Df	0.22	0/576	0.35	0/777
4	Dp	0.22	0/576	0.33	0/777
4	Dz	0.22	0/576	0.35	0/777
4	Ej	0.22	0/576	0.37	0/777
4	Et	0.22	0/576	0.38	0/777
5	Af	0.16	0/456	0.33	0/615
5	Ap	0.15	0/456	0.31	0/615
5	Az	0.12	0/456	0.32	0/615
5	Bj	0.13	0/456	0.34	0/615
5	Bt	0.14	0/456	0.34	0/615
5	Cd	0.17	0/456	0.37	0/615
5	Cn	0.17	0/456	0.33	0/615
5	Cx	0.17	0/456	0.31	0/615
5	Dh	0.17	0/456	0.36	0/615
5	Dr	0.16	0/456	0.36	0/615
5	Eb	0.16	0/456	0.34	0/615
5	El	0.15	0/456	0.36	0/615

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	Ev	0.15	0/456	0.33	0/615
6	Ag	0.24	0/708	0.37	0/963
6	Aq	0.25	0/708	0.39	0/963
6	Ba	0.25	0/708	0.37	0/963
6	Bk	0.24	0/708	0.37	0/963
6	Bu	0.24	0/708	0.34	0/963
6	Ce	0.24	0/708	0.38	0/963
6	Co	0.24	0/708	0.37	0/963
6	Cy	0.25	0/708	0.38	0/963
6	Di	0.24	0/708	0.37	0/963
6	Ds	0.24	0/708	0.35	0/963
6	Ec	0.24	0/708	0.36	0/963
6	Em	0.24	0/708	0.36	0/963
6	Ew	0.25	0/708	0.36	0/963
7	Ah	0.19	0/1530	0.35	0/2068
7	Ar	0.19	0/1530	0.35	0/2068
7	Bb	0.19	0/1530	0.33	0/2068
7	Bl	0.19	0/1530	0.34	0/2068
7	Bv	0.20	0/1530	0.34	0/2068
7	Cf	0.19	0/1530	0.33	0/2068
7	Cp	0.19	0/1530	0.36	0/2068
7	Cz	0.19	0/1530	0.36	0/2068
7	Dj	0.19	0/1530	0.34	0/2068
7	Dt	0.19	0/1530	0.36	0/2068
7	Ed	0.19	0/1530	0.37	0/2068
7	En	0.19	0/1530	0.35	0/2068
7	Ex	0.19	0/1530	0.36	0/2068
8	Ai	0.20	0/2006	0.33	0/2718
8	As	0.21	0/2006	0.33	0/2718
8	Bc	0.20	0/2006	0.32	0/2718
8	Bm	0.21	0/2006	0.31	0/2718
8	Bw	0.21	0/2006	0.34	0/2718
8	Cg	0.20	0/2006	0.30	0/2718
8	Cq	0.20	0/2006	0.31	0/2718
8	Da	0.20	0/2006	0.31	0/2718
8	Dk	0.20	0/2006	0.33	0/2718
8	Du	0.20	0/2006	0.33	0/2718
8	Ee	0.20	0/2006	0.31	0/2718
8	Eo	0.21	0/2006	0.31	0/2718
8	Ey	0.21	0/2006	0.33	0/2718
9	Aj	0.17	0/574	0.38	0/778
9	At	0.17	0/574	0.38	0/778
9	Bd	0.16	0/574	0.39	0/778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	Bn	0.18	0/574	0.42	0/778
9	Bx	0.18	0/574	0.41	0/778
9	Ch	0.18	0/574	0.43	0/778
9	Cr	0.18	0/574	0.39	0/778
9	Db	0.17	0/574	0.41	0/778
9	Dl	0.18	0/574	0.41	0/778
9	Dv	0.16	0/574	0.38	0/778
9	Ef	0.19	0/574	0.43	0/778
9	Ep	0.18	0/574	0.44	0/778
9	Ez	0.20	0/574	0.46	0/778
All	All	0.19	0/150254	0.35	0/203320

