



Full wwPDB EM Validation Report ⓘ

Sep 8, 2025 – 12:33 PM EDT

PDB ID : 9NGV / pdb_00009ngv
EMDB ID : EMD-49394
Title : In situ cryo-EM structure of periplasmic ring (PR) of the Legionella Dot/Icm T4SS machine.
Authors : Yue, J.; Jun, L.
Deposited on : 2025-02-22
Resolution : 3.04 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

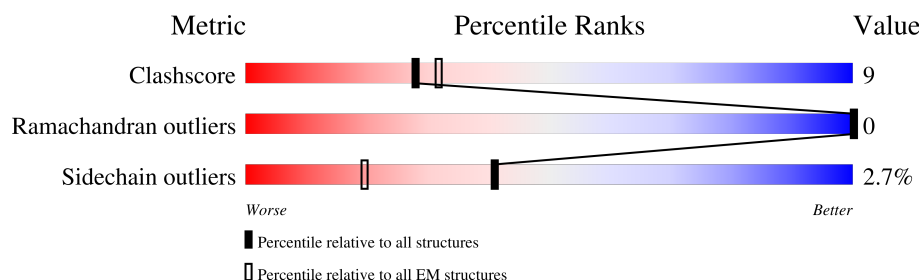
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 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	16	<div> <div>12%</div> <div>69%</div> <div>31%</div> </div>
1	Ah	16	<div> <div>19%</div> <div>81%</div> <div>19%</div> </div>
1	Ao	16	<div> <div>19%</div> <div>62%</div> <div>38%</div> </div>
1	Av	16	<div> <div>6%</div> <div>81%</div> <div>19%</div> </div>
1	Bc	16	<div> <div>12%</div> <div>75%</div> <div>25%</div> </div>
1	Bj	16	<div> <div>6%</div> <div>75%</div> <div>25%</div> </div>
1	Bq	16	<div> <div>6%</div> <div>81%</div> <div>19%</div> </div>
1	Bx	16	<div> <div>19%</div> <div>88%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	Ce	16	
1	Cl	16	
1	Cs	16	
1	Cz	16	
1	Dg	16	
1	Dn	16	
1	Du	16	
1	Eb	16	
1	Ei	16	
1	Ep	16	
2	Ab	9	
2	Ai	9	
2	Ap	9	
2	Aw	9	
2	Bd	9	
2	Bk	9	
2	Br	9	
2	By	9	
2	Cf	9	
2	Cm	9	
2	Ct	9	
2	Da	9	
2	Dh	9	
2	Do	9	
2	Dv	9	

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Mol	Chain	Length	Quality of chain
2	Ec	9	
2	Ej	9	
2	Eq	9	
3	Ac	16	
3	Aj	16	
3	Aq	16	
3	Ax	16	
3	Be	16	
3	Bl	16	
3	Bs	16	
3	Bz	16	
3	Cg	16	
3	Cn	16	
3	Cu	16	
3	Db	16	
3	Di	16	
3	Dp	16	
3	Dw	16	
3	Ed	16	
3	Ek	16	
3	Er	16	
4	Ad	5	
4	Ak	5	
4	Ar	5	
4	Ay	5	














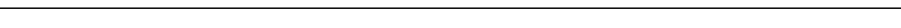

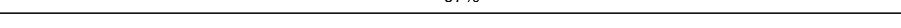
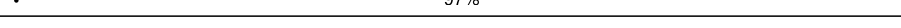
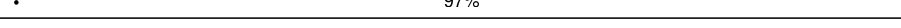
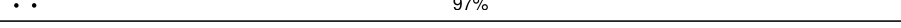
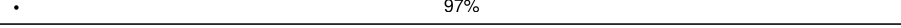
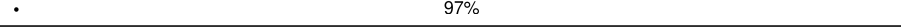
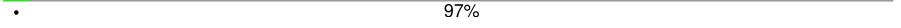
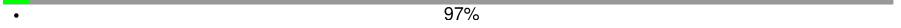
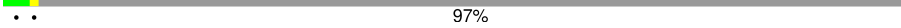
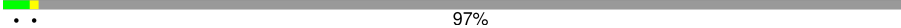
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Mol	Chain	Length	Quality of chain
4	Bf	5	
4	Bm	5	
4	Bt	5	
4	Ca	5	
4	Ch	5	
4	Co	5	
4	Cv	5	
4	Dc	5	
4	Dj	5	
4	Dq	5	
4	Dx	5	
4	Ee	5	
4	El	5	
4	Es	5	
5	Ae	269	
5	Al	269	
5	As	269	
5	Az	269	
5	Bg	269	
5	Bn	269	
5	Bu	269	
5	Cb	269	
5	Ci	269	
5	Cp	269	
5	Cw	269	















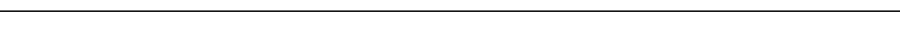
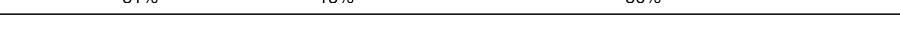


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Mol	Chain	Length	Quality of chain
5	Dd	269	 19% 5% 77%
5	Dk	269	 18% 5% 77%
5	Dr	269	 19% 5% 77%
5	Dy	269	 18% 5% 77%
5	Ef	269	 18% 5% 77%
5	Em	269	 18% 5% 77%
5	Et	269	 19% 5% 77%
6	Af	1048	 97%
6	Am	1048	 97%
6	At	1048	 97%
6	Ba	1048	 97%
6	Bh	1048	 97%
6	Bo	1048	 97%
6	Bv	1048	 97%
6	Cc	1048	 97%
6	Cj	1048	 97%
6	Cq	1048	 97%
6	Cx	1048	 97%
6	De	1048	 97%
6	Dl	1048	 97%
6	Ds	1048	 97%
6	Dz	1048	 97%
6	Eg	1048	 97%
6	En	1048	 97%
6	Eu	1048	 97%

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Mol	Chain	Length	Quality of chain
7	Ag	361	 33% 10% 56%
7	An	361	 35% 9% 56%
7	Au	361	 34% 10% 56%
7	Bb	361	 36% 9% 56%
7	Bi	361	 35% 9% 56%
7	Bp	361	 32% 12% 56%
7	Bw	361	 37% 7% 56%
7	Cd	361	 34% 10% 56%
7	Ck	361	 37% 7% 56%
7	Cr	361	 34% 9% 56%
7	Cy	361	 35% 9% 56%
7	Df	361	 34% 9% 56%
7	Dm	361	 35% 9% 56%
7	Dt	361	 34% 9% 56%
7	Ea	361	 31% 13% 56%
7	Eh	361	 35% 9% 56%
7	Eo	361	 34% 10% 56%
7	Ev	361	 36% 8% 56%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 42066 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 unknown peptide A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Ah	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Ao	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Av	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Bc	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Bj	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Bq	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Bx	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Ce	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Cl	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Cs	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Cz	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Dg	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Dn	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Du	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Eb	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Ei	16	Total	C	N	O	S	0	0
			117	71	20	25	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ep	16	Total	C	N	O	S	0	0
			117	71	20	25	1		

- Molecule 2 is a protein called unknown peptide B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Ai	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Ap	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Aw	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Bd	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Bk	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Br	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	By	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Cf	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Cm	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Ct	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Da	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Dh	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Do	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Dv	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Ec	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Ej	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Eq	9	Total	C	N	O	S	0	0
			61	35	12	12	2		

- Molecule 3 is a protein called unknown peptide C.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Ac	16	Total	C	N	O	0	0
			125	78	21	26		
3	Aj	16	Total	C	N	O	0	0
			125	78	21	26		
3	Aq	16	Total	C	N	O	0	0
			125	78	21	26		
3	Ax	16	Total	C	N	O	0	0
			125	78	21	26		
3	Be	16	Total	C	N	O	0	0
			125	78	21	26		
3	Bl	16	Total	C	N	O	0	0
			125	78	21	26		
3	Bs	16	Total	C	N	O	0	0
			125	78	21	26		
3	Bz	16	Total	C	N	O	0	0
			125	78	21	26		
3	Cg	16	Total	C	N	O	0	0
			125	78	21	26		
3	Cn	16	Total	C	N	O	0	0
			125	78	21	26		
3	Cu	16	Total	C	N	O	0	0
			125	78	21	26		
3	Db	16	Total	C	N	O	0	0
			125	78	21	26		
3	Di	16	Total	C	N	O	0	0
			125	78	21	26		
3	Dp	16	Total	C	N	O	0	0
			125	78	21	26		
3	Dw	16	Total	C	N	O	0	0
			125	78	21	26		
3	Ed	16	Total	C	N	O	0	0
			125	78	21	26		
3	Ek	16	Total	C	N	O	0	0
			125	78	21	26		
3	Er	16	Total	C	N	O	0	0
			125	78	21	26		

- Molecule 4 is a protein called unknown peptide D.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Ad	5	Total	C	N	O	0	0
			36	23	5	8		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	Ak	5	Total	C	N	O	0	0
			36	23	5	8		
4	Ar	5	Total	C	N	O	0	0
			36	23	5	8		
4	Ay	5	Total	C	N	O	0	0
			36	23	5	8		
4	Bf	5	Total	C	N	O	0	0
			36	23	5	8		
4	Bm	5	Total	C	N	O	0	0
			36	23	5	8		
4	Bt	5	Total	C	N	O	0	0
			36	23	5	8		
4	Ca	5	Total	C	N	O	0	0
			36	23	5	8		
4	Ch	5	Total	C	N	O	0	0
			36	23	5	8		
4	Co	5	Total	C	N	O	0	0
			36	23	5	8		
4	Cv	5	Total	C	N	O	0	0
			36	23	5	8		
4	Dc	5	Total	C	N	O	0	0
			36	23	5	8		
4	Dj	5	Total	C	N	O	0	0
			36	23	5	8		
4	Dq	5	Total	C	N	O	0	0
			36	23	5	8		
4	Dx	5	Total	C	N	O	0	0
			36	23	5	8		
4	Ee	5	Total	C	N	O	0	0
			36	23	5	8		
4	El	5	Total	C	N	O	0	0
			36	23	5	8		
4	Es	5	Total	C	N	O	0	0
			36	23	5	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ae	63	Total	C	N	O	S	0	0
			484	308	84	91	1		
5	Al	63	Total	C	N	O	S	0	0
			484	308	84	91	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	As	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Az	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Bg	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Bn	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Bu	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Cb	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Ci	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Cp	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Cw	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Dd	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Dk	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Dr	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Dy	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Ef	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Em	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Et	63	Total 484	C 308	N 84	O 91	S 1	0	0

- Molecule 6 is a protein called IcmE (DotG).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Af	34	Total 276	C 168	N 47	O 60	S 1	0	0
6	Am	34	Total 276	C 168	N 47	O 60	S 1	0	0
6	At	34	Total 276	C 168	N 47	O 60	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	Ba	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	Bh	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	Bo	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	Bv	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	Cc	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	Cj	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	Cq	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	Cx	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	De	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	Dl	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	Ds	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	Dz	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	Eg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	En	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
6	Eu	34	Total	C	N	O	S	0	0
			276	168	47	60	1		

- Molecule 7 is a protein called IcmK (DotH).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ag	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	An	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Au	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Bb	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		

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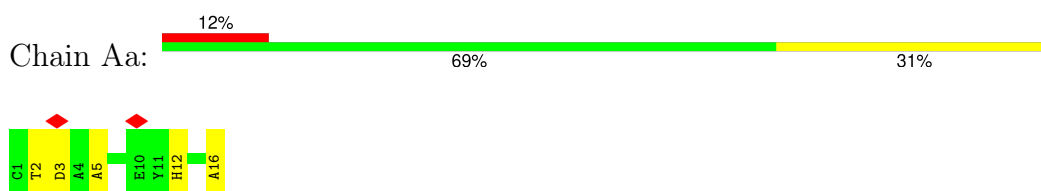
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Mol	Chain	Residues	Atoms					AltConf	Trace
7	Bi	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Bp	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Bw	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Cd	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Ck	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Cr	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Cy	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Df	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Dm	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Dt	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Ea	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Eh	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Eo	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
7	Ev	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		

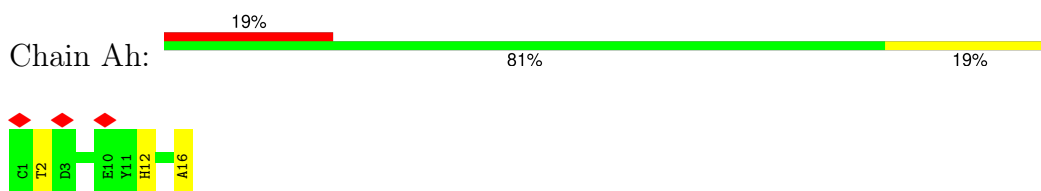
3 Residue-property plots [i](#)

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.

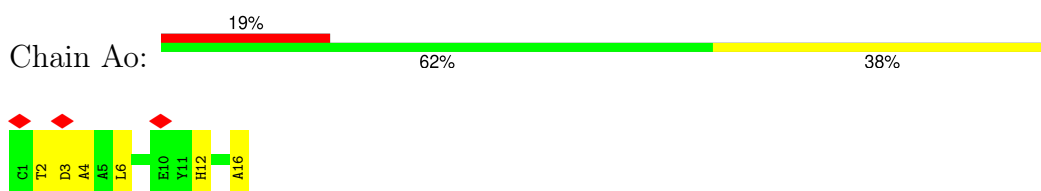
- Molecule 1: unknown peptide A



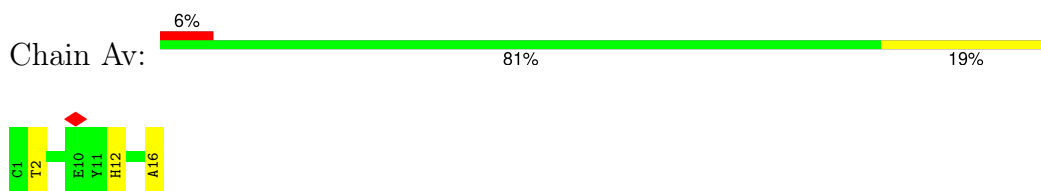
- Molecule 1: unknown peptide A



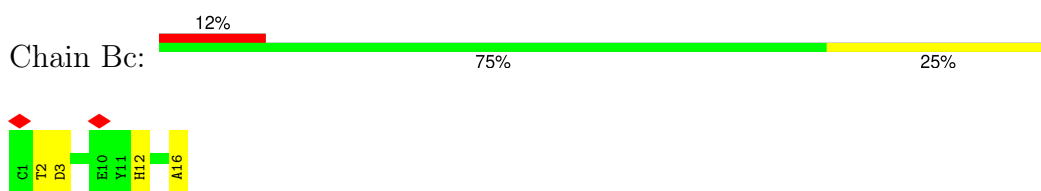
- Molecule 1: unknown peptide A



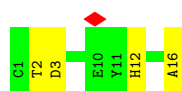
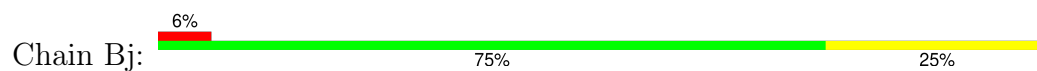
- Molecule 1: unknown peptide A



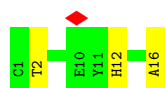
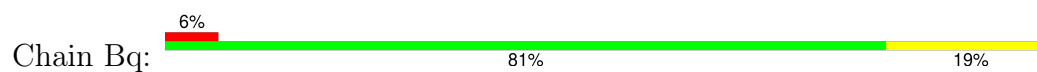
- Molecule 1: unknown peptide A



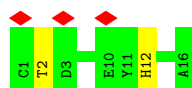
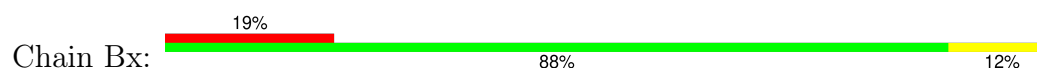
- Molecule 1: unknown peptide A



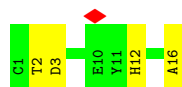
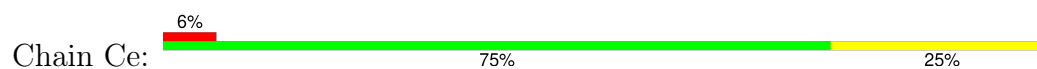
- Molecule 1: unknown peptide A



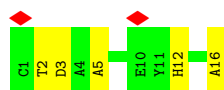
- Molecule 1: unknown peptide A



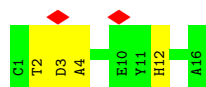
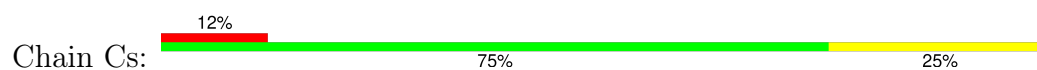
- Molecule 1: unknown peptide A



- Molecule 1: unknown peptide A

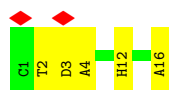


- Molecule 1: unknown peptide A

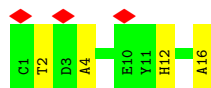
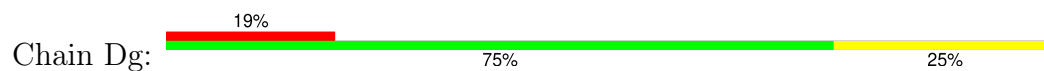


- Molecule 1: unknown peptide A

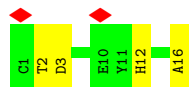
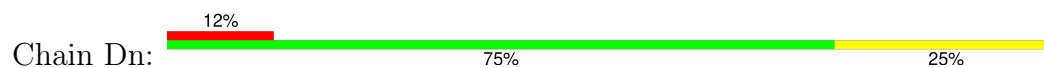




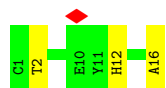
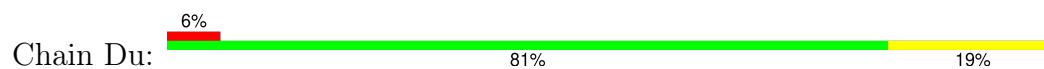
- Molecule 1: unknown peptide A



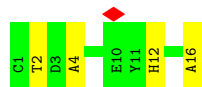
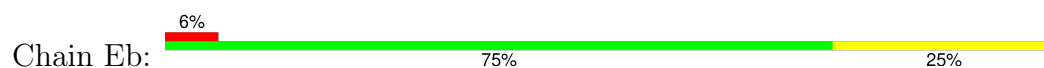
- Molecule 1: unknown peptide A



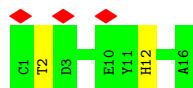
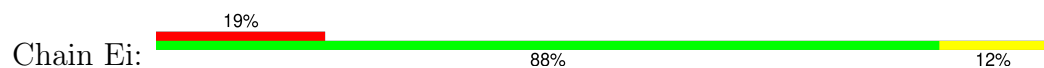
- Molecule 1: unknown peptide A



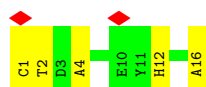
- Molecule 1: unknown peptide A



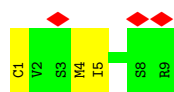
- Molecule 1: unknown peptide A



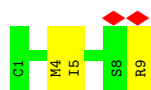
- Molecule 1: unknown peptide A



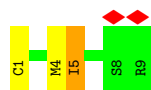
- Molecule 2: unknown peptide B



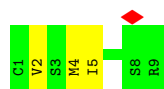
- Molecule 2: unknown peptide B



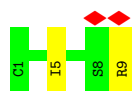
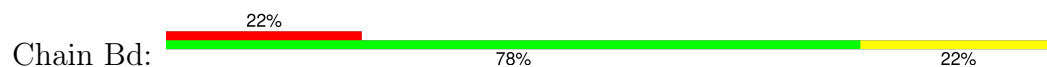
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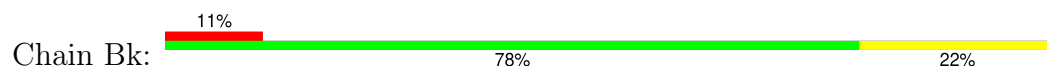
- Molecule 2: unknown peptide B



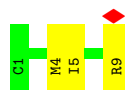
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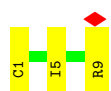
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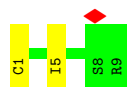
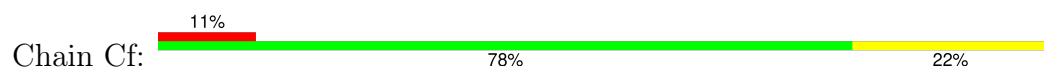
- Molecule 2: unknown peptide B



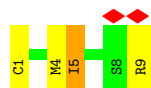
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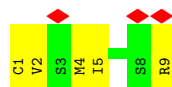
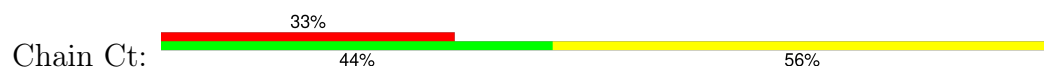
- Molecule 2: unknown peptide B



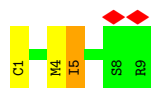
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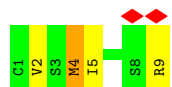
- Molecule 2: unknown peptide B



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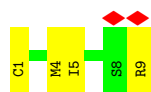


- Molecule 2: unknown peptide B

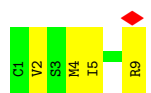


- Molecule 2: unknown peptide B

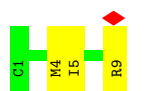




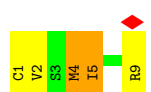
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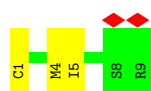
- Molecule 2: unknown peptide B



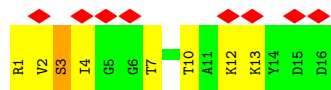
- Molecule 2: unknown peptide B



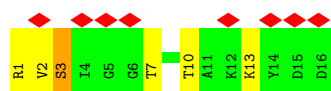
- Molecule 2: unknown peptide B



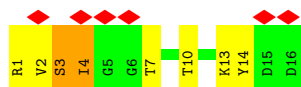
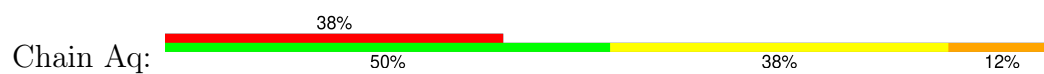
- Molecule 3: unknown peptide C



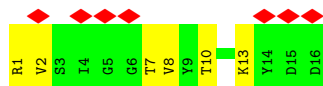
- Molecule 3: unknown peptide C



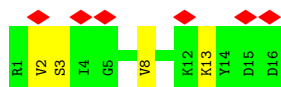
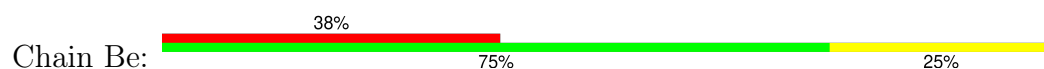
- Molecule 3: unknown peptide C



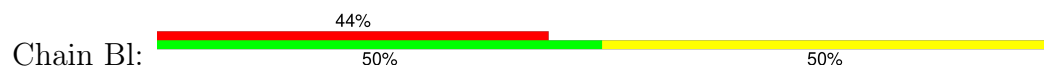
- Molecule 3: unknown peptide C



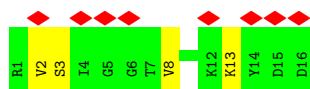
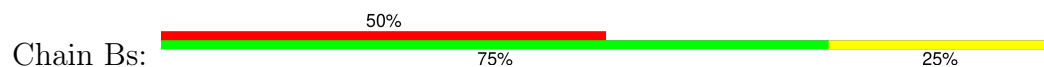
- Molecule 3: unknown peptide C



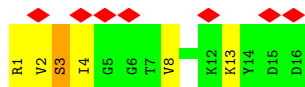
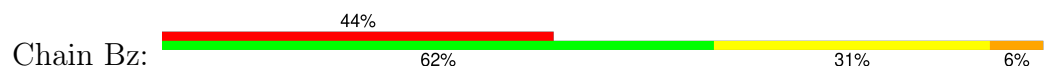
- Molecule 3: unknown peptide C



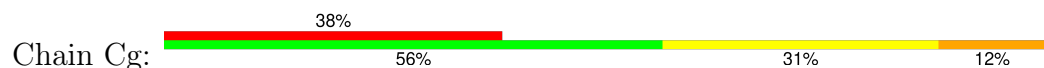
- Molecule 3: unknown peptide C

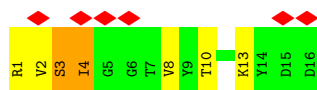


- Molecule 3: unknown peptide C

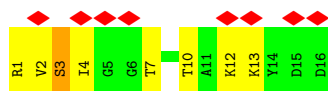


- Molecule 3: unknown peptide C

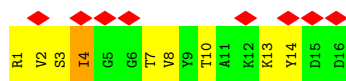




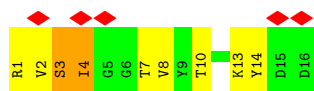
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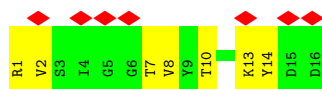
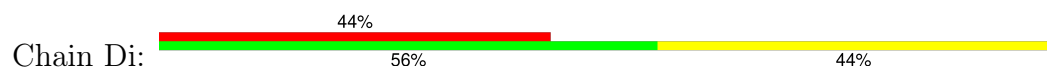
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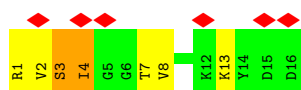
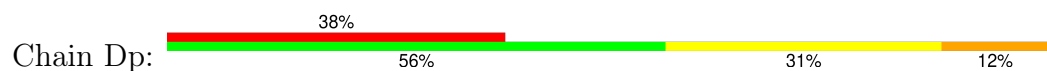
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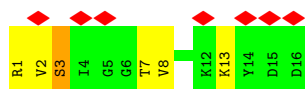
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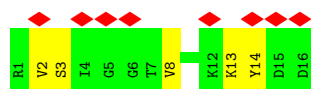
- Molecule 3: unknown peptide C



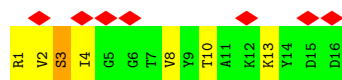
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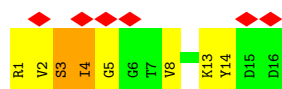
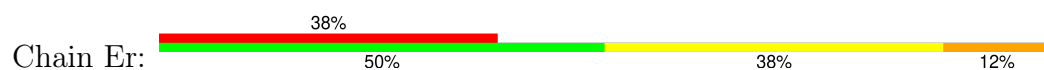
- Molecule 3: unknown peptide C



