



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2025 – 06:14 PM EDT

PDB ID : 9EA9 / pdb_00009ea9
Title : Crystal structure of BoNT/A-NTNH-HA70 -VHH_F12-VHH_H7-Fab_NTN
H complex
Authors : Lam, K.H.; Gao, L.; Jin, R.
Deposited on : 2024-11-10
Resolution : 2.93 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

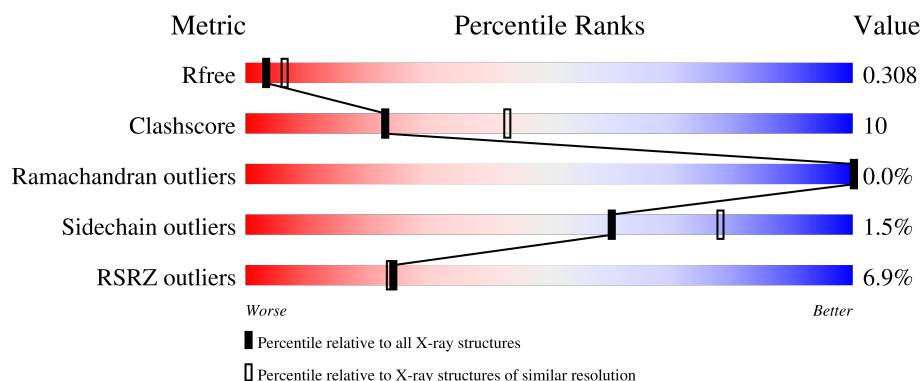
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1067 (2.96-2.92)
Clashscore	180529	1122 (2.96-2.92)
Ramachandran outliers	177936	1075 (2.96-2.92)
Sidechain outliers	177891	1075 (2.96-2.92)
RSRZ outliers	164620	1067 (2.96-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1296	<div> <div>4%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
2	B	1194	<div> <div>3%</div> <div>75%</div> <div>23%</div> <div>..</div> </div>
3	C	128	<div> <div>10%</div> <div>64%</div> <div>27%</div> <div>9%</div> </div>
4	F	121	<div> <div>3%</div> <div>74%</div> <div>19%</div> <div>6%</div> </div>
5	D	626	<div> <div>%</div> <div>20%</div> <div>8%</div> <div>72%</div> </div>

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Mol	Chain	Length	Quality of chain
5	G	626	
5	H	626	
5	I	626	
5	J	626	
6	E	626	
7	K	105	
8	M	117	
9	N	94	
10	L	103	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	SO4	A	1301	-	-	X	-
11	SO4	E	701	-	-	X	-
13	MG	E	705	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 39218 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1276	Total	C	N	O	S	0	0	0
			10371	6651	1716	1971	33			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	VAL	variant	UNP P0DPI0
A	224	GLN	GLU	conflict	UNP P0DPI0
A	363	ALA	ARG	conflict	UNP P0DPI0
A	366	PHE	TYR	conflict	UNP P0DPI0

- Molecule 2 is a protein called Non-toxic nonhemagglutinin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1187	Total	C	N	O	S	0	0	0
			9671	6194	1553	1892	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	426	SER	THR	conflict	UNP Q45914
B	1194	PRO	-	expression tag	UNP Q45914

- Molecule 3 is a protein called Nanobody ciA-F12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	117	Total	C	N	O	S	0	0	0
			873	540	153	176	4			

- Molecule 4 is a protein called Nanobody ciA-H7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	114	Total	C	N	O	S	0	0	0
			853	529	151	168	5			

- Molecule 5 is a protein called HA-70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	169	Total	C	N	O	S	0	0	0
			1376	891	223	260	2			
5	J	421	Total	C	N	O	S	0	0	0
			3366	2121	564	676	5			
5	D	174	Total	C	N	O	S	0	0	0
			1409	914	228	265	2			
5	G	169	Total	C	N	O	S	0	0	0
			1382	894	223	263	2			
5	H	421	Total	C	N	O	S	0	0	0
			3363	2120	562	676	5			

- Molecule 6 is a protein called HA70/A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	421	Total	C	N	O	S	0	0	0
			3358	2115	561	677	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	575	ASP	ILE	conflict	UNP Q8KHU9
E	576	ALA	ASP	conflict	UNP Q8KHU9

- Molecule 7 is a protein called anti-NTNH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	K	105	Total	C	N	O	S	0	0	0
			803	505	134	162	2			

- Molecule 8 is a protein called anti-NTNH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	117	Total	C	N	O	S	0	0	0
			881	557	144	176	4			

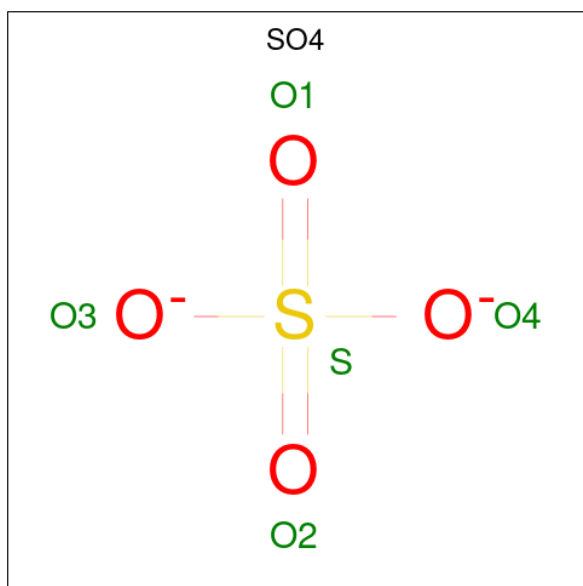
- Molecule 9 is a protein called anti-NTNH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	94	Total	C	N	O	S	8	0	0
			634	399	104	129	2			

- Molecule 10 is a protein called anti-NTNH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	103	Total	C	N	O	S	0	0	0
			752	460	129	160	3			

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total	O	S	0	0
			5	4	1		
11	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Zn	0	0
			1	1		

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	Mg	0	0
			1	1		
13	B	1	Total	Mg	0	0
			1	1		
13	J	1	Total	Mg	0	0
			1	1		
13	E	6	Total	Mg	0	0
			6	6		
13	H	1	Total	Mg	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	25	Total	O	0	0
			25	25		
14	B	15	Total	O	0	0
			15	15		
14	F	4	Total	O	0	0
			4	4		
14	I	3	Total	O	0	0
			3	3		
14	J	2	Total	O	0	0
			2	2		
14	D	3	Total	O	0	0
			3	3		
14	E	8	Total	O	0	0
			8	8		

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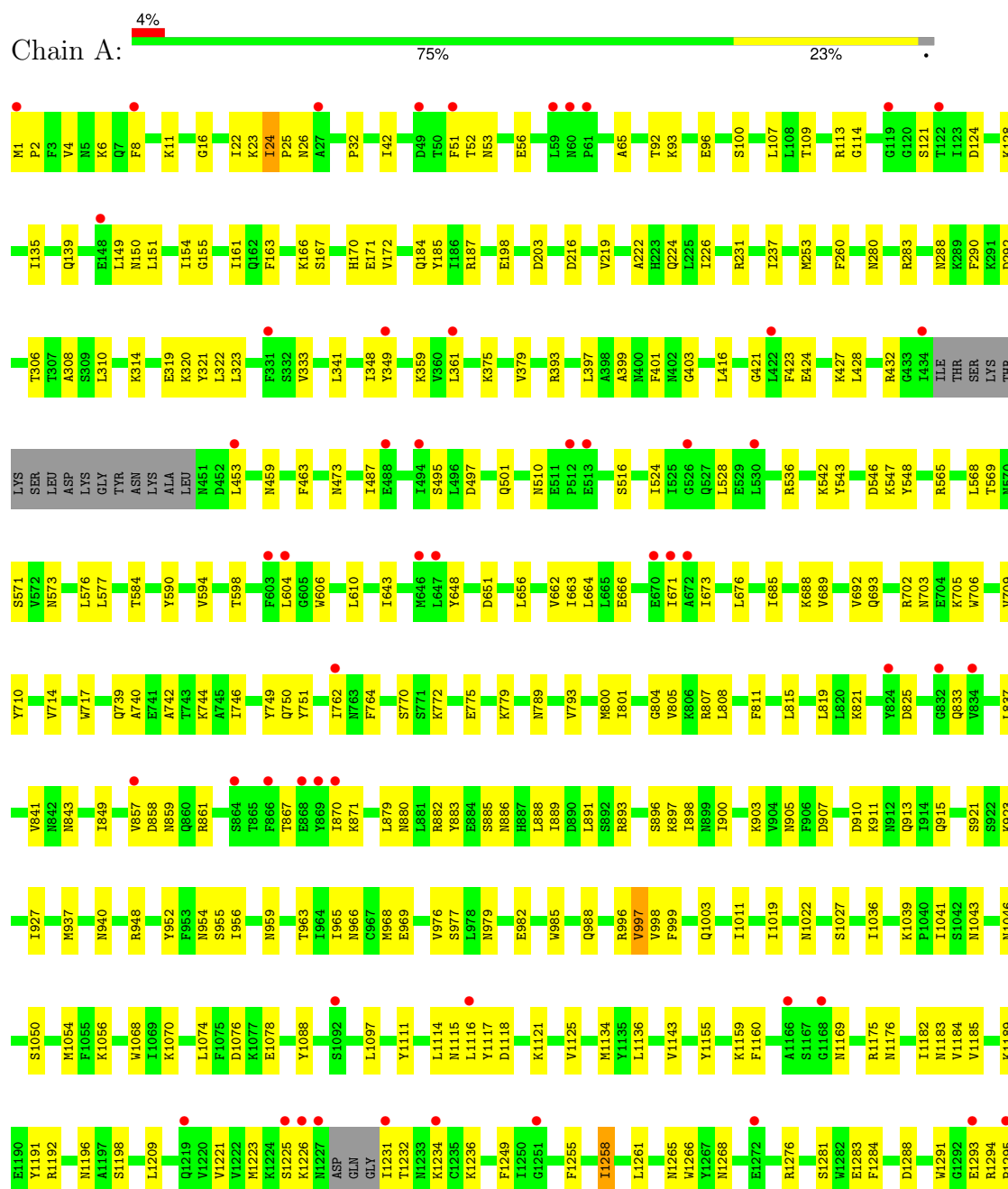
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	G	2	Total	O	0	0
			2	2		
14	H	2	Total	O	0	0
			2	2		
14	M	1	Total	O	0	0
			1	1		

3 Residue-property plots

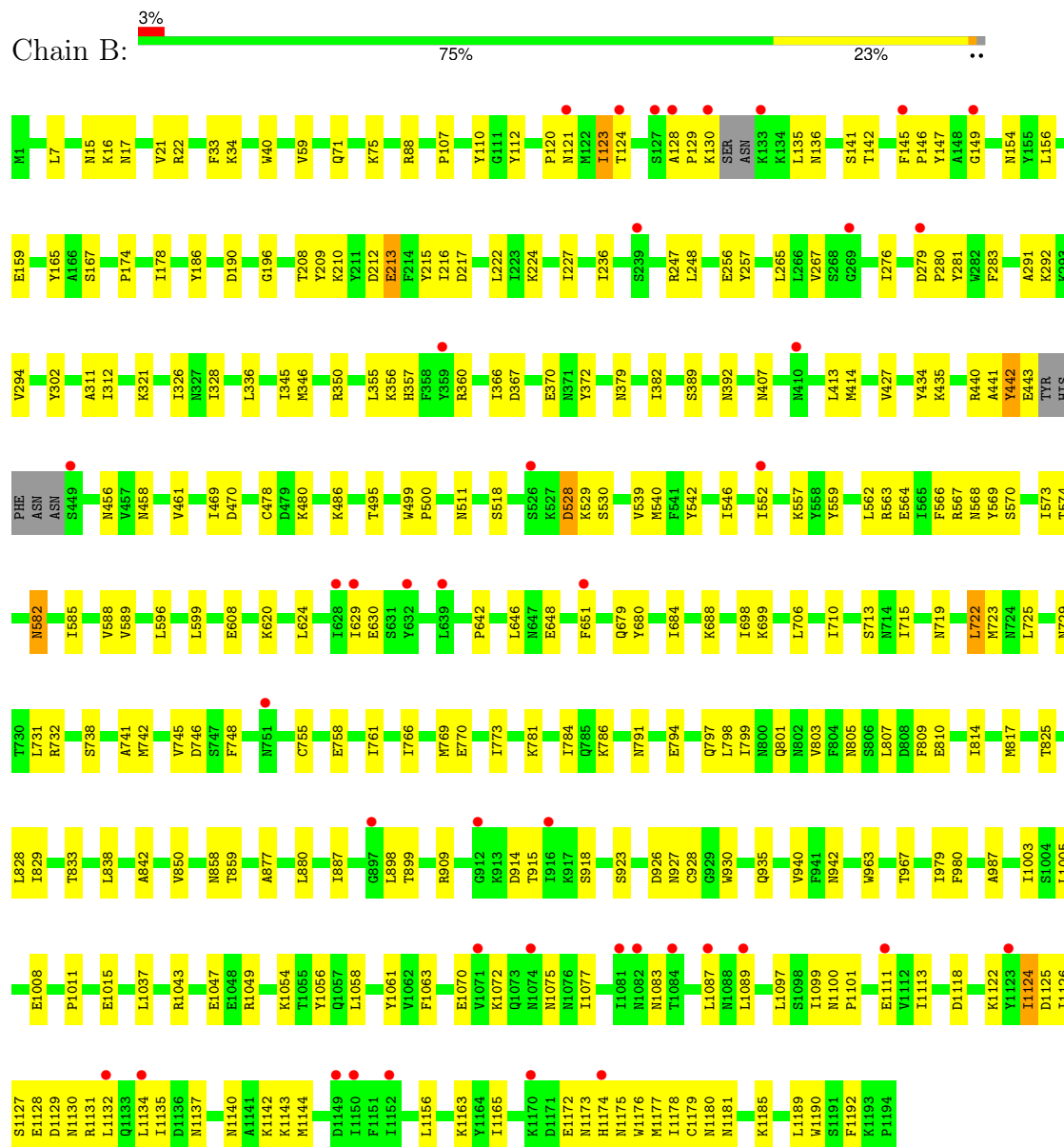
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Botulinum neurotoxin type A

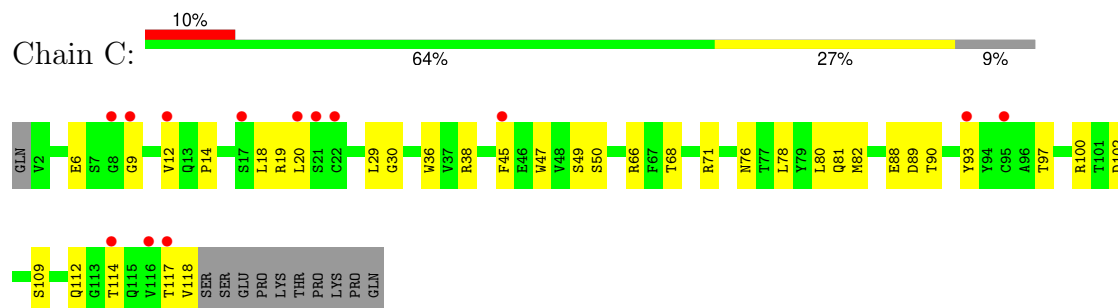


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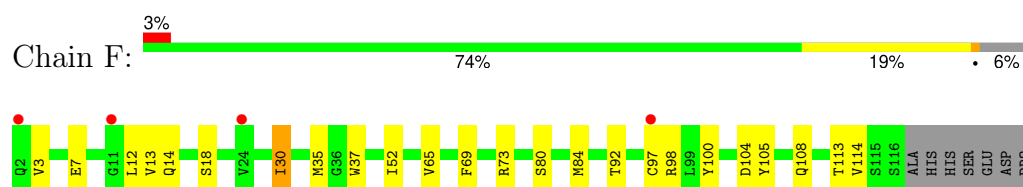
- Molecule 2: Non-toxic nonhemagglutinin type A