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	1078	0	1112	30	0
1	Ae	1049	0	1079	25	0
1	Ak	1078	0	1112	26	0
1	Ao	1049	0	1079	23	0
1	Au	1078	0	1112	23	0
1	Ay	1049	0	1079	31	0
1	Be	1078	0	1112	31	0
1	Bi	1049	0	1079	26	0
1	Bo	1078	0	1112	23	0
1	Bs	1049	0	1079	25	0
1	By	1078	0	1112	31	0
1	Cc	1049	0	1079	23	0
1	Ci	1078	0	1112	23	0
1	Cm	1049	0	1079	21	0
1	Cs	1078	0	1112	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Cw	1049	0	1079	19	0
1	Dc	1078	0	1112	28	0
1	Dg	1049	0	1079	18	0
1	Dm	1078	0	1112	25	0
1	Dq	1049	0	1079	24	0
1	Dw	1078	0	1112	26	0
1	Ea	1049	0	1079	24	0
1	Eg	1078	0	1112	29	0
1	Ek	1049	0	1079	30	0
1	Eq	1078	0	1112	26	0
1	Eu	1049	0	1079	20	0
2	Ab	1161	0	1205	26	0
2	Al	1161	0	1205	26	0
2	Av	1161	0	1205	26	0
2	Bf	1161	0	1205	29	0
2	Bp	1161	0	1205	23	0
2	Bz	1161	0	1205	25	0
2	Cj	1161	0	1205	33	0
2	Ct	1161	0	1205	24	0
2	Dd	1161	0	1205	30	0
2	Dn	1161	0	1205	24	0
2	Dx	1161	0	1205	23	0
2	Eh	1161	0	1205	26	0
2	Er	1161	0	1205	22	0
3	Ac	2321	0	2343	48	0
3	Am	2321	0	2343	47	0
3	Aw	2321	0	2343	47	0
3	Bg	2321	0	2343	45	0
3	Bq	2321	0	2343	46	0
3	Ca	2321	0	2343	42	0
3	Ck	2321	0	2343	45	0
3	Cu	2321	0	2343	42	0
3	De	2321	0	2343	41	0
3	Do	2321	0	2343	38	0
3	Dy	2321	0	2343	53	0
3	Ei	2321	0	2343	45	0
3	Es	2321	0	2343	42	0
4	Ad	565	0	513	9	0
4	An	565	0	513	9	0
4	Ax	565	0	513	14	0
4	Bh	565	0	513	13	0
4	Br	565	0	513	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Cb	565	0	513	7	0
4	Cl	565	0	513	11	0
4	Cv	565	0	513	15	0
4	Df	565	0	513	10	0
4	Dp	565	0	513	12	0
4	Dz	565	0	513	11	0
4	Ej	565	0	513	13	0
4	Et	565	0	513	12	0
5	Af	449	0	474	11	0
5	Ap	449	0	474	11	0
5	Az	449	0	474	11	0
5	Bj	449	0	474	13	0
5	Bt	449	0	474	7	0
5	Cd	449	0	474	15	0
5	Cn	449	0	474	12	0
5	Cx	449	0	474	8	0
5	Dh	449	0	474	10	0
5	Dr	449	0	474	10	0
5	Eb	449	0	474	9	0
5	El	449	0	474	13	0
5	Ev	449	0	474	12	0
6	Ag	691	0	703	13	0
6	Aq	691	0	703	16	0
6	Ba	691	0	703	15	0
6	Bk	691	0	703	14	0
6	Bu	691	0	703	14	0
6	Ce	691	0	703	16	0
6	Co	691	0	703	17	0
6	Cy	691	0	703	19	0
6	Di	691	0	703	14	0
6	Ds	691	0	703	15	0
6	Ec	691	0	703	16	0
6	Em	691	0	703	16	0
6	Ew	691	0	703	17	0
7	Ah	1500	0	1499	32	0
7	Ar	1500	0	1499	29	0
7	Bb	1500	0	1499	28	0
7	Bl	1500	0	1499	34	0
7	Bv	1500	0	1499	32	0
7	Cf	1500	0	1499	26	0
7	Cp	1500	0	1499	34	0
7	Cz	1500	0	1499	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Dj	1500	0	1499	28	0
7	Dt	1500	0	1499	34	0
7	Ed	1500	0	1499	32	0
7	En	1500	0	1499	29	0
7	Ex	1500	0	1499	30	0
8	Ai	1970	0	1980	43	0
8	As	1970	0	1980	53	0
8	Bc	1970	0	1980	43	0
8	Bm	1970	0	1980	51	0
8	Bw	1970	0	1980	44	0
8	Cg	1970	0	1980	38	0
8	Cq	1970	0	1980	37	0
8	Da	1970	0	1980	51	0
8	Dk	1970	0	1980	44	0
8	Du	1970	0	1980	43	0
8	Ee	1970	0	1980	43	0
8	Eo	1970	0	1980	42	0
8	Ey	1970	0	1980	35	0
9	Aj	562	0	545	16	0
9	At	562	0	545	17	0
9	Bd	562	0	545	12	0
9	Bn	562	0	545	16	0
9	Bx	562	0	545	22	0
9	Ch	562	0	545	17	0
9	Cr	562	0	545	15	0
9	Db	562	0	545	22	0
9	Dl	562	0	545	19	0
9	Dv	562	0	545	16	0
9	Ef	562	0	545	17	0
9	Ep	562	0	545	15	0
9	Ez	562	0	545	21	0
All	All	147498	0	148889	2688	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (2688) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:As:107:PRO:HG2	8:As:209:MET:HG2	1.52	0.89
8:Ai:107:PRO:HG2	8:Ai:209:MET:HG2	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bi:75:ASN:HD22	1:Bi:75:ASN:C	1.78	0.89
4:Cv:45:MET:HB3	4:Cv:62:ASN:HD21	1.38	0.88
3: Ei:149:ASN:O	3: Ei:149:ASN:ND2	2.06	0.88
1:Bi:75:ASN:O	1:Bi:75:ASN:ND2	2.06	0.87
2:Ct:50:ASP:HB3	4:Cv:45:MET:HE3	1.54	0.86
8:Cg:107:PRO:HG2	8:Cg:209:MET:HG2	1.57	0.86
3:Dy:115:ARG:HD3	3:Dy:117:ARG:HH22	1.41	0.86
8:Ee:107:PRO:HG2	8:Ee:209:MET:HG2	1.57	0.85
4:Ad:45:MET:HB3	4:Ad:62:ASN:HD21	1.40	0.85
8:Du:107:PRO:HG2	8:Du:209:MET:HG2	1.55	0.85
8:As:218:MET:HE3	8:As:220:MET:HE3	1.59	0.85
8:Da:107:PRO:HG2	8:Da:209:MET:HG2	1.59	0.84
9:Aj:27:LYS:HZ2	9:Aj:29:ARG:H	1.26	0.84
9:Db:27:LYS:HZ2	9:Db:29:ARG:H	1.26	0.83
9:Ez:46:LEU:HD11	9:Ez:59:LYS:HD3	1.60	0.83
3:Ac:196:MET:HE3	3:Ac:220:ALA:HB1	1.61	0.82
9:Dl:27:LYS:HZ2	9:Dl:29:ARG:H	1.26	0.82
9:Cr:27:LYS:HZ2	9:Cr:29:ARG:H	1.27	0.82
3:Ei:267:ASN:HB3	3:Ei:268:HIS:HD2	1.45	0.82
1:Be:62:ILE:HD13	8:Bm:263:ARG:HE	1.43	0.82
9:At:27:LYS:HZ2	9:At:29:ARG:H	1.26	0.82
9:Bx:27:LYS:HZ2	9:Bx:29:ARG:H	1.27	0.82
4:Ej:63:GLY:HA3	1:Eq:27:LYS:HB2	1.60	0.81
9:Bd:27:LYS:HZ2	9:Bd:29:ARG:H	1.28	0.81
8:Bw:107:PRO:HG2	8:Bw:209:MET:HG2	1.62	0.81
9:Ch:27:LYS:HZ2	9:Ch:29:ARG:H	1.28	0.81
1:Ci:62:ILE:HD13	8:Cq:263:ARG:HE	1.45	0.81
4:Cb:76:MET:HG3	6:Ce:299:GLY:HA2	1.61	0.81
2:Er:166:THR:HG22	2:Er:168:TYR:H	1.45	0.81
4:An:63:GLY:HA3	1:Au:27:LYS:HB2	1.63	0.81
9:Dv:27:LYS:HZ2	9:Dv:29:ARG:H	1.28	0.80
9:Ef:27:LYS:HZ2	9:Ef:29:ARG:H	1.30	0.80
6:Em:275:SER:HA	8:Ey:126:ARG:HG2	1.64	0.80
9:Ep:27:LYS:HZ2	9:Ep:29:ARG:H	1.28	0.80
2:Dn:166:THR:HG22	2:Dn:168:TYR:H	1.45	0.80
4:Dp:63:GLY:HA3	1:Dw:27:LYS:HB2	1.63	0.80
4:Ej:76:MET:HG3	6:Em:299:GLY:HA2	1.63	0.80
1:Cs:29:PRO:HG2	7:Cz:225:GLN:HA	1.64	0.79
4:Ax:63:GLY:HA3	1:Be:27:LYS:HB2	1.64	0.79
1:Aa:27:LYS:HB2	4:Et:63:GLY:HA3	1.64	0.79
4:Br:76:MET:HG3	6:Bu:299:GLY:HA2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3: Ei:149:ASN:HD22	3: Ei:149:ASN:C	1.91	0.78
9: Bn:27:LYS:HZ2	9: Bn:29:ARG:H	1.31	0.78
2: Bp:166:THR:HG22	2: Bp:168:TYR:H	1.47	0.78
5: El:233:ARG:HD3	5: El:234:GLU:H	1.48	0.78
9: Aj:47:LEU:HB3	9: Aj:91:ALA:HB3	1.65	0.78
4: Ad:76:MET:HG3	6: Ag:299:GLY:HA2	1.65	0.77
4: Bh:63:GLY:HA3	1: Bo:27:LYS:HB2	1.67	0.77
1: By:29:PRO:HG2	7: Cf:225:GLN:HA	1.66	0.77
2: Av:166:THR:HG22	2: Av:168:TYR:H	1.50	0.77
4: Br:63:GLY:HA3	1: By:27:LYS:HB2	1.65	0.77
6: Cy:324:TRP:HA	6: Cy:339:MET:HB3	1.65	0.77
2: Bz:166:THR:HG22	2: Bz:168:TYR:H	1.47	0.77
4: Dp:76:MET:HG3	6: Ds:299:GLY:HA2	1.67	0.76
4: Df:63:GLY:HA3	1: Dm:27:LYS:HB2	1.66	0.76
2: Ab:50:ASP:HB3	4: Ad:45:MET:HE3	1.65	0.76
4: Cv:63:GLY:HA3	1: Dc:27:LYS:HB2	1.67	0.76
4: Ad:63:GLY:HA3	1: Ak:27:LYS:HB2	1.66	0.76
8: Bc:271:ASN:HB2	9: Bd:53:SER:HA	1.67	0.76
5: Bj:233:ARG:HD3	5: Bj:234:GLU:H	1.49	0.75
4: Cl:63:GLY:HA3	1: Cs:27:LYS:HB2	1.69	0.75
2: Bp:50:ASP:HB3	4: Br:45:MET:HE3	1.67	0.75
2: Cj:65:ILE:HD12	2: Cj:78:ILE:HG23	1.68	0.75
4: Df:76:MET:HG3	6: Di:299:GLY:HA2	1.67	0.75
4: Ej:45:MET:HB3	4: Ej:62:ASN:HD21	1.50	0.75
1: Dw:62:ILE:HD12	8: Ee:263:ARG:HE	1.52	0.74
2: Eh:166:THR:HG22	2: Eh:168:TYR:H	1.52	0.74
7: Bb:118:GLU:HG3	7: Bb:123:ARG:HG2	1.67	0.74
8: Bw:276:PHE:HE2	9: Bx:79:ILE:HG21	1.52	0.74
2: Dd:50:ASP:HB3	4: Df:45:MET:HE3	1.67	0.74
4: Cv:76:MET:HG3	6: Cy:299:GLY:HA2	1.69	0.74
8: Bw:271:ASN:HB2	9: Bx:53:SER:HA	1.71	0.73
1: Eq:62:ILE:HD13	8: Ey:263:ARG:HE	1.52	0.73
4: Dz:63:GLY:HA3	1: Eg:27:LYS:HB2	1.71	0.73
1: Be:29:PRO:HG2	7: Bl:225:GLN:HA	1.68	0.73
1: Dw:55:MET:HE1	1: Ea:55:MET:HG3	1.69	0.73
4: Cb:63:GLY:HA3	1: Ci:27:LYS:HB2	1.69	0.73
2: Av:65:ILE:HD12	2: Av:78:ILE:HG23	1.70	0.72
4: Dp:62:ASN:HB3	1: Dw:26:LYS:HG2	1.71	0.71
1: Dm:85:VAL:HG12	2: Dn:153:ILE:HG23	1.71	0.71
1: Cs:62:ILE:HD12	8: Da:263:ARG:HE	1.56	0.71
4: Dp:45:MET:HB3	4: Dp:62:ASN:HD21	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Da:146:THR:HG23	8:Da:148:ARG:H	1.56	0.71
8:Bw:273:LEU:HG	8:Bw:274:GLU:HG2	1.73	0.70
1:Ak:29:PRO:HG2	7:Ar:225:GLN:HA	1.72	0.70
3:Am:280:TYR:HB3	3:Am:301:MET:HG3	1.74	0.70
3:De:110:THR:HG22	3:De:112:PHE:H	1.57	0.70
6:Ag:297:VAL:HG22	6:Ag:358:VAL:HG22	1.73	0.70
8:Ee:225:TYR:HB2	8:Ee:251:ALA:HB3	1.72	0.70
7:Ex:54:ARG:HB3	7:Ex:57:VAL:HG22	1.74	0.70
3:Ei:110:THR:HG22	3:Ei:112:PHE:H	1.57	0.70
1:Be:75:ASN:HD22	1:Be:80:GLN:HE21	1.40	0.69
8:Cg:225:TYR:HB2	8:Cg:251:ALA:HB3	1.74	0.69
9:Db:47:LEU:HB3	9:Db:91:ALA:HB3	1.73	0.69
3:Am:110:THR:HG22	3:Am:112:PHE:H	1.57	0.69
7:Cp:55:ARG:HH12	7:Cp:153:ARG:CZ	2.05	0.69
9:Ep:46:LEU:HD11	9:Ep:59:LYS:HD3	1.73	0.69
6:Bu:275:SER:HA	8:Cg:126:ARG:HD3	1.74	0.69
8:Da:225:TYR:HB2	8:Da:251:ALA:HB3	1.74	0.69
8:Ey:273:LEU:HG	8:Ey:274:GLU:HG2	1.74	0.69
1:Ay:97:ARG:HD2	8:Bm:263:ARG:HH22	1.55	0.69
7:Ar:54:ARG:HB3	7:Ar:57:VAL:HG22	1.75	0.69
3:Do:228:VAL:HG11	3:Do:231:LEU:HB2	1.75	0.69
2:Dx:56:MET:HE1	2:Dx:108:GLN:HG3	1.74	0.69
8:Ey:146:THR:HG23	8:Ey:148:ARG:H	1.58	0.69
6:Ba:275:SER:HA	8:Bm:126:ARG:HD3	1.75	0.69
3:De:280:TYR:HB3	3:De:301:MET:HG3	1.74	0.69
3:Ei:280:TYR:HB3	3:Ei:301:MET:HG3	1.75	0.69
2:Bf:166:THR:HG22	2:Bf:168:TYR:H	1.58	0.68
2:Bp:65:ILE:HD12	2:Bp:78:ILE:HG23	1.75	0.68
3:Ac:110:THR:HG22	3:Ac:112:PHE:H	1.58	0.68
2:Bf:56:MET:HE1	2:Bf:108:GLN:HG3	1.73	0.68
6:Ba:328:MET:HG2	8:Bm:116:THR:HG22	1.74	0.68
8:Bm:146:THR:HG23	8:Bm:148:ARG:H	1.59	0.68
4:Et:76:MET:HE3	6:Ew:299:GLY:HA2	1.76	0.68
8:Ai:273:LEU:HG	8:Ai:274:GLU:HG2	1.76	0.68
8:Ai:126:ARG:HD3	6:Ew:275:SER:HA	1.76	0.68
8:Dk:146:THR:HG23	8:Dk:148:ARG:H	1.58	0.68
3:Bq:110:THR:HG22	3:Bq:112:PHE:H	1.59	0.68
8:Du:146:THR:HG23	8:Du:148:ARG:H	1.59	0.68
8:Eo:273:LEU:HG	8:Eo:274:GLU:HG2	1.75	0.68
8:As:225:TYR:HB2	8:As:251:ALA:HB3	1.74	0.68
3:Ca:110:THR:HG22	3:Ca:112:PHE:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Cz:54:ARG:HB3	7:Cz:57:VAL:HG22	1.74	0.68
3:Dy:110:THR:HG22	3:Dy:112:PHE:H	1.58	0.68
3:Dy:117:ARG:NH1	3:Dy:117:ARG:HB2	2.09	0.68
3:Aw:110:THR:HG22	3:Aw:112:PHE:H	1.59	0.68
8:Bm:273:LEU:HG	8:Bm:274:GLU:HG2	1.75	0.68
8:Da:273:LEU:HG	8:Da:274:GLU:HG2	1.76	0.68
8:Cq:195:LEU:O	8:Cq:199:ILE:HG13	1.94	0.67
3:Do:303:GLU:HB2	3:Do:306:GLN:HG3	1.76	0.67
7:Cp:118:GLU:HG3	7:Cp:123:ARG:HG2	1.76	0.67
1:Dw:162:TYR:HD1	8:Ee:247:LEU:HD11	1.59	0.67
7:En:60:VAL:O	7:En:64:THR:HG23	1.93	0.67
1:Eq:162:TYR:HD1	8:Ey:247:LEU:HD11	1.58	0.67
6:Aq:275:SER:HA	8:Bc:126:ARG:HD3	1.75	0.67
3:Es:110:THR:HG22	3:Es:112:PHE:H	1.60	0.67
8:Bw:225:TYR:HB2	8:Bw:251:ALA:HB3	1.77	0.67
7:Cp:212:ASN:HD22	8:Cq:295:TRP:HZ3	1.40	0.67
8:Ai:225:TYR:HB2	8:Ai:251:ALA:HB3	1.75	0.67
4:Bh:99:GLY:HA3	4:Bh:114:LEU:HB2	1.76	0.67
3:Ck:84:ILE:HG13	3:Ck:86:LYS:HZ2	1.60	0.67
8:Cq:273:LEU:HG	8:Cq:274:GLU:HG2	1.77	0.67
4:Cv:62:ASN:HB3	1:Dc:26:LYS:HG2	1.77	0.67
7:Ah:54:ARG:HB3	7:Ah:57:VAL:HG22	1.76	0.67
7:Ar:60:VAL:O	7:Ar:64:THR:HG23	1.94	0.67
8:Dk:225:TYR:HB2	8:Dk:251:ALA:HB3	1.76	0.67
7:Bl:212:ASN:HD22	8:Bm:295:TRP:HZ3	1.43	0.67
7:Dt:54:ARG:HB3	7:Dt:57:VAL:HG22	1.77	0.67
7:Bb:54:ARG:HB3	7:Bb:57:VAL:HG22	1.76	0.67
8:Du:273:LEU:HG	8:Du:274:GLU:HG2	1.77	0.67
3:Cu:110:THR:HG22	3:Cu:112:PHE:H	1.60	0.67
2:Dn:65:ILE:HD12	2:Dn:78:ILE:HG23	1.76	0.67
6:Ds:284:LEU:HD22	6:Ds:330:SER:HB3	1.77	0.67
3:Ei:267:ASN:HB3	3:Ei:268:HIS:CD2	2.29	0.67
6:Ce:275:SER:HA	8:Cq:126:ARG:HD3	1.77	0.66
8:Bc:273:LEU:HG	8:Bc:274:GLU:HG2	1.77	0.66
1:Bo:85:VAL:HG12	2:Bp:153:ILE:HG23	1.77	0.66
1:Dc:162:TYR:HD1	8:Dk:247:LEU:HD11	1.60	0.66
3:Ck:110:THR:HG22	3:Ck:112:PHE:H	1.60	0.66
2:Dx:65:ILE:HD12	2:Dx:78:ILE:HG23	1.77	0.66
3:Bg:110:THR:HG22	3:Bg:112:PHE:H	1.59	0.66
7:En:54:ARG:HB3	7:En:57:VAL:HG22	1.77	0.66
7:Bl:54:ARG:HB3	7:Bl:57:VAL:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Bq:303:GLU:HB2	3:Bq:306:GLN:HG3	1.77	0.66
4:Br:99:GLY:HA3	4:Br:114:LEU:HB2	1.76	0.66
5:Cd:233:ARG:HD3	5:Cd:234:GLU:H	1.60	0.66
4:Df:99:GLY:HA3	4:Df:114:LEU:HB2	1.78	0.66
3:Dy:313:ASP:H	3:Dy:316:ASN:HB2	1.59	0.66
8:Eo:225:TYR:HB2	8:Eo:251:ALA:HB3	1.76	0.66
8:Ai:146:THR:HG23	8:Ai:148:ARG:H	1.59	0.66
3:Bg:84:ILE:HG13	3:Bg:86:LYS:HZ2	1.61	0.66
8:Cg:273:LEU:HG	8:Cg:274:GLU:HG2	1.78	0.66
4:Et:99:GLY:HA3	4:Et:114:LEU:HB2	1.77	0.66
4:Ax:99:GLY:HA3	4:Ax:114:LEU:HB2	1.76	0.66
8:Bm:225:TYR:HB2	8:Bm:251:ALA:HB3	1.77	0.66
7:Cf:118:GLU:HG3	7:Cf:123:ARG:HG2	1.78	0.66
3:Cu:303:GLU:HB2	3:Cu:306:GLN:HG3	1.78	0.66
3:De:84:ILE:HG13	3:De:86:LYS:HZ2	1.60	0.66
3:Do:313:ASP:H	3:Do:316:ASN:HB2	1.61	0.66
4:Dz:99:GLY:HA3	4:Dz:114:LEU:HB2	1.78	0.66
4:An:99:GLY:HA3	4:An:114:LEU:HB2	1.76	0.66
1:Bs:39:ILE:O	1:Bs:43:GLU:HG3	1.96	0.66
1:By:62:ILE:HD12	8:Cg:263:ARG:HE	1.61	0.66
8:Ee:273:LEU:HG	8:Ee:274:GLU:HG2	1.76	0.66
2:Eh:130:ARG:HH11	2:Eh:130:ARG:HG3	1.60	0.66
8:As:273:LEU:HG	8:As:274:GLU:HG2	1.78	0.66
1:Dc:98:ILE:HG23	1:Dc:128:LEU:HD22	1.78	0.66
3:Cu:196:MET:HE3	3:Cu:220:ALA:HB1	1.77	0.65
6:Cy:328:MET:HG2	8:Dk:116:THR:HG22	1.77	0.65
8:Bc:146:THR:HG23	8:Bc:148:ARG:H	1.61	0.65
3:Ck:176:VAL:HG22	3:Ck:195:ASP:HB2	1.78	0.65
3:Do:110:THR:HG22	3:Do:112:PHE:H	1.62	0.65
7:Ah:60:VAL:O	7:Ah:64:THR:HG23	1.97	0.65
8:Bc:225:TYR:HB2	8:Bc:251:ALA:HB3	1.78	0.65
1:Bo:162:TYR:HD1	8:Bw:247:LEU:HD11	1.61	0.65
2:Cj:75:LEU:HD12	2:Cj:183:THR:HG22	1.79	0.65
9:Db:48:VAL:HG21	9:Db:57:ILE:HD11	1.78	0.65
1:Eq:29:PRO:HG3	7:Ex:225:GLN:HA	1.79	0.65
3:Ck:250:ARG:HD3	3:Ck:268:HIS:HB2	1.79	0.65
4:Cv:99:GLY:HA3	4:Cv:114:LEU:HB2	1.78	0.65
6:Ce:297:VAL:HG22	6:Ce:358:VAL:HG22	1.79	0.65
1:Cw:121:ILE:HG21	1:Cw:131:ILE:HG23	1.78	0.65
8:Eo:146:THR:HG23	8:Eo:148:ARG:H	1.60	0.65
1:Cs:94:LEU:HD23	1:Cs:119:ILE:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Ds:275:SER:HA	8:Ee:126:ARG:HD3	1.78	0.65
1:Eg:52:MET:HE2	1:Ek:52:MET:SD	2.37	0.65
2:Ab:65:ILE:HD12	2:Ab:78:ILE:HG23	1.78	0.65
5:Ap:223:ILE:HD11	5:Ap:227:GLY:HA2	1.79	0.65
6:Co:275:SER:HA	8:Da:126:ARG:HD3	1.78	0.65
2:Er:65:ILE:HD12	2:Er:78:ILE:HG23	1.77	0.65
7:Ah:118:GLU:HG3	7:Ah:123:ARG:HG2	1.77	0.65
2:Cj:51:ALA:HB1	4:Cl:44:LYS:HE3	1.79	0.65
2:Dd:75:LEU:HD12	2:Dd:183:THR:HG22	1.77	0.65
6:Di:275:SER:HA	8:Du:126:ARG:HD3	1.79	0.65
7:Dj:54:ARG:HB3	7:Dj:57:VAL:HG22	1.77	0.65
1:Dm:162:TYR:HD1	8:Du:247:LEU:HD11	1.61	0.65
6:Bk:275:SER:HA	8:Bw:126:ARG:HD3	1.79	0.65
6:Co:297:VAL:HG22	6:Co:358:VAL:HG22	1.79	0.65
7:Dj:51:GLN:HG3	7:Dj:52:PRO:HD2	1.78	0.65
1:Be:87:TRP:O	1:Be:120:SER:HA	1.97	0.65
7:Dt:60:VAL:O	7:Dt:64:THR:HG23	1.97	0.65
1:Aa:75:ASN:HD22	1:Aa:80:GLN:HE21	1.44	0.64
8:Cq:146:THR:HG23	8:Cq:148:ARG:H	1.62	0.64
3:Dy:84:ILE:HG13	3:Dy:86:LYS:HZ2	1.61	0.64
7:Ed:54:ARG:HB3	7:Ed:57:VAL:HG22	1.77	0.64
7:Ar:212:ASN:HD22	8:As:295:TRP:HZ3	1.43	0.64
2:Bf:50:ASP:HB3	4:Bh:45:MET:HE3	1.78	0.64
2:Bf:65:ILE:HD12	2:Bf:78:ILE:HG23	1.79	0.64
7:Cf:54:ARG:HB3	7:Cf:57:VAL:HG22	1.77	0.64
4:Cl:99:GLY:HA3	4:Cl:114:LEU:HB2	1.79	0.64
8:Du:225:TYR:HB2	8:Du:251:ALA:HB3	1.79	0.64
6:Ec:275:SER:HA	8:Eo:126:ARG:HD3	1.78	0.64
3:Ac:199:LYS:HG2	3:Ac:219:ALA:HB3	1.80	0.64
1:Ak:162:TYR:HD1	8:As:247:LEU:HD11	1.62	0.64
6:Aq:284:LEU:HD22	6:Aq:330:SER:HB3	1.80	0.64
1:Bi:75:ASN:C	1:Bi:75:ASN:ND2	2.54	0.64
8:Cq:225:TYR:HB2	8:Cq:251:ALA:HB3	1.79	0.64
3:Do:280:TYR:HB3	3:Do:301:MET:HG3	1.78	0.64
1:Au:162:TYR:HD1	8:Bc:247:LEU:HD11	1.61	0.64
3:Bq:84:ILE:HG13	3:Bq:86:LYS:HZ2	1.62	0.64
6:Bu:284:LEU:HD22	6:Bu:330:SER:HB3	1.80	0.64
7:Cz:212:ASN:HD22	8:Da:295:TRP:HZ3	1.45	0.64
1:Dc:52:MET:HE2	1:Dg:52:MET:SD	2.38	0.64
1:Eg:87:TRP:O	1:Eg:120:SER:HA	1.97	0.64
3:Ck:313:ASP:H	3:Ck:316:ASN:HB2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dc:67:LYS:HB3	1:Dg:62:ILE:HD11	1.79	0.64
1:Aa:87:TRP:O	1:Aa:120:SER:HA	1.97	0.64
1:Ci:87:TRP:O	1:Ci:120:SER:HA	1.97	0.64
3:Ac:313:ASP:H	3:Ac:316:ASN:HB2	1.63	0.64
7:Ex:60:VAL:O	7:Ex:64:THR:HG23	1.97	0.64
2:Dn:67:VAL:HG22	2:Dn:76:ILE:HG23	1.80	0.64
1:Ea:160:LYS:HD3	1:Ea:160:LYS:H	1.62	0.64
2:Eh:65:ILE:HD12	2:Eh:78:ILE:HG23	1.80	0.64
4:Ej:99:GLY:HA3	4:Ej:114:LEU:HB2	1.80	0.64
1:Eq:87:TRP:O	1:Eq:120:SER:HA	1.97	0.64
6:Ba:284:LEU:HD22	6:Ba:330:SER:HB3	1.79	0.64
7:Bb:212:ASN:HD22	8:Bc:295:TRP:HZ3	1.45	0.64
2:Bp:45:VAL:HG23	2:Bp:48:ALA:HB3	1.80	0.63
2:Ct:65:ILE:HD12	2:Ct:78:ILE:HG23	1.80	0.63
1:Aa:162:TYR:HD1	8:Ai:247:LEU:HD11	1.61	0.63
6:Bk:297:VAL:HG22	6:Bk:358:VAL:HG22	1.80	0.63
7:Dt:118:GLU:HG3	7:Dt:123:ARG:HG2	1.79	0.63
8:Ee:146:THR:HG23	8:Ee:148:ARG:H	1.63	0.63
8:Cg:224:PRO:HB3	8:Cg:253:PRO:HD3	1.80	0.63
3:Es:199:LYS:HG2	3:Es:219:ALA:HB3	1.81	0.63
8:As:146:THR:HG23	8:As:148:ARG:H	1.62	0.63
6:Ce:284:LEU:HD22	6:Ce:330:SER:HB3	1.80	0.63
3:Cu:300:ASP:OD1	3:Cu:302:ARG:HG3	1.99	0.63
3:Aw:199:LYS:HG2	3:Aw:219:ALA:HB3	1.80	0.63
6:Bk:285:GLU:HG3	8:Bw:204:GLU:HG3	1.80	0.63
3:Bq:292:MET:HE2	3:Bq:298:VAL:H	1.63	0.63
7:Cp:54:ARG:HB3	7:Cp:57:VAL:HG22	1.80	0.63
3:Cu:84:ILE:HG13	3:Cu:86:LYS:HZ2	1.62	0.63
8:Ey:225:TYR:HB2	8:Ey:251:ALA:HB3	1.79	0.63
1:Be:98:ILE:HG23	1:Be:128:LEU:HD22	1.81	0.63
8:Dk:273:LEU:HG	8:Dk:274:GLU:HG2	1.80	0.63
1:Bo:87:TRP:O	1:Bo:120:SER:HA	1.98	0.63
6:Bu:285:GLU:HG3	8:Cg:204:GLU:HG3	1.79	0.63
8:Cg:146:THR:HG23	8:Cg:148:ARG:H	1.64	0.63
1:Cm:39:ILE:O	1:Cm:43:GLU:HG3	1.98	0.63
5:Bj:210:TYR:HB2	5:Bj:241:TYR:HE2	1.64	0.63
1:By:98:ILE:HG23	1:By:128:LEU:HD22	1.81	0.63
6:Em:284:LEU:HD22	6:Em:330:SER:HB3	1.81	0.63
8:As:288:ILE:HA	9:At:79:ILE:HG12	1.81	0.62
1:Cc:44:ALA:O	1:Cc:48:VAL:HG23	1.99	0.62
3:Dy:176:VAL:HG22	3:Dy:195:ASP:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:85:VAL:HG12	2:Al:153:ILE:HG23	1.80	0.62
3:De:313:ASP:H	3:De:316:ASN:HB2	1.62	0.62
1:Dm:87:TRP:O	1:Dm:120:SER:HA	1.99	0.62
4:Ad:99:GLY:HA3	4:Ad:114:LEU:HB2	1.80	0.62
4:Ax:45:MET:HG2	4:Ax:62:ASN:HD21	1.64	0.62
2:Bp:67:VAL:HG22	2:Bp:76:ILE:HG23	1.81	0.62
5:Cd:210:TYR:HB2	5:Cd:241:TYR:HE2	1.64	0.62
2:Dd:65:ILE:HD12	2:Dd:78:ILE:HG23	1.81	0.62
1:Au:87:TRP:O	1:Au:120:SER:HA	2.00	0.62
7:Bl:51:GLN:HG3	7:Bl:52:PRO:HD2	1.80	0.62
2:Er:45:VAL:HG23	2:Er:48:ALA:HB3	1.81	0.62
1:Bi:39:ILE:O	1:Bi:43:GLU:HG3	2.00	0.62
2:Bz:52:THR:O	2:Bz:56:MET:HG3	1.99	0.62
1:Cs:162:TYR:HD1	8:Da:247:LEU:HD11	1.63	0.62
4:Dp:99:GLY:HA3	4:Dp:114:LEU:HB2	1.82	0.62
1:Au:62:ILE:HD13	8:Bc:263:ARG:HE	1.65	0.62
2:Dx:114:ILE:HG23	2:Dx:184:PHE:HB3	1.80	0.62
3:Ei:313:ASP:H	3:Ei:316:ASN:HB2	1.65	0.62
7:Bl:134:MET:HE2	7:Bl:141:ASN:HA	1.81	0.62
6:Bu:297:VAL:HG22	6:Bu:358:VAL:HG22	1.81	0.62
2:Bz:65:ILE:HD12	2:Bz:78:ILE:HG23	1.80	0.62
1:Cc:97:ARG:HH11	1:Cc:100:LYS:HZ3	1.46	0.62
1:Dg:97:ARG:HH11	1:Dg:100:LYS:HZ3	1.46	0.62
5:Dr:210:TYR:HB2	5:Dr:241:TYR:HE2	1.65	0.62
2:Al:75:LEU:HD12	2:Al:183:THR:HG22	1.82	0.62
3:Bq:228:VAL:HG11	3:Bq:231:LEU:HB2	1.81	0.62
1:Dc:87:TRP:O	1:Dc:120:SER:HA	1.99	0.61
3:Ei:196:MET:HE3	3:Ei:220:ALA:HB1	1.82	0.61
3:Bq:313:ASP:H	3:Bq:316:ASN:HB2	1.63	0.61
3:Ca:313:ASP:H	3:Ca:316:ASN:HB2	1.63	0.61
1:Cw:74:PRO:HD2	1:Cw:129:ALA:HB1	1.83	0.61
3:Ca:176:VAL:HG22	3:Ca:195:ASP:HB2	1.81	0.61
4:Cb:99:GLY:HA3	4:Cb:114:LEU:HB2	1.82	0.61
2:Dx:166:THR:HG22	2:Dx:168:TYR:H	1.65	0.61
1:Eg:67:LYS:HB3	1:Ek:62:ILE:HD11	1.81	0.61
3:Ei:300:ASP:OD1	3:Ei:302:ARG:HG3	2.00	0.61
1:Eq:98:ILE:HG23	1:Eq:128:LEU:HD22	1.82	0.61
2:Ab:166:THR:HG22	2:Ab:168:TYR:H	1.65	0.61
6:Co:328:MET:HE2	8:Da:116:THR:HG23	1.80	0.61
6:Ec:284:LEU:HD22	6:Ec:330:SER:HB3	1.82	0.61
6:Ag:275:SER:HA	8:As:126:ARG:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Bx:48:VAL:HG21	9:Bx:57:ILE:HD11	1.81	0.61
1:Cm:74:PRO:HD2	1:Cm:129:ALA:HB1	1.82	0.61
2:Ct:166:THR:HG22	2:Ct:168:TYR:H	1.65	0.61
5:Ap:210:TYR:HB2	5:Ap:241:TYR:HE2	1.65	0.61
6:Bk:284:LEU:HD22	6:Bk:330:SER:HB3	1.83	0.61
8:Bw:146:THR:HG23	8:Bw:148:ARG:H	1.64	0.61
3:Ca:250:ARG:HD3	3:Ca:268:HIS:HB2	1.82	0.61
5:Dh:210:TYR:HB2	5:Dh:241:TYR:HE2	1.66	0.61
3:Do:253:VAL:HG21	3:Do:263:ILE:HG21	1.82	0.61
1:Dw:29:PRO:HG3	7:Ed:225:GLN:HA	1.83	0.61
9:Ez:27:LYS:HZ2	9:Ez:29:ARG:H	1.49	0.61
8:Ai:271:ASN:HB2	9:Aj:53:SER:HA	1.82	0.61
1:Ci:162:TYR:HD1	8:Cq:247:LEU:HD11	1.64	0.61
1:Dw:85:VAL:HG12	2:Dx:153:ILE:HG23	1.82	0.61
8:Ey:271:ASN:HB2	9:Ez:53:SER:HA	1.80	0.61
2:Bf:75:LEU:HD12	2:Bf:183:THR:HG22	1.82	0.61
1:Eq:94:LEU:HD23	1:Eq:119:ILE:HD11	1.83	0.61
7:Ex:234:PHE:CE2	9:Ez:29:ARG:HG2	2.36	0.61
2:Al:65:ILE:HD12	2:Al:78:ILE:HG23	1.80	0.61
1:By:65:PRO:HD3	1:Cc:58:VAL:HG22	1.82	0.61
4:Ej:46:GLY:HA3	4:Ej:61:ASN:HB2	1.82	0.61
1:Cw:160:LYS:HD3	1:Cw:160:LYS:H	1.65	0.61
3:Ac:117:ARG:HB3	3:Ac:117:ARG:NH1	2.16	0.60
2:Av:45:VAL:HG23	2:Av:48:ALA:HB3	1.82	0.60
1:Be:28:PRO:HD3	7:Bl:115:GLN:HB2	1.83	0.60
1:Ea:121:ILE:HG21	1:Ea:131:ILE:HG23	1.83	0.60
3:Aw:84:ILE:HG13	3:Aw:86:LYS:HZ2	1.66	0.60
7:Bb:165:VAL:HG13	7:Bb:231:ILE:HG12	1.83	0.60
5:Ev:223:ILE:HD12	5:Ev:224:GLY:H	1.65	0.60
3:Es:191:LEU:HD21	3:Es:194:LEU:HD12	1.83	0.60
3:Es:313:ASP:H	3:Es:316:ASN:HB2	1.66	0.60
1:Ao:74:PRO:HD2	1:Ao:129:ALA:HB1	1.83	0.60
1:Au:94:LEU:HD23	1:Au:119:ILE:HD11	1.83	0.60
3:Ca:84:ILE:HG13	3:Ca:86:LYS:HZ2	1.65	0.60
8:Cg:271:ASN:HB2	9:Ch:53:SER:HA	1.83	0.60
1:Ci:94:LEU:HD23	1:Ci:119:ILE:HD11	1.83	0.60
3:Ei:199:LYS:HG2	3:Ei:219:ALA:HB3	1.84	0.60
1:Ek:75:ASN:HA	1:Ek:80:GLN:HE22	1.66	0.60
3:Ca:228:VAL:HG11	3:Ca:231:LEU:HB2	1.84	0.60
3:Cu:199:LYS:HG2	3:Cu:219:ALA:HB3	1.83	0.60
6:Cy:284:LEU:HD22	6:Cy:330:SER:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Eq:85:VAL:HG12	2:Er:153:ILE:HG23	1.83	0.60
2:Ab:152:ARG:HD2	6:Ag:352:LYS:HB2	1.82	0.60
3:Am:199:LYS:HG2	3:Am:219:ALA:HB3	1.84	0.60
1:By:87:TRP:O	1:By:120:SER:HA	2.01	0.60
1:Dw:87:TRP:O	1:Dw:120:SER:HA	2.02	0.60
3:Bg:228:VAL:HG11	3:Bg:231:LEU:HB2	1.83	0.60
1:Bs:74:PRO:HD2	1:Bs:129:ALA:HB1	1.84	0.60
8:Bw:108:PRO:HD3	8:Bw:138:ALA:HB2	1.83	0.60
2:Dx:67:VAL:HG22	2:Dx:76:ILE:HG23	1.83	0.60
6:Ag:284:LEU:HD22	6:Ag:330:SER:HB3	1.83	0.60
6:Cy:275:SER:HA	8:Dk:126:ARG:HD3	1.83	0.60
1:Dc:94:LEU:HD23	1:Dc:119:ILE:HD11	1.83	0.60
6:Ds:346:LEU:HD12	6:Ds:355:GLN:HG2	1.83	0.60
3:Dy:260:VAL:HG22	3:Dy:278:ASP:HB2	1.83	0.60
7:Ex:212:ASN:HD22	8:Ey:295:TRP:HZ3	1.48	0.60
7:Bv:134:MET:HE2	7:Bv:141:ASN:HA	1.83	0.60
1:By:28:PRO:HD3	7:Cf:115:GLN:HB2	1.84	0.60
5:Dh:233:ARG:HD3	5:Dh:234:GLU:H	1.67	0.60
1:Dq:97:ARG:HD2	8:Ee:263:ARG:HH22	1.66	0.60
5:Cn:223:ILE:HD11	5:Cn:227:GLY:HA2	1.84	0.60
1:Dq:74:PRO:HD2	1:Dq:129:ALA:HB1	1.84	0.60
8:Bm:214:LYS:O	8:Bm:218:MET:HG3	2.02	0.59
6:Aq:285:GLU:HG3	8:Bc:204:GLU:HG3	1.84	0.59
5:Bj:247:ILE:HG22	5:Bj:254:ILE:HG13	1.83	0.59
8:Bm:99:LEU:HD13	8:Bm:209:MET:HB2	1.84	0.59
1:Ci:98:ILE:HG23	1:Ci:128:LEU:HD22	1.85	0.59
2:Dx:45:VAL:HG11	4:Dz:57:ARG:HH22	1.67	0.59
7:Cz:165:VAL:HG13	7:Cz:231:ILE:HG12	1.82	0.59
3:De:253:VAL:HG21	3:De:263:ILE:HG21	1.82	0.59
9:Ef:76:VAL:HG12	9:Ef:86:SER:HA	1.83	0.59
8:Bc:224:PRO:HB3	8:Bc:253:PRO:HD3	1.83	0.59
1:Eg:94:LEU:HD23	1:Eg:119:ILE:HD11	1.83	0.59
4:Ej:62:ASN:HB3	1:Eq:26:LYS:HG2	1.84	0.59
1:Ek:121:ILE:HG21	1:Ek:131:ILE:HG23	1.85	0.59
6:Ew:284:LEU:HD22	6:Ew:330:SER:HB3	1.84	0.59
8:As:224:PRO:HB3	8:As:253:PRO:HD3	1.84	0.59
4:Ax:62:ASN:HB3	1:Be:26:LYS:HG2	1.83	0.59
6:Ba:346:LEU:HD12	6:Ba:355:GLN:HG2	1.85	0.59
5:Cn:210:TYR:HB2	5:Cn:241:TYR:HE2	1.67	0.59
3:Cu:313:ASP:H	3:Cu:316:ASN:HB2	1.66	0.59
5:Cx:210:TYR:HB2	5:Cx:241:TYR:HE2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:94:LEU:HD23	1:Aa:119:ILE:HD11	1.84	0.59
1:Ak:87:TRP:O	1:Ak:120:SER:HA	2.02	0.59
1:Be:65:PRO:HD3	1:Bi:58:VAL:HG22	1.85	0.59
1:Be:94:LEU:HD23	1:Be:119:ILE:HD11	1.84	0.59
1:Ci:85:VAL:HG12	2:Cj:153:ILE:HG23	1.83	0.59
4:Dz:56:GLY:HA2	4:Dz:71:THR:HG22	1.85	0.59
1:Eu:74:PRO:HD2	1:Eu:129:ALA:HB1	1.85	0.59
5:Ev:233:ARG:HD3	5:Ev:234:GLU:H	1.66	0.59
6:Ag:285:GLU:HG3	8:As:204:GLU:HG3	1.84	0.59
3:Am:29:GLU:HB3	3:Am:99:PRO:HG3	1.82	0.59
3:Aw:209:SER:HB3	3:Aw:228:VAL:HG22	1.85	0.59
3:Bq:199:LYS:HG2	3:Bq:219:ALA:HB3	1.85	0.59
1:Cc:74:PRO:HD2	1:Cc:129:ALA:HB1	1.85	0.59
6:Co:324:TRP:HA	6:Co:339:MET:HB3	1.84	0.59
1:Cs:87:TRP:O	1:Cs:120:SER:HA	2.02	0.59
3:Am:313:ASP:H	3:Am:316:ASN:HB2	1.67	0.59
1:Bi:74:PRO:HD2	1:Bi:129:ALA:HB1	1.85	0.59
6:Ew:297:VAL:HG11	6:Ew:302:ALA:HB3	1.84	0.59
7:Ex:169:THR:HG23	7:Ex:182:SER:HB3	1.84	0.59
1:Be:85:VAL:HG12	2:Bf:153:ILE:HG23	1.84	0.59
6:Ec:297:VAL:HG22	6:Ec:358:VAL:HG22	1.85	0.59
2:Eh:106:LEU:HD22	2:Eh:114:ILE:HD13	1.85	0.59
3:Es:176:VAL:HG22	3:Es:195:ASP:HB2	1.84	0.59
5:Bj:223:ILE:HD12	5:Bj:224:GLY:H	1.68	0.59
7:Bv:60:VAL:O	7:Bv:64:THR:HG23	2.03	0.59
5:Cd:223:ILE:HD11	5:Cd:227:GLY:HA2	1.84	0.59
1:Ea:74:PRO:HD2	1:Ea:129:ALA:HB1	1.85	0.59
3:Ei:250:ARG:HD3	3:Ei:268:HIS:HB2	1.85	0.59
3:Am:84:ILE:HG13	3:Am:86:LYS:HZ2	1.68	0.58
8:Bw:137:GLN:HG2	8:Bw:252:LEU:HD13	1.85	0.58
1:Dm:98:ILE:HG23	1:Dm:128:LEU:HD22	1.85	0.58
4:Et:46:GLY:HA3	4:Et:61:ASN:HB2	1.85	0.58
1:Ae:74:PRO:HD2	1:Ae:129:ALA:HB1	1.85	0.58
3:Am:253:VAL:HG21	3:Am:263:ILE:HG21	1.84	0.58
7:Bl:169:THR:HG23	7:Bl:182:SER:HB3	1.85	0.58
2:Cj:106:LEU:HD22	2:Cj:114:ILE:HD13	1.85	0.58
1:Dw:94:LEU:HD23	1:Dw:119:ILE:HD11	1.84	0.58
3:Es:292:MET:HE1	3:Es:320:PRO:HB3	1.84	0.58
3:Ac:209:SER:HB3	3:Ac:228:VAL:HG22	1.85	0.58
1:Au:85:VAL:HG12	2:Av:153:ILE:HG23	1.84	0.58
5:Az:230:LEU:HD12	5:Az:231:THR:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Bk:284:LEU:HD11	6:Bk:328:MET:HB3	1.85	0.58
1:Ek:74:PRO:HD2	1:Ek:129:ALA:HB1	1.85	0.58
1:Cc:39:ILE:O	1:Cc:43:GLU:HG3	2.02	0.58
1:Dc:41:LEU:HD22	8:Dk:90:LEU:HD21	1.85	0.58
1:By:162:TYR:CD2	8:Cg:247:LEU:HD11	2.38	0.58
2:Dn:45:VAL:HG11	4:Dp:57:ARG:HH22	1.69	0.58
8:Du:205:ASP:O	8:Du:209:MET:HE3	2.04	0.58
1:Au:65:PRO:HD3	1:Ay:58:VAL:HG22	1.85	0.58
3:Bg:313:ASP:H	3:Bg:316:ASN:HB2	1.69	0.58
5:Bt:210:TYR:HB2	5:Bt:241:TYR:HE2	1.69	0.58
9:Bx:76:VAL:HG12	9:Bx:86:SER:HA	1.85	0.58
8:Dk:137:GLN:HG2	8:Dk:252:LEU:HD13	1.86	0.58
6:Ag:284:LEU:HD11	6:Ag:328:MET:HB3	1.85	0.58
2:Bz:67:VAL:HG22	2:Bz:76:ILE:HG23	1.85	0.58
1:Cs:65:PRO:HD3	1:Cw:58:VAL:HG22	1.84	0.58
2:Er:106:LEU:HD22	2:Er:114:ILE:HD13	1.86	0.58
3:Ac:280:TYR:HB3	3:Ac:301:MET:HG3	1.85	0.58
8:Ai:299:ILE:HD12	2:Er:75:LEU:HB2	1.85	0.58
4:An:46:GLY:HA3	4:An:61:ASN:HB2	1.86	0.58
8:As:271:ASN:HB2	9:At:53:SER:HA	1.84	0.58
3:Ck:209:SER:HB3	3:Ck:228:VAL:HG22	1.85	0.58
3:Cu:253:VAL:HG21	3:Cu:263:ILE:HG21	1.84	0.58
1:Cw:119:ILE:HD12	1:Cw:135:ILE:HG12	1.86	0.58
6:Ba:320:LEU:HD11	6:Ba:348:SER:HB3	1.84	0.58
3:Bg:199:LYS:HG2	3:Bg:219:ALA:HB3	1.86	0.58
1:Ao:97:ARG:HH11	1:Ao:100:LYS:HZ3	1.51	0.58
4:Cv:84:CYS:HA	8:Da:154:ASP:HB3	1.86	0.58
2:Ct:45:VAL:HG11	4:Cv:57:ARG:HH22	1.69	0.57
3:De:257:ASP:HA	3:De:275:ASP:O	2.04	0.57
6:Di:346:LEU:HD12	6:Di:355:GLN:HG2	1.84	0.57
1:Dm:147:VAL:HG22	1:Dm:154:VAL:HG22	1.85	0.57
2:Dn:45:VAL:HG23	2:Dn:48:ALA:HB3	1.86	0.57
1:Dq:76:ALA:O	1:Dq:80:GLN:HG2	2.04	0.57
8:Du:271:ASN:HB2	9:Dv:53:SER:HA	1.85	0.57
3:Dy:173:LEU:HD12	3:Dy:174:GLN:N	2.19	0.57
4:Ej:56:GLY:HA2	4:Ej:71:THR:HG22	1.86	0.57
9:Ep:25:LEU:HG	9:Ep:67:ARG:CZ	2.34	0.57
1:Dq:39:ILE:O	1:Dq:43:GLU:HG3	2.04	0.57
3:Dy:250:ARG:HD3	3:Dy:268:HIS:HB2	1.85	0.57
3:Dy:280:TYR:HB3	3:Dy:301:MET:HG3	1.86	0.57
3:Am:52:VAL:HG13	3:Am:92:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:As:108:PRO:HD3	8:As:138:ALA:HB2	1.84	0.57
5:Az:223:ILE:HD12	5:Az:224:GLY:H	1.70	0.57
3:Ca:253:VAL:HG21	3:Ca:263:ILE:HG21	1.85	0.57
1:Eg:62:ILE:HD12	8:Eo:263:ARG:HE	1.69	0.57
1:Ek:119:ILE:HD12	1:Ek:135:ILE:HG12	1.86	0.57
1:Eq:55:MET:HE1	1:Eu:55:MET:HG3	1.85	0.57
2:Av:45:VAL:HG11	4:Ax:57:ARG:HH22	1.69	0.57
6:Ce:346:LEU:HD12	6:Ce:355:GLN:HG2	1.85	0.57
1:Dc:57:LYS:O	1:Dc:61:VAL:HG23	2.05	0.57
1:Dq:105:ARG:HB2	1:Dq:153:VAL:HG22	1.87	0.57
6:Aq:346:LEU:HD12	6:Aq:355:GLN:HG2	1.86	0.57
1:By:94:LEU:HD23	1:By:119:ILE:HD11	1.85	0.57
6:Cy:346:LEU:HD12	6:Cy:355:GLN:HG2	1.86	0.57
8:Eo:224:PRO:HB3	8:Eo:253:PRO:HD3	1.87	0.57
7:Ex:165:VAL:HG13	7:Ex:231:ILE:HG12	1.85	0.57
5:Az:216:ILE:HG13	5:Az:217:PRO:HD2	1.86	0.57
3:Bg:173:LEU:HD12	3:Bg:174:GLN:N	2.18	0.57
7:Cp:51:GLN:HG3	7:Cp:52:PRO:HD2	1.87	0.57
9:Cr:76:VAL:HG12	9:Cr:86:SER:HA	1.86	0.57
1:Aa:65:PRO:HD3	1:Ae:58:VAL:HG22	1.86	0.57
2:Ab:106:LEU:HD22	2:Ab:114:ILE:HD13	1.87	0.57
3:Ac:260:VAL:HG22	3:Ac:278:ASP:HB2	1.86	0.57
7:Ah:51:GLN:HG3	7:Ah:52:PRO:HD2	1.87	0.57
8:As:62:THR:O	8:As:66:VAL:HG12	2.04	0.57
1:By:54:GLU:O	1:By:58:VAL:HG12	2.05	0.57
1:Cs:85:VAL:HG12	2:Ct:153:ILE:HG23	1.86	0.57
1:Cs:147:VAL:HG22	1:Cs:154:VAL:HG22	1.86	0.57
6:Cy:284:LEU:HD11	6:Cy:328:MET:HB3	1.87	0.57
9:Db:25:LEU:HG	9:Db:67:ARG:CZ	2.35	0.57
1:Ak:65:PRO:HD3	1:Ao:58:VAL:HG22	1.86	0.57
1:Dm:77:TYR:OH	2:Dn:130:ARG:HD3	2.05	0.57
2:Dn:75:LEU:HD12	2:Dn:183:THR:HG22	1.87	0.57
8:Ee:214:LYS:O	8:Ee:218:MET:HG3	2.04	0.57
6:Em:297:VAL:HG22	6:Em:358:VAL:HG22	1.85	0.57
5:Ev:210:TYR:HB2	5:Ev:241:TYR:HE2	1.69	0.57
8:Bw:275:ARG:C	8:Bw:276:PHE:HD1	2.13	0.57
5:Dh:223:ILE:HD11	5:Dh:227:GLY:HA2	1.87	0.57
2:Ab:45:VAL:HG23	2:Ab:48:ALA:HB3	1.86	0.57
8:Ai:108:PRO:HD3	8:Ai:138:ALA:HB2	1.86	0.57
1:Ak:28:PRO:HD3	7:Ar:115:GLN:HB2	1.87	0.57
3:Aw:176:VAL:HG22	3:Aw:195:ASP:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ca:280:TYR:HB3	3:Ca:301:MET:HG3	1.87	0.57
2:Cj:114:ILE:HG23	2:Cj:184:PHE:HB3	1.87	0.57
3:Cu:292:MET:HE1	3:Cu:320:PRO:HB3	1.86	0.57
6:Di:285:GLU:HG3	8:Du:204:GLU:HG3	1.86	0.57
9:Ef:25:LEU:HG	9:Ef:67:ARG:CZ	2.34	0.57
1:Eg:65:PRO:HD3	1:Ek:58:VAL:HG22	1.87	0.57
7:Ah:169:THR:HG23	7:Ah:182:SER:HB3	1.85	0.56
7:Bb:169:THR:HG23	7:Bb:182:SER:HB3	1.87	0.56
8:Bm:271:ASN:HB2	9:Bn:53:SER:HA	1.86	0.56
6:Co:346:LEU:HD12	6:Co:355:GLN:HG2	1.85	0.56
1:Ek:97:ARG:HH11	1:Ek:100:LYS:HZ3	1.52	0.56
8:Eo:108:PRO:HD3	8:Eo:138:ALA:HB2	1.87	0.56
1:Aa:85:VAL:HG12	2:Ab:153:ILE:HG23	1.86	0.56
3:Ck:191:LEU:HD21	3:Ck:194:LEU:HD12	1.87	0.56
7:Cz:51:GLN:HG3	7:Cz:52:PRO:HD2	1.86	0.56
2:Dd:45:VAL:HG22	4:Df:67:THR:HB	1.88	0.56
8:Du:137:GLN:HG2	8:Du:252:LEU:HD13	1.87	0.56
3:Dy:214:ILE:HD11	3:Dy:224:LEU:HD11	1.86	0.56
8:Ey:108:PRO:HD3	8:Ey:138:ALA:HB2	1.86	0.56
4:Ad:62:ASN:HB3	1:Ak:26:LYS:HG2	1.88	0.56
8:Ai:62:THR:O	8:Ai:66:VAL:HG12	2.05	0.56
7:Ar:118:GLU:HG3	7:Ar:123:ARG:HG2	1.85	0.56
8:As:214:LYS:O	8:As:218:MET:HG3	2.05	0.56
3:Aw:52:VAL:HG13	3:Aw:92:VAL:HB	1.87	0.56
2:Cj:67:VAL:HG22	2:Cj:76:ILE:HG23	1.85	0.56
2:Ct:45:VAL:HG23	2:Ct:48:ALA:HB3	1.87	0.56
8:Da:108:PRO:HD3	8:Da:138:ALA:HB2	1.87	0.56
1:Dm:29:PRO:HG3	7:Dt:225:GLN:HA	1.88	0.56
1:Dm:62:ILE:HD12	8:Du:263:ARG:HE	1.71	0.56
5:Dr:216:ILE:HG13	5:Dr:217:PRO:HD2	1.86	0.56
5:El:210:TYR:HB2	5:El:241:TYR:HE2	1.69	0.56
8:Eo:271:ASN:HB2	9:Ep:53:SER:HA	1.86	0.56
1:Eq:41:LEU:HD22	8:Ey:90:LEU:HD21	1.88	0.56
3:Es:280:TYR:HB3	3:Es:301:MET:HG3	1.86	0.56
5:Ev:216:ILE:HG13	5:Ev:217:PRO:HD2	1.86	0.56
1:Ae:76:ALA:O	1:Ae:80:GLN:HG2	2.05	0.56
2:Bf:152:ARG:HD2	6:Bk:352:LYS:HB2	1.86	0.56
4:Bh:46:GLY:HA3	4:Bh:61:ASN:HB2	1.87	0.56
8:Cg:214:LYS:O	8:Cg:218:MET:HG3	2.06	0.56
5:Dr:213:GLN:HG3	5:Dr:223:ILE:HB	1.87	0.56
3:Dy:117:ARG:HG3	3:Dy:137:TYR:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:En:118:GLU:HG3	7:En:123:ARG:HG2	1.87	0.56
8:EO:62:THR:O	8:EO:66:VAL:HG12	2.06	0.56
4:Et:111:GLU:HG2	8:Ey:153:MET:HE2	1.88	0.56
2:Ab:75:LEU:HD12	2:Ab:183:THR:HG22	1.87	0.56
8:AI:224:PRO:HB3	8:AI:253:PRO:HD3	1.88	0.56
3:Bg:52:VAL:HG13	3:Bg:92:VAL:HB	1.88	0.56
6:Bk:346:LEU:HD12	6:Bk:355:GLN:HG2	1.87	0.56
1:By:147:VAL:HG22	1:By:154:VAL:HG22	1.87	0.56
1:Cs:28:PRO:HD3	7:Cz:115:GLN:HB2	1.85	0.56
3:De:199:LYS:HG2	3:De:219:ALA:HB3	1.87	0.56
1:Eg:85:VAL:HG12	2:Eh:153:ILE:HG23	1.88	0.56
7:En:212:ASN:HD22	8:EO:295:TRP:HZ3	1.52	0.56
2:Er:45:VAL:HG11	4:Et:57:ARG:HH22	1.71	0.56
2:Al:45:VAL:HG23	2:Al:48:ALA:HB3	1.86	0.56
9:At:46:LEU:HD11	9:At:59:LYS:HD2	1.87	0.56
4:Ax:46:GLY:HA3	4:Ax:61:ASN:HB2	1.87	0.56
1:Ay:74:PRO:HD2	1:Ay:129:ALA:HB1	1.88	0.56
1:Dg:74:PRO:HD2	1:Dg:129:ALA:HB1	1.88	0.56
3:Do:191:LEU:HD21	3:Do:194:LEU:HD12	1.87	0.56
7:Ed:169:THR:HG23	7:Ed:182:SER:HB3	1.86	0.56
8:AI:214:LYS:O	8:AI:218:MET:HG3	2.06	0.56
1:Ak:94:LEU:HD23	1:Ak:119:ILE:HD11	1.87	0.56
1:Bo:29:PRO:HG3	7:Bv:225:GLN:HA	1.86	0.56
5:Bt:216:ILE:HG13	5:Bt:217:PRO:HD2	1.88	0.56
3:Cu:257:ASP:HA	3:Cu:275:ASP:O	2.06	0.56
2:Dd:75:LEU:HB2	8:Du:299:ILE:HD12	1.86	0.56
1:Dw:162:TYR:CD1	8:Ee:247:LEU:HD11	2.41	0.56
2:Cj:45:VAL:HG23	2:Cj:48:ALA:HB3	1.88	0.56
8:Bm:62:THR:O	8:Bm:66:VAL:HG12	2.06	0.56
3:Bq:176:VAL:HG22	3:Bq:195:ASP:HB2	1.88	0.56
8:Cg:62:THR:O	8:Cg:66:VAL:HG12	2.05	0.56
1:CI:117:VAL:HG13	1:CI:142:LYS:HD3	1.87	0.56
1:Cw:105:ARG:HB2	1:Cw:153:VAL:HG22	1.88	0.56
2:Dn:152:ARG:HD2	6:Ds:352:LYS:HB2	1.87	0.56
3:Dy:253:VAL:HG21	3:Dy:263:ILE:HG21	1.88	0.56
6:Ec:346:LEU:HD12	6:Ec:355:GLN:HG2	1.87	0.56
9:Ez:76:VAL:HG12	9:Ez:86:SER:HA	1.88	0.56
7:Ar:165:VAL:HG13	7:Ar:231:ILE:HG12	1.88	0.56
3:Aw:280:TYR:HB3	3:Aw:301:MET:HG3	1.87	0.56
1:Ay:105:ARG:HB2	1:Ay:153:VAL:HG22	1.87	0.56
5:Az:210:TYR:HB2	5:Az:241:TYR:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Be:77:TYR:OH	2:Bf:130:ARG:HD3	2.06	0.56
5:Dh:221:TRP:HE1	5:Dh:229:THR:HG23	1.70	0.56
8:Dk:224:PRO:HB3	8:Dk:253:PRO:HD3	1.87	0.56
3:Dy:52:VAL:HG13	3:Dy:92:VAL:HB	1.87	0.56
3:Dy:199:LYS:HG2	3:Dy:219:ALA:HB3	1.87	0.56
5:Eb:210:TYR:HB2	5:Eb:241:TYR:HE2	1.71	0.56
6:Ec:285:GLU:HG3	8:Eo:204:GLU:HG3	1.87	0.56
2:Eh:45:VAL:HG23	2:Eh:48:ALA:HB3	1.87	0.56
9:Aj:76:VAL:HG12	9:Aj:86:SER:HA	1.88	0.55
7:Ar:169:THR:HG23	7:Ar:182:SER:HB3	1.88	0.55
8:Bc:62:THR:O	8:Bc:66:VAL:HG12	2.05	0.55
1:Bo:54:GLU:O	1:Bo:58:VAL:HG12	2.04	0.55
2:Bz:114:ILE:HG23	2:Bz:184:PHE:HB3	1.88	0.55
2:Cj:45:VAL:HG11	4:Cl:57:ARG:HH22	1.71	0.55
3:Ck:199:LYS:HG2	3:Ck:219:ALA:HB3	1.87	0.55
8:Cq:214:LYS:O	8:Cq:218:MET:HG3	2.05	0.55
7:Ed:118:GLU:HG3	7:Ed:123:ARG:HG2	1.87	0.55
1:Eg:162:TYR:CD2	8:Eo:247:LEU:HD11	2.41	0.55
2:Er:75:LEU:HD12	2:Er:183:THR:HG22	1.88	0.55
3:Bq:257:ASP:HA	3:Bq:275:ASP:O	2.07	0.55
5:Cx:216:ILE:HG13	5:Cx:217:PRO:HD2	1.87	0.55
7:Cz:169:THR:HG23	7:Cz:182:SER:HB3	1.89	0.55
8:Ee:271:ASN:HB2	9:Ef:53:SER:HA	1.87	0.55
5:Af:216:ILE:HG13	5:Af:217:PRO:HD2	1.88	0.55
9:Aj:40:PRO:HB3	9:Aj:56:TYR:CE1	2.42	0.55
1:Ao:94:LEU:HD23	1:Ao:119:ILE:HD11	1.88	0.55
3:Aw:292:MET:HE2	3:Aw:298:VAL:H	1.71	0.55
7:Bv:118:GLU:HG3	7:Bv:123:ARG:HG2	1.88	0.55
2:Bz:45:VAL:HG23	2:Bz:48:ALA:HB3	1.88	0.55
3:Ca:173:LEU:HD12	3:Ca:174:GLN:N	2.22	0.55
3:Ca:260:VAL:HG22	3:Ca:278:ASP:HB2	1.88	0.55
5:Cn:230:LEU:HD12	5:Cn:231:THR:N	2.21	0.55
2:Ct:152:ARG:HD2	6:Cy:352:LYS:HB2	1.89	0.55
4:Df:46:GLY:HA3	4:Df:61:ASN:HB2	1.88	0.55
2:Dn:106:LEU:HD22	2:Dn:114:ILE:HD13	1.88	0.55
5:Af:230:LEU:HD12	5:Af:231:THR:N	2.21	0.55
6:Ba:297:VAL:HG11	6:Ba:302:ALA:HB3	1.87	0.55
1:Be:162:TYR:CD2	8:Bm:247:LEU:HD11	2.40	0.55
4:Cb:46:GLY:HA3	4:Cb:61:ASN:HB2	1.87	0.55
3:Ck:257:ASP:HA	3:Ck:275:ASP:O	2.06	0.55
3:Cu:52:VAL:HG13	3:Cu:92:VAL:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Di:284:LEU:HD11	6:Di:328:MET:HB3	1.89	0.55
9:Dv:76:VAL:HG12	9:Dv:86:SER:HA	1.87	0.55
5:Af:230:LEU:HD21	5:Af:238:ILE:HG22	1.88	0.55
5:Bj:216:ILE:HG13	5:Bj:217:PRO:HD2	1.89	0.55
3:Ca:52:VAL:HG13	3:Ca:92:VAL:HB	1.89	0.55
9:Ch:23:CYS:HB2	9:Ch:64:ILE:HD11	1.89	0.55
1:Cs:55:MET:HE1	1:Cw:55:MET:HG3	1.88	0.55
8:Da:62:THR:O	8:Da:66:VAL:HG12	2.05	0.55
3:De:176:VAL:HG22	3:De:195:ASP:HB2	1.89	0.55
9:Dv:23:CYS:HB2	9:Dv:64:ILE:HD11	1.88	0.55
3:Dy:257:ASP:HA	3:Dy:275:ASP:O	2.07	0.55
6:Em:285:GLU:HG3	8:Ey:204:GLU:HG3	1.88	0.55
6:Em:320:LEU:HD11	6:Em:348:SER:HB3	1.87	0.55
8:Ai:99:LEU:HD13	8:Ai:209:MET:HB3	1.89	0.55
1:Be:162:TYR:HD2	8:Bm:247:LEU:HD11	1.72	0.55
3:Bq:173:LEU:HD23	3:Bq:174:GLN:N	2.21	0.55
1:Ci:54:GLU:O	1:Ci:58:VAL:HG12	2.07	0.55
1:Ci:65:PRO:HD3	1:Cm:58:VAL:HG22	1.87	0.55
3:Ck:52:VAL:HG13	3:Ck:92:VAL:HB	1.88	0.55
4:Cv:46:GLY:HA3	4:Cv:61:ASN:HB2	1.88	0.55
8:Du:62:THR:O	8:Du:66:VAL:HG12	2.06	0.55
8:Ey:224:PRO:HB3	8:Ey:253:PRO:HD3	1.89	0.55
7:Cf:165:VAL:HG13	7:Cf:231:ILE:HG12	1.88	0.55
4:Dz:46:GLY:HA3	4:Dz:61:ASN:HB2	1.89	0.55
5:Eb:230:LEU:HD21	5:Eb:238:ILE:HG22	1.86	0.55
3:Ei:52:VAL:HG13	3:Ei:92:VAL:HB	1.88	0.55
3:Es:84:ILE:HG13	3:Es:86:LYS:HZ2	1.70	0.55
7:Ex:125:LEU:HD11	7:Ex:154:LEU:HD23	1.89	0.55
5:Ap:216:ILE:HG13	5:Ap:217:PRO:HD2	1.89	0.55
8:Bw:62:THR:O	8:Bw:66:VAL:HG12	2.06	0.55
6:Ce:284:LEU:HD11	6:Ce:328:MET:HB3	1.88	0.55
2:Ct:126:VAL:HA	2:Ct:129:GLU:OE1	2.06	0.55
2:Dd:67:VAL:HG22	2:Dd:76:ILE:HG23	1.89	0.55
3:Do:52:VAL:HG13	3:Do:92:VAL:HB	1.88	0.55
6:Ds:297:VAL:HG22	6:Ds:358:VAL:HG22	1.89	0.55
3:Ac:253:VAL:HG21	3:Ac:263:ILE:HG21	1.89	0.55
4:Ad:46:GLY:HA3	4:Ad:61:ASN:HB2	1.89	0.55
8:As:276:PHE:CE2	9:At:79:ILE:HG21	2.42	0.55
3:Aw:313:ASP:H	3:Aw:316:ASN:HB2	1.71	0.55
7:Bl:165:VAL:HG13	7:Bl:231:ILE:HG12	1.89	0.55
3:Bq:267:ASN:HB3	3:Bq:268:HIS:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Ch:48:VAL:HG21	9:Ch:57:ILE:HD11	1.88	0.55
6:Co:294:ARG:HD2	8:Da:197:GLU:OE2	2.07	0.55
8:Cq:62:THR:O	8:Cq:66:VAL:HG12	2.06	0.55
1:Cs:98:ILE:HG23	1:Cs:128:LEU:HD22	1.89	0.55
2:Dn:55:LYS:HB2	4:Dp:44:LYS:NZ	2.21	0.55
6:Ew:346:LEU:HD12	6:Ew:355:GLN:HG2	1.89	0.55
8:Ai:137:GLN:HG2	8:Ai:252:LEU:HD13	1.89	0.55
1:Au:41:LEU:HD22	8:Bc:90:LEU:HD21	1.88	0.55
2:Av:90:ARG:HD3	3:Aw:292:MET:HB3	1.88	0.55
7:Bv:169:THR:HG23	7:Bv:182:SER:HB3	1.88	0.55
1:By:68:ASP:HB3	1:By:70:THR:HG22	1.89	0.55
7:Cf:107:ARG:O	7:Cf:111:LYS:HG3	2.07	0.55
1:Cw:76:ALA:O	1:Cw:80:GLN:HG2	2.06	0.55
1:Dc:65:PRO:HD3	1:Dg:58:VAL:HG22	1.88	0.55
1:Dq:97:ARG:HD2	8:Ee:263:ARG:NH2	2.22	0.55
1:Dw:98:ILE:HG23	1:Dw:128:LEU:HD22	1.89	0.55
1:Eg:55:MET:HE3	8:Eo:213:ARG:HB3	1.89	0.55
3:Bq:209:SER:HB3	3:Bq:228:VAL:HG22	1.89	0.54
2:Bz:111:LYS:HD2	2:Bz:114:ILE:HG12	1.89	0.54
6:Co:280:LEU:HB3	6:Co:328:MET:HG3	1.88	0.54
7:Cp:125:LEU:HD11	7:Cp:154:LEU:HD23	1.88	0.54
6:Cy:285:GLU:HG3	8:Dk:204:GLU:HG3	1.89	0.54
3:Do:257:ASP:HA	3:Do:275:ASP:O	2.07	0.54
1:Dq:75:ASN:HA	1:Dq:80:GLN:NE2	2.22	0.54
2:Eh:152:ARG:HD2	6:Em:352:LYS:HB2	1.88	0.54
3:Ei:257:ASP:HA	3:Ei:275:ASP:O	2.06	0.54
1:Ek:39:ILE:O	1:Ek:43:GLU:HG3	2.07	0.54
8:Ey:62:THR:O	8:Ey:66:VAL:HG12	2.07	0.54
1:Ak:98:ILE:HG23	1:Ak:128:LEU:HD22	1.89	0.54
8:As:276:PHE:HE2	9:At:79:ILE:HG21	1.70	0.54
1:Bi:97:ARG:HH11	1:Bi:100:LYS:HZ3	1.54	0.54
3:Ca:257:ASP:HA	3:Ca:275:ASP:O	2.07	0.54
6:Ce:285:GLU:HG3	8:Cq:204:GLU:HG3	1.90	0.54
8:Cg:108:PRO:HD3	8:Cg:138:ALA:HB2	1.88	0.54
1:Dg:119:ILE:HD12	1:Dg:135:ILE:HG12	1.88	0.54
1:Dm:65:PRO:HD3	1:Dq:58:VAL:HG22	1.89	0.54
2:Dx:152:ARG:HD2	6:Ec:352:LYS:HB2	1.87	0.54
6:Em:283:VAL:HG21	6:Em:312:TYR:HB3	1.89	0.54
2:Ab:67:VAL:HG22	2:Ab:76:ILE:HG23	1.88	0.54
3:Ac:191:LEU:HD21	3:Ac:194:LEU:HD12	1.89	0.54
2:Av:111:LYS:HD2	2:Av:114:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:97:ARG:HD2	8:Bm:263:ARG:NH2	2.22	0.54
1:By:77:TYR:OH	2:Bz:130:ARG:HD3	2.07	0.54
1:By:124:LYS:HE2	2:Bz:142:GLU:OE1	2.07	0.54
5:Cd:216:ILE:HG13	5:Cd:217:PRO:HD2	1.89	0.54
5:El:223:ILE:HD12	5:El:224:GLY:H	1.72	0.54
1:Ak:67:LYS:HB3	1:Ao:62:ILE:HD11	1.90	0.54
5:Az:233:ARG:HD3	5:Az:234:GLU:H	1.73	0.54
6:Ba:285:GLU:HG3	8:Bm:204:GLU:HG3	1.90	0.54
1:Bo:147:VAL:HG22	1:Bo:154:VAL:HG22	1.89	0.54
2:Bz:106:LEU:HD22	2:Bz:114:ILE:HD13	1.89	0.54
6:Ce:311:MET:HE2	6:Ce:341:LYS:HA	1.90	0.54
5:Cn:216:ILE:HG13	5:Cn:217:PRO:HD2	1.90	0.54
1:Dc:85:VAL:HG12	2:Dd:153:ILE:HG23	1.89	0.54
3:Dy:250:ARG:HH11	7:Ed:190:MET:HE1	1.71	0.54
5:Af:210:TYR:HB2	5:Af:241:TYR:HE2	1.73	0.54
8:Ai:275:ARG:C	8:Ai:276:PHE:HD1	2.16	0.54
1:Cc:26:LYS:HG2	7:Cf:143:ILE:HD11	1.90	0.54
8:Dk:62:THR:O	8:Dk:66:VAL:HG12	2.06	0.54
7:Dt:212:ASN:HD22	8:Du:295:TRP:HZ3	1.53	0.54
8:Du:109:VAL:HG13	8:Du:208:GLY:HA3	1.89	0.54
3:Dy:118:TYR:OH	3:Dy:122:GLY:HA3	2.08	0.54
2:Eh:45:VAL:HG11	4:Ej:57:ARG:HH22	1.72	0.54
3:Es:257:ASP:HA	3:Es:275:ASP:O	2.08	0.54
3:Ac:257:ASP:HA	3:Ac:275:ASP:O	2.08	0.54
8:Ai:247:LEU:HB2	8:As:125:ILE:HG12	1.89	0.54
3:Bq:280:TYR:HB3	3:Bq:301:MET:HG3	1.89	0.54
9:Cr:23:CYS:HB2	9:Cr:64:ILE:HD11	1.90	0.54
1:Dc:29:PRO:HG3	7:Dj:225:GLN:HA	1.88	0.54
6:Ew:297:VAL:HG22	6:Ew:358:VAL:HG22	1.90	0.54
3:Aw:292:MET:HG2	3:Aw:296:GLY:O	2.06	0.54
1:Bi:76:ALA:O	1:Bi:80:GLN:HG2	2.08	0.54
1:Bo:62:ILE:HD12	8:Bw:263:ARG:HE	1.73	0.54
1:Dg:105:ARG:HB2	1:Dg:153:VAL:HG22	1.90	0.54
3:Do:84:ILE:HG13	3:Do:86:LYS:HZ2	1.72	0.54
2:Eh:67:VAL:HG22	2:Eh:76:ILE:HG23	1.88	0.54
6:Aq:283:VAL:HG21	6:Aq:312:TYR:HB3	1.89	0.54
2:Cj:53:ILE:HG22	2:Cj:57:MET:HE2	1.90	0.54
3:De:52:VAL:HG13	3:De:92:VAL:HB	1.88	0.54
7:Dj:165:VAL:HG13	7:Dj:231:ILE:HG12	1.88	0.54
3:Ei:173:LEU:HD12	3:Ei:174:GLN:N	2.23	0.54
8:Eo:246:VAL:HG22	8:Ey:126:ARG:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:105:ARG:HB2	1:Ao:153:VAL:HG22	1.89	0.54
2:Bf:45:VAL:HG11	4:Bh:57:ARG:HH22	1.73	0.54
3:Bg:173:LEU:HD12	3:Bg:174:GLN:H	1.73	0.54
9:Bn:76:VAL:HG12	9:Bn:86:SER:HA	1.90	0.54
2:Bp:45:VAL:HG11	4:Br:57:ARG:HH22	1.73	0.54
2:Bz:152:ARG:HD2	6:Ce:352:LYS:HB2	1.89	0.54
6:Ce:283:VAL:HG21	6:Ce:312:TYR:HB3	1.89	0.54
3:Dy:228:VAL:HG11	3:Dy:231:LEU:HB2	1.89	0.54
5:Eb:230:LEU:HD12	5:Eb:231:THR:N	2.22	0.54
2:Ab:114:ILE:HG23	2:Ab:184:PHE:HB3	1.89	0.54
1:Ao:76:ALA:O	1:Ao:80:GLN:HG2	2.07	0.54
8:As:137:GLN:HG2	8:As:252:LEU:HD13	1.90	0.54
1:Cw:80:GLN:NE2	9:Dl:47:LEU:HD11	2.22	0.54
3:Dy:250:ARG:HH21	9:Ef:82:GLU:HG2	1.73	0.54
5:El:233:ARG:HD3	5:El:234:GLU:N	2.21	0.54
5:Ev:223:ILE:HD11	5:Ev:227:GLY:HA2	1.90	0.54
7:Ex:53:ASP:OD1	7:Ex:55:ARG:HD2	2.08	0.54
3:Ac:176:VAL:HG22	3:Ac:195:ASP:HB3	1.90	0.53
8:Bm:137:GLN:HG2	8:Bm:252:LEU:HD13	1.91	0.53
2:Bz:45:VAL:HG11	4:Cb:57:ARG:HH22	1.72	0.53
8:Cq:224:PRO:HB3	8:Cq:253:PRO:HD3	1.89	0.53
1:Cw:97:ARG:HD2	8:Dk:263:ARG:HH12	1.73	0.53
8:Du:298:ILE:H	8:Du:298:ILE:HD12	1.73	0.53
8:Ey:109:VAL:HG13	8:Ey:208:GLY:HA3	1.90	0.53
1:Aa:98:ILE:HG23	1:Aa:128:LEU:HD22	1.90	0.53
8:As:109:VAL:HG13	8:As:208:GLY:HA3	1.90	0.53
3:Bq:52:VAL:HG13	3:Bq:92:VAL:HB	1.90	0.53
8:Cg:137:GLN:HG2	8:Cg:252:LEU:HD13	1.90	0.53
8:Cq:292:ASN:HD21	9:Cr:31:ASP:HA	1.73	0.53
2:Dd:66:LYS:HD3	7:Dt:119:TYR:HD2	1.72	0.53
1:Dw:41:LEU:HD22	8:Ee:90:LEU:HD21	1.90	0.53
1:Ea:33:PRO:HB2	1:Ea:39:ILE:HG12	1.90	0.53
1:Aa:29:PRO:HG3	7:Ah:225:GLN:HA	1.90	0.53
6:Bu:284:LEU:HD11	6:Bu:328:MET:HB3	1.90	0.53
3:De:209:SER:HB3	3:De:228:VAL:HG22	1.89	0.53
7:Dt:165:VAL:HG13	7:Dt:231:ILE:HG12	1.89	0.53
7:Dt:169:THR:HG23	7:Dt:182:SER:HB3	1.90	0.53
6:Ec:324:TRP:HA	6:Ec:339:MET:HB3	1.90	0.53
8:Ey:137:GLN:HG2	8:Ey:252:LEU:HD13	1.89	0.53
2:Bp:45:VAL:HG22	4:Br:67:THR:HB	1.90	0.53
1:Cc:76:ALA:O	1:Cc:80:GLN:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Cd:233:ARG:CD	5:Cd:234:GLU:H	2.20	0.53
3:Ck:280:TYR:HB3	3:Ck:301:MET:HG3	1.89	0.53
8:Cq:215:LEU:HG	8:Cq:220:MET:HB2	1.90	0.53
2:Ct:106:LEU:HD22	2:Ct:114:ILE:HD13	1.90	0.53
2:Ct:114:ILE:HG23	2:Ct:184:PHE:HB3	1.90	0.53
2:Dd:106:LEU:HD22	2:Dd:114:ILE:HD13	1.91	0.53
3:Es:228:VAL:HG11	3:Es:231:LEU:HB2	1.90	0.53
7:Ah:165:VAL:HG13	7:Ah:231:ILE:HG12	1.90	0.53
3:Am:250:ARG:HD3	3:Am:268:HIS:HB2	1.89	0.53
9:Bd:76:VAL:HG12	9:Bd:86:SER:HA	1.89	0.53
1:By:151:SER:HB3	9:Cr:92:GLU:HG2	1.91	0.53
5:Eb:216:ILE:HG13	5:Eb:217:PRO:HD2	1.89	0.53
8:Bc:137:GLN:HG2	8:Bc:252:LEU:HD13	1.91	0.53
1:Bs:119:ILE:HD12	1:Bs:135:ILE:HG12	1.90	0.53
7:Cp:165:VAL:HG13	7:Cp:231:ILE:HG12	1.91	0.53
8:Cq:108:PRO:HD3	8:Cq:138:ALA:HB2	1.90	0.53
2:Dd:45:VAL:HG23	2:Dd:48:ALA:HB3	1.91	0.53
9:Dl:60:GLN:O	9:Dl:64:ILE:HG22	2.09	0.53
1:Eq:65:PRO:HD3	1:Eu:58:VAL:HG22	1.89	0.53
8:As:99:LEU:HD13	8:As:209:MET:HB3	1.91	0.53
2:Av:114:ILE:HG23	2:Av:184:PHE:HB3	1.90	0.53
2:Av:164:PRO:HB2	2:Av:177:ASN:HD22	1.74	0.53
2:Bf:67:VAL:HG22	2:Bf:76:ILE:HG23	1.90	0.53
3:Bg:257:ASP:HA	3:Bg:275:ASP:O	2.08	0.53
2:Bp:106:LEU:HD22	2:Bp:114:ILE:HD13	1.90	0.53
3:Bq:191:LEU:HG	3:Bq:212:LEU:HD21	1.91	0.53
1:By:162:TYR:HD2	8:Cg:247:LEU:HD11	1.71	0.53
3:Ck:250:ARG:HH21	9:Cr:82:GLU:HG2	1.74	0.53
2:Dd:45:VAL:HG11	4:Df:57:ARG:HH22	1.72	0.53
3:De:260:VAL:HG22	3:De:278:ASP:HB2	1.90	0.53
1:Dm:94:LEU:HD23	1:Dm:119:ILE:HD11	1.90	0.53
1:Eg:29:PRO:HG3	7:En:225:GLN:HA	1.91	0.53
1:Eq:68:ASP:HB3	1:Eq:70:THR:HG22	1.90	0.53
2:Av:106:LEU:HD22	2:Av:114:ILE:HD13	1.89	0.53
2:Bf:45:VAL:HG23	2:Bf:48:ALA:HB3	1.89	0.53
7:Bl:190:MET:HG2	7:Bl:203:LEU:HD13	1.89	0.53
1:By:85:VAL:HG12	2:Bz:153:ILE:HG23	1.90	0.53
8:Da:271:ASN:HB2	9:Db:53:SER:HA	1.90	0.53
6:Ec:297:VAL:HG11	6:Ec:302:ALA:HB3	1.90	0.53
6:Aq:297:VAL:HG11	6:Aq:302:ALA:HB3	1.91	0.53
6:Bu:346:LEU:HD12	6:Bu:355:GLN:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Cg:99:LEU:HD13	8:Cg:209:MET:HB3	1.91	0.53
2:Cj:152:ARG:HD2	6:Co:352:LYS:HB2	1.90	0.53
6:Co:320:LEU:O	8:Cq:143:THR:HB	2.08	0.53
1:Dq:74:PRO:O	1:Dq:75:ASN:ND2	2.33	0.53
1:Dq:74:PRO:C	1:Dq:75:ASN:HD22	2.14	0.53
5:El:216:ILE:HG13	5:El:217:PRO:HD2	1.90	0.53
2:Er:152:ARG:HD2	6:Ew:352:LYS:HB2	1.90	0.53
3:Ac:52:VAL:HG13	3:Ac:92:VAL:HB	1.90	0.53
3:Am:176:VAL:HG22	3:Am:195:ASP:HB2	1.90	0.53
1:Au:55:MET:HE3	8:Bc:213:ARG:HB3	1.91	0.53
3:Aw:51:VAL:HG22	3:Aw:117:ARG:HG3	1.91	0.53
3:Aw:250:ARG:HD3	3:Aw:268:HIS:HB2	1.91	0.53
7:Bb:140:LEU:HD13	7:Bb:188:THR:HG22	1.91	0.53
3:Ca:199:LYS:HG2	3:Ca:219:ALA:HB3	1.91	0.53
7:Cf:169:THR:HG23	7:Cf:182:SER:HB3	1.90	0.53
5:Cx:223:ILE:HD12	5:Cx:224:GLY:H	1.73	0.53
1:Ea:105:ARG:HB2	1:Ea:153:VAL:HG22	1.90	0.53
1:Ae:119:ILE:HD12	1:Ae:135:ILE:HG12	1.91	0.52
2:Al:45:VAL:HG11	4:An:57:ARG:HH22	1.74	0.52
7:Bl:125:LEU:HD11	7:Bl:154:LEU:HD23	1.90	0.52
7:Bv:165:VAL:HG13	7:Bv:231:ILE:HG12	1.91	0.52
9:Ch:62:TYR:HD1	9:Ch:62:TYR:O	1.92	0.52
2:Ct:45:VAL:HG22	4:Cv:67:THR:HB	1.91	0.52
1:Dc:147:VAL:HG22	1:Dc:154:VAL:HG22	1.92	0.52
5:El:233:ARG:CD	5:El:234:GLU:H	2.18	0.52
5:Az:230:LEU:HD12	5:Az:231:THR:N	2.23	0.52
2:Bz:75:LEU:HD11	2:Bz:181:GLU:HG2	1.90	0.52
1:Cs:41:LEU:HD22	8:Da:90:LEU:HD21	1.92	0.52
2:Dx:45:VAL:HG22	4:Dz:67:THR:HB	1.91	0.52
1:Ek:97:ARG:HH11	1:Ek:100:LYS:NZ	2.07	0.52
8:Bc:108:PRO:HD3	8:Bc:138:ALA:HB2	1.89	0.52
8:Cq:109:VAL:HG13	8:Cq:208:GLY:HA3	1.91	0.52
3:Do:199:LYS:HG2	3:Do:219:ALA:HB3	1.91	0.52