- Molecule 3: unknown peptide C



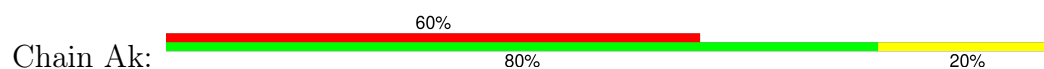
- Molecule 3: unknown peptide C



- Molecule 4: unknown peptide D



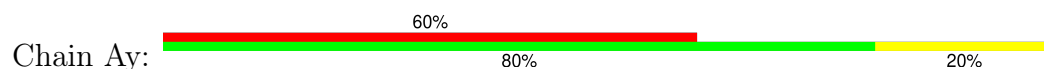
- Molecule 4: unknown peptide D



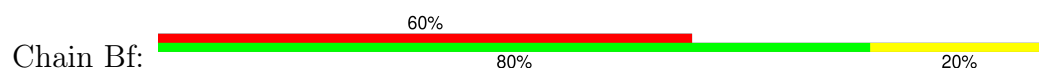
- Molecule 4: unknown peptide D



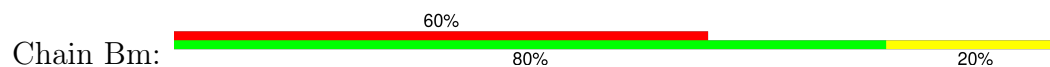
- Molecule 4: unknown peptide D



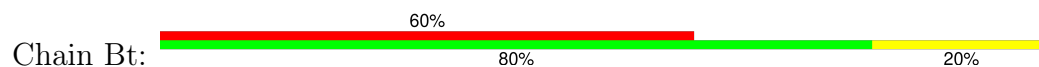
- Molecule 4: unknown peptide D



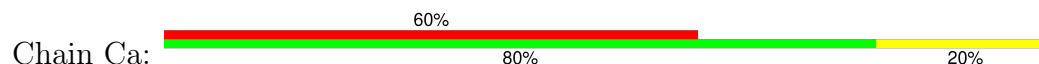
- Molecule 4: unknown peptide D



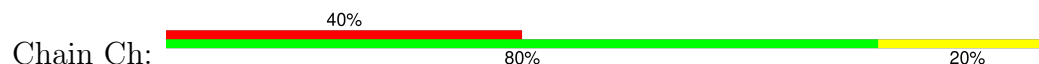
- Molecule 4: unknown peptide D



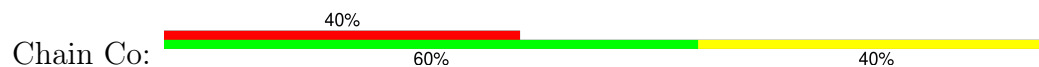
- Molecule 4: unknown peptide D



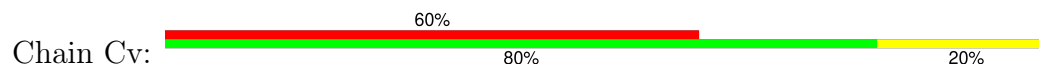
- Molecule 4: unknown peptide D



- Molecule 4: unknown peptide D



- Molecule 4: unknown peptide D



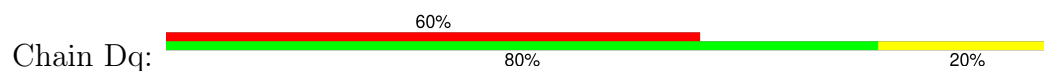
- Molecule 4: unknown peptide D



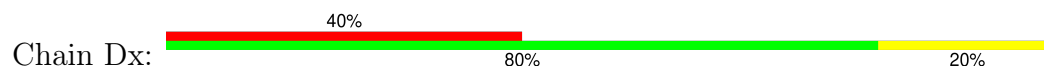
- Molecule 4: unknown peptide D



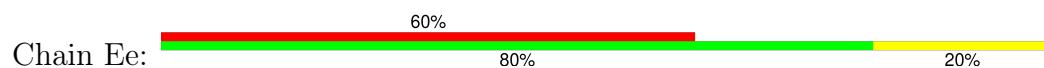
- Molecule 4: unknown peptide D



- Molecule 4: unknown peptide D



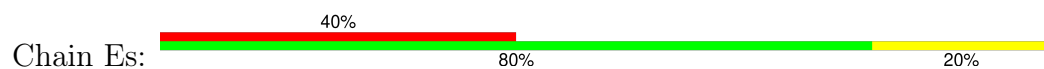
- Molecule 4: unknown peptide D



- Molecule 4: unknown peptide D



- Molecule 4: unknown peptide D



- Molecule 5: IcmG (DotF)

Response	Percentage
Yes, the U.S. is a democracy	19%
No, the U.S. is not a democracy	5%
Don't know	77%

- Molecule 5: IcmG (DotF)

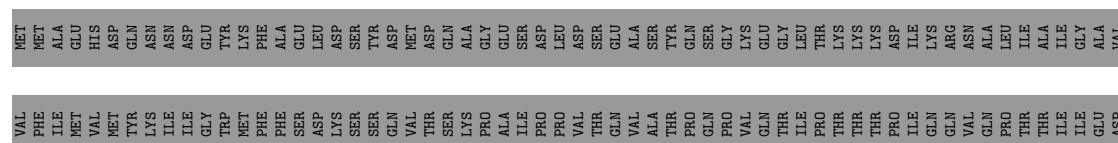
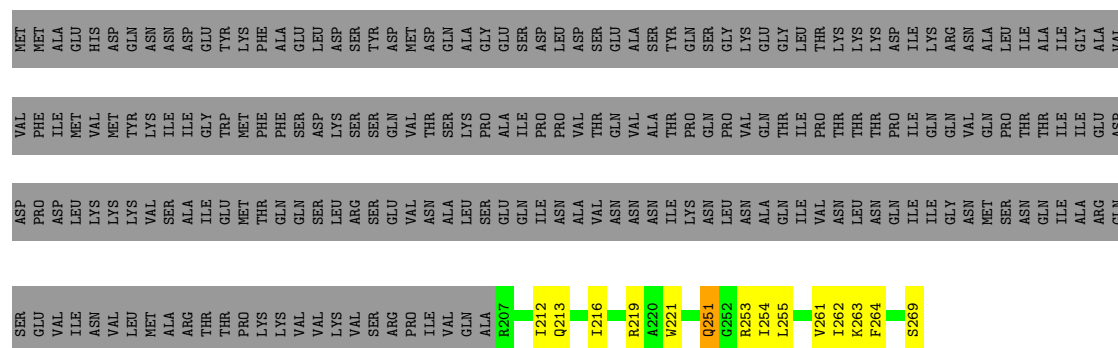
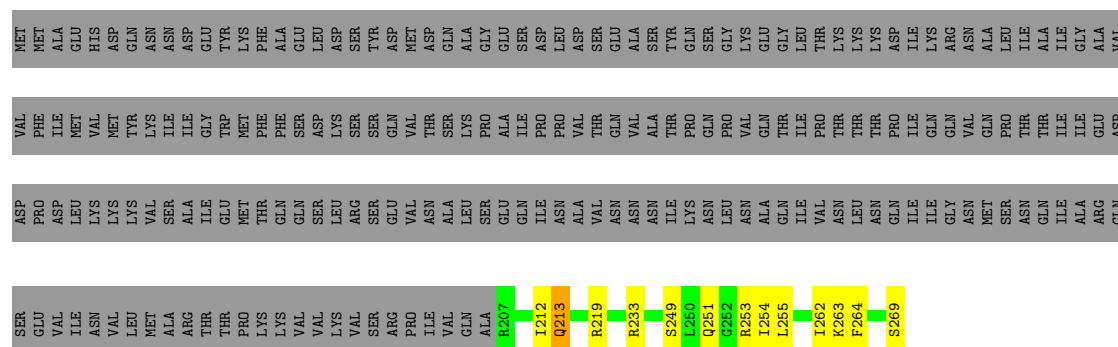
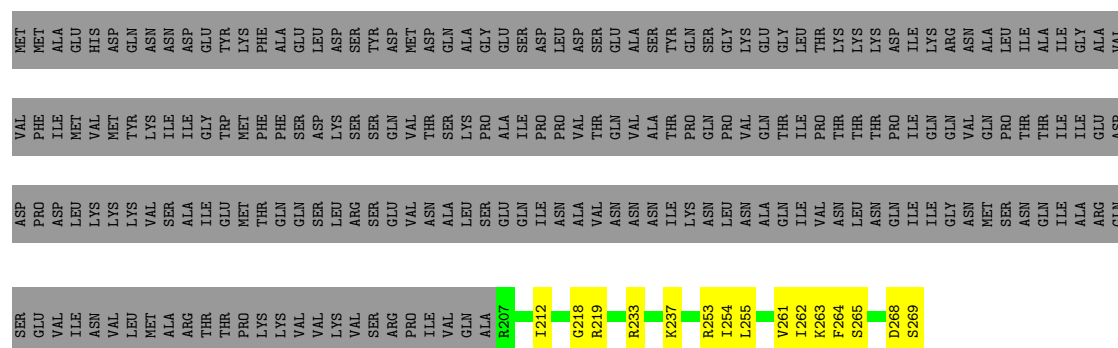
Device Type	Percentage
Smartphones	19%
Tablets	5%
Other mobile devices	77%

- Molecule 5: IcmG (DotF)

Response	Percentage
Yes	19%
No	5%
Don't know	77%

- Molecule 5: IcmG (DotF)

Response	Percentage
Yes, the U.S. is a democracy	18%
No, the U.S. is not a democracy	6%
Don't know	77%



- Molecule 5: IcmG (DotF)



SER	ASP	VAL	MET
GJU	PRO	PHE	MET
VAL	ASP	ILE	ALA
ILE	LEU	MET	GLU
ASN	LYS	VAL	HIS
VAL	LYS	MET	ASP
LEU	LYS	TYR	GLN
MET	VAL	LYS	ASN
ALA	SER	ILE	ASN
ARG	ALA	ILE	ASP
THR	ILE	GLY	GIJ
THR	GLI	TRP	TYR
PRO	MET	MET	LYS
LYS	THR	PHE	PHE
LYS	GLN	PHE	ALA
VAL	GLN	SER	GLU
VAL	SER	ASP	LEU
LYS	LEU	LYS	ASP
VAL	ARG	SER	SER
SER	SER	SER	TYR
ARG	GIJ	GLN	ASP
PRO	VAL	VAL	MET
ILE	ASN	THR	ASP
ILE	ALA	SER	GLN
GLN	LEU	LYS	ALA
R207	SER	PRO	GLY
L212	GLN	ILE	SER
L219	ILE	PRO	ASP
L233	ASN	PRO	LEU
L250	ALA	VAL	SER
R253	ASN	VAL	ALA
L254	ASN	GLN	SER
L255	LEU	THR	GLN
L261	ASN	PRO	GLY
L262	ASN	VAL	LYS
K263	ALA	GLN	LYS
F264	GLN	THR	GLY
D268	ILE	ILE	GLY
S269	ASN	THR	LYS
	GLN	PRO	LYS
	ILE	ILE	ASP
	ILE	GLN	LYS
	GLY	VAL	ARG
	ASN	GLN	ASN
	MET	GLN	ALA
	SER	PRO	LEU
	ASN	THR	ALA
	GLN	THR	ILE
	ILE	ILE	ILE
	GLY	ILE	GLY
	ASN	ILE	ALA
	ARG	GLU	ALA

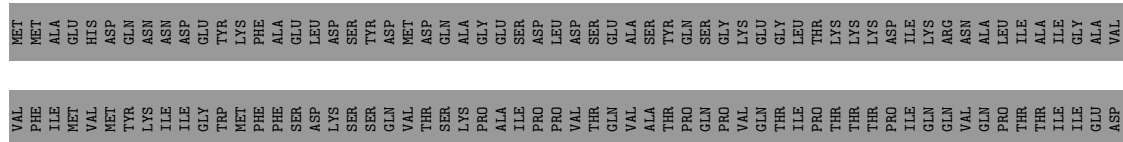
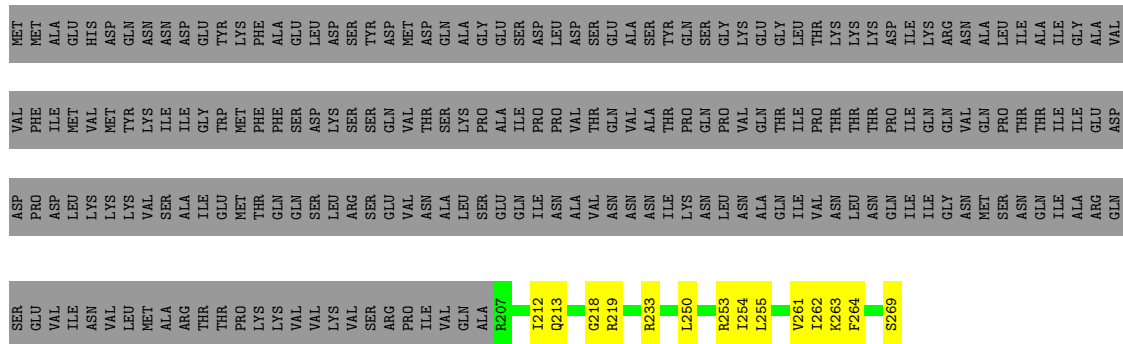
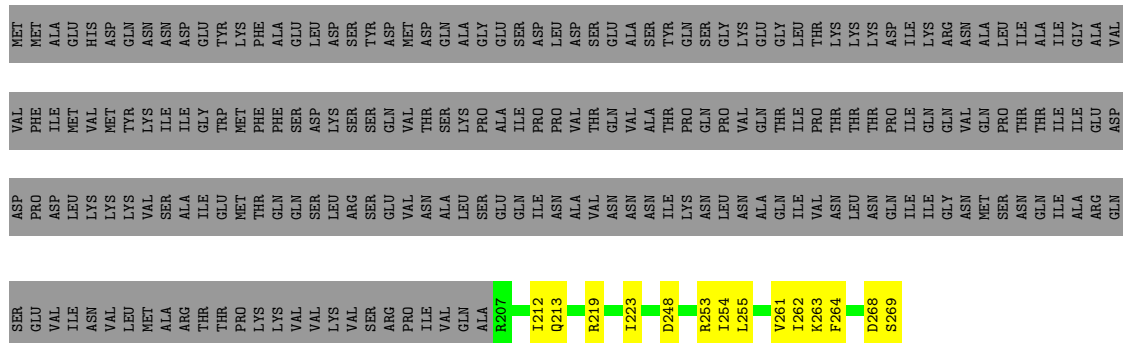
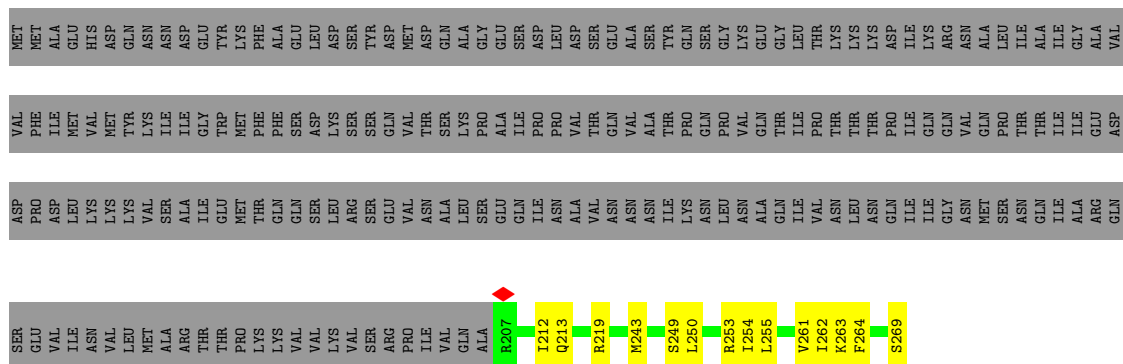
- Molecule 5: IcmG (DotF)

[illegible]

- Molecule 5: IcmG (DotF)

[illegible]

- Molecule 5: IcmG (DotF)



- Molecule 6: IcmE (DotG)

Chain Af: 97%

[illegible]

- Molecule 6: IcmE (DotG)

Chain At: 97%

[illegible]

THR	GLN	ASP	VAL	THR	THR	ILE	GLY	THR	THR	GLY	ASN	ASN	ILE	VAL	VAL	ALA	ALA	ASN	GLY	VAL	GLY	ARG	SER	THR	LEU	GLU	ASN	ALA	VAL	ILE	GLY	LEU	ALA	THR	THR	VAL	GLY	LYS	ALA	SER	SER	GLN	GLN	ALA	GLN	GLN	LEU	PHE	ASN	THR	THR	PRO	THR	THR	VAL	GLU	VAL	THR	TTR	VAL	GLY	SER	GLY	GLY	GLY	LEU	ILE	LEU	PHE
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- Molecule 6: IcmE (DotG)

Chain Bh:  97%

[illegible]

THR	GLN	ASP	VAL	THR	THR	ILE	GLY	GLY	THR	GLY	ASN	ASN	ILE	THR	VAL	ALA	ALA	ASN	GLY	VAL	GLY	ARG	SER	THR	LEU	GLU	ASN	ALA	VAL	ILE	GLY	LEU	ALA	THR	VAL	GLY	LYS	SER	GLN	GLN	ALA	GLN	GLN	GLN	LEU	PHE	ASN	THR	PRO	THR	THR	THR	VAL	GLU	VAL	VAL	TYR	SER	GLY	THR	GLY	LEU	ILE	GLY	LEU	PHE
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- Molecule 6: IcmE (DotG)

Chain Bo: 97%

[illegible]

- Molecule 6: IcmE (DotG)

Chain Bv:  97%

[illegible]

PHE	THR	GLN	ASP	VAL	THR	THR	ILE	THR	GLY	ASN	ASN	ILE	THR	VAL	ALA	ASN	GLY	VAL	GLY	ARG	SER	THR	THR	LEU	GLU	ASN	ALA	VAL	ILE	GLY	GLY	ALA	GLN	THR	VAL	GLY	LYS	ALA	TRP	SER	SER	GLN	GLN	GLN	GLN	LEU	PHE	ASN	THR	PRO	THR	THR	THR	VAL	GLU	VAL	THR	GLY	GLY	ILE	LEU
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- Molecule 6: IcmE (DotG)

Chain Cc: 97%

[illegible]

ASP	VAL	THR	THR	ILE	THR	GLY	ASN	ILE	THR	THR	VAL	ALA	ASN	GLY	VAL	ARG	GLY	SER	THR	LEU	GLU	ASN	ALA	VAL	ILE	GLY	LEU	ALA	THR	THR	VAL	GLY	LYS	ALA	SER	GLN	GLN	ALA	GLN	GLN	LEU	PHE	ASN	THR	PRO	THR	THR	VAL	GLU	VAL	THR	THR	GLN	THR	GLY	LEU	ILE	GLY	PHE	THR	GLN
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- Molecule 6: IcmE (DotG)

Chain Cj: 97%

[illegible]

ASP	VAL	THR	THR	ILE	THR	GLY	GLY	ASN	ASN	ILE	THR	VAL	ALA	ASN	GLY	VAL	GLY	ARG	SER	THR	LEU	GLU	ASN	ALA	VAL	ILE	GLY	LEU	ALA	THR	THR	VAL	GLY	LYS	ALA	THR	SER	GLN	GLN	ALA	GLN	GLN	LEU	PHE	ASN	THR	PRO	THR	THR	VAL	GLU	VAL	THR	GLY	GLY	LEU	ILE	LEU	PHE	THR	GLN
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- Molecule 6: IcmE (DotG)

Chain Cq: 97%

[illegible]

[illegible]

- Molecule 6: IcmE (DotG)

Chain Cx: 97%

[illegible]

GLN	ASP	VAL	THR	THR	ILE	GLY	THR	GLY	GLY	ASN	ASN	ILE	THR	THR	VAL	ALA	ASN	GLY	VAL	GLY	ARG	SER	THR	THR	LEU	GLU	ASN	ALA	ALA	LEU	GLY	ILE	VAL	VAL	GLY	LYS	THR	TRP	SER	SER	GLN	GLN	ALA	GLN	GLN	GLN	LEU	PHE	ASN	THR	PHO	THR	THR	THR	VAL	GLU	VAL	TYR	SER	SER	GLY	THR	THR	GLY	LEU	GLY	GLY	ILE	GLY	LEU	PHE	THR
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- Molecule 6: IcmE (DotG)

Chain De: 97%

[illegible]

VAL	THR	THR	ILE	GLY	GLY	ASN	ASN	ASN	ILE	THR	VAL	ALA	ASN	GLY	VAL	GLY	ARG	SER	THR	LEU	GLU	ASN	ALA	VAL	ILE	ILE	GLY	LEU	ALA	THR	SER	GLN	GLN	ALA	GLN	GLN	LEU	PHE	ASN	THR	PRO	THR	THR	VAL	GLU	VAL	THR	GLY	GLY	LEU	GLY	ILE	LEU	PHE	THR	THR	GLN	ASN
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- Molecule 6: IcmE (DotG)

Chain D1: 97%

[illegible]

THR	GLN	ASP	VAL	THR	THR	ILE	GLY	GLY	THR	GLY	ASN	ASN	ILE	THR	VAL	ALA	ALA	ASN	GLY	VAL	GLY	ARG	SER	THR	LEU	GLU	ASN	ALA	VAL	ILE	GLY	LEU	ALA	THR	VAL	GLY	LYS	SER	GLN	GLN	ALA	GLN	GLN	GLN	LEU	PHE	ASN	THR	PRO	THR	THR	THR	VAL	GLU	VAL	VAL	TYR	SER	GLY	THR	GLY	LEU	ILE	GLY	LEU	PHE
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- Molecule 6: IcmE (DotG)

Chain Ds:

[illegible]

THR	GLN	ASP	VAL	THR	THR	ILE	GLY	GLY	THR	THR	GLY	ASN	ASN	ALA	ASN	GLY	VAL	GLY	ARG	SER	THR	LEU	GLU	ASN	ALA	VAL	ILE	GLY	LEU	ALA	THR	THR	VAL	GLY	LYS	ALA	SER	GLN	GLN	ALA	GLN	LEU	PHE	ASN	THR	PRO	THR	THR	VAL	GLU	VAL	THR	THR	VAL	THR	THR	THR	LEU	GLY	ILE	LEU	PHE
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- Molecule 6: IcmE (DotG)

Chain Dz: 97%

[illegible]

GLN	ASP	VAL	THR	THR	ILE	GLY	THR	GLY	GLY	ASN	ASN	ILE	THR	THR	VAL	ALA	ASN	GLY	VAL	GLY	ARG	SER	THR	LEU	GLU	ASN	ALA	ALA	LEU	GLY	ILE	VAL	VAL	GLY	LYS	THR	TRP	SER	GLN	GLN	ALA	GLN	GLN	LEU	PHE	ASN	THR	PRO	THR	THR	THR	VAL	GLU	VAL	TYR	SER	SER	GLY	THR	THR	GLY	LEU	GLY	GLY	ILE	GLY	LEU	PHE	THR
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- Molecule 6: IcmE (DotG)

Chain Eg: 97%

[illegible]

- Molecule 6: IcmE (DotG)

Chain En: 97%

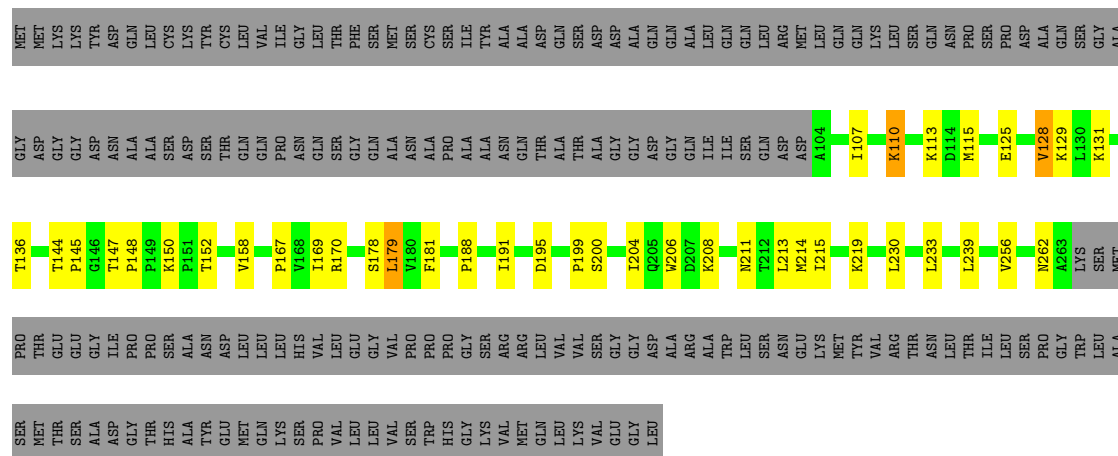
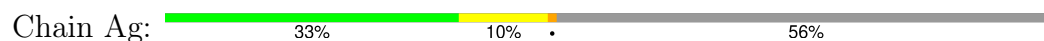


- Molecule 6: IcmE (DotG)

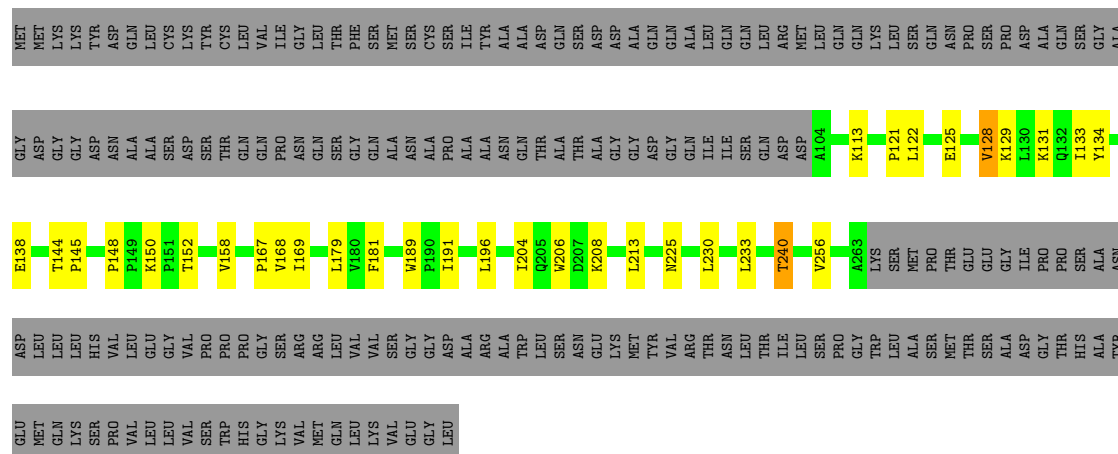
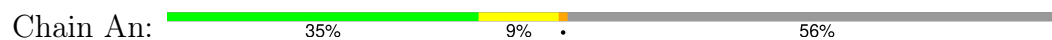
Chain Eu: 97%



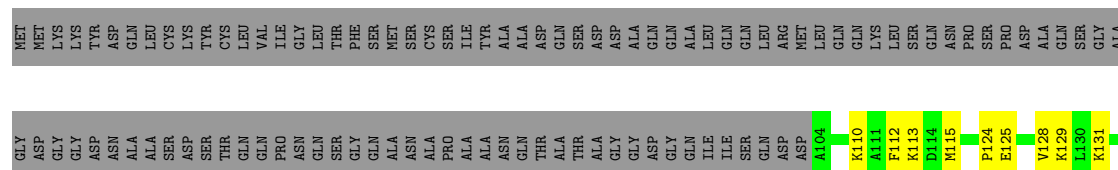
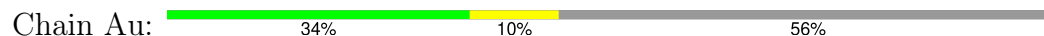
- Molecule 7: IcmK (DotH)