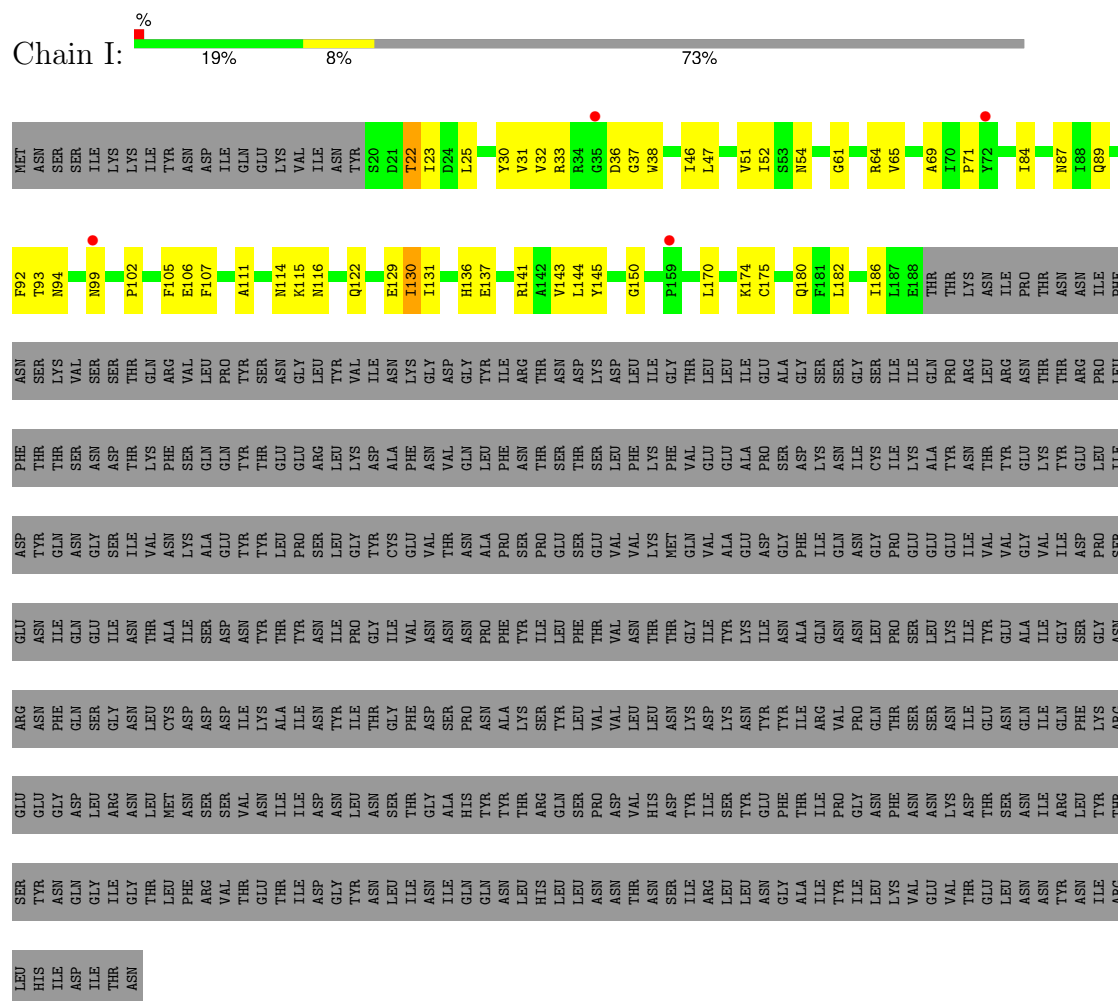
- Molecule 3: Nanobody ciA-F12



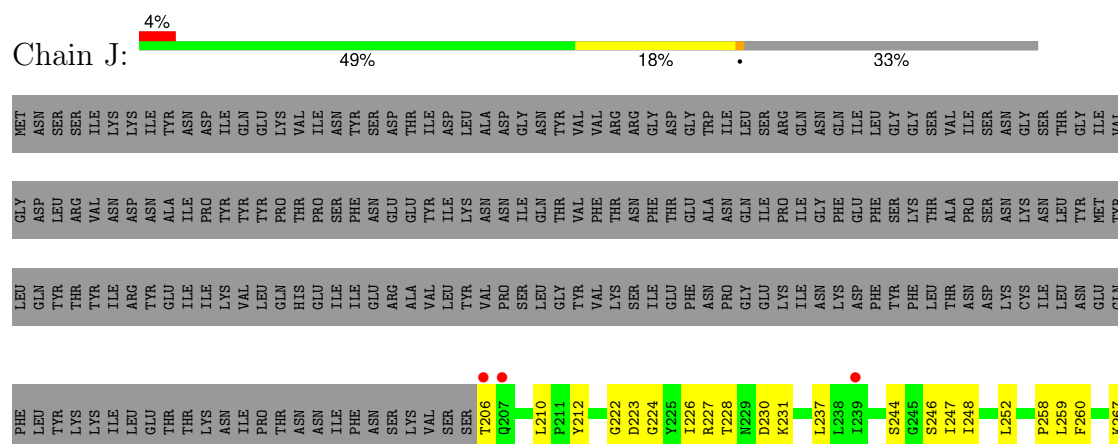
- Molecule 4: Nanobody ciA-H7

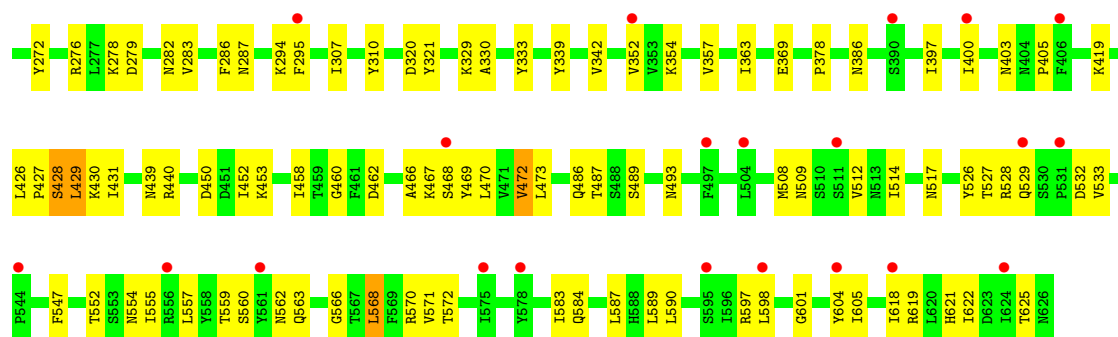


- Molecule 5: HA-70

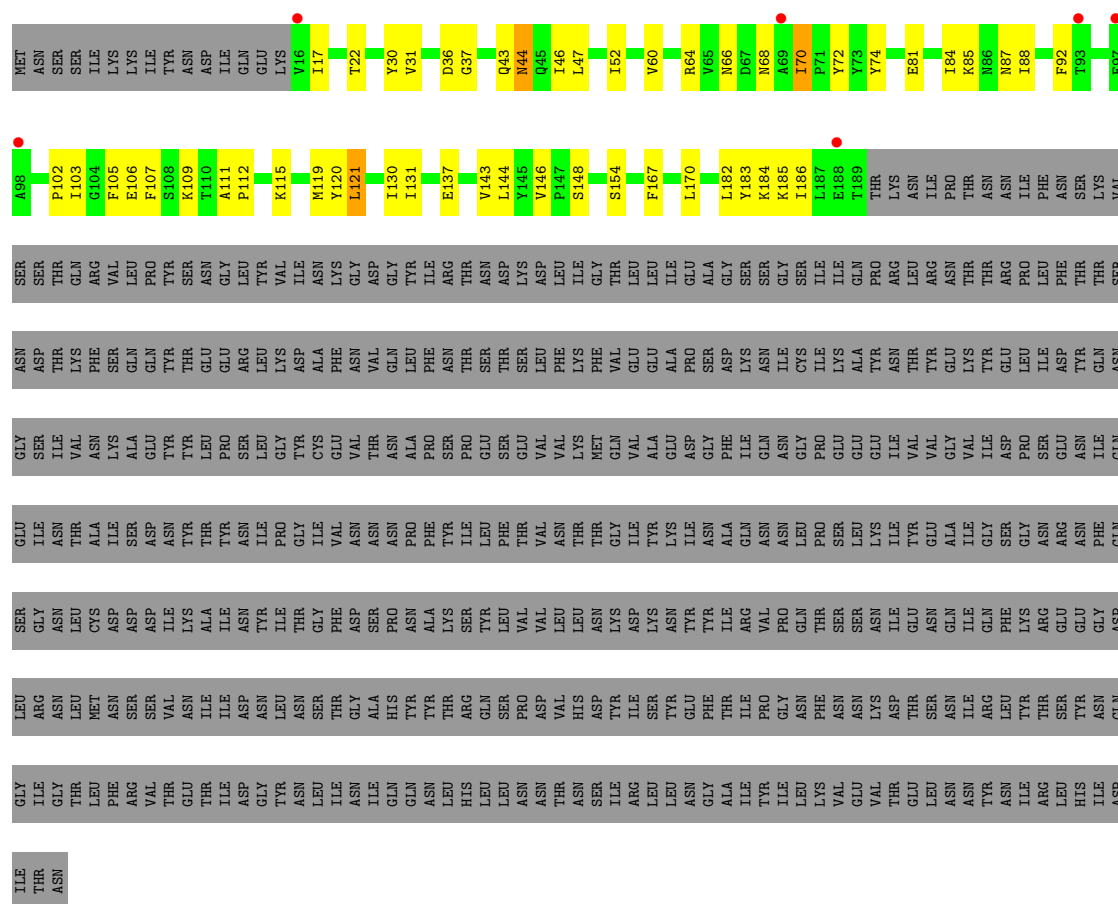


- Molecule 5: HA-70



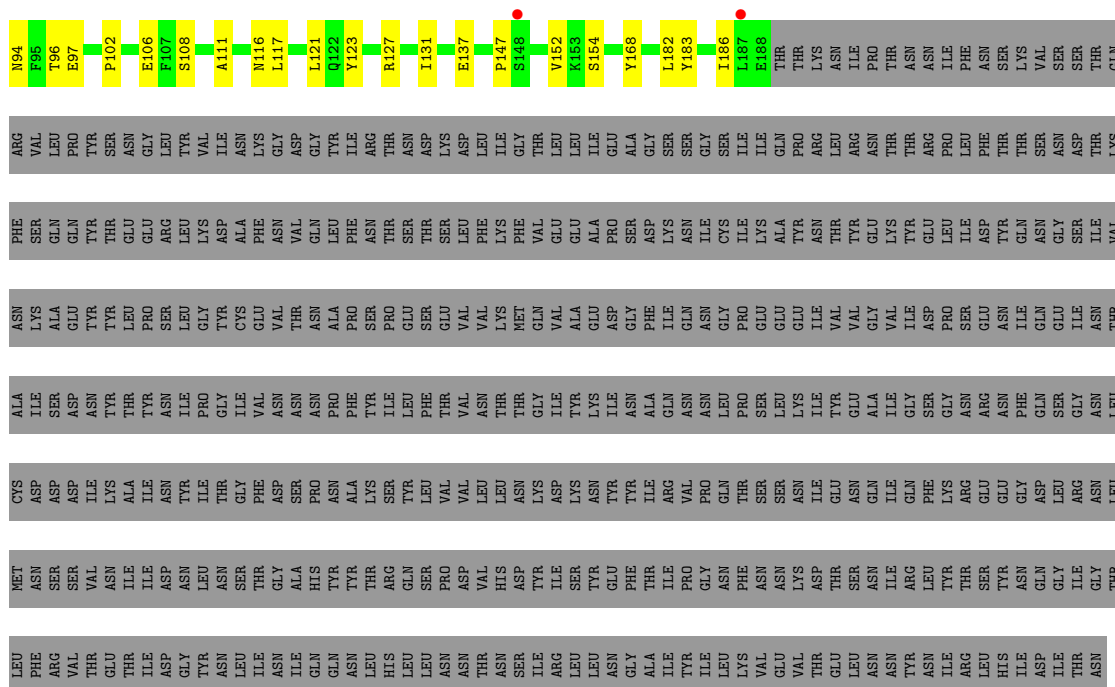


● Molecule 5: HA-70

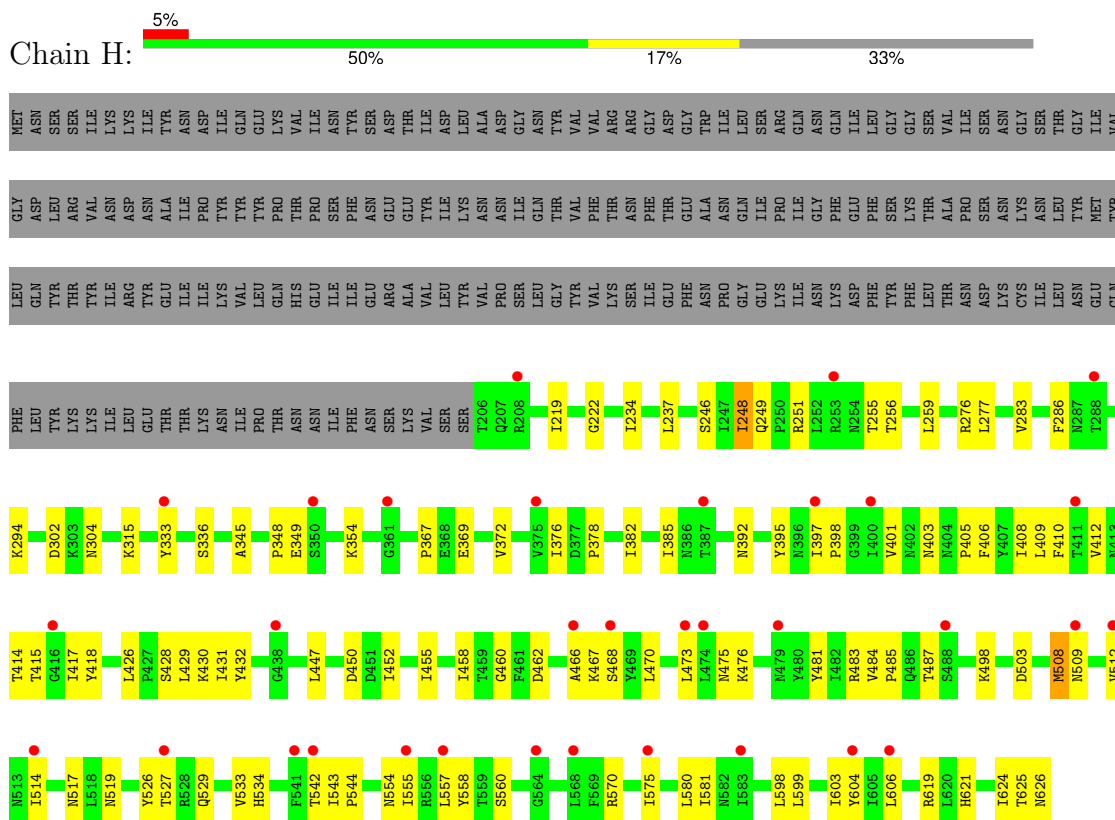


● Molecule 5: HA-70



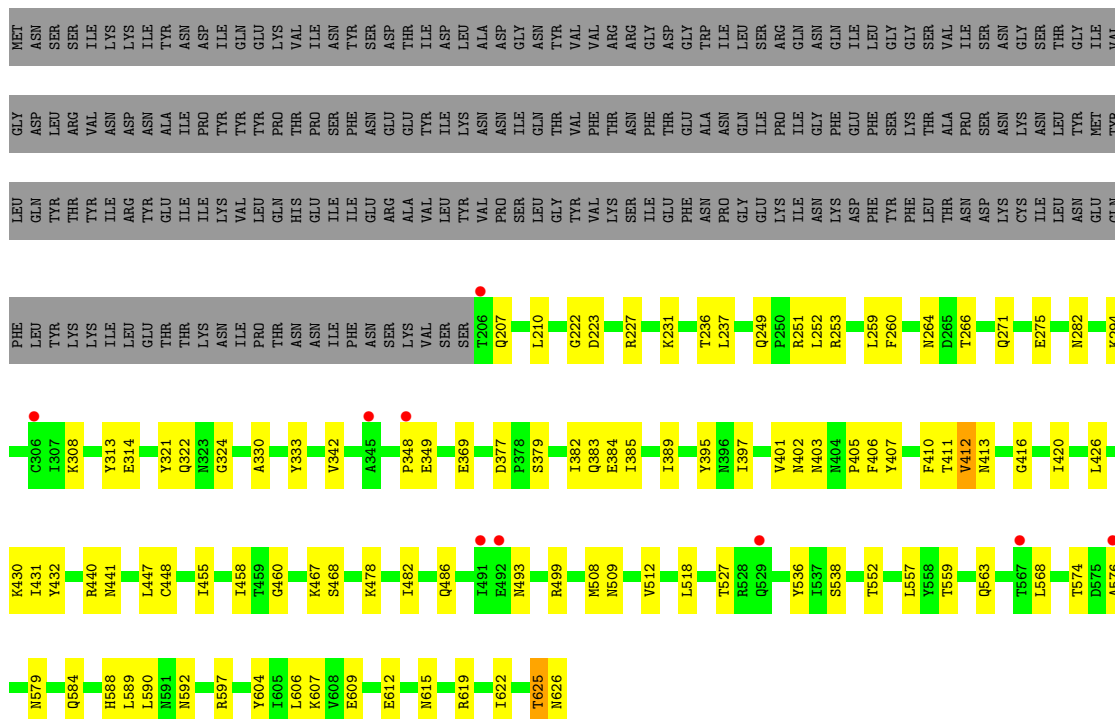


- Molecule 5: HA-70

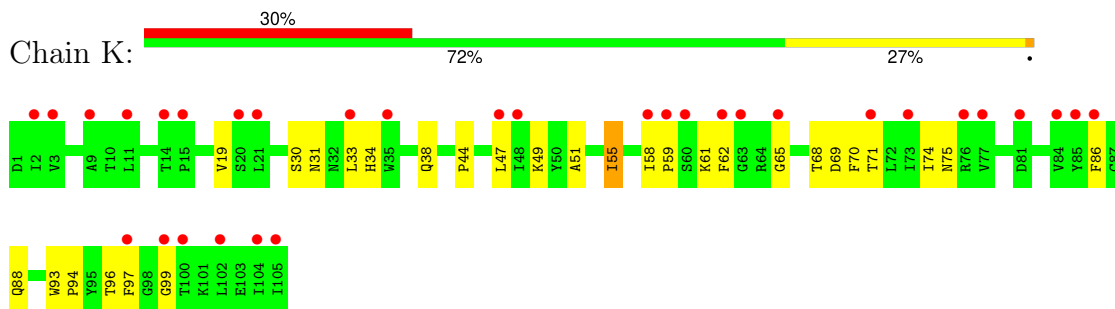


- Molecule 6: HA70/A1

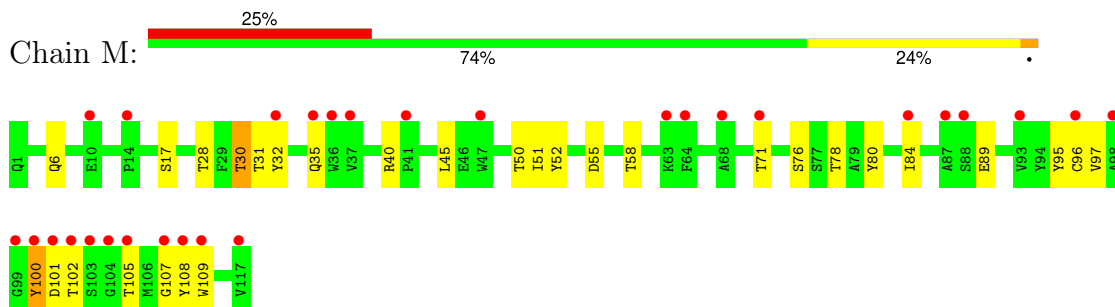




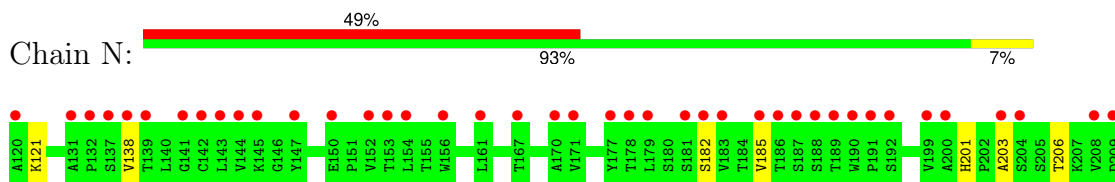
- Molecule 7: anti-NTNH Fab

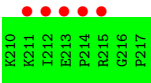


- Molecule 8: anti-NTNH Fab

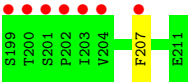
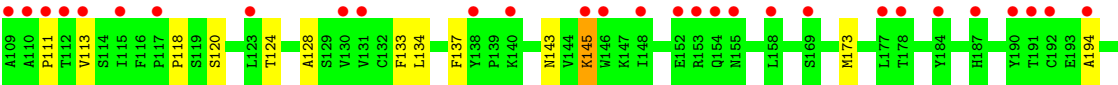
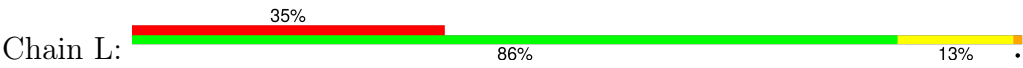


- Molecule 9: anti-NTNH Fab





● Molecule 10: anti-NTNH Fab



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	203.65Å 203.65Å 479.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.61 – 2.93 99.61 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (99.61-2.93) 99.9 (99.61-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5107	Depositor
R, R_{free}	0.286 , 0.308 0.287 , 0.308	Depositor DCC
R_{free} test set	2000 reflections (0.93%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	39218	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, SO4

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	A	0.14	0/10590	0.32	0/14338
2	B	0.15	0/9876	0.34	0/13390
3	C	0.16	0/893	0.34	0/1213
4	F	0.15	0/867	0.35	0/1167
5	D	0.16	0/1442	0.37	0/1959
5	G	0.11	0/1414	0.32	0/1919
5	H	0.14	0/3426	0.36	0/4662
5	I	0.13	0/1408	0.36	0/1911
5	J	0.13	0/3429	0.36	0/4667
6	E	0.13	0/3421	0.35	0/4657
7	K	0.29	0/821	0.50	0/1116
8	M	0.15	0/902	0.34	0/1226
9	N	0.11	0/650	0.33	0/900
10	L	0.13	0/768	0.31	0/1047
All	All	0.14	0/39907	0.34	0/54172

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	A	10371	0	10228	199	0
2	B	9671	0	9434	189	0
3	C	873	0	812	20	0
4	F	853	0	830	17	0
5	D	1409	0	1375	41	0
5	G	1382	0	1357	38	0
5	H	3363	0	3265	73	0
5	I	1376	0	1348	35	0
5	J	3366	0	3267	84	0
6	E	3358	0	3253	69	0
7	K	803	0	766	30	0
8	M	881	0	834	23	0
9	N	634	0	579	4	0
10	L	752	0	650	10	0
11	A	20	0	0	3	0
11	B	20	0	0	1	0
11	D	5	0	0	0	0
11	E	5	0	0	4	0
12	A	1	0	0	0	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	E	6	0	0	0	0
13	H	1	0	0	0	0
13	J	1	0	0	0	0
14	A	25	0	0	4	0
14	B	15	0	0	3	0
14	D	3	0	0	1	0
14	E	8	0	0	3	0
14	F	4	0	0	0	0
14	G	2	0	0	0	0
14	H	2	0	0	1	0
14	I	3	0	0	0	0
14	J	2	0	0	0	0
14	M	1	0	0	0	0
All	All	39218	0	37998	785	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 10.