5:Dr:250:LEU:H	5:Dr:250:LEU:HD22	1.74	0.52
1:Dw:62:ILE:CD1	8:Ee:263:ARG:HE	2.21	0.52
6:Ec:320:LEU:HD11	6:Ec:348:SER:HB3	1.91	0.52
8:Ee:215:LEU:HB3	8:Ee:221:VAL:HG22	1.90	0.52
1:Aa:77:TYR:OH	2:Ab:130:ARG:HD3	2.10	0.52
1:Be:117:VAL:HG13	1:Be:142:LYS:HD3	1.91	0.52
1:Bo:69:ASN:HD21	1:Bo:133:ARG:HA	1.73	0.52
8:Bc:247:LEU:HB2	8:Bm:125:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bo:98:ILE:HG23	1:Bo:128:LEU:HD22	1.92	0.52
1:Dg:75:ASN:O	1:Dg:75:ASN:ND2	2.43	0.52
1:Dg:87:TRP:CD1	1:Dg:94:LEU:HD22	2.45	0.52
7:Dj:125:LEU:HD11	7:Dj:154:LEU:HD23	1.92	0.52
3:Ac:303:GLU:HB2	3:Ac:306:GLN:HG3	1.92	0.52
6:Ag:346:LEU:HD12	6:Ag:355:GLN:HG2	1.89	0.52
4:Br:46:GLY:HA3	4:Br:61:ASN:HB2	1.92	0.52
4:Dp:46:GLY:HA3	4:Dp:61:ASN:HB2	1.91	0.52
2:Eh:45:VAL:HG22	4:Ej:67:THR:HB	1.92	0.52
3:Es:303:GLU:HB2	3:Es:306:GLN:HG3	1.92	0.52
1:Ay:75:ASN:HA	1:Ay:80:GLN:NE2	2.25	0.52
1:Bs:105:ARG:HB2	1:Bs:153:VAL:HG22	1.90	0.52
6:Di:284:LEU:HD22	6:Di:330:SER:HB3	1.91	0.52
2:Dn:55:LYS:HB2	4:Dp:44:LYS:HZ1	1.72	0.52
1:Ea:109:LEU:HD23	1:Ea:157:ARG:HG3	1.91	0.52
6:Em:284:LEU:HD11	6:Em:328:MET:HB3	1.92	0.52
3:Es:52:VAL:HG13	3:Es:92:VAL:HB	1.90	0.52
3:Am:209:SER:HB3	3:Am:228:VAL:HG22	1.91	0.52
1:Au:69:ASN:HD21	1:Au:133:ARG:HA	1.75	0.52
3:Aw:303:GLU:HB2	3:Aw:306:GLN:HG3	1.92	0.52
1:Ay:76:ALA:O	1:Ay:80:GLN:HG2	2.09	0.52
8:Bw:224:PRO:HB3	8:Bw:253:PRO:HD3	1.91	0.52
9:Bx:60:GLN:O	9:Bx:64:ILE:HG22	2.10	0.52
2:Bz:115:THR:HG23	2:Bz:155:PHE:HB2	1.92	0.52
3:Ca:65:ASN:HB2	3:Ca:109:LYS:HG2	1.92	0.52
2:Dd:114:ILE:HG23	2:Dd:184:PHE:HB3	1.91	0.52
7:Dj:169:THR:HG23	7:Dj:182:SER:HB3	1.91	0.52
3:Do:176:VAL:HG22	3:Do:195:ASP:HB2	1.91	0.52
9:Ef:46:LEU:HB3	9:Ef:62:TYR:HD1	1.75	0.52
3:Bg:253:VAL:HG21	3:Bg:263:ILE:HG21	1.90	0.52
8:Cq:137:GLN:HG2	8:Cq:252:LEU:HD13	1.91	0.52
8:Ee:108:PRO:HD3	8:Ee:138:ALA:HB2	1.92	0.52
8:Ee:242:ILE:HG13	8:Ee:130:ARG:HB2	1.90	0.52
7:En:169:THR:HG23	7:En:182:SER:HB3	1.92	0.52
3:Am:196:MET:HE3	3:Am:220:ALA:HB1	1.92	0.52
3:Am:257:ASP:HA	3:Am:275:ASP:O	2.09	0.52
3:Bq:163:THR:HB	3:Bq:183:VAL:HG23	1.91	0.52
1:Cs:162:TYR:CD1	8:Da:247:LEU:HD11	2.43	0.52
1:Dm:41:LEU:HD22	8:Du:90:LEU:HD21	1.92	0.52
1:Dq:97:ARG:HH11	1:Dq:100:LYS:HZ3	1.58	0.52
8:Eo:109:VAL:HG13	8:Eo:208:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:75:LEU:HB2	8:As:299:ILE:HD12	1.92	0.51
1:Bo:162:TYR:CD1	8:Bw:247:LEU:HD11	2.43	0.51
7:En:55:ARG:HH21	7:En:153:ARG:NH1	2.08	0.51
7:En:125:LEU:HD11	7:En:154:LEU:HD23	1.93	0.51
2:Al:126:VAL:HA	2:Al:129:GLU:OE2	2.09	0.51
6:Aq:284:LEU:HD11	6:Aq:328:MET:HB3	1.93	0.51
2:Bf:106:LEU:HD22	2:Bf:114:ILE:HD13	1.91	0.51
8:Bw:276:PHE:CE2	9:Bx:79:ILE:HG21	2.39	0.51
1:Dc:77:TYR:OH	2:Dd:130:ARG:HD3	2.10	0.51
7:Dj:167:GLY:HA2	7:Dj:229:ILE:HD13	1.92	0.51
3:Es:191:LEU:HG	3:Es:212:LEU:HD21	1.91	0.51
7:Ar:125:LEU:HD11	7:Ar:154:LEU:HD23	1.92	0.51
4:Ax:62:ASN:HD22	4:Ax:64:PHE:HD2	1.58	0.51
9:Bd:23:CYS:HB2	9:Bd:64:ILE:HD11	1.91	0.51
1:Bo:77:TYR:OH	2:Bp:130:ARG:HD3	2.10	0.51
1:Bs:160:LYS:H	1:Bs:160:LYS:HD3	1.74	0.51
8:Bw:38:ALA:HB1	8:Bw:173:LYS:HD2	1.91	0.51
5:Dh:216:ILE:HG13	5:Dh:217:PRO:HD2	1.91	0.51
8:Dk:214:LYS:O	8:Dk:218:MET:HG3	2.11	0.51
8:Ee:109:VAL:HG13	8:Ee:208:GLY:HA3	1.92	0.51
3:Ei:209:SER:HB3	3:Ei:228:VAL:HG22	1.91	0.51
8:Ai:109:VAL:HG13	8:Ai:208:GLY:HA3	1.93	0.51
4:Bh:84:CYS:HB3	8:Bm:154:ASP:HB3	1.91	0.51
6:Bk:283:VAL:HG21	6:Bk:312:TYR:HB3	1.91	0.51
3:De:65:ASN:HB2	3:De:109:LYS:HG2	1.92	0.51
3:De:271:SER:HB3	3:De:279:ILE:HD13	1.92	0.51
6:Ds:283:VAL:HG21	6:Ds:312:TYR:HB3	1.91	0.51
1:Ea:39:ILE:O	1:Ea:43:GLU:HG3	2.11	0.51
4:Et:69:TYR:CE2	4:Et:76:MET:HG2	2.45	0.51
6:Ew:283:VAL:HG21	6:Ew:312:TYR:HB3	1.92	0.51
6:Ag:283:VAL:HG21	6:Ag:312:TYR:HB3	1.91	0.51
3:Bg:280:TYR:HB3	3:Bg:301:MET:HG3	1.92	0.51
3:Bq:275:ASP:HB3	3:Bq:294:PHE:HB2	1.93	0.51
9:Bx:40:PRO:HB3	9:Bx:56:TYR:CE1	2.45	0.51
1:By:62:ILE:CD1	8:Cg:263:ARG:HE	2.23	0.51
1:Ci:29:PRO:HG3	7:Cp:225:GLN:HA	1.91	0.51
3:Cu:209:SER:HB3	3:Cu:228:VAL:HG22	1.91	0.51
2:Dn:93:TRP:HB2	7:Dt:46:PRO:HD3	1.93	0.51
3:Do:231:LEU:HD12	3:Do:232:ASP:N	2.26	0.51
2:Eh:50:ASP:HB3	4:Ej:45:MET:HE3	1.91	0.51
3:Ei:65:ASN:HB2	3:Ei:109:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ek:105:ARG:HB2	1:Ek:153:VAL:HG22	1.92	0.51
6:Bk:317:LEU:HD22	6:Bk:349:TRP:HA	1.93	0.51
3:Ck:65:ASN:HB2	3:Ck:109:LYS:HG2	1.92	0.51
3:Ck:260:VAL:HG22	3:Ck:278:ASP:HB2	1.92	0.51
6:Di:283:VAL:HG21	6:Di:312:TYR:HB3	1.92	0.51
4:Ax:58:LEU:HB2	4:Ax:66:SER:HB3	1.93	0.51
1:Bi:160:LYS:H	1:Bi:160:LYS:HD3	1.76	0.51
7:Bl:167:GLY:HA2	7:Bl:229:ILE:HD13	1.92	0.51
1:Cc:105:ARG:HB2	1:Cc:153:VAL:HG22	1.91	0.51
1:Ci:162:TYR:CD1	8:Cq:247:LEU:HD11	2.44	0.51
9:Db:76:VAL:HG12	9:Db:86:SER:HA	1.92	0.51
5:Ev:219:ARG:HD3	5:Ev:233:ARG:HH21	1.76	0.51
9:Ez:60:GLN:O	9:Ez:64:ILE:HG22	2.10	0.51
3:Aw:191:LEU:HG	3:Aw:212:LEU:HD21	1.92	0.51
6:Ec:283:VAL:HG21	6:Ec:312:TYR:HB3	1.92	0.51
3:Ei:84:ILE:HG13	3:Ei:86:LYS:HZ2	1.74	0.51
9:Ez:62:TYR:HD2	9:Ez:62:TYR:O	1.93	0.51
1:Aa:55:MET:HE1	1:Ae:55:MET:HE2	1.93	0.51
3:Ac:118:TYR:OH	3:Ac:122:GLY:HA3	2.10	0.51
1:Ae:39:ILE:O	1:Ae:43:GLU:HG3	2.11	0.51
9:Bn:60:GLN:O	9:Bn:64:ILE:HG22	2.11	0.51
3:Cu:191:LEU:HG	3:Cu:212:LEU:HD21	1.93	0.51
8:Dk:108:PRO:HD3	8:Dk:138:ALA:HB2	1.93	0.51
3:Do:250:ARG:HD3	3:Do:268:HIS:HB2	1.92	0.51
3:Dy:250:ARG:NH1	7:Ed:190:MET:HE1	2.25	0.51
3:Ei:118:TYR:OH	3:Ei:122:GLY:HA3	2.11	0.51
7:En:165:VAL:HG13	7:En:231:ILE:HG12	1.92	0.51
2:Al:117:THR:HG23	2:Al:157:GLN:HG3	1.93	0.51
2:Bf:45:VAL:HG22	4:Bh:67:THR:HB	1.92	0.51
3:Bq:65:ASN:HB2	3:Bq:109:LYS:HG2	1.93	0.51
3:Bq:118:TYR:OH	3:Bq:122:GLY:HA3	2.11	0.51
7:Cf:125:LEU:HD11	7:Cf:154:LEU:HD23	1.92	0.51
1:Cm:160:LYS:H	1:Cm:160:LYS:HD3	1.76	0.51
2:Dd:152:ARG:HD2	6:Di:352:LYS:HB2	1.93	0.51
3:Do:118:TYR:OH	3:Do:122:GLY:HA3	2.11	0.51
6:Ew:320:LEU:O	8:Ey:143:THR:HB	2.11	0.51
2:Ab:45:VAL:HG11	4:Ad:57:ARG:HH22	1.76	0.50
3:Am:292:MET:HE1	3:Am:320:PRO:HB3	1.93	0.50
9:Ch:76:VAL:HG12	9:Ch:86:SER:HA	1.93	0.50
2:Cj:45:VAL:HG22	4:Cl:67:THR:HB	1.92	0.50
3:De:118:TYR:OH	3:De:122:GLY:HA3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Dj:163:ILE:HD11	7:Dj:202:ARG:HH21	1.76	0.50
7:Dt:167:GLY:HA2	7:Dt:229:ILE:HD13	1.94	0.50
8:Du:247:LEU:HB2	8:Ee:125:ILE:HG12	1.92	0.50
7:Ed:167:GLY:HA2	7:Ed:229:ILE:HD13	1.92	0.50
1:Eg:147:VAL:HG22	1:Eg:154:VAL:HG22	1.93	0.50
3:Es:118:TYR:OH	3:Es:122:GLY:HA3	2.11	0.50
3:Es:260:VAL:HG22	3:Es:278:ASP:HB2	1.93	0.50
3:Am:65:ASN:HB2	3:Am:109:LYS:HG2	1.92	0.50
3:Aw:257:ASP:HA	3:Aw:275:ASP:O	2.10	0.50
3:Bg:51:VAL:HG22	3:Bg:117:ARG:HG3	1.93	0.50
1:Bi:80:GLN:NE2	9:Bx:47:LEU:HD11	2.26	0.50
9:Dv:25:LEU:HD23	9:Dv:68:TYR:CZ	2.46	0.50
8:Ee:215:LEU:HG	8:Ee:220:MET:HB2	1.93	0.50
2:Ab:118:SER:HB2	2:Ab:133:THR:HB	1.93	0.50
1:Ay:97:ARG:HH11	1:Ay:100:LYS:HZ3	1.57	0.50
3:Bg:65:ASN:HB2	3:Bg:109:LYS:HG2	1.92	0.50
3:Bg:118:TYR:OH	3:Bg:122:GLY:HA3	2.11	0.50
7:Bv:140:LEU:HD23	7:Bv:148:LEU:HD13	1.93	0.50
7:Cz:234:PHE:CE1	9:Db:29:ARG:HG2	2.46	0.50
6:Em:346:LEU:HD12	6:Em:355:GLN:HG2	1.94	0.50
1:Eq:147:VAL:HG22	1:Eq:154:VAL:HG22	1.93	0.50
8:As:275:ARG:C	8:As:276:PHE:HD1	2.18	0.50
3:Aw:228:VAL:HG11	3:Aw:231:LEU:HB2	1.92	0.50
1:Ay:160:LYS:HD3	1:Ay:160:LYS:H	1.76	0.50
1:Bo:65:PRO:HD3	1:Bs:58:VAL:HG22	1.93	0.50
1:Cc:160:LYS:HD3	1:Cc:160:LYS:H	1.77	0.50
7:Cf:167:GLY:HA2	7:Cf:229:ILE:HD13	1.93	0.50
2:Cj:90:ARG:HD3	3:Ck:292:MET:HB2	1.93	0.50
6:Co:285:GLU:HG3	8:Da:204:GLU:HG3	1.93	0.50
3:De:196:MET:HE3	3:De:220:ALA:HB1	1.91	0.50
7:En:140:LEU:HD13	7:En:188:THR:HG22	1.92	0.50
7:En:219:ILE:HG13	7:En:222:GLY:H	1.76	0.50
8:Eo:119:LEU:HD12	8:Eo:125:ILE:HG22	1.93	0.50
2:Er:111:LYS:HD2	2:Er:114:ILE:HG12	1.93	0.50
3:Es:253:VAL:HG21	3:Es:263:ILE:HG21	1.93	0.50
1:Eu:105:ARG:HB2	1:Eu:153:VAL:HG22	1.93	0.50
1:Aa:147:VAL:HG22	1:Aa:154:VAL:HG22	1.93	0.50
7:Ah:208:TYR:CD2	9:Aj:86:SER:HB2	2.46	0.50
5:Bj:250:LEU:HD22	5:Bj:250:LEU:H	1.76	0.50
9:Cr:25:LEU:HD23	9:Cr:68:TYR:CZ	2.47	0.50
2:Ct:93:TRP:HB2	7:Cz:46:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Cy:306:LEU:HD11	6:Cy:341:LYS:HE2	1.94	0.50
7:Cz:167:GLY:HA2	7:Cz:229:ILE:HD13	1.93	0.50
5:Dh:223:ILE:HD12	5:Dh:224:GLY:H	1.77	0.50
2:Dx:106:LEU:HD22	2:Dx:114:ILE:HD13	1.94	0.50
1:Aa:162:TYR:CD1	8:Ai:247:LEU:HD11	2.43	0.50
3:Ac:250:ARG:HH21	9:Aj:82:GLU:HG2	1.76	0.50
3:Ac:275:ASP:HB3	3:Ac:294:PHE:HB2	1.94	0.50
8:Ai:125:ILE:HG12	8:Ey:247:LEU:HB2	1.93	0.50
1:Au:162:TYR:CD1	8:Bc:247:LEU:HD11	2.44	0.50
6:Ba:283:VAL:HG21	6:Ba:312:TYR:HB3	1.93	0.50
2:Bf:126:VAL:HA	2:Bf:129:GLU:OE1	2.11	0.50
1:Bs:121:ILE:HG21	1:Bs:131:ILE:HG23	1.93	0.50
2:Bz:117:THR:HG23	2:Bz:157:GLN:HG3	1.94	0.50
1:Ci:55:MET:SD	1:Cm:55:MET:HE2	2.52	0.50
5:Cn:230:LEU:HD21	5:Cn:238:ILE:HG22	1.93	0.50
3:Cu:280:TYR:HB3	3:Cu:301:MET:HG3	1.94	0.50
9:Db:60:GLN:O	9:Db:64:ILE:HG22	2.11	0.50
6:Ds:285:GLU:HG3	8:Ee:204:GLU:HG3	1.93	0.50
3:Ei:275:ASP:HB3	3:Ei:294:PHE:HB2	1.94	0.50
7:Ah:140:LEU:HD13	7:Ah:188:THR:HG22	1.93	0.50
2:Al:52:THR:O	2:Al:56:MET:HG3	2.11	0.50
3:Aw:118:TYR:OH	3:Aw:122:GLY:HA3	2.11	0.50
3:De:275:ASP:HB3	3:De:294:PHE:HB2	1.94	0.50
7:Dj:134:MET:HE2	7:Dj:141:ASN:HA	1.94	0.50
9:Ep:62:TYR:HD2	9:Ep:62:TYR:O	1.94	0.50
3:Es:250:ARG:HH21	9:Ez:82:GLU:HG2	1.75	0.50
9:Aj:46:LEU:HB3	9:Aj:62:TYR:HD2	1.77	0.50
3:Ca:51:VAL:HG22	3:Ca:117:ARG:HG3	1.94	0.50
3:Cu:118:TYR:OH	3:Cu:122:GLY:HA3	2.11	0.50
3:Cu:250:ARG:HD3	3:Cu:268:HIS:HB2	1.94	0.50
6:Ds:324:TRP:HA	6:Ds:339:MET:HB3	1.94	0.50
3:Dy:65:ASN:HB2	3:Dy:109:LYS:HG2	1.94	0.50
8:Ee:137:GLN:HG2	8:Ee:252:LEU:HD13	1.94	0.50
3:Bg:176:VAL:HG22	3:Bg:195:ASP:HB2	1.94	0.50
3:Bq:253:VAL:HG21	3:Bq:263:ILE:HG21	1.94	0.50
4:Cl:76:MET:SD	6:Co:299:GLY:HA2	2.52	0.50
8:Dk:99:LEU:HD13	8:Dk:209:MET:HB3	1.94	0.50
2:Dn:164:PRO:HB2	2:Dn:177:ASN:HD22	1.77	0.50
1:Dq:147:VAL:HG22	1:Dq:154:VAL:HG22	1.94	0.50
5:Dr:236:SER:H	5:Dr:244:VAL:HG22	1.76	0.50
2:Er:67:VAL:HG22	2:Er:76:ILE:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:117:VAL:HG13	1:Aa:142:LYS:HD3	1.94	0.49
6:Ag:320:LEU:O	8:Ai:143:THR:HB	2.11	0.49
2:Al:51:ALA:HB1	4:An:44:LYS:HD3	1.94	0.49
1:Ay:119:ILE:HD12	1:Ay:135:ILE:HG12	1.94	0.49
2:Bf:114:ILE:HG23	2:Bf:184:PHE:HB3	1.93	0.49
3:Bg:275:ASP:HB3	3:Bg:294:PHE:HB2	1.94	0.49
3:Ck:244:LYS:HD3	3:Ck:282:TYR:CD2	2.46	0.49
3:Cu:65:ASN:HB2	3:Cu:109:LYS:HG2	1.94	0.49
3:Cu:250:ARG:HH21	9:Db:82:GLU:HG2	1.77	0.49
7:En:148:LEU:HB3	7:En:192:PHE:CE2	2.46	0.49
3:Ac:292:MET:HG2	3:Ac:296:GLY:O	2.13	0.49
3:Bg:70:MET:HG3	3:Bg:107:ASP:HB3	1.93	0.49
7:Bl:148:LEU:HB3	7:Bl:192:PHE:CE2	2.47	0.49
3:Ca:303:GLU:HB2	3:Ca:306:GLN:HG3	1.93	0.49
3:Cu:176:VAL:HG22	3:Cu:195:ASP:HB2	1.94	0.49
3:Cu:275:ASP:HB3	3:Cu:294:PHE:HB2	1.94	0.49
4:Cv:92:TYR:CE2	4:Cv:94:GLN:HB3	2.46	0.49
1:Ek:75:ASN:HA	1:Ek:80:GLN:NE2	2.27	0.49
2:Er:45:VAL:HG22	4:Et:67:THR:HB	1.94	0.49
2:Er:118:SER:HB2	2:Er:133:THR:HB	1.93	0.49
7:Ah:166:ALA:HA	7:Ah:206:GLU:O	2.12	0.49
1:Bi:30:ILE:HD12	1:Bi:31:ASN:N	2.28	0.49
2:Bz:126:VAL:HA	2:Bz:129:GLU:OE1	2.11	0.49
3:Ca:118:TYR:OH	3:Ca:122:GLY:HA3	2.11	0.49
5:Cd:246:LEU:HG	5:Cd:255:LEU:HD23	1.94	0.49
7:Cp:167:GLY:HA2	7:Cp:229:ILE:HD13	1.94	0.49
3:Cu:228:VAL:HG11	3:Cu:231:LEU:HB2	1.95	0.49
2:Ab:45:VAL:HG22	4:Ad:67:THR:HB	1.94	0.49
3:Am:177:LEU:HD13	3:Am:181:PRO:HG2	1.94	0.49
8:Bm:108:PRO:HD3	8:Bm:138:ALA:HB2	1.94	0.49
1:Bo:125:ASP:OD1	3:Bq:319:PHE:HE1	1.94	0.49
2:Cj:148:GLY:HA3	1:Cm:30:ILE:HD11	1.94	0.49
1:Eg:143:ALA:HB1	1:Eg:156:LEU:HD11	1.93	0.49
9:Ez:27:LYS:NZ	9:Ez:28:PHE:H	2.10	0.49
3:Ac:65:ASN:HB2	3:Ac:109:LYS:HG2	1.94	0.49
7:Ah:147:GLY:O	7:Ah:151:VAL:HG23	2.12	0.49
7:Ar:167:GLY:HA2	7:Ar:229:ILE:HD13	1.94	0.49
1:Au:29:PRO:HG3	7:Bb:225:GLN:HA	1.94	0.49
2:Cj:75:LEU:HB2	8:Da:299:ILE:HD12	1.93	0.49
2:Dx:75:LEU:HD12	2:Dx:183:THR:HG22	1.95	0.49
7:Ed:51:GLN:HG3	7:Ed:52:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3: Ei:303:GLU:HB2	3: Ei:306:GLN:HG3	1.93	0.49
1: Ak:162:TYR:CD1	8: As:247:LEU:HD11	2.45	0.49
8: Bc:271:ASN:HD21	8: Bc:273:LEU:HB2	1.77	0.49
7: Bl:163:ILE:HD11	7: Bl:202:ARG:HH21	1.78	0.49
8: Cg:246:VAL:HG22	8: Cq:126:ARG:HG3	1.93	0.49
1: Dc:54:GLU:O	1: Dc:58:VAL:HG12	2.13	0.49
1: Dw:28:PRO:HD3	7: Ed:115:GLN:HB2	1.94	0.49
3: Ei:49:GLN:HB3	3: Ei:89:THR:HG22	1.95	0.49
3: Ac:292:MET:HE2	3: Ac:298:VAL:H	1.77	0.49
3: Aw:268:HIS:HB3	7: Bb:187:GLU:OE1	2.13	0.49
1: Be:58:VAL:HG11	8: Bm:214:LYS:HG3	1.94	0.49
7: Bl:140:LEU:HD13	7: Bl:188:THR:HG22	1.95	0.49
7: Bv:54:ARG:HB3	7: Bv:57:VAL:HG22	1.93	0.49
1: By:121:ILE:HG22	1: By:123:THR:HG23	1.94	0.49
3: Ck:275:ASP:HB3	3: Ck:294:PHE:HB2	1.95	0.49
8: Cq:271:ASN:HB2	9: Cr:53:SER:HA	1.93	0.49
2: Ct:67:VAL:HG22	2: Ct:76:ILE:HG23	1.94	0.49
4: Dz:76:MET:SD	6: Ec:299:GLY:HA2	2.52	0.49
1: Ea:97:ARG:HH11	1: Ea:100:LYS:NZ	2.11	0.49
3: Am:118:TYR:OH	3: Am:122:GLY:HA3	2.11	0.49
7: Bl:118:GLU:HG3	7: Bl:123:ARG:HG2	1.94	0.49
9: Ch:40:PRO:HB3	9: Ch:56:TYR:CE1	2.48	0.49
8: Cq:99:LEU:HD13	8: Cq:209:MET:HB2	1.95	0.49
3: Do:191:LEU:HG	3: Do:212:LEU:HD21	1.94	0.49
3: Do:275:ASP:HB3	3: Do:294:PHE:HB2	1.95	0.49
9: Dv:62:TYR:HD2	9: Dv:62:TYR:O	1.95	0.49
7: En:161:SER:HB2	7: En:233:TRP:HB2	1.94	0.49
3: Ac:117:ARG:HB3	3: Ac:117:ARG:HH11	1.75	0.49
1: Ak:55:MET:HE1	1: Ao:55:MET:HE2	1.93	0.49
3: Am:303:GLU:HB2	3: Am:306:GLN:HG3	1.94	0.49
8: Bc:170:LYS:HG3	8: Bc:171:ALA:H	1.77	0.49
9: Bn:40:PRO:HB3	9: Bn:56:TYR:CE2	2.48	0.49
1: Cc:97:ARG:HD2	8: Cq:263:ARG:HH22	1.78	0.49
3: Ck:250:ARG:NH1	7: Cp:190:MET:HE1	2.27	0.49
1: Cm:87:TRP:CD1	1: Cm:94:LEU:HD22	2.48	0.49
3: De:292:MET:HE1	3: De:320:PRO:HB3	1.95	0.49
3: Ei:191:LEU:HG	3: Ei:212:LEU:HD21	1.94	0.49
8: Eo:137:GLN:HG2	8: Eo:252:LEU:HD13	1.95	0.49
1: Be:69:ASN:HD21	1: Be:133:ARG:HA	1.77	0.49
2: Bf:66:LYS:HD3	7: Bv:119:TYR:HD1	1.78	0.49
2: Bp:93:TRP:HB2	7: Bv:46:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Br:45:MET:HB3	4:Br:62:ASN:HD21	1.78	0.49
1:Cc:80:GLN:NE2	9:Cr:47:LEU:HD11	2.27	0.49
1:Ci:69:ASN:HD21	1:Ci:133:ARG:HA	1.77	0.49
8:Da:38:ALA:HB1	8:Da:173:LYS:HD2	1.94	0.49
3:De:228:VAL:HG11	3:De:231:LEU:HB2	1.94	0.49
1:Dg:76:ALA:O	1:Dg:80:GLN:HG2	2.13	0.49
9:Dl:46:LEU:HD11	9:Dl:59:LYS:HD3	1.94	0.49
9:Dl:48:VAL:HG21	9:Dl:57:ILE:HD11	1.95	0.49
3:Dy:163:THR:HB	3:Dy:183:VAL:HG23	1.95	0.49
8:Eo:276:PHE:HB2	8:Eo:288:ILE:HD11	1.95	0.49
7:Ah:167:GLY:HA2	7:Ah:229:ILE:HD13	1.94	0.48
1:Au:147:VAL:HG22	1:Au:154:VAL:HG22	1.94	0.48
8:Bm:247:LEU:HB2	8:Bw:125:ILE:HG12	1.95	0.48
3:Ck:118:TYR:OH	3:Ck:122:GLY:HA3	2.11	0.48
2:Dd:52:THR:O	2:Dd:56:MET:HG3	2.13	0.48
2:Dd:56:MET:HE1	2:Dd:105:PHE:HA	1.94	0.48
3:De:303:GLU:HB2	3:De:306:GLN:HG3	1.95	0.48
7:Dt:125:LEU:HD11	7:Dt:154:LEU:HD23	1.95	0.48
3:Ei:228:VAL:HG11	3:Ei:231:LEU:HB2	1.95	0.48
5:El:233:ARG:HG2	5:El:233:ARG:HH11	1.78	0.48
1:Eq:136:ASP:OD2	1:Eu:60:LYS:HE2	2.12	0.48
7:Ar:148:LEU:HB3	7:Ar:192:PHE:CE2	2.48	0.48
2:Bf:117:THR:HG23	2:Bf:157:GLN:HG3	1.95	0.48
1:By:136:ASP:OD2	1:Cc:60:LYS:HE2	2.12	0.48
6:Ce:324:TRP:HA	6:Ce:339:MET:HB3	1.94	0.48
7:Cf:51:GLN:HG3	7:Cf:52:PRO:HD2	1.95	0.48
7:Cz:148:LEU:HB3	7:Cz:192:PHE:CE2	2.48	0.48
8:Da:137:GLN:HG2	8:Da:252:LEU:HD13	1.95	0.48
9:Dl:39:LYS:HD3	9:Dl:40:PRO:CD	2.42	0.48
2:Dn:111:LYS:HD2	2:Dn:114:ILE:HG12	1.94	0.48
1:Dq:119:ILE:HD12	1:Dq:135:ILE:HG12	1.95	0.48
1:Dw:117:VAL:HG13	1:Dw:142:LYS:HD3	1.93	0.48
2:Eh:93:TRP:HB2	7:En:46:PRO:HD3	1.95	0.48
2:Eh:117:THR:HG23	2:Eh:157:GLN:HG3	1.94	0.48
3:Ac:84:ILE:HG13	3:Ac:86:LYS:HZ2	1.78	0.48
3:Aw:65:ASN:HB2	3:Aw:109:LYS:HG2	1.94	0.48
3:Aw:274:THR:O	3:Aw:293:ALA:HB3	2.13	0.48
4:Br:84:CYS:HB3	8:Bw:154:ASP:HB3	1.94	0.48
6:Bu:283:VAL:HG21	6:Bu:312:TYR:HB3	1.95	0.48
3:Ck:274:THR:O	3:Ck:293:ALA:HB3	2.14	0.48
3:Ck:292:MET:HE1	3:Ck:320:PRO:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Co:284:LEU:HD22	6:Co:330:SER:HB3	1.96	0.48
1:Cw:87:TRP:CD1	1:Cw:94:LEU:HB2	2.48	0.48
7:Ex:167:GLY:HA2	7:Ex:229:ILE:HD13	1.94	0.48
9:Ez:40:PRO:HB3	9:Ez:56:TYR:CE2	2.49	0.48
1:Ae:97:ARG:HH11	1:Ae:100:LYS:NZ	2.10	0.48
2:Al:106:LEU:HD22	2:Al:114:ILE:HD13	1.94	0.48
2:Bf:56:MET:HE3	2:Bf:105:PHE:HD1	1.77	0.48
9:Bn:62:TYR:O	9:Bn:62:TYR:HD2	1.95	0.48
2:Bp:111:LYS:HD2	2:Bp:114:ILE:HG12	1.95	0.48
3:De:228:VAL:HG23	3:De:246:LEU:HD11	1.95	0.48
7:En:167:GLY:HA2	7:En:229:ILE:HD13	1.94	0.48
9:Ez:25:LEU:HD23	9:Ez:68:TYR:CZ	2.48	0.48
3:Ac:228:VAL:HG11	3:Ac:231:LEU:HB2	1.95	0.48
1:Ae:40:LYS:HG2	7:Ah:172:VAL:HG21	1.96	0.48
3:Aw:70:MET:HG3	3:Aw:107:ASP:HB3	1.96	0.48
9:Bd:27:LYS:NZ	9:Bd:29:ARG:H	2.07	0.48
3:Bq:250:ARG:HD3	3:Bq:268:HIS:HB2	1.94	0.48
3:Cu:191:LEU:HD21	3:Cu:194:LEU:HD12	1.95	0.48
3:Dy:228:VAL:HG23	3:Dy:246:LEU:HD11	1.95	0.48
3:Es:51:VAL:HG22	3:Es:117:ARG:HG3	1.96	0.48
3:Es:65:ASN:HB2	3:Es:109:LYS:HG2	1.95	0.48
4:Et:91:VAL:HG13	4:Et:101:VAL:HG13	1.95	0.48
6:Ce:320:LEU:O	8:Cg:143:THR:HB	2.14	0.48
1:Cm:75:ASN:O	1:Cm:75:ASN:OD1	2.31	0.48
9:Db:62:TYR:HD2	9:Db:62:TYR:O	1.96	0.48
1:Eq:162:TYR:CD1	8:Ey:247:LEU:HD11	2.44	0.48
8:Ai:60:LYS:HD3	8:Ai:179:TYR:CZ	2.48	0.48
1:Ak:147:VAL:HG22	1:Ak:154:VAL:HG22	1.94	0.48
2:Av:118:SER:HB2	2:Av:133:THR:HB	1.94	0.48
1:Be:125:ASP:C	1:Be:125:ASP:OD1	2.57	0.48
2:Bp:117:THR:HG23	2:Bp:157:GLN:HG3	1.95	0.48
1:Eu:40:LYS:HG2	7:Ex:172:VAL:HG21	1.96	0.48
6:Ew:324:TRP:HA	6:Ew:339:MET:HB3	1.95	0.48
9:Aj:27:LYS:NZ	9:Aj:29:ARG:H	2.06	0.48
1:Ak:28:PRO:HG2	1:Ak:29:PRO:HD3	1.96	0.48
3:Bg:134:LEU:HD21	3:Bg:150:ILE:HG23	1.96	0.48
1:Ci:124:LYS:HE2	2:Cj:142:GLU:OE2	2.13	0.48
6:Co:283:VAL:HG21	6:Co:312:TYR:HB3	1.96	0.48
3:Cu:173:LEU:HD23	3:Cu:174:GLN:N	2.29	0.48
5:Cx:223:ILE:HD11	5:Cx:227:GLY:HA2	1.96	0.48
2:Dd:93:TRP:HB2	7:Dj:46:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Eh:75:LEU:HD12	2:Eh:183:THR:HG22	1.96	0.48
1:Eu:87:TRP:CD1	1:Eu:94:LEU:HB2	2.48	0.48
1:Ae:75:ASN:HA	1:Ae:80:GLN:NE2	2.29	0.48
2:Av:126:VAL:HA	2:Av:129:GLU:OE2	2.14	0.48
1:Ay:160:LYS:H	1:Ay:160:LYS:CD	2.27	0.48
7:Cf:234:PHE:CE2	9:Ch:29:ARG:HG2	2.48	0.48
5:Cx:233:ARG:HA	5:Cx:233:ARG:HD3	1.67	0.48
2:Dn:50:ASP:HB3	4:Dp:45:MET:SD	2.54	0.48
8:Du:224:PRO:HB3	8:Du:253:PRO:HD3	1.94	0.48
3:Dy:275:ASP:HB3	3:Dy:294:PHE:HB2	1.96	0.48
6:Ec:320:LEU:O	8:Ee:143:THR:HB	2.13	0.48
8:Ee:99:LEU:HD13	8:Ee:209:MET:HB3	1.96	0.48
9:Ef:25:LEU:O	9:Ef:25:LEU:HD13	2.13	0.48
1:Aa:41:LEU:HD22	8:Ai:90:LEU:HD21	1.95	0.48
8:Ai:197:GLU:OE2	6:Ew:294:ARG:HD2	2.14	0.48
4:An:76:MET:SD	6:Aq:299:GLY:HA2	2.53	0.48
9:At:27:LYS:NZ	9:At:29:ARG:H	2.06	0.48
8:Bc:38:ALA:HB1	8:Bc:173:LYS:HD2	1.96	0.48
3:Bg:292:MET:HE1	3:Bg:320:PRO:HB3	1.95	0.48
6:Bk:297:VAL:HG11	6:Bk:302:ALA:HB3	1.96	0.48
6:Bk:320:LEU:O	8:Bm:143:THR:HB	2.14	0.48
3:Ca:196:MET:HE1	3:Ca:202:LEU:HB3	1.96	0.48
1:Dg:160:LYS:H	1:Dg:160:LYS:HD3	1.79	0.48
1:Dm:162:TYR:CD1	8:Du:247:LEU:HD11	2.45	0.48
3:Do:117:ARG:HE	3:Do:117:ARG:HB3	1.46	0.48
9:Ef:62:TYR:HD2	9:Ef:62:TYR:O	1.96	0.48
3:Ei:253:VAL:HG21	3:Ei:263:ILE:HG21	1.96	0.48
5:El:234:GLU:OE1	5:El:247:ILE:HG12	2.14	0.48
2:Al:55:LYS:HB2	4:An:44:LYS:NZ	2.29	0.47
1:Ao:75:ASN:HA	1:Ao:80:GLN:NE2	2.29	0.47
9:Bn:26:THR:O	9:Bn:27:LYS:C	2.57	0.47
3:Bq:31:LYS:HG3	3:Bq:33:GLN:H	1.80	0.47
3:Ck:253:VAL:HG21	3:Ck:263:ILE:HG21	1.96	0.47
3:Cu:228:VAL:HG23	3:Cu:246:LEU:HD11	1.96	0.47
8:Da:292:ASN:OD1	9:Db:31:ASP:HA	2.14	0.47
9:Db:25:LEU:O	9:Db:25:LEU:HD13	2.13	0.47
1:Dc:58:VAL:HG23	8:Dk:265:ALA:HB3	1.96	0.47
1:Eg:41:LEU:HD22	8:Eo:90:LEU:HD21	1.95	0.47
2:Av:57:MET:HG2	2:Av:67:VAL:CG1	2.44	0.47
6:Ce:297:VAL:HG11	6:Ce:302:ALA:HB3	1.95	0.47
2:Dx:45:VAL:HG23	2:Dx:48:ALA:HB3	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Es:118:TYR:HB3	3:Es:138:LEU:HD13	1.97	0.47
7:Bv:51:GLN:HG3	7:Bv:52:PRO:HD2	1.96	0.47
5:Cd:223:ILE:HD12	5:Cd:224:GLY:H	1.80	0.47
2:Cj:55:LYS:HB2	4:Cl:44:LYS:NZ	2.29	0.47
3:Ck:228:VAL:HG23	3:Ck:246:LEU:HD11	1.96	0.47
4:Cl:46:GLY:HA3	4:Cl:61:ASN:HB2	1.95	0.47
7:Cp:148:LEU:HB3	7:Cp:192:PHE:CE2	2.50	0.47
1:Dc:69:ASN:HD21	1:Dc:133:ARG:HA	1.78	0.47
3:De:119:GLU:HG2	3:De:139:ALA:HB3	1.97	0.47
8:Du:218:MET:HE3	8:Du:220:MET:HE1	1.96	0.47
1:Aa:58:VAL:HG23	8:Ai:265:ALA:HB3	1.96	0.47
2:Ab:93:TRP:HB2	7:Ah:46:PRO:HD3	1.95	0.47
1:Ak:62:ILE:HD12	8:As:263:ARG:HE	1.78	0.47
2:Av:75:LEU:HB2	8:Bm:299:ILE:HD12	1.95	0.47
7:Bb:161:SER:HB2	7:Bb:233:TRP:HB2	1.97	0.47
3:Bg:292:MET:HE2	3:Bg:298:VAL:H	1.79	0.47
4:Bh:111:GLU:HG3	8:Bm:154:ASP:HB2	1.97	0.47
3:Bq:119:GLU:HG2	3:Bq:139:ALA:HB3	1.95	0.47
3:Bq:274:THR:O	3:Bq:293:ALA:HB3	2.14	0.47
8:Bw:109:VAL:HG13	8:Bw:208:GLY:HA3	1.97	0.47
8:Bw:247:LEU:HB2	8:Cg:125:ILE:HG12	1.96	0.47
6:Cy:283:VAL:HG21	6:Cy:312:TYR:HB3	1.96	0.47
8:Da:99:LEU:HD13	8:Da:209:MET:HB3	1.96	0.47
8:Da:247:LEU:HB2	8:Dk:125:ILE:HG12	1.96	0.47
6:Di:312:TYR:HA	6:Di:337:TYR:O	2.15	0.47
1:Dm:117:VAL:HG13	1:Dm:142:LYS:HD3	1.95	0.47
1:Dw:143:ALA:HB1	1:Dw:156:LEU:HD11	1.95	0.47
3:Dy:191:LEU:HG	3:Dy:212:LEU:HD21	1.96	0.47
1:Eg:125:ASP:OD1	3:Ei:319:PHE:HE1	1.97	0.47
7:Ex:132:TYR:CE2	7:Ex:144:CYS:HB3	2.49	0.47
7:Ex:140:LEU:HD13	7:Ex:188:THR:HG22	1.97	0.47
2:Al:117:THR:HA	2:Al:157:GLN:O	2.15	0.47
2:Av:45:VAL:HG22	4:Ax:67:THR:HB	1.95	0.47
6:Ba:320:LEU:O	8:Bc:143:THR:HB	2.14	0.47
8:Bc:246:VAL:HG22	8:Bm:126:ARG:HG3	1.96	0.47
9:Bd:62:TYR:HD1	9:Bd:62:TYR:O	1.96	0.47
3:Bq:231:LEU:HD12	3:Bq:232:ASP:N	2.29	0.47
2:Bz:118:SER:HB2	2:Bz:133:THR:HB	1.96	0.47
5:Cd:233:ARG:HD3	5:Cd:234:GLU:N	2.26	0.47
3:Cu:111:LYS:HE3	3:Cu:111:LYS:HB3	1.68	0.47
3:Cu:119:GLU:HG2	3:Cu:139:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dc:55:MET:HE1	1:Dg:55:MET:SD	2.55	0.47
6:Di:320:LEU:O	8:Dk:143:THR:HB	2.13	0.47
1:Dq:160:LYS:H	1:Dq:160:LYS:HD3	1.79	0.47
1:Dw:77:TYR:OH	2:Dx:130:ARG:HD3	2.14	0.47
3:Dy:119:GLU:HG2	3:Dy:139:ALA:HB3	1.97	0.47
9:Ep:25:LEU:HD13	9:Ep:25:LEU:O	2.14	0.47
2:Ab:117:THR:HG23	2:Ab:157:GLN:HG3	1.96	0.47
1:Ae:105:ARG:HB2	1:Ae:153:VAL:HG22	1.96	0.47
7:Ar:51:GLN:HG3	7:Ar:52:PRO:HD2	1.97	0.47
3:Ca:214:ILE:HD11	3:Ca:224:LEU:HD11	1.97	0.47
3:Ca:274:THR:O	3:Ca:293:ALA:HB3	2.14	0.47
2:Cj:93:TRP:HB2	7:Cp:46:PRO:HD3	1.96	0.47
3:Cu:301:MET:HE3	3:Cu:301:MET:HB3	1.83	0.47
3:De:173:LEU:HD23	3:De:174:GLN:N	2.29	0.47
3:De:250:ARG:HD3	3:De:268:HIS:HB2	1.95	0.47
1:Dg:39:ILE:O	1:Dg:43:GLU:HG3	2.15	0.47
2:Dx:113:ALA:HA	2:Dx:153:ILE:O	2.14	0.47
3:Dy:134:LEU:HD21	3:Dy:150:ILE:HG23	1.96	0.47
8:Ee:178:ILE:HG13	8:Ee:179:TYR:N	2.29	0.47
3:Ei:51:VAL:HG22	3:Ei:117:ARG:HG3	1.97	0.47
1:Ek:100:LYS:HB3	1:Ek:100:LYS:HE2	1.68	0.47
2:Al:45:VAL:HG22	4:An:67:THR:HB	1.96	0.47
2:Av:50:ASP:HB3	4:Ax:45:MET:SD	2.54	0.47
3:Aw:253:VAL:HG21	3:Aw:263:ILE:HG21	1.96	0.47
1:Ay:97:ARG:NH1	8:Bm:263:ARG:HH12	2.13	0.47
5:Az:223:ILE:HD11	5:Az:227:GLY:HA2	1.96	0.47
1:Be:28:PRO:HG2	1:Be:29:PRO:HD3	1.97	0.47
7:Bl:55:ARG:HH21	7:Bl:153:ARG:NH1	2.13	0.47
3:Ck:228:VAL:HG11	3:Ck:231:LEU:HB2	1.97	0.47
5:Cn:230:LEU:HD12	5:Cn:231:THR:H	1.78	0.47
8:Cq:247:LEU:HB2	8:Da:125:ILE:HG12	1.94	0.47
6:Cy:297:VAL:HG11	6:Cy:302:ALA:HB3	1.96	0.47
7:Dt:163:ILE:HD11	7:Dt:202:ARG:HH21	1.80	0.47
6:Ew:306:LEU:HD11	6:Ew:341:LYS:HE2	1.97	0.47
1:Aa:58:VAL:HG11	8:Ai:214:LYS:HG3	1.96	0.47
6:Ag:297:VAL:HG11	6:Ag:302:ALA:HB3	1.97	0.47
1:Ao:97:ARG:HD2	8:Bc:263:ARG:NH2	2.30	0.47
3:Aw:228:VAL:HG23	3:Aw:246:LEU:HD11	1.97	0.47
7:Bb:167:GLY:HA2	7:Bb:229:ILE:HD13	1.96	0.47
1:Be:41:LEU:HD22	8:Bm:90:LEU:HD21	1.97	0.47
3:Bq:292:MET:HE1	3:Bq:320:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Bv:234:PHE:CE1	9:Bx:29:ARG:HG2	2.49	0.47
3:Ca:119:GLU:HG2	3:Ca:139:ALA:HB3	1.95	0.47
2:Cj:117:THR:HA	2:Cj:157:GLN:O	2.15	0.47
2:Cj:166:THR:HG22	2:Cj:168:TYR:H	1.80	0.47
1:Cm:119:ILE:HD13	1:Cm:135:ILE:HG23	1.96	0.47
1:Cw:26:LYS:HG2	7:Cz:143:ILE:HD11	1.97	0.47
3:Do:31:LYS:HG3	3:Do:33:GLN:H	1.80	0.47
3:Dy:31:LYS:HG3	3:Dy:33:GLN:H	1.79	0.47
1:Eu:160:LYS:CD	1:Eu:160:LYS:H	2.28	0.47
9:At:76:VAL:HG12	9:At:86:SER:HA	1.97	0.47
3:Bg:260:VAL:HG22	3:Bg:278:ASP:HB2	1.97	0.47
9:Bn:27:LYS:NZ	9:Bn:29:ARG:H	2.09	0.47
7:Bv:167:GLY:HA2	7:Bv:229:ILE:HD13	1.97	0.47
7:Bv:234:PHE:CZ	9:Bx:29:ARG:HG2	2.50	0.47
3:Ca:196:MET:HE3	3:Ca:222:ILE:HG12	1.96	0.47
1:Cc:33:PRO:HB2	1:Cc:39:ILE:HG12	1.97	0.47
2:Cj:117:THR:HG23	2:Cj:157:GLN:HG3	1.96	0.47
1:Dc:162:TYR:CD1	8:Dk:247:LEU:HD11	2.44	0.47
6:Ds:320:LEU:O	8:Du:143:THR:HB	2.15	0.47
8:Du:108:PRO:HD3	8:Du:138:ALA:HB2	1.97	0.47
1:Ea:87:TRP:CD1	1:Ea:94:LEU:HD22	2.50	0.47
7:Ed:140:LEU:HD13	7:Ed:188:THR:HG22	1.97	0.47
8:Ee:247:LEU:HB2	8:Eo:125:ILE:HG12	1.95	0.47
3:Es:275:ASP:HB3	3:Es:294:PHE:HB2	1.97	0.47
8:Ai:271:ASN:HD21	8:Ai:273:LEU:HB2	1.79	0.47
1:Ak:58:VAL:HG23	8:As:265:ALA:HB3	1.96	0.47
8:Bc:109:VAL:HG13	8:Bc:208:GLY:HA3	1.97	0.47
8:Bm:116:THR:HG21	8:Bm:131:THR:HG23	1.97	0.47
6:Bu:320:LEU:O	8:Bw:143:THR:HB	2.15	0.47
9:Bx:62:TYR:HD2	9:Bx:62:TYR:O	1.98	0.47
3:Ca:270:SER:HB3	7:Cf:191:THR:HG23	1.96	0.47
1:Cc:100:LYS:HB3	1:Cc:100:LYS:HE2	1.60	0.47
2:Ct:111:LYS:HD2	2:Ct:114:ILE:HG12	1.96	0.47
8:Da:243:ASP:O	8:Dk:128:SER:HA	2.15	0.47
7:Dj:234:PHE:CE1	9:Dl:29:ARG:HG2	2.50	0.47
7:Ex:234:PHE:N	7:Ex:234:PHE:CD1	2.83	0.47
1:Ae:76:ALA:HB3	1:Ae:79:LEU:HD12	1.97	0.46
3:Aw:31:LYS:HG3	3:Aw:33:GLN:H	1.80	0.46
7:Bb:190:MET:HG2	7:Bb:203:LEU:HD13	1.98	0.46
1:Be:75:ASN:HD22	1:Be:80:GLN:NE2	2.11	0.46
3:Ca:209:SER:HB3	3:Ca:228:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Da:298:ILE:H	8:Da:298:ILE:HD12	1.78	0.46
3:De:118:TYR:HB3	3:De:138:LEU:HD13	1.98	0.46
2:Dx:111:LYS:HD2	2:Dx:114:ILE:HG12	1.96	0.46
1:Eg:69:ASN:HD21	1:Eg:133:ARG:HA	1.79	0.46
3: Ei:166:ASN:HA	3: Ei:186:SER:HB3	1.97	0.46
3: Ei:191:LEU:HD21	3: Ei:194:LEU:HD12	1.97	0.46
9:Ep:26:THR:O	9:Ep:27:LYS:C	2.58	0.46
3:Ac:274:THR:O	3:Ac:293:ALA:HB3	2.14	0.46
9:Bd:26:THR:O	9:Bd:27:LYS:C	2.58	0.46
1:Bi:97:ARG:HH11	1:Bi:100:LYS:NZ	2.13	0.46
8:Bm:224:PRO:HB3	8:Bm:253:PRO:HD3	1.97	0.46
8:Bw:298:ILE:H	8:Bw:298:ILE:HD12	1.81	0.46
8:Cg:298:ILE:HD12	8:Cg:298:ILE:H	1.81	0.46
7:Cp:163:ILE:HD11	7:Cp:202:ARG:HH21	1.80	0.46
7:Cp:234:PHE:CE1	9:Cr:29:ARG:HG2	2.50	0.46
7:Dj:212:ASN:HD22	8:Dk:295:TRP:HZ3	1.64	0.46
1:Dw:65:PRO:HD3	1:Ea:58:VAL:HG22	1.97	0.46
9:Ef:26:THR:O	9:Ef:27:LYS:C	2.58	0.46
3:Es:31:LYS:HG3	3:Es:33:GLN:H	1.80	0.46
7:Ex:57:VAL:HA	7:Ex:60:VAL:HG22	1.96	0.46
7:Ah:170:ASP:OD2	7:Ah:227:ARG:HD3	2.15	0.46
3:Am:31:LYS:HG3	3:Am:33:GLN:H	1.80	0.46
3:Bq:70:MET:HG3	3:Bq:107:ASP:HB3	1.96	0.46
3:Bq:166:ASN:HA	3:Bq:186:SER:HB3	1.98	0.46
9:Ch:26:THR:O	9:Ch:27:LYS:C	2.58	0.46
3:Cu:31:LYS:HG3	3:Cu:33:GLN:H	1.80	0.46
8:Da:77:LYS:O	8:Da:81:GLU:HG3	2.16	0.46
3:Dy:155:LEU:HD23	3:Dy:155:LEU:HA	1.78	0.46
5:Ev:236:SER:H	5:Ev:244:VAL:HG22	1.80	0.46
1:Ak:77:TYR:OH	2:Al:130:ARG:HD3	2.15	0.46
2:Al:118:SER:HB2	2:Al:133:THR:HB	1.97	0.46
7:Ar:53:ASP:OD1	7:Ar:55:ARG:HD2	2.15	0.46
7:Bl:53:ASP:OD1	7:Bl:55:ARG:HG3	2.14	0.46
9:Bx:27:LYS:NZ	9:Bx:29:ARG:H	2.07	0.46
1:By:137:TYR:CZ	1:Cc:57:LYS:HG3	2.50	0.46
1:By:160:LYS:HE3	1:By:160:LYS:HB3	1.84	0.46
3:Ca:275:ASP:HB3	3:Ca:294:PHE:HB2	1.98	0.46
7:Cp:55:ARG:HH12	7:Cp:153:ARG:NE	2.13	0.46
9:Cr:40:PRO:HB3	9:Cr:56:TYR:CE1	2.49	0.46
9:Db:27:LYS:NZ	9:Db:29:ARG:H	2.05	0.46
1:Dg:40:LYS:HG2	7:Dj:172:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Dh:236:SER:H	5:Dh:244:VAL:HG22	1.80	0.46
3:Dy:274:THR:O	3:Dy:293:ALA:HB3	2.15	0.46
1:Eg:98:ILE:HG23	1:Eg:128:LEU:HD22	1.98	0.46
2:Eh:56:MET:HE1	2:Eh:105:PHE:HA	1.97	0.46
2:Eh:111:LYS:HD2	2:Eh:114:ILE:HG12	1.96	0.46
2:Eh:117:THR:HA	2:Eh:157:GLN:O	2.16	0.46
6:Em:306:LEU:HD11	6:Em:341:LYS:HE2	1.98	0.46
1:Eq:126:GLU:OE2	1:Eq:130:GLU:HB3	2.15	0.46
3:Es:205:TYR:O	3:Es:225:ALA:HB3	2.16	0.46
1:Aa:28:PRO:HD3	7:Ah:115:GLN:HB2	1.97	0.46
3:Bg:31:LYS:HG3	3:Bg:33:GLN:H	1.80	0.46
4:Bh:84:CYS:HA	8:Bm:154:ASP:HB3	1.98	0.46
9:Bn:25:LEU:HD23	9:Bn:68:TYR:CZ	2.50	0.46
2:Bz:93:TRP:HB2	7:Cf:46:PRO:HD3	1.98	0.46
8:Cg:109:VAL:HG13	8:Cg:208:GLY:HA3	1.98	0.46
3:Ck:217:LYS:HA	3:Ck:236:TRP:HB2	1.98	0.46
1:Dw:58:VAL:O	1:Dw:62:ILE:HG12	2.15	0.46
1:Aa:55:MET:HA	1:Aa:58:VAL:HG12	1.97	0.46
2:Al:152:ARG:HD2	6:Aq:352:LYS:HB2	1.97	0.46
1:Ay:97:ARG:HH11	1:Ay:100:LYS:NZ	2.14	0.46
4:Bh:76:MET:SD	6:Bk:299:GLY:HA2	2.55	0.46
2:Cj:98:LEU:HA	2:Cj:101:GLU:OE2	2.16	0.46
1:Cm:76:ALA:O	1:Cm:80:GLN:HG2	2.15	0.46
7:Cp:140:LEU:HD13	7:Cp:188:THR:HG22	1.98	0.46
8:Cq:243:ASP:O	8:Da:128:SER:HA	2.16	0.46
1:Cs:69:ASN:HD21	1:Cs:133:ARG:HA	1.79	0.46
8:Da:224:PRO:HB3	8:Da:253:PRO:HD3	1.96	0.46
4:Df:58:LEU:HB2	4:Df:66:SER:HB3	1.97	0.46
6:Di:320:LEU:HD11	6:Di:348:SER:HB3	1.97	0.46
8:Dk:247:LEU:HB2	8:Du:125:ILE:HG12	1.97	0.46
8:Dk:271:ASN:HD22	9:Dl:54:TYR:H	1.63	0.46
6:Em:281:LEU:O	6:Em:285:GLU:HG2	2.16	0.46
8:Eo:292:ASN:HD21	9:Ep:30:TRP:HE3	1.63	0.46
2:Av:93:TRP:HB2	7:Bb:46:PRO:HD3	1.98	0.46
3:Bq:51:VAL:HG22	3:Bq:117:ARG:HG3	1.98	0.46
2:Ct:113:ALA:HA	2:Ct:153:ILE:O	2.16	0.46
1:Cw:141:LYS:HB3	1:Cw:141:LYS:HE3	1.71	0.46
3:Dy:173:LEU:HD12	3:Dy:174:GLN:H	1.80	0.46
9:Ef:40:PRO:HB3	9:Ef:56:TYR:CE2	2.50	0.46
1:Ek:80:GLN:NE2	9:Ez:47:LEU:HD11	2.31	0.46
8:Eo:38:ALA:HB1	8:Eo:173:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Eu:26:LYS:HG2	7:Ex:143:ILE:HD11	1.98	0.46
2:Ab:98:LEU:HA	2:Ab:101:GLU:OE1	2.15	0.46
8:Ai:177:CYS:HA	8:Ai:180:THR:HG22	1.96	0.46
9:At:26:THR:O	9:At:27:LYS:C	2.59	0.46
8:Bc:178:ILE:HG13	8:Bc:179:TYR:N	2.30	0.46
2:Bf:183:THR:HB	8:Bw:299:ILE:HG23	1.97	0.46
8:Bm:231:LEU:HB2	8:Bm:244:ASP:HB3	1.98	0.46
1:Bs:76:ALA:O	1:Bs:80:GLN:HG2	2.16	0.46
8:Cg:243:ASP:O	8:Cq:128:SER:HA	2.16	0.46
1:Ci:147:VAL:HG22	1:Ci:154:VAL:HG22	1.96	0.46
2:Cj:50:ASP:HB3	4:Cl:45:MET:SD	2.56	0.46
2:Dn:45:VAL:HG22	4:Dp:67:THR:HB	1.98	0.46
3:Do:65:ASN:HB2	3:Do:109:LYS:HG2	1.98	0.46
1:Dq:35:ASP:O	1:Dq:39:ILE:HG13	2.16	0.46
8:Du:298:ILE:HD12	8:Du:298:ILE:N	2.31	0.46
2:Dx:126:VAL:HA	2:Dx:129:GLU:OE2	2.15	0.46
7:Ed:161:SER:HB2	7:Ed:233:TRP:HB2	1.98	0.46
8:Ee:153:MET:HE2	8:Ee:153:MET:HB3	1.82	0.46
9:Ep:27:LYS:NZ	9:Ep:29:ARG:H	2.06	0.46
3:Ac:119:GLU:HG2	3:Ac:139:ALA:HB3	1.97	0.46
3:Aw:275:ASP:HB3	3:Aw:294:PHE:HB2	1.98	0.46
2:Bp:148:GLY:HA3	1:Bs:30:ILE:HD11	1.98	0.46
7:Bv:148:LEU:HB3	7:Bv:192:PHE:CE2	2.51	0.46
3:Ck:119:GLU:HG2	3:Ck:139:ALA:HB3	1.98	0.46
1:Cm:30:ILE:HD12	1:Cm:31:ASN:N	2.31	0.46
1:Cm:160:LYS:H	1:Cm:160:LYS:CD	2.29	0.46
3:Cu:242:LYS:HE2	3:Cu:242:LYS:HB2	1.78	0.46
6:Cy:320:LEU:O	8:Da:143:THR:HB	2.15	0.46
3:De:31:LYS:HG3	3:De:33:GLN:H	1.80	0.46
9:Dv:26:THR:O	9:Dv:27:LYS:C	2.58	0.46
8:Ee:38:ALA:HB1	8:Ee:173:LYS:HD2	1.98	0.46
1:Ek:26:LYS:HG2	7:En:143:ILE:HD11	1.98	0.46
2:Er:114:ILE:HG23	2:Er:184:PHE:HB3	1.97	0.46
2:Ab:56:MET:HE1	2:Ab:105:PHE:HA	1.98	0.46
2:Al:50:ASP:HB3	4:An:45:MET:HE3	1.98	0.46
2:Al:93:TRP:HB2	7:Ar:46:PRO:HD3	1.99	0.46
1:Ay:107:ARG:NH1	1:Ay:153:VAL:HG11	2.31	0.46
7:Bb:60:VAL:O	7:Bb:64:THR:HG23	2.16	0.46
2:Bf:111:LYS:HD2	2:Bf:114:ILE:HG12	1.98	0.46
5:Bj:219:ARG:HD3	5:Bj:233:ARG:HH21	1.81	0.46
7:Bl:219:ILE:HG13	7:Bl:222:GLY:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Bv:57:VAL:HA	7:Bv:60:VAL:HG22	1.98	0.46
5:Cn:236:SER:H	5:Cn:244:VAL:HG22	1.81	0.46
6:Co:319:ILE:HG23	6:Co:322:PRO:HD2	1.98	0.46
7:Cp:105:ILE:HD13	7:Cp:153:ARG:HG2	1.97	0.46
9:Dl:26:THR:O	9:Dl:27:LYS:C	2.58	0.46
3:Do:111:LYS:HB3	3:Do:111:LYS:HE3	1.68	0.46
3:Do:119:GLU:HG2	3:Do:139:ALA:HB3	1.98	0.46
1:Eu:105:ARG:NH2	1:Eu:152:GLN:HB2	2.31	0.46
3:Ac:202:LEU:HD23	3:Ac:222:ILE:HG23	1.97	0.45
3:Am:228:VAL:HG11	3:Am:231:LEU:HB2	1.97	0.45
2:Bf:66:LYS:HD3	7:Bv:119:TYR:CD1	2.51	0.45
3:Bg:119:GLU:HG2	3:Bg:139:ALA:HB3	1.97	0.45
1:Bs:87:TRP:CD1	1:Bs:94:LEU:HD22	2.51	0.45
1:Cc:160:LYS:H	1:Cc:160:LYS:CD	2.29	0.45
7:Dt:140:LEU:HD13	7:Dt:188:THR:HG22	1.97	0.45
2:Er:93:TRP:HB2	7:Ex:46:PRO:HD3	1.98	0.45
8:Ey:299:ILE:HG22	8:Ey:302:VAL:HG23	1.98	0.45
9:Ez:26:THR:O	9:Ez:27:LYS:C	2.59	0.45
2:Ab:159:LEU:HB3	2:Ab:162:ASP:HB2	1.97	0.45
3:Ac:111:LYS:HE3	3:Ac:111:LYS:HB3	1.67	0.45
3:Ac:270:SER:HB3	7:Ah:191:THR:HG23	1.98	0.45
2:Al:67:VAL:HG22	2:Al:76:ILE:HG23	1.98	0.45
1:Ao:80:GLN:NE2	9:Bd:47:LEU:HD11	2.30	0.45
8:As:38:ALA:HB1	8:As:173:LYS:HD2	1.98	0.45
8:As:298:ILE:HG22	8:As:299:ILE:HD13	1.97	0.45
2:Bf:118:SER:HB2	2:Bf:133:THR:HB	1.98	0.45
1:Bs:97:ARG:HH11	1:Bs:100:LYS:HZ3	1.64	0.45
3:Ck:242:LYS:HE2	3:Ck:242:LYS:HB2	1.78	0.45
9:Cr:62:TYR:O	9:Cr:62:TYR:HD1	1.99	0.45
2:Ct:66:LYS:HE2	7:Dj:118:GLU:O	2.16	0.45
3:Cv:274:THR:O	3:Cv:293:ALA:HB3	2.16	0.45
6:Cy:312:TYR:HA	6:Cy:337:TYR:O	2.16	0.45
7:Cz:161:SER:HB2	7:Cz:233:TRP:HB2	1.98	0.45
8:Dk:146:THR:HG23	8:Dk:148:ARG:N	2.28	0.45
8:Dk:177:CYS:HA	8:Dk:180:THR:HG22	1.99	0.45
3:Do:208:LYS:HD3	3:Do:227:ILE:HD11	1.98	0.45
3:Do:270:SER:HB3	7:Dt:191:THR:HG23	1.98	0.45
3:Do:274:THR:O	3:Do:293:ALA:HB3	2.15	0.45
1:Dw:58:VAL:HG11	8:Ee:214:LYS:HG3	1.98	0.45
5:Eb:238:ILE:HG13	5:Eb:241:TYR:HB2	1.98	0.45
7:Ed:187:GLU:HG2	7:Ed:190:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Es:146:THR:HG23	8:Es:148:ARG:N	2.30	0.45
3:Es:274:THR:O	3:Es:293:ALA:HB3	2.16	0.45
1:Ae:87:TRP:CD1	1:Ae:94:LEU:HD22	2.51	0.45
5:Af:236:SER:H	5:Af:244:VAL:HG22	1.81	0.45
9:Aj:26:THR:O	9:Aj:27:LYS:C	2.59	0.45
3:Bg:274:THR:O	3:Bg:293:ALA:HB3	2.16	0.45
3:Bq:242:LYS:HE2	3:Bq:242:LYS:HB2	1.77	0.45
2:Bz:45:VAL:HG22	4:Cb:67:THR:HB	1.97	0.45
2:Bz:56:MET:HE1	2:Bz:105:PHE:HA	1.98	0.45
2:Bz:75:LEU:HD12	2:Bz:183:THR:HG22	1.97	0.45
5:Cd:247:ILE:HG13	5:Cd:247:ILE:O	2.17	0.45
2:Cj:113:ALA:HA	2:Cj:153:ILE:O	2.16	0.45
3:Ck:303:GLU:HB2	3:Ck:306:GLN:HG3	1.96	0.45
9:Cr:27:LYS:NZ	9:Cr:29:ARG:H	2.05	0.45
9:Db:26:THR:O	9:Db:27:LYS:C	2.58	0.45
2:Dd:117:THR:HA	2:Dd:157:GLN:O	2.15	0.45
8:Dk:38:ALA:HB1	8:Dk:173:LYS:HD2	1.98	0.45
1:Dm:69:ASN:HD21	1:Dm:133:ARG:HA	1.80	0.45
7:Ed:163:ILE:HD11	7:Ed:202:ARG:HH21	1.82	0.45
9:Ep:40:PRO:HB3	9:Ep:56:TYR:CE2	2.51	0.45
3:Am:51:VAL:HG22	3:Am:117:ARG:HG3	1.99	0.45
3:Am:274:THR:O	3:Am:293:ALA:HB3	2.16	0.45
8:As:243:ASP:O	8:Bc:128:SER:HA	2.17	0.45
1:Be:147:VAL:HG22	1:Be:154:VAL:HG22	1.97	0.45
1:Bi:119:ILE:HD13	1:Bi:135:ILE:HG12	1.98	0.45
8:Bm:109:VAL:HG13	8:Bm:208:GLY:HA3	1.98	0.45
8:Bm:119:LEU:HD12	8:Bm:125:ILE:HG22	1.98	0.45
2:Bp:118:SER:HB2	2:Bp:133:THR:HB	1.98	0.45
6:Bu:297:VAL:HG11	6:Bu:302:ALA:HB3	1.98	0.45
3:Ca:70:MET:HG3	3:Ca:107:ASP:HB3	1.99	0.45
3:Ck:31:LYS:HG3	3:Ck:33:GLN:H	1.81	0.45
8:Cq:38:ALA:HB1	8:Cq:173:LYS:HD2	1.97	0.45
4:Df:84:CYS:HA	8:Dk:154:ASP:HB3	1.98	0.45
3:Do:164:GLN:HE21	3:Do:184:LEU:HD11	1.81	0.45
1:Dq:40:LYS:HG2	7:Dt:172:VAL:HG21	1.98	0.45
8:Du:119:LEU:HD12	8:Du:125:ILE:HG22	1.99	0.45
8:Du:243:ASP:O	8:Ee:128:SER:HA	2.17	0.45
3:Ei:119:GLU:HG2	3:Ei:139:ALA:HB3	1.98	0.45
7:En:98:TYR:C	7:En:98:TYR:CD1	2.95	0.45
7:En:108:ASP:HA	7:En:111:LYS:HG3	1.98	0.45
8:Es:99:LEU:HD13	8:Es:209:MET:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Ex:234:PHE:CZ	9:Ez:29:ARG:HG2	2.50	0.45
1:Ae:87:TRP:CD1	1:Ae:94:LEU:HB2	2.52	0.45
1:Ao:120:SER:HB3	8:Bc:129:ASP:OD1	2.16	0.45
8:As:247:LEU:HB2	8:Bc:125:ILE:HG12	1.98	0.45
1:Au:117:VAL:HG13	1:Au:142:LYS:HD3	1.97	0.45
3:Aw:270:SER:HB3	7:Bb:191:THR:HG23	1.98	0.45
1:Ay:147:VAL:HG22	1:Ay:154:VAL:HG22	1.97	0.45
8:Bc:243:ASP:O	8:Bm:128:SER:HA	2.16	0.45
3:Bg:94:LEU:HD23	3:Bg:94:LEU:H	1.82	0.45
1:Bo:117:VAL:HG13	1:Bo:142:LYS:HD3	1.98	0.45
1:Bs:35:ASP:O	1:Bs:39:ILE:HG13	2.16	0.45
1:Bs:97:ARG:NH1	8:Cg:263:ARG:HH12	2.14	0.45
5:Bt:243:MET:HE2	5:Bt:244:VAL:O	2.17	0.45
1:Cs:62:ILE:CD1	8:Da:263:ARG:HE	2.28	0.45
8:Da:298:ILE:HD12	8:Da:298:ILE:N	2.31	0.45
2:Dx:99:LEU:HD23	2:Dx:99:LEU:HA	1.81	0.45
7:Ed:148:LEU:HB3	7:Ed:192:PHE:CE2	2.51	0.45
3:Ei:274:THR:O	3:Ei:293:ALA:HB3	2.16	0.45
1:Ek:35:ASP:O	1:Ek:39:ILE:HG13	2.15	0.45
5:El:238:ILE:HG13	5:El:241:TYR:HB2	1.99	0.45
2:Er:117:THR:HG23	2:Er:157:GLN:HG3	1.97	0.45
1:Eu:30:ILE:HD12	1:Eu:31:ASN:N	2.30	0.45
6:Ew:354:MET:HE2	6:Ew:354:MET:HB3	1.79	0.45
1:Ae:26:LYS:HG2	7:Ah:143:ILE:HD11	1.99	0.45
7:Ah:125:LEU:HD11	7:Ah:154:LEU:HD23	1.99	0.45
8:Ai:128:SER:HA	8:Ey:243:ASP:O	2.17	0.45
8:As:79:ILE:HG21	8:As:153:MET:HG3	1.98	0.45
2:Av:148:GLY:HA3	1:Ay:30:ILE:HD11	1.98	0.45
1:Bs:30:ILE:HD12	1:Bs:31:ASN:N	2.32	0.45
3:Ca:242:LYS:HE2	3:Ca:242:LYS:HB2	1.77	0.45
7:Cf:148:LEU:HB3	7:Cf:192:PHE:CE2	2.52	0.45
5:Cn:254:ILE:HB	5:Cn:262:ILE:HG12	1.99	0.45
7:Cp:55:ARG:HH12	7:Cp:153:ARG:NH2	2.14	0.45
8:Da:177:CYS:HA	8:Da:180:THR:HG22	1.98	0.45
8:Da:231:LEU:HB2	8:Da:244:ASP:HB3	1.98	0.45
3:De:217:LYS:HA	3:De:236:TRP:HB2	1.99	0.45
6:Ds:284:LEU:HD11	6:Ds:328:MET:HB3	1.97	0.45
1:Ea:105:ARG:NH2	1:Ea:152:GLN:HB2	2.32	0.45
1:Ae:77:TYR:HE2	8:As:273:LEU:HD13	1.82	0.45
9:Bd:40:PRO:HB3	9:Bd:56:TYR:CE2	2.52	0.45
2:Bf:93:TRP:HB2	7:Bl:46:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Br:62:ASN:HB2	1:By:26:LYS:HA	1.99	0.45
7:Bv:208:TYR:CD2	9:Bx:86:SER:HB2	2.51	0.45
9:Bx:26:THR:O	9:Bx:27:LYS:C	2.59	0.45
7:Cf:60:VAL:O	7:Cf:64:THR:HG23	2.17	0.45
7:Cp:105:ILE:HD12	7:Cp:157:PHE:HE2	1.82	0.45
7:Cz:163:ILE:HD11	7:Cz:202:ARG:HH21	1.82	0.45
8:Dk:271:ASN:ND2	9:Dl:54:TYR:H	2.15	0.45
1:Dq:26:LYS:HG2	7:Dt:143:ILE:HD11	1.99	0.45
3:El:31:LYS:HG3	3:El:33:GLN:H	1.82	0.45
1:Ek:87:TRP:CD1	1:Ek:94:LEU:HB2	2.52	0.45
1:Ek:105:ARG:NH2	1:Ek:152:GLN:HB2	2.32	0.45
5:Ev:238:ILE:HG13	5:Ev:241:TYR:HB2	1.99	0.45
8:As:119:LEU:HD12	8:As:125:ILE:HG22	1.99	0.45
1:Au:125:ASP:OD1	3:Aw:319:PHE:HE1	1.99	0.45
8:Bw:99:LEU:HD13	8:Bw:209:MET:HB3	1.99	0.45
8:Da:218:MET:HE3	8:Da:220:MET:HE3	1.98	0.45
2:Dd:118:SER:HB2	2:Dd:133:THR:HB	1.99	0.45
3:Do:94:LEU:HD23	3:Do:94:LEU:H	1.82	0.45
5:Dr:230:LEU:HD12	5:Dr:232:VAL:HG13	1.99	0.45
7:Dt:208:TYR:HD2	9:Dv:86:SER:HB2	1.82	0.45
3:Dy:217:LYS:HA	3:Dy:236:TRP:HB2	1.99	0.45
7:Ed:60:VAL:O	7:Ed:64:THR:HG23	2.17	0.45
7:Ed:166:ALA:HA	7:Ed:206:GLU:O	2.16	0.45
1:Eq:52:MET:HE2	1:Eu:52:MET:SD	2.56	0.45
1:Ak:39:ILE:O	1:Ak:43:GLU:HG3	2.17	0.45
1:Ao:39:ILE:O	1:Ao:43:GLU:HG3	2.17	0.45
5:Ap:210:TYR:CE2	5:Ap:224:GLY:HA2	2.52	0.45
1:Au:54:GLU:O	1:Au:58:VAL:HG12	2.17	0.45
1:Be:125:ASP:OD2	3:Bg:319:PHE:HE1	1.99	0.45
9:Bx:25:LEU:HD23	9:Bx:68:TYR:CZ	2.52	0.45
8:Cg:119:LEU:HD12	8:Cg:125:ILE:HG22	1.98	0.45
9:Ch:25:LEU:HD23	9:Ch:68:TYR:CZ	2.52	0.45
2:Cj:118:SER:HB2	2:Cj:133:THR:HB	1.99	0.45
3:Cu:235:LEU:HD11	3:Cu:241:PHE:HB3	1.99	0.45
7:Cz:219:ILE:HG13	7:Cz:222:GLY:H	1.82	0.45
2:Dd:111:LYS:HD2	2:Dd:114:ILE:HG12	1.99	0.45
7:Dj:60:VAL:O	7:Dj:64:THR:HG23	2.17	0.45
8:Dk:153:MET:HE2	8:Dk:153:MET:HB3	1.70	0.45
7:Dt:51:GLN:HG3	7:Dt:52:PRO:HD2	1.99	0.45
3:Dy:270:SER:HB3	7:Ed:191:THR:HG23	1.99	0.45
6:Ba:284:LEU:HD11	6:Ba:328:MET:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bo:94:LEU:HD23	1:Bo:119:ILE:HD11	1.98	0.45
7:Bv:53:ASP:OD1	7:Bv:55:ARG:HD2	2.17	0.45
8:Bw:119:LEU:HD12	8:Bw:125:ILE:HG22	1.99	0.45
3:Ca:138:LEU:HD13	3:Ca:138:LEU:HA	1.87	0.45
2:Cj:126:VAL:HA	2:Cj:129:GLU:OE1	2.17	0.45
3:Cu:117:ARG:HE	3:Cu:117:ARG:HB3	1.67	0.45
1:Dc:151:SER:HB3	9:Dv:92:GLU:HG2	1.99	0.45
8:Dk:243:ASP:O	8:Du:128:SER:HA	2.17	0.45
1:Dm:54:GLU:O	1:Dm:58:VAL:HG12	2.17	0.45
3:Dy:292:MET:HE2	3:Dy:298:VAL:H	1.81	0.45
4:Dz:45:MET:HG2	4:Dz:62:ASN:HD21	1.81	0.45
2:Eh:113:ALA:HA	2:Eh:153:ILE:O	2.17	0.45
2:Eh:114:ILE:HG23	2:Eh:184:PHE:HB3	1.98	0.45
6:Em:297:VAL:HG11	6:Em:302:ALA:HB3	1.99	0.45
7:En:53:ASP:OD1	7:En:55:ARG:HG3	2.16	0.45
2:Ab:113:ALA:HA	2:Ab:153:ILE:O	2.18	0.44
3:Ac:31:LYS:HG3	3:Ac:33:GLN:H	1.82	0.44
7:Ah:142:GLU:H	7:Ah:142:GLU:HG2	1.61	0.44
3:Am:119:GLU:HG2	3:Am:139:ALA:HB3	1.98	0.44
2:Av:135:ALA:O	2:Av:139:VAL:HG23	2.17	0.44
7:Bl:57:VAL:HA	7:Bl:60:VAL:HG22	1.99	0.44
2:Cj:66:LYS:HD3	7:Cz:119:TYR:CD1	2.52	0.44
7:Cp:60:VAL:O	7:Cp:64:THR:HG23	2.16	0.44
6:Cy:319:ILE:HG23	6:Cy:322:PRO:HD2	1.99	0.44
8:Da:153:MET:HE2	8:Da:153:MET:HB3	1.81	0.44
3:Do:224:LEU:HB2	3:Do:246:LEU:HD22	1.99	0.44
3:Dy:303:GLU:HB2	3:Dy:306:GLN:HG3	1.98	0.44
1:Eu:105:ARG:HH21	1:Eu:152:GLN:HB2	1.82	0.44
3:Ac:166:ASN:HA	3:Ac:186:SER:HB3	1.99	0.44
1:Ae:141:LYS:HB3	1:Ae:141:LYS:NZ	2.32	0.44
6:Aq:297:VAL:HG22	6:Aq:358:VAL:HG22	2.00	0.44
2:Av:75:LEU:HD12	2:Av:183:THR:HG22	1.98	0.44
2:Bf:135:ALA:O	2:Bf:139:VAL:HG23	2.16	0.44
3:Bg:111:LYS:HE3	3:Bg:111:LYS:HB3	1.68	0.44
3:Bg:116:PHE:HB3	3:Bg:136:LEU:HD23	1.99	0.44
4:Br:62:ASN:HB3	1:By:26:LYS:HG2	2.00	0.44
7:Bv:163:ILE:HD11	7:Bv:202:ARG:HH21	1.82	0.44
8:Bw:299:ILE:HG22	8:Bw:302:VAL:HG23	1.99	0.44
2:Bz:164:PRO:HB2	2:Bz:177:ASN:HD22	1.82	0.44
1:Cm:148:TYR:O	1:Cm:152:GLN:HA	2.17	0.44
7:Cz:60:VAL:O	7:Cz:64:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:De:166:ASN:HA	3:De:186:SER:HB3	1.99	0.44
3:Dy:209:SER:HB3	3:Dy:228:VAL:HG22	1.99	0.44
3:Ac:180:ASP:OD1	3:Ac:199:LYS:HB2	2.17	0.44
1:Ae:80:GLN:NE2	9:At:47:LEU:HD11	2.32	0.44
3:Am:217:LYS:HA	3:Am:236:TRP:HB2	1.99	0.44
3:Am:275:ASP:HB3	3:Am:294:PHE:HB2	1.99	0.44
5:Ap:250:LEU:H	5:Ap:250:LEU:HD22	1.82	0.44
3:Aw:111:LYS:HE3	3:Aw:111:LYS:HB3	1.68	0.44
8:Bc:99:LEU:HD13	8:Bc:209:MET:HB2	1.99	0.44
8:Bc:146:THR:HG23	8:Bc:148:ARG:N	2.30	0.44
3:Bg:303:GLU:HB2	3:Bg:306:GLN:HG3	1.98	0.44
8:Bw:170:LYS:HE3	8:Bw:174:GLU:OE1	2.17	0.44
1:Cc:30:ILE:HD12	1:Cc:31:ASN:N	2.32	0.44
5:Cd:230:LEU:HD23	5:Cd:231:THR:N	2.33	0.44
1:Ci:28:PRO:HD3	7:Cp:115:GLN:HB2	1.99	0.44
3:Ck:250:ARG:HH11	7:Cp:190:MET:HE1	1.82	0.44
1:Cw:87:TRP:CD1	1:Cw:94:LEU:HD22	2.53	0.44
5:Cx:236:SER:H	5:Cx:244:VAL:HG22	1.82	0.44
3:Do:250:ARG:HH21	9:Dv:82:GLU:HG2	1.82	0.44
1:Dq:141:LYS:NZ	1:Dq:141:LYS:HB3	2.32	0.44
5:Dr:230:LEU:HD13	5:Dr:231:THR:N	2.32	0.44
3:Dy:117:ARG:HB2	3:Dy:117:ARG:HH11	1.80	0.44
3:Dy:166:ASN:HA	3:Dy:186:SER:HB3	2.00	0.44
1:Ea:30:ILE:HD12	1:Ea:31:ASN:N	2.31	0.44
1:Ea:141:LYS:HB3	1:Ea:141:LYS:NZ	2.32	0.44
3:Es:164:GLN:HE21	3:Es:184:LEU:HD11	1.82	0.44
2:Ab:126:VAL:HA	2:Ab:129:GLU:OE1	2.17	0.44
8:Ai:88:ARG:HA	8:Ai:88:ARG:HD2	1.78	0.44
3:Aw:158:VAL:O	3:Aw:179:GLY:HA3	2.18	0.44
9:Bd:25:LEU:HD23	9:Bd:68:TYR:CZ	2.53	0.44
3:Bg:242:LYS:HE2	3:Bg:242:LYS:HB2	1.78	0.44
1:Bs:97:ARG:HD2	8:Cg:263:ARG:HH22	1.82	0.44
8:Cq:270:GLU:O	8:Cq:270:GLU:HG3	2.17	0.44
8:Da:290:ILE:HG22	9:Db:75:MET:HE3	1.99	0.44
4:Dz:84:CYS:HA	8:Ee:154:ASP:HB3	1.99	0.44
6:Ec:354:MET:HE2	6:Ec:354:MET:HB3	1.74	0.44
1:Eq:58:VAL:HG23	8:Ey:265:ALA:HB3	1.99	0.44
9:Ez:25:LEU:HD12	9:Ez:67:ARG:NH2	2.33	0.44
1:Aa:75:ASN:HD22	1:Aa:80:GLN:NE2	2.14	0.44
1:Aa:137:TYR:CZ	1:Ae:57:LYS:HG3	2.53	0.44
1:Ae:35:ASP:O	1:Ae:39:ILE:HG13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:143:ALA:HB1	1:Ak:156:LEU:HD11	2.00	0.44
3:Am:166:ASN:HA	3:Am:186:SER:HB3	1.99	0.44
3:Aw:217:LYS:HA	3:Aw:236:TRP:HB2	1.99	0.44
7:Bb:163:ILE:HD11	7:Bb:202:ARG:HH21	1.82	0.44
8:Bc:88:ARG:HA	8:Bc:88:ARG:HD2	1.77	0.44
1:Be:82:ARG:NH2	1:Be:126:GLU:HA	2.32	0.44
2:Bf:148:GLY:HA3	1:Bi:30:ILE:HD11	2.00	0.44
8:Bm:146:THR:HG23	8:Bm:148:ARG:N	2.30	0.44
2:Bp:152:ARG:HD2	6:Bu:352:LYS:HB2	1.98	0.44
3:Bq:94:LEU:HD23	3:Bq:94:LEU:H	1.82	0.44
9:Db:40:PRO:HB3	9:Db:56:TYR:CE2	2.52	0.44
1:Dc:160:LYS:HE3	1:Dc:160:LYS:HB3	1.82	0.44
7:Dj:234:PHE:CZ	9:Dl:29:ARG:HG2	2.53	0.44
8:Dk:77:LYS:O	8:Dk:81:GLU:HG3	2.18	0.44
2:Dx:93:TRP:HB2	7:Ed:46:PRO:HD3	1.99	0.44
8:Ee:243:ASP:O	8:Eo:128:SER:HA	2.16	0.44
3:Ei:94:LEU:HD23	3:Ei:94:LEU:H	1.82	0.44
8:Eo:247:LEU:HB2	8:Ey:125:ILE:HG12	1.98	0.44
5:Ev:233:ARG:HD3	5:Ev:234:GLU:N	2.33	0.44
8:Ai:38:ALA:HB1	8:Ai:173:LYS:HD2	2.00	0.44
8:Ai:153:MET:HE2	8:Ai:153:MET:HB3	1.94	0.44
3:Am:173:LEU:HD22	3:Am:175:ILE:HD12	2.00	0.44
1:Ao:87:TRP:CD1	1:Ao:94:LEU:HD22	2.52	0.44
3:Aw:118:TYR:HB3	3:Aw:138:LEU:HD13	1.99	0.44
3:Aw:119:GLU:HG2	3:Aw:139:ALA:HB3	1.99	0.44
8:Bc:146:THR:HG22	8:Bc:149:GLN:HG3	1.99	0.44
2:Bf:113:ALA:HA	2:Bf:153:ILE:O	2.17	0.44
1:Bi:33:PRO:HB3	1:Bi:38:THR:HG22	2.00	0.44
8:Bw:288:ILE:HA	9:Bx:79:ILE:HG12	2.00	0.44
6:Ce:320:LEU:HD11	6:Ce:348:SER:HB3	1.99	0.44
2:Ct:118:SER:HB2	2:Ct:133:THR:HB	2.00	0.44
7:Dj:57:VAL:HA	7:Dj:60:VAL:HG22	1.99	0.44
7:Dj:140:LEU:HD13	7:Dj:188:THR:HG22	1.99	0.44
7:Dt:234:PHE:CE1	9:Dv:29:ARG:HG2	2.53	0.44
5:Eb:247:ILE:O	5:Eb:247:ILE:HG13	2.18	0.44
6:Ec:317:LEU:HD22	6:Ec:349:TRP:HA	1.99	0.44
2:Eh:188:VAL:HG13	4:Ej:55:ALA:HB1	1.99	0.44
8:Eo:243:ASP:O	8:Ey:128:SER:HA	2.18	0.44
1:Eu:37:ALA:HA	7:Ex:220:ILE:HD12	1.99	0.44
2:Al:111:LYS:HD2	2:Al:114:ILE:HG12	2.00	0.44
3:Am:181:PRO:C	3:Am:182:LYS:HD2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:75:ASN:HA	1:Ao:80:GLN:HE22	1.82	0.44
9:At:62:TYR:HD2	9:At:62:TYR:O	2.01	0.44
1:Bi:126:GLU:HG2	1:Bi:130:GLU:HB2	1.98	0.44
5:Bj:223:ILE:HD11	5:Bj:227:GLY:HA2	1.99	0.44
7:Bl:60:VAL:O	7:Bl:64:THR:HG23	2.17	0.44
1:Bs:26:LYS:HG2	7:Bv:143:ILE:HD11	2.00	0.44
1:Bs:160:LYS:H	1:Bs:160:LYS:CD	2.29	0.44
1:By:126:GLU:OE1	1:By:130:GLU:HB3	2.18	0.44
7:Cf:98:TYR:CD1	7:Cf:98:TYR:C	2.96	0.44
3:Ck:111:LYS:HB3	3:Ck:111:LYS:HE3	1.68	0.44
2:Ct:52:THR:O	2:Ct:56:MET:HG3	2.18	0.44
3:Cu:94:LEU:HD23	3:Cu:94:LEU:H	1.83	0.44
7:Dj:193:LEU:HD11	7:Dj:231:ILE:HD13	2.00	0.44
9:Di:46:LEU:HD13	9:Di:62:TYR:HD1	1.83	0.44
1:Ek:40:LYS:HG2	7:En:172:VAL:HG21	2.00	0.44
3:Aw:94:LEU:HD23	3:Aw:94:LEU:H	1.83	0.44
3:Bg:209:SER:HB3	3:Bg:228:VAL:HG22	1.99	0.44
9:Bn:64:ILE:HD11	9:Bn:68:TYR:CE2	2.53	0.44
8:Bw:218:MET:HE2	8:Bw:220:MET:HE3	2.00	0.44