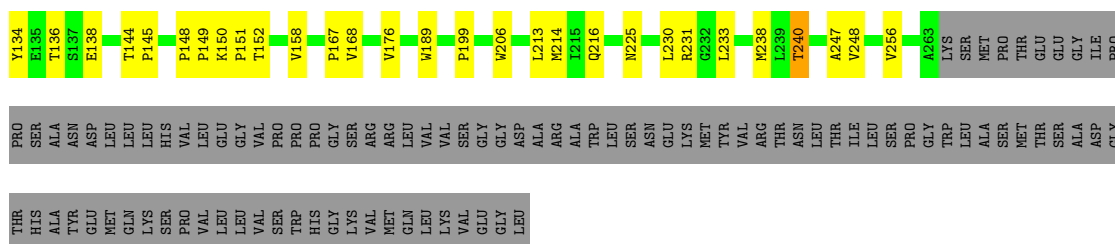


- Molecule 7: IcmK (DotH)

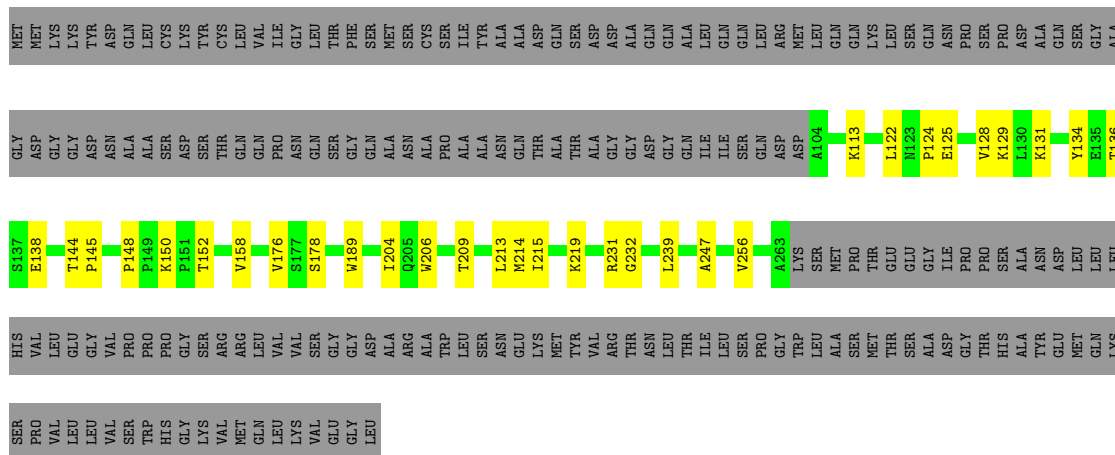
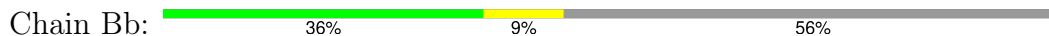


- Molecule 7: IcmK (DotH)

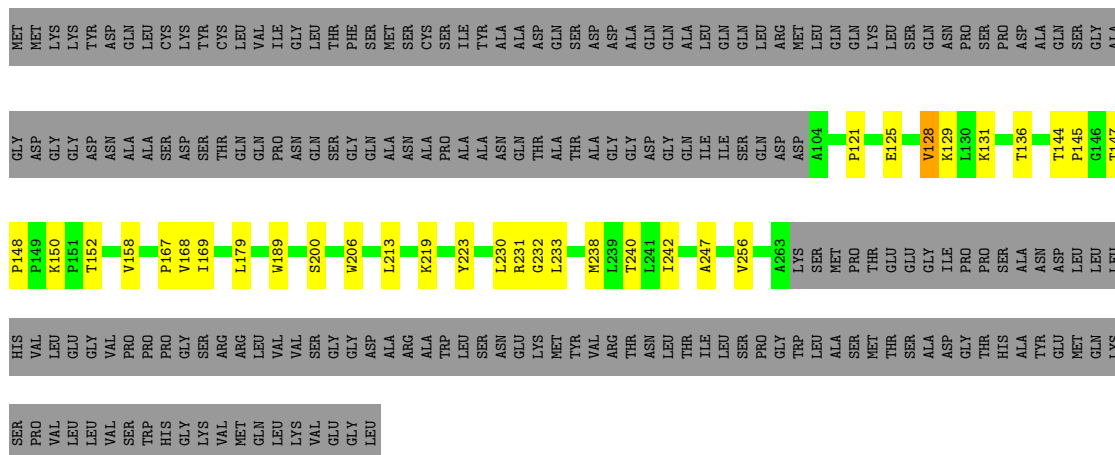
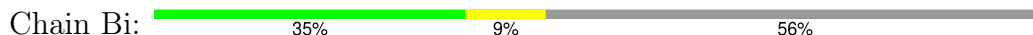




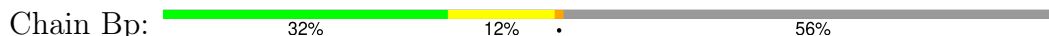
- Molecule 7: IcmK (DotH)

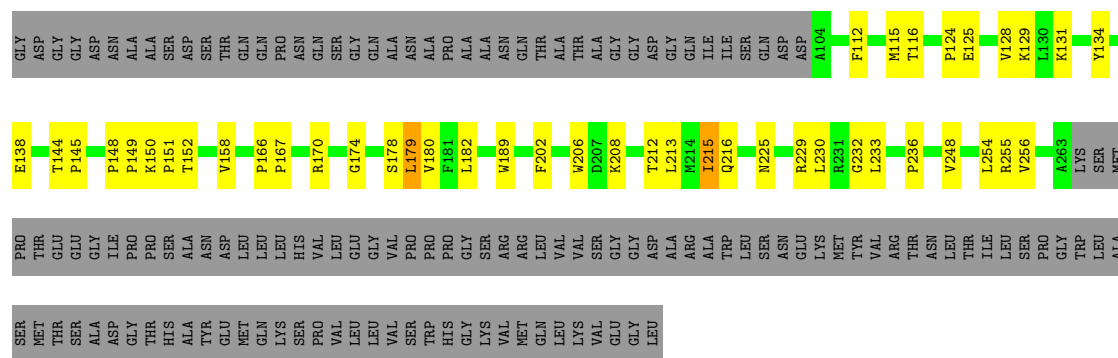


- Molecule 7: IcmK (DotH)



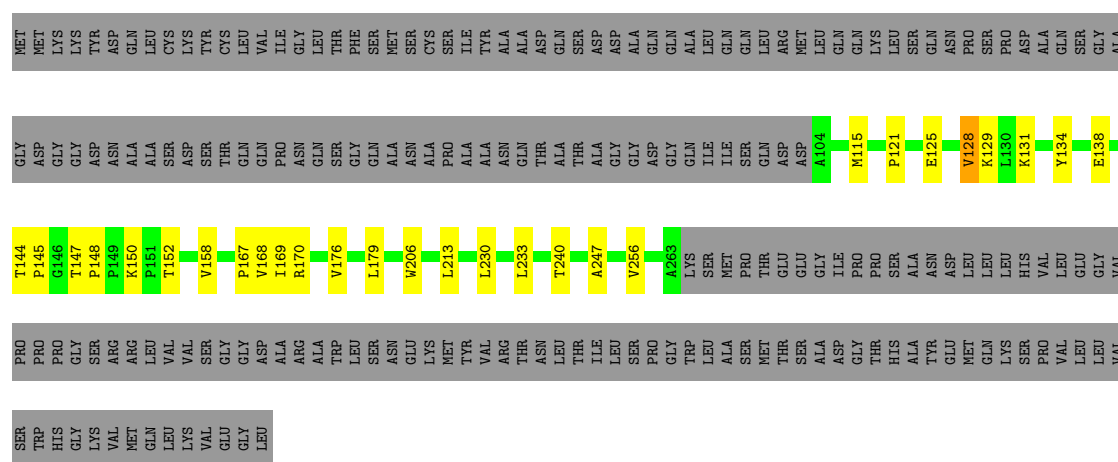
- Molecule 7: IcmK (DotH)





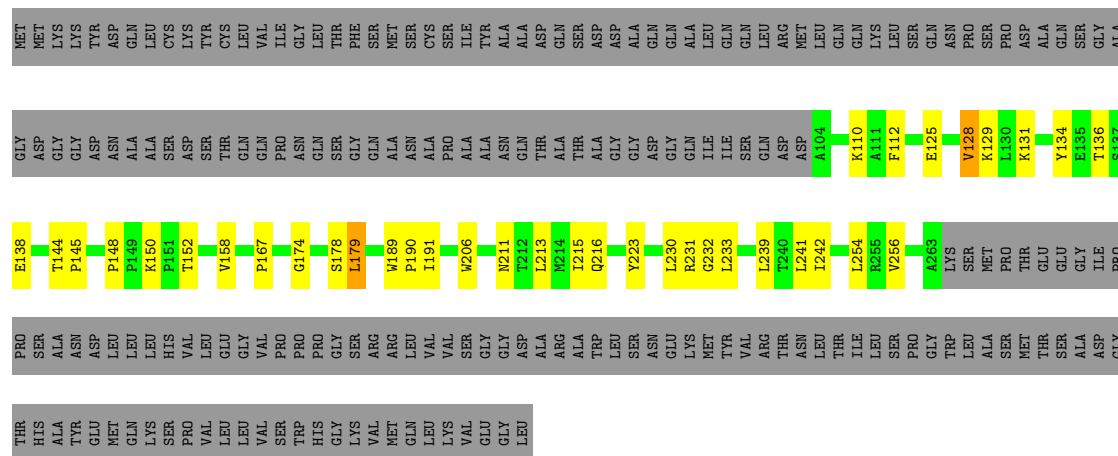
• Molecule 7: IcmK (DotH)

Chain Bw: 37% 7% 56%



• Molecule 7: IcmK (DotH)

Chain Cd: 34% 10% 56%



• Molecule 7: IcmK (DotH)

Chain Ck: 37% 7% 56%

Chain Ea: 31% 13% 56%

Position	Most Conserved AA	Information Content (bits)
1	ASP	0.251
2	ILE	0.136
3	LEU	0.137
4	SER	0.138
5	PRO	0.256
6	GLY	0.263
7	LYS	0.135
8	LEU	0.148
9	ALA	0.149
10	SER	0.150
11	PRO	0.151
12	THR	0.152
13	GLU	0.158
14	SER	0.167
15	ILE	0.170
16	ASP	0.174
17	ASN	0.178
18	LEU	0.179
19	GLN	0.180
20	HIS	0.181
21	PRO	0.182
22	VAL	0.189
23	LEU	0.196
24	GLY	0.203
25	PRO	0.204
26	HIS	0.205
27	GLY	0.206
28	SER	0.207
29	ARG	0.208
30	MET	0.212
31	LEU	0.213
32	VAL	0.214
33	SER	0.215
34	GLY	0.216
35	GLY	0.225
36	ASP	0.229
37	ALA	0.230
38	ARG	0.231
39	ALA	0.232
40	TRP	0.233
41	SER	0.236
42	LEU	0.241
43	ASN	0.246
44	THR	0.247
45	ASN	0.248

[illegible]

Chain Eo:

34% 10% 56%

MET MET LYS TYR ASP GLN LEU CYS TYR CYS LEU VAL ILE GLY THR PHE SER MET CYS ILE TYR ALA ALA ASP GLN SER ASP GLN LEU ARG MET GLN GLN LEU LEU ARG MET GLN PRO SER PRO ASP ALA GLN GLY

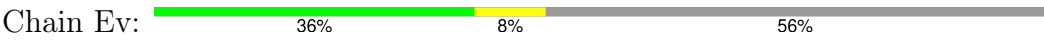
GLY ASP GLY ASP ASN ALA ALA SER SER THR GLN GLN PRO ASN GLN SER GLY ALA ASN ALA PRO ALA THR ALA GLN ILE ILE SER GLN ASP ASP I194 K113 P121 E125 V128 K129 L130 K131 Y134 E135 T136 S137

E138 T144 P145 P148 P149 K150 P151 T152 V158 P167 R170 S178 L179 W189 P190 I191 W206 N211 T212 T213 W214 I215 L230 R231 G232 L233 L239 F240 L241 V248 L254 R255 V256 A263 Lys Ser Met Pro Thr Glu Gly Ile Pro Gly Ser

ALA ASP ASP LEU LEU HIS LEU LEU GLY VAL PRO PRO PRO GLY SER ANG ARG LEU VAL VAL SER SER GLY ASP ASP ALA ARG ALA TRP LEU SER ASN GLU THR LEU THR LEU LEU ILE LEU SER PRO GLY TRP LEU ALA SER MET THR SER ALA ASP GLY THR

ALA
TYR
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● Molecule 7: IcmK (DotH)



MET
MET
LYS
LYS
TYR
ASP
GLN
LEU
CYS
LYS
TYR
CYS
LEU
VAL
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A104
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P121
E125
V128
K129
L130
K131
T136
T144
P145

G146
T147
P149
K150
P151
T152
V158
P167
R170
W189
P190
I191
D195
W206
N211
T212
L213
R231
G232
L233
N234
V237
N238
L239
T240
V248
V256
A263
LYS
SER
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VAL
LEU
LEU
VAL
SER
TRP
HIS
GLY
VAL
MET
GLN
LEU
VAL
VAL
GLY
GLY
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76406	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	2.503	Depositor
Minimum map value	-1.764	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.049	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

5.1 Standard geometry

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	0.10	0/118	0.26	0/158
1	Ah	0.09	0/118	0.23	0/158
1	Ao	0.09	0/118	0.26	0/158
1	Av	0.07	0/118	0.21	0/158
1	Bc	0.07	0/118	0.22	0/158
1	Bj	0.07	0/118	0.22	0/158
1	Bq	0.06	0/118	0.20	0/158
1	Bx	0.08	0/118	0.23	0/158
1	Ce	0.08	0/118	0.23	0/158
1	Cl	0.08	0/118	0.21	0/158
1	Cs	0.07	0/118	0.21	0/158
1	Cz	0.07	0/118	0.23	0/158
1	Dg	0.07	0/118	0.21	0/158
1	Dn	0.07	0/118	0.20	0/158
1	Du	0.13	0/118	0.32	0/158
1	Eb	0.06	0/118	0.22	0/158
1	Ei	0.08	0/118	0.24	0/158
1	Ep	0.10	0/118	0.24	0/158
2	Ab	0.10	0/60	0.26	0/76
2	Ai	0.07	0/60	0.23	0/76
2	Ap	0.09	0/60	0.30	0/76
2	Aw	0.09	0/60	0.29	0/76
2	Bd	0.10	0/60	0.32	0/76
2	Bk	0.12	0/60	0.45	0/76
2	Br	0.11	0/60	0.25	0/76
2	By	0.12	0/60	0.39	0/76
2	Cf	0.11	0/60	0.36	0/76
2	Cm	0.09	0/60	0.27	0/76
2	Ct	0.11	0/60	0.27	0/76
2	Da	0.08	0/60	0.30	0/76
2	Dh	0.08	0/60	0.30	0/76
2	Do	0.08	0/60	0.26	0/76
2	Dv	0.17	0/60	0.56	0/76
2	Ec	0.11	0/60	0.27	0/76

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Ej	0.08	0/60	0.31	0/76
2	Eq	0.09	0/60	0.29	0/76
3	Ac	0.15	0/126	0.39	0/167
3	Aj	0.09	0/126	0.31	0/167
3	Aq	0.10	0/126	0.35	0/167
3	Ax	0.09	0/126	0.30	0/167
3	Be	0.10	0/126	0.31	0/167
3	Bl	0.12	0/126	0.35	0/167
3	Bs	0.12	0/126	0.31	0/167
3	Bz	0.14	0/126	0.37	0/167
3	Cg	0.12	0/126	0.36	0/167
3	Cn	0.12	0/126	0.40	0/167
3	Cu	0.10	0/126	0.36	0/167
3	Db	0.10	0/126	0.37	0/167
3	Di	0.08	0/126	0.29	0/167
3	Dp	0.14	0/126	0.34	0/167
3	Dw	0.13	0/126	0.32	0/167
3	Ed	0.12	0/126	0.31	0/167
3	Ek	0.13	0/126	0.37	0/167
3	Er	0.11	0/126	0.37	0/167
4	Ad	0.14	0/37	0.25	0/47
4	Ak	0.07	0/37	0.16	0/47
4	Ar	0.09	0/37	0.23	0/47
4	Ay	0.09	0/37	0.23	0/47
4	Bf	0.07	0/37	0.17	0/47
4	Bm	0.08	0/37	0.27	0/47
4	Bt	0.06	0/37	0.17	0/47
4	Ca	0.07	0/37	0.18	0/47
4	Ch	0.08	0/37	0.23	0/47
4	Co	0.08	0/37	0.27	0/47
4	Cv	0.06	0/37	0.17	0/47
4	Dc	0.07	0/37	0.22	0/47
4	Dj	0.09	0/37	0.23	0/47
4	Dq	0.07	0/37	0.18	0/47
4	Dx	0.09	0/37	0.22	0/47
4	Ee	0.06	0/37	0.17	0/47
4	El	0.07	0/37	0.19	0/47
4	Es	0.07	0/37	0.19	0/47
5	Ae	0.11	0/491	0.27	0/660
5	Al	0.19	0/491	0.35	0/660
5	As	0.11	0/491	0.27	0/660
5	Az	0.11	0/491	0.30	0/660
5	Bg	0.10	0/491	0.27	0/660

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	Bn	0.11	0/491	0.32	0/660
5	Bu	0.11	0/491	0.27	0/660
5	Cb	0.12	0/491	0.30	0/660
5	Ci	0.13	0/491	0.31	0/660
5	Cp	0.11	0/491	0.29	0/660
5	Cw	0.11	0/491	0.29	0/660
5	Dd	0.11	0/491	0.29	0/660
5	Dk	0.12	0/491	0.31	0/660
5	Dr	0.11	0/491	0.27	0/660
5	Dy	0.11	0/491	0.31	0/660
5	Ef	0.11	0/491	0.27	0/660
5	Em	0.12	0/491	0.29	0/660
5	Et	0.12	0/491	0.30	0/660
6	Af	0.13	0/278	0.29	0/377
6	Am	0.10	0/278	0.24	0/377
6	At	0.13	0/278	0.33	0/377
6	Ba	0.10	0/278	0.23	0/377
6	Bh	0.10	0/278	0.20	0/377
6	Bo	0.11	0/278	0.25	0/377
6	Bv	0.11	0/278	0.23	0/377
6	Cc	0.10	0/278	0.23	0/377
6	Cj	0.12	0/278	0.24	0/377
6	Cq	0.12	0/278	0.26	0/377
6	Cx	0.11	0/278	0.26	0/377
6	De	0.11	0/278	0.29	0/377
6	Dl	0.10	0/278	0.26	0/377
6	Ds	0.11	0/278	0.23	0/377
6	Dz	0.11	0/278	0.21	0/377
6	Eg	0.10	0/278	0.24	0/377
6	En	0.09	0/278	0.23	0/377
6	Eu	0.11	0/278	0.25	0/377
7	Ag	0.15	0/1269	0.29	0/1734
7	An	0.13	0/1269	0.31	0/1734
7	Au	0.12	0/1269	0.27	0/1734
7	Bb	0.12	0/1269	0.29	0/1734
7	Bi	0.13	0/1269	0.28	0/1734
7	Bp	0.15	0/1269	0.31	0/1734
7	Bw	0.13	0/1269	0.33	0/1734
7	Cd	0.12	0/1269	0.28	0/1734
7	Ck	0.13	0/1269	0.30	0/1734
7	Cr	0.13	0/1269	0.29	0/1734
7	Cy	0.13	0/1269	0.30	0/1734
7	Df	0.13	0/1269	0.27	0/1734

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	Dm	0.14	0/1269	0.31	0/1734
7	Dt	0.13	0/1269	0.28	0/1734
7	Ea	0.14	0/1269	0.29	0/1734
7	Eh	0.13	0/1269	0.32	0/1734
7	Eo	0.12	0/1269	0.28	0/1734
7	Ev	0.14	0/1269	0.30	0/1734
All	All	0.12	0/42822	0.29	0/57942

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 [i](#)