All (785) 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)
10:L:143:ASN:HB3	10:L:145:LYS:HE2	1.47	0.96
5:J:584:GLN:HG3	5:J:587:LEU:HD11	1.48	0.92
5:I:54:ASN:HD22	5:I:114:ASN:H	1.22	0.87
1:A:903:LYS:HG3	1:A:921:SER:HB2	1.55	0.87
2:B:120:PRO:HB3	2:B:146:PRO:HD2	1.57	0.87
7:K:55:ILE:HG13	8:M:100:TYR:OH	1.77	0.84
1:A:709:VAL:HG21	1:A:808:LEU:HD21	1.61	0.82
1:A:717:TRP:HB2	1:A:800:MET:HE1	1.61	0.82
5:G:89:GLN:HG2	5:G:94:ASN:HA	1.63	0.81
1:A:952:TYR:H	1:A:1003:GLN:HE22	1.29	0.81
2:B:528:ASP:HB2	2:B:530:SER:H	1.51	0.76
5:J:562:ASN:HB2	5:J:618:ILE:HD13	1.66	0.74
1:A:24:ILE:HD11	1:A:51:PHE:CE2	2.23	0.74
5:G:92:PHE:HE1	5:G:182:LEU:HD23	1.52	0.74
5:D:84:ILE:O	5:D:88:ILE:HG12	1.89	0.73
5:H:415:THR:HG22	5:H:475:ASN:HA	1.70	0.73
1:A:880:ASN:OD1	1:A:882:ARG:NH1	2.22	0.73
5:G:117:LEU:HD21	5:G:154:SER:HB2	1.70	0.73
1:A:948:ARG:HB3	1:A:1068:TRP:HB2	1.71	0.72
2:B:59:VAL:HG12	2:B:486:LYS:HD2	1.71	0.72
6:E:568:LEU:HB3	6:E:584:GLN:HB3	1.71	0.72
1:A:648:TYR:N	1:A:651:ASP:OD2	2.23	0.71
1:A:1088:TYR:HH	1:A:1231:ILE:N	1.87	0.71
5:G:94:ASN:HD21	5:G:97:GLU:HB2	1.55	0.71
5:H:529:GLN:HB3	14:H:802:HOH:O	1.91	0.70
2:B:360:ARG:HE	2:B:360:ARG:HA	1.55	0.70
7:K:47:LEU:HD22	7:K:58:ILE:CG2	2.22	0.69
1:A:473:ASN:HB2	14:A:1403:HOH:O	1.91	0.69
7:K:44:PRO:HG2	8:M:45:LEU:HD11	1.74	0.69
5:H:542:THR:HG22	5:H:603:ILE:HG12	1.74	0.69
1:A:709:VAL:CG2	1:A:808:LEU:HD21	2.23	0.69
2:B:379:ASN:HD21	2:B:858:ASN:HD21	1.40	0.68
2:B:145:PHE:HB3	2:B:146:PRO:HD3	1.76	0.68
2:B:511:ASN:HD22	2:B:530:SER:HA	1.59	0.68
5:H:259:LEU:HB2	5:H:333:TYR:HB2	1.74	0.68
6:E:249:GLN:HE21	6:E:251:ARG:H	1.42	0.68
2:B:442:TYR:HD1	2:B:443:GLU:HG3	1.59	0.68
2:B:22:ARG:NH1	2:B:159:GLU:O	2.26	0.68
5:I:52:ILE:HG13	5:I:111:ALA:HB2	1.77	0.67
7:K:34:HIS:HD2	7:K:88:GLN:HE21	1.41	0.67
5:D:44:ASN:HD21	5:D:170:LEU:HB2	1.58	0.67
5:G:89:GLN:NE2	5:G:94:ASN:OD1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:17:SER:HB3	8:M:84:ILE:HG13	1.76	0.67
1:A:24:ILE:HD11	1:A:51:PHE:HE2	1.57	0.67
2:B:486:LYS:NZ	11:B:1202:SO4:O4	2.28	0.66
5:D:183:TYR:HE2	5:H:354:LYS:HB3	1.60	0.66
5:H:543:ILE:HD12	5:H:543:ILE:H	1.60	0.66
7:K:55:ILE:HG22	7:K:58:ILE:HG12	1.77	0.66
5:G:46:ILE:HG22	5:H:283:VAL:HG12	1.76	0.66
5:D:81:GLU:CD	5:D:81:GLU:H	2.01	0.65
2:B:212:ASP:OD2	2:B:688:LYS:NZ	2.27	0.65
5:H:349:GLU:OE1	5:H:349:GLU:N	2.26	0.65
2:B:1173:ASN:O	2:B:1174:HIS:ND1	2.29	0.65
2:B:1135:ILE:HD12	2:B:1137:ASN:H	1.61	0.65
1:A:598:THR:O	1:A:750:GLN:NE2	2.29	0.65
5:G:31:VAL:HG21	5:G:91:VAL:HG21	1.79	0.65
2:B:719:ASN:O	2:B:723:MET:HG3	1.96	0.65
10:L:134:LEU:HD22	10:L:173:MET:HE1	1.79	0.65
5:D:52:ILE:HG13	5:D:111:ALA:HB2	1.79	0.64
3:C:82:MET:HE1	3:C:93:TYR:CE2	2.32	0.64
1:A:888:LEU:HB3	1:A:900:ILE:HD11	1.77	0.64
5:H:395:TYR:HE1	5:H:398:PRO:HD3	1.63	0.64
2:B:706:LEU:O	2:B:710:ILE:HG13	1.98	0.64
1:A:705:LYS:O	1:A:709:VAL:HG22	1.98	0.64
5:J:259:LEU:HB2	5:J:333:TYR:HB2	1.80	0.64
2:B:1132:LEU:HD11	2:B:1165:ILE:HD13	1.78	0.64
2:B:435:LYS:NZ	14:B:1301:HOH:O	2.31	0.64
5:I:84:ILE:HG12	5:I:130:ILE:HG13	1.79	0.64
7:K:49:LYS:H	7:K:55:ILE:HD13	1.63	0.64
2:B:784:ILE:HD13	2:B:798:LEU:HB3	1.78	0.63
2:B:979:ILE:HB	2:B:987:ALA:HB3	1.79	0.63
5:I:115:LYS:HD3	5:I:116:ASN:H	1.62	0.63
5:D:22:THR:HA	5:D:137:GLU:HA	1.79	0.63
6:E:625:THR:OG1	6:E:626:ASN:ND2	2.32	0.63
7:K:47:LEU:HD22	7:K:58:ILE:HG23	1.80	0.63
5:H:555:ILE:HD12	5:H:624:ILE:HG12	1.81	0.63
2:B:770:GLU:HA	2:B:773:ILE:HG12	1.80	0.63
1:A:673:ILE:HG22	1:A:807:ARG:HG3	1.81	0.63
6:E:405:PRO:HD3	6:E:486:GLN:HB2	1.80	0.63
4:F:98:ARG:NH2	4:F:104:ASP:OD1	2.23	0.62
1:A:1114:LEU:HB3	1:A:1283:GLU:HB2	1.81	0.62
5:J:467:LYS:HB3	5:J:514:ILE:HB	1.81	0.62
7:K:51:ALA:HB1	7:K:65:GLY:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:473:LEU:H	5:H:509:ASN:ND2	1.98	0.61
2:B:1172:GLU:H	2:B:1173:ASN:HA	1.65	0.61
5:I:170:LEU:HD21	5:I:174:LYS:HG2	1.81	0.61
6:E:385:ILE:HD11	6:E:395:TYR:HD2	1.66	0.61
2:B:914:ASP:OD1	2:B:915:THR:N	2.32	0.61
4:F:108:GLN:N	4:F:108:GLN:OE1	2.34	0.61
1:A:1115:ASN:HD21	1:A:1117:TYR:HB3	1.66	0.61
2:B:528:ASP:HB2	2:B:530:SER:N	2.15	0.61
1:A:985:TRP:HB3	1:A:997:VAL:HG22	1.82	0.61
5:J:466:ALA:HB2	5:J:528:ARG:HH21	1.66	0.61
8:M:102:THR:HB	8:M:105:THR:HG23	1.83	0.60
1:A:198:GLU:HG2	1:A:361:LEU:HD11	1.83	0.60
2:B:518:SER:HB3	2:B:540:MET:HE1	1.83	0.60
2:B:1178:ILE:HD12	2:B:1180:ASN:HB3	1.83	0.60
5:J:517:ASN:HD21	5:J:526:TYR:HE1	1.50	0.60
5:D:36:ASP:OD1	5:D:37:GLY:N	2.35	0.60
6:E:397:ILE:HD12	6:E:493:ASN:HB3	1.83	0.60
5:J:231:LYS:NZ	5:G:91:VAL:O	2.34	0.60
8:M:97:VAL:HG11	8:M:109:TRP:CE3	2.36	0.60
5:G:94:ASN:ND2	5:G:97:GLU:HB2	2.17	0.60
5:H:557:LEU:HD13	5:H:606:LEU:HD22	1.82	0.60
5:D:92:PHE:HE1	5:D:182:LEU:HD23	1.65	0.60
7:K:61:LYS:HB2	7:K:75:ASN:H	1.66	0.60
2:B:7:LEU:HD13	2:B:33:PHE:HB3	1.84	0.59
1:A:573:ASN:O	1:A:577:LEU:HD12	2.01	0.59
1:A:937:MET:HE3	1:A:1046:ASN:HB2	1.83	0.59
6:E:260:PHE:HE1	6:E:330:ALA:HB1	1.67	0.59
2:B:1072:LYS:HE2	2:B:1075:ASN:HA	1.83	0.59
5:J:428:SER:HB2	5:J:466:ALA:HB3	1.85	0.59
5:J:230:ASP:O	5:G:93:THR:OG1	2.21	0.59
8:M:6:GLN:HE22	8:M:95:TYR:HA	1.65	0.59
2:B:1070:GLU:HB2	2:B:1077:ILE:HD11	1.84	0.59
2:B:1140:ASN:O	2:B:1142:LYS:NZ	2.36	0.59
2:B:880:LEU:O	2:B:1011:PRO:HA	2.03	0.58
1:A:959:ASN:ND2	2:B:801:GLN:O	2.32	0.58
2:B:208:THR:HB	2:B:366:ILE:HD11	1.85	0.58
5:J:267:LYS:NZ	5:J:320:ASP:OD2	2.33	0.58
1:A:954:ASN:OD1	1:A:956:ILE:N	2.29	0.58
1:A:996:ARG:HD3	2:B:807:LEU:HD21	1.83	0.58
1:A:1294:ARG:HD3	1:A:1295:PRO:HD2	1.83	0.58
2:B:624:LEU:HD11	2:B:761:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1097:LEU:HB2	2:B:1113:ILE:HG12	1.85	0.58
1:A:710:TYR:O	1:A:714:VAL:HG23	2.03	0.58
1:A:913:GLN:HG2	1:A:1070:LYS:HD3	1.85	0.58
1:A:1265:ASN:OD1	1:A:1268:ASN:ND2	2.37	0.58
5:J:462:ASP:OD2	5:J:529:GLN:NE2	2.36	0.58
1:A:1115:ASN:HD22	1:A:1118:ASP:H	1.52	0.58
5:H:543:ILE:HD11	5:H:604:TYR:CD2	2.39	0.58
6:E:207:GLN:NE2	14:E:802:HOH:O	2.33	0.58
2:B:838:LEU:HD13	2:B:859:THR:HG21	1.85	0.58
5:D:30:TYR:HB2	5:D:131:ILE:HG13	1.86	0.57
5:J:559:THR:HB	5:J:618:ILE:HD11	1.86	0.57
3:C:68:THR:HG22	3:C:81:GLN:HB3	1.86	0.57
5:D:70:ILE:HD13	5:D:72:TYR:HE1	1.70	0.57
1:A:1097:LEU:HD21	1:A:1223:MET:HB3	1.86	0.57
5:H:554:ASN:HB3	5:H:625:THR:HG23	1.86	0.57
3:C:97:THR:HG21	3:C:109:SER:H	1.70	0.57
10:L:113:VAL:HG22	10:L:134:LEU:HG	1.87	0.57
5:I:47:LEU:HD23	5:I:122:GLN:HA	1.87	0.56
5:J:469:TYR:CE1	5:J:512:VAL:HB	2.40	0.56
5:I:61:GLY:HA3	5:I:106:GLU:HG3	1.86	0.56
1:A:393:ARG:NH1	14:A:1401:HOH:O	2.38	0.56
5:J:222:GLY:HA2	5:J:369:GLU:HB3	1.87	0.56
5:J:431:ILE:HG21	5:J:472:VAL:HG11	1.87	0.56
5:H:560:SER:OG	5:H:621:HIS:NE2	2.39	0.56
5:J:431:ILE:HG23	5:J:458:ILE:HB	1.86	0.56
6:E:557:LEU:HD13	6:E:606:LEU:HD22	1.86	0.56
1:A:676:LEU:HB3	1:A:705:LYS:HE2	1.87	0.56
1:A:742:ALA:O	1:A:746:ILE:HG13	2.06	0.56
5:J:557:LEU:HD23	5:J:622:ILE:HG12	1.86	0.56
5:D:144:LEU:HD11	5:D:146:VAL:HG23	1.86	0.56
5:I:31:VAL:HG13	5:I:186:ILE:HD11	1.86	0.56
4:F:92:THR:HG23	4:F:113:THR:HA	1.88	0.56
5:I:71:PRO:HB2	5:I:144:LEU:HD11	1.88	0.56
1:A:779:LYS:NZ	11:A:1301:SO4:S	2.71	0.55
5:D:31:VAL:HG13	5:D:186:ILE:HD11	1.87	0.55
8:M:51:ILE:HD13	8:M:58:THR:HG22	1.88	0.55
6:E:559:THR:HG23	6:E:589:LEU:HB3	1.88	0.55
8:M:71:THR:HG23	8:M:80:TYR:HB2	1.88	0.55
1:A:24:ILE:HG22	1:A:135:ILE:HG22	1.88	0.55
6:E:249:GLN:NE2	6:E:251:ARG:H	2.05	0.55
5:J:227:ARG:HD2	5:J:259:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:55:ASP:OD1	8:M:55:ASP:N	2.38	0.55
1:A:114:GLY:HA2	1:A:320:LYS:HG3	1.89	0.55
2:B:589:VAL:HG21	2:B:745:VAL:HG12	1.87	0.55
1:A:858:ASP:O	1:A:861:ARG:NH1	2.40	0.55
5:J:252:LEU:HB2	5:G:102:PRO:HG2	1.89	0.55
5:J:570:ARG:HH21	5:J:572:THR:HG22	1.72	0.55
5:D:105:PHE:HE2	5:D:121:LEU:HD11	1.71	0.55
6:E:615:ASN:OD1	11:E:701:SO4:S	2.64	0.55
2:B:350:ARG:NH2	2:B:746:ASP:OD1	2.40	0.54
2:B:469:ILE:HG13	6:E:253:ARG:HH11	1.72	0.54
5:J:426:LEU:HD21	5:J:467:LYS:HG2	1.89	0.54
5:G:89:GLN:HE22	5:G:96:THR:HB	1.72	0.54
5:H:527:THR:HG22	5:H:619:ARG:HG2	1.89	0.54
1:A:954:ASN:OD1	1:A:955:SER:N	2.41	0.54
2:B:470:ASP:HB2	6:E:253:ARG:HD3	1.89	0.54
5:H:430:LYS:HD3	5:H:483:ARG:HD3	1.89	0.54
2:B:147:TYR:CD2	6:E:252:LEU:HB3	2.43	0.54
2:B:773:ILE:HD13	2:B:809:PHE:HE2	1.71	0.54
1:A:1:MET:N	1:A:2:PRO:HD3	2.22	0.54
1:A:23:LYS:HD2	1:A:32:PRO:HG3	1.89	0.54
2:B:1099:ILE:HD11	2:B:1111:GLU:HB3	1.88	0.54
7:K:49:LYS:HB3	7:K:55:ILE:HD11	1.90	0.54
1:A:149:LEU:C	1:A:150:ASN:HD22	2.15	0.54
7:K:19:VAL:HG22	7:K:74:ILE:HB	1.90	0.54
5:J:223:ASP:OD1	5:J:224:GLY:N	2.40	0.54
1:A:453:LEU:HD23	1:A:453:LEU:H	1.73	0.54
3:C:90:THR:HG23	3:C:117:THR:HA	1.89	0.54
5:G:52:ILE:HG13	5:G:111:ALA:HB2	1.89	0.54
5:I:33:ARG:HH11	5:I:180:GLN:HE22	1.54	0.54
5:J:260:PHE:HE1	5:J:330:ALA:HB1	1.72	0.53
6:E:411:THR:HB	6:E:447:LEU:HD13	1.90	0.53
1:A:280:ASN:OD1	1:A:283:ARG:NH1	2.31	0.53
8:M:97:VAL:HG12	8:M:109:TRP:HA	1.89	0.53
1:A:167:SER:HB3	1:A:184:GLN:HE22	1.74	0.53
7:K:47:LEU:HD22	7:K:58:ILE:HG21	1.88	0.53
2:B:511:ASN:ND2	2:B:530:SER:HA	2.21	0.53
5:H:409:LEU:HG	5:H:447:LEU:HD21	1.90	0.53
5:D:88:ILE:HD11	5:D:130:ILE:HD11	1.90	0.53
1:A:1155:TYR:CD2	1:A:1293:GLU:HG2	2.43	0.53