7:Cf:57:VAL:HA	7:Cf:60:VAL:HG22	2.00	0.44
7:Cp:170:ASP:OD1	7:Cp:227:ARG:HD3	2.17	0.44
7:Cz:90:THR:O	7:Cz:94:VAL:HG12	2.18	0.44
8:Dk:271:ASN:CG	8:Dk:272:ALA:N	2.76	0.44
1:Ea:26:LYS:HG2	7:Ed:143:ILE:HD11	2.00	0.44
6:Ec:284:LEU:HD11	6:Ec:328:MET:HB3	1.99	0.44
7:Ed:125:LEU:HD11	7:Ed:154:LEU:HD23	1.99	0.44
7:Ed:219:ILE:HG13	7:Ed:222:GLY:H	1.83	0.44
8:Ee:290:ILE:HG22	9:Ef:75:MET:HE3	1.99	0.44
6:Em:324:TRP:HA	6:Em:339:MET:HB3	1.99	0.44
8:Eo:214:LYS:O	8:Eo:218:MET:HG3	2.17	0.44
1:Be:151:SER:OG	9:Bx:92:GLU:HG2	2.18	0.44
3:Bg:235:LEU:HD11	3:Bg:241:PHE:HB3	1.99	0.44
3:Bq:39:ARG:HD3	3:Bq:39:ARG:HA	1.80	0.44
8:Bw:88:ARG:HA	8:Bw:88:ARG:HD2	1.83	0.44
9:Ch:27:LYS:NZ	9:Ch:29:ARG:H	2.08	0.44
9:Cr:26:THR:O	9:Cr:27:LYS:C	2.61	0.44
2:Ct:55:LYS:HB2	4:Cv:44:LYS:NZ	2.33	0.44
8:Da:170:LYS:HB2	8:Da:170:LYS:HE2	1.72	0.44
2:Dd:65:ILE:HG13	2:Dd:98:LEU:HD11	1.99	0.44
3:De:274:THR:O	3:De:293:ALA:HB3	2.17	0.44
8:Dk:246:VAL:HG22	8:Du:126:ARG:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dn:117:THR:HA	2:Dn:157:GLN:O	2.17	0.44
7:Dt:190:MET:HG2	7:Dt:203:LEU:HD13	2.00	0.44
7:Ed:98:TYR:CD1	7:Ed:98:TYR:C	2.96	0.44
8:Eo:88:ARG:HD2	8:Eo:88:ARG:HA	1.80	0.44
1:Ae:75:ASN:OD1	1:Ae:75:ASN:C	2.62	0.43
5:Af:238:ILE:HG13	5:Af:241:TYR:HB2	2.00	0.43
3:Am:173:LEU:HD23	3:Am:174:GLN:N	2.33	0.43
1:Ao:141:LYS:NZ	1:Ao:141:LYS:HB3	2.32	0.43
7:Ar:166:ALA:HA	7:Ar:206:GLU:O	2.17	0.43
8:As:146:THR:HG23	8:As:148:ARG:N	2.32	0.43
8:As:170:LYS:HG3	8:As:171:ALA:N	2.32	0.43
8:As:290:ILE:HG22	9:At:75:MET:HE3	1.99	0.43
8:Bc:77:LYS:O	8:Bc:81:GLU:HG3	2.18	0.43
3:Bg:205:TYR:O	3:Bg:225:ALA:HB3	2.18	0.43
1:Bi:141:LYS:NZ	1:Bi:141:LYS:HB3	2.32	0.43
8:Bm:106:LEU:HD13	8:Bm:141:ILE:HD13	1.99	0.43
3:Bq:217:LYS:HA	3:Bq:236:TRP:HB2	1.99	0.43
3:Bq:233:VAL:HG21	3:Bq:241:PHE:CE2	2.53	0.43
8:Bw:77:LYS:O	8:Bw:81:GLU:HG3	2.18	0.43
3:Ca:94:LEU:HD23	3:Ca:94:LEU:H	1.83	0.43
3:Ca:196:MET:SD	3:Ca:220:ALA:HB1	2.58	0.43
3:Ca:250:ARG:HH21	9:Ch:82:GLU:HG2	1.82	0.43
5:Cd:236:SER:H	5:Cd:244:VAL:HG22	1.82	0.43
4:Cl:64:PHE:CD2	1:Cs:27:LYS:HE3	2.52	0.43
7:Cp:57:VAL:HA	7:Cp:60:VAL:HG22	2.00	0.43
7:Cp:234:PHE:N	7:Cp:234:PHE:CD2	2.85	0.43
2:Ct:99:LEU:HD23	2:Ct:99:LEU:HA	1.84	0.43
1:Dm:151:SER:OG	9:Ef:92:GLU:HG2	2.18	0.43
9:Dv:27:LYS:NZ	9:Dv:29:ARG:H	2.07	0.43
1:Ea:97:ARG:HD3	1:Ea:100:LYS:NZ	2.32	0.43
9:Ef:27:LYS:NZ	9:Ef:29:ARG:H	2.10	0.43
3:Ac:173:LEU:HD23	3:Ac:174:GLN:N	2.33	0.43
7:Ah:57:VAL:HA	7:Ah:60:VAL:HG22	1.99	0.43
9:Aj:62:TYR:O	9:Aj:62:TYR:HD1	2.00	0.43
1:Ao:97:ARG:HD2	8:Bc:263:ARG:HH22	1.83	0.43
9:At:23:CYS:HB2	9:At:64:ILE:HD11	1.99	0.43
7:Bb:152:ILE:HD13	7:Bb:152:ILE:HA	1.85	0.43
8:Bw:185:LYS:HA	8:Bw:185:LYS:HD3	1.86	0.43
2:Bz:113:ALA:HA	2:Bz:153:ILE:O	2.18	0.43
3:Ca:111:LYS:HE3	3:Ca:111:LYS:HB3	1.68	0.43
3:Ck:164:GLN:HE21	3:Ck:184:LEU:HD11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cu:194:LEU:HD11	3:Cu:202:LEU:HD21	2.00	0.43
8:Dk:298:ILE:H	8:Dk:298:ILE:HD12	1.83	0.43
1:Dq:100:LYS:HB3	1:Dq:100:LYS:HE2	1.77	0.43
3:Dy:111:LYS:HE3	3:Dy:111:LYS:HB3	1.68	0.43
7:En:57:VAL:HA	7:En:60:VAL:HG22	1.99	0.43
8:Eo:170:LYS:HG3	8:Eo:171:ALA:N	2.33	0.43
3:Es:177:LEU:HD13	3:Es:181:PRO:HG2	2.00	0.43
7:Ex:140:LEU:HD23	7:Ex:148:LEU:HD13	1.98	0.43
3:Am:52:VAL:HB	3:Am:118:TYR:CD2	2.53	0.43
3:Am:228:VAL:HG23	3:Am:246:LEU:HD11	2.01	0.43
8:As:291:THR:HG22	8:As:293:LYS:N	2.33	0.43
5:Az:236:SER:H	5:Az:244:VAL:HG22	1.83	0.43
1:Bo:136:ASP:OD1	1:Bs:60:LYS:HE2	2.18	0.43
1:By:28:PRO:HG2	1:By:29:PRO:HD3	2.00	0.43
6:Cy:341:LYS:HB2	6:Cy:361:LEU:HD22	2.00	0.43
2:Dd:135:ALA:O	2:Dd:139:VAL:HG23	2.18	0.43
1:Dw:69:ASN:HD21	1:Dw:133:ARG:HA	1.83	0.43
7:En:51:GLN:HG3	7:En:52:PRO:HD2	2.01	0.43
7:En:138:PRO:HB3	7:En:184:ALA:HB1	1.99	0.43
2:Ab:117:THR:HA	2:Ab:157:GLN:O	2.18	0.43
3:Ac:164:GLN:HE21	3:Ac:184:LEU:HD11	1.83	0.43
8:Ai:56:GLU:O	8:Ai:60:LYS:HG3	2.18	0.43
1:Be:58:VAL:HG23	8:Bm:265:ALA:HB3	1.99	0.43
8:Bm:177:CYS:HA	8:Bm:180:THR:HG22	2.00	0.43
5:Cn:247:ILE:HG22	5:Cn:254:ILE:HG13	2.00	0.43
7:Cp:166:ALA:HA	7:Cp:206:GLU:O	2.17	0.43
5:Dh:247:ILE:O	5:Dh:247:ILE:HG13	2.19	0.43
2:Dn:148:GLY:HA3	1:Dq:30:ILE:HD11	2.01	0.43
8:Du:88:ARG:HA	8:Du:88:ARG:HD2	1.78	0.43
7:Ex:208:TYR:CD2	9:Ez:86:SER:HB2	2.53	0.43
1:Aa:69:ASN:HD21	1:Aa:133:ARG:HA	1.83	0.43
8:Ai:264:ALA:H	1:Eu:93:GLU:HG3	1.82	0.43
1:Au:58:VAL:HG23	8:Bc:265:ALA:HB3	2.01	0.43
8:Bc:170:LYS:CG	8:Bc:171:ALA:H	2.31	0.43
1:Be:137:TYR:CZ	1:Bi:57:LYS:HG3	2.53	0.43
5:Bj:247:ILE:HG13	5:Bj:247:ILE:O	2.19	0.43
8:Cg:146:THR:HG22	8:Cg:149:GLN:HG3	2.00	0.43
1:Cm:141:LYS:NZ	1:Cm:141:LYS:HB3	2.33	0.43
4:Cv:86:LEU:HD23	6:Cy:343:PRO:HG2	1.99	0.43
1:Cw:75:ASN:HA	1:Cw:80:GLN:NE2	2.33	0.43
8:Dk:287:LYS:HE3	8:Dk:289:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Eg:78:ASN:HB3	9:Ez:70:ARG:HD3	2.00	0.43
4:Et:45:MET:HG2	4:Et:62:ASN:HD21	1.82	0.43
1:Aa:151:SER:HB3	9:At:92:GLU:HG2	2.01	0.43
8:Ai:77:LYS:O	8:Ai:81:GLU:HG3	2.19	0.43
3:Aw:203:SER:HA	3:Aw:223:GLN:O	2.18	0.43
1:Be:77:TYR:C	1:Be:79:LEU:H	2.26	0.43
8:Bm:153:MET:HB3	8:Bm:153:MET:HE2	1.72	0.43
3:Bq:98:TYR:HE1	3:Bq:101:TYR:H	1.67	0.43
8:Bw:243:ASP:O	8:Cg:128:SER:HA	2.18	0.43
5:Cd:255:LEU:HD13	5:Cd:261:VAL:HG13	2.00	0.43
3:Ck:134:LEU:HD21	3:Ck:150:ILE:HG23	1.99	0.43
1:Cm:35:ASP:O	1:Cm:39:ILE:HG13	2.19	0.43
1:Cm:97:ARG:HD2	8:Da:263:ARG:HH22	1.83	0.43
1:Cs:84:SER:HB3	1:Cs:124:LYS:HA	2.01	0.43
2:Ct:183:THR:HB	8:Dk:299:ILE:HG23	2.00	0.43
7:Cz:57:VAL:HA	7:Cz:60:VAL:HG22	2.00	0.43
7:Cz:212:ASN:ND2	8:Da:295:TRP:HZ3	2.15	0.43
3:De:94:LEU:HD23	3:De:94:LEU:H	1.82	0.43
5:Dr:238:ILE:HG13	5:Dr:241:TYR:HB2	2.01	0.43
3:Dy:70:MET:HE2	3:Dy:70:MET:HB3	1.84	0.43
3:Dy:292:MET:HE1	3:Dy:320:PRO:HB3	2.00	0.43
3:Ei:217:LYS:HA	3:Ei:236:TRP:HB2	2.00	0.43
1:Eq:69:ASN:HD21	1:Eq:133:ARG:HA	1.84	0.43
1:Eu:141:LYS:NZ	1:Eu:141:LYS:HB3	2.33	0.43
5:Af:230:LEU:HD12	5:Af:231:THR:H	1.81	0.43
7:Ah:163:ILE:HD11	7:Ah:202:ARG:HH21	1.84	0.43
7:Ah:208:TYR:HD2	9:Aj:86:SER:HB2	1.84	0.43
1:Ao:26:LYS:HG2	7:Ar:143:ILE:HD11	2.01	0.43
7:Bb:57:VAL:HA	7:Bb:60:VAL:HG22	2.00	0.43
8:Bm:38:ALA:HB1	8:Bm:173:LYS:HD2	2.00	0.43
8:Bm:243:ASP:O	8:Bw:128:SER:HA	2.19	0.43
7:Cf:140:LEU:HD13	7:Cf:188:THR:HG22	2.01	0.43
1:Ci:79:LEU:HD23	1:Ci:79:LEU:HA	1.89	0.43
1:Ci:151:SER:HB3	9:Db:92:GLU:HG2	2.00	0.43
1:Ci:160:LYS:HE3	1:Ci:160:LYS:HB3	1.86	0.43
6:Ds:319:ILE:HG23	6:Ds:322:PRO:HD2	2.00	0.43
3:Es:70:MET:HG3	3:Es:107:ASP:HB3	2.00	0.43
1:Ao:48:VAL:HG11	8:As:93:ILE:HA	2.00	0.43
5:Ap:247:ILE:O	5:Ap:247:ILE:HG13	2.19	0.43
7:Ar:98:TYR:C	7:Ar:98:TYR:CD2	2.96	0.43
5:Az:233:ARG:CD	5:Az:234:GLU:H	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Bg:166:ASN:HA	3:Bg:186:SER:HB3	2.01	0.43
7:Bl:145:TYR:CD1	7:Bl:146:PRO:HD3	2.54	0.43
8:Bm:77:LYS:O	8:Bm:81:GLU:HG3	2.19	0.43
4:Br:111:GLU:HG3	8:Bw:154:ASP:HB2	2.00	0.43
4:Cb:102:VAL:HG22	4:Cb:108:VAL:HG22	2.01	0.43
6:Co:297:VAL:HG11	6:Co:302:ALA:HB3	2.00	0.43
8:Cq:298:ILE:H	8:Cq:298:ILE:HD12	1.84	0.43
2:Dd:113:ALA:HA	2:Dd:153:ILE:O	2.18	0.43
5:Dh:233:ARG:CD	5:Dh:234:GLU:H	2.30	0.43
3:Do:242:LYS:HE2	3:Do:242:LYS:HB2	1.79	0.43
1:Eg:137:TYR:CZ	1:Ek:57:LYS:HG3	2.53	0.43
8:Eo:231:LEU:HB2	8:Eo:244:ASP:HB3	2.01	0.43
6:Ew:322:PRO:HG2	6:Ew:345:LEU:HD23	2.00	0.43
9:Ez:57:ILE:HD12	9:Ez:61:GLN:HB3	2.00	0.43
1:Ae:148:TYR:O	1:Ae:152:GLN:HA	2.19	0.43
7:Ah:219:ILE:HG13	7:Ah:222:GLY:H	1.84	0.43
3:Am:208:LYS:HD3	3:Am:227:ILE:HD11	2.00	0.43
2:Bp:115:THR:HG23	2:Bp:155:PHE:HB2	2.01	0.43
5:Cd:247:ILE:HG22	5:Cd:254:ILE:HG13	2.00	0.43
3:Cu:141:GLU:HA	3:Cu:161:GLY:HA2	2.01	0.43
3:Cu:270:SER:HB3	7:Cz:191:THR:HG23	2.01	0.43
1:Dc:143:ALA:HB1	1:Dc:156:LEU:HD11	2.01	0.43
6:Di:341:LYS:HB2	6:Di:361:LEU:HD22	2.00	0.43
7:Dt:105:ILE:HD12	7:Dt:157:PHE:HE2	1.84	0.43
3:Dy:301:MET:HE3	3:Dy:301:MET:HB3	1.84	0.43
1:Ea:48:VAL:HG11	8:Ee:93:ILE:HA	1.99	0.43
7:Ed:57:VAL:HA	7:Ed:60:VAL:HG22	1.99	0.43
2:Eh:99:LEU:HD23	2:Eh:99:LEU:HA	1.78	0.43
3:Ei:212:LEU:HD12	3:Ei:228:VAL:HG21	2.01	0.43
7:En:234:PHE:CZ	9:Ep:29:ARG:HG2	2.54	0.43
2:Er:126:VAL:HA	2:Er:129:GLU:OE2	2.19	0.43
7:Ah:98:TYR:C	7:Ah:98:TYR:CD2	2.97	0.43
7:Ah:148:LEU:HB3	7:Ah:192:PHE:CE2	2.54	0.43
3:Am:250:ARG:HH21	9:At:82:GLU:HG2	1.84	0.43
3:Bg:217:LYS:HA	3:Bg:236:TRP:HB2	2.00	0.43
5:Bj:230:LEU:HD22	5:Bj:232:VAL:HG13	2.00	0.43
5:Bj:236:SER:H	5:Bj:244:VAL:HG22	1.83	0.43
9:Bn:46:LEU:HB3	9:Bn:62:TYR:HD1	1.84	0.43
5:Bt:230:LEU:HD22	5:Bt:232:VAL:HG13	2.00	0.43
5:Bt:238:ILE:HG13	5:Bt:241:TYR:HB2	2.01	0.43
1:By:62:ILE:HD13	8:Cg:263:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cc:105:ARG:NH2	1:Cc:152:GLN:HB2	2.34	0.43
8:Cg:146:THR:HG23	8:Cg:148:ARG:N	2.33	0.43
3:Ck:94:LEU:HD23	3:Ck:94:LEU:H	1.83	0.43
5:Cn:247:ILE:O	5:Cn:247:ILE:HG13	2.19	0.43
3:Cu:166:ASN:HA	3:Cu:186:SER:HB3	2.01	0.43
8:Da:146:THR:HG23	8:Da:148:ARG:N	2.29	0.43
2:Dd:65:ILE:HG23	2:Dd:78:ILE:HA	2.01	0.43
7:Dj:105:ILE:O	7:Dj:109:LEU:HD12	2.19	0.43
7:Dj:107:ARG:HG3	7:Dj:107:ARG:HH11	1.84	0.43
9:Dl:39:LYS:HD3	9:Dl:40:PRO:HD2	2.01	0.43
1:Dm:77:TYR:C	1:Dm:79:LEU:H	2.27	0.43
3:Dy:94:LEU:HD23	3:Dy:94:LEU:H	1.82	0.43
7:Ed:170:ASP:OD1	7:Ed:227:ARG:HD3	2.19	0.43
8:Ee:224:PRO:HB3	8:Ee:253:PRO:HD3	2.00	0.43
9:Ep:76:VAL:HG12	9:Ep:86:SER:HA	2.01	0.43
3:Es:119:GLU:HG2	3:Es:139:ALA:HB3	2.01	0.43
3:Ac:94:LEU:HD23	3:Ac:94:LEU:H	1.83	0.42
9:Aj:25:LEU:HD23	9:Aj:68:TYR:CZ	2.54	0.42
5:Ap:230:LEU:HD23	5:Ap:231:THR:N	2.34	0.42
7:Ar:57:VAL:HA	7:Ar:60:VAL:HG22	2.00	0.42
3:Aw:301:MET:HE3	3:Aw:301:MET:HB3	1.81	0.42
1:Ay:30:ILE:HD12	1:Ay:31:ASN:N	2.34	0.42
1:Ay:87:TRP:O	1:Ay:120:SER:HA	2.19	0.42
7:Bb:148:LEU:HB3	7:Bb:192:PHE:CE2	2.54	0.42
3:Bg:98:TYR:HE1	3:Bg:101:TYR:H	1.67	0.42
1:Bo:143:ALA:HB1	1:Bo:156:LEU:HD11	2.01	0.42
2:Bp:114:ILE:HG23	2:Bp:184:PHE:HB3	2.01	0.42
5:Bt:247:ILE:O	5:Bt:247:ILE:HG13	2.19	0.42
1:By:69:ASN:HD21	1:By:133:ARG:HA	1.84	0.42
1:Cw:93:GLU:HG3	8:Dk:264:ALA:H	1.84	0.42
5:Cx:247:ILE:O	5:Cx:247:ILE:HG13	2.18	0.42
8:Da:109:VAL:HG13	8:Da:208:GLY:HA3	2.01	0.42
9:Db:75:MET:HE3	9:Db:75:MET:HB3	1.94	0.42
2:Dd:174:ARG:H	2:Dd:174:ARG:HG2	1.67	0.42
8:Du:38:ALA:HB1	8:Du:173:LYS:HD2	2.01	0.42
8:Du:146:THR:HG23	8:Du:148:ARG:N	2.32	0.42
3:Dy:233:VAL:HG21	3:Dy:241:PHE:CE2	2.53	0.42
1:Ea:160:LYS:H	1:Ea:160:LYS:CD	2.29	0.42
1:Ek:76:ALA:O	1:Ek:80:GLN:HG2	2.18	0.42
8:Eo:292:ASN:HB2	9:Ep:75:MET:HE1	2.01	0.42
2:Er:90:ARG:HD3	3:Es:292:MET:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:170:LEU:H	2:Ab:170:LEU:HD22	1.83	0.42
5:Af:218:GLY:H	5:Af:247:ILE:HD11	1.84	0.42
1:Ak:69:ASN:HD21	1:Ak:133:ARG:HA	1.83	0.42
4:Ax:79:GLN:HE22	6:Ba:354:MET:HA	1.84	0.42
4:Ax:91:VAL:HG13	4:Ax:101:VAL:HG13	2.01	0.42
1:Ay:141:LYS:NZ	1:Ay:141:LYS:HB3	2.33	0.42
6:Ba:319:ILE:HG23	6:Ba:322:PRO:HD2	2.01	0.42
4:Bh:91:VAL:HG13	4:Bh:101:VAL:HG13	2.02	0.42
8:Bm:270:GLU:O	8:Bm:270:GLU:HG3	2.18	0.42
1:Bo:28:PRO:HD3	7:Bv:115:GLN:HB2	2.00	0.42
3:Bq:250:ARG:HH21	9:Bx:82:GLU:HG2	1.83	0.42
2:Cj:111:LYS:HD2	2:Cj:114:ILE:HG12	2.01	0.42
7:Cp:98:TYR:C	7:Cp:98:TYR:CD1	2.95	0.42
2:Ct:170:LEU:HD22	2:Ct:170:LEU:H	1.85	0.42
5:Cx:218:GLY:H	5:Cx:247:ILE:HD11	1.83	0.42
8:Da:218:MET:CE	8:Da:220:MET:HE3	2.48	0.42
2:Dd:165:ILE:HG21	7:Dt:119:TYR:CE1	2.54	0.42
7:Dj:148:LEU:HB3	7:Dj:192:PHE:CE2	2.54	0.42
8:Dk:106:LEU:HD12	8:Dk:106:LEU:HA	1.92	0.42
2:Dn:113:ALA:HA	2:Dn:153:ILE:O	2.19	0.42
3:Do:98:TYR:HE1	3:Do:101:TYR:H	1.66	0.42
7:Ed:165:VAL:HG23	7:Ed:231:ILE:HG12	2.01	0.42
7:Ed:208:TYR:CD2	9:Ef:86:SER:HB2	2.54	0.42
8:Ee:72:LEU:HD12	8:Ee:191:ALA:HB2	2.01	0.42
3:Ei:164:GLN:HE21	3:Ei:184:LEU:HD11	1.83	0.42
7:Ah:114:ILE:HG12	7:Ah:127:ILE:HG23	2.00	0.42
6:Aq:285:GLU:OE1	6:Aq:285:GLU:HA	2.19	0.42
7:Ar:201:LYS:H	7:Ar:201:LYS:HG2	1.64	0.42
7:Bb:219:ILE:HG13	7:Bb:222:GLY:H	1.84	0.42
3:Bq:111:LYS:HE3	3:Bq:111:LYS:HB3	1.68	0.42
7:Bv:124:THR:OG1	7:Bv:232:GLN:HG2	2.19	0.42
3:Ca:31:LYS:HG3	3:Ca:33:GLN:H	1.83	0.42
1:Cs:117:VAL:HG13	1:Cs:142:LYS:HD3	2.01	0.42
3:Cu:98:TYR:HE1	3:Cu:101:TYR:H	1.68	0.42
2:Dd:45:VAL:HG12	2:Dd:110:ARG:NH2	2.35	0.42
5:Dr:223:ILE:HD12	5:Dr:223:ILE:HA	1.84	0.42
7:Dt:152:ILE:HD13	7:Dt:152:ILE:HA	1.86	0.42
3:Dy:141:GLU:HA	3:Dy:161:GLY:HA2	2.01	0.42
3:Ei:111:LYS:HE3	3:Ei:111:LYS:HB3	1.68	0.42
2:Er:148:GLY:HA3	1:Eu:30:ILE:HD11	2.01	0.42
3:Es:270:SER:HB3	7:Ex:191:THR:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ac:214:ILE:HD11	3:Ac:224:LEU:HD11	2.02	0.42
5:Af:254:ILE:HD12	5:Af:254:ILE:N	2.34	0.42
1:Ao:97:ARG:HH11	1:Ao:100:LYS:NZ	2.17	0.42
8:As:298:ILE:H	8:As:298:ILE:HD12	1.85	0.42
3:Aw:268:HIS:ND1	7:Bb:187:GLU:OE2	2.53	0.42
1:Ay:75:ASN:HA	1:Ay:80:GLN:HE22	1.84	0.42
1:Ay:105:ARG:NH2	1:Ay:152:GLN:HB2	2.34	0.42
1:Bi:26:LYS:HG2	7:Bl:143:ILE:HD11	2.02	0.42
1:Bi:55:MET:HE2	1:Bi:55:MET:HB3	1.89	0.42
5:Bj:238:ILE:HG13	5:Bj:241:TYR:HB2	2.02	0.42
1:Bo:72:THR:HG23	1:Bs:62:ILE:HD12	2.01	0.42
2:Bp:174:ARG:HE	2:Bp:174:ARG:HB3	1.63	0.42
3:Bq:164:GLN:HE21	3:Bq:184:LEU:HD11	1.84	0.42
9:Bx:64:ILE:HD11	9:Bx:68:TYR:CE2	2.54	0.42
3:Ca:52:VAL:HB	3:Ca:118:TYR:CD2	2.54	0.42
3:Ca:278:ASP:HB3	3:Ca:280:TYR:CZ	2.54	0.42
2:Cj:56:MET:HE2	2:Cj:56:MET:HB2	1.83	0.42
8:Da:119:LEU:HD12	8:Da:125:ILE:HG22	2.01	0.42
7:Dt:126:ILE:HG12	7:Dt:230:GLU:HG2	2.01	0.42
7:Dt:208:TYR:CD2	9:Dv:86:SER:HB2	2.54	0.42
7:Dt:234:PHE:CZ	9:Dv:29:ARG:HG2	2.54	0.42
1:Ek:98:ILE:HG13	8:Ey:266:VAL:HG21	2.01	0.42
1:Ek:105:ARG:HH21	1:Ek:152:GLN:HB2	1.84	0.42
1:Eq:160:LYS:HE3	1:Eq:160:LYS:HB3	1.85	0.42
3:Es:235:LEU:HD11	3:Es:241:PHE:HB3	2.01	0.42
7:Ex:148:LEU:HB3	7:Ex:192:PHE:CE2	2.55	0.42
8:Ey:88:ARG:HA	8:Ey:88:ARG:HD2	1.78	0.42
1:Ae:33:PRO:HB2	1:Ae:39:ILE:HG12	2.02	0.42
1:Ak:70:THR:HG22	1:Ak:133:ARG:CZ	2.50	0.42
2:Al:99:LEU:HD23	2:Al:99:LEU:HA	1.82	0.42
3:Am:94:LEU:HD23	3:Am:94:LEU:H	1.83	0.42
6:Aq:306:LEU:HD11	6:Aq:341:LYS:HE2	2.02	0.42
7:Ar:140:LEU:HD13	7:Ar:188:THR:HG22	2.00	0.42
8:As:177:CYS:O	8:As:180:THR:HG22	2.20	0.42
1:Ay:87:TRP:CD1	1:Ay:94:LEU:HD22	2.54	0.42
5:Az:247:ILE:O	5:Az:247:ILE:HG13	2.19	0.42
7:Bb:98:TYR:C	7:Bb:98:TYR:CD2	2.97	0.42
1:Bi:35:ASP:O	1:Bi:39:ILE:HG13	2.20	0.42
3:Ck:98:TYR:HE1	3:Ck:101:TYR:H	1.67	0.42
1:Cs:28:PRO:HG2	1:Cs:29:PRO:HD3	2.01	0.42
1:Cs:136:ASP:OD1	1:Cw:60:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Du:300:ALA:HB3	8:Du:301:PRO:HD3	2.02	0.42
1:Eg:115:VAL:HG13	8:Eo:142:THR:O	2.19	0.42
9:Ep:50:CYS:HB2	9:Ep:77:LEU:HD12	2.01	0.42
3:Es:94:LEU:H	3:Es:94:LEU:HD23	1.83	0.42
7:Ex:98:TYR:C	7:Ex:98:TYR:CD2	2.97	0.42
3:Ac:217:LYS:HA	3:Ac:236:TRP:HB2	2.01	0.42
8:Ai:245:ARG:HE	8:As:127:ILE:HD11	1.84	0.42
2:Al:135:ALA:O	2:Al:139:VAL:HG23	2.20	0.42
1:Au:55:MET:HE1	1:Ay:55:MET:HG3	2.01	0.42
1:Ay:35:ASP:O	1:Ay:39:ILE:HG13	2.20	0.42
2:Bf:117:THR:HA	2:Bf:157:GLN:O	2.20	0.42
3:Bg:164:GLN:HE21	3:Bg:184:LEU:HD11	1.84	0.42
7:Bl:145:TYR:CG	7:Bl:146:PRO:HD3	2.55	0.42
7:Bl:206:GLU:OE2	8:Bm:294:SER:HB2	2.19	0.42
5:Bt:233:ARG:HA	5:Bt:233:ARG:HD3	1.79	0.42
7:Bv:44:HIS:HB2	7:Bv:48:ASN:HA	2.02	0.42
8:Bw:246:VAL:HG22	8:Cg:126:ARG:HG3	2.01	0.42
9:Ch:39:LYS:HD3	9:Ch:40:PRO:HD2	2.01	0.42
3:Ck:118:TYR:HB3	3:Ck:138:LEU:HD13	2.02	0.42
3:Ck:235:LEU:HD11	3:Ck:241:PHE:HB3	2.02	0.42
1:Cm:97:ARG:HD2	8:Da:263:ARG:NH2	2.35	0.42
3:Cu:52:VAL:HB	3:Cu:118:TYR:CD2	2.55	0.42
3:De:203:SER:HA	3:De:223:GLN:O	2.19	0.42
3:De:242:LYS:HE2	3:De:242:LYS:HB2	1.78	0.42
3:De:270:SER:HB3	7:Dj:191:THR:HG23	2.01	0.42
6:Di:352:LYS:HD3	6:Di:354:MET:HE3	2.00	0.42
8:Du:293:LYS:HE2	8:Du:293:LYS:HB2	1.85	0.42
1:Ea:105:ARG:HH21	1:Ea:152:GLN:HB2	1.84	0.42
7:Ed:102:LYS:HD3	7:Ed:158:TYR:OH	2.20	0.42
8:Eo:177:CYS:O	8:Eo:180:THR:HG22	2.20	0.42
1:Aa:72:THR:HG23	1:Ae:62:ILE:HD12	2.00	0.42
3:Am:98:TYR:HE1	3:Am:101:TYR:H	1.66	0.42
1:Au:62:ILE:CD1	8:Bc:263:ARG:HE	2.31	0.42
2:Av:56:MET:HE1	2:Av:105:PHE:HA	2.00	0.42
6:Bu:341:LYS:HB2	6:Bu:361:LEU:HD22	2.02	0.42
7:Bv:166:ALA:HA	7:Bv:206:GLU:O	2.18	0.42
7:Bv:219:ILE:HG13	7:Bv:222:GLY:H	1.84	0.42
3:Ca:228:VAL:HG23	3:Ca:246:LEU:HD11	2.02	0.42
8:Cg:177:CYS:O	8:Cg:180:THR:HG22	2.20	0.42
3:Ck:166:ASN:HA	3:Ck:186:SER:HB3	2.02	0.42
7:Cp:169:THR:HG23	7:Cp:182:SER:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ct:174:ARG:HE	2:Ct:174:ARG:HB3	1.68	0.42
7:Cz:98:TYR:CD1	7:Cz:98:TYR:C	2.96	0.42
3:De:164:GLN:HE21	3:De:184:LEU:HD11	1.84	0.42
1:Dg:160:LYS:H	1:Dg:160:LYS:CD	2.33	0.42
7:Dj:161:SER:HB2	7:Dj:233:TRP:HB2	2.02	0.42
9:Dl:27:LYS:NZ	9:Dl:29:ARG:H	2.08	0.42
3:Do:166:ASN:HA	3:Do:186:SER:HB3	2.02	0.42
3:Do:217:LYS:HA	3:Do:236:TRP:HB2	2.02	0.42
7:Dt:212:ASN:ND2	8:Du:295:TRP:HZ3	2.17	0.42
2:Dx:75:LEU:HB2	8:Eo:299:ILE:HD12	2.02	0.42
5:El:250:LEU:HD13	5:El:250:LEU:HA	1.93	0.42
7:En:166:ALA:HA	7:En:206:GLU:O	2.19	0.42
5:Ev:247:ILE:O	5:Ev:247:ILE:HG13	2.19	0.42
1:Aa:82:ARG:NH2	1:Aa:126:GLU:HA	2.34	0.42
2:Ab:56:MET:HE1	2:Ab:108:GLN:HG3	2.01	0.42
3:Ac:173:LEU:HD22	3:Ac:175:ILE:HD11	2.02	0.42
6:Ag:294:ARG:HD2	8:As:197:GLU:OE2	2.20	0.42
9:Aj:46:LEU:HD13	9:Aj:93:ARG:HD3	2.01	0.42
6:Aq:319:ILE:HD13	6:Aq:339:MET:HE1	2.01	0.42
8:As:153:MET:HE3	8:As:153:MET:HB3	1.78	0.42
8:As:291:THR:HG22	8:As:293:LYS:H	1.85	0.42
3:Ca:98:TYR:HE1	3:Ca:101:TYR:H	1.68	0.42
8:Cg:38:ALA:HB1	8:Cg:173:LYS:HD2	2.01	0.42
3:Ck:173:LEU:HD23	3:Ck:174:GLN:N	2.34	0.42
7:Cp:142:GLU:H	7:Cp:142:GLU:HG3	1.66	0.42
1:Cw:75:ASN:HA	1:Cw:80:GLN:HE22	1.84	0.42
8:Da:88:ARG:HD2	8:Da:88:ARG:HA	1.81	0.42
3:Dy:158:VAL:O	3:Dy:179:GLY:HA3	2.19	0.42
1:Eg:55:MET:HE1	1:Ek:55:MET:SD	2.59	0.42
2:Eh:126:VAL:HG23	2:Eh:130:ARG:NH1	2.34	0.42
3:Ac:173:LEU:HD22	3:Ac:175:ILE:CD1	2.50	0.42
7:Ar:102:LYS:HB2	7:Ar:102:LYS:HE2	1.71	0.42
3:Aw:141:GLU:HA	3:Aw:161:GLY:HA2	2.00	0.42
7:Bl:193:LEU:HD11	7:Bl:231:ILE:HD13	2.02	0.42
7:Bv:134:MET:HB2	7:Bv:137:SER:OG	2.19	0.42
1:Cc:97:ARG:HD2	8:Cq:263:ARG:NH2	2.34	0.42
3:Ck:270:SER:HB3	7:Cp:191:THR:HG23	2.02	0.42
2:Ct:122:LYS:HA	2:Ct:129:GLU:OE2	2.20	0.42
6:Cy:289:PRO:HA	6:Cy:290:PRO:HD3	1.96	0.42
8:Da:300:ALA:HB3	8:Da:301:PRO:HD3	2.02	0.42
2:Dd:188:VAL:HG13	4:Df:55:ALA:HB1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:De:233:VAL:HG21	3:De:241:PHE:CE2	2.55	0.42
6:Di:321:SER:HB2	6:Di:346:LEU:HD22	2.02	0.42
8:Dk:88:ARG:HD2	8:Dk:88:ARG:HA	1.81	0.42
1:Dm:136:ASP:OD2	1:Dq:60:LYS:HE2	2.20	0.42
1:Dw:151:SER:HB3	9:Ep:92:GLU:HG2	2.01	0.42
1:Ea:94:LEU:HD23	1:Ea:119:ILE:HD11	2.01	0.42
8:Ee:300:ALA:HB3	8:Ee:301:PRO:HD3	2.01	0.42
1:Eg:28:PRO:HD3	7:En:115:GLN:HB2	2.02	0.42
1:Eg:52:MET:HE1	8:Eo:99:LEU:HD21	2.01	0.42
1:Ek:160:LYS:H	1:Ek:160:LYS:CD	2.33	0.42
8:Eo:270:GLU:O	8:Eo:270:GLU:HG3	2.18	0.42
4:Et:58:LEU:HB2	4:Et:66:SER:HB3	2.02	0.42
7:Ex:219:ILE:HG13	7:Ex:222:GLY:H	1.84	0.42
3:Ac:177:LEU:HD22	3:Ac:196:MET:SD	2.60	0.42
3:Ac:242:LYS:HE2	3:Ac:242:LYS:HB2	1.78	0.42
6:Ag:354:MET:HE2	6:Ag:354:MET:HB3	1.78	0.42
7:Ah:134:MET:HB2	7:Ah:137:SER:OG	2.18	0.42
3:Am:111:LYS:HB3	3:Am:111:LYS:HE3	1.67	0.42
3:Am:270:SER:HB3	7:Ar:191:THR:HG23	2.02	0.42
5:Ap:243:MET:HE3	5:Ap:243:MET:HB3	1.98	0.42
7:Ar:234:PHE:CZ	9:At:29:ARG:HG2	2.54	0.42
2:Av:166:THR:HG22	2:Av:168:TYR:N	2.27	0.42
3:Aw:250:ARG:HH21	9:Bd:82:GLU:HG2	1.83	0.42
1:Ay:57:LYS:HB2	1:Ay:57:LYS:HE2	1.91	0.42
1:Bi:109:LEU:HD23	1:Bi:157:ARG:HG3	2.02	0.42
7:Bl:98:TYR:C	7:Bl:98:TYR:CD2	2.98	0.42
3:Bq:30:VAL:HG23	3:Bq:76:ARG:HD3	2.02	0.42
3:Bq:235:LEU:HD11	3:Bq:241:PHE:HB3	2.02	0.42
5:Cd:246:LEU:HD12	5:Cd:247:ILE:N	2.35	0.42
2:Cj:135:ALA:O	2:Cj:139:VAL:HG23	2.20	0.42
3:Ck:141:GLU:HA	3:Ck:161:GLY:HA2	2.02	0.42
8:Cq:116:THR:HG21	8:Cq:131:THR:HG23	2.02	0.42
1:Dc:41:LEU:HD23	8:Dk:199:ILE:HD11	2.02	0.42
1:Dq:126:GLU:HG2	1:Dq:130:GLU:HB2	2.02	0.42
7:Dt:152:ILE:HD11	7:Dt:193:LEU:HA	2.01	0.42
7:Dt:166:ALA:HA	7:Dt:206:GLU:O	2.20	0.42
8:Du:182:ARG:HE	8:Du:182:ARG:HB2	1.78	0.42
3:Es:244:LYS:HB3	3:Es:244:LYS:HE2	1.86	0.42
5:Af:247:ILE:O	5:Af:247:ILE:HG13	2.19	0.41
3:Am:164:GLN:HE21	3:Am:184:LEU:HD11	1.85	0.41
8:Bc:177:CYS:HA	8:Bc:180:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Be:78:ASN:C	1:Be:78:ASN:OD1	2.63	0.41
1:Bi:87:TRP:CD1	1:Bi:94:LEU:HB2	2.55	0.41
7:Bv:145:TYR:CG	7:Bv:146:PRO:HD3	2.55	0.41
8:Cg:231:LEU:HB2	8:Cg:244:ASP:HB3	2.02	0.41
1:Cm:97:ARG:HH11	1:Cm:100:LYS:NZ	2.18	0.41
8:Da:270:GLU:O	8:Da:270:GLU:HG3	2.20	0.41
1:Dm:62:ILE:HD13	1:Dm:62:ILE:HA	1.92	0.41
2:Dn:46:ASP:OD1	2:Dn:46:ASP:N	2.53	0.41
3:Dy:164:GLN:HE21	3:Dy:184:LEU:HD11	1.85	0.41
1:Ea:87:TRP:CD1	1:Ea:94:LEU:HB2	2.55	0.41
2:Er:113:ALA:HA	2:Er:153:ILE:O	2.20	0.41
8:Ey:38:ALA:HB1	8:Ey:173:LYS:HD2	2.02	0.41
9:Aj:92:GLU:HG2	1:Eq:151:SER:HB3	2.01	0.41
1:Ak:55:MET:HA	1:Ak:58:VAL:HG12	2.03	0.41
1:Ao:33:PRO:HB3	1:Ao:38:THR:HG22	2.02	0.41
3:Aw:242:LYS:HE2	3:Aw:242:LYS:HB2	1.79	0.41
2:Bf:174:ARG:H	2:Bf:174:ARG:HG2	1.63	0.41
3:Bg:39:ARG:HA	3:Bg:39:ARG:HD3	1.81	0.41
1:Bo:120:SER:H	1:Bo:138:GLN:NE2	2.18	0.41
3:Ca:217:LYS:HA	3:Ca:236:TRP:HB2	2.01	0.41
3:Ca:233:VAL:HG21	3:Ca:241:PHE:CE2	2.56	0.41
8:Cg:72:LEU:HD12	8:Cg:191:ALA:HB2	2.01	0.41
2:Cj:66:LYS:HD3	7:Cz:119:TYR:HD1	1.85	0.41
5:Cn:238:ILE:HG13	5:Cn:241:TYR:HB2	2.03	0.41
7:Cz:125:LEU:HD11	7:Cz:154:LEU:HD23	2.01	0.41
9:Db:46:LEU:HD13	9:Db:62:TYR:HD1	1.85	0.41
1:Dc:55:MET:HA	1:Dc:58:VAL:HG12	2.02	0.41
8:Dk:107:PRO:HG2	8:Dk:209:MET:CG	2.50	0.41
1:Dm:28:PRO:HD3	7:Dt:115:GLN:HB2	2.02	0.41
7:Ed:152:ILE:HD13	7:Ed:152:ILE:HA	1.85	0.41
8:Ee:231:LEU:HB2	8:Ee:244:ASP:HB3	2.02	0.41
1:Eg:63:THR:HG23	1:Eg:63:THR:O	2.20	0.41
2:Eh:46:ASP:OD1	2:Eh:46:ASP:N	2.54	0.41
3:Ei:39:ARG:HA	3:Ei:39:ARG:HD3	1.81	0.41
3:Ei:155:LEU:HD12	3:Ei:155:LEU:HA	1.83	0.41
4:Ej:86:LEU:HD23	6:Em:343:PRO:HG2	2.02	0.41
1:Ek:87:TRP:CD1	1:Ek:94:LEU:HD22	2.55	0.41
1:Ek:97:ARG:HD2	8:Ey:263:ARG:HH22	1.85	0.41
1:Eq:117:VAL:HG13	1:Eq:142:LYS:HD3	2.02	0.41
7:Ex:145:TYR:CG	7:Ex:146:PRO:HD3	2.55	0.41
9:Ez:27:LYS:HZ3	9:Ez:28:PHE:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Al:174:ARG:H	2:Al:174:ARG:HG2	1.64	0.41
3:Am:233:VAL:HG21	3:Am:241:PHE:CE2	2.54	0.41
4:Ax:111:GLU:HG2	8:Bc:153:MET:CE	2.50	0.41
3:Bg:278:ASP:HB3	3:Bg:280:TYR:CZ	2.56	0.41
3:Bg:301:MET:HE3	3:Bg:301:MET:HB3	1.81	0.41
7:Bl:234:PHE:CZ	9:Bn:29:ARG:HG2	2.55	0.41
2:Bp:52:THR:O	2:Bp:56:MET:HG3	2.20	0.41
2:Bz:117:THR:HA	2:Bz:157:GLN:O	2.20	0.41
9:Cr:46:LEU:HD13	9:Cr:62:TYR:HD2	1.85	0.41
8:Dk:272:ALA:HA	8:Dk:275:ARG:CZ	2.50	0.41
3:Do:260:VAL:HG22	3:Do:278:ASP:HB2	2.01	0.41
6:Ds:297:VAL:HG11	6:Ds:302:ALA:HB3	2.02	0.41
6:Ds:321:SER:HB2	6:Ds:346:LEU:HD22	2.02	0.41
7:Dt:98:TYR:CD2	7:Dt:98:TYR:C	2.98	0.41
8:Du:77:LYS:O	8:Du:81:GLU:HG3	2.20	0.41
8:Du:153:MET:HE2	8:Du:153:MET:HB3	1.84	0.41
1:Ea:76:ALA:O	1:Ea:80:GLN:HG2	2.19	0.41
1:Eg:39:ILE:O	1:Eg:43:GLU:HG3	2.20	0.41
7:En:145:TYR:CG	7:En:146:PRO:HD3	2.55	0.41
1:Aa:39:ILE:O	1:Aa:43:GLU:HG3	2.21	0.41
1:Aa:78:ASN:OD1	1:Aa:78:ASN:C	2.63	0.41
1:Aa:136:ASP:OD2	1:Ae:60:LYS:HE2	2.20	0.41
8:Ai:106:LEU:HD12	8:Ai:106:LEU:HA	1.95	0.41
1:Au:98:ILE:HG23	1:Au:128:LEU:HD22	2.03	0.41
1:Ay:80:GLN:NE2	9:Bn:47:LEU:HD11	2.34	0.41
7:Bb:138:PRO:HB3	7:Bb:184:ALA:HB1	2.03	0.41
4:Bh:84:CYS:CB	8:Bm:154:ASP:HB3	2.50	0.41
7:Bl:161:SER:HB2	7:Bl:233:TRP:HB2	2.02	0.41
1:Bo:78:ASN:HB3	9:Ch:70:ARG:HD3	2.01	0.41
2:Bp:75:LEU:HB2	8:Cg:299:ILE:HG23	2.02	0.41
1:Bs:87:TRP:CD1	1:Bs:94:LEU:HB2	2.55	0.41
1:Cc:75:ASN:HA	1:Cc:80:GLN:HE22	1.85	0.41
3:Ck:287:THR:HG21	7:Cp:184:ALA:HA	2.01	0.41
9:Dl:64:ILE:HD11	9:Dl:68:TYR:CE2	2.54	0.41
2:Dn:114:ILE:HG23	2:Dn:184:PHE:HB3	2.01	0.41
6:Ds:311:MET:HE3	6:Ds:311:MET:HB3	1.97	0.41
4:Dz:62:ASN:HB2	1:Eg:26:LYS:HA	2.02	0.41
3: Ei:98:TYR:HE1	3: Ei:101:TYR:H	1.67	0.41
1:Ek:48:VAL:HG11	8:Eo:93:ILE:HA	2.02	0.41
4:Et:87:TRP:HH2	6:Ew:346:LEU:HB2	1.86	0.41
5:Ev:255:LEU:HD13	5:Ev:261:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Ex:128:PRO:HD2	7:Ex:132:TYR:CD1	2.56	0.41
1:Aa:143:ALA:HB1	1:Aa:156:LEU:HD11	2.02	0.41
8:Ai:243:ASP:O	8:As:128:SER:HA	2.21	0.41
8:Ai:270:GLU:HG3	8:Ai:270:GLU:O	2.20	0.41
3:Am:260:VAL:HG22	3:Am:278:ASP:HB2	2.03	0.41
6:Aq:289:PRO:HA	6:Aq:290:PRO:HD3	1.97	0.41
8:As:185:LYS:HA	8:As:185:LYS:HD3	1.87	0.41
3:Aw:164:GLN:HE21	3:Aw:184:LEU:HD11	1.85	0.41
3:Aw:173:LEU:HD22	3:Aw:191:LEU:HD13	2.02	0.41
7:Bb:145:TYR:CD1	7:Bb:146:PRO:HD3	2.55	0.41
1:Bo:78:ASN:C	1:Bo:78:ASN:OD1	2.63	0.41
6:Bu:289:PRO:HA	6:Bu:290:PRO:HD3	1.96	0.41
9:Bx:46:LEU:HD13	9:Bx:93:ARG:HD3	2.01	0.41
1:Cc:35:ASP:O	1:Cc:39:ILE:HG13	2.21	0.41
8:Cg:293:LYS:HE2	8:Cg:293:LYS:HB2	1.87	0.41
3:Ck:244:LYS:HE2	3:Ck:244:LYS:HB3	1.82	0.41
6:Co:289:PRO:HA	6:Co:290:PRO:HD3	1.96	0.41
6:Co:306:LEU:HD11	6:Co:341:LYS:HE2	2.02	0.41
6:Cy:322:PRO:HG2	6:Cy:345:LEU:HD23	2.03	0.41
3:De:51:VAL:HG22	3:De:117:ARG:HG3	2.01	0.41
3:De:205:TYR:O	3:De:225:ALA:HB3	2.21	0.41
5:Eb:230:LEU:HD12	5:Eb:231:THR:H	1.85	0.41
1:Eg:77:TYR:O	1:Eg:78:ASN:OD1	2.37	0.41
2:Eh:130:ARG:HG3	2:Eh:130:ARG:NH1	2.32	0.41
3: Ei:292:MET:HE1	3: Ei:320:PRO:HB3	2.02	0.41
3:Es:130:ARG:HE	3:Es:130:ARG:HB2	1.78	0.41
1:Eu:87:TRP:CD1	1:Eu:94:LEU:HD22	2.56	0.41
5:Ev:233:ARG:CD	5:Ev:234:GLU:H	2.32	0.41
3:Ac:141:GLU:HA	3:Ac:161:GLY:HA2	2.02	0.41
7:Ah:145:TYR:CG	7:Ah:146:PRO:HD3	2.55	0.41
8:Ai:56:GLU:HG3	8:Ai:171:ALA:HB2	2.01	0.41
2:Al:174:ARG:HE	2:Al:174:ARG:HB3	1.61	0.41
1:Au:78:ASN:OD1	1:Au:78:ASN:C	2.64	0.41
1:Ay:40:LYS:HG2	7:Bb:172:VAL:HG21	2.03	0.41
8:Bc:182:ARG:HE	8:Bc:182:ARG:HB2	1.76	0.41
9:Bd:46:LEU:HD13	9:Bd:93:ARG:HD3	2.03	0.41
2:Bf:174:ARG:HE	2:Bf:174:ARG:HB3	1.66	0.41
3:Bq:203:SER:HA	3:Bq:223:GLN:O	2.20	0.41
1:Bs:97:ARG:HD3	1:Bs:100:LYS:NZ	2.35	0.41
8:Bw:170:LYS:CG	8:Bw:171:ALA:H	2.33	0.41
8:Bw:293:LYS:HE2	8:Bw:293:LYS:HB2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cc:40:LYS:HG2	7:Cf:172:VAL:HG21	2.01	0.41
7:Cf:145:TYR:CG	7:Cf:146:PRO:HD3	2.55	0.41
2:Cj:188:VAL:HG12	4:Cl:57:ARG:HE	1.85	0.41
1:Cm:97:ARG:NH1	8:Da:263:ARG:HH12	2.18	0.41
5:Cn:255:LEU:HD13	5:Cn:261:VAL:HG13	2.02	0.41
7:Cp:145:TYR:CG	7:Cp:146:PRO:HD3	2.55	0.41
7:Cz:102:LYS:HB2	7:Cz:102:LYS:HE2	1.70	0.41
9:Db:64:ILE:HD11	9:Db:68:TYR:CE2	2.56	0.41
3:Do:194:LEU:HD11	3:Do:202:LEU:HD21	2.02	0.41
1:Dq:97:ARG:HD3	1:Dq:100:LYS:NZ	2.36	0.41
3:Dy:235:LEU:HD11	3:Dy:241:PHE:HB3	2.03	0.41
1:Ea:40:LYS:HG2	7:Ed:172:VAL:HG21	2.01	0.41
5:Eb:218:GLY:H	5:Eb:247:ILE:HD11	1.85	0.41
6:Ec:283:VAL:HG13	6:Ec:305:TRP:HZ3	1.84	0.41
8:Ee:146:THR:HG23	8:Ee:148:ARG:N	2.34	0.41
1:Ek:97:ARG:NH1	8:Ey:263:ARG:HH12	2.19	0.41
3:Es:141:GLU:HA	3:Es:161:GLY:HA2	2.01	0.41
2:Ab:142:GLU:HG3	3:Ac:319:PHE:CD2	2.56	0.41
3:Ac:155:LEU:HA	3:Ac:155:LEU:HD23	1.84	0.41
3:Ac:205:TYR:O	3:Ac:225:ALA:HB3	2.21	0.41
5:Af:250:LEU:HD13	5:Af:250:LEU:HA	1.92	0.41
3:Am:194:LEU:HD11	3:Am:202:LEU:HD21	2.02	0.41
7:Bl:105:ILE:HD12	7:Bl:157:PHE:HE2	1.86	0.41
6:Ce:289:PRO:HA	6:Ce:290:PRO:HD3	1.97	0.41
1:Cs:151:SER:HB3	9:Dl:92:GLU:HG2	2.02	0.41
1:Dc:136:ASP:OD1	1:Dg:60:LYS:HE2	2.21	0.41
2:Dd:127:LYS:HB3	2:Dd:127:LYS:HE3	1.89	0.41
2:Dd:142:GLU:HG3	3:De:319:PHE:CD2	2.55	0.41
3:De:52:VAL:HB	3:De:118:TYR:CD2	2.56	0.41
3:De:141:GLU:HA	3:De:161:GLY:HA2	2.03	0.41
1:Dm:82:ARG:NH2	1:Dm:126:GLU:HA	2.36	0.41
3:Do:52:VAL:HB	3:Do:118:TYR:CD2	2.55	0.41
5:El:233:ARG:HG2	5:El:233:ARG:NH1	2.34	0.41
2:Er:117:THR:HA	2:Er:157:GLN:O	2.21	0.41
8:Ai:126:ARG:HG3	8:Ey:246:VAL:HG22	2.02	0.41
8:Ai:300:ALA:HB3	8:Ai:301:PRO:HD3	2.02	0.41
3:Am:176:VAL:C	3:Am:177:LEU:HD23	2.45	0.41
3:Am:242:LYS:HE2	3:Am:242:LYS:HB2	1.77	0.41
1:Ao:160:LYS:CD	1:Ao:160:LYS:H	2.34	0.41
5:Ap:223:ILE:HD12	5:Ap:224:GLY:H	1.85	0.41
7:Ar:163:ILE:HD11	7:Ar:202:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Bg:271:SER:HB3	3:Bg:279:ILE:HD13	2.03	0.41
7:Bl:208:TYR:CD2	9:Bn:86:SER:HB2	2.56	0.41
7:Bl:208:TYR:HD2	9:Bn:86:SER:HB2	1.85	0.41
3:Bq:212:LEU:HD12	3:Bq:228:VAL:HG21	2.03	0.41
3:Bq:270:SER:HB3	7:Bv:191:THR:HG23	2.02	0.41
2:Cj:66:LYS:HE2	7:Cz:118:GLU:O	2.20	0.41
7:Cp:152:ILE:HD11	7:Cp:193:LEU:HA	2.02	0.41
8:Cq:78:ILE:O	8:Cq:82:GLN:HG2	2.20	0.41
1:Cs:160:LYS:HE3	1:Cs:160:LYS:HB3	1.84	0.41
3:Cu:177:LEU:HD13	3:Cu:181:PRO:HG2	2.02	0.41
9:Db:29:ARG:C	9:Db:30:TRP:CG	2.99	0.41
9:Dl:40:PRO:HB3	9:Dl:56:TYR:CE2	2.56	0.41
1:Dw:67:LYS:HB3	1:Ea:62:ILE:HD11	2.03	0.41
2:Dx:135:ALA:O	2:Dx:139:VAL:HG23	2.20	0.41
4:Dz:58:LEU:HB2	4:Dz:66:SER:HB3	2.02	0.41
7:Ed:145:TYR:CG	7:Ed:146:PRO:HD3	2.56	0.41
2:Eh:159:LEU:HB3	2:Eh:162:ASP:HB2	2.02	0.41
1:Eu:119:ILE:HD12	1:Eu:135:ILE:HG12	2.03	0.41
9:Aj:23:CYS:HB2	9:Aj:64:ILE:HD11	2.03	0.41
3:Am:134:LEU:HD21	3:Am:150:ILE:HG23	2.02	0.41
5:Ap:236:SER:H	5:Ap:244:VAL:HG22	1.86	0.41
6:Aq:321:SER:HB2	6:Aq:346:LEU:HD22	2.03	0.41
6:Aq:341:LYS:HB2	6:Aq:361:LEU:HD22	2.03	0.41
7:Ar:161:SER:HB2	7:Ar:233:TRP:HB2	2.02	0.41
8:As:300:ALA:HB3	8:As:301:PRO:HD3	2.03	0.41
1:Au:137:TYR:CZ	1:Ay:57:LYS:HG3	2.55	0.41
6:Ba:289:PRO:HA	6:Ba:290:PRO:HD3	1.97	0.41
7:Bb:125:LEU:HD11	7:Bb:154:LEU:HD23	2.03	0.41
1:Be:55:MET:HE3	8:Bm:213:ARG:HB3	2.02	0.41
3:Bg:141:GLU:HA	3:Bg:161:GLY:HA2	2.02	0.41
1:Bi:120:SER:HB2	8:Bw:129:ASP:OD2	2.20	0.41
6:Bk:322:PRO:HG2	6:Bk:345:LEU:HD23	2.03	0.41
1:Bs:57:LYS:HB2	1:Bs:57:LYS:HE2	1.94	0.41
7:Bv:125:LEU:HD11	7:Bv:154:LEU:HD23	2.02	0.41
9:Bx:29:ARG:C	9:Bx:30:TRP:CG	2.99	0.41
7:Cp:161:SER:HB2	7:Cp:233:TRP:HB2	2.02	0.41
8:Cq:246:VAL:HG22	8:Da:126:ARG:HG3	2.03	0.41
1:Cs:78:ASN:OD1	1:Cs:78:ASN:C	2.63	0.41
3:Cu:212:LEU:HD12	3:Cu:228:VAL:HG21	2.03	0.41
1:Cw:40:LYS:HG2	7:Cz:172:VAL:HG21	2.02	0.41
3:De:98:TYR:HE1	3:De:101:TYR:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dg:105:ARG:NH2	1:Dg:152:GLN:HB2	2.36	0.41
7:Dj:145:TYR:CG	7:Dj:146:PRO:HD3	2.56	0.41
7:Dj:170:ASP:OD1	7:Dj:227:ARG:HD3	2.21	0.41
9:Dl:57:ILE:HD12	9:Dl:61:GLN:HB3	2.03	0.41
2:Dn:51:ALA:HB1	4:Dp:44:LYS:HE3	2.03	0.41
7:Dt:57:VAL:HA	7:Dt:60:VAL:HG22	2.01	0.41
7:Dt:161:SER:HB2	7:Dt:233:TRP:HB2	2.03	0.41
8:Du:213:ARG:HD2	8:Du:213:ARG:HA	1.91	0.41
8:Du:246:VAL:HG22	8:Ee:126:ARG:HG3	2.03	0.41
1:Dw:39:ILE:O	1:Dw:43:GLU:HG3	2.20	0.41
3:Dy:242:LYS:HB2	3:Dy:242:LYS:HE2	1.78	0.41
5:Eb:236:SER:H	5:Eb:244:VAL:HG22	1.85	0.41
7:Ed:145:TYR:CD1	7:Ed:146:PRO:HD3	2.55	0.41
8:Ee:77:LYS:O	8:Ee:81:GLU:HG3	2.21	0.41
1:Eg:79:LEU:HD11	1:Eg:147:VAL:HG11	2.03	0.41
3:Ei:141:GLU:HA	3:Ei:161:GLY:HA2	2.02	0.41
1:Eq:28:PRO:HD3	7:Ex:115:GLN:HB2	2.01	0.41
1:Eq:78:ASN:OD1	1:Eq:78:ASN:C	2.64	0.41
1:Eq:115:VAL:HG13	8:Ey:142:THR:O	2.21	0.41
3:Es:217:LYS:HA	3:Es:236:TRP:HB2	2.02	0.41
1:Eu:94:LEU:HD23	1:Eu:119:ILE:HD11	2.03	0.41
7:Ex:193:LEU:HD11	7:Ex:231:ILE:HD13	2.02	0.41
3:Ac:52:VAL:HB	3:Ac:118:TYR:CD2	2.56	0.41
3:Ac:244:LYS:HB3	3:Ac:244:LYS:HE2	1.85	0.41
3:Aw:202:LEU:HD11	3:Aw:204:LEU:CD1	2.51	0.41
7:Bb:134:MET:HB2	7:Bb:137:SER:OG	2.21	0.41
3:Bg:270:SER:HB3	7:Bl:191:THR:HG23	2.02	0.41
8:Bm:300:ALA:HB3	8:Bm:301:PRO:HD3	2.03	0.41
1:Bs:77:TYR:HE2	8:Cg:273:LEU:HD13	1.86	0.41
1:Bs:80:GLN:HG3	9:Ch:47:LEU:HD11	2.03	0.41
7:Bv:98:TYR:CD2	7:Bv:98:TYR:C	2.99	0.41
1:By:39:ILE:O	1:By:43:GLU:HG3	2.21	0.41
1:Cc:93:GLU:HG3	8:Cq:264:ALA:H	1.86	0.41
7:Cf:90:THR:O	7:Cf:94:VAL:HG22	2.21	0.41
1:Ci:78:ASN:OD1	1:Ci:78:ASN:C	2.64	0.41
3:Ck:52:VAL:HB	3:Ck:118:TYR:CD2	2.56	0.41
3:Ck:250:ARG:HE	3:Ck:250:ARG:HB2	1.78	0.41
1:Cm:105:ARG:HB2	1:Cm:153:VAL:HG22	2.02	0.41
8:Cq:300:ALA:HB3	8:Cq:301:PRO:HD3	2.03	0.41
4:Cv:56:GLY:HA2	4:Cv:71:THR:CG2	2.51	0.41
4:Cv:92:TYR:HE2	4:Cv:94:GLN:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Dm:53:LEU:HD23	1:Dm:53:LEU:HA	1.84	0.41
1:Dm:55:MET:HE1	1:Dm:59:GLU:OE1	2.21	0.41
8:Du:177:CYS:O	8:Du:180:THR:HG22	2.21	0.41
8:Du:292:ASN:OD1	9:Dv:31:ASP:HA	2.20	0.41
8:Ee:213:ARG:HA	8:Ee:213:ARG:HD2	1.90	0.41
3:Ei:178:LYS:HD2	3:Ei:197:TYR:CD1	2.56	0.41
6:Em:354:MET:HE2	6:Em:354:MET:HB3	1.82	0.41
3:Ac:228:VAL:HG23	3:Ac:246:LEU:HD11	2.02	0.40
3:Ac:235:LEU:HD11	3:Ac:241:PHE:HB3	2.02	0.40
1:Ao:40:LYS:HG2	7:Ar:172:VAL:HG21	2.03	0.40
2:Av:66:LYS:HD3	7:Bl:119:TYR:CD1	2.56	0.40
8:Bc:170:LYS:CG	8:Bc:171:ALA:N	2.83	0.40
4:Br:95:LEU:HD23	4:Br:95:LEU:HA	1.97	0.40
7:Bv:145:TYR:CD1	7:Bv:146:PRO:HD3	2.56	0.40
1:By:78:ASN:C	1:By:78:ASN:OD1	2.64	0.40
1:By:102:ALA:HB2	1:By:128:LEU:HD13	2.03	0.40
3:Ca:212:LEU:HD12	3:Ca:228:VAL:HG21	2.03	0.40
6:Ce:319:ILE:HG23	6:Ce:322:PRO:HD2	2.03	0.40
7:Cf:142:GLU:H	7:Cf:142:GLU:HG2	1.59	0.40
1:Ci:143:ALA:HB1	1:Ci:156:LEU:HD11	2.04	0.40
1:Dc:78:ASN:OD1	1:Dc:78:ASN:C	2.63	0.40
3:De:117:ARG:HE	3:De:117:ARG:HB3	1.77	0.40
2:Dn:75:LEU:HB2	8:Ee:299:ILE:HD12	2.02	0.40
3:Do:141:GLU:HA	3:Do:161:GLY:HA2	2.03	0.40
3:Do:235:LEU:HD11	3:Do:241:PHE:HB3	2.04	0.40
9:Dv:25:LEU:HD12	9:Dv:67:ARG:NH2	2.36	0.40
3:Dy:30:VAL:HG23	3:Dy:76:ARG:HD3	2.03	0.40
3:Ei:52:VAL:HB	3:Ei:118:TYR:CD2	2.55	0.40
7:En:107:ARG:O	7:En:111:LYS:HG3	2.21	0.40
3:Es:52:VAL:HB	3:Es:118:TYR:CD2	2.56	0.40
3:Es:279:ILE:O	3:Es:298:VAL:HA	2.22	0.40
6:Ew:312:TYR:HA	6:Ew:337:TYR:O	2.21	0.40
7:Ah:190:MET:HE2	7:Ah:190:MET:HB3	1.78	0.40
8:Ai:204:GLU:HG3	6:Ew:285:GLU:HG3	2.02	0.40
1:Ak:115:VAL:HG13	8:As:142:THR:O	2.20	0.40
3:Am:39:ARG:HD3	3:Am:39:ARG:HA	1.89	0.40
7:Ar:62:VAL:O	7:Ar:66:ILE:HG12	2.22	0.40
8:As:60:LYS:HG2	8:As:179:TYR:CE2	2.57	0.40
8:As:246:VAL:HG22	8:Bc:126:ARG:HG3	2.02	0.40
8:As:288:ILE:HG22	9:At:36:VAL:HB	2.03	0.40
3:Aw:52:VAL:HB	3:Aw:118:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Aw:98:TYR:HE1	3:Aw:101:TYR:H	1.68	0.40
3:Aw:244:LYS:HD3	3:Aw:282:TYR:CD2	2.56	0.40
4:Ax:87:TRP:HH2	6:Ba:346:LEU:HB2	1.87	0.40
7:Bb:145:TYR:CG	7:Bb:146:PRO:HD3	2.56	0.40
3:Bg:52:VAL:HB	3:Bg:118:TYR:CD2	2.56	0.40
5:Bj:255:LEU:HD13	5:Bj:261:VAL:HG13	2.03	0.40
8:Bm:78:ILE:O	8:Bm:82:GLN:HG2	2.21	0.40
2:Bp:117:THR:HA	2:Bp:157:GLN:O	2.21	0.40
2:Bp:174:ARG:H	2:Bp:174:ARG:HG2	1.66	0.40
3:Bq:228:VAL:HG23	3:Bq:246:LEU:HD11	2.04	0.40
1:Bs:108:VAL:HG22	1:Bs:156:LEU:HB3	2.03	0.40
1:Bi:78:ASN:HB3	9:Db:70:ARG:HD3	2.03	0.40
8:Cq:231:LEU:HB2	8:Cq:244:ASP:HB3	2.03	0.40
1:Dc:39:ILE:O	1:Dc:43:GLU:HG3	2.21	0.40
1:Dq:80:GLN:NE2	9:Ef:47:LEU:HD11	2.35	0.40
1:Dw:78:ASN:OD1	1:Dw:78:ASN:C	2.64	0.40
2:Dx:117:THR:HA	2:Dx:157:GLN:O	2.20	0.40
2:Eh:127:LYS:HB3	2:Eh:127:LYS:HE3	1.92	0.40
4:Ej:58:LEU:HB2	4:Ej:66:SER:HB3	2.02	0.40
1:Ek:73:ILE:H	1:Ek:73:ILE:HG12	1.76	0.40
5:El:236:SER:H	5:El:244:VAL:HG22	1.86	0.40
5:El:247:ILE:O	5:El:247:ILE:HG13	2.20	0.40
8:Eo:300:ALA:HB3	8:Eo:301:PRO:HD3	2.02	0.40
2:Er:107:LYS:HG3	2:Er:149:VAL:HG12	2.03	0.40
8:Ey:293:LYS:HB2	8:Ey:293:LYS:HE2	1.81	0.40
1:Aa:100:LYS:NZ	8:As:303:SER:HA	2.37	0.40
7:Ah:152:ILE:HD13	7:Ah:152:ILE:HA	1.85	0.40
2:Al:46:ASP:OD1	2:Al:46:ASP:N	2.54	0.40
7:Ar:145:TYR:CG	7:Ar:146:PRO:HD3	2.56	0.40
7:Ar:212:ASN:ND2	8:As:295:TRP:HZ3	2.16	0.40
1:Ay:37:ALA:HA	7:Bb:220:ILE:HD12	2.04	0.40
1:Ay:87:TRP:CD1	1:Ay:94:LEU:HB2	2.56	0.40
6:Ba:317:LEU:HD22	6:Ba:349:TRP:HA	2.03	0.40
6:Bk:321:SER:HB2	6:Bk:346:LEU:HD22	2.03	0.40
9:Bn:25:LEU:HG	9:Bn:67:ARG:HE	1.86	0.40
4:Br:82:MET:HE2	8:Bw:155:TYR:CE2	2.56	0.40
3:Ca:164:GLN:HE21	3:Ca:184:LEU:HD11	1.86	0.40
5:Cd:210:TYR:CE1	5:Cd:224:GLY:HA2	2.57	0.40
1:Dg:107:ARG:NH2	1:Dg:153:VAL:HG11	2.35	0.40
5:Dh:223:ILE:HD12	5:Dh:224:GLY:N	2.36	0.40
7:Dt:148:LEU:HB3	7:Dt:192:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dx:65:ILE:HG23	2:Dx:78:ILE:HA	2.04	0.40
3:Dy:86:LYS:HE2	3:Dy:86:LYS:HB2	2.01	0.40
3:Ei:70:MET:HG3	3:Ei:107:ASP:HB3	2.04	0.40
3:Ei:278:ASP:HB3	3:Ei:280:TYR:CZ	2.56	0.40
7:En:152:ILE:HD13	7:En:152:ILE:HA	1.86	0.40
3:Es:176:VAL:C	3:Es:177:LEU:HD23	2.46	0.40
8:Ey:288:ILE:HG22	9:Ez:36:VAL:HB	2.02	0.40
7:Ah:161:SER:HB2	7:Ah:233:TRP:HB2	2.03	0.40
1:Ak:63:THR:HG23	1:Ak:63:THR:O	2.22	0.40
1:Ak:117:VAL:HG13	1:Ak:142:LYS:HD3	2.01	0.40
2:Al:56:MET:HE1	2:Al:105:PHE:HA	2.02	0.40
5:Ap:238:ILE:HG13	5:Ap:241:TYR:HB2	2.03	0.40
1:Au:52:MET:HE2	1:Ay:52:MET:SD	2.62	0.40
2:Av:99:LEU:HD23	2:Av:99:LEU:HA	1.82	0.40
5:Az:255:LEU:HD13	5:Az:261:VAL:HG13	2.04	0.40
4:Bh:110:GLU:HG2	8:Bm:194:ILE:HD11	2.02	0.40
4:Br:58:LEU:HB2	4:Br:66:SER:HB3	2.03	0.40
8:Bw:275:ARG:C	8:Bw:276:PHE:CD1	2.98	0.40
3:Ca:202:LEU:HD11	3:Ca:204:LEU:CD1	2.52	0.40
7:Cf:166:ALA:HA	7:Cf:206:GLU:O	2.21	0.40
7:Cf:234:PHE:CZ	9:Ch:29:ARG:HG2	2.55	0.40
9:Ch:39:LYS:HD3	9:Ch:40:PRO:CD	2.52	0.40
1:Cm:57:LYS:HB2	1:Cm:57:LYS:HE2	1.88	0.40
7:Cz:224:ALA:HA	7:Cz:227:ARG:CZ	2.52	0.40
8:Da:173:LYS:HA	8:Da:176:TRP:HB3	2.02	0.40
8:Dk:299:ILE:HG22	8:Dk:302:VAL:HG23	2.02	0.40
9:Dl:29:ARG:C	9:Dl:30:TRP:CG	3.00	0.40
1:Dm:161:ILE:H	1:Dm:161:ILE:HG13	1.68	0.40
5:Dr:254:ILE:N	5:Dr:254:ILE:HD12	2.37	0.40
3:Dy:52:VAL:HB	3:Dy:118:TYR:CD2	2.56	0.40
7:Ed:208:TYR:HD2	9:Ef:86:SER:HB2	1.86	0.40
9:Ef:46:LEU:HD13	9:Ef:93:ARG:HD3	2.04	0.40
8:Eo:213:ARG:HA	8:Eo:213:ARG:HD2	1.93	0.40
3:Es:30:VAL:HG23	3:Es:76:ARG:HD3	2.03	0.40
3:Es:98:TYR:HE1	3:Es:101:TYR:H	1.68	0.40
1:Ae:48:VAL:HG11	8:Ai:93:ILE:HA	2.03	0.40
3:Am:174:GLN:OE1	3:Am:176:VAL:HG23	2.22	0.40
3:Am:244:LYS:HE2	3:Am:244:LYS:HB3	1.85	0.40
2:Av:57:MET:HG2	2:Av:67:VAL:HG11	2.02	0.40
2:Av:113:ALA:HA	2:Av:153:ILE:O	2.21	0.40
3:Aw:130:ARG:HE	3:Aw:130:ARG:HB2	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Be:136:ASP:OD2	1:Bi:60:LYS:HE2	2.22	0.40
3:Bg:206:TRP:HA	3:Bg:206:TRP:CE3	2.56	0.40
1:Bi:75:ASN:HA	1:Bi:80:GLN:HE22	1.86	0.40
8:Bm:272:ALA:HA	8:Bm:275:ARG:CZ	2.51	0.40
3:Bq:141:GLU:HA	3:Bq:161:GLY:HA2	2.03	0.40
4:Br:84:CYS:CB	8:Bw:154:ASP:HB3	2.50	0.40
6:Bu:312:TYR:HA	6:Bu:337:TYR:O	2.20	0.40
7:Cf:102:LYS:HD2	7:Cf:158:TYR:OH	2.22	0.40
8:Cq:137:GLN:HG3	8:Cq:252:LEU:HD22	2.03	0.40
3:Cu:205:TYR:O	3:Cu:225:ALA:HB3	2.21	0.40
7:Cz:152:ILE:HD13	7:Cz:152:ILE:HA	1.87	0.40
7:Dj:189:MET:O	7:Dj:193:LEU:HG	2.21	0.40
7:Dj:219:ILE:HG13	7:Dj:222:GLY:H	1.86	0.40
8:Dk:291:THR:HG22	8:Dk:293:LYS:N	2.36	0.40
8:Du:231:LEU:HB2	8:Du:244:ASP:HB3	2.04	0.40
1:Dw:124:LYS:HE2	2:Dx:142:GLU:OE1	2.21	0.40
1:Eg:126:GLU:OE2	1:Eg:130:GLU:HB3	2.22	0.40
8:Eo:77:LYS:O	8:Eo:81:GLU:HG3	2.22	0.40
3:Es:111:LYS:HE3	3:Es:111:LYS:HB3	1.67	0.40
7:Ex:166:ALA:HA	7:Ex:206:GLU:O	2.22	0.40
8:Ey:276:PHE:CE2	9:Ez:79:ILE:HD13	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Ae	134/163 (82%)	131 (98%)	3 (2%)	0	100	100
1	Ak	137/163 (84%)	130 (95%)	7 (5%)	0	100	100
1	Ao	134/163 (82%)	130 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Au	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Ay	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
1	Be	137/163 (84%)	130 (95%)	7 (5%)	0	100	100
1	Bi	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
1	Bo	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Bs	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
1	By	137/163 (84%)	131 (96%)	6 (4%)	0	100	100
1	Cc	134/163 (82%)	130 (97%)	4 (3%)	0	100	100
1	Ci	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Cm	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
1	Cs	137/163 (84%)	130 (95%)	7 (5%)	0	100	100
1	Cw	134/163 (82%)	130 (97%)	4 (3%)	0	100	100
1	Dc	137/163 (84%)	130 (95%)	7 (5%)	0	100	100
1	Dg	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
1	Dm	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Dq	134/163 (82%)	130 (97%)	4 (3%)	0	100	100
1	Dw	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Ea	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
1	Eg	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Ek	134/163 (82%)	131 (98%)	3 (2%)	0	100	100
1	Eq	137/163 (84%)	130 (95%)	7 (5%)	0	100	100
1	Eu	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
2	Ab	147/189 (78%)	145 (99%)	2 (1%)	0	100	100
2	Al	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
2	Av	147/189 (78%)	143 (97%)	4 (3%)	0	100	100
2	Bf	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
2	Bp	147/189 (78%)	145 (99%)	2 (1%)	0	100	100
2	Bz	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
2	Cj	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
2	Ct	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
2	Dd	147/189 (78%)	145 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Dn	147/189 (78%)	145 (99%)	2 (1%)	0	100	100
2	Dx	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
2	Eh	147/189 (78%)	143 (97%)	4 (3%)	0	100	100
2	Er	147/189 (78%)	145 (99%)	2 (1%)	0	100	100
3	Ac	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
3	Am	290/320 (91%)	270 (93%)	20 (7%)	0	100	100
3	Aw	290/320 (91%)	270 (93%)	20 (7%)	0	100	100
3	Bg	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
3	Bq	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
3	Ca	290/320 (91%)	272 (94%)	18 (6%)	0	100	100
3	Ck	290/320 (91%)	271 (93%)	19 (7%)	0	100	100
3	Cu	290/320 (91%)	271 (93%)	19 (7%)	0	100	100
3	De	290/320 (91%)	270 (93%)	20 (7%)	0	100	100
3	Do	290/320 (91%)	267 (92%)	23 (8%)	0	100	100
3	Dy	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
3	Ei	290/320 (91%)	270 (93%)	20 (7%)	0	100	100
3	Es	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
4	Ad	74/124 (60%)	68 (92%)	6 (8%)	0	100	100
4	An	74/124 (60%)	68 (92%)	6 (8%)	0	100	100
4	Ax	74/124 (60%)	67 (90%)	7 (10%)	0	100	100
4	Bh	74/124 (60%)	67 (90%)	7 (10%)	0	100	100
4	Br	74/124 (60%)	68 (92%)	6 (8%)	0	100	100
4	Cb	74/124 (60%)	67 (90%)	7 (10%)	0	100	100
4	Cl	74/124 (60%)	69 (93%)	5 (7%)	0	100	100
4	Cv	74/124 (60%)	69 (93%)	5 (7%)	0	100	100
4	Df	74/124 (60%)	67 (90%)	7 (10%)	0	100	100
4	Dp	74/124 (60%)	70 (95%)	4 (5%)	0	100	100
4	Dz	74/124 (60%)	70 (95%)	4 (5%)	0	100	100
4	Ej	74/124 (60%)	68 (92%)	6 (8%)	0	100	100
4	Et	74/124 (60%)	67 (90%)	7 (10%)	0	100	100
5	Af	57/269 (21%)	55 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Ap	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
5	Az	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
5	Bj	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
5	Bt	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
5	Cd	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
5	Cn	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
5	Cx	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
5	Dh	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
5	Dr	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
5	Eb	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
5	El	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
5	Ev	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
6	Ag	89/361 (25%)	83 (93%)	6 (7%)	0	100	100
6	Aq	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Ba	89/361 (25%)	83 (93%)	6 (7%)	0	100	100
6	Bk	89/361 (25%)	83 (93%)	6 (7%)	0	100	100
6	Bu	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Ce	89/361 (25%)	85 (96%)	4 (4%)	0	100	100
6	Co	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Cy	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Di	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Ds	89/361 (25%)	83 (93%)	6 (7%)	0	100	100
6	Ec	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Em	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Ew	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
7	Ah	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Ar	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Bb	191/249 (77%)	185 (97%)	6 (3%)	0	100	100
7	Bl	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Bv	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Cf	191/249 (77%)	184 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Cp	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Cz	191/249 (77%)	183 (96%)	8 (4%)	0	100	100
7	Dj	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Dt	191/249 (77%)	185 (97%)	6 (3%)	0	100	100
7	Ed	191/249 (77%)	186 (97%)	5 (3%)	0	100	100
7	En	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Ex	191/249 (77%)	183 (96%)	8 (4%)	0	100	100
8	Ai	241/303 (80%)	224 (93%)	17 (7%)	0	100	100
8	As	241/303 (80%)	225 (93%)	16 (7%)	0	100	100
8	Bc	241/303 (80%)	228 (95%)	13 (5%)	0	100	100
8	Bm	241/303 (80%)	225 (93%)	16 (7%)	0	100	100
8	Bw	241/303 (80%)	226 (94%)	15 (6%)	0	100	100
8	Cg	241/303 (80%)	226 (94%)	15 (6%)	0	100	100
8	Cq	241/303 (80%)	226 (94%)	15 (6%)	0	100	100
8	Da	241/303 (80%)	225 (93%)	16 (7%)	0	100	100
8	Dk	241/303 (80%)	228 (95%)	13 (5%)	0	100	100
8	Du	241/303 (80%)	226 (94%)	15 (6%)	0	100	100
8	Ee	241/303 (80%)	227 (94%)	14 (6%)	0	100	100
8	Eo	241/303 (80%)	227 (94%)	14 (6%)	0	100	100
8	Ey	241/303 (80%)	225 (93%)	16 (7%)	0	100	100
9	Aj	69/93 (74%)	62 (90%)	6 (9%)	1 (1%)	9	25
9	At	69/93 (74%)	61 (88%)	7 (10%)	1 (1%)	9	25
9	Bd	69/93 (74%)	62 (90%)	6 (9%)	1 (1%)	9	25
9	Bn	69/93 (74%)	61 (88%)	7 (10%)	1 (1%)	9	25
9	Bx	69/93 (74%)	60 (87%)	8 (12%)	1 (1%)	9	25
9	Ch	69/93 (74%)	59 (86%)	9 (13%)	1 (1%)	9	25
9	Cr	69/93 (74%)	62 (90%)	6 (9%)	1 (1%)	9	25
9	Db	69/93 (74%)	62 (90%)	6 (9%)	1 (1%)	9	25
9	Dl	69/93 (74%)	60 (87%)	8 (12%)	1 (1%)	9	25
9	Dv	69/93 (74%)	62 (90%)	6 (9%)	1 (1%)	9	25
9	Ef	69/93 (74%)	61 (88%)	7 (10%)	1 (1%)	9	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Ep	69/93 (74%)	62 (90%)	6 (9%)	1 (1%)	9	25
9	Ez	69/93 (74%)	61 (88%)	7 (10%)	1 (1%)	9	25
All	All	18577/29042 (64%)	17556 (94%)	1008 (5%)	13 (0%)	50	72