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	117	0	111	4	0
1	Ah	117	0	111	3	0
1	Ao	117	0	111	4	0
1	Av	117	0	111	3	0
1	Bc	117	0	111	3	0
1	Bj	117	0	111	5	0
1	Bq	117	0	111	3	0
1	Bx	117	0	111	2	0
1	Ce	117	0	111	4	0
1	Cl	117	0	111	4	0
1	Cs	117	0	111	4	0
1	Cz	117	0	111	4	0
1	Dg	117	0	111	4	0
1	Dn	117	0	111	3	0
1	Du	117	0	111	3	0
1	Eb	117	0	111	4	0
1	Ei	117	0	111	2	0
1	Ep	117	0	111	6	0
2	Ab	61	0	65	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ai	61	0	65	3	0
2	Ap	61	0	65	5	0
2	Aw	61	0	65	4	0
2	Bd	61	0	65	2	0
2	Bk	61	0	65	2	0
2	Br	61	0	65	3	0
2	By	61	0	65	3	0
2	Cf	61	0	65	2	0
2	Cm	61	0	65	5	0
2	Ct	61	0	65	6	0
2	Da	61	0	65	4	0
2	Dh	61	0	65	6	0
2	Do	61	0	65	5	0
2	Dv	61	0	65	7	0
2	Ec	61	0	65	3	0
2	Ej	61	0	65	7	0
2	Eq	61	0	65	4	0
3	Ac	125	0	126	4	0
3	Aj	125	0	126	3	0
3	Aq	125	0	126	5	0
3	Ax	125	0	126	4	0
3	Be	125	0	126	4	0
3	Bl	125	0	126	7	0
3	Bs	125	0	126	3	0
3	Bz	125	0	126	6	0
3	Cg	125	0	126	5	0
3	Cn	125	0	126	4	0
3	Cu	125	0	126	7	0
3	Db	125	0	126	6	0
3	Di	125	0	126	5	0
3	Dp	125	0	126	6	0
3	Dw	125	0	126	6	0
3	Ed	125	0	126	5	0
3	Ek	125	0	126	7	0
3	Er	125	0	126	7	0
4	Ad	36	0	30	3	0
4	Ak	36	0	30	1	0
4	Ar	36	0	30	3	0
4	Ay	36	0	30	2	0
4	Bf	36	0	30	1	0
4	Bm	36	0	30	1	0
4	Bt	36	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Ca	36	0	30	1	0
4	Ch	36	0	30	1	0
4	Co	36	0	30	2	0
4	Cv	36	0	30	1	0
4	Dc	36	0	30	2	0
4	Dj	36	0	30	4	0
4	Dq	36	0	30	1	0
4	Dx	36	0	30	1	0
4	Ee	36	0	30	1	0
4	El	36	0	30	2	0
4	Es	36	0	30	1	0
5	Ae	484	0	502	11	0
5	Al	484	0	502	11	0
5	As	484	0	502	14	0
5	Az	484	0	502	13	0
5	Bg	484	0	502	10	0
5	Bn	484	0	502	12	0
5	Bu	484	0	502	11	0
5	Cb	484	0	502	13	0
5	Ci	484	0	502	13	0
5	Cp	484	0	502	12	0
5	Cw	484	0	502	13	0
5	Dd	484	0	502	13	0
5	Dk	484	0	502	13	0
5	Dr	484	0	502	11	0
5	Dy	484	0	502	14	0
5	Ef	484	0	502	12	0
5	Em	484	0	502	14	0
5	Et	484	0	502	14	0
6	Af	276	0	263	7	0
6	Am	276	0	263	6	0
6	At	276	0	263	3	0
6	Ba	276	0	263	4	0
6	Bh	276	0	263	4	0
6	Bo	276	0	263	6	0
6	Bv	276	0	263	4	0
6	Cc	276	0	263	4	0
6	Cj	276	0	263	3	0
6	Cq	276	0	263	4	0
6	Cx	276	0	263	6	0
6	De	276	0	263	4	0
6	Dl	276	0	263	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Ds	276	0	263	4	0
6	Dz	276	0	263	3	0
6	Eg	276	0	263	5	0
6	En	276	0	263	6	0
6	Eu	276	0	263	2	0
7	Ag	1238	0	1252	36	0
7	An	1238	0	1252	28	0
7	Au	1238	0	1252	35	0
7	Bb	1238	0	1252	24	0
7	Bi	1238	0	1252	26	0
7	Bp	1238	0	1252	38	0
7	Bw	1238	0	1252	24	0
7	Cd	1238	0	1252	29	0
7	Ck	1238	0	1252	22	0
7	Cr	1238	0	1252	30	0
7	Cy	1238	0	1252	30	0
7	Df	1238	0	1252	31	0
7	Dm	1238	0	1252	27	0
7	Dt	1238	0	1252	29	0
7	Ea	1238	0	1252	40	0
7	Eh	1238	0	1252	28	0
7	Eo	1238	0	1252	29	0
7	Ev	1238	0	1252	29	0
All	All	42066	0	42282	794	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 (794) 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)
2:Ec:5:ILE:HD11	7:Eo:136:THR:HG23	1.61	0.82
2:Br:5:ILE:HD11	7:Cd:136:THR:HG23	1.61	0.82
7:Ag:136:THR:HG23	2:Eq:5:ILE:HD11	1.62	0.81
2:Ai:5:ILE:HD11	7:Au:136:THR:HG23	1.66	0.77
2:Dv:5:ILE:HD11	7:Eh:136:THR:HG23	1.67	0.76
2:Aw:5:ILE:HD11	7:Bi:136:THR:HG23	1.67	0.76
7:Ag:144:THR:HG21	7:Ag:148:PRO:HG3	1.69	0.74
2:Dh:5:ILE:HD11	7:Dt:136:THR:HG23	1.70	0.72
7:Ag:145:PRO:HG3	7:An:131:LYS:HG2	1.71	0.71
7:Cr:144:THR:HG21	7:Cr:148:PRO:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Bw:145:PRO:HG3	7:Cd:131:LYS:HG2	1.72	0.71
2:Do:4:MET:HG3	5:Dr:248:ASP:HA	1.73	0.71
6:Cj:797:ARG:O	6:Cj:801:MET:HG3	1.90	0.70
6:Bh:797:ARG:O	6:Bh:801:MET:HG3	1.92	0.70
7:Cr:200:SER:HB3	6:Cx:816:GLU:HG3	1.74	0.70
2:Cf:5:ILE:HD12	2:Cf:5:ILE:H	1.57	0.70
1:Bq:16:ALA:HB3	2:By:9:ARG:HD2	1.74	0.70
7:Ck:145:PRO:HG3	7:Cr:131:LYS:HG2	1.73	0.69
7:Ev:144:THR:HG21	7:Ev:148:PRO:HG3	1.73	0.69
7:Cd:145:PRO:HG3	7:Ck:131:LYS:HG2	1.75	0.69
7:Ag:131:LYS:HG2	7:Ev:145:PRO:HG3	1.75	0.69
5:Dk:233:ARG:HB2	7:Dt:147:THR:HG21	1.75	0.68
6:Ds:797:ARG:O	6:Ds:801:MET:HG3	1.92	0.68
7:Eo:145:PRO:HG3	7:Ev:131:LYS:HG2	1.76	0.68
7:Cr:145:PRO:HG3	7:Cy:131:LYS:HG2	1.75	0.68
2:Ej:5:ILE:HD11	7:Ev:136:THR:HG23	1.75	0.68
2:Bk:5:ILE:HD12	2:Bk:5:ILE:H	1.59	0.68
2:Do:5:ILE:HD11	7:Ea:136:THR:HG23	1.76	0.67
1:Dg:16:ALA:HB3	2:Do:9:ARG:HD2	1.76	0.67
6:Cj:791:GLN:HG3	6:Cj:794:ILE:HD12	1.77	0.67
7:Ag:200:SER:HB3	6:Am:816:GLU:HG3	1.75	0.67
7:Dm:145:PRO:HG3	7:Dt:131:LYS:HG2	1.77	0.67
1:Eb:16:ALA:HB3	2:Ej:9:ARG:HD2	1.77	0.67
7:Dt:145:PRO:HG3	7:Ea:131:LYS:HG2	1.77	0.67
6:Dz:797:ARG:O	6:Dz:801:MET:HG3	1.95	0.67
7:An:145:PRO:HG3	7:Au:131:LYS:HG2	1.77	0.66
7:Bb:145:PRO:HG3	7:Bi:131:LYS:HG2	1.77	0.66
7:Bp:145:PRO:HG3	7:Bw:131:LYS:HG2	1.76	0.66
5:Cw:254:ILE:HB	5:Cw:262:ILE:HB	1.76	0.66
1:Av:16:ALA:HB3	2:Bd:9:ARG:HD2	1.76	0.66
5:Em:253:ARG:HD2	5:Em:263:LYS:HE2	1.76	0.66
6:Bo:801:MET:HG2	7:Bw:121:PRO:HB2	1.78	0.66
7:Bp:179:LEU:HD11	7:Bp:215:ILE:HD11	1.78	0.66
7:Ck:144:THR:HG21	7:Ck:148:PRO:HG3	1.77	0.66
5:Cb:253:ARG:HD2	5:Cb:263:LYS:HE2	1.78	0.66
3:Ed:2:VAL:HG22	3:Ed:8:VAL:HG23	1.77	0.66
7:Bi:145:PRO:HG3	7:Bp:131:LYS:HG2	1.77	0.65
1:Aa:16:ALA:HB3	2:Ai:9:ARG:HD2	1.79	0.65
7:Eh:145:PRO:HG3	7:Eo:131:LYS:HG2	1.78	0.65
7:Cy:145:PRO:HG3	7:Df:131:LYS:HG2	1.77	0.65
5:Dd:253:ARG:HD2	5:Dd:263:LYS:HE2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Ag:178:SER:HA	7:Ag:213:LEU:O	1.97	0.65
1:Ce:16:ALA:HB3	2:Cm:9:ARG:HD2	1.78	0.65
7:Au:144:THR:HG21	7:Au:148:PRO:HG3	1.78	0.64
7:Eh:144:THR:HG21	7:Eh:148:PRO:HG3	1.79	0.64
5:Bu:253:ARG:HD2	5:Bu:263:LYS:HE2	1.80	0.64
5:Cp:253:ARG:HD2	5:Cp:263:LYS:HE2	1.79	0.64
5:Cb:264:PHE:HB3	5:Cb:269:SER:HB3	1.79	0.64
2:Bd:5:ILE:HD12	2:Bd:5:ILE:H	1.62	0.64
7:Cd:179:LEU:HD22	7:Cd:254:LEU:HD11	1.78	0.64
7:Ag:199:PRO:HD2	6:Am:816:GLU:HB3	1.80	0.64
5:Cp:254:ILE:HB	5:Cp:262:ILE:HB	1.80	0.64
5:Ef:253:ARG:HD2	5:Ef:263:LYS:HE2	1.79	0.64
7:Df:145:PRO:HG3	7:Dm:131:LYS:HG2	1.80	0.63
5:Ae:254:ILE:HB	5:Ae:262:ILE:HB	1.81	0.63
1:Du:2:THR:HG21	5:Dy:253:ARG:HH21	1.63	0.63
3:Bl:2:VAL:HG22	3:Bl:8:VAL:HG23	1.80	0.63
5:Ci:219:ARG:H	7:Cr:148:PRO:HD2	1.64	0.63
1:Aa:2:THR:HG21	5:Ae:253:ARG:HH21	1.63	0.63
5:Bn:264:PHE:HB3	5:Bn:269:SER:HB3	1.80	0.63
7:Au:150:LYS:HG2	7:Au:152:THR:HG23	1.80	0.63
3:Ek:2:VAL:HG22	3:Ek:8:VAL:HG23	1.80	0.63
5:Ci:254:ILE:HB	5:Ci:262:ILE:HB	1.80	0.62
6:Bh:801:MET:HB2	7:Bw:115:MET:HG3	1.79	0.62
6:Cq:805:ALA:HB2	7:Cy:122:LEU:HD11	1.81	0.62
1:Dg:2:THR:HG21	5:Dk:253:ARG:HH21	1.64	0.62
5:Cp:264:PHE:HB3	5:Cp:269:SER:HB3	1.82	0.62
5:Dy:254:ILE:HB	5:Dy:262:ILE:HB	1.82	0.62
5:As:253:ARG:HD2	5:As:263:LYS:HE2	1.82	0.62
2:Ap:5:ILE:HD11	7:Bb:136:THR:HG23	1.80	0.62
5:Ae:253:ARG:HD2	5:Ae:263:LYS:HE2	1.80	0.62
7:Eo:179:LEU:HD22	7:Eo:254:LEU:HD11	1.81	0.62
7:Au:145:PRO:HG3	7:Bb:131:LYS:HG2	1.80	0.62
5:Az:233:ARG:HB2	7:Bi:147:THR:HG21	1.81	0.61
1:Ao:2:THR:HG21	5:As:253:ARG:HH21	1.65	0.61
6:Cq:797:ARG:O	6:Cq:801:MET:HG3	2.00	0.61
6:Af:797:ARG:O	6:Af:801:MET:HG3	1.99	0.61
7:Df:150:LYS:HG2	7:Df:152:THR:HG23	1.81	0.61
3:Dw:2:VAL:HG22	3:Dw:8:VAL:HG23	1.81	0.61
5:Dy:264:PHE:HB3	5:Dy:269:SER:HB3	1.81	0.61
3:Be:2:VAL:HG22	3:Be:8:VAL:HG23	1.82	0.61
3:Bz:2:VAL:HG22	3:Bz:8:VAL:HG23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Bw:144:THR:HG21	7:Bw:148:PRO:HG3	1.82	0.61
6:Cj:791:GLN:HG2	6:Cj:795:GLN:HE22	1.65	0.61
5:Et:254:ILE:HB	5:Et:262:ILE:HB	1.83	0.61
5:Bn:254:ILE:HB	5:Bn:262:ILE:HB	1.82	0.61
7:Cr:199:PRO:HD2	6:Cx:816:GLU:HB3	1.83	0.61
5:Ef:264:PHE:HB3	5:Ef:269:SER:HB3	1.83	0.61
7:Ag:150:LYS:HG2	7:Ag:152:THR:HG23	1.83	0.60
1:Ah:2:THR:HG21	5:Al:253:ARG:HH21	1.67	0.60
1:Cz:2:THR:HG21	5:Dd:253:ARG:HH21	1.66	0.60
4:Co:2:PHE:HD2	5:Cp:251:GLN:HE22	1.48	0.60
6:Ds:801:MET:HB2	7:Eh:115:MET:HG3	1.84	0.60
5:As:254:ILE:HB	5:As:262:ILE:HB	1.83	0.60
2:By:5:ILE:HD12	2:By:5:ILE:H	1.67	0.60
6:Af:805:ALA:HB2	7:An:122:LEU:HD11	1.84	0.60
7:Ea:145:PRO:HG3	7:Eh:131:LYS:HG2	1.83	0.60
1:Bc:2:THR:HG21	5:Bg:253:ARG:HH21	1.67	0.60
1:Cl:2:THR:HG21	5:Cp:253:ARG:HH21	1.66	0.60
6:Dl:797:ARG:O	6:Dl:801:MET:HG3	2.02	0.59
7:Dm:144:THR:HG21	7:Dm:148:PRO:HG3	1.83	0.59
7:Dt:150:LYS:HG2	7:Dt:152:THR:HG23	1.84	0.59
7:Ev:150:LYS:HG2	7:Ev:152:THR:HG23	1.84	0.59
5:Ae:264:PHE:HB3	5:Ae:269:SER:HB3	1.83	0.59
5:Al:254:ILE:HB	5:Al:262:ILE:HB	1.84	0.59
7:Bb:144:THR:HG21	7:Bb:148:PRO:HG3	1.84	0.59
1:Bx:2:THR:HG21	5:Cb:253:ARG:HH21	1.68	0.59
5:Dy:253:ARG:HD2	5:Dy:263:LYS:HE2	1.84	0.59
5:Em:264:PHE:HB3	5:Em:269:SER:HB3	1.84	0.59
5:Dd:254:ILE:HB	5:Dd:262:ILE:HB	1.85	0.59
7:Eo:150:LYS:HG2	7:Eo:152:THR:HG23	1.84	0.59
6:Ba:797:ARG:O	6:Ba:801:MET:HG3	2.02	0.59
3:Cn:1:ARG:HH22	3:Cn:3:SER:HB2	1.68	0.59
1:Av:2:THR:HG21	5:Az:253:ARG:HH21	1.67	0.59
2:Da:5:ILE:HD11	7:Dm:136:THR:HG23	1.83	0.59
1:Dn:2:THR:HG21	5:Dr:253:ARG:HH21	1.68	0.59
3:Er:1:ARG:HH22	3:Er:3:SER:HB2	1.67	0.59
5:Bn:253:ARG:HD2	5:Bn:263:LYS:HE2	1.84	0.59
7:Bw:150:LYS:HG2	7:Bw:152:THR:HG23	1.85	0.59
7:Cr:150:LYS:HG2	7:Cr:152:THR:HG23	1.83	0.59
2:Ct:5:ILE:HD12	2:Ct:5:ILE:H	1.66	0.58
1:Bx:12:HIS:CE1	4:Ch:3:GLY:HA2	2.37	0.58
7:An:129:LYS:O	7:An:133:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Cd:150:LYS:HG2	7:Cd:152:THR:HG23	1.85	0.58
3:Cu:1:ARG:HH22	3:Cu:3:SER:HB2	1.69	0.58
1:Et:2:THR:HG21	5:Em:253:ARG:HH21	1.68	0.58
1:Et:12:HIS:CE1	4:Es:3:GLY:HA2	2.39	0.58
5:Al:219:ARG:HG3	7:Au:148:PRO:HB2	1.86	0.58
7:Bb:150:LYS:HG2	7:Bb:152:THR:HG23	1.84	0.58
1:Bc:16:ALA:HB3	2:Bk:9:ARG:HD2	1.85	0.58
2:Al:4:MET:HG3	5:Al:248:ASP:HA	1.85	0.58
7:Bp:112:PHE:O	7:Bp:116:THR:HG22	2.03	0.58
7:Bi:150:LYS:HG2	7:Bi:152:THR:HG23	1.85	0.58
6:Af:820:TYR:HE1	6:Af:822:GLU:HG2	1.69	0.58
1:Bc:12:HIS:CE1	4:Bm:3:GLY:HA2	2.39	0.58
3:Bs:2:VAL:HG22	3:Bs:8:VAL:HG23	1.85	0.58
7:An:150:LYS:HG2	7:An:152:THR:HG23	1.86	0.57
1:Bq:2:THR:HG21	5:Bu:253:ARG:HH21	1.69	0.57
2:Do:5:ILE:HA	5:Dr:250:LEU:HD11	1.85	0.57
6:Af:801:MET:HG2	7:An:121:PRO:HB2	1.85	0.57
5:Al:264:PHE:HB3	5:Al:269:SER:HB3	1.87	0.57
6:Bo:797:ARG:O	6:Bo:801:MET:HG3	2.05	0.57
7:Ck:150:LYS:HG2	7:Ck:152:THR:HG23	1.85	0.57
3:Dp:2:VAL:HG22	3:Dp:8:VAL:HG23	1.86	0.57
1:Av:12:HIS:CE1	4:Bf:3:GLY:HA2	2.39	0.57
7:Dm:150:LYS:HG2	7:Dm:152:THR:HG23	1.84	0.57
7:Ag:115:MET:HG2	6:En:802:LEU:HD23	1.87	0.57
5:Az:219:ARG:HG3	7:Bi:148:PRO:HB2	1.87	0.57
5:Ci:233:ARG:HB2	7:Cr:147:THR:HG21	1.86	0.57
7:Eh:150:LYS:HG2	7:Eh:152:THR:HG23	1.84	0.57
5:Az:264:PHE:HB3	5:Az:269:SER:HB3	1.86	0.57
5:Dk:219:ARG:HG3	7:Dt:148:PRO:HB2	1.85	0.57
6:En:797:ARG:O	6:En:801:MET:HG3	2.04	0.57
7:Ev:191:ILE:HG13	7:Ev:211:ASN:HA	1.86	0.57
5:Ef:212:ILE:HG13	5:Ef:262:ILE:HG22	1.85	0.57
7:Cy:150:LYS:HG2	7:Cy:152:THR:HG23	1.86	0.56
1:Dg:12:HIS:CE1	4:Dq:3:GLY:HA2	2.40	0.56
5:Dk:264:PHE:HB3	5:Dk:269:SER:HB3	1.86	0.56
5:Ci:264:PHE:HB3	5:Ci:269:SER:HB3	1.87	0.56
7:Cr:178:SER:HA	7:Cr:213:LEU:O	2.04	0.56
7:Ck:191:ILE:HG13	7:Ck:211:ASN:HA	1.86	0.56
7:Dt:145:PRO:HD3	7:Ea:131:LYS:HE2	1.87	0.56
7:Ea:150:LYS:HG2	7:Ea:152:THR:HG23	1.86	0.56
6:Cc:797:ARG:O	6:Cc:801:MET:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Eb:2:THR:HG21	5:Ef:253:ARG:HH21	1.69	0.56
5:Cw:264:PHE:HB3	5:Cw:269:SER:HB3	1.87	0.56
1:Bj:2:THR:HG21	5:Bn:253:ARG:HH21	1.72	0.55
7:Bp:150:LYS:HG2	7:Bp:152:THR:HG23	1.87	0.55
5:Bu:212:ILE:HG13	5:Bu:262:ILE:HG22	1.88	0.55
7:Cy:129:LYS:O	7:Cy:133:ILE:HG13	2.06	0.55
5:Bu:254:ILE:HB	5:Bu:262:ILE:HB	1.88	0.55
5:Ef:254:ILE:HB	5:Ef:262:ILE:HB	1.88	0.55
3:Ek:1:ARG:HH22	3:Ek:3:SER:HB2	1.72	0.55
5:Ci:253:ARG:HH21	5:Ci:255:LEU:HD21	1.72	0.55
1:Cl:16:ALA:HB3	2:Ct:9:ARG:HD2	1.89	0.55
7:Dt:230:LEU:HD12	7:Dt:233:LEU:HD12	1.88	0.55
7:Cy:225:ASN:HD21	7:Df:176:VAL:H	1.54	0.55
5:Dd:219:ARG:H	7:Dm:148:PRO:HD2	1.72	0.55
5:Et:253:ARG:HH21	5:Et:255:LEU:HD21	1.72	0.55
5:As:264:PHE:HB3	5:As:269:SER:HB3	1.88	0.55
3:Di:2:VAL:HG11	7:Ea:129:LYS:HG2	1.89	0.55
3:Er:2:VAL:HG22	3:Er:8:VAL:HG23	1.89	0.55
5:Ae:213:GLN:O	7:Ag:170:ARG:HD2	2.08	0.54
5:Bn:219:ARG:HG3	7:Bw:148:PRO:HB2	1.89	0.54
5:Cb:254:ILE:HB	5:Cb:262:ILE:HB	1.89	0.54
5:Em:254:ILE:HB	5:Em:262:ILE:HB	1.89	0.54
7:Ag:204:ILE:HG12	7:Ag:215:ILE:HG13	1.88	0.54
6:Ba:801:MET:HG2	7:Bi:121:PRO:HB2	1.89	0.54
5:Dr:219:ARG:H	7:Ea:148:PRO:HD2	1.71	0.54
5:Dr:264:PHE:HB3	5:Dr:269:SER:HB3	1.90	0.54
3:Ax:2:VAL:HG11	7:Bp:129:LYS:HG2	1.88	0.54
7:Bi:230:LEU:HD12	7:Bi:233:LEU:HD12	1.90	0.54
3:Bl:2:VAL:HG11	7:Cd:129:LYS:HG2	1.90	0.54
7:Bw:145:PRO:HD3	7:Cd:131:LYS:HE2	1.90	0.54
2:Dv:4:MET:HG3	5:Dy:249:SER:H	1.72	0.54
5:Cb:219:ARG:H	7:Ck:148:PRO:HD2	1.72	0.54
6:At:805:ALA:HB2	7:Bb:122:LEU:HD11	1.90	0.54
3:Db:1:ARG:HH22	3:Db:3:SER:HB2	1.72	0.54
5:Dd:264:PHE:HB3	5:Dd:269:SER:HB3	1.88	0.54
6:Cx:805:ALA:HB2	7:Df:122:LEU:HD11	1.90	0.53
7:Eo:191:ILE:HG13	7:Eo:211:ASN:HA	1.90	0.53
5:Em:212:ILE:HD11	5:Em:254:ILE:HG13	1.91	0.53
6:Ba:802:LEU:HD13	7:Bp:115:MET:HG2	1.89	0.53
6:Cc:802:LEU:HD23	7:Cr:115:MET:HG2	1.89	0.53
7:An:225:ASN:HD21	7:Au:176:VAL:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Aq:1:ARG:HH22	3:Aq:3:SER:HB2	1.72	0.53
1:Bj:12:HIS:CE1	4:Bt:3:GLY:HA2	2.43	0.53
5:Ef:219:ARG:HG3	7:Eo:148:PRO:HB2	1.89	0.53
3:Bl:11:ALA:HB1	3:Bl:14:TYR:CE1	2.43	0.53
1:Dn:12:HIS:NE2	4:Dx:3:GLY:HA2	2.23	0.53
7:Ea:204:ILE:HG12	7:Ea:215:ILE:HG12	1.91	0.53
6:En:820:TYR:HE1	6:En:822:GLU:HG2	1.72	0.53
5:Bu:219:ARG:HG3	7:Cd:148:PRO:HB2	1.91	0.53
7:Cr:204:ILE:HG12	7:Cr:215:ILE:HG13	1.90	0.53
5:Dy:219:ARG:HG3	7:Eh:148:PRO:HB2	1.91	0.53
5:Cw:219:ARG:HG3	7:Df:148:PRO:HB2	1.90	0.53
7:An:168:VAL:HG23	7:An:240:THR:HG23	1.90	0.53
5:As:219:ARG:H	7:Bb:148:PRO:HD2	1.72	0.53
5:Cw:255:LEU:HD13	5:Cw:261:VAL:HG22	1.91	0.53
6:Dl:802:LEU:HD13	7:Ea:115:MET:HG2	1.89	0.53
7:Eo:158:VAL:HB	7:Eo:256:VAL:HA	1.90	0.53
7:Ev:158:VAL:HG22	7:Ev:167:PRO:HG2	1.91	0.53
1:Aa:5:ALA:HB2	2:Ab:4:MET:HE1	1.91	0.53
7:Ag:148:PRO:HD2	5:Et:219:ARG:H	1.73	0.53
6:At:818:GLN:HE21	7:Au:216:GLN:HB2	1.74	0.53
7:Cd:191:ILE:HG13	7:Cd:211:ASN:HA	1.91	0.53
5:Cp:213:GLN:O	7:Cr:170:ARG:HD2	2.09	0.53
5:Ae:219:ARG:HG3	7:An:148:PRO:HB2	1.91	0.52
5:Bn:255:LEU:HD13	5:Bn:261:VAL:HG22	1.91	0.52
6:Cx:802:LEU:HD13	7:Dm:115:MET:HG2	1.90	0.52
5:Et:264:PHE:HB3	5:Et:269:SER:HB3	1.90	0.52
7:Bp:179:LEU:HD11	7:Bp:215:ILE:CD1	2.39	0.52
5:Dd:219:ARG:HG3	7:Dm:148:PRO:HB2	1.92	0.52
5:Az:212:ILE:HD11	5:Az:254:ILE:HG13	1.91	0.52
5:Bg:264:PHE:HB3	5:Bg:269:SER:HB3	1.91	0.52
7:Cd:206:TRP:HB2	7:Cd:213:LEU:HD23	1.92	0.52
7:Eh:145:PRO:HD3	7:Eo:131:LYS:HE2	1.91	0.52
5:Dk:212:ILE:HD11	5:Dk:254:ILE:HG13	1.92	0.52
6:Cq:801:MET:HG2	7:Cy:121:PRO:HB2	1.90	0.52
7:Cy:145:PRO:HD3	7:Df:131:LYS:HE2	1.91	0.52
5:Dy:219:ARG:H	7:Eh:148:PRO:HD2	1.73	0.52
6:Eg:797:ARG:O	6:Eg:801:MET:HG3	2.10	0.52
3:Cg:1:ARG:HH22	3:Cg:3:SER:HB2	1.73	0.52
5:Cp:219:ARG:HG3	7:Cy:148:PRO:HB2	1.91	0.52
7:An:230:LEU:HD12	7:An:233:LEU:HD12	1.92	0.52
7:Cr:206:TRP:HB2	7:Cr:213:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:An:158:VAL:HG22	7:An:167:PRO:HG2	1.91	0.52
7:Cy:230:LEU:HD12	7:Cy:233:LEU:HD12	1.91	0.52
1:Cz:12:HIS:CE1	4:Dj:3:GLY:HA2	2.45	0.52
6:De:805:ALA:HB2	7:Dm:122:LEU:HD11	1.91	0.52
7:Ea:230:LEU:HD12	7:Ea:233:LEU:HD12	1.91	0.52
3:Bz:1:ARG:HH22	3:Bz:3:SER:HB2	1.74	0.51
7:Cy:158:VAL:HG22	7:Cy:167:PRO:HG2	1.91	0.51
7:Df:158:VAL:HG22	7:Df:167:PRO:HG2	1.90	0.51
3:Dp:1:ARG:HH22	3:Dp:3:SER:HB2	1.75	0.51
5:Dy:255:LEU:HD13	5:Dy:261:VAL:HG22	1.91	0.51
5:Em:219:ARG:HG3	7:Ev:148:PRO:HB2	1.93	0.51
7:Eo:206:TRP:HB2	7:Eo:213:LEU:HD23	1.93	0.51
1:Ep:2:THR:HG21	5:Et:253:ARG:HH21	1.75	0.51
2:Ap:4:MET:HG3	4:Ar:2:PHE:HE2	1.75	0.51
7:Ea:206:TRP:HB2	7:Ea:213:LEU:HD23	1.93	0.51
5:Al:219:ARG:H	7:Au:148:PRO:HD2	1.74	0.51
1:Bq:12:HIS:CE1	4:Ca:3:GLY:HA2	2.45	0.51
7:Cy:168:VAL:HG23	7:Cy:240:THR:HG23	1.93	0.51
3:Dp:2:VAL:HG11	7:Eh:129:LYS:HG2	1.92	0.51
3:Ed:2:VAL:HG11	7:Ev:129:LYS:HG2	1.93	0.51
7:An:145:PRO:HD3	7:Au:131:LYS:HE2	1.93	0.51
2:Aw:5:ILE:HA	5:Az:250:LEU:HD11	1.93	0.51
6:Bo:794:ILE:HG21	7:Cd:110:LYS:HE3	1.92	0.51
1:Dn:16:ALA:HB3	2:Dv:9:ARG:HD2	1.93	0.51
1:Ao:12:HIS:CE1	4:Ay:3:GLY:HA2	2.45	0.51
5:Et:251:GLN:HB2	5:Et:253:ARG:HG3	1.93	0.51
5:Ae:212:ILE:HD11	5:Ae:254:ILE:HG13	1.93	0.51
7:Bp:134:TYR:O	7:Bp:138:GLU:HG2	2.11	0.51
5:Em:219:ARG:H	7:Ev:148:PRO:HD2	1.74	0.51
7:Bi:158:VAL:HB	7:Bi:256:VAL:HA	1.93	0.51
6:Dl:801:MET:HG2	7:Dt:121:PRO:HB2	1.92	0.51
2:Ct:4:MET:HB3	5:Cw:250:LEU:HD13	1.93	0.51
7:Bi:145:PRO:HD3	7:Bp:131:LYS:HE2	1.93	0.50
5:Cb:212:ILE:HD11	5:Cb:254:ILE:HG13	1.93	0.50
5:Em:213:GLN:O	7:Eo:170:ARG:HD3	2.10	0.50
6:Eu:797:ARG:O	6:Eu:801:MET:HG3	2.11	0.50
7:Ag:148:PRO:HB2	5:Et:219:ARG:HG3	1.93	0.50
5:As:219:ARG:HG3	7:Bb:148:PRO:HB2	1.93	0.50
7:Ea:134:TYR:O	7:Ea:138:GLU:HG2	2.11	0.50
3:Be:2:VAL:HG11	7:Bw:129:LYS:HG2	1.92	0.50
7:Ag:129:LYS:HG2	3:Ek:2:VAL:HG11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Bz:2:VAL:HG11	7:Cr:129:LYS:HG2	1.94	0.50
7:Cy:206:TRP:HB2	7:Cy:213:LEU:HD23	1.94	0.50
1:Ce:2:THR:HG21	5:Ci:253:ARG:HH21	1.75	0.50
5:Ci:219:ARG:HG3	7:Cr:148:PRO:HB2	1.93	0.50
7:Cr:238:MET:HE2	7:Cy:178:SER:HB3	1.94	0.50
5:Cw:212:ILE:HG13	5:Cw:262:ILE:HG22	1.92	0.50
7:Dt:206:TRP:HB2	7:Dt:213:LEU:HD23	1.94	0.50
5:Al:255:LEU:HD13	5:Al:261:VAL:HG22	1.94	0.50
5:Bg:219:ARG:H	7:Bp:148:PRO:HD2	1.75	0.50
7:Bw:158:VAL:HG22	7:Bw:167:PRO:HG2	1.93	0.50
1:Cs:12:HIS:NE2	4:Dc:3:GLY:HA2	2.27	0.50
1:Cz:16:ALA:HB3	2:Dh:9:ARG:HD2	1.92	0.50
7:Bp:206:TRP:HB2	7:Bp:213:LEU:HD23	1.94	0.50
7:Eo:145:PRO:HD3	7:Ev:131:LYS:HE2	1.94	0.50
5:Bu:264:PHE:HB3	5:Bu:269:SER:HB3	1.93	0.50
7:Au:158:VAL:HG22	7:Au:167:PRO:HG2	1.93	0.50
7:Ck:158:VAL:HG22	7:Ck:167:PRO:HG2	1.94	0.50
7:Dt:158:VAL:HB	7:Dt:256:VAL:HA	1.93	0.50
3:Aj:2:VAL:HG11	7:Bb:129:LYS:HG2	1.92	0.49
5:Ci:251:GLN:HB2	5:Ci:253:ARG:HG3	1.93	0.49
5:Cw:219:ARG:H	7:Df:148:PRO:HD2	1.75	0.49
6:En:801:MET:HG2	7:Ev:121:PRO:HB2	1.94	0.49
1:Ce:12:HIS:NE2	4:Co:3:GLY:HA2	2.26	0.49
2:Ct:4:MET:HG3	5:Cw:248:ASP:HA	1.93	0.49
3:Dw:2:VAL:HG11	7:Eo:129:LYS:HG2	1.94	0.49
7:Eo:230:LEU:HD12	7:Eo:233:LEU:HD12	1.94	0.49
7:Ag:211:ASN:HD21	7:Ev:234:ASN:HD21	1.59	0.49
5:Bg:254:ILE:HB	5:Bg:262:ILE:HB	1.94	0.49
3:Cu:2:VAL:HG11	7:Dm:129:LYS:HG2	1.94	0.49
3:Di:2:VAL:HG22	3:Di:8:VAL:HG23	1.93	0.49
5:Dr:254:ILE:HB	5:Dr:262:ILE:HB	1.94	0.49
7:An:206:TRP:HB2	7:An:213:LEU:HD23	1.94	0.49
7:Cr:169:ILE:HG13	7:Cr:179:LEU:HD21	1.95	0.49
5:Ae:219:ARG:H	7:An:148:PRO:HD2	1.78	0.49
1:Eb:12:HIS:CE1	4:El:3:GLY:HA2	2.47	0.49
7:Cd:158:VAL:HB	7:Cd:256:VAL:HA	1.94	0.49
5:Cp:212:ILE:HD11	5:Cp:254:ILE:HG13	1.95	0.49
2:Ec:4:MET:HG3	5:Ef:248:ASP:HA	1.95	0.49
7:Ag:199:PRO:HG3	6:Am:819:VAL:HG13	1.95	0.49
7:Bp:145:PRO:HD3	7:Bw:131:LYS:HE2	1.95	0.49
2:By:1:CYS:HA	3:Bz:4:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dh:2:VAL:HG23	3:Di:1:ARG:HG3	1.95	0.49
3:Ax:2:VAL:HG22	3:Ax:8:VAL:HG23	1.95	0.49
5:Cb:265:SER:HB3	5:Cb:268:ASP:HB3	1.94	0.49
7:Cd:145:PRO:HD3	7:Ck:131:LYS:HE2	1.95	0.49
3:Cg:2:VAL:HG22	3:Cg:8:VAL:HG23	1.95	0.49
7:Bp:230:LEU:HD12	7:Bp:233:LEU:HD12	1.94	0.49
5:Ci:213:GLN:O	7:Ck:170:ARG:HD2	2.12	0.49
2:Cm:1:CYS:HA	3:Cn:4:ILE:HD13	1.95	0.49
7:Ag:169:ILE:HG13	7:Ag:179:LEU:HD21	1.95	0.49
7:Bp:158:VAL:HB	7:Bp:256:VAL:HA	1.95	0.49
7:Dt:158:VAL:HG22	7:Dt:167:PRO:HG2	1.95	0.49
7:Eh:158:VAL:HG22	7:Eh:167:PRO:HG2	1.94	0.49
7:Ev:206:TRP:HB2	7:Ev:213:LEU:HD23	1.94	0.49
4:Ad:3:GLY:HA2	1:Ep:12:HIS:NE2	2.28	0.48
3:Aj:1:ARG:HH22	3:Aj:3:SER:HB2	1.78	0.48
7:Bp:225:ASN:HD21	7:Bw:176:VAL:H	1.61	0.48
7:Cd:230:LEU:HD12	7:Cd:233:LEU:HD12	1.95	0.48
2:Ap:5:ILE:HD13	5:As:250:LEU:HD21	1.95	0.48
7:Bi:206:TRP:HB2	7:Bi:213:LEU:HD23	1.94	0.48
7:Cd:167:PRO:HB2	7:Cd:239:LEU:HD23	1.94	0.48
5:Et:213:GLN:O	7:Ev:170:ARG:HD2	2.13	0.48
7:Ag:206:TRP:HB2	7:Ag:213:LEU:HD23	1.95	0.48
6:Bv:820:TYR:HE1	6:Bv:822:GLU:HG2	1.78	0.48
7:An:134:TYR:O	7:An:138:GLU:HG2	2.14	0.48
5:Cb:219:ARG:HG3	7:Ck:148:PRO:HB2	1.95	0.48
7:Cy:134:TYR:O	7:Cy:138:GLU:HG2	2.13	0.48
7:Ea:225:ASN:HD21	7:Eh:176:VAL:H	1.62	0.48
1:Ah:12:HIS:NE2	4:Ar:3:GLY:HA2	2.28	0.48
3:Bs:2:VAL:HG11	7:Ck:129:LYS:HG2	1.96	0.48
7:Bw:206:TRP:HB2	7:Bw:213:LEU:HD23	1.96	0.48
1:Cl:5:ALA:HB2	2:Cm:4:MET:HE1	1.96	0.48
7:Dm:204:ILE:HG12	7:Dm:215:ILE:HG12	1.95	0.48
1:Ce:2:THR:HG21	5:Ci:253:ARG:NH2	2.29	0.48
4:Dj:2:PHE:HB3	5:Dk:251:GLN:HE21	1.79	0.48
2:Dv:4:MET:HE3	2:Dv:4:MET:HA	1.94	0.48
7:Ea:158:VAL:HB	7:Ea:256:VAL:HA	1.95	0.48
5:As:233:ARG:HG2	5:As:233:ARG:HH11	1.79	0.48
7:Ck:206:TRP:HB2	7:Ck:213:LEU:HD23	1.96	0.48
5:Dy:212:ILE:HD11	5:Dy:254:ILE:HG13	1.96	0.48
7:Ea:208:LYS:HB3	6:Eg:824:THR:H	1.79	0.48
4:Ad:3:GLY:H	1:Ep:16:ALA:HB1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Am:791:GLN:HA	6:Am:794:ILE:HD12	1.96	0.48
5:Dy:213:GLN:O	7:Ea:170:ARG:HD2	2.14	0.48
7:Eh:238:MET:HE3	7:Eo:178:SER:HB3	1.96	0.48
7:Au:145:PRO:HD3	7:Bb:131:LYS:HE2	1.96	0.47
7:Bp:179:LEU:HD23	7:Bp:254:LEU:HD11	1.96	0.47
7:Ag:131:LYS:HE2	7:Ev:145:PRO:HD3	1.97	0.47
5:Bg:253:ARG:HD2	5:Bg:263:LYS:HE2	1.96	0.47
7:Bp:178:SER:HA	7:Bp:213:LEU:O	2.14	0.47
6:Cx:791:GLN:HA	6:Cx:794:ILE:HD12	1.95	0.47
5:Dr:219:ARG:HG3	7:Ea:148:PRO:HB2	1.95	0.47
2:Ej:1:CYS:HA	3:Ek:4:ILE:HD13	1.96	0.47
3:Bl:13:LYS:HA	3:Bl:13:LYS:HD3	1.67	0.47
7:Df:168:VAL:HG23	7:Df:240:THR:HG23	1.95	0.47
3:Di:13:LYS:HD3	3:Di:13:LYS:HA	1.65	0.47
5:Dr:263:LYS:HB2	5:Dr:263:LYS:NZ	2.30	0.47
7:Ev:158:VAL:HG11	7:Ev:237:VAL:HG13	1.95	0.47
5:Al:213:GLN:HB2	5:Al:223:ILE:HG22	1.97	0.47
2:Aw:2:VAL:HG23	3:Ax:1:ARG:HG3	1.96	0.47
7:Bi:158:VAL:HG22	7:Bi:167:PRO:HG2	1.96	0.47
5:Bn:212:ILE:HD11	5:Bn:254:ILE:HG13	1.97	0.47
5:Cw:212:ILE:HD11	5:Cw:254:ILE:HG13	1.95	0.47
7:Dt:200:SER:HB3	6:Dz:816:GLU:HG3	1.97	0.47
7:Eh:206:TRP:HB2	7:Eh:213:LEU:HD23	1.97	0.47
5:Em:212:ILE:HG13	5:Em:262:ILE:HG22	1.97	0.47
3:Ac:1:ARG:HH22	3:Ac:3:SER:HB2	1.78	0.47
7:An:169:ILE:HG21	7:An:179:LEU:HD21	1.97	0.47
7:Bb:158:VAL:HB	7:Bb:256:VAL:HA	1.97	0.47
3:Cg:13:LYS:HD3	3:Cg:13:LYS:HA	1.66	0.47
5:Cp:219:ARG:H	7:Cy:148:PRO:HD2	1.78	0.47
7:Cr:190:PRO:HA	7:Cr:211:ASN:HB3	1.97	0.47
1:Cs:2:THR:HG21	5:Cw:253:ARG:HH21	1.79	0.47
5:Dd:233:ARG:HH11	5:Dd:233:ARG:HG2	1.80	0.47
5:Dk:254:ILE:HB	5:Dk:262:ILE:HB	1.97	0.47
7:Ea:115:MET:HE3	7:Ea:115:MET:HB3	1.78	0.47
2:Ej:4:MET:HG3	4:El:2:PHE:HE2	1.79	0.47
1:Ah:16:ALA:HB1	4:Ar:3:GLY:H	1.79	0.47
5:Al:212:ILE:HG13	5:Al:262:ILE:HG22	1.97	0.47
7:Au:158:VAL:HB	7:Au:256:VAL:HA	1.97	0.47
3:Be:13:LYS:HA	3:Be:13:LYS:HD3	1.65	0.47
3:Db:2:VAL:HG22	3:Db:8:VAL:HG23	1.97	0.47
2:Dv:5:ILE:HA	5:Dy:250:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Eo:167:PRO:HB2	7:Eo:239:LEU:HD23	1.95	0.47
7:Ag:145:PRO:HD3	7:An:131:LYS:HE2	1.97	0.47
7:Bi:231:ARG:HD3	7:Bi:231:ARG:HA	1.79	0.47
7:Cy:158:VAL:HB	7:Cy:256:VAL:HA	1.97	0.47
7:Df:230:LEU:HD12	7:Df:233:LEU:HD12	1.97	0.47
2:Dh:4:MET:HG3	4:Dj:2:PHE:HE2	1.79	0.47
3:Aj:13:LYS:HD3	3:Aj:13:LYS:HA	1.67	0.46
5:Az:254:ILE:HB	5:Az:262:ILE:HB	1.97	0.46
3:Cn:12:LYS:O	3:Cn:13:LYS:HD2	2.15	0.46
2:Da:4:MET:HG3	4:Dc:2:PHE:HE2	1.80	0.46
7:Df:225:ASN:HD21	7:Dm:176:VAL:H	1.63	0.46
7:Dt:144:THR:OG1	7:Dt:148:PRO:HG3	2.16	0.46
5:Dy:212:ILE:HG13	5:Dy:262:ILE:HG22	1.97	0.46
7:Ev:158:VAL:HB	7:Ev:256:VAL:HA	1.97	0.46
3:Ac:12:LYS:O	3:Ac:13:LYS:HD2	2.14	0.46
7:Bi:168:VAL:HG23	7:Bi:240:THR:HG23	1.96	0.46
5:Al:253:ARG:HD2	5:Al:263:LYS:HE2	1.97	0.46
7:An:158:VAL:HB	7:An:256:VAL:HA	1.98	0.46
5:Bg:219:ARG:HG3	7:Bp:148:PRO:HB2	1.97	0.46
7:Bp:125:GLU:O	7:Bp:128:VAL:HG22	2.16	0.46
7:Cr:125:GLU:O	7:Cr:128:VAL:HG22	2.15	0.46
7:Cr:238:MET:HE3	7:Cy:250:TYR:O	2.15	0.46
7:Dt:168:VAL:HG23	7:Dt:240:THR:HG23	1.96	0.46
2:Ej:5:ILE:HA	5:Em:250:LEU:HD11	1.98	0.46
6:Af:798:THR:HG23	7:Au:115:MET:HB2	1.97	0.46
5:Al:212:ILE:HD11	5:Al:254:ILE:HG13	1.98	0.46
7:Au:230:LEU:HD12	7:Au:233:LEU:HD12	1.97	0.46
3:Ax:13:LYS:HA	3:Ax:13:LYS:HD3	1.66	0.46
5:Ci:212:ILE:HG13	5:Ci:262:ILE:HG22	1.97	0.46
7:Dt:223:TYR:HB3	7:Dt:242:ILE:HG23	1.98	0.46
2:Eq:5:ILE:HA	5:Et:250:LEU:HD11	1.98	0.46
5:Bn:213:GLN:O	7:Bp:170:ARG:HD2	2.15	0.46
6:Bv:813:LYS:HD3	7:Cd:134:TYR:HE1	1.81	0.46
5:Dd:212:ILE:HD11	5:Dd:254:ILE:HG13	1.98	0.46
6:De:794:ILE:HG21	7:Dt:110:LYS:HD2	1.98	0.46
6:Eu:791:GLN:HA	6:Eu:794:ILE:HD12	1.96	0.46
6:Af:794:ILE:HG21	7:Au:110:LYS:HD2	1.98	0.46
6:Cc:801:MET:HG2	7:Ck:121:PRO:HB2	1.97	0.46
7:Cr:145:PRO:HD3	7:Cy:131:LYS:HE2	1.98	0.46
7:Cy:208:LYS:HB3	6:De:824:THR:H	1.81	0.46
7:Dm:158:VAL:HB	7:Dm:256:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:An:144:THR:OG1	7:An:148:PRO:HG3	2.16	0.46
7:Au:206:TRP:HB2	7:Au:213:LEU:HD23	1.98	0.46
7:Au:225:ASN:HD21	7:Bb:176:VAL:H	1.64	0.46
1:Cl:12:HIS:NE2	4:Cv:3:GLY:HA2	2.30	0.46
7:Cy:144:THR:OG1	7:Cy:148:PRO:HG3	2.16	0.46
7:Cy:169:ILE:HG21	7:Cy:179:LEU:HD21	1.98	0.46
7:Df:145:PRO:HD3	7:Dm:131:LYS:HE2	1.98	0.46
7:Ev:231:ARG:HD3	7:Ev:231:ARG:HA	1.79	0.46
7:Ag:115:MET:HE3	7:Ag:115:MET:HB3	1.85	0.46
7:Au:134:TYR:O	7:Au:138:GLU:HG2	2.16	0.46
5:Az:255:LEU:HD13	5:Az:261:VAL:HG22	1.97	0.46
5:Bu:268:ASP:O	7:Bw:247:ALA:HB2	2.16	0.46
7:Eh:125:GLU:O	7:Eh:128:VAL:HG22	2.16	0.46
1:Ep:2:THR:HG21	5:Et:253:ARG:NH2	2.30	0.46
7:An:208:LYS:HB3	6:At:824:THR:H	1.81	0.46
7:Ck:158:VAL:HB	7:Ck:256:VAL:HA	1.97	0.46
7:Cy:125:GLU:O	7:Cy:128:VAL:HG22	2.16	0.46
7:Df:158:VAL:HB	7:Df:256:VAL:HA	1.98	0.46
5:Az:212:ILE:HG13	5:Az:262:ILE:HG22	1.99	0.45
7:Au:151:PRO:HA	7:Au:248:VAL:HG13	1.97	0.45
2:Cm:5:ILE:HD13	2:Cm:5:ILE:HA	1.79	0.45
7:Df:206:TRP:HB2	7:Df:213:LEU:HD23	1.98	0.45
7:Ag:158:VAL:HB	7:Ag:256:VAL:HA	1.99	0.45
7:Bb:206:TRP:HB2	7:Bb:213:LEU:HD23	1.98	0.45
5:Bn:219:ARG:H	7:Bw:148:PRO:HD2	1.80	0.45
3:Bz:13:LYS:HD3	3:Bz:13:LYS:HA	1.66	0.45
6:En:795:GLN:H	6:En:795:GLN:HG2	1.56	0.45
6:Bh:802:LEU:HD12	6:Bh:802:LEU:HA	1.84	0.45