2:B:326:ILE:HD13	2:B:456:ASN:HB2	1.91	0.53
2:B:442:TYR:CD1	2:B:443:GLU:HG3	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:382:ILE:HG23	6:E:407:TYR:HB2	1.91	0.53
1:A:124:ASP:OD1	1:A:124:ASP:N	2.34	0.53
5:I:102:PRO:HB2	6:E:252:LEU:HD12	1.90	0.53
5:J:354:LYS:H	5:J:354:LYS:HD2	1.74	0.53
1:A:548:TYR:HE2	1:A:576:LEU:HD12	1.73	0.53
1:A:1226:LYS:O	1:A:1234:LYS:HB2	2.08	0.52
6:E:389:ILE:HB	6:E:412:VAL:HA	1.90	0.52
6:E:468:SER:HA	6:E:512:VAL:O	2.09	0.52
1:A:656:LEU:HD13	1:A:663:ILE:HD11	1.90	0.52
1:A:998:VAL:HB	2:B:807:LEU:HD12	1.91	0.52
6:E:402:ASN:OD1	6:E:403:ASN:ND2	2.42	0.52
1:A:319:GLU:OE2	1:A:510:ASN:ND2	2.41	0.52
2:B:283:PHE:HA	2:B:434:TYR:OH	2.09	0.52
2:B:1131:ARG:HD3	2:B:1176:TRP:HB3	1.92	0.52
4:F:7:GLU:H	4:F:108:GLN:HE22	1.56	0.52
2:B:495:THR:HG21	2:B:499:TRP:CD1	2.45	0.52
5:J:571:VAL:HG21	5:J:605:ILE:HG13	1.91	0.52
2:B:755:CYS:SG	14:B:1309:HOH:O	2.59	0.52
1:A:1176:ASN:HD22	1:A:1225:SER:H	1.56	0.52
5:H:276:ARG:NH1	5:H:378:PRO:HG3	2.25	0.52
7:K:49:LYS:HD3	7:K:55:ILE:HD11	1.90	0.52
2:B:210:LYS:HE3	2:B:213:GLU:HA	1.90	0.52
5:H:468:SER:HA	5:H:512:VAL:O	2.09	0.52
1:A:751:TYR:CE2	1:A:764:PHE:HB3	2.44	0.52
2:B:1172:GLU:N	2:B:1173:ASN:HA	2.24	0.52
2:B:1083:ASN:ND2	2:B:1175:ASN:OD1	2.36	0.51
5:D:102:PRO:O	5:H:249:GLN:NE2	2.43	0.51
5:H:429:LEU:HB2	5:H:470:LEU:HD11	1.92	0.51
7:K:55:ILE:HG13	8:M:100:TYR:HH	1.74	0.51
8:M:107:GLY:C	8:M:108:TYR:HD1	2.19	0.51
1:A:1125:VAL:HG22	1:A:1134:MET:HG2	1.93	0.51
4:F:65:VAL:HB	4:F:69:PHE:CD2	2.44	0.51
7:K:49:LYS:HE3	8:M:101:ASP:OD2	2.10	0.51
2:B:1130:ASN:O	2:B:1179:CYS:N	2.37	0.51
10:L:134:LEU:HD21	10:L:194:ALA:HB2	1.92	0.51
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	1.92	0.51
2:B:311:ALA:O	2:B:312:ILE:HD13	2.10	0.51
5:D:183:TYR:CE2	5:H:354:LYS:HB3	2.43	0.51
1:A:940:ASN:HB2	11:A:1301:SO4:O2	2.10	0.51
2:B:21:VAL:HG21	2:B:156:LEU:HD13	1.93	0.51
3:C:45:PHE:HB2	3:C:102:ASP:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:36:ASP:OD1	5:I:37:GLY:N	2.44	0.51
6:E:210:LEU:HB2	6:E:321:TYR:OH	2.10	0.51
2:B:781:LYS:HG3	2:B:799:ILE:HD13	1.92	0.51
4:F:14:GLN:OE1	4:F:14:GLN:N	2.44	0.51
5:H:503:ASP:HB3	5:H:580:LEU:HB2	1.93	0.51
1:A:590:TYR:O	1:A:594:VAL:HG12	2.11	0.51
4:F:12:LEU:H	4:F:12:LEU:HD23	1.75	0.51
5:H:219:ILE:HG12	5:H:372:VAL:HG13	1.93	0.51
5:H:432:TYR:HB3	5:H:455:ILE:HB	1.92	0.51
1:A:184:GLN:NE2	1:A:231:ARG:HD3	2.25	0.51
3:C:9:GLY:H	3:C:18:LEU:HD21	1.75	0.51
1:A:897:LYS:HB3	1:A:927:ILE:HB	1.92	0.50
7:K:31:ASN:HB2	7:K:51:ALA:HB2	1.93	0.50
10:L:120:SER:O	10:L:124:THR:HG23	2.12	0.50
1:A:121:SER:HB2	1:A:128:LYS:HB2	1.93	0.50
1:A:1266:TRP:HH2	1:A:1276:ARG:HB3	1.77	0.50
5:D:112:PRO:HB2	5:D:115:LYS:HD2	1.93	0.50
5:H:462:ASP:OD2	5:H:529:GLN:NE2	2.43	0.50
3:C:36:TRP:CD2	3:C:80:LEU:HD12	2.47	0.50
5:D:84:ILE:HG12	5:D:130:ILE:HG13	1.93	0.50
5:G:67:ASP:HB2	5:H:286:PHE:CZ	2.46	0.50
1:A:1196:ASN:OD1	1:A:1198:SER:OG	2.24	0.50
6:E:410:PHE:HE1	6:E:482:ILE:HG13	1.76	0.50
5:H:405:PRO:HB3	5:H:485:PRO:HA	1.94	0.50
1:A:1097:LEU:HD12	1:A:1225:SER:HB3	1.93	0.50
2:B:1124:ILE:HG23	2:B:1132:LEU:HD22	1.94	0.50
5:J:427:PRO:HG3	5:J:487:THR:HG22	1.93	0.50
6:E:574:THR:HG23	6:E:576:ALA:H	1.76	0.50
7:K:49:LYS:CD	7:K:55:ILE:HD11	2.41	0.50
8:M:30:THR:O	8:M:30:THR:OG1	2.29	0.50
1:A:709:VAL:HG21	1:A:808:LEU:HD11	1.93	0.50
1:A:568:LEU:HD22	1:A:594:VAL:HG11	1.93	0.50
1:A:569:THR:HG22	1:A:571:SER:H	1.77	0.50
2:B:389:SER:O	2:B:392:ASN:ND2	2.45	0.50
6:E:615:ASN:OD1	11:E:701:SO4:O2	2.29	0.50
2:B:346:MET:HB3	2:B:825:THR:HG23	1.92	0.50
3:C:29:LEU:HD21	3:C:78:LEU:HB2	1.93	0.50
5:J:466:ALA:CB	5:J:528:ARG:HH21	2.25	0.50
9:N:201:HIS:CE1	9:N:203:ALA:HB3	2.47	0.50
2:B:458:ASN:HB3	2:B:461:VAL:HG22	1.94	0.49
2:B:1125:ASP:OD1	2:B:1126:ILE:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:81:GLU:OE1	5:D:81:GLU:N	2.34	0.49
5:H:392:ASN:OD1	5:H:498:LYS:HD3	2.12	0.49
5:H:450:ASP:HB2	5:H:452:ILE:HG13	1.93	0.49
1:A:643:ILE:HG21	1:A:664:LEU:HD23	1.94	0.49
2:B:599:LEU:HB3	2:B:608:GLU:HG2	1.94	0.49
2:B:1061:TYR:HB2	2:B:1189:LEU:HB2	1.93	0.49
3:C:29:LEU:H	3:C:76:ASN:ND2	2.10	0.49
5:I:54:ASN:ND2	5:I:114:ASN:H	2.02	0.49
1:A:96:GLU:O	1:A:100:SER:OG	2.30	0.49
1:A:821:LYS:NZ	1:A:825:ASP:OD2	2.46	0.49
1:A:969:GLU:HG3	1:A:1050:SER:HA	1.95	0.49
2:B:112:TYR:CD1	2:B:149:GLY:HA3	2.47	0.49
2:B:1172:GLU:H	2:B:1174:HIS:H	1.60	0.49
14:A:1420:HOH:O	2:B:585:ILE:HD11	2.13	0.49
2:B:256:GLU:HG3	2:B:427:VAL:HG12	1.94	0.49
5:J:554:ASN:HB3	5:J:625:THR:OG1	2.13	0.49
2:B:877:ALA:HB2	2:B:1015:GLU:HB2	1.94	0.49
3:C:14:PRO:HG3	3:C:118:VAL:HG12	1.94	0.49
5:J:429:LEU:HB2	5:J:470:LEU:HD11	1.94	0.49
5:J:560:SER:HG	5:J:621:HIS:HE2	1.60	0.49
5:H:414:THR:O	5:H:418:TYR:OH	2.25	0.49
1:A:815:LEU:HD23	1:A:819:LEU:HD13	1.94	0.49
5:I:22:THR:HA	5:I:137:GLU:HA	1.95	0.49
5:H:417:ILE:HD13	5:H:508:MET:HG2	1.94	0.49
2:B:539:VAL:HG11	2:B:698:ILE:HD11	1.95	0.49
5:J:587:LEU:HB3	5:J:589:LEU:HD21	1.95	0.49
6:E:512:VAL:HG22	6:E:538:SER:HB2	1.93	0.49
5:G:62:ASP:OD1	5:G:63:LEU:N	2.42	0.49
1:A:288:ASN:HB2	4:F:100:TYR:HD2	1.78	0.49
1:A:292:ASP:CG	4:F:98:ARG:HH12	2.21	0.49
5:J:559:THR:HG23	5:J:589:LEU:HB3	1.95	0.49
5:D:60:VAL:HG13	5:D:119:MET:HE2	1.95	0.49
5:H:401:VAL:HG21	5:H:406:PHE:CD2	2.48	0.49
2:B:582:ASN:OD1	2:B:582:ASN:N	2.46	0.48
2:B:786:LYS:HG3	8:M:52:TYR:CD2	2.48	0.48
3:C:112:GLN:OE1	3:C:112:GLN:N	2.39	0.48
5:J:210:LEU:HD23	5:J:212:TYR:CE2	2.48	0.48
2:B:291:ALA:HA	2:B:294:VAL:HG22	1.94	0.48
2:B:552:ILE:HD12	2:B:557:LYS:HB3	1.96	0.48
2:B:528:ASP:OD1	2:B:528:ASP:N	2.45	0.48
2:B:224:LYS:HB2	2:B:336:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:805:ASN:OD1	2:B:807:LEU:HB2	2.13	0.48
5:D:109:LYS:HE3	5:D:154:SER:HB3	1.96	0.48
2:B:15:ASN:OD1	2:B:165:TYR:OH	2.27	0.48
2:B:699:LYS:HG2	2:B:731:LEU:HD22	1.95	0.48
5:I:31:VAL:HG12	5:I:130:ILE:HD13	1.95	0.48
7:K:86:PHE:CD1	7:K:99:GLY:HA2	2.48	0.48
1:A:52:THR:HG23	1:A:528:LEU:HD21	1.95	0.48
1:A:306:THR:OG1	1:A:516:SER:O	2.26	0.48
2:B:142:THR:HG21	5:J:248:ILE:HG21	1.96	0.48
2:B:480:LYS:H	2:B:480:LYS:HD2	1.77	0.48
2:B:738:SER:O	2:B:742:MET:HG3	2.13	0.48
5:J:570:ARG:HB2	5:J:583:ILE:HD13	1.96	0.48
1:A:965:ILE:HB	1:A:976:VAL:HB	1.95	0.48
5:D:70:ILE:HD12	5:D:70:ILE:O	2.14	0.48
5:D:92:PHE:CE1	5:D:182:LEU:HD23	2.46	0.48
1:A:24:ILE:HD12	1:A:185:TYR:CE2	2.49	0.48
1:A:1266:TRP:CH2	1:A:1276:ARG:HB3	2.49	0.48
2:B:217:ASP:OD1	2:B:372:TYR:OH	2.28	0.48
9:N:182:SER:HB3	10:L:133:PHE:CD2	2.48	0.48
1:A:167:SER:HB3	1:A:184:GLN:NE2	2.29	0.48
2:B:435:LYS:HE2	2:B:630:GLU:HB2	1.94	0.48
5:J:419:LYS:HE3	5:J:469:TYR:CD2	2.48	0.48
5:J:473:LEU:H	5:J:509:ASN:ND2	2.12	0.48
5:H:543:ILE:HD13	5:H:599:LEU:O	2.14	0.48
1:A:885:SER:OG	1:A:886:ASN:N	2.47	0.47
1:A:1169:ASN:HD21	1:A:1175:ARG:HH22	1.60	0.47
5:H:415:THR:HG23	5:H:476:LYS:HG2	1.94	0.47
1:A:915:GLN:HB2	1:A:1068:TRP:CH2	2.48	0.47
2:B:356:LYS:H	2:B:356:LYS:HD2	1.79	0.47
2:B:367:ASP:HB3	2:B:370:GLU:OE1	2.14	0.47
2:B:799:ILE:O	2:B:803:VAL:HG13	2.15	0.47
2:B:1118:ASP:HB2	2:B:1122:LYS:HG2	1.95	0.47
5:H:625:THR:OG1	5:H:626:ASN:N	2.47	0.47
10:L:111:PRO:HB3	10:L:137:PHE:HB3	1.96	0.47
2:B:1135:ILE:HD12	2:B:1137:ASN:N	2.28	0.47
1:A:397:LEU:HD12	1:A:403:GLY:HA2	1.95	0.47
2:B:1127:SER:OG	2:B:1128:GLU:N	2.47	0.47
6:E:321:TYR:CE2	6:E:324:GLY:HA2	2.49	0.47
7:K:30:SER:OG	7:K:31:ASN:N	2.45	0.47
1:A:968:MET:HE1	1:A:988:GLN:HB3	1.96	0.47
1:A:979:ASN:HB3	1:A:982:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ILE:HG12	2:B:124:THR:N	2.30	0.47
1:A:42:ILE:HD13	1:A:151:LEU:HB3	1.96	0.47
1:A:804:GLY:O	1:A:808:LEU:HD12	2.15	0.47
2:B:209:TYR:CZ	2:B:216:ILE:HG13	2.49	0.47
5:H:543:ILE:HD11	5:H:604:TYR:HD2	1.77	0.47
7:K:59:PRO:HB2	7:K:62:PHE:HE2	1.79	0.47
1:A:107:LEU:HA	1:A:349:TYR:CZ	2.50	0.47
1:A:375:LYS:HB2	1:A:416:LEU:HD11	1.97	0.47
1:A:428:LEU:HD23	1:A:542:LYS:HD2	1.96	0.47
2:B:1087:LEU:HB3	2:B:1089:LEU:HD12	1.96	0.47
5:J:563:GLN:HB2	5:J:590:LEU:HD22	1.96	0.47
6:E:377:ASP:OD1	6:E:379:SER:OG	2.27	0.47
6:E:478:LYS:HD2	14:E:803:HOH:O	2.14	0.47
6:E:563:GLN:HA	6:E:590:LEU:HB2	1.96	0.47
5:G:168:TYR:OH	5:H:367:PRO:HB2	2.15	0.47
7:K:47:LEU:HA	7:K:47:LEU:HD23	1.58	0.47
2:B:128:ALA:HB3	2:B:136:ASN:HB2	1.97	0.47
5:H:304:ASN:HB2	5:H:345:ALA:HB2	1.97	0.47
5:H:403:ASN:HB3	5:H:487:THR:O	2.15	0.47
1:A:702:ARG:HH21	1:A:703:ASN:HD21	1.63	0.47
2:B:360:ARG:HA	2:B:360:ARG:NE	2.28	0.47
5:H:376:ILE:HG21	5:H:382:ILE:HD11	1.96	0.47
1:A:306:THR:HG23	1:A:308:ALA:H	1.80	0.47
1:A:915:GLN:HB2	1:A:1068:TRP:CZ3	2.50	0.47
2:B:1054:LYS:HB3	2:B:1056:TYR:CE1	2.49	0.47
5:J:279:ASP:HB3	5:J:453:LYS:HB2	1.97	0.47
1:A:867:THR:HG22	1:A:871:LYS:HD2	1.96	0.46
2:B:588:VAL:HG22	2:B:748:PHE:CE1	2.50	0.46
2:B:829:ILE:O	2:B:833:THR:OG1	2.26	0.46
5:D:44:ASN:OD1	5:D:44:ASN:N	2.48	0.46
6:E:264:ASN:OD1	6:E:266:THR:HG22	2.15	0.46
6:E:348:PRO:HA	6:E:349:GLU:HA	1.45	0.46
5:H:348:PRO:HA	5:H:349:GLU:HA	1.54	0.46
5:H:426:LEU:HD21	5:H:467:LYS:HG2	1.96	0.46
1:A:1160:PHE:CE1	1:A:1184:VAL:HG22	2.50	0.46
2:B:16:LYS:HE2	2:B:17:ASN:OD1	2.15	0.46
2:B:570:SER:O	2:B:574:THR:OG1	2.25	0.46
5:I:23:ILE:HG23	5:I:25:LEU:HB2	1.97	0.46