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	Aj	27	LYS
9	At	27	LYS
9	Bd	27	LYS
9	Bn	27	LYS
9	Bx	27	LYS
9	Ch	27	LYS
9	Cr	27	LYS
9	Db	27	LYS
9	Dl	27	LYS
9	Dv	27	LYS
9	Ef	27	LYS
9	Ep	27	LYS
9	Ez	27	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aa	120/139 (86%)	118 (98%)	2 (2%)	56	76
1	Ae	117/139 (84%)	115 (98%)	2 (2%)	56	76
1	Ak	120/139 (86%)	118 (98%)	2 (2%)	56	76
1	Ao	117/139 (84%)	114 (97%)	3 (3%)	41	65
1	Au	120/139 (86%)	118 (98%)	2 (2%)	56	76
1	Ay	117/139 (84%)	113 (97%)	4 (3%)	32	57
1	Be	120/139 (86%)	117 (98%)	3 (2%)	42	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bi	117/139 (84%)	112 (96%)	5 (4%)	25	49
1	Bo	120/139 (86%)	120 (100%)	0	100	100
1	Bs	117/139 (84%)	112 (96%)	5 (4%)	25	49
1	By	120/139 (86%)	118 (98%)	2 (2%)	56	76
1	Cc	117/139 (84%)	111 (95%)	6 (5%)	20	43
1	Ci	120/139 (86%)	118 (98%)	2 (2%)	56	76
1	Cm	117/139 (84%)	116 (99%)	1 (1%)	75	86
1	Cs	120/139 (86%)	117 (98%)	3 (2%)	42	66
1	Cw	117/139 (84%)	113 (97%)	4 (3%)	32	57
1	Dc	120/139 (86%)	117 (98%)	3 (2%)	42	66
1	Dg	117/139 (84%)	115 (98%)	2 (2%)	56	76
1	Dm	120/139 (86%)	120 (100%)	0	100	100
1	Dq	117/139 (84%)	113 (97%)	4 (3%)	32	57
1	Dw	120/139 (86%)	119 (99%)	1 (1%)	79	88
1	Ea	117/139 (84%)	115 (98%)	2 (2%)	56	76
1	Eg	120/139 (86%)	119 (99%)	1 (1%)	79	88
1	Ek	117/139 (84%)	114 (97%)	3 (3%)	41	65
1	Eq	120/139 (86%)	116 (97%)	4 (3%)	33	58
1	Eu	117/139 (84%)	113 (97%)	4 (3%)	32	57
2	Ab	127/163 (78%)	123 (97%)	4 (3%)	35	59
2	Al	127/163 (78%)	123 (97%)	4 (3%)	35	59
2	Av	127/163 (78%)	123 (97%)	4 (3%)	35	59
2	Bf	127/163 (78%)	122 (96%)	5 (4%)	27	52
2	Bp	127/163 (78%)	123 (97%)	4 (3%)	35	59
2	Bz	127/163 (78%)	124 (98%)	3 (2%)	44	68
2	Cj	127/163 (78%)	123 (97%)	4 (3%)	35	59
2	Ct	127/163 (78%)	124 (98%)	3 (2%)	44	68
2	Dd	127/163 (78%)	126 (99%)	1 (1%)	79	88
2	Dn	127/163 (78%)	124 (98%)	3 (2%)	44	68
2	Dx	127/163 (78%)	123 (97%)	4 (3%)	35	59
2	Eh	127/163 (78%)	125 (98%)	2 (2%)	58	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Er	127/163 (78%)	122 (96%)	5 (4%)	27	52
3	Ac	251/276 (91%)	243 (97%)	8 (3%)	34	59
3	Am	251/276 (91%)	245 (98%)	6 (2%)	44	68
3	Aw	251/276 (91%)	245 (98%)	6 (2%)	44	68
3	Bg	251/276 (91%)	244 (97%)	7 (3%)	38	63
3	Bq	251/276 (91%)	244 (97%)	7 (3%)	38	63
3	Ca	251/276 (91%)	242 (96%)	9 (4%)	30	55
3	Ck	251/276 (91%)	246 (98%)	5 (2%)	50	72
3	Cu	251/276 (91%)	246 (98%)	5 (2%)	50	72
3	De	251/276 (91%)	243 (97%)	8 (3%)	34	59
3	Do	251/276 (91%)	242 (96%)	9 (4%)	30	55
3	Dy	251/276 (91%)	245 (98%)	6 (2%)	44	68
3	Ei	251/276 (91%)	242 (96%)	9 (4%)	30	55
3	Es	251/276 (91%)	241 (96%)	10 (4%)	27	51
4	Ad	64/107 (60%)	61 (95%)	3 (5%)	22	46
4	An	64/107 (60%)	63 (98%)	1 (2%)	58	77
4	Ax	64/107 (60%)	62 (97%)	2 (3%)	35	59
4	Bh	64/107 (60%)	63 (98%)	1 (2%)	58	77
4	Br	64/107 (60%)	63 (98%)	1 (2%)	58	77
4	Cb	64/107 (60%)	63 (98%)	1 (2%)	58	77
4	Cl	64/107 (60%)	63 (98%)	1 (2%)	58	77
4	Cv	64/107 (60%)	63 (98%)	1 (2%)	58	77
4	Df	64/107 (60%)	63 (98%)	1 (2%)	58	77
4	Dp	64/107 (60%)	61 (95%)	3 (5%)	22	46
4	Dz	64/107 (60%)	63 (98%)	1 (2%)	58	77
4	Ej	64/107 (60%)	62 (97%)	2 (3%)	35	59
4	Et	64/107 (60%)	63 (98%)	1 (2%)	58	77
5	Af	49/237 (21%)	47 (96%)	2 (4%)	26	51
5	Ap	49/237 (21%)	47 (96%)	2 (4%)	26	51
5	Az	49/237 (21%)	48 (98%)	1 (2%)	50	72
5	Bj	49/237 (21%)	48 (98%)	1 (2%)	50	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Bt	49/237 (21%)	48 (98%)	1 (2%)	50	72
5	Cd	49/237 (21%)	47 (96%)	2 (4%)	26	51
5	Cn	49/237 (21%)	49 (100%)	0	100	100
5	Cx	49/237 (21%)	49 (100%)	0	100	100
5	Dh	49/237 (21%)	48 (98%)	1 (2%)	50	72
5	Dr	49/237 (21%)	45 (92%)	4 (8%)	9	24
5	Eb	49/237 (21%)	48 (98%)	1 (2%)	50	72
5	El	49/237 (21%)	48 (98%)	1 (2%)	50	72
5	Ev	49/237 (21%)	49 (100%)	0	100	100
6	Ag	76/300 (25%)	75 (99%)	1 (1%)	65	80
6	Aq	76/300 (25%)	76 (100%)	0	100	100
6	Ba	76/300 (25%)	75 (99%)	1 (1%)	65	80
6	Bk	76/300 (25%)	76 (100%)	0	100	100
6	Bu	76/300 (25%)	75 (99%)	1 (1%)	65	80
6	Ce	76/300 (25%)	74 (97%)	2 (3%)	41	65
6	Co	76/300 (25%)	74 (97%)	2 (3%)	41	65
6	Cy	76/300 (25%)	75 (99%)	1 (1%)	65	80
6	Di	76/300 (25%)	76 (100%)	0	100	100
6	Ds	76/300 (25%)	75 (99%)	1 (1%)	65	80
6	Ec	76/300 (25%)	75 (99%)	1 (1%)	65	80
6	Em	76/300 (25%)	75 (99%)	1 (1%)	65	80
6	Ew	76/300 (25%)	74 (97%)	2 (3%)	41	65
7	Ah	155/203 (76%)	152 (98%)	3 (2%)	52	73
7	Ar	155/203 (76%)	152 (98%)	3 (2%)	52	73
7	Bb	155/203 (76%)	149 (96%)	6 (4%)	27	52
7	Bl	155/203 (76%)	152 (98%)	3 (2%)	52	73
7	Bv	155/203 (76%)	152 (98%)	3 (2%)	52	73
7	Cf	155/203 (76%)	149 (96%)	6 (4%)	27	52
7	Cp	155/203 (76%)	152 (98%)	3 (2%)	52	73
7	Cz	155/203 (76%)	153 (99%)	2 (1%)	65	80
7	Dj	155/203 (76%)	152 (98%)	3 (2%)	52	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	Dt	155/203 (76%)	153 (99%)	2 (1%)	65	80
7	Ed	155/203 (76%)	150 (97%)	5 (3%)	34	59
7	En	155/203 (76%)	151 (97%)	4 (3%)	41	65
7	Ex	155/203 (76%)	151 (97%)	4 (3%)	41	65
8	Ai	208/257 (81%)	205 (99%)	3 (1%)	62	79
8	As	208/257 (81%)	204 (98%)	4 (2%)	52	73
8	Bc	208/257 (81%)	205 (99%)	3 (1%)	62	79
8	Bm	208/257 (81%)	204 (98%)	4 (2%)	52	73
8	Bw	208/257 (81%)	201 (97%)	7 (3%)	32	57
8	Cg	208/257 (81%)	206 (99%)	2 (1%)	73	85
8	Cq	208/257 (81%)	203 (98%)	5 (2%)	44	68
8	Da	208/257 (81%)	204 (98%)	4 (2%)	52	73
8	Dk	208/257 (81%)	203 (98%)	5 (2%)	44	68
8	Du	208/257 (81%)	199 (96%)	9 (4%)	25	49
8	Ee	208/257 (81%)	205 (99%)	3 (1%)	62	79
8	Eo	208/257 (81%)	202 (97%)	6 (3%)	37	61
8	Ey	208/257 (81%)	204 (98%)	4 (2%)	52	73
9	Aj	63/80 (79%)	60 (95%)	3 (5%)	21	46
9	At	63/80 (79%)	61 (97%)	2 (3%)	34	59
9	Bd	63/80 (79%)	60 (95%)	3 (5%)	21	46
9	Bn	63/80 (79%)	62 (98%)	1 (2%)	58	77
9	Bx	63/80 (79%)	61 (97%)	2 (3%)	34	59
9	Ch	63/80 (79%)	61 (97%)	2 (3%)	34	59
9	Cr	63/80 (79%)	61 (97%)	2 (3%)	34	59
9	Db	63/80 (79%)	62 (98%)	1 (2%)	58	77
9	Dl	63/80 (79%)	61 (97%)	2 (3%)	34	59
9	Dv	63/80 (79%)	61 (97%)	2 (3%)	34	59
9	Ef	63/80 (79%)	61 (97%)	2 (3%)	34	59
9	Ep	63/80 (79%)	62 (98%)	1 (2%)	58	77
9	Ez	63/80 (79%)	60 (95%)	3 (5%)	21	46
All	All	15990/24713 (65%)	15599 (98%)	391 (2%)	45	68