7:Cd:125:GLU:O	7:Cd:128:VAL:HG22	2.16	0.45
7:Df:151:PRO:HA	7:Df:248:VAL:HG13	1.98	0.45
7:Bw:125:GLU:O	7:Bw:128:VAL:HG22	2.17	0.45
2:Da:5:ILE:HA	5:Dd:250:LEU:HD11	1.97	0.45
7:Df:134:TYR:O	7:Df:138:GLU:HG2	2.17	0.45
5:As:212:ILE:HD11	5:As:254:ILE:HG13	1.98	0.45
5:Dk:255:LEU:HD13	5:Dk:261:VAL:HG22	1.97	0.45
7:Ea:144:THR:OG1	7:Ea:148:PRO:HG3	2.16	0.45
7:Bp:151:PRO:HA	7:Bp:248:VAL:HG13	1.99	0.45
7:Ck:145:PRO:HD3	7:Cr:131:LYS:HE2	1.99	0.45
5:Et:212:ILE:HD11	5:Et:254:ILE:HG13	1.99	0.45
2:Cm:5:ILE:HG21	7:Cy:140:ALA:HB2	1.98	0.45
7:Df:125:GLU:O	7:Df:128:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Dl:794:ILE:HG23	7:Ea:110:LYS:HZ3	1.82	0.45
7:Ea:125:GLU:O	7:Ea:128:VAL:HG22	2.16	0.45
7:Ea:174:GLY:HA2	7:Ea:216:GLN:HE21	1.82	0.45
7:Ea:203:ASN:O	7:Ea:215:ILE:HA	2.16	0.45
7:Ea:231:ARG:HD3	7:Ea:231:ARG:HA	1.79	0.45
7:Eo:144:THR:OG1	7:Eo:148:PRO:HG3	2.17	0.45
2:Ap:1:CYS:HA	3:Aq:4:ILE:HD13	1.98	0.45
7:Au:125:GLU:O	7:Au:128:VAL:HG22	2.17	0.45
7:Bb:145:PRO:HD3	7:Bi:131:LYS:HE2	1.99	0.45
7:Bp:115:MET:HE3	7:Bp:115:MET:HB3	1.79	0.45
7:Bp:149:PRO:HB2	7:Bp:248:VAL:HG12	1.99	0.45
1:Cs:4:ALA:HB2	3:Cu:14:TYR:HB2	1.99	0.45
2:Dh:5:ILE:HA	5:Dk:250:LEU:HD11	1.99	0.45
7:Bb:134:TYR:O	7:Bb:138:GLU:HG2	2.17	0.45
7:Cd:189:TRP:HE1	7:Cd:232:GLY:H	1.64	0.45
7:Eh:124:PRO:O	7:Eh:128:VAL:HG13	2.17	0.45
7:Ev:113:LYS:HA	7:Ev:113:LYS:HD3	1.81	0.45
7:Ev:167:PRO:HD2	7:Ev:238:MET:O	2.17	0.45
5:Ae:216:ILE:HG12	5:Ae:221:TRP:HZ3	1.83	0.44
7:Bi:144:THR:OG1	7:Bi:148:PRO:HG3	2.17	0.44
1:Bj:16:ALA:HB3	2:Br:9:ARG:HD2	1.98	0.44
7:Ea:145:PRO:HD3	7:Eh:131:LYS:HE2	1.99	0.44
7:Eh:113:LYS:HA	7:Eh:113:LYS:HD3	1.82	0.44
1:Aa:12:HIS:NE2	4:Ak:3:GLY:HA2	2.32	0.44
7:Ag:125:GLU:O	7:Ag:128:VAL:HG22	2.17	0.44
7:Cd:144:THR:OG1	7:Cd:148:PRO:HG3	2.17	0.44
2:Cf:1:CYS:HA	3:Cg:4:ILE:HD13	1.99	0.44
7:Ck:125:GLU:O	7:Ck:128:VAL:HG22	2.16	0.44
7:Cy:225:ASN:HD21	7:Df:176:VAL:N	2.16	0.44
2:Da:1:CYS:HA	3:Db:4:ILE:HD13	1.99	0.44
7:Dm:124:PRO:O	7:Dm:128:VAL:HG13	2.17	0.44
2:Do:1:CYS:HA	3:Dp:4:ILE:HD13	2.00	0.44
2:Dv:2:VAL:HG23	3:Dw:1:ARG:HG3	1.98	0.44
7:Ea:178:SER:O	7:Ea:251:ARG:HA	2.17	0.44
5:Et:212:ILE:HG13	5:Et:262:ILE:HG22	1.99	0.44
5:Ae:255:LEU:HD13	5:Ae:261:VAL:HG22	1.99	0.44
7:Ag:230:LEU:HD12	7:Ag:233:LEU:HD12	1.99	0.44
7:An:113:LYS:HA	7:An:113:LYS:HD3	1.81	0.44
5:Bu:213:GLN:O	7:Bw:170:ARG:HD2	2.17	0.44
7:Cr:230:LEU:HD12	7:Cr:233:LEU:HD12	1.99	0.44
5:Bu:255:LEU:HD13	5:Bu:261:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Dm:145:PRO:HD3	7:Dt:131:LYS:HE2	1.99	0.44
2:Br:4:MET:HG3	5:Bu:248:ASP:HA	1.98	0.44
7:Cy:231:ARG:HD3	7:Cy:231:ARG:HA	1.81	0.44
2:Ej:5:ILE:HD13	5:Em:250:LEU:HD21	1.99	0.44
7:Eo:125:GLU:O	7:Eo:128:VAL:HG22	2.17	0.44
2:Ab:1:CYS:HA	3:Ac:4:ILE:HD13	1.99	0.44
2:Ap:5:ILE:HA	5:As:250:LEU:HD11	1.99	0.44
7:Au:225:ASN:HD21	7:Bb:176:VAL:N	2.16	0.44
7:Ag:208:LYS:HB3	6:Am:824:THR:H	1.82	0.44
3:Dp:13:LYS:HA	3:Dp:13:LYS:HD3	1.65	0.44
5:Ef:213:GLN:O	7:Eh:170:ARG:HD2	2.18	0.44
7:Ev:125:GLU:O	7:Ev:128:VAL:HG22	2.17	0.44
1:Ao:4:ALA:HB2	3:Aq:14:TYR:HB2	1.98	0.44
7:Bb:189:TRP:HE1	7:Bb:232:GLY:H	1.66	0.44
5:Bn:212:ILE:HG13	5:Bn:262:ILE:HG22	1.98	0.44
7:Cr:158:VAL:HB	7:Cr:256:VAL:HA	2.00	0.44
5:Dr:243:MET:HE2	5:Dr:243:MET:HB3	1.80	0.44
5:Ef:255:LEU:HD13	5:Ef:261:VAL:HG22	1.99	0.44
2:Eq:1:CYS:HA	3:Er:4:ILE:HD13	1.99	0.44
3:Bs:13:LYS:HA	3:Bs:13:LYS:HD3	1.65	0.44
6:Eg:813:LYS:HD3	7:Eo:134:TYR:HE1	1.82	0.44
7:Eh:134:TYR:O	7:Eh:138:GLU:HG2	2.18	0.44
7:Eh:158:VAL:HB	7:Eh:256:VAL:HA	1.99	0.44
7:Eo:189:TRP:HE1	7:Eo:232:GLY:H	1.66	0.44
7:An:129:LYS:HG2	3:Er:2:VAL:HG11	1.99	0.43
7:Bp:180:VAL:HG12	7:Bp:212:THR:OG1	2.18	0.43
3:Db:13:LYS:HD3	3:Db:13:LYS:HA	1.65	0.43
4:Ad:1:PRO:HA	3:Er:5:GLY:CA	2.48	0.43
7:Ag:214:MET:HE3	7:Ev:195:ASP:HB2	2.00	0.43
7:An:125:GLU:O	7:An:128:VAL:HG22	2.18	0.43
7:Bp:158:VAL:HG22	7:Bp:167:PRO:HG2	1.99	0.43
6:Cq:798:THR:HG23	7:Df:115:MET:HB2	1.99	0.43
7:Cr:158:VAL:HG22	7:Cr:167:PRO:HG2	2.00	0.43
3:Dw:2:VAL:HG21	7:Eo:129:LYS:CG	2.48	0.43
5:Em:255:LEU:HD13	5:Em:261:VAL:HG22	1.99	0.43
2:Eq:4:MET:HG3	5:Et:248:ASP:HA	2.00	0.43
7:Au:233:LEU:HD23	7:Au:233:LEU:HA	1.91	0.43
5:Bu:213:GLN:HB2	5:Bu:223:ILE:HG22	2.00	0.43
3:Dw:13:LYS:HD3	3:Dw:13:LYS:HA	1.67	0.43
6:Dz:791:GLN:HA	6:Dz:794:ILE:HD12	2.00	0.43
7:Ea:196:LEU:HD13	7:Ea:204:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ef:268:ASP:O	7:Eh:247:ALA:HB2	2.17	0.43
2:Ej:2:VAL:HG23	3:Ek:1:ARG:HG3	2.00	0.43
1:Du:12:HIS:NE2	4:Ee:3:GLY:HA2	2.33	0.43
7:Ea:151:PRO:HA	7:Ea:248:VAL:HG13	1.99	0.43
7:Ea:189:TRP:HE1	7:Ea:232:GLY:H	1.66	0.43
3:Aq:13:LYS:HA	3:Aq:13:LYS:HD3	1.65	0.43
7:Cd:179:LEU:HD12	7:Cd:215:ILE:HD11	2.00	0.43
7:Ck:151:PRO:HA	7:Ck:248:VAL:HG13	2.01	0.43
7:Dt:113:LYS:HA	7:Dt:113:LYS:HD3	1.83	0.43
3:Er:13:LYS:HD3	3:Er:13:LYS:HA	1.65	0.43
5:As:233:ARG:HG2	5:As:233:ARG:NH1	2.34	0.43
6:Bv:797:ARG:O	6:Bv:801:MET:HG3	2.18	0.43
5:Cp:255:LEU:HD13	5:Cp:261:VAL:HG22	2.00	0.43
6:Eg:820:TYR:HE1	6:Eg:822:GLU:HG2	1.82	0.43
7:Eo:190:PRO:HB2	7:Eo:231:ARG:HG2	2.00	0.43
5:Az:243:MET:HE2	5:Az:243:MET:HB3	1.90	0.43
7:Cy:189:TRP:CZ2	7:Cy:233:LEU:HG	2.54	0.43
5:Dk:212:ILE:HG13	5:Dk:262:ILE:HG22	2.00	0.43
7:Dm:189:TRP:HE1	7:Dm:232:GLY:H	1.67	0.43
7:Ea:124:PRO:O	7:Ea:128:VAL:HG13	2.18	0.43
5:Ef:213:GLN:HB2	5:Ef:223:ILE:HG22	2.00	0.43
1:Ep:1:CYS:HB3	1:Ep:2:THR:H	1.61	0.43
5:Ae:212:ILE:HG13	5:Ae:262:ILE:HG22	1.99	0.43
7:Au:124:PRO:O	7:Au:128:VAL:HG13	2.19	0.43
7:Bi:125:GLU:O	7:Bi:128:VAL:HG22	2.19	0.43
7:Cd:190:PRO:HB2	7:Cd:231:ARG:HG2	2.00	0.43
5:Cw:263:LYS:HE3	5:Cw:263:LYS:HB3	1.77	0.43
7:Dt:134:TYR:O	7:Dt:138:GLU:HG2	2.18	0.43
7:Eh:230:LEU:HD12	7:Eh:233:LEU:HD12	2.00	0.43
5:Bg:268:ASP:O	7:Bi:247:ALA:HB2	2.19	0.43
7:Bp:229:ARG:HG2	7:Bp:236:PRO:HB3	2.00	0.43
7:Cd:134:TYR:O	7:Cd:138:GLU:HG2	2.19	0.43
7:Cd:178:SER:HA	7:Cd:213:LEU:O	2.18	0.43
7:Dm:134:TYR:O	7:Dm:138:GLU:HG2	2.18	0.43
7:Dt:125:GLU:O	7:Dt:128:VAL:HG22	2.19	0.43
2:Dv:5:ILE:HD13	5:Dy:250:LEU:HD21	2.00	0.43
7:Ag:181:PHE:CE2	7:Ag:191:ILE:HD11	2.54	0.43
5:Cb:212:ILE:HG13	5:Cb:262:ILE:HG22	2.00	0.43
6:Cc:795:GLN:H	6:Cc:795:GLN:HG2	1.56	0.43
7:Cd:231:ARG:HD3	7:Cd:231:ARG:HA	1.82	0.43
3:Ed:13:LYS:HA	3:Ed:13:LYS:HD3	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Eg:801:MET:HG2	7:Eo:121:PRO:HB2	2.01	0.43
7:Au:238:MET:HE3	7:Bb:178:SER:HB3	2.01	0.42
5:Bg:222:LEU:HD21	5:Bg:254:ILE:HD12	2.00	0.42
7:Cy:233:LEU:HD23	7:Cy:233:LEU:HA	1.89	0.42
7:Dm:195:ASP:HB3	7:Dm:227:ALA:HB3	2.00	0.42
7:Dt:151:PRO:HA	7:Dt:248:VAL:HG13	2.01	0.42
3:Ed:2:VAL:HG21	7:Ev:129:LYS:CG	2.49	0.42
3:Ek:13:LYS:HA	3:Ek:13:LYS:HD3	1.66	0.42
7:Eo:158:VAL:HG22	7:Eo:167:PRO:HG2	2.00	0.42
3:Ac:2:VAL:HG11	7:Au:129:LYS:HG2	2.00	0.42
7:An:189:TRP:CZ2	7:An:233:LEU:HG	2.54	0.42
7:Au:113:LYS:HA	7:Au:113:LYS:HD3	1.82	0.42
7:Bb:125:GLU:O	7:Bb:128:VAL:HG22	2.20	0.42
1:Bj:3:ASP:OD2	3:Bl:16:ASP:HB2	2.19	0.42
3:Bl:2:VAL:HG21	7:Cd:129:LYS:CG	2.49	0.42
6:Bo:801:MET:HE1	7:Cd:112:PHE:HA	2.00	0.42
7:Bp:189:TRP:HE1	7:Bp:232:GLY:H	1.66	0.42
5:Cb:255:LEU:HD13	5:Cb:261:VAL:HG22	1.99	0.42
5:Ci:212:ILE:HD11	5:Ci:254:ILE:HG13	2.01	0.42
5:Cp:216:ILE:HG12	5:Cp:221:TRP:HZ3	1.83	0.42
5:Dr:268:ASP:O	7:Dt:247:ALA:HB2	2.19	0.42
7:Ea:180:VAL:HG12	7:Ea:212:THR:OG1	2.18	0.42
7:Bp:124:PRO:O	7:Bp:128:VAL:HG13	2.19	0.42
7:Cr:181:PHE:CE2	7:Cr:191:ILE:HD11	2.54	0.42
7:Cr:208:LYS:HB3	6:Cx:824:THR:H	1.85	0.42
1:Cs:2:THR:HG21	5:Cw:253:ARG:NH2	2.34	0.42
5:Dk:268:ASP:O	7:Dm:247:ALA:HB2	2.20	0.42
7:Dt:149:PRO:HB2	7:Dt:248:VAL:HG12	2.00	0.42
7:Ea:233:LEU:HD23	7:Ea:233:LEU:HA	1.89	0.42
7:Ag:188:PRO:HB3	7:Ag:211:ASN:ND2	2.34	0.42
7:Ag:204:ILE:HG12	7:Ag:215:ILE:CG1	2.48	0.42
7:Bp:182:LEU:HD12	7:Bp:255:ARG:HD3	2.00	0.42
5:Cb:233:ARG:HB2	7:Ck:147:THR:HG21	2.00	0.42
5:Em:233:ARG:HB2	7:Ev:147:THR:HG21	2.02	0.42
7:Dt:189:TRP:HE1	7:Dt:232:GLY:H	1.67	0.42
7:Ea:182:LEU:HD12	7:Ea:255:ARG:HD3	2.01	0.42
5:As:212:ILE:HG13	5:As:262:ILE:HG22	2.02	0.42
5:Az:268:ASP:O	7:Bb:247:ALA:HB2	2.20	0.42
7:Bb:124:PRO:O	7:Bb:128:VAL:HG13	2.20	0.42
7:Bp:144:THR:OG1	7:Bp:148:PRO:HG3	2.19	0.42
7:Bp:208:LYS:HB3	6:Bv:824:THR:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Df:144:THR:OG1	7:Df:148:PRO:HG3	2.19	0.42
7:Dm:125:GLU:O	7:Dm:128:VAL:HG22	2.19	0.42
7:Eo:134:TYR:O	7:Eo:138:GLU:HG2	2.20	0.42
5:As:255:LEU:HD13	5:As:261:VAL:HG22	2.01	0.42
5:Bg:243:MET:HE2	5:Bg:243:MET:HB3	1.80	0.42
7:Bp:179:LEU:O	7:Bp:212:THR:HA	2.20	0.42
5:Dd:233:ARG:HG2	5:Dd:233:ARG:NH1	2.35	0.42
7:Df:238:MET:HE3	7:Dm:178:SER:HB3	2.02	0.42
7:Dm:208:LYS:HA	7:Dm:208:LYS:HD2	1.91	0.42
7:Bi:189:TRP:CZ2	7:Bi:233:LEU:HG	2.55	0.42
7:Bp:174:GLY:HA2	7:Bp:216:GLN:HE21	1.85	0.42
7:Bw:158:VAL:HB	7:Bw:256:VAL:HA	2.02	0.42
7:Ck:167:PRO:HD2	7:Ck:238:MET:O	2.20	0.42
5:Cp:212:ILE:HG13	5:Cp:262:ILE:HG22	2.01	0.42
3:Cu:13:LYS:HA	3:Cu:13:LYS:HD3	1.66	0.42
5:Bg:212:ILE:HD11	5:Bg:254:ILE:HG13	2.01	0.42
7:Bi:189:TRP:HE1	7:Bi:232:GLY:H	1.66	0.42
7:Bi:200:SER:HB3	6:Bo:816:GLU:HG3	2.02	0.42
7:Bw:169:ILE:HG21	7:Bw:179:LEU:HD21	2.02	0.42
7:Df:225:ASN:HD21	7:Dm:176:VAL:N	2.17	0.42
6:Ds:802:LEU:HD12	6:Ds:802:LEU:HA	1.84	0.42
7:Ev:151:PRO:HA	7:Ev:248:VAL:HG13	2.01	0.42
7:Bb:113:LYS:HA	7:Bb:113:LYS:HD3	1.83	0.42
7:Ea:149:PRO:HB2	7:Ea:248:VAL:HG12	2.00	0.42
7:Eh:169:ILE:HG21	7:Eh:179:LEU:HD21	2.01	0.42
7:Eh:233:LEU:HD23	7:Eh:233:LEU:HA	1.89	0.42
7:Eo:149:PRO:HB2	7:Eo:248:VAL:HG12	2.02	0.42
1:Ao:16:ALA:HA	4:Ay:3:GLY:HA3	2.02	0.41
7:Ea:225:ASN:HD21	7:Eh:176:VAL:N	2.18	0.41
6:En:820:TYR:CE1	6:En:822:GLU:HG2	2.54	0.41
7:Ev:233:LEU:HD23	7:Ev:233:LEU:HA	1.91	0.41
7:An:225:ASN:HD21	7:Au:176:VAL:N	2.17	0.41
7:Au:231:ARG:HD3	7:Au:231:ARG:HA	1.77	0.41
7:Bi:167:PRO:HD2	7:Bi:238:MET:O	2.20	0.41
7:Ck:158:VAL:HG11	7:Ck:237:VAL:HG13	2.02	0.41
5:Dk:243:MET:HE2	5:Dk:243:MET:HB3	1.85	0.41
7:Ev:189:TRP:CZ2	7:Ev:233:LEU:HG	2.55	0.41
7:Bb:231:ARG:HD3	7:Bb:231:ARG:HA	1.94	0.41
7:Bi:169:ILE:HG21	7:Bi:179:LEU:HD21	2.03	0.41
3:Cg:2:VAL:HG11	7:Cy:129:LYS:HG2	2.02	0.41
5:Dd:268:ASP:O	7:Df:247:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dh:4:MET:HE3	4:Dj:2:PHE:CZ	2.55	0.41
7:Dm:181:PHE:CD2	7:Dm:191:ILE:HD11	2.55	0.41
7:Eo:113:LYS:HA	7:Eo:113:LYS:HD3	1.85	0.41
7:Ag:107:ILE:HA	7:Ag:110:LYS:HE2	2.02	0.41
7:Bp:166:PRO:HA	7:Bp:167:PRO:HD3	1.97	0.41
6:De:805:ALA:HA	6:De:808:LEU:HB2	2.02	0.41
7:Df:149:PRO:HB2	7:Df:248:VAL:HG12	2.02	0.41
5:As:268:ASP:O	7:Au:247:ALA:HB2	2.21	0.41
1:Bj:2:THR:HG21	5:Bn:253:ARG:NH2	2.34	0.41
7:Bp:225:ASN:HD21	7:Bw:176:VAL:N	2.19	0.41
5:Ci:263:LYS:HB3	5:Ci:263:LYS:HE3	1.86	0.41
7:Ck:149:PRO:HB2	7:Ck:248:VAL:HG12	2.03	0.41
7:Cr:215:ILE:HD12	7:Cr:215:ILE:N	2.35	0.41
7:Df:233:LEU:HD23	7:Df:233:LEU:HA	1.91	0.41
6:Dl:794:ILE:CG2	7:Ea:110:LYS:HZ3	2.33	0.41
7:Dt:189:TRP:CZ2	7:Dt:233:LEU:HG	2.55	0.41
5:Dy:243:MET:HE2	5:Dy:243:MET:HB3	1.76	0.41
7:Ea:229:ARG:HG2	7:Ea:236:PRO:HB3	2.02	0.41
7:Ag:167:PRO:HB2	7:Ag:239:LEU:HD23	2.02	0.41
7:Au:199:PRO:HG2	6:Ba:816:GLU:HG2	2.01	0.41
2:Aw:4:MET:HG2	5:Az:248:ASP:HA	2.03	0.41
7:Bw:230:LEU:HD12	7:Bw:233:LEU:HD12	2.03	0.41
1:Cz:4:ALA:HB2	3:Db:14:TYR:HB2	2.03	0.41
7:Dm:158:VAL:HG22	7:Dm:167:PRO:HG2	2.03	0.41
7:Ea:113:LYS:HA	7:Ea:113:LYS:HD3	1.82	0.41
7:Ag:113:LYS:HA	7:Ag:113:LYS:HD3	1.84	0.41
7:Au:189:TRP:CZ2	7:Au:233:LEU:HG	2.56	0.41
5:Az:219:ARG:H	7:Bi:148:PRO:HD2	1.84	0.41
7:Cr:115:MET:HE3	7:Cr:115:MET:HB3	1.92	0.41
7:Dm:166:PRO:HA	7:Dm:167:PRO:HD3	1.98	0.41
7:Eo:151:PRO:HA	7:Eo:248:VAL:HG13	2.01	0.41
7:Bp:202:PHE:HB3	7:Bp:215:ILE:CG2	2.50	0.41
3:Bz:2:VAL:HG21	7:Cr:129:LYS:CG	2.51	0.41
7:Cd:174:GLY:HA2	7:Cd:216:GLN:HE21	1.86	0.41
3:Cn:2:VAL:HG11	7:Df:129:LYS:HG2	2.02	0.41
5:Dd:212:ILE:HG13	5:Dd:262:ILE:HG22	2.02	0.41
7:Eh:231:ARG:HD3	7:Eh:231:ARG:HA	1.79	0.41
6:Af:801:MET:HE1	7:Au:112:PHE:HA	2.03	0.41
7:Ag:195:ASP:HB2	6:Am:820:TYR:HD1	1.86	0.41
7:An:181:PHE:CD2	7:An:191:ILE:HD11	2.56	0.41
7:Bb:204:ILE:HG12	7:Bb:215:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Bh:820:TYR:HE1	6:Bh:822:GLU:HG2	1.86	0.41
7:Bi:223:TYR:HB3	7:Bi:242:ILE:HG23	2.02	0.41
3:Bl:1:ARG:HG2	3:Bl:2:VAL:N	2.35	0.41
6:Bo:820:TYR:HE1	6:Bo:822:GLU:HG2	1.85	0.41
7:Bp:189:TRP:CZ2	7:Bp:233:LEU:HG	2.56	0.41
7:Bw:134:TYR:O	7:Bw:138:GLU:HG2	2.21	0.41
5:Cb:237:LYS:HA	5:Cb:237:LYS:HD3	1.95	0.41
7:Cy:181:PHE:CD2	7:Cy:191:ILE:HD11	2.56	0.41
3:Db:2:VAL:HG11	7:Dt:129:LYS:HG2	2.03	0.41
7:Df:195:ASP:O	7:Df:226:LEU:HD12	2.21	0.41
5:Dr:212:ILE:HD11	5:Dr:254:ILE:HG13	2.03	0.41
7:Ea:189:TRP:CZ2	7:Ea:233:LEU:HG	2.56	0.41
7:Ag:178:SER:HB3	7:Ag:214:MET:SD	2.61	0.41
7:An:196:LEU:HD22	7:An:204:ILE:HG13	2.03	0.41
7:An:233:LEU:HD23	7:An:233:LEU:HA	1.89	0.41
5:Dd:255:LEU:HD13	5:Dd:261:VAL:HG22	2.02	0.41
7:Df:166:PRO:HA	7:Df:167:PRO:HD3	1.99	0.41
1:Dg:4:ALA:HB2	3:Di:14:TYR:HB2	2.03	0.41
7:Au:149:PRO:HB2	7:Au:248:VAL:HG12	2.03	0.40
5:Cb:218:GLY:HA3	7:Ck:148:PRO:HD3	2.03	0.40
2:Ct:1:CYS:HA	3:Cu:4:ILE:HD13	2.02	0.40
2:Ct:2:VAL:HG23	3:Cu:1:ARG:HD2	2.04	0.40
7:Df:189:TRP:CZ2	7:Df:233:LEU:HG	2.56	0.40
6:Ds:820:TYR:HE1	6:Ds:822:GLU:HG2	1.86	0.40
3:Aq:2:VAL:HG11	7:Bi:129:LYS:HG2	2.03	0.40
5:Dk:219:ARG:H	7:Dt:148:PRO:HD2	1.85	0.40
3:Dp:2:VAL:HG13	3:Dp:8:VAL:HA	2.03	0.40
3:Dw:1:ARG:HH22	3:Dw:3:SER:HB2	1.86	0.40
5:Ef:219:ARG:H	7:Eo:148:PRO:HD2	1.87	0.40
1:Ep:4:ALA:HB2	3:Er:14:TYR:HB2	2.03	0.40
7:Ag:129:LYS:CG	3:Ek:2:VAL:HG21	2.51	0.40
3:Be:2:VAL:HG21	7:Bw:129:LYS:CG	2.51	0.40
5:Cw:213:GLN:HB2	5:Cw:223:ILE:HG22	2.04	0.40
7:Ea:158:VAL:HG22	7:Ea:167:PRO:HG2	2.02	0.40
7:Ag:147:THR:HG21	5:Et:233:ARG:HB2	2.03	0.40
7:Au:168:VAL:HA	7:Au:240:THR:HG23	2.03	0.40
7:Cd:158:VAL:HG22	7:Cd:167:PRO:HG2	2.04	0.40
7:Cd:223:TYR:HB3	7:Cd:242:ILE:HG23	2.03	0.40
7:Dt:129:LYS:O	7:Dt:133:ILE:HG13	2.21	0.40
1:Eb:4:ALA:HB2	3:Ed:14:TYR:HB2	2.03	0.40
5:Bn:233:ARG:HB2	7:Bw:147:THR:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cu:2:VAL:HG22	3:Cu:8:VAL:HG23	2.04	0.40
7:Df:181:PHE:CE2	7:Df:191:ILE:HD11	2.57	0.40
1:Du:16:ALA:HB3	2:Ec:9:ARG:HD2	2.03	0.40
7:Eh:192:ALA:HB2	7:Eh:231:ARG:HD3	2.04	0.40
5:Em:218:GLY:HA3	7:Ev:148:PRO:HD3	2.04	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	14/16 (88%)	14 (100%)	0	0	100	100
1	Ah	14/16 (88%)	14 (100%)	0	0	100	100
1	Ao	14/16 (88%)	14 (100%)	0	0	100	100
1	Av	14/16 (88%)	14 (100%)	0	0	100	100
1	Bc	14/16 (88%)	14 (100%)	0	0	100	100
1	Bj	14/16 (88%)	14 (100%)	0	0	100	100
1	Bq	14/16 (88%)	14 (100%)	0	0	100	100
1	Bx	14/16 (88%)	14 (100%)	0	0	100	100
1	Ce	14/16 (88%)	14 (100%)	0	0	100	100
1	Cl	14/16 (88%)	14 (100%)	0	0	100	100
1	Cs	14/16 (88%)	14 (100%)	0	0	100	100
1	Cz	14/16 (88%)	14 (100%)	0	0	100	100
1	Dg	14/16 (88%)	14 (100%)	0	0	100	100
1	Dn	14/16 (88%)	14 (100%)	0	0	100	100
1	Du	14/16 (88%)	14 (100%)	0	0	100	100
1	Eb	14/16 (88%)	14 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ei	14/16 (88%)	14 (100%)	0	0	100	100
1	Ep	14/16 (88%)	14 (100%)	0	0	100	100
2	Ab	7/9 (78%)	7 (100%)	0	0	100	100
2	Ai	7/9 (78%)	7 (100%)	0	0	100	100
2	Ap	7/9 (78%)	7 (100%)	0	0	100	100
2	Aw	7/9 (78%)	7 (100%)	0	0	100	100
2	Bd	7/9 (78%)	7 (100%)	0	0	100	100
2	Bk	7/9 (78%)	7 (100%)	0	0	100	100
2	Br	7/9 (78%)	7 (100%)	0	0	100	100
2	By	7/9 (78%)	7 (100%)	0	0	100	100
2	Cf	7/9 (78%)	7 (100%)	0	0	100	100
2	Cm	7/9 (78%)	7 (100%)	0	0	100	100
2	Ct	7/9 (78%)	7 (100%)	0	0	100	100
2	Da	7/9 (78%)	7 (100%)	0	0	100	100
2	Dh	7/9 (78%)	7 (100%)	0	0	100	100
2	Do	7/9 (78%)	7 (100%)	0	0	100	100
2	Dv	7/9 (78%)	7 (100%)	0	0	100	100
2	Ec	7/9 (78%)	7 (100%)	0	0	100	100
2	Ej	7/9 (78%)	7 (100%)	0	0	100	100
2	Eq	7/9 (78%)	7 (100%)	0	0	100	100
3	Ac	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Aj	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Aq	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Ax	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Be	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Bl	14/16 (88%)	12 (86%)	2 (14%)	0	100	100
3	Bs	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Bz	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Cg	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Cn	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Cu	14/16 (88%)	13 (93%)	1 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Db	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Di	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Dp	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Dw	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Ed	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Ek	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Er	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
4	Ad	3/5 (60%)	3 (100%)	0	0	100	100
4	Ak	3/5 (60%)	3 (100%)	0	0	100	100
4	Ar	3/5 (60%)	3 (100%)	0	0	100	100
4	Ay	3/5 (60%)	3 (100%)	0	0	100	100
4	Bf	3/5 (60%)	3 (100%)	0	0	100	100
4	Bm	3/5 (60%)	3 (100%)	0	0	100	100
4	Bt	3/5 (60%)	3 (100%)	0	0	100	100
4	Ca	3/5 (60%)	3 (100%)	0	0	100	100
4	Ch	3/5 (60%)	3 (100%)	0	0	100	100
4	Co	3/5 (60%)	3 (100%)	0	0	100	100
4	Cv	3/5 (60%)	3 (100%)	0	0	100	100
4	Dc	3/5 (60%)	3 (100%)	0	0	100	100
4	Dj	3/5 (60%)	3 (100%)	0	0	100	100
4	Dq	3/5 (60%)	3 (100%)	0	0	100	100
4	Dx	3/5 (60%)	3 (100%)	0	0	100	100
4	Ee	3/5 (60%)	3 (100%)	0	0	100	100
4	El	3/5 (60%)	3 (100%)	0	0	100	100
4	Es	3/5 (60%)	3 (100%)	0	0	100	100
5	Ae	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
5	Al	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	As	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Az	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Bg	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Bn	61/269 (23%)	61 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Bu	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
5	Cb	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Ci	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Cp	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
5	Cw	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
5	Dd	61/269 (23%)	61 (100%)	0	0	100	100
5	Dk	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Dr	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
5	Dy	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Ef	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
5	Em	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Et	61/269 (23%)	61 (100%)	0	0	100	100
6	Af	32/1048 (3%)	32 (100%)	0	0	100	100
6	Am	32/1048 (3%)	32 (100%)	0	0	100	100
6	At	32/1048 (3%)	32 (100%)	0	0	100	100
6	Ba	32/1048 (3%)	32 (100%)	0	0	100	100
6	Bh	32/1048 (3%)	32 (100%)	0	0	100	100
6	Bo	32/1048 (3%)	32 (100%)	0	0	100	100
6	Bv	32/1048 (3%)	32 (100%)	0	0	100	100
6	Cc	32/1048 (3%)	32 (100%)	0	0	100	100
6	Cj	32/1048 (3%)	32 (100%)	0	0	100	100
6	Cq	32/1048 (3%)	32 (100%)	0	0	100	100
6	Cx	32/1048 (3%)	32 (100%)	0	0	100	100
6	De	32/1048 (3%)	32 (100%)	0	0	100	100
6	Dl	32/1048 (3%)	32 (100%)	0	0	100	100
6	Ds	32/1048 (3%)	32 (100%)	0	0	100	100
6	Dz	32/1048 (3%)	32 (100%)	0	0	100	100
6	Eg	32/1048 (3%)	32 (100%)	0	0	100	100
6	En	32/1048 (3%)	32 (100%)	0	0	100	100
6	Eu	32/1048 (3%)	32 (100%)	0	0	100	100
7	Ag	158/361 (44%)	155 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	An	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Au	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Bb	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Bi	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
7	Bp	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Bw	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Cd	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Ck	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Cr	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Cy	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Df	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Dm	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Dt	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Ea	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Eh	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Eo	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Ev	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
All	All	5202/31032 (17%)	5105 (98%)	97 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	11/11 (100%)	10 (91%)	1 (9%)	7	27
1	Ah	11/11 (100%)	11 (100%)	0	100	100
1	Ao	11/11 (100%)	9 (82%)	2 (18%)	1	6
1	Av	11/11 (100%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bc	11/11 (100%)	10 (91%)	1 (9%)	7	27
1	Bj	11/11 (100%)	11 (100%)	0	100	100
1	Bq	11/11 (100%)	11 (100%)	0	100	100
1	Bx	11/11 (100%)	11 (100%)	0	100	100
1	Ce	11/11 (100%)	10 (91%)	1 (9%)	7	27
1	Cl	11/11 (100%)	10 (91%)	1 (9%)	7	27
1	Cs	11/11 (100%)	10 (91%)	1 (9%)	7	27
1	Cz	11/11 (100%)	10 (91%)	1 (9%)	7	27
1	Dg	11/11 (100%)	11 (100%)	0	100	100
1	Dn	11/11 (100%)	10 (91%)	1 (9%)	7	27
1	Du	11/11 (100%)	11 (100%)	0	100	100
1	Eb	11/11 (100%)	11 (100%)	0	100	100
1	Ei	11/11 (100%)	11 (100%)	0	100	100
1	Ep	11/11 (100%)	11 (100%)	0	100	100
2	Ab	7/7 (100%)	6 (86%)	1 (14%)	2	12
2	Ai	7/7 (100%)	7 (100%)	0	100	100
2	Ap	7/7 (100%)	6 (86%)	1 (14%)	2	12
2	Aw	7/7 (100%)	7 (100%)	0	100	100
2	Bd	7/7 (100%)	7 (100%)	0	100	100
2	Bk	7/7 (100%)	7 (100%)	0	100	100
2	Br	7/7 (100%)	7 (100%)	0	100	100
2	By	7/7 (100%)	7 (100%)	0	100	100
2	Cf	7/7 (100%)	7 (100%)	0	100	100
2	Cm	7/7 (100%)	6 (86%)	1 (14%)	2	12
2	Ct	7/7 (100%)	7 (100%)	0	100	100
2	Da	7/7 (100%)	6 (86%)	1 (14%)	2	12
2	Dh	7/7 (100%)	6 (86%)	1 (14%)	2	12
2	Do	7/7 (100%)	7 (100%)	0	100	100
2	Dv	7/7 (100%)	7 (100%)	0	100	100
2	Ec	7/7 (100%)	7 (100%)	0	100	100
2	Ej	7/7 (100%)	5 (71%)	2 (29%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Eq	7/7 (100%)	7 (100%)	0	100	100
3	Ac	13/13 (100%)	10 (77%)	3 (23%)	0	3
3	Aj	13/13 (100%)	10 (77%)	3 (23%)	0	3
3	Aq	13/13 (100%)	9 (69%)	4 (31%)	0	1
3	Ax	13/13 (100%)	11 (85%)	2 (15%)	2	10
3	Be	13/13 (100%)	12 (92%)	1 (8%)	10	34
3	Bl	13/13 (100%)	12 (92%)	1 (8%)	10	34
3	Bs	13/13 (100%)	12 (92%)	1 (8%)	10	34
3	Bz	13/13 (100%)	12 (92%)	1 (8%)	10	34
3	Cg	13/13 (100%)	10 (77%)	3 (23%)	0	3
3	Cn	13/13 (100%)	10 (77%)	3 (23%)	0	3
3	Cu	13/13 (100%)	10 (77%)	3 (23%)	0	3
3	Db	13/13 (100%)	9 (69%)	4 (31%)	0	1
3	Di	13/13 (100%)	11 (85%)	2 (15%)	2	10
3	Dp	13/13 (100%)	10 (77%)	3 (23%)	0	3
3	Dw	13/13 (100%)	11 (85%)	2 (15%)	2	10
3	Ed	13/13 (100%)	12 (92%)	1 (8%)	10	34
3	Ek	13/13 (100%)	11 (85%)	2 (15%)	2	10
3	Er	13/13 (100%)	11 (85%)	2 (15%)	2	10
4	Ad	3/3 (100%)	3 (100%)	0	100	100
4	Ak	3/3 (100%)	3 (100%)	0	100	100
4	Ar	3/3 (100%)	3 (100%)	0	100	100
4	Ay	3/3 (100%)	3 (100%)	0	100	100
4	Bf	3/3 (100%)	3 (100%)	0	100	100
4	Bm	3/3 (100%)	3 (100%)	0	100	100
4	Bt	3/3 (100%)	3 (100%)	0	100	100
4	Ca	3/3 (100%)	3 (100%)	0	100	100
4	Ch	3/3 (100%)	3 (100%)	0	100	100
4	Co	3/3 (100%)	3 (100%)	0	100	100
4	Cv	3/3 (100%)	3 (100%)	0	100	100
4	Dc	3/3 (100%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Dj	3/3 (100%)	3 (100%)	0	100	100
4	Dq	3/3 (100%)	3 (100%)	0	100	100
4	Dx	3/3 (100%)	3 (100%)	0	100	100
4	Ee	3/3 (100%)	3 (100%)	0	100	100
4	El	3/3 (100%)	3 (100%)	0	100	100
4	Es	3/3 (100%)	3 (100%)	0	100	100
5	Ae	53/237 (22%)	53 (100%)	0	100	100
5	Al	53/237 (22%)	53 (100%)	0	100	100
5	As	53/237 (22%)	53 (100%)	0	100	100
5	Az	53/237 (22%)	52 (98%)	1 (2%)	52	76
5	Bg	53/237 (22%)	52 (98%)	1 (2%)	52	76
5	Bn	53/237 (22%)	53 (100%)	0	100	100
5	Bu	53/237 (22%)	52 (98%)	1 (2%)	52	76
5	Cb	53/237 (22%)	53 (100%)	0	100	100
5	Ci	53/237 (22%)	51 (96%)	2 (4%)	28	59
5	Cp	53/237 (22%)	52 (98%)	1 (2%)	52	76
5	Cw	53/237 (22%)	53 (100%)	0	100	100
5	Dd	53/237 (22%)	53 (100%)	0	100	100
5	Dk	53/237 (22%)	53 (100%)	0	100	100
5	Dr	53/237 (22%)	52 (98%)	1 (2%)	52	76
5	Dy	53/237 (22%)	53 (100%)	0	100	100
5	Ef	53/237 (22%)	53 (100%)	0	100	100
5	Em	53/237 (22%)	53 (100%)	0	100	100
5	Et	53/237 (22%)	52 (98%)	1 (2%)	52	76
6	Af	31/765 (4%)	30 (97%)	1 (3%)	34	64
6	Am	31/765 (4%)	31 (100%)	0	100	100
6	At	31/765 (4%)	30 (97%)	1 (3%)	34	64
6	Ba	31/765 (4%)	30 (97%)	1 (3%)	34	64
6	Bh	31/765 (4%)	31 (100%)	0	100	100
6	Bo	31/765 (4%)	30 (97%)	1 (3%)	34	64
6	Bv	31/765 (4%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Cc	31/765 (4%)	31 (100%)	0	100	100
6	Cj	31/765 (4%)	31 (100%)	0	100	100
6	Cq	31/765 (4%)	30 (97%)	1 (3%)	34	64
6	Cx	31/765 (4%)	31 (100%)	0	100	100
6	De	31/765 (4%)	31 (100%)	0	100	100
6	Dl	31/765 (4%)	30 (97%)	1 (3%)	34	64
6	Ds	31/765 (4%)	31 (100%)	0	100	100
6	Dz	31/765 (4%)	31 (100%)	0	100	100
6	Eg	31/765 (4%)	31 (100%)	0	100	100
6	En	31/765 (4%)	31 (100%)	0	100	100
6	Eu	31/765 (4%)	31 (100%)	0	100	100
7	Ag	137/300 (46%)	132 (96%)	5 (4%)	30	61
7	An	137/300 (46%)	135 (98%)	2 (2%)	60	80
7	Au	137/300 (46%)	135 (98%)	2 (2%)	60	80
7	Bb	137/300 (46%)	133 (97%)	4 (3%)	37	67
7	Bi	137/300 (46%)	135 (98%)	2 (2%)	60	80
7	Bp	137/300 (46%)	135 (98%)	2 (2%)	60	80
7	Bw	137/300 (46%)	134 (98%)	3 (2%)	47	73
7	Cd	137/300 (46%)	134 (98%)	3 (2%)	47	73
7	Ck	137/300 (46%)	134 (98%)	3 (2%)	47	73
7	Cr	137/300 (46%)	130 (95%)	7 (5%)	20	50
7	Cy	137/300 (46%)	135 (98%)	2 (2%)	60	80
7	Df	137/300 (46%)	134 (98%)	3 (2%)	47	73
7	Dm	137/300 (46%)	135 (98%)	2 (2%)	60	80
7	Dt	137/300 (46%)	133 (97%)	4 (3%)	37	67
7	Ea	137/300 (46%)	135 (98%)	2 (2%)	60	80
7	Eh	137/300 (46%)	133 (97%)	4 (3%)	37	67
7	Eo	137/300 (46%)	134 (98%)	3 (2%)	47	73
7	Ev	137/300 (46%)	135 (98%)	2 (2%)	60	80
All	All	4590/24048 (19%)	4464 (97%)	126 (3%)	41	68