5:J:212:TYR:HB2	5:J:321:TYR:CD2	2.50	0.46
5:J:247:ILE:HG13	5:J:307:ILE:HD11	1.98	0.46
5:D:112:PRO:HG2	5:D:115:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:527:THR:HG22	6:E:619:ARG:HG2	1.96	0.46
8:M:35:GLN:HB3	8:M:50:THR:HG23	1.98	0.46
1:A:4:VAL:HG21	1:A:92:THR:HG23	1.96	0.46
2:B:34:LYS:HB2	2:B:40:TRP:CZ3	2.50	0.46
5:I:105:PHE:CZ	5:I:150:GLY:HA3	2.49	0.46
5:H:251:ARG:NH2	5:H:336:SER:O	2.49	0.46
1:A:6:LYS:HB3	1:A:8:PHE:CE2	2.50	0.46
5:J:552:THR:HG23	5:J:597:ARG:HH21	1.80	0.46
5:D:143:VAL:HG21	6:E:440:ARG:HA	1.98	0.46
5:H:401:VAL:HG11	5:H:406:PHE:CE2	2.51	0.46
1:A:171:GLU:HG2	1:A:172:VAL:HG13	1.98	0.46
1:A:772:LYS:HA	1:A:775:GLU:OE1	2.16	0.46
3:C:6:GLU:HB2	3:C:114:THR:OG1	2.15	0.46
5:J:405:PRO:HD3	5:J:486:GLN:HB2	1.96	0.46
1:A:361:LEU:HB2	1:A:401:PHE:CD2	2.51	0.46
1:A:879:LEU:HB3	1:A:1074:LEU:HB3	1.97	0.46
4:F:7:GLU:N	4:F:108:GLN:HE22	2.13	0.46
4:F:37:TRP:CH2	4:F:97:CYS:HB2	2.51	0.46
6:E:389:ILE:O	6:E:413:ASN:HB2	2.16	0.46
5:G:47:LEU:HD11	5:G:123:TYR:CZ	2.51	0.46
1:A:689:VAL:O	1:A:693:GLN:HG3	2.15	0.46
2:B:248:LEU:HD12	2:B:257:TYR:CZ	2.51	0.46
2:B:620:LYS:HB2	2:B:679:GLN:HE22	1.81	0.46
5:D:144:LEU:CD1	5:D:146:VAL:HG23	2.45	0.46
6:E:563:GLN:HB2	6:E:590:LEU:HD22	1.98	0.46
5:G:31:VAL:HG11	5:G:87:ASN:HB3	1.98	0.46
5:H:598:LEU:HD22	5:H:604:TYR:CZ	2.51	0.46
2:B:1043:ARG:HB3	2:B:1047:GLU:HA	1.98	0.46
5:I:64:ARG:NH1	5:I:99:ASN:OD1	2.48	0.46
6:E:222:GLY:HA2	6:E:369:GLU:HB3	1.98	0.46
6:E:432:TYR:HB3	6:E:455:ILE:HB	1.96	0.46
5:H:431:ILE:HG23	5:H:458:ILE:HB	1.96	0.46
1:A:93:LYS:NZ	1:A:379:VAL:O	2.50	0.46
2:B:713:SER:OG	2:B:715:ILE:HG13	2.15	0.46
5:I:141:ARG:NH2	5:J:439:ASN:O	2.49	0.46
5:J:248:ILE:HG12	5:J:294:LYS:HG3	1.96	0.46
5:J:272:TYR:O	5:J:276:ARG:HG2	2.16	0.46
5:G:89:GLN:NE2	5:G:96:THR:H	2.14	0.46
10:L:118:PRO:HG2	10:L:128:ALA:HB1	1.97	0.46
1:A:948:ARG:NH2	1:A:1288:ASP:OD2	2.44	0.45
2:B:935:GLN:OE1	2:B:940:VAL:HG21	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:313:TYR:HB3	6:E:333:TYR:HB3	1.97	0.45
6:E:431:ILE:HG23	6:E:458:ILE:HB	1.97	0.45
6:E:563:GLN:HB3	6:E:612:GLU:HB3	1.98	0.45
5:G:65:VAL:N	5:G:68:ASN:OD1	2.47	0.45
1:A:688:LYS:O	1:A:692:VAL:HG13	2.17	0.45
1:A:801:ILE:O	1:A:805:VAL:HG23	2.16	0.45
1:A:1121:LYS:HB3	1:A:1136:LEU:HB3	1.97	0.45
2:B:559:TYR:OH	2:B:722:LEU:HD23	2.17	0.45
4:F:30:ILE:O	4:F:30:ILE:HG13	2.16	0.45
5:G:85:LYS:HB3	5:G:85:LYS:HE3	1.70	0.45
1:A:789:ASN:O	1:A:793:VAL:HG23	2.15	0.45
1:A:1134:MET:HE3	1:A:1261:LEU:HD12	1.99	0.45
4:F:35:MET:SD	4:F:80:SER:HB2	2.56	0.45
5:H:558:TYR:CE1	5:H:621:HIS:HB2	2.51	0.45
4:F:52:ILE:HG23	4:F:73:ARG:HD2	1.99	0.45
5:D:184:LYS:NZ	14:D:801:HOH:O	2.40	0.45
1:A:11:LYS:HA	1:A:11:LYS:HD2	1.68	0.45
2:B:265:LEU:HD21	2:B:276:ILE:HG13	1.98	0.45
2:B:918:SER:HB3	2:B:1008:GLU:HB2	1.97	0.45
2:B:1132:LEU:HD12	2:B:1177:MET:HB3	1.97	0.45
5:G:30:TYR:HB2	5:G:131:ILE:HG13	1.99	0.45
5:H:508:MET:HA	5:H:509:ASN:HA	1.60	0.45
1:A:25:PRO:HA	1:A:524:ILE:HB	1.99	0.45
2:B:129:PRO:O	2:B:130:LYS:HG2	2.16	0.45
2:B:236:ILE:HG21	2:B:328:ILE:HD11	1.98	0.45
2:B:1165:ILE:HG22	2:B:1190:TRP:CZ2	2.51	0.45
5:J:227:ARG:HH21	5:J:231:LYS:HD2	1.82	0.45
1:A:751:TYR:OH	1:A:762:ILE:O	2.33	0.45
1:A:779:LYS:NZ	11:A:1301:SO4:O3	2.49	0.45
1:A:1182:ILE:HD12	1:A:1221:VAL:HG21	1.98	0.45
1:A:1189:LYS:HG2	5:J:400:ILE:HA	1.99	0.45
1:A:1236:LYS:HB3	1:A:1249:PHE:HE2	1.81	0.45
2:B:124:THR:OG1	5:G:106:GLU:OE2	2.27	0.45
5:J:563:GLN:HA	5:J:590:LEU:HB2	1.98	0.45
2:B:794:GLU:HA	2:B:797:GLN:HG2	1.98	0.45
3:C:30:GLY:HA2	3:C:71:ARG:NH1	2.32	0.45
5:J:428:SER:CB	5:J:466:ALA:HB3	2.47	0.45
6:E:223:ASP:CG	6:E:314:GLU:HG3	2.42	0.45
2:B:1144:MET:HE2	2:B:1144:MET:HB2	1.88	0.45
5:G:121:LEU:HB2	5:G:152:VAL:HG12	1.98	0.45
1:A:22:ILE:HD12	1:A:24:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ILE:HG21	1:A:260:PHE:HB2	1.99	0.45
1:A:1111:TYR:CG	1:A:1284:PHE:HB3	2.52	0.45
2:B:186:TYR:CE2	2:B:478:CYS:HB3	2.52	0.45
2:B:440:ARG:N	2:B:442:TYR:CE2	2.76	0.45
3:C:38:ARG:NH2	3:C:88:GLU:O	2.50	0.45
4:F:18:SER:HA	4:F:84:MET:O	2.16	0.45
5:I:69:ALA:O	5:I:99:ASN:ND2	2.50	0.45
5:J:226:ILE:HG21	5:J:310:TYR:HB3	1.99	0.45
5:J:587:LEU:HB3	5:J:589:LEU:CD2	2.46	0.45
5:D:103:ILE:HD11	5:H:234:ILE:HG23	1.99	0.45
6:E:568:LEU:HD11	6:E:604:TYR:HB3	1.97	0.45
1:A:26:ASN:ND2	1:A:51:PHE:O	2.50	0.44
2:B:414:MET:HE2	2:B:414:MET:HB3	1.62	0.44
2:B:722:LEU:HA	2:B:725:LEU:HD12	1.99	0.44
6:E:420:ILE:HD13	6:E:482:ILE:HD11	1.98	0.44
1:A:749:TYR:CD1	1:A:749:TYR:C	2.95	0.44
2:B:528:ASP:H	2:B:529:LYS:HA	1.82	0.44
5:I:129:GLU:HG2	5:I:143:VAL:HG22	1.99	0.44
5:J:386:ASN:OD1	5:J:386:ASN:N	2.47	0.44
6:E:383:GLN:HG2	6:E:395:TYR:OH	2.17	0.44
6:E:518:LEU:HD21	6:E:622:ILE:HG21	1.98	0.44
5:G:87:ASN:O	5:G:91:VAL:HG23	2.17	0.44
5:H:517:ASN:HD21	5:H:526:TYR:HE2	1.64	0.44
10:L:134:LEU:HD13	10:L:173:MET:SD	2.57	0.44
1:A:16:GLY:HA3	1:A:139:GLN:OE1	2.17	0.44
1:A:547:LYS:HD2	1:A:547:LYS:HA	1.82	0.44
1:A:565:ARG:HB2	1:A:749:TYR:CE2	2.52	0.44
5:J:508:MET:HA	5:J:509:ASN:HA	1.65	0.44
5:J:468:SER:HA	5:J:512:VAL:O	2.18	0.44
5:J:568:LEU:HD21	5:J:604:TYR:HB3	2.00	0.44
1:A:671:ILE:HG13	1:A:673:ILE:HD13	1.99	0.44
1:A:883:TYR:CE1	1:A:911:LYS:HE3	2.52	0.44
2:B:909:ARG:HD3	2:B:963:TRP:CD1	2.52	0.44
5:J:527:THR:HG23	5:J:619:ARG:HG3	1.99	0.44
5:J:570:ARG:NH2	5:J:572:THR:HG22	2.33	0.44
6:E:536:TYR:CE1	6:E:609:GLU:HB2	2.53	0.44
5:H:467:LYS:HB2	5:H:514:ILE:HB	2.00	0.44
1:A:1159:LYS:HB2	1:A:1185:VAL:HB	2.00	0.44
2:B:741:ALA:O	2:B:745:VAL:HG13	2.17	0.44
3:C:49:SER:OG	3:C:50:SER:N	2.50	0.44
5:I:38:TRP:CE2	5:I:175:CYS:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:258:PRO:HG3	5:J:286:PHE:O	2.18	0.44
5:J:532:ASP:OD1	5:J:533:VAL:N	2.48	0.44
5:D:46:ILE:HG13	5:D:47:LEU:HD22	2.00	0.44
6:E:508:MET:HA	6:E:509:ASN:HA	1.64	0.44
2:B:141:SER:OG	6:E:294:LYS:NZ	2.49	0.44
2:B:742:MET:O	2:B:745:VAL:HG22	2.18	0.44
5:G:69:ALA:C	5:G:147:PRO:HG2	2.42	0.44
2:B:758:GLU:OE2	2:B:814:ILE:HG12	2.18	0.44
2:B:798:LEU:HD23	2:B:798:LEU:HA	1.88	0.44
5:J:397:ILE:HD12	5:J:493:ASN:HB3	2.00	0.44
6:E:227:ARG:HE	6:E:231:LYS:HD3	1.83	0.44
5:H:234:ILE:HD11	5:H:249:GLN:HG3	2.00	0.44
5:H:385:ILE:HD13	5:H:385:ILE:HA	1.87	0.44
1:A:427:LYS:HD3	1:A:543:TYR:HE2	1.82	0.43
5:J:246:SER:HA	5:J:295:PHE:O	2.18	0.43
6:E:401:VAL:HG21	6:E:406:PHE:CD1	2.52	0.43
6:E:430:LYS:HA	6:E:460:GLY:HA3	2.00	0.43
5:H:248:ILE:HG22	5:H:294:LYS:HB2	2.00	0.43
1:A:706:TRP:CE3	1:A:849:ILE:HB	2.54	0.43
1:A:896:SER:HB3	1:A:927:ILE:O	2.18	0.43
2:B:247:ARG:CZ	2:B:357:HIS:HD2	2.31	0.43
5:I:22:THR:HB	5:I:137:GLU:OE2	2.18	0.43
5:I:33:ARG:HB2	5:I:92:PHE:CZ	2.54	0.43
5:I:145:TYR:HE2	5:J:440:ARG:HG2	1.82	0.43
5:D:112:PRO:HB2	5:D:115:LYS:NZ	2.32	0.43
1:A:53:ASN:OD1	1:A:56:GLU:N	2.51	0.43
1:A:216:ASP:HB3	1:A:219:VAL:HG23	1.99	0.43
1:A:501:GLN:HG3	2:B:1063:PHE:CE1	2.53	0.43
1:A:843:ASN:HB3	2:B:935:GLN:NE2	2.33	0.43
5:D:120:TYR:OH	5:D:167:PHE:O	2.34	0.43
1:A:432:ARG:NH1	1:A:546:ASP:OD2	2.52	0.43
1:A:717:TRP:HZ3	1:A:857:VAL:HG21	1.82	0.43
2:B:121:ASN:O	2:B:121:ASN:ND2	2.52	0.43
2:B:469:ILE:HG13	2:B:470:ASP:H	1.83	0.43
2:B:569:TYR:CD1	2:B:698:ILE:HG13	2.54	0.43
2:B:923:SER:HB2	2:B:1003:ILE:HG12	2.00	0.43
7:K:96:THR:OG1	7:K:97:PHE:N	2.51	0.43
1:A:1043:ASN:OD1	1:A:1043:ASN:N	2.48	0.43
3:C:18:LEU:HD23	3:C:19:ARG:H	1.83	0.43
3:C:20:LEU:N	3:C:20:LEU:HD12	2.34	0.43
5:J:555:ILE:HG13	5:J:598:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:74:TYR:O	6:E:441:ASN:HB3	2.18	0.43
6:E:207:GLN:CD	14:E:802:HOH:O	2.61	0.43
6:E:588:HIS:O	6:E:592:ASN:HB2	2.19	0.43
5:H:599:LEU:HD12	5:H:604:TYR:OH	2.18	0.43
1:A:253:MET:HG2	1:A:459:ASN:O	2.18	0.43
1:A:322:LEU:HD23	1:A:341:LEU:HD13	2.01	0.43
1:A:463:PHE:CE1	1:A:666:GLU:HG3	2.54	0.43
2:B:1129:ASP:OD2	2:B:1131:ARG:NH2	2.51	0.43
5:J:403:ASN:O	5:J:486:GLN:NE2	2.51	0.43
5:D:107:PHE:CZ	5:H:237:LEU:HD22	2.53	0.43
6:E:615:ASN:ND2	11:E:701:SO4:O4	2.52	0.43
1:A:222:ALA:O	1:A:226:ILE:HG13	2.19	0.43
1:A:997:VAL:HG12	1:A:1039:LYS:HB2	2.00	0.43
1:A:1291:TRP:NE1	1:A:1293:GLU:OE1	2.48	0.43
2:B:107:PRO:HB3	2:B:196:GLY:C	2.44	0.43
2:B:842:ALA:HA	2:B:850:VAL:O	2.19	0.43
8:M:32:TYR:OH	8:M:100:TYR:O	2.36	0.43
1:A:1176:ASN:ND2	1:A:1225:SER:H	2.16	0.43
2:B:926:ASP:O	2:B:927:ASN:C	2.61	0.43
2:B:967:THR:HB	2:B:980:PHE:HB2	2.01	0.43
1:A:907:ASP:HB3	1:A:910:ASP:O	2.19	0.43
1:A:999:PHE:HD1	1:A:1036:ILE:HG21	1.82	0.43
2:B:210:LYS:HB2	2:B:215:TYR:CE1	2.54	0.43
4:F:13:VAL:O	4:F:114:VAL:HA	2.19	0.43
6:E:384:GLU:HG2	6:E:447:LEU:HD23	2.01	0.43
5:H:401:VAL:HG21	5:H:406:PHE:HD2	1.83	0.43
7:K:93:TRP:N	7:K:94:PRO:HD2	2.34	0.43
1:A:24:ILE:HG22	1:A:135:ILE:CG2	2.49	0.43
1:A:226:ILE:HD13	1:A:349:TYR:C	2.44	0.43
2:B:769:MET:O	2:B:773:ILE:HG23	2.18	0.43
2:B:926:ASP:O	2:B:928:CYS:HB2	2.18	0.43
2:B:1049:ARG:H	2:B:1049:ARG:HG3	1.69	0.43
5:J:287:ASN:OD1	5:J:287:ASN:N	2.49	0.43
5:J:528:ARG:HA	5:J:528:ARG:HD3	1.64	0.43
5:J:570:ARG:HG3	5:J:604:TYR:CE2	2.54	0.43
5:J:450:ASP:HB3	5:J:452:ILE:HG13	2.00	0.42
6:E:619:ARG:NH2	11:E:701:SO4:O4	2.52	0.42
2:B:123:ILE:HG12	2:B:124:THR:H	1.84	0.42
2:B:573:ILE:HD12	2:B:573:ILE:HA	1.94	0.42
2:B:786:LYS:HG3	8:M:52:TYR:HD2	1.84	0.42