All (391) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	49	SER
1	Aa	160	LYS
2	Ab	55	LYS
2	Ab	78	ILE
2	Ab	129	GLU
2	Ab	183	THR
3	Ac	85	VAL
3	Ac	136	LEU
3	Ac	138	LEU
3	Ac	155	LEU
3	Ac	183	VAL
3	Ac	307	SER
3	Ac	309	LEU
3	Ac	315	TYR
4	Ad	51	CYS
4	Ad	62	ASN
4	Ad	81	LEU
1	Ae	72	THR
1	Ae	144	SER
5	Af	236	SER
5	Af	250	LEU
6	Ag	311	MET
7	Ah	55	ARG
7	Ah	57	VAL
7	Ah	110	GLN
8	Ai	221	VAL
8	Ai	228	HIS
8	Ai	263	ARG
9	Aj	25	LEU
9	Aj	30	TRP
9	Aj	38	VAL
1	Ak	49	SER
1	Ak	151	SER
2	Al	55	LYS
2	Al	125	SER
2	Al	129	GLU
2	Al	170	LEU
3	Am	85	VAL
3	Am	117	ARG
3	Am	129	LEU
3	Am	155	LEU
3	Am	183	VAL

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Mol	Chain	Res	Type
3	Am	299	LEU
4	An	94	GLN
1	Ao	34	SER
1	Ao	75	ASN
1	Ao	144	SER
5	Ap	212	ILE
5	Ap	243	MET
7	Ar	57	VAL
7	Ar	110	GLN
7	Ar	206	GLU
8	As	221	VAL
8	As	228	HIS
8	As	263	ARG
8	As	289	VAL
9	At	30	TRP
9	At	53	SER
1	Au	49	SER
1	Au	85	VAL
2	Av	55	LYS
2	Av	75	LEU
2	Av	78	ILE
2	Av	129	GLU
3	Aw	85	VAL
3	Aw	117	ARG
3	Aw	129	LEU
3	Aw	183	VAL
3	Aw	277	SER
3	Aw	297	SER
4	Ax	51	CYS
4	Ax	62	ASN
1	Ay	30	ILE
1	Ay	63	THR
1	Ay	72	THR
1	Ay	144	SER
5	Az	210	TYR
6	Ba	275	SER
7	Bb	57	VAL
7	Bb	110	GLN
7	Bb	142	GLU
7	Bb	177	HIS
7	Bb	206	GLU
7	Bb	225	GLN