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	3	ASP
2	Ab	5	ILE
3	Ac	3	SER
3	Ac	7	THR
3	Ac	10	THR
6	Af	814	GLN
7	Ag	110	LYS
7	Ag	128	VAL
7	Ag	179	LEU
7	Ag	219	LYS
7	Ag	262	ASN
3	Aj	3	SER
3	Aj	7	THR
3	Aj	10	THR
7	An	128	VAL
7	An	240	THR
1	Ao	3	ASP
1	Ao	6	LEU
2	Ap	5	ILE
3	Aq	3	SER
3	Aq	4	ILE
3	Aq	7	THR
3	Aq	10	THR
6	At	814	GLN
7	Au	214	MET
7	Au	240	THR
3	Ax	7	THR
3	Ax	10	THR
5	Az	226	ASN
6	Ba	814	GLN
7	Bb	209	THR
7	Bb	214	MET
7	Bb	219	LYS
7	Bb	239	LEU
1	Bc	3	ASP
3	Be	3	SER
5	Bg	267	GLU
7	Bi	128	VAL
7	Bi	219	LYS
3	Bl	7	THR
6	Bo	822	GLU
7	Bp	179	LEU
7	Bp	215	ILE

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Mol	Chain	Res	Type
3	Bs	3	SER
5	Bu	226	ASN
7	Bw	128	VAL
7	Bw	168	VAL
7	Bw	240	THR
3	Bz	3	SER
7	Cd	128	VAL
7	Cd	179	LEU
7	Cd	241	LEU
1	Ce	3	ASP
3	Cg	3	SER
3	Cg	4	ILE
3	Cg	10	THR
5	Ci	213	GLN
5	Ci	249	SER
7	Ck	128	VAL
7	Ck	214	MET
7	Ck	240	THR
1	Cl	3	ASP
2	Cm	5	ILE
3	Cn	3	SER
3	Cn	7	THR
3	Cn	10	THR
5	Cp	251	GLN
6	Cq	814	GLN
7	Cr	128	VAL
7	Cr	178	SER
7	Cr	179	LEU
7	Cr	219	LYS
7	Cr	240	THR
7	Cr	241	LEU
7	Cr	262	ASN
1	Cs	3	ASP
3	Cu	4	ILE
3	Cu	7	THR
3	Cu	10	THR
7	Cy	128	VAL
7	Cy	240	THR
1	Cz	3	ASP
2	Da	5	ILE
3	Db	3	SER
3	Db	4	ILE