5:I:22:THR:HA	5:I:136:HIS:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:428:SER:OG	5:H:466:ALA:O	2.35	0.42
9:N:121:LYS:HB3	9:N:121:LYS:HE2	1.78	0.42
3:C:47:TRP:CD1	3:C:100:ARG:HA	2.54	0.42
5:J:244:SER:HB2	5:G:108:SER:HB3	2.00	0.42
6:E:385:ILE:HD11	6:E:395:TYR:CD2	2.49	0.42
5:G:24:ASP:O	5:G:25:LEU:HD23	2.18	0.42
1:A:740:ALA:O	1:A:744:LYS:HG3	2.19	0.42
1:A:837:LEU:O	1:A:841:VAL:HG23	2.19	0.42
2:B:1100:ASN:OD1	2:B:1101:PRO:HD2	2.20	0.42
7:K:55:ILE:HG22	7:K:55:ILE:O	2.19	0.42
2:B:110:TYR:OH	2:B:190:ASP:OD1	2.30	0.42
2:B:642:PRO:O	2:B:646:LEU:HB2	2.20	0.42
5:I:51:VAL:HB	5:J:339:TYR:HD1	1.84	0.42
5:G:36:ASP:OD1	5:G:37:GLY:N	2.51	0.42
5:H:410:PHE:HA	5:H:447:LEU:HD22	2.01	0.42
1:A:224:GLN:OE1	1:A:224:GLN:HA	2.20	0.42
1:A:584:THR:HA	1:A:739:GLN:HE22	1.83	0.42
2:B:71:GLN:O	2:B:75:LYS:HG3	2.19	0.42
2:B:112:TYR:HD1	2:B:149:GLY:HA3	1.85	0.42
2:B:500:PRO:HB3	2:B:596:LEU:HB3	2.01	0.42
5:I:22:THR:H	5:I:137:GLU:HG3	1.83	0.42
1:A:421:GLY:N	1:A:424:GLU:HG3	2.34	0.42
1:A:1182:ILE:O	1:A:1192:ARG:HD3	2.20	0.42
5:I:46:ILE:HB	5:J:283:VAL:HG12	2.02	0.42
5:I:107:PHE:CZ	6:E:237:LEU:HG	2.55	0.42
5:H:408:ILE:O	5:H:481:TYR:HA	2.20	0.42
1:A:1116:LEU:HD12	1:A:1281:SER:HB3	2.01	0.42
2:B:292:LYS:HE3	2:B:292:LYS:HB2	1.82	0.42
2:B:321:LYS:HE2	14:B:1305:HOH:O	2.20	0.42
2:B:648:GLU:HA	2:B:651:PHE:CD2	2.55	0.42
2:B:729:ASN:ND2	2:B:732:ARG:HH12	2.17	0.42
5:J:547:PHE:HB2	5:J:601:GLY:HA3	2.00	0.42
5:J:566:GLY:O	5:J:587:LEU:HB2	2.20	0.42
5:D:31:VAL:HG11	5:D:87:ASN:HB3	2.00	0.42
5:H:255:THR:O	5:H:256:THR:OG1	2.35	0.42
7:K:68:THR:OG1	7:K:69:ASP:OD1	2.35	0.42
7:K:69:ASP:N	7:K:69:ASP:OD1	2.53	0.42
8:M:28:THR:O	8:M:31:THR:HG22	2.19	0.42
1:A:473:ASN:CB	14:A:1403:HOH:O	2.60	0.42
1:A:689:VAL:O	1:A:692:VAL:HG22	2.20	0.42
2:B:407:ASN:HB3	2:B:413:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1156:LEU:HD11	2:B:1192:PHE:HE2	1.85	0.42
1:A:166:LYS:HE3	1:A:187:ARG:NH2	2.34	0.42
2:B:88:ARG:HH21	2:B:345:ILE:HD11	1.85	0.42
2:B:279:ASP:HB3	2:B:280:PRO:HD3	2.02	0.42
2:B:1058:LEU:HD21	2:B:1190:TRP:HB3	2.01	0.42
6:E:426:LEU:HG	6:E:467:LYS:HG2	2.02	0.42
7:K:33:LEU:HD22	7:K:70:PHE:CG	2.55	0.42
7:K:34:HIS:CD2	7:K:88:GLN:HE21	2.28	0.42
1:A:150:ASN:HD22	1:A:150:ASN:N	2.16	0.41
1:A:423:PHE:N	1:A:423:PHE:CD1	2.87	0.41
1:A:706:TRP:HA	1:A:808:LEU:CD2	2.50	0.41
1:A:923:LYS:HB3	1:A:1056:LYS:HG3	2.00	0.41
2:B:302:TYR:CD1	2:B:302:TYR:C	2.97	0.41
2:B:564:GLU:O	2:B:568:ASN:ND2	2.37	0.41
2:B:1163:LYS:HA	2:B:1181:ASN:OD1	2.20	0.41
5:G:83:TYR:O	5:G:87:ASN:ND2	2.35	0.41
1:A:870:ILE:HD13	1:A:870:ILE:HA	1.85	0.41
1:A:889:ILE:HA	1:A:898:ILE:HD13	2.02	0.41
1:A:1255:PHE:O	1:A:1258:ILE:HG12	2.20	0.41
2:B:154:ASN:OD1	2:B:154:ASN:N	2.53	0.41
2:B:281:TYR:HB2	2:B:441:ALA:HB1	2.02	0.41
2:B:1113:ILE:HG22	2:B:1143:LYS:HG3	2.02	0.41
5:D:30:TYR:CZ	5:D:185:LYS:HD2	2.55	0.41
5:D:85:LYS:HB3	5:D:85:LYS:HE3	1.76	0.41
5:D:106:GLU:HG2	5:H:246:SER:HB2	2.02	0.41
1:A:290:PHE:HB3	1:A:333:VAL:HG21	2.01	0.41
2:B:1163:LYS:HB2	2:B:1179:CYS:SG	2.60	0.41
1:A:606:TRP:O	1:A:610:LEU:HD23	2.20	0.41
1:A:709:VAL:HG21	1:A:808:LEU:CD2	2.40	0.41
1:A:744:LYS:HD3	1:A:770:SER:HA	2.02	0.41
1:A:857:VAL:HG12	1:A:859:ASN:H	1.84	0.41
1:A:963:THR:HA	1:A:977:SER:HA	2.02	0.41
2:B:1135:ILE:HD11	2:B:1137:ASN:O	2.20	0.41
6:E:236:THR:HG23	6:E:308:LYS:HG2	2.02	0.41
5:H:519:ASN:HA	5:H:544:PRO:HB3	2.02	0.41
1:A:833:GLN:N	1:A:833:GLN:OE1	2.53	0.41
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.55	0.41
2:B:154:ASN:HB2	2:B:167:SER:O	2.21	0.41
2:B:1129:ASP:OD1	2:B:1129:ASP:N	2.49	0.41
5:I:89:GLN:HG2	5:I:94:ASN:HA	2.01	0.41
5:J:237:LEU:HD23	5:J:237:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:237:LEU:HB2	5:J:307:ILE:HG12	2.02	0.41
5:J:276:ARG:NH1	5:J:378:PRO:HG3	2.35	0.41
6:E:518:LEU:HD12	6:E:518:LEU:HA	1.93	0.41
5:G:34:ARG:HB2	5:G:127:ARG:HB3	2.03	0.41
1:A:321:TYR:HB2	1:A:323:LEU:CD1	2.51	0.41
1:A:811:PHE:CZ	1:A:815:LEU:HD12	2.55	0.41
1:A:882:ARG:HB2	1:A:891:LEU:HD13	2.02	0.41
1:A:1027:SER:HB2	1:A:1041:ILE:HD13	2.02	0.41
2:B:766:ILE:O	2:B:770:GLU:HG2	2.20	0.41
5:J:278:LYS:O	5:J:282:ASN:HA	2.21	0.41
1:A:905:ASN:HB3	1:A:915:GLN:HB3	2.02	0.41
2:B:147:TYR:O	2:B:147:TYR:CG	2.73	0.41
2:B:817:MET:HB3	2:B:817:MET:HE3	1.82	0.41
6:E:259:LEU:HB2	6:E:333:TYR:HB2	2.02	0.41
5:G:116:ASN:OD1	5:G:116:ASN:N	2.54	0.41
5:H:397:ILE:HA	5:H:398:PRO:HD3	1.95	0.41
1:A:203:ASP:N	1:A:203:ASP:OD1	2.53	0.41
1:A:310:LEU:O	1:A:314:LYS:HG3	2.21	0.41
1:A:819:LEU:HD23	1:A:841:VAL:HG22	2.01	0.41
6:E:552:THR:HG23	6:E:597:ARG:HH21	1.85	0.41
5:G:31:VAL:O	5:G:183:TYR:HA	2.21	0.41
1:A:163:PHE:O	1:A:224:GLN:NE2	2.54	0.41
1:A:676:LEU:HB2	1:A:811:PHE:HB2	2.02	0.41
1:A:966:ASN:HB3	1:A:1054:MET:HB3	2.02	0.41
1:A:1022:ASN:HB2	1:A:1078:GLU:CD	2.46	0.41
2:B:542:TYR:O	2:B:546:ILE:HG12	2.21	0.41
2:B:563:ARG:O	2:B:567:ARG:HG3	2.21	0.41
2:B:680:TYR:O	2:B:684:ILE:HG13	2.21	0.41
2:B:1122:LYS:HB3	2:B:1134:LEU:HB3	2.02	0.41
2:B:1185:LYS:H	2:B:1185:LYS:HG2	1.67	0.41
3:C:12:VAL:O	3:C:118:VAL:HA	2.21	0.41
5:J:228:THR:HG22	5:J:363:ILE:HD11	2.03	0.41
5:J:357:VAL:HG12	5:G:182:LEU:HG	2.02	0.41
5:J:430:LYS:HA	5:J:460:GLY:HA3	2.03	0.41
5:D:43:GLN:OE1	6:E:282:ASN:ND2	2.51	0.41
6:E:271:GLN:O	6:E:275:GLU:HG2	2.21	0.41
7:K:65:GLY:HA3	7:K:70:PHE:HA	2.02	0.41
8:M:51:ILE:HD12	8:M:51:ILE:HA	1.87	0.41
1:A:109:THR:O	1:A:113:ARG:HG2	2.20	0.41
1:A:154:ILE:HG13	1:A:155:GLY:O	2.21	0.41
1:A:1134:MET:HE3	1:A:1134:MET:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:PRO:CB	2:B:178:ILE:HA	2.51	0.41
2:B:791:ASN:HA	8:M:101:ASP:O	2.21	0.41
4:F:3:VAL:HB	4:F:105:TYR:CE1	2.56	0.41
5:H:315:LYS:HG3	5:H:333:TYR:CE2	2.56	0.41
5:H:430:LYS:HA	5:H:460:GLY:HA3	2.03	0.41
1:A:1183:ASN:HA	1:A:1191:TYR:O	2.20	0.40
2:B:566:PHE:CD2	2:B:899:THR:HB	2.57	0.40
2:B:930:TRP:HA	2:B:942:ASN:O	2.22	0.40
5:J:462:ASP:CG	5:J:529:GLN:HE22	2.28	0.40
6:E:416:GLY:HA3	6:E:499:ARG:NH1	2.36	0.40
6:E:536:TYR:CD1	6:E:607:LYS:HE2	2.56	0.40
5:G:67:ASP:HB2	5:H:286:PHE:CE2	2.56	0.40
5:G:83:TYR:OH	5:G:186:ILE:HG21	2.21	0.40
5:H:533:VAL:HG12	5:H:534:HIS:ND1	2.36	0.40
1:A:1191:TYR:HB3	1:A:1209:LEU:O	2.22	0.40
3:C:66:ARG:HH22	3:C:89:ASP:CG	2.29	0.40
5:G:38:TRP:CZ2	5:G:127:ARG:HD3	2.57	0.40
5:H:222:GLY:HA2	5:H:369:GLU:HB3	2.03	0.40
7:K:38:GLN:OE1	7:K:44:PRO:HG3	2.21	0.40
1:A:399:ALA:HB2	1:A:893:ARG:HB2	2.02	0.40
1:A:685:ILE:HD12	1:A:685:ILE:H	1.86	0.40
2:B:562:LEU:HD23	2:B:898:LEU:HD23	2.03	0.40
5:I:30:TYR:HB2	5:I:131:ILE:HG12	2.03	0.40
5:I:32:VAL:HA	5:I:182:LEU:O	2.21	0.40
5:J:329:LYS:HB3	5:J:329:LYS:HE2	1.87	0.40
5:G:22:THR:HG22	5:G:137:GLU:HG3	2.04	0.40
5:H:277:LEU:HB3	5:H:283:VAL:CG2	2.50	0.40
1:A:1236:LYS:HB3	1:A:1249:PHE:CE2	2.56	0.40
2:B:227:ILE:HG22	2:B:267:VAL:HG22	2.03	0.40
2:B:1037:LEU:HA	2:B:1037:LEU:HD23	1.84	0.40
5:I:31:VAL:HG11	5:I:87:ASN:HB3	2.03	0.40
5:I:64:ARG:O	5:I:64:ARG:HD2	2.21	0.40
5:D:64:ARG:HG2	5:D:66:ASN:HB2	2.03	0.40
1:A:65:ALA:O	1:A:536:ARG:NH1	2.45	0.40
1:A:170:HIS:CG	1:A:171:GLU:N	2.89	0.40
1:A:306:THR:HG23	1:A:308:ALA:N	2.36	0.40
1:A:495:SER:OG	1:A:497:ASP:OD1	2.38	0.40
1:A:1189:LYS:HG2	5:J:400:ILE:HG23	2.03	0.40
2:B:213:GLU:HG3	2:B:382:ILE:CD1	2.52	0.40
2:B:887:ILE:HG23	2:B:1005:LEU:HB3	2.03	0.40
5:D:70:ILE:H	5:D:70:ILE:HG13	1.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:570:ARG:O	5:H:581:ILE:HD12	2.22	0.40
8:M:40:ARG:HH21	8:M:89:GLU:C	2.30	0.40
8:M:76:SER:OG	8:M:78:THR:OG1	2.29	0.40
9:N:201:HIS:HB3	9:N:206:THR:HB	2.03	0.40
10:L:133:PHE:C	10:L:134:LEU:HD12	2.47	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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	1270/1296 (98%)	1236 (97%)	34 (3%)	0	100	100
2	B	1181/1194 (99%)	1133 (96%)	48 (4%)	0	100	100
3	C	115/128 (90%)	113 (98%)	2 (2%)	0	100	100
4	F	112/121 (93%)	110 (98%)	1 (1%)	1 (1%)	14	35
5	D	172/626 (28%)	164 (95%)	8 (5%)	0	100	100
5	G	167/626 (27%)	161 (96%)	6 (4%)	0	100	100
5	H	419/626 (67%)	399 (95%)	20 (5%)	0	100	100
5	I	167/626 (27%)	156 (93%)	11 (7%)	0	100	100
5	J	419/626 (67%)	401 (96%)	18 (4%)	0	100	100
6	E	419/626 (67%)	403 (96%)	16 (4%)	0	100	100
7	K	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
8	M	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
9	N	90/94 (96%)	88 (98%)	2 (2%)	0	100	100
10	L	101/103 (98%)	101 (100%)	0	0	100	100
All	All	4850/6914 (70%)	4664 (96%)	185 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	30	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	1152/1177 (98%)	1140 (99%)	12 (1%)	73	84
2	B	1101/1113 (99%)	1088 (99%)	13 (1%)	67	81
3	C	90/103 (87%)	90 (100%)	0	100	100
4	F	90/97 (93%)	90 (100%)	0	100	100
5	D	153/572 (27%)	147 (96%)	6 (4%)	27	52
5	G	153/572 (27%)	153 (100%)	0	100	100
5	H	381/572 (67%)	375 (98%)	6 (2%)	58	77
5	I	151/572 (26%)	147 (97%)	4 (3%)	41	65
5	J	381/572 (67%)	373 (98%)	8 (2%)	48	71
6	E	380/571 (66%)	374 (98%)	6 (2%)	58	77
7	K	91/94 (97%)	89 (98%)	2 (2%)	47	70
8	M	90/94 (96%)	87 (97%)	3 (3%)	33	57
9	N	68/83 (82%)	66 (97%)	2 (3%)	37	62
10	L	79/95 (83%)	77 (98%)	2 (2%)	42	66
All	All	4360/6287 (69%)	4296 (98%)	64 (2%)	60	78