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Mol	Chain	Res	Type
8	Bc	226	VAL
8	Bc	228	HIS
8	Bc	231	LEU
9	Bd	25	LEU
9	Bd	30	TRP
9	Bd	86	SER
1	Be	62	ILE
1	Be	75	ASN
1	Be	84	SER
2	Bf	75	LEU
2	Bf	78	ILE
2	Bf	129	GLU
2	Bf	170	LEU
2	Bf	183	THR
3	Bg	85	VAL
3	Bg	117	ARG
3	Bg	129	LEU
3	Bg	152	LEU
3	Bg	155	LEU
3	Bg	183	VAL
3	Bg	228	VAL
4	Bh	76	MET
1	Bi	30	ILE
1	Bi	34	SER
1	Bi	59	GLU
1	Bi	75	ASN
1	Bi	144	SER
5	Bj	243	MET
7	Bl	57	VAL
7	Bl	206	GLU
7	Bl	223	SER
8	Bm	221	VAL
8	Bm	228	HIS
8	Bm	231	LEU
8	Bm	289	VAL
9	Bn	30	TRP
2	Bp	55	LYS
2	Bp	75	LEU
2	Bp	78	ILE
2	Bp	174	ARG
3	Bq	85	VAL
3	Bq	129	LEU

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Mol	Chain	Res	Type
3	Bq	155	LEU
3	Bq	180	ASP
3	Bq	212	LEU
3	Bq	307	SER
3	Bq	315	TYR
4	Br	51	CYS
1	Bs	30	ILE
1	Bs	63	THR
1	Bs	71	LEU
1	Bs	75	ASN
1	Bs	144	SER
5	Bt	253	ARG
6	Bu	348	SER
7	Bv	57	VAL
7	Bv	110	GLN
7	Bv	165	VAL
8	Bw	178	ILE
8	Bw	228	HIS
8	Bw	231	LEU
8	Bw	244	ASP
8	Bw	263	ARG
8	Bw	288	ILE
8	Bw	289	VAL
9	Bx	25	LEU
9	Bx	30	TRP
1	By	49	SER
1	By	151	SER
2	Bz	55	LYS
2	Bz	101	GLU
2	Bz	129	GLU
3	Ca	85	VAL
3	Ca	117	ARG
3	Ca	138	LEU
3	Ca	183	VAL
3	Ca	212	LEU
3	Ca	292	MET
3	Ca	299	LEU
3	Ca	307	SER
3	Ca	315	TYR
4	Cb	104	ASN
1	Cc	30	ILE
1	Cc	34	SER

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Mol	Chain	Res	Type
1	Cc	41	LEU
1	Cc	52	MET
1	Cc	55	MET
1	Cc	75	ASN
5	Cd	236	SER
5	Cd	243	MET
6	Ce	311	MET
6	Ce	348	SER
7	Cf	57	VAL
7	Cf	93	LEU
7	Cf	110	GLN
7	Cf	142	GLU
7	Cf	189	MET
7	Cf	206	GLU
8	Cg	228	HIS
8	Cg	299	ILE
9	Ch	30	TRP
9	Ch	47	LEU
1	Ci	62	ILE
1	Ci	63	THR
2	Cj	66	LYS
2	Cj	75	LEU
2	Cj	78	ILE
2	Cj	170	LEU
3	Ck	85	VAL
3	Ck	129	LEU
3	Ck	183	VAL
3	Ck	292	MET
3	Ck	315	TYR
4	Cl	51	CYS
1	Cm	72	THR
6	Co	275	SER
6	Co	348	SER
7	Cp	57	VAL
7	Cp	110	GLN
7	Cp	225	GLN
8	Cq	34	LEU
8	Cq	228	HIS
8	Cq	231	LEU
8	Cq	289	VAL
8	Cq	299	ILE
9	Cr	30	TRP

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Mol	Chain	Res	Type
9	Cr	32	CYS
1	Cs	49	SER
1	Cs	84	SER
1	Cs	151	SER
2	Ct	55	LYS
2	Ct	75	LEU
2	Ct	78	ILE
3	Cu	85	VAL
3	Cu	129	LEU
3	Cu	183	VAL
3	Cu	292	MET
3	Cu	315	TYR
4	Cv	62	ASN
1	Cw	72	THR
1	Cw	75	ASN
1	Cw	120	SER
1	Cw	144	SER
6	Cy	342	SER
7	Cz	57	VAL
7	Cz	93	LEU
8	Da	221	VAL
8	Da	228	HIS
8	Da	231	LEU
8	Da	289	VAL
9	Db	30	TRP
1	Dc	49	SER
1	Dc	63	THR
1	Dc	151	SER
2	Dd	78	ILE
3	De	85	VAL
3	De	117	ARG
3	De	129	LEU
3	De	136	LEU
3	De	180	ASP
3	De	183	VAL
3	De	299	LEU
3	De	315	TYR
4	Df	108	VAL
1	Dg	34	SER
1	Dg	72	THR
5	Dh	229	THR
7	Dj	57	VAL

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Mol	Chain	Res	Type
7	Dj	110	GLN
7	Dj	225	GLN
8	Dk	170	LYS
8	Dk	221	VAL
8	Dk	228	HIS
8	Dk	271	ASN
8	Dk	288	ILE
9	Dl	30	TRP
9	Dl	31	ASP
2	Dn	78	ILE
2	Dn	101	GLU
2	Dn	146	SER
3	Do	85	VAL
3	Do	129	LEU
3	Do	136	LEU
3	Do	183	VAL
3	Do	194	LEU
3	Do	212	LEU
3	Do	228	VAL
3	Do	299	LEU
3	Do	315	TYR
4	Dp	51	CYS
4	Dp	62	ASN
4	Dp	108	VAL
1	Dq	61	VAL
1	Dq	63	THR
1	Dq	67	LYS
1	Dq	75	ASN
5	Dr	230	LEU
5	Dr	236	SER
5	Dr	243	MET
5	Dr	253	ARG
6	Ds	275	SER
7	Dt	57	VAL
7	Dt	110	GLN
8	Du	34	LEU
8	Du	180	THR
8	Du	209	MET
8	Du	220	MET
8	Du	228	HIS
8	Du	244	ASP
8	Du	263	ARG

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Mol	Chain	Res	Type
8	Du	288	ILE
8	Du	289	VAL
9	Dv	25	LEU
9	Dv	30	TRP
1	Dw	151	SER
2	Dx	55	LYS
2	Dx	75	LEU
2	Dx	78	ILE
2	Dx	129	GLU
3	Dy	85	VAL
3	Dy	129	LEU
3	Dy	138	LEU
3	Dy	175	ILE
3	Dy	180	ASP
3	Dy	315	TYR
4	Dz	51	CYS
1	Ea	75	ASN
1	Ea	144	SER
5	Eb	243	MET
6	Ec	275	SER
7	Ed	57	VAL
7	Ed	93	LEU
7	Ed	110	GLN
7	Ed	206	GLU
7	Ed	225	GLN
8	Ee	221	VAL
8	Ee	228	HIS
8	Ee	289	VAL
9	Ef	30	TRP
9	Ef	65	LEU
1	Eg	54	GLU
2	Eh	78	ILE
2	Eh	156	THR
3	Ei	85	VAL
3	Ei	117	ARG
3	Ei	136	LEU
3	Ei	149	ASN
3	Ei	175	ILE
3	Ei	183	VAL
3	Ei	292	MET
3	Ei	307	SER
3	Ei	315	TYR

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Mol	Chain	Res	Type
4	Ej	51	CYS
4	Ej	62	ASN
1	Ek	72	THR
1	Ek	144	SER
1	Ek	155	GLU
5	El	253	ARG
6	Em	310	LYS
7	En	57	VAL
7	En	110	GLN
7	En	177	HIS
7	En	225	GLN
8	Eo	124	SER
8	Eo	180	THR
8	Eo	221	VAL
8	Eo	228	HIS
8	Eo	263	ARG
8	Eo	289	VAL
9	Ep	30	TRP
1	Eq	53	LEU
1	Eq	63	THR
1	Eq	85	VAL
1	Eq	151	SER
2	Er	55	LYS
2	Er	78	ILE
2	Er	101	GLU
2	Er	129	GLU
2	Er	170	LEU
3	Es	85	VAL
3	Es	117	ARG
3	Es	129	LEU
3	Es	155	LEU
3	Es	183	VAL
3	Es	194	LEU
3	Es	290	ASP
3	Es	292	MET
3	Es	307	SER
3	Es	315	TYR
4	Et	51	CYS
1	Eu	61	VAL
1	Eu	72	THR
1	Eu	75	ASN
1	Eu	155	GLU

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Mol	Chain	Res	Type
6	Ew	275	SER
6	Ew	314	ARG
7	Ex	53	ASP
7	Ex	57	VAL
7	Ex	110	GLN
7	Ex	206	GLU
8	Ey	170	LYS
8	Ey	221	VAL
8	Ey	228	HIS
8	Ey	244	ASP
9	Ez	25	LEU
9	Ez	30	TRP
9	Ez	31	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	69	ASN
1	Aa	75	ASN
2	Ab	147	GLN
3	Ac	96	GLN
3	Ac	164	GLN
3	Ac	269	GLN
4	Ad	61	ASN
4	Ad	62	ASN
4	Ad	94	GLN
1	Ae	146	HIS
6	Ag	308	ASN
6	Ag	350	HIS
8	Ai	97	ASN
8	Ai	137	GLN
8	Ai	271	ASN
1	Ak	69	ASN
1	Ak	80	GLN
2	Al	147	GLN
3	Am	61	HIS
3	Am	166	ASN
3	Am	269	GLN
6	Aq	277	ASN
6	Aq	316	ASN
6	Aq	350	HIS
7	Ar	212	ASN

Continued on next page...

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Mol	Chain	Res	Type
7	Ar	232	GLN
8	As	97	ASN
8	As	123	GLN
8	As	137	GLN
8	As	285	GLN
1	Au	75	ASN
2	Av	147	GLN
3	Aw	59	ASN
3	Aw	61	HIS
3	Aw	164	GLN
3	Aw	269	GLN
4	Ax	79	GLN
4	Ax	94	GLN
1	Ay	146	HIS
1	Ay	152	GLN
6	Ba	277	ASN
6	Ba	316	ASN
6	Ba	350	HIS
8	Bc	137	GLN
8	Bc	271	ASN
8	Bc	285	GLN
1	Be	69	ASN
1	Be	75	ASN
2	Bf	147	GLN
3	Bg	96	GLN
3	Bg	164	GLN
3	Bg	172	ASN
3	Bg	269	GLN
4	Bh	88	HIS
1	Bi	75	ASN
1	Bi	78	ASN
6	Bk	350	HIS
7	Bl	51	GLN
7	Bl	212	ASN
7	Bl	232	GLN
8	Bm	97	ASN
8	Bm	137	GLN
8	Bm	228	HIS
8	Bm	285	GLN
1	Bo	75	ASN
1	Bo	80	GLN
1	Bo	138	GLN

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Mol	Chain	Res	Type
1	Bo	152	GLN
2	Bp	147	GLN
3	Bq	96	GLN
3	Bq	166	ASN
3	Bq	269	GLN
1	Bs	146	HIS
6	Bu	316	ASN
6	Bu	350	HIS
7	Bv	232	GLN
8	Bw	97	ASN
8	Bw	103	HIS
8	Bw	137	GLN
8	Bw	139	HIS
8	Bw	228	HIS
8	Bw	285	GLN
1	By	103	HIS
1	By	152	GLN
2	Bz	147	GLN
3	Ca	59	ASN
3	Ca	61	HIS
3	Ca	164	GLN
3	Ca	172	ASN
3	Ca	269	GLN
1	Cc	146	HIS
6	Ce	316	ASN
8	Cg	97	ASN
8	Cg	103	HIS
8	Cg	137	GLN
8	Cg	228	HIS
8	Cg	285	GLN
9	Ch	69	GLN
1	Ci	69	ASN
1	Ci	80	GLN
1	Ci	103	HIS
1	Ci	146	HIS
2	Cj	147	GLN
3	Ck	164	GLN
1	Cm	75	ASN
1	Cm	78	ASN
7	Cp	212	ASN
8	Cq	97	ASN
8	Cq	103	HIS

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Mol	Chain	Res	Type
8	Cq	123	GLN
8	Cq	228	HIS
8	Cq	285	GLN
8	Cq	292	ASN
1	Cs	103	HIS
2	Ct	147	GLN
3	Cu	166	ASN
3	Cu	269	GLN
4	Cv	62	ASN
1	Cw	146	HIS
5	Cx	251	GLN
6	Cy	277	ASN
6	Cy	316	ASN
6	Cy	350	HIS
7	Cz	212	ASN
8	Da	97	ASN
8	Da	137	GLN
1	Dc	69	ASN
1	Dc	80	GLN
1	Dc	103	HIS
2	Dd	147	GLN
3	De	164	GLN
3	De	269	GLN
4	Df	61	ASN
7	Dj	51	GLN
7	Dj	232	GLN
8	Dk	97	ASN
8	Dk	103	HIS
8	Dk	104	ASN
8	Dk	139	HIS
8	Dk	228	HIS
8	Dk	271	ASN
8	Dk	285	GLN
8	Dk	292	ASN
1	Dm	75	ASN
1	Dm	103	HIS
2	Dn	147	GLN
3	Do	164	GLN
3	Do	269	GLN
3	Do	318	GLN
4	Dp	61	ASN
6	Ds	316	ASN

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Mol	Chain	Res	Type
7	Dt	177	HIS
8	Du	137	GLN
8	Du	228	HIS
8	Du	285	GLN
1	Dw	80	GLN
2	Dx	147	GLN
3	Dy	61	HIS
3	Dy	164	GLN
3	Dy	269	GLN
4	Dz	88	HIS
1	Ea	152	GLN
6	Ec	316	ASN
6	Ec	350	HIS
8	Ee	89	ASN
8	Ee	123	GLN
8	Ee	228	HIS
1	Eg	146	HIS
2	Uh	147	GLN
3	Ei	96	GLN
3	Ei	164	GLN
3	Ei	172	ASN
3	Ei	268	HIS
3	Ei	269	GLN
4	Ej	62	ASN
4	Ej	88	HIS
6	Em	350	HIS
7	En	51	GLN
8	Eu	97	ASN
8	Eu	137	GLN
8	Eu	292	ASN
1	Eq	75	ASN
1	Eq	80	GLN
1	Eq	152	GLN
2	Er	147	GLN
3	Es	61	HIS
3	Es	166	ASN
3	Es	172	ASN
3	Es	269	GLN
1	Eu	146	HIS
6	Ew	277	ASN
6	Ew	350	HIS
7	Ex	212	ASN

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Mol	Chain	Res	Type
7	Ex	232	GLN
8	Ey	97	ASN
8	Ey	139	HIS
8	Ey	285	GLN
8	Ey	292	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

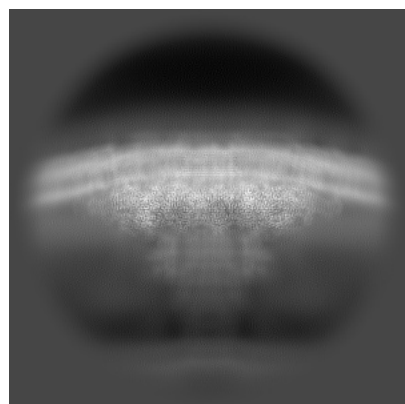
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49393. These allow visual inspection of the internal detail of the map and identification of artifacts.