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Mol	Chain	Res	Type
3	Db	7	THR
3	Db	10	THR
7	Df	128	VAL
7	Df	214	MET
7	Df	240	THR
2	Dh	4	MET
3	Di	7	THR
3	Di	10	THR
6	Dl	814	GLN
7	Dm	209	THR
7	Dm	219	LYS
1	Dn	3	ASP
3	Dp	3	SER
3	Dp	4	ILE
3	Dp	7	THR
5	Dr	267	GLU
7	Dt	110	LYS
7	Dt	128	VAL
7	Dt	219	LYS
7	Dt	240	THR
3	Dw	3	SER
3	Dw	7	THR
7	Ea	241	LEU
7	Ea	246	LYS
3	Ed	3	SER
7	Eh	168	VAL
7	Eh	209	THR
7	Eh	214	MET
7	Eh	240	THR
2	Ej	4	MET
2	Ej	5	ILE
3	Ek	3	SER
3	Ek	10	THR
7	Eo	128	VAL
7	Eo	215	ILE
7	Eo	241	LEU
3	Er	3	SER
3	Er	4	ILE
5	Et	213	GLN
7	Ev	128	VAL
7	Ev	240	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77)

such sidechains are listed below:

Mol	Chain	Res	Type
7	Ag	123	ASN
7	Ag	126	GLN
7	Ag	132	GLN
7	Ag	222	ASN
7	Ag	234	ASN
7	Ag	245	GLN
5	Al	213	GLN
5	Al	251	GLN
7	An	123	ASN
7	An	126	GLN
7	An	203	ASN
7	An	222	ASN
7	An	262	ASN
7	Au	132	GLN
7	Au	203	ASN
7	Au	222	ASN
7	Au	262	ASN
5	Az	251	GLN
7	Bb	159	ASN
7	Bb	203	ASN
7	Bb	222	ASN
7	Bb	257	GLN
5	Bg	251	GLN
7	Bi	123	ASN
7	Bi	126	GLN
7	Bi	203	ASN
7	Bi	222	ASN
7	Bp	203	ASN
7	Bp	222	ASN
7	Bp	245	GLN
5	Bu	213	GLN
7	Bw	262	ASN
7	Cd	126	GLN
7	Cd	159	ASN
7	Cd	257	GLN
7	Cd	262	ASN
7	Ck	123	ASN
7	Ck	126	GLN
7	Ck	222	ASN
7	Ck	262	ASN
5	Cp	213	GLN
7	Cr	132	GLN

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Mol	Chain	Res	Type
7	Cr	211	ASN
7	Cr	222	ASN
7	Cr	234	ASN
7	Cr	245	GLN
5	Cw	213	GLN
7	Cy	132	GLN
7	Cy	222	ASN
7	Cy	262	ASN
5	Dd	251	GLN
7	Df	222	ASN
5	Dk	251	GLN
7	Dm	159	ASN
7	Dm	257	GLN
7	Dm	262	ASN
7	Dt	123	ASN
7	Dt	126	GLN
7	Dt	159	ASN
7	Dt	222	ASN
7	Dt	257	GLN
5	Dy	251	GLN
7	Ea	222	ASN
7	Ea	245	GLN
7	Eh	123	ASN
7	Eh	126	GLN
7	Eh	132	GLN
5	Em	213	GLN
5	Em	251	GLN
6	En	818	GLN
7	Eo	123	ASN
7	Eo	126	GLN
7	Eo	159	ASN
7	Eo	203	ASN
7	Eo	257	GLN
7	Ev	234	ASN
7	Ev	262	ASN

5.3.3 RNA ⓘ

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.

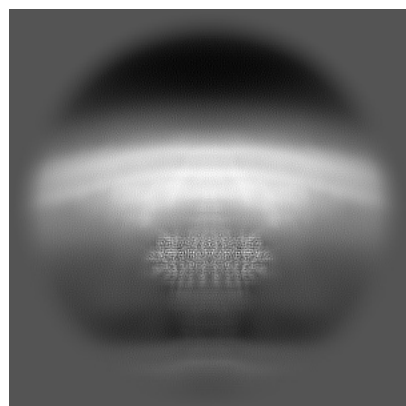
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49394. These allow visual inspection of the internal detail of the map and identification of artifacts.

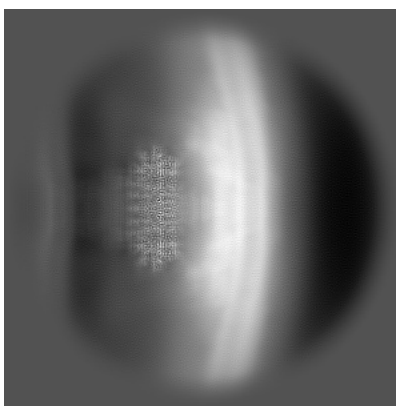
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

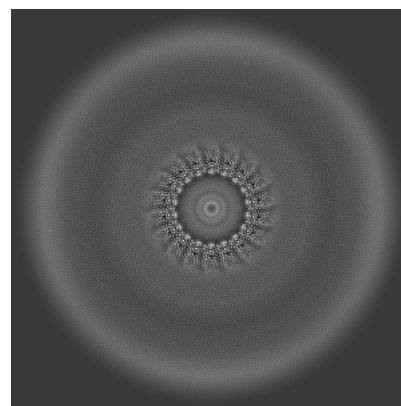
6.1.1 Primary map



X

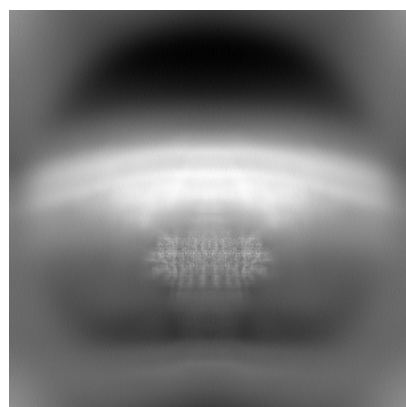


Y

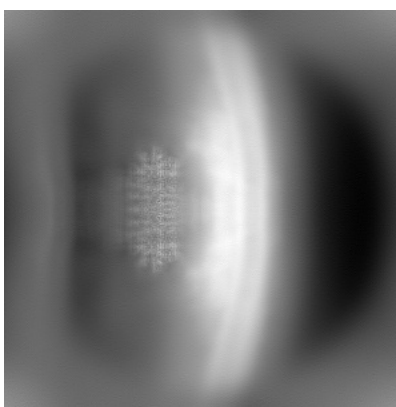


Z

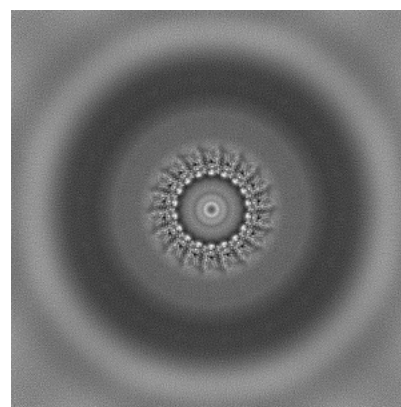
6.1.2 Raw map



X



Y

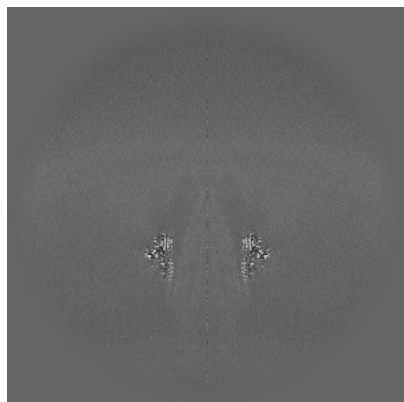


Z

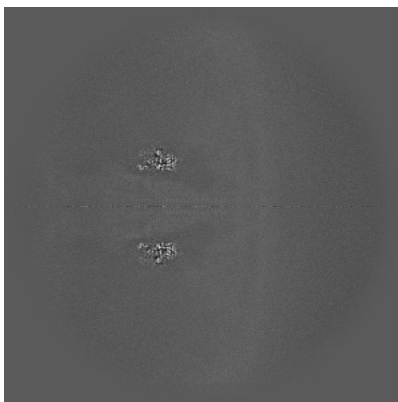
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

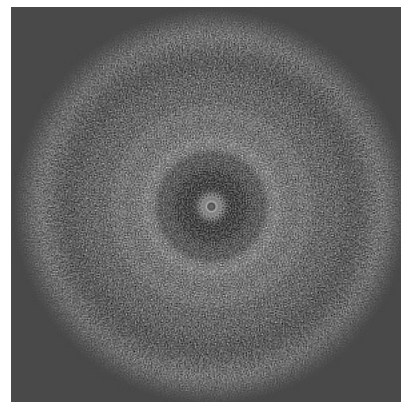
6.2.1 Primary map



X Index: 224

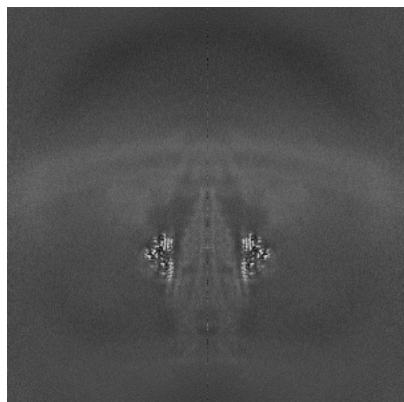


Y Index: 224

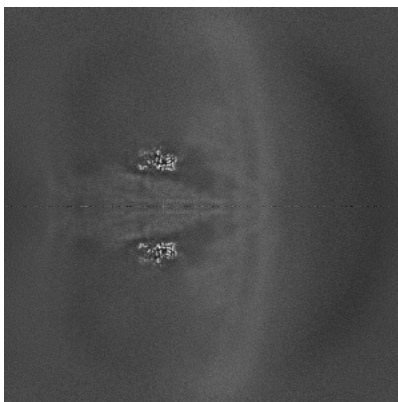


Z Index: 224

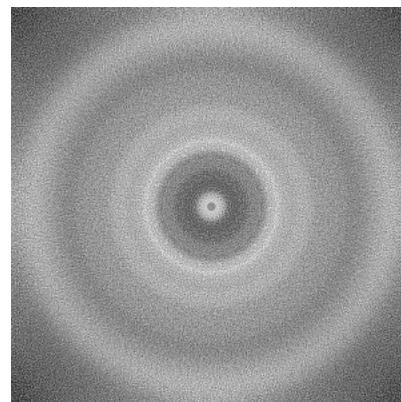
6.2.2 Raw map



X Index: 224



Y Index: 224

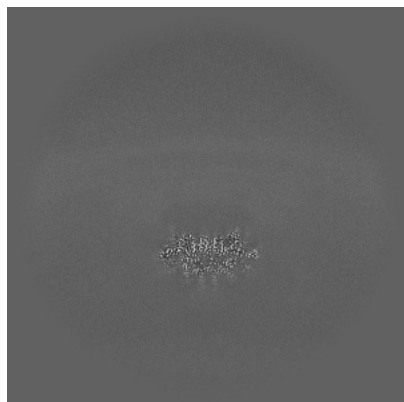


Z Index: 224

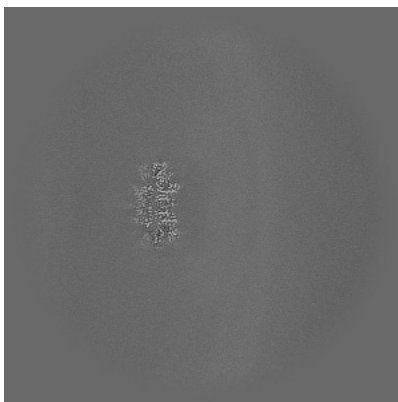
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

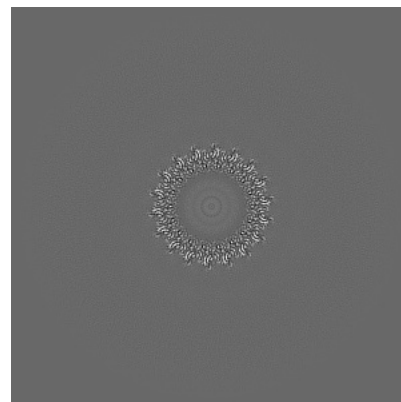
6.3.1 Primary map



X Index: 181

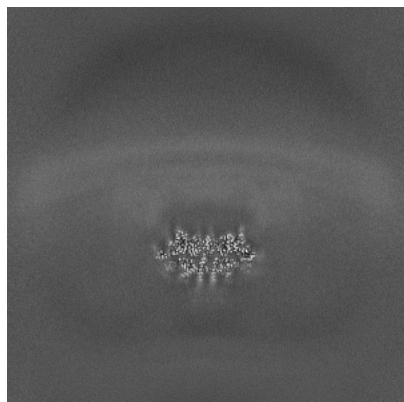


Y Index: 269

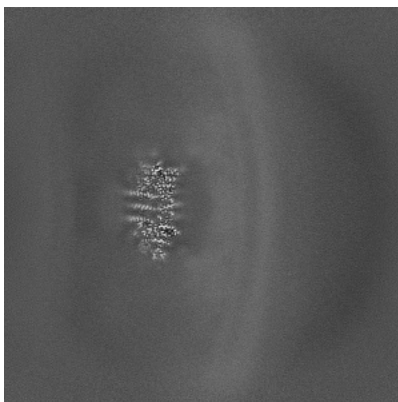


Z Index: 174

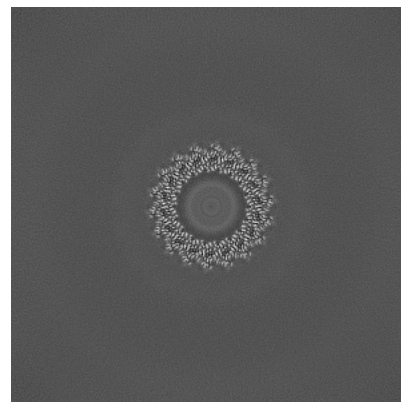
6.3.2 Raw map



X Index: 266



Y Index: 264

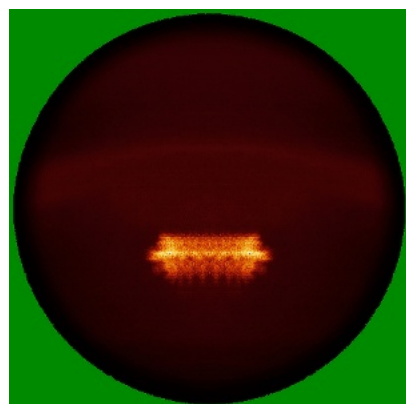


Z Index: 175

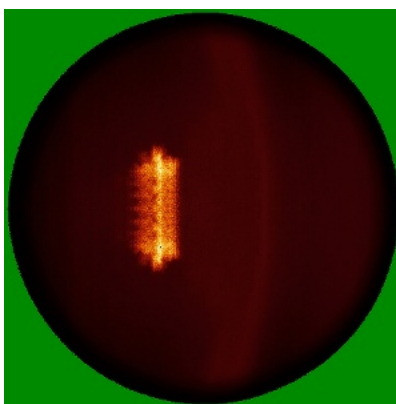
The images above show the largest variance slices of the map in three orthogonal directions.

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

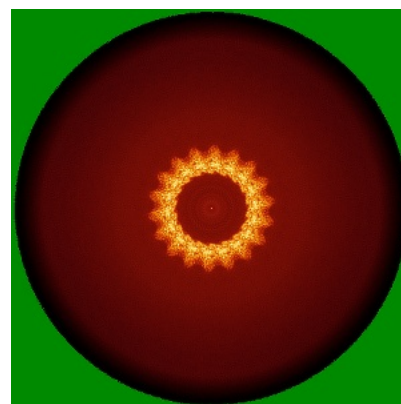
6.4.1 Primary map



X

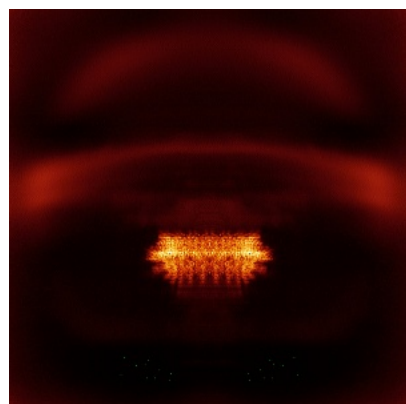


Y

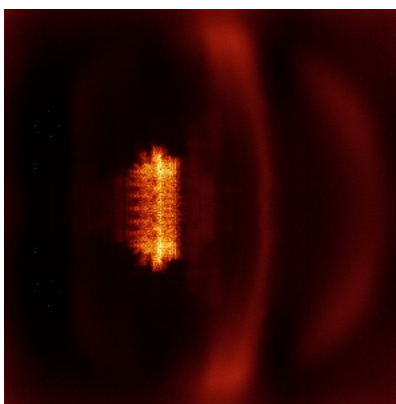


Z

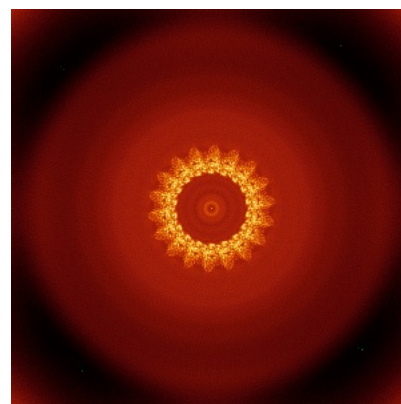
6.4.2 Raw map



X



Y

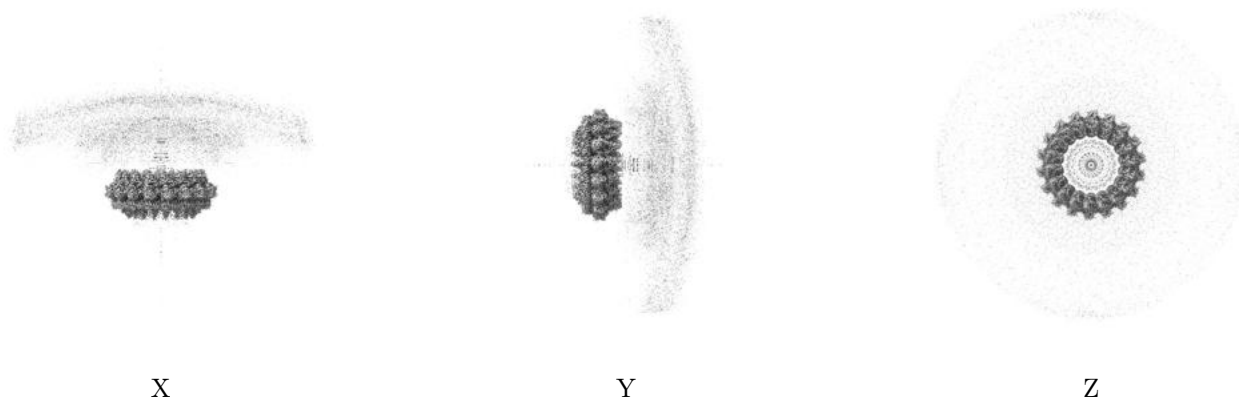


Z

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.

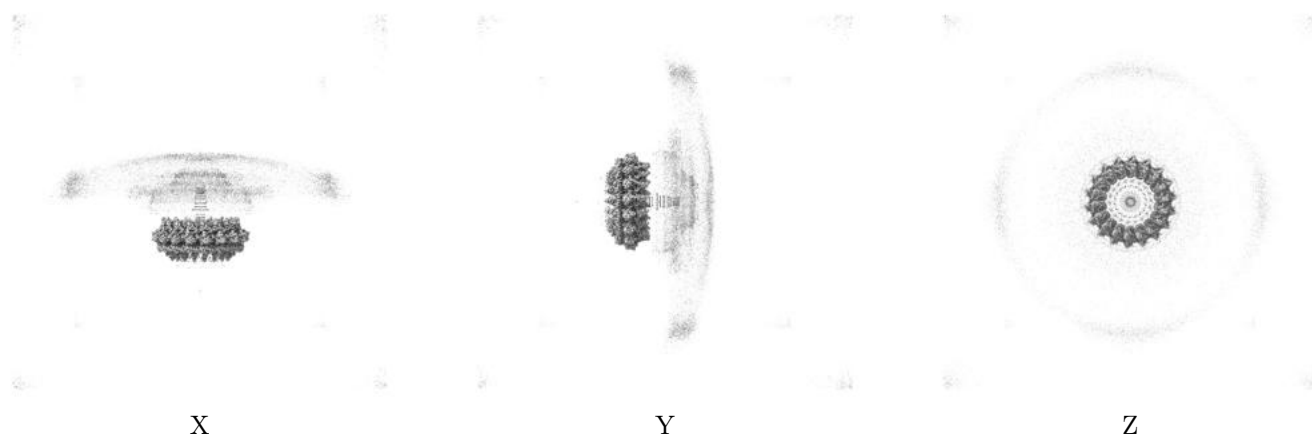
6.5 Orthogonal surface views [i](#)

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.