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	161	ILE
1	A	348	ILE
1	A	359	LYS
1	A	487	ILE

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Mol	Chain	Res	Type
1	A	604	LEU
1	A	662	VAL
1	A	997	VAL
1	A	1076	ASP
1	A	1143	VAL
1	A	1232	THR
1	A	1258	ILE
2	B	123	ILE
2	B	135	LEU
2	B	213	GLU
2	B	222	LEU
2	B	355	LEU
2	B	442	TYR
2	B	528	ASP
2	B	582	ASN
2	B	629	ILE
2	B	722	LEU
2	B	810	GLU
2	B	828	LEU
2	B	1124	ILE
5	I	22	THR
5	I	65	VAL
5	I	93	THR
5	I	130	ILE
5	J	206	THR
5	J	342	VAL
5	J	352	VAL
5	J	428	SER
5	J	429	LEU
5	J	472	VAL
5	J	489	SER
5	J	568	LEU
5	D	17	ILE
5	D	44	ASN
5	D	68	ASN
5	D	70	ILE
5	D	121	LEU
5	D	148	SER
6	E	322	GLN
6	E	342	VAL
6	E	412	VAL
6	E	448	CYS

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Mol	Chain	Res	Type
6	E	579	ASN
6	E	625	THR
5	H	248	ILE
5	H	302	ASP
5	H	412	VAL
5	H	484	VAL
5	H	508	MET
5	H	575	ILE
7	K	55	ILE
7	K	71	THR
8	M	30	THR
8	M	96	CYS
8	M	100	TYR
9	N	138	VAL
9	N	185	VAL
10	L	145	LYS
10	L	207	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	174	ASN
1	A	184	GLN
1	A	278	GLN
1	A	315	ASN
1	A	514	ASN
1	A	573	ASN
1	A	609	GLN
1	A	703	ASN
1	A	739	GLN
1	A	753	GLN
1	A	852	GLN
1	A	859	ASN
1	A	1003	GLN
1	A	1115	ASN
1	A	1238	ASN
1	A	1257	ASN
1	A	1265	ASN
1	A	1268	ASN
2	B	93	ASN
2	B	254	ASN