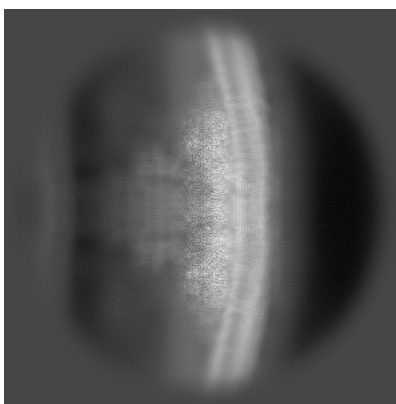
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

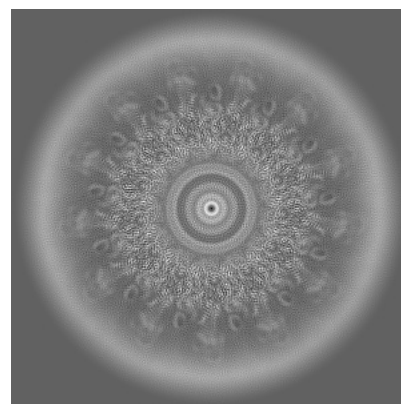
6.1.1 Primary map



X

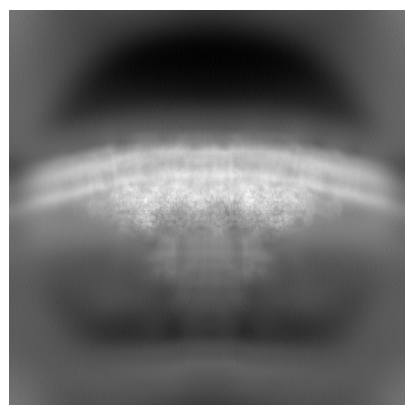


Y

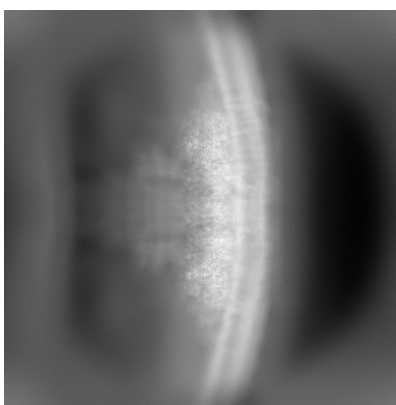


Z

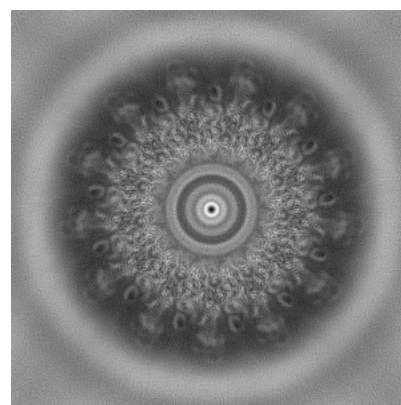
6.1.2 Raw map



X



Y

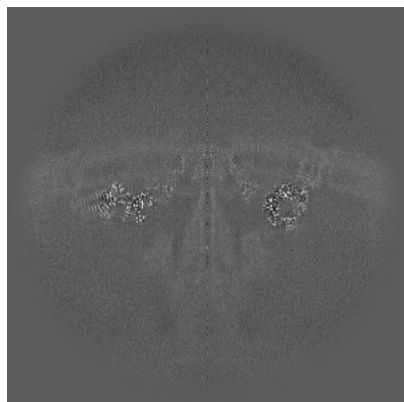


Z

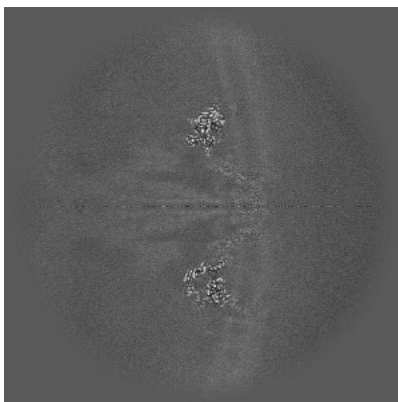
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

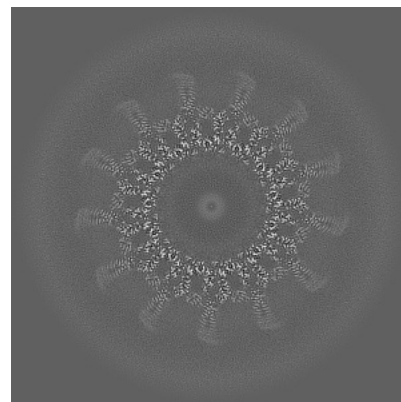
6.2.1 Primary map



X Index: 224

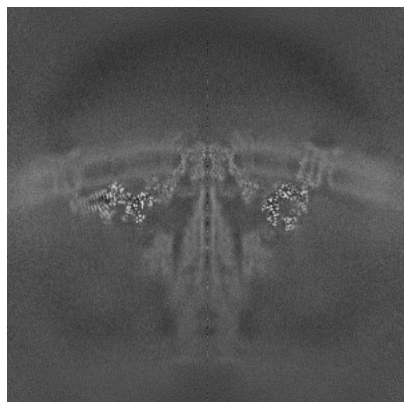


Y Index: 224

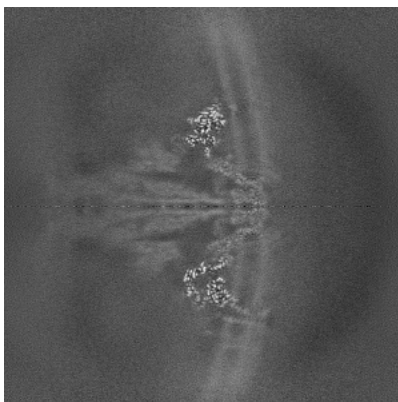


Z Index: 224

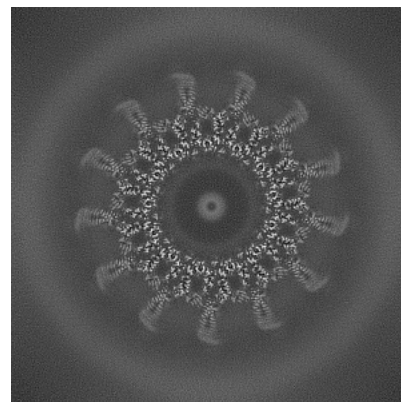
6.2.2 Raw map



X Index: 224



Y Index: 224

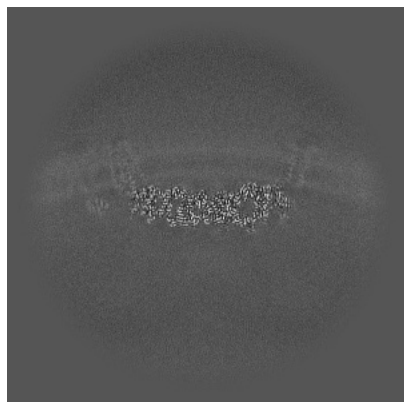


Z Index: 224

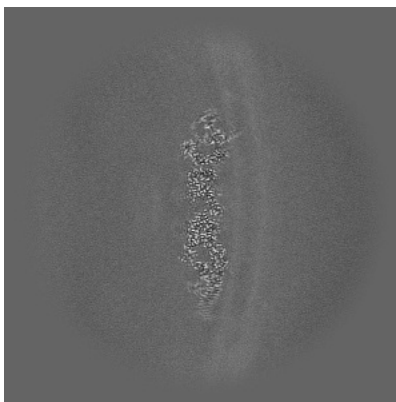
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

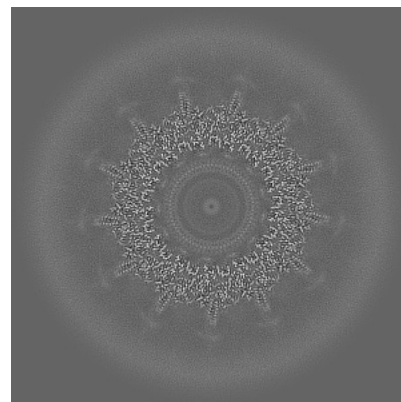
6.3.1 Primary map



X Index: 152

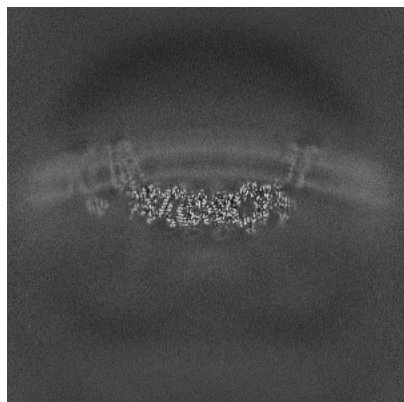


Y Index: 155

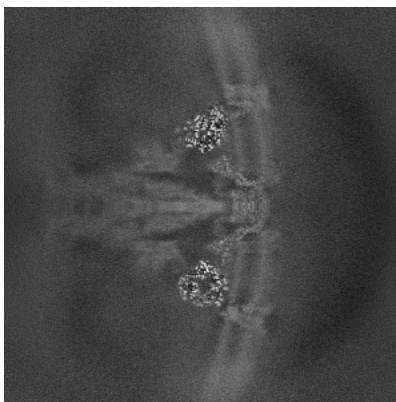


Z Index: 235

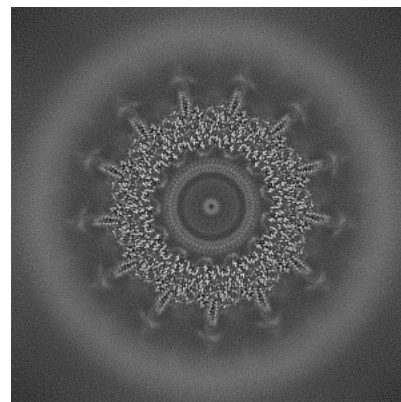
6.3.2 Raw map



X Index: 152



Y Index: 230

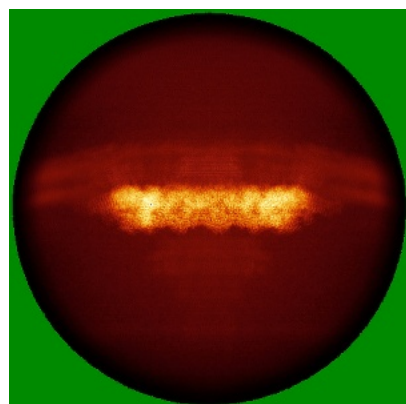


Z Index: 235

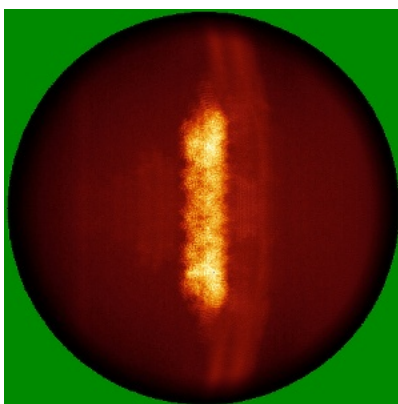
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

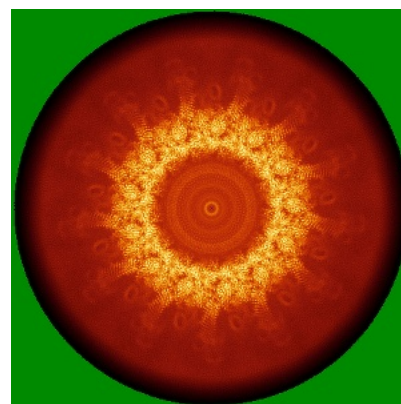
6.4.1 Primary map



X

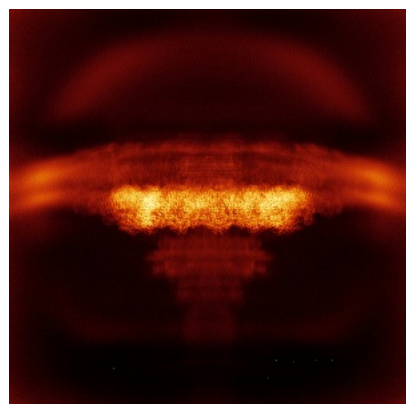


Y

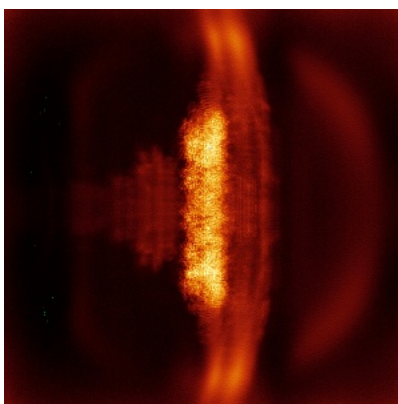


Z

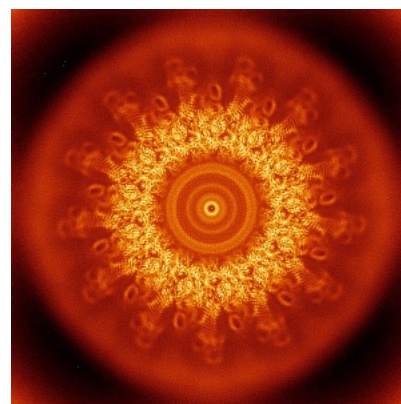
6.4.2 Raw map



X



Y

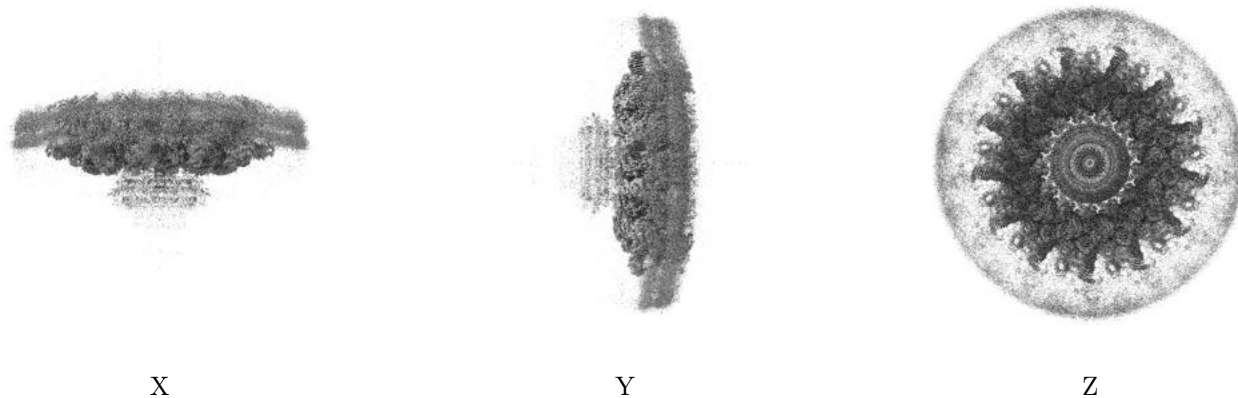


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

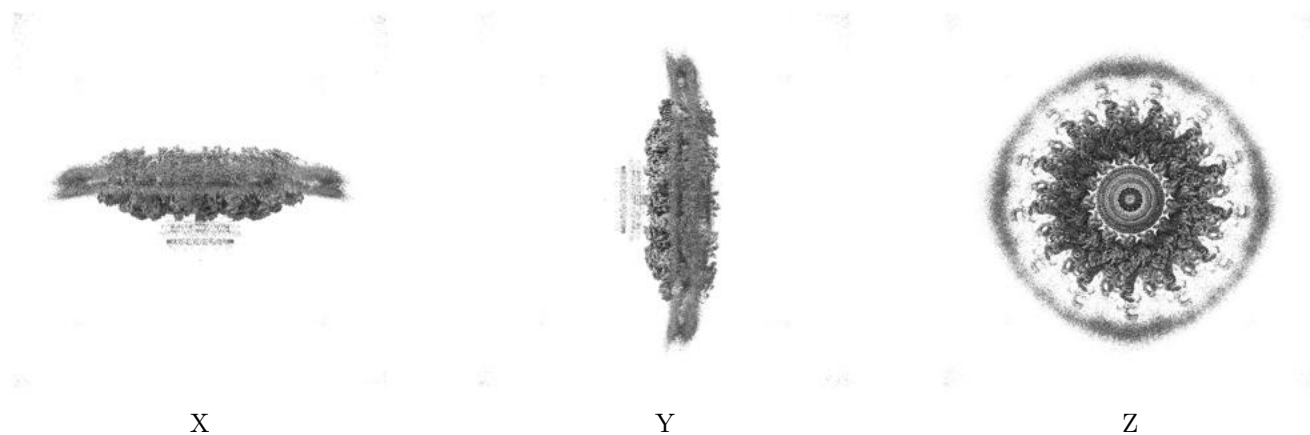
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

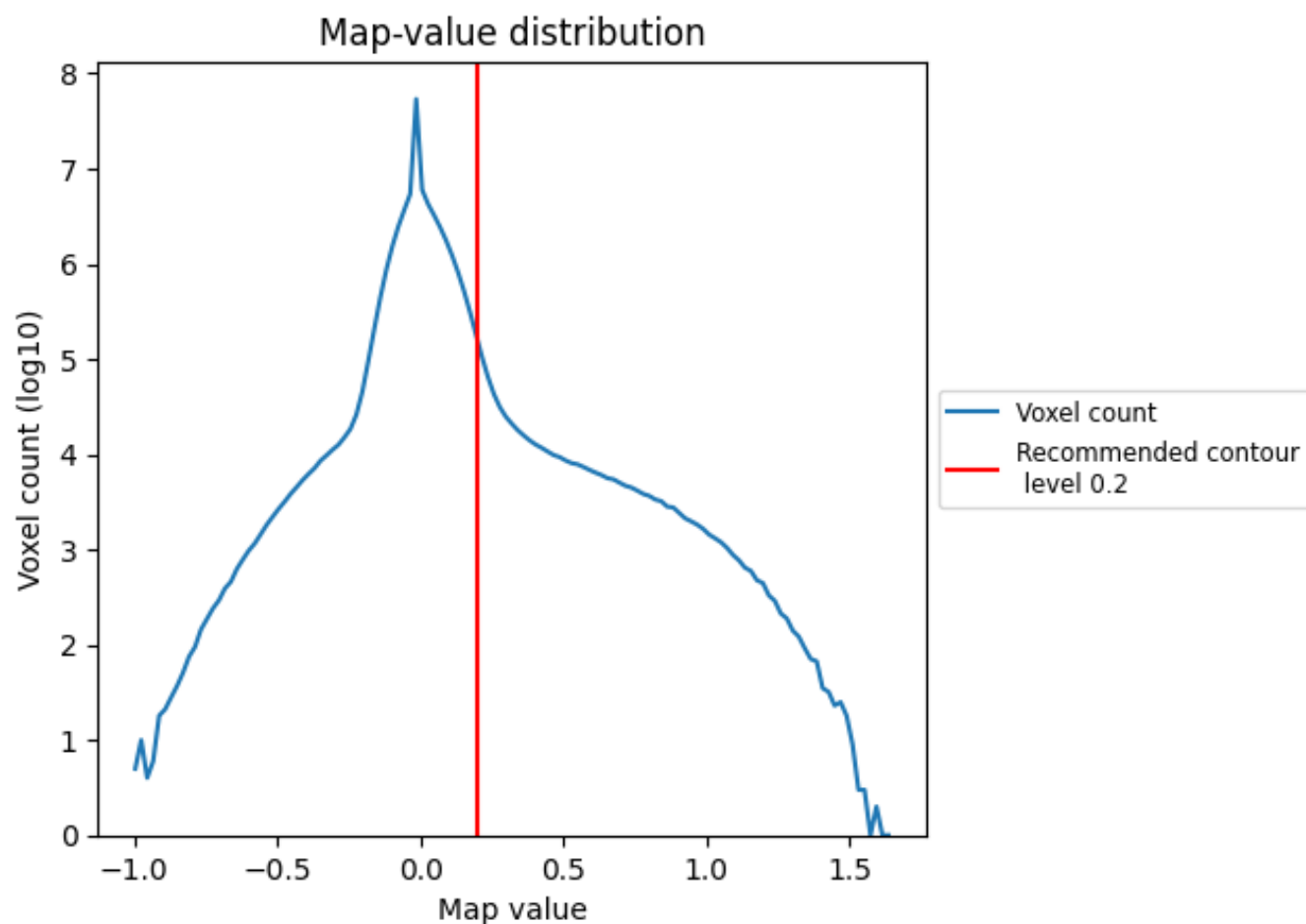
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

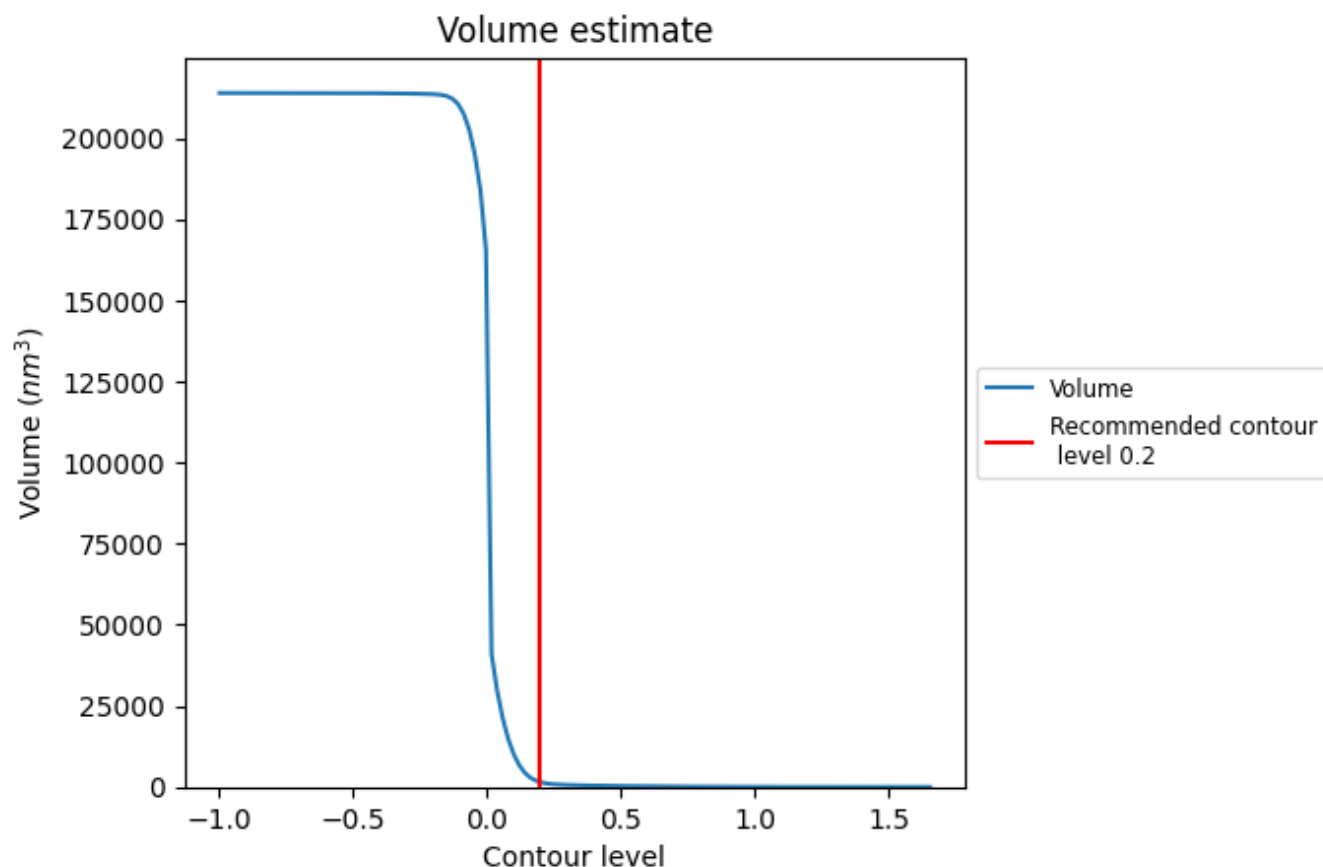
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

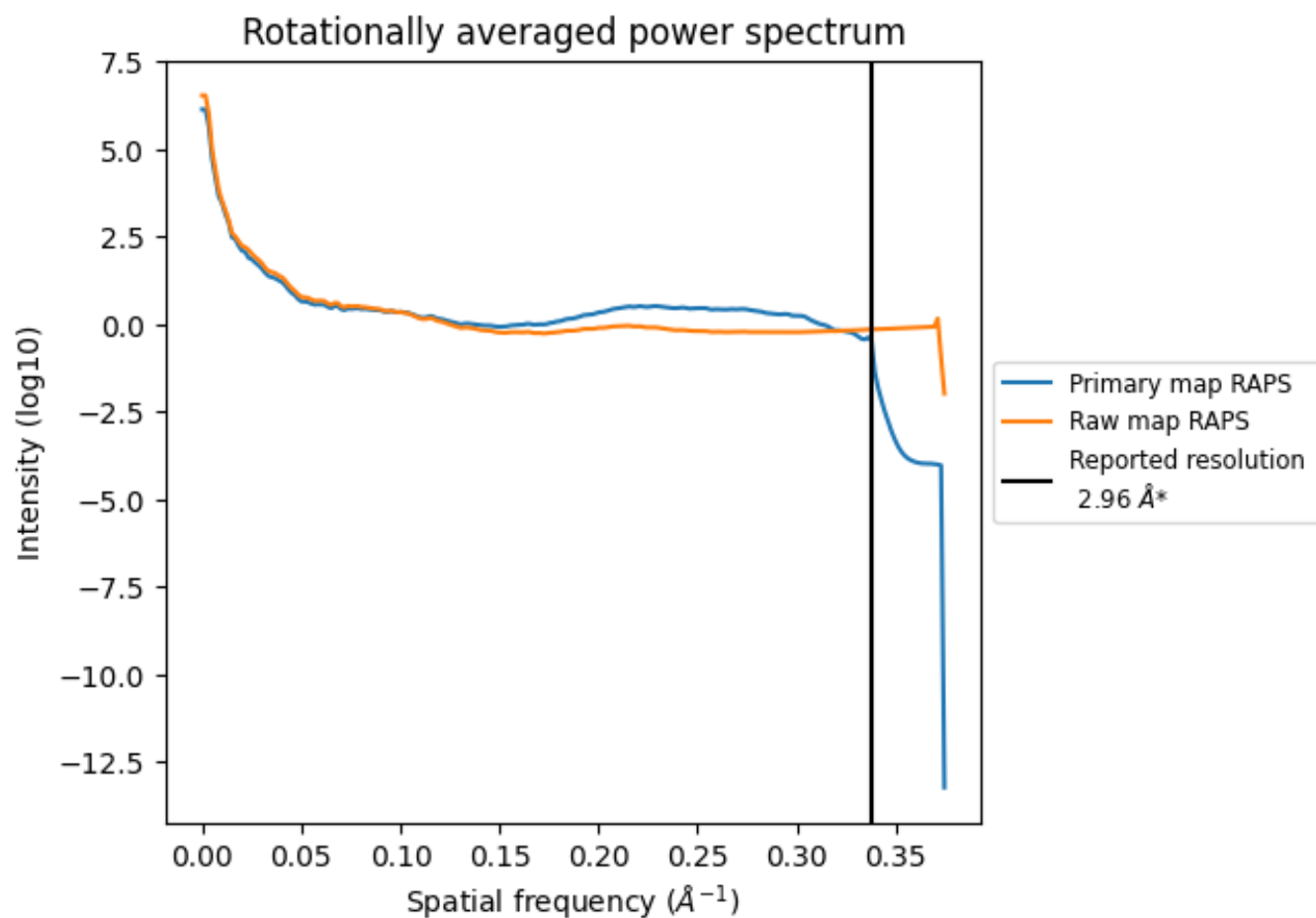
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1548 nm^3 ; this corresponds to an approximate mass of 1398 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

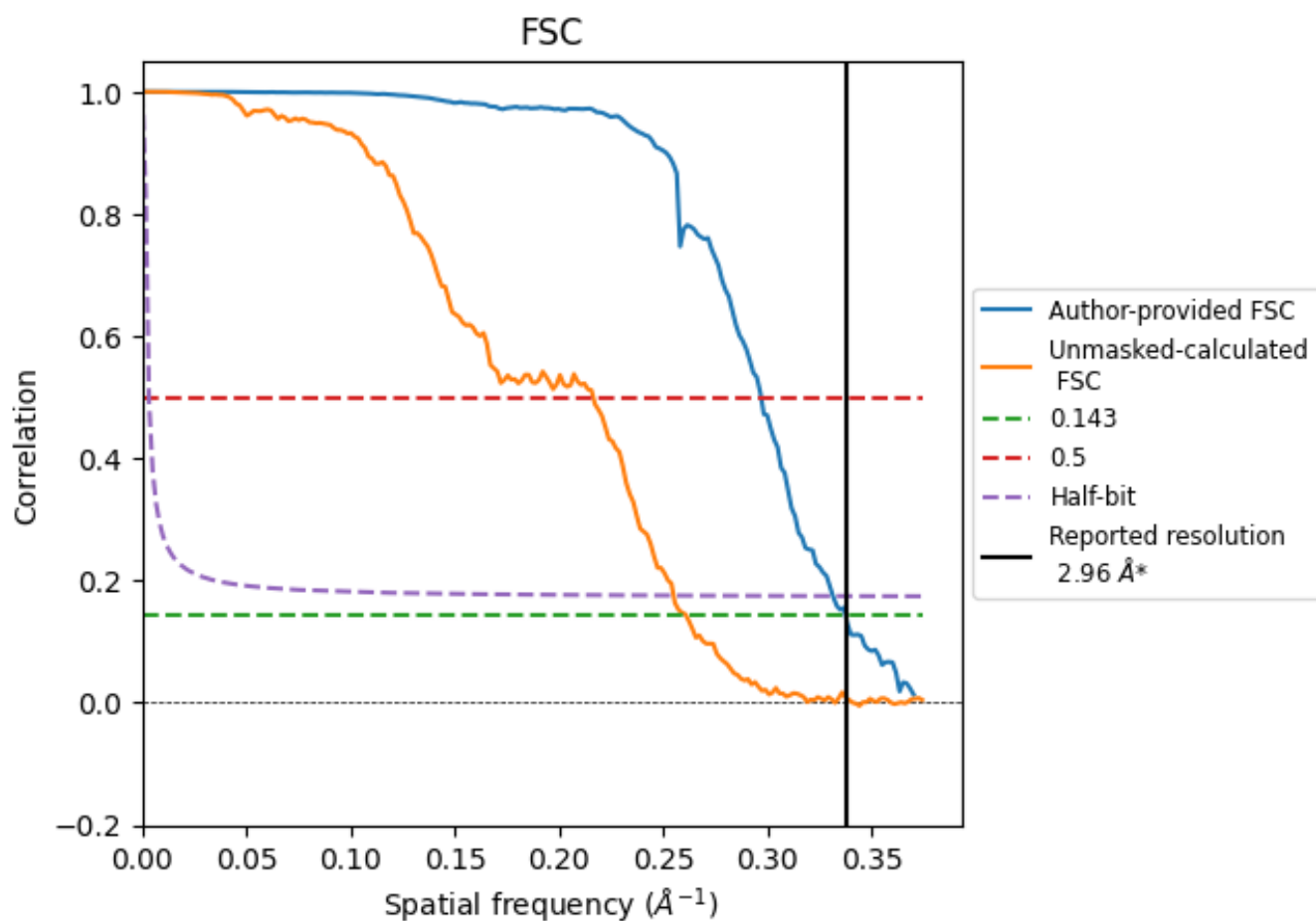


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.338 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.36	3.01
Unmasked-calculated*	3.83	4.62	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49393 and PDB model 9NGU. Per-residue inclusion information can be found in section [3](#) on page [17](#).

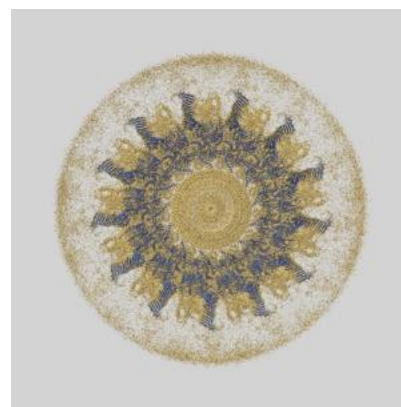
9.1 Map-model overlay [i](#)



X



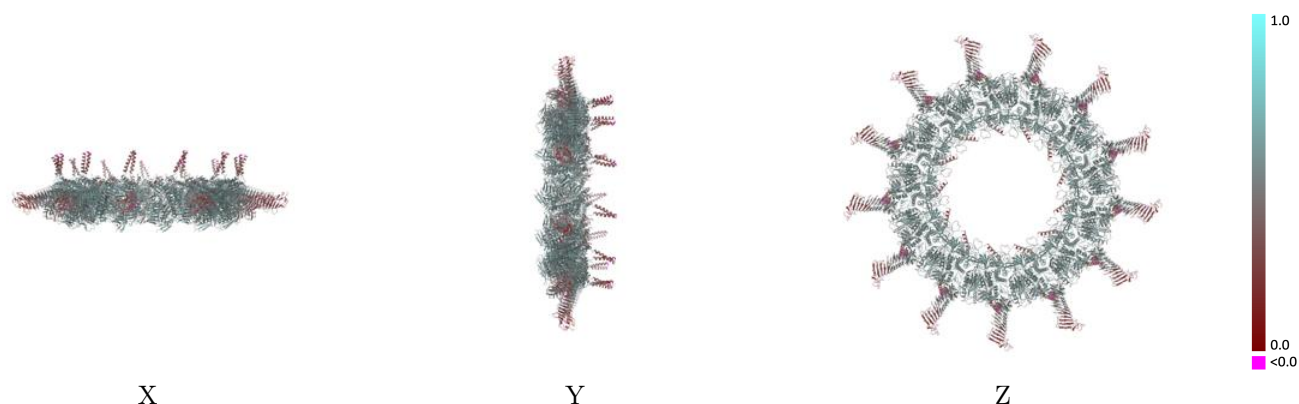
Y



Z

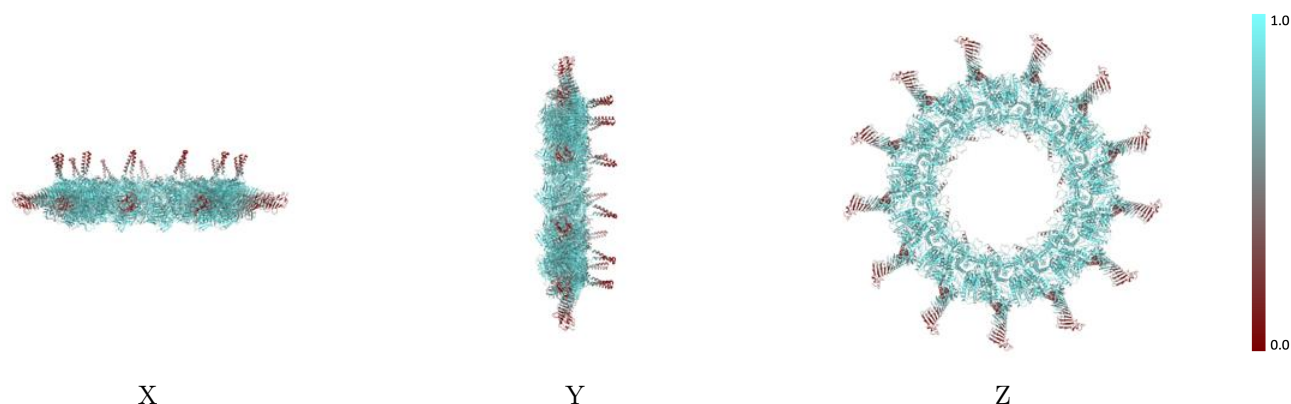
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



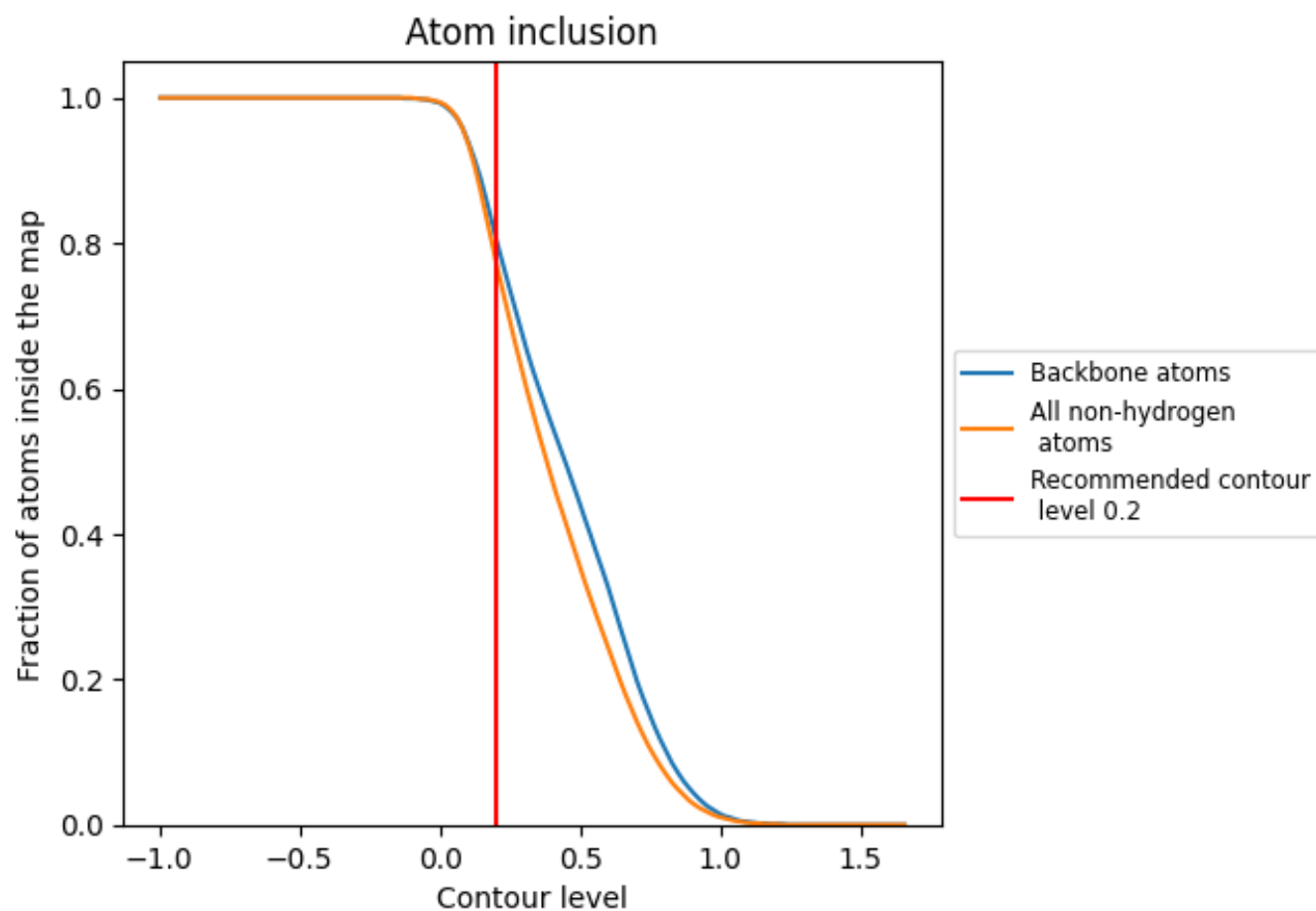
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7750	 0.5120
Aa	 0.8750	 0.5600
Ab	 0.8780	 0.5500
Ac	 0.5520	 0.4120
Ad	 0.8740	 0.5550
Ae	 0.8510	 0.5520
Af	 0.6700	 0.4700
Ag	 0.9370	 0.5980
Ah	 0.7860	 0.5120
Ai	 0.8350	 0.5430
Aj	 0.7040	 0.4820
Ak	 0.8790	 0.5610
Al	 0.8840	 0.5530
Am	 0.5560	 0.4100
An	 0.8720	 0.5540
Ao	 0.8660	 0.5490
Ap	 0.6560	 0.4660
Aq	 0.9260	 0.5920
Ar	 0.7770	 0.5100
As	 0.8350	 0.5400
At	 0.7060	 0.4760
Au	 0.8850	 0.5630
Av	 0.8750	 0.5510
Aw	 0.5490	 0.4080
Ax	 0.8880	 0.5560
Ay	 0.8550	 0.5510
Az	 0.6760	 0.4690
Ba	 0.9310	 0.5910
Bb	 0.7830	 0.5090
Bc	 0.8310	 0.5400
Bd	 0.6980	 0.4780
Be	 0.8750	 0.5610
Bf	 0.8790	 0.5520
Bg	 0.5490	 0.4080
Bh	 0.8760	 0.5510























































































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Chain	Atom inclusion	Q-score
Bi	 0.8600	 0.5550
Bj	 0.6760	 0.4670
Bk	 0.9250	 0.5940
Bl	 0.7840	 0.5130
Bm	 0.8340	 0.5430
Bn	 0.7090	 0.4800
Bo	 0.8710	 0.5610
Bp	 0.8890	 0.5520
Bq	 0.5460	 0.4090
Br	 0.8720	 0.5520
Bs	 0.8590	 0.5540
Bt	 0.6650	 0.4700
Bu	 0.9310	 0.5900
Bv	 0.7800	 0.5080
Bw	 0.8340	 0.5410
Bx	 0.6980	 0.4820
By	 0.8770	 0.5620
Bz	 0.8820	 0.5520
Ca	 0.5520	 0.4050
Cb	 0.8770	 0.5540
Cc	 0.8570	 0.5520
Cd	 0.6700	 0.4720
Ce	 0.9290	 0.5910
Cf	 0.7750	 0.5080
Cg	 0.8340	 0.5410
Ch	 0.6950	 0.4740
Ci	 0.8790	 0.5580
Cj	 0.8900	 0.5500
Ck	 0.5520	 0.4080
Cl	 0.8740	 0.5540
Cm	 0.8610	 0.5480
Cn	 0.6650	 0.4710
Co	 0.9250	 0.5910
Cp	 0.7850	 0.5110
Cq	 0.8340	 0.5420
Cr	 0.6890	 0.4790
Cs	 0.8800	 0.5580
Ct	 0.8860	 0.5520
Cu	 0.5490	 0.4060
Cv	 0.8770	 0.5500
Cw	 0.8630	 0.5500
Cx	 0.6560	 0.4710

























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Chain	Atom inclusion	Q-score
Cy	 0.9160	 0.5900
Cz	 0.7810	 0.5120
Da	 0.8310	 0.5400
Db	 0.7110	 0.4750
Dc	 0.8720	 0.5580
Dd	 0.8820	 0.5490
De	 0.5480	 0.4120
Df	 0.8760	 0.5570
Dg	 0.8540	 0.5490
Dh	 0.6670	 0.4690
Di	 0.9250	 0.5930
Dj	 0.7760	 0.5100
Dk	 0.8360	 0.5440
Dl	 0.7000	 0.4740
Dm	 0.8770	 0.5610
Dn	 0.8730	 0.5510
Do	 0.5520	 0.4100
Dp	 0.8810	 0.5510
Dq	 0.8620	 0.5530
Dr	 0.6560	 0.4700
Ds	 0.9320	 0.5900
Dt	 0.7830	 0.5080
Du	 0.8310	 0.5400
Dv	 0.6890	 0.4810
Dw	 0.8750	 0.5580
Dx	 0.8860	 0.5540
Dy	 0.5550	 0.4140
Dz	 0.8810	 0.5530
Ea	 0.8610	 0.5510
Eb	 0.6580	 0.4690
Ec	 0.9310	 0.5950
Ed	 0.7760	 0.5100
Ee	 0.8310	 0.5410
Ef	 0.7060	 0.4740
Eg	 0.8900	 0.5580
Eh	 0.8730	 0.5510
Ei	 0.5530	 0.4120
Ej	 0.8790	 0.5510
Ek	 0.8570	 0.5540
El	 0.6630	 0.4690
Em	 0.9250	 0.5930
En	 0.7780	 0.5100

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Chain	Atom inclusion	Q-score
Eo	 0.8370	 0.5400
Ep	 0.6890	 0.4760
Eq	 0.8770	 0.5620
Er	 0.8760	 0.5510
Es	 0.5550	 0.4130
Et	 0.8740	 0.5530
Eu	 0.8650	 0.5540
Ev	 0.6610	 0.4680
Ew	 0.9250	 0.5940
Ex	 0.7800	 0.5110
Ey	 0.8350	 0.5430
Ez	 0.6950	 0.4780