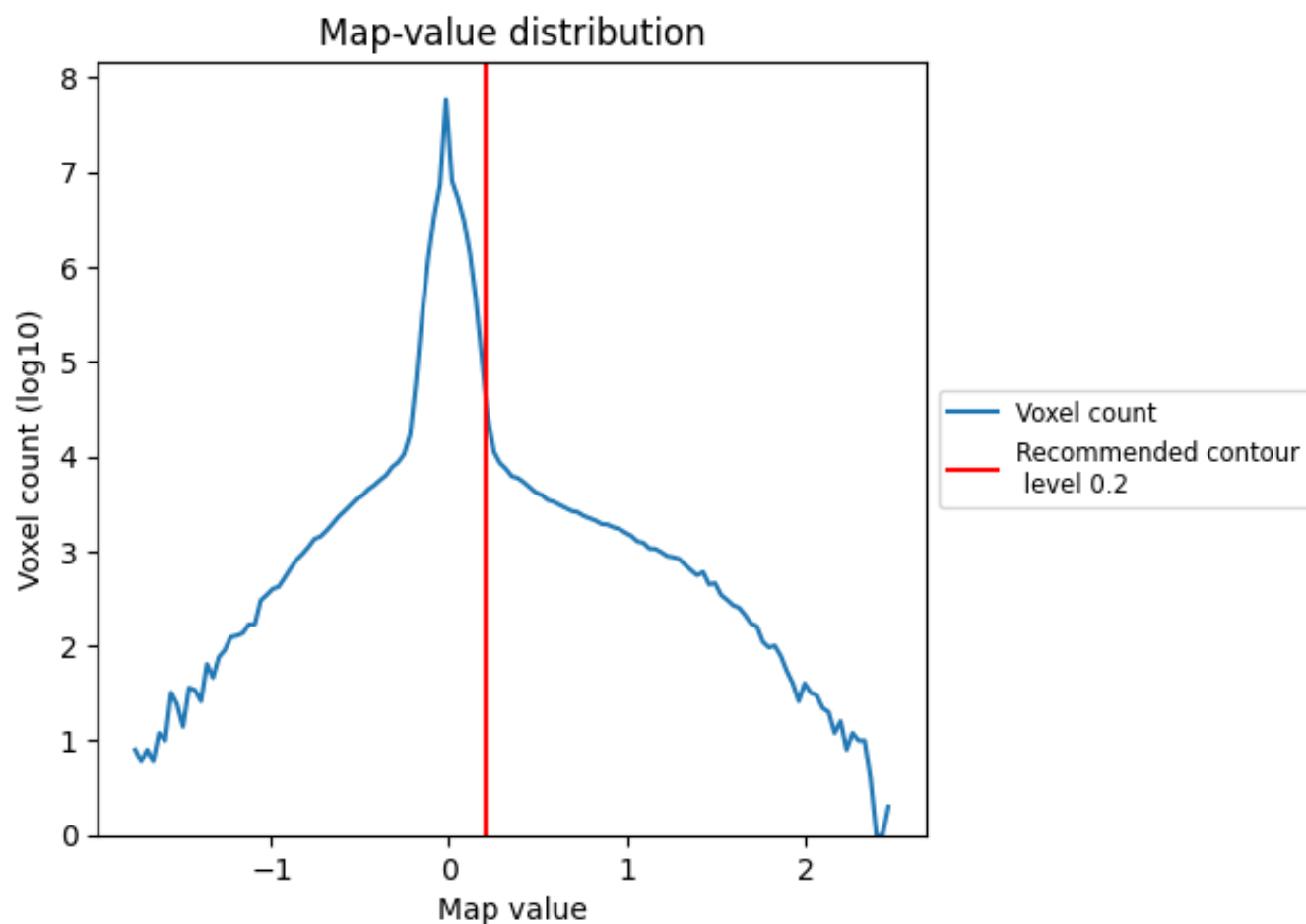
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

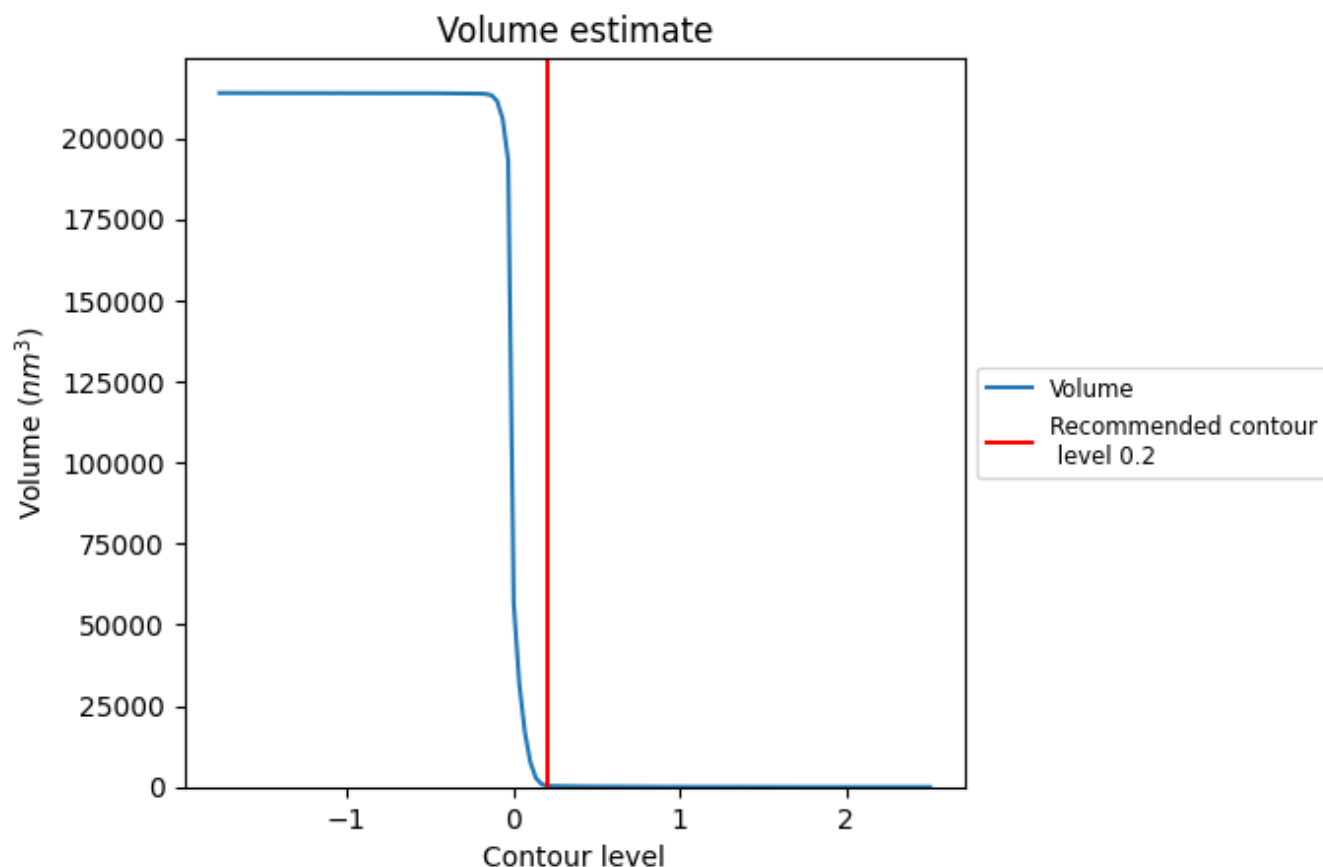
This section contains the results of statistical analysis of the map.

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.

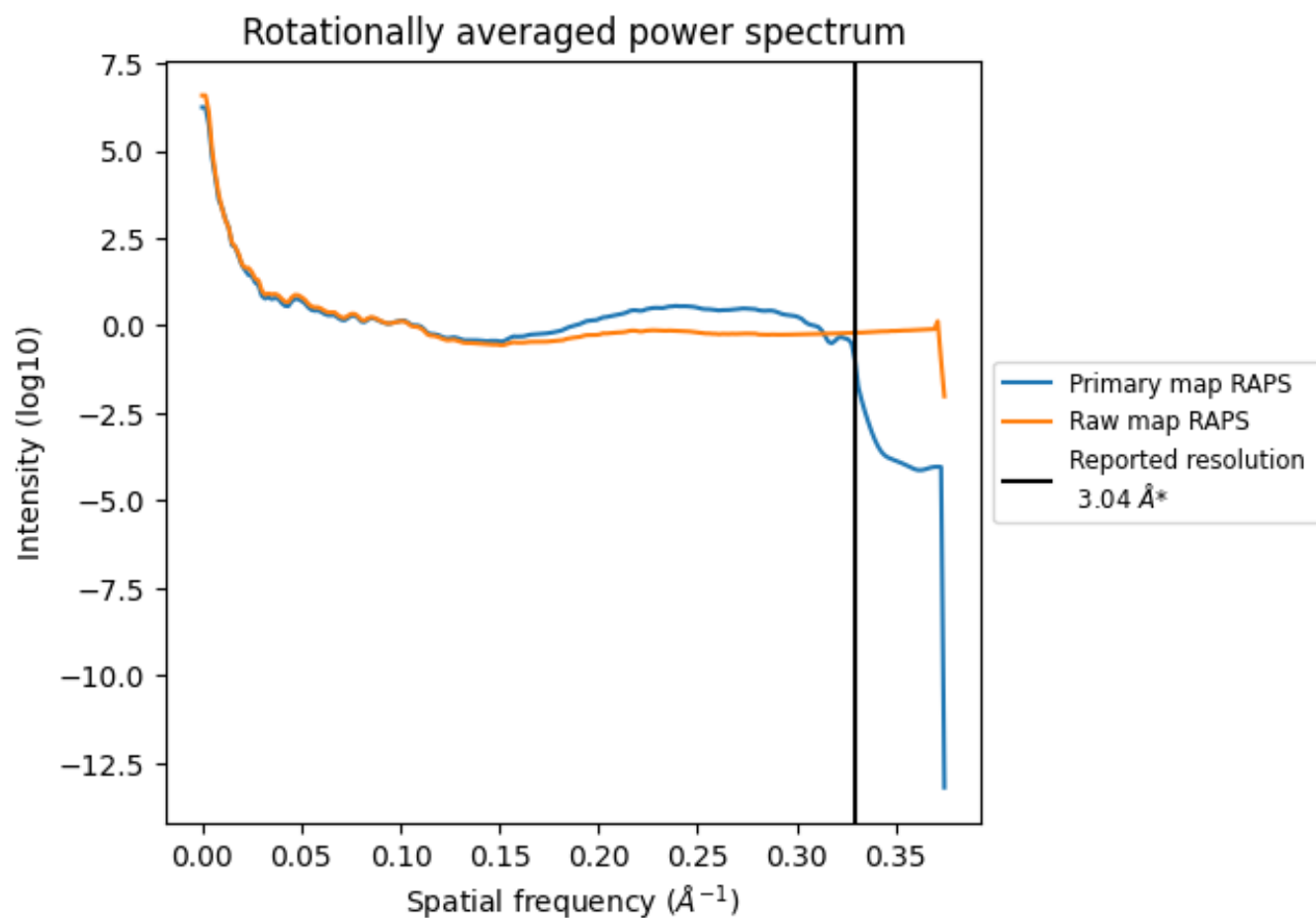
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 428 nm³; this corresponds to an approximate mass of 387 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 ⓘ

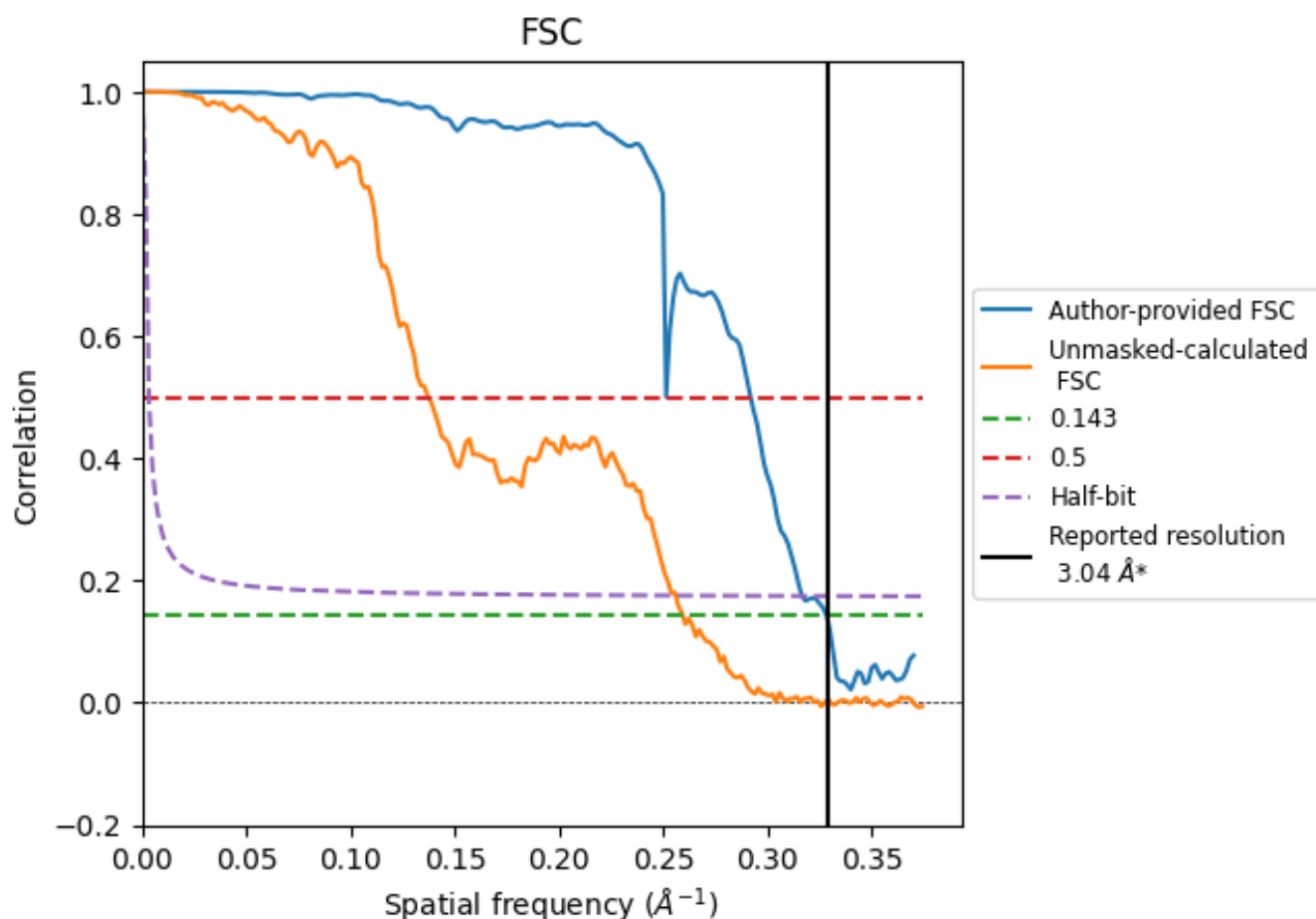


*Reported resolution corresponds to spatial frequency of 0.329 \AA^{-1}

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 0.329 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.42	3.16
Unmasked-calculated*	3.85	7.28	3.90

*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 3.85 differs from the reported value 3.04 by more than 10 %

9 Map-model fit [i](#)

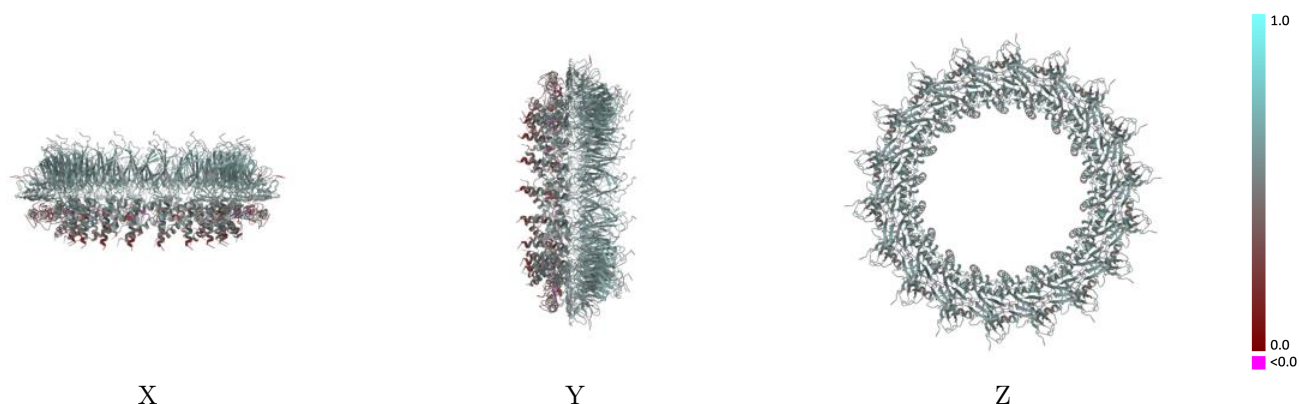
This section contains information regarding the fit between EMDB map EMD-49394 and PDB model 9NGV. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



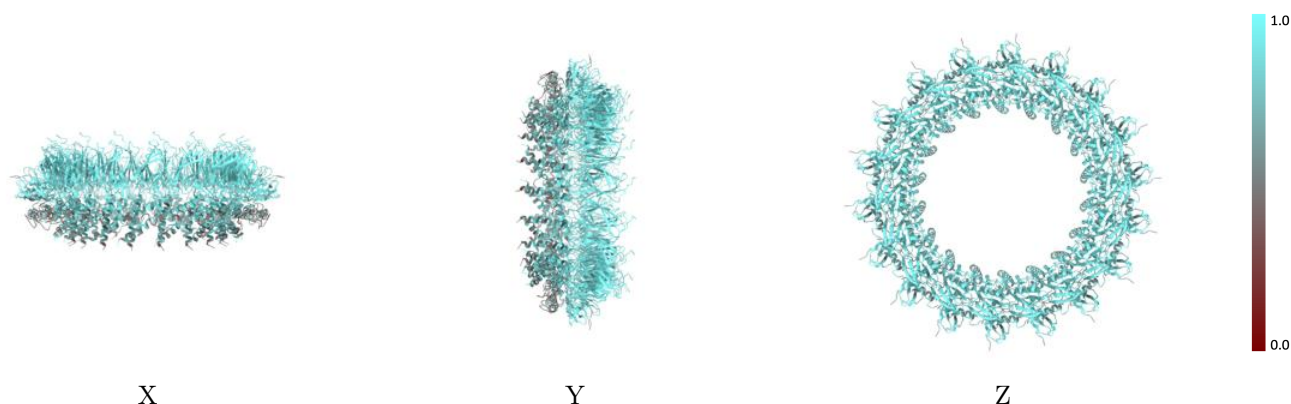
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



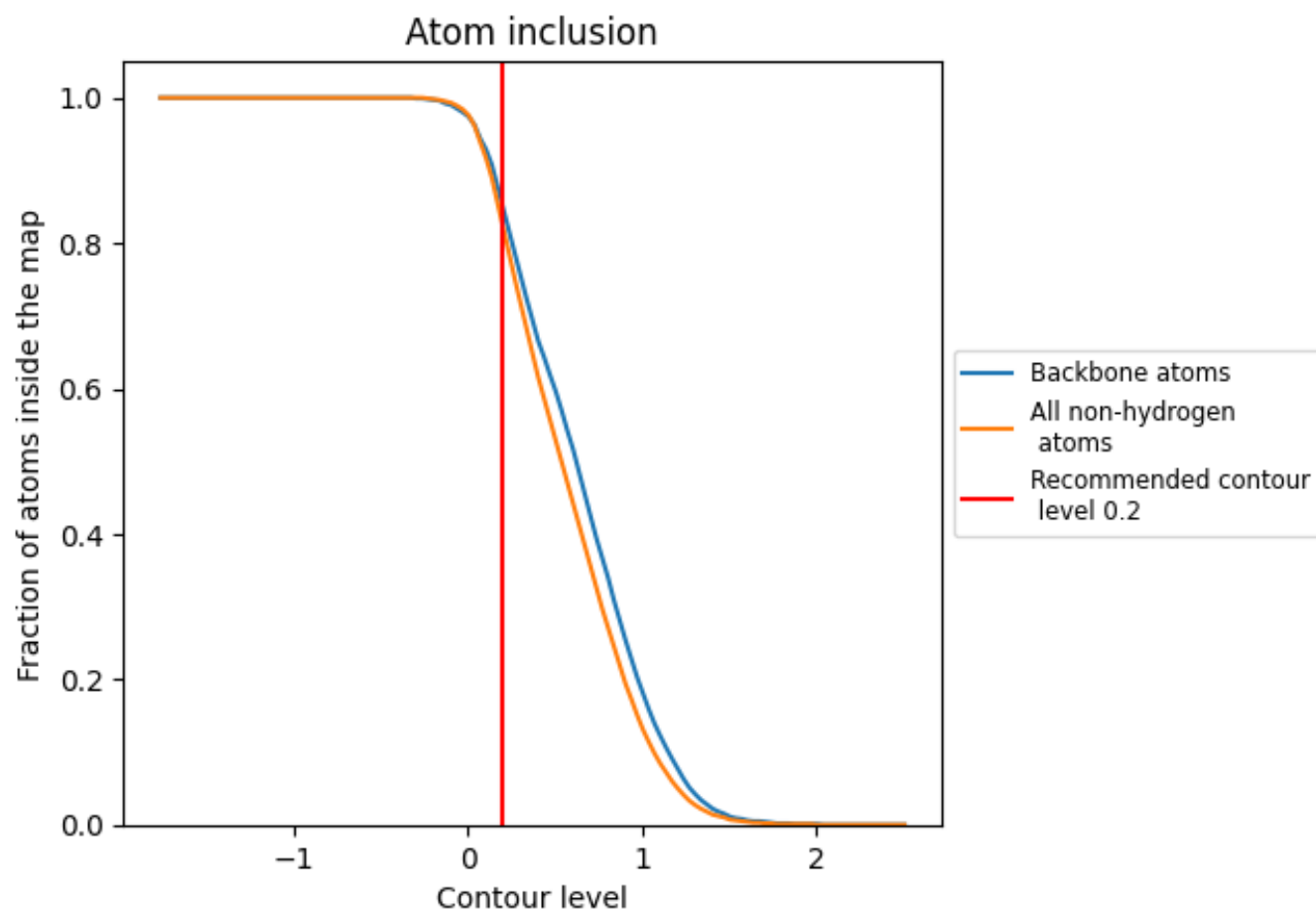
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 85% of all backbone atoms, 82% 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	0.8220	0.5110
Aa	0.5950	0.4440
Ab	0.6100	0.3260
Ac	0.4380	0.2980
Ad	0.2780	0.1990
Ae	0.8410	0.5190
Af	0.7900	0.5080
Ag	0.9090	0.5550
Ah	0.5950	0.4260
Ai	0.6610	0.3410
Aj	0.4380	0.3090
Ak	0.3330	0.2090
Al	0.8620	0.5210
Am	0.7900	0.5070
An	0.9060	0.5560
Ao	0.5520	0.4530
Ap	0.6270	0.3520
Aq	0.4460	0.3000
Ar	0.3060	0.1960
As	0.8560	0.5210
At	0.7980	0.5060
Au	0.9070	0.5550
Av	0.5690	0.4400
Aw	0.6780	0.3570
Ax	0.4300	0.3060
Ay	0.3330	0.1840
Az	0.8500	0.5180
Ba	0.7980	0.4970
Bb	0.9040	0.5540
Bc	0.5860	0.4370
Bd	0.6440	0.3430
Be	0.4460	0.3240
Bf	0.3330	0.1970
Bg	0.8430	0.5170
Bh	0.7760	0.4920























































































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Chain	Atom inclusion	Q-score
Bi	 0.8960	 0.5530
Bj	 0.5950	 0.4470
Bk	 0.6270	 0.3460
Bl	 0.4460	 0.3210
Bm	 0.2500	 0.1680
Bn	 0.8500	 0.5150
Bo	 0.8160	 0.5030
Bp	 0.8960	 0.5540
Bq	 0.5780	 0.4310
Br	 0.6780	 0.3610
Bs	 0.4130	 0.3090
Bt	 0.3060	 0.2320
Bu	 0.8410	 0.5190
Bv	 0.8200	 0.5050
Bw	 0.8990	 0.5540
Bx	 0.5600	 0.4370
By	 0.6440	 0.3440
Bz	 0.4550	 0.3000
Ca	 0.3330	 0.1850
Cb	 0.8430	 0.5160
Cc	 0.7870	 0.5030
Cd	 0.8960	 0.5510
Ce	 0.5950	 0.4420
Cf	 0.6100	 0.3350
Cg	 0.4460	 0.3070
Ch	 0.3060	 0.2080
Ci	 0.8540	 0.5190
Cj	 0.7830	 0.5040
Ck	 0.9000	 0.5550
Cl	 0.5860	 0.4370
Cm	 0.6100	 0.3360
Cn	 0.4380	 0.2910
Co	 0.3060	 0.1780
Cp	 0.8350	 0.5170
Cq	 0.7980	 0.5000
Cr	 0.9050	 0.5550
Cs	 0.6210	 0.4420
Ct	 0.6440	 0.3340
Cu	 0.4460	 0.3040
Cv	 0.3330	 0.2120
Cw	 0.8620	 0.5220
Cx	 0.7980	 0.5050

















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Chain	Atom inclusion	Q-score
Cy	 0.9090	 0.5560
Cz	 0.5690	 0.4530
Da	 0.6610	 0.3470
Db	 0.4550	 0.3060
Dc	 0.3060	 0.1860
Dd	 0.8560	 0.5190
De	 0.7940	 0.5060
Df	 0.9050	 0.5560
Dg	 0.5600	 0.4330
Dh	 0.6610	 0.3490
Di	 0.4300	 0.3110
Dj	 0.2780	 0.1890
Dk	 0.8500	 0.5240
Dl	 0.8010	 0.4980
Dm	 0.9050	 0.5540
Dn	 0.6030	 0.4280
Do	 0.6100	 0.3410
Dp	 0.4710	 0.3130
Dq	 0.3330	 0.1920
Dr	 0.8410	 0.5180
Ds	 0.7760	 0.4950
Dt	 0.9000	 0.5550
Du	 0.6120	 0.4330
Dv	 0.6100	 0.3440
Dw	 0.4550	 0.3160
Dx	 0.3060	 0.1690
Dy	 0.8450	 0.5180
Dz	 0.8120	 0.5120
Ea	 0.9000	 0.5550
Eb	 0.5690	 0.4170
Ec	 0.6440	 0.3610
Ed	 0.4130	 0.3100
Ee	 0.3060	 0.2330
Ef	 0.8390	 0.5190
Eg	 0.8160	 0.5120
Eh	 0.8960	 0.5550
Ei	 0.5780	 0.4320
Ej	 0.6950	 0.3560
Ek	 0.4630	 0.3050
El	 0.3060	 0.2070
Em	 0.8450	 0.5200
En	 0.7900	 0.5050

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Chain	Atom inclusion	Q-score
Eo	 0.8960	 0.5530
Ep	 0.5950	 0.4380
Eq	 0.6440	 0.3420
Er	 0.4550	 0.3100
Es	 0.3060	 0.2300
Et	 0.8540	 0.5190
Eu	 0.7830	 0.5020
Ev	 0.9000	 0.5560