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Mol	Chain	Res	Type
2	B	450	ASN
2	B	485	GLN
2	B	507	GLN
2	B	694	GLN
2	B	729	ASN
2	B	739	GLN
2	B	760	ASN
2	B	858	ASN
2	B	1010	ASN
2	B	1140	ASN
3	C	86	GLN
4	F	40	GLN
4	F	75	ASN
5	I	54	ASN
5	I	180	GLN
5	J	322	GLN
5	J	396	ASN
5	J	486	GLN
5	J	563	GLN
5	J	579	ASN
5	J	617	ASN
5	D	116	ASN
6	E	249	GLN
6	E	284	GLN
6	E	365	ASN
6	E	403	ASN
6	E	423	GLN
6	E	439	ASN
6	E	475	ASN
6	E	479	ASN
6	E	513	ASN
6	E	549	ASN
5	G	89	GLN
5	G	172	ASN
5	G	180	GLN
5	H	282	ASN
5	H	365	ASN
5	H	439	ASN
5	H	446	ASN
5	H	479	ASN
5	H	486	GLN
5	H	614	ASN

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Mol	Chain	Res	Type
7	K	88	GLN
8	M	1	GLN
8	M	35	GLN
8	M	62	GLN
10	L	135	ASN
10	L	159	ASN
10	L	188	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 11 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	SO4	D	701	-	4,4,4	0.68	0	6,6,6	0.38	0
11	SO4	B	1204	-	4,4,4	0.73	0	6,6,6	0.42	0
11	SO4	A	1304	-	4,4,4	0.72	0	6,6,6	0.39	0
11	SO4	B	1202	-	4,4,4	0.66	0	6,6,6	0.22	0
11	SO4	A	1302	-	4,4,4	0.67	0	6,6,6	0.18	0
11	SO4	A	1301	-	4,4,4	0.64	0	6,6,6	0.09	0
11	SO4	B	1201	-	4,4,4	0.67	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SO4	E	701	-	4,4,4	1.04	0	6,6,6	1.39	1 (16%)
11	SO4	B	1203	-	4,4,4	0.67	0	6,6,6	0.08	0
11	SO4	A	1303	-	4,4,4	0.67	0	6,6,6	0.05	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	701	SO4	O4-S-O3	3.06	125.39	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1202	SO4	1	0
11	A	1301	SO4	3	0
11	E	701	SO4	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	132:PRO	C	137:SER	N	10.71

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1276/1296 (98%)	0.45	54 (4%) 41 38	35, 63, 101, 165	0
2	B	1187/1194 (99%)	0.32	41 (3%) 47 44	27, 53, 95, 176	0
3	C	117/128 (91%)	0.81	13 (11%) 12 14	56, 94, 129, 158	0
4	F	114/121 (94%)	0.35	4 (3%) 47 44	55, 68, 90, 95	0
5	D	174/626 (27%)	0.38	6 (3%) 48 45	28, 48, 87, 133	0
5	G	169/626 (26%)	0.55	5 (2%) 52 49	40, 61, 92, 113	0
5	H	421/626 (67%)	0.73	33 (7%) 20 21	32, 82, 127, 170	0
5	I	169/626 (26%)	0.36	4 (2%) 59 57	28, 49, 79, 107	0
5	J	421/626 (67%)	0.70	24 (5%) 30 29	36, 71, 124, 159	0
6	E	421/626 (67%)	0.34	9 (2%) 63 61	24, 42, 86, 169	0
7	K	105/105 (100%)	1.57	32 (30%) 1 2	96, 141, 175, 214	0
8	M	117/117 (100%)	1.26	29 (24%) 2 3	84, 116, 146, 155	0
9	N	93/94 (98%)	2.16	46 (49%) 0 1	131, 179, 209, 218	0
10	L	103/103 (100%)	1.74	36 (34%) 1 1	168, 206, 234, 274	0
All	All	4887/6914 (70%)	0.56	336 (6%) 24 24	24, 62, 150, 274	0

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	L	201	SER	6.4
9	N	188	SER	5.9
10	L	111	PRO	5.4
7	K	102	LEU	5.0
1	A	1225	SER	4.9
9	N	132	PRO	4.8
9	N	150	GLU	4.7
9	N	153	THR	4.7

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Mol	Chain	Res	Type	RSRZ
9	N	199	VAL	4.7
9	N	208	VAL	4.7
9	N	152	VAL	4.5
1	A	1227	ASN	4.4
10	L	138	TYR	4.2
9	N	147	TYR	4.2
9	N	213	GLU	4.2
9	N	200	ALA	4.2
2	B	629	ILE	4.1
10	L	117	PRO	4.1
10	L	155	ASN	4.0
10	L	109	ALA	4.0
7	K	105	ILE	4.0
1	A	51	PHE	3.9
5	D	16	VAL	3.9
9	N	189	THR	3.9
5	H	575	ILE	3.9
2	B	1084	THR	3.7
1	A	832	GLY	3.7
7	K	48	ILE	3.7
1	A	1295	PRO	3.7
1	A	672	ALA	3.6
5	J	468	SER	3.6
8	M	107	GLY	3.6
10	L	112	THR	3.6
1	A	647	LEU	3.6
7	K	11	LEU	3.6
1	A	119	GLY	3.5
8	M	117	VAL	3.5
2	B	1087	LEU	3.5
8	M	100	TYR	3.5
9	N	179	LEU	3.5
7	K	85	TYR	3.5
7	K	2	ILE	3.5
10	L	154	GLN	3.5
9	N	185	VAL	3.5
10	L	200	THR	3.5
5	J	529	GLN	3.4
7	K	86	PHE	3.4
5	H	438	GLY	3.4
7	K	62	PHE	3.4
5	G	64	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
9	N	191	PRO	3.3
2	B	121	ASN	3.3
6	E	348	PRO	3.3
7	K	59	PRO	3.3
3	C	12	VAL	3.3
1	A	1226	LYS	3.2
5	J	400	ILE	3.2
5	G	187	LEU	3.2
9	N	183	VAL	3.2
7	K	77	VAL	3.2
8	M	87	ALA	3.2
8	M	93	VAL	3.2
10	L	153	ARG	3.2
6	E	491	ILE	3.1
8	M	99	GLY	3.1
5	J	406	PHE	3.1
10	L	148	ILE	3.1
1	A	512	PRO	3.1
10	L	203	ILE	3.1
1	A	1092	SER	3.1
1	A	434	ILE	3.1
9	N	144	VAL	3.1
1	A	869	TYR	3.1
3	C	114	THR	3.1
5	J	206	THR	3.1
10	L	146	TRP	3.1
2	B	127	SER	3.0
2	B	526	SER	3.0
9	N	131	ALA	3.0
9	N	142	CYS	3.0
6	E	529	GLN	3.0
8	M	108	TYR	3.0
10	L	202	PRO	3.0
5	J	239	ILE	3.0
3	C	9	GLY	3.0
5	H	541	PHE	3.0
1	A	27	ALA	3.0
9	N	190	TRP	3.0
9	N	177	TYR	2.9
5	H	253	ARG	2.9
7	K	15	PRO	2.9
8	M	14	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
8	M	41	PRO	2.9
10	L	177	LEU	2.9
1	A	857	VAL	2.9
9	N	143	LEU	2.9
1	A	824	TYR	2.9
9	N	154	LEU	2.8
5	I	99	ASN	2.8
9	N	192	SER	2.8
10	L	190	TYR	2.8
8	M	105	THR	2.8
10	L	191	THR	2.8
5	J	497	PHE	2.8
10	L	158	LEU	2.8
7	K	9	ALA	2.8
7	K	81	ASP	2.8
9	N	120	ALA	2.8
9	N	186	THR	2.8
5	J	544	PRO	2.8
9	N	214	PRO	2.8
2	B	1071	VAL	2.8
5	D	98	ALA	2.8
10	L	110	ALA	2.8
10	L	140	LYS	2.8
2	B	651	PHE	2.8
7	K	73	ILE	2.8
1	A	61	PRO	2.7
2	B	1082	ASN	2.7
5	H	542	THR	2.7
3	C	22	CYS	2.7
1	A	1166	ALA	2.7
7	K	104	ILE	2.7
8	M	64	PHE	2.7
2	B	916	ILE	2.7
3	C	93	TYR	2.7
1	A	1168	GLY	2.7
1	A	834	VAL	2.7
9	N	138	VAL	2.7
2	B	1150	ILE	2.7
8	M	10	GLU	2.7
2	B	145	PHE	2.6
2	B	1081	ILE	2.6
5	H	555	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
5	D	97	GLU	2.6
9	N	182	SER	2.6
9	N	187	SER	2.6
2	B	751	ASN	2.6
2	B	1152	ILE	2.6
10	L	115	ILE	2.6
2	B	133	LYS	2.6
5	H	514	ILE	2.6
5	H	509	ASN	2.6
2	B	1111	GLU	2.6
10	L	192	CYS	2.6
2	B	410	ASN	2.6
2	B	1174	HIS	2.6
5	H	288	THR	2.6
7	K	60	SER	2.6
5	H	400	ILE	2.5
1	A	1272	GLU	2.5
5	H	361	GLY	2.5
5	H	564	GLY	2.5
5	H	411	THR	2.5
10	L	131	VAL	2.5
1	A	604	LEU	2.5
2	B	359	TYR	2.5
10	L	169	SER	2.5
6	E	306	CYS	2.5
5	J	618	ILE	2.5
9	N	209	ASP	2.5
8	M	36	TRP	2.5
2	B	269	GLY	2.5
1	A	530	LEU	2.5
9	N	171	VAL	2.5
10	L	204	VAL	2.5
2	B	130	LYS	2.5
7	K	35	TRP	2.5
2	B	149	GLY	2.5
1	A	361	LEU	2.5
7	K	84	VAL	2.5
9	N	139	THR	2.5
3	C	21	SER	2.4
7	K	20	SER	2.4
9	N	156	TRP	2.4
2	B	912	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	8	GLY	2.4
5	H	474	LEU	2.4
1	A	60	ASN	2.4
1	A	870	ILE	2.4
9	N	212	ILE	2.4
9	N	181	SER	2.4
2	B	1134	LEU	2.4
9	N	141	GLY	2.4
9	N	170	ALA	2.4
5	H	527	THR	2.4
1	A	864	SER	2.4
2	B	279	ASP	2.4
2	B	1149	ASP	2.4
5	H	350	SER	2.4
7	K	47	LEU	2.4
9	N	161	LEU	2.4
1	A	513	GLU	2.4
1	A	866	PHE	2.4
5	J	604	TYR	2.4
5	H	473	LEU	2.4
1	A	49	ASP	2.4
5	J	511	SER	2.4
1	A	868	GLU	2.4
3	C	95	CYS	2.4
7	K	71	THR	2.4
10	L	178	THR	2.4
1	A	646	MET	2.3
3	C	17	SER	2.3
8	M	88	SER	2.3
9	N	204	SER	2.3
5	H	583	ILE	2.3
7	K	58	ILE	2.3
6	E	345	ALA	2.3
6	E	576	ALA	2.3
2	B	124	THR	2.3
5	J	578	TYR	2.3
1	A	148	GLU	2.3
5	G	148	SER	2.3
8	M	101	ASP	2.3
1	A	331	PHE	2.3
1	A	603	PHE	2.3
8	M	71	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.3
2	B	639	LEU	2.3
4	F	97	CYS	2.3
5	J	561	TYR	2.3
10	L	145	LYS	2.3
4	F	24	VAL	2.3
8	M	104	GLY	2.3
2	B	552	ILE	2.3
5	J	575	ILE	2.3
8	M	109	TRP	2.3
1	A	670	GLU	2.3
1	A	1293	GLU	2.3
2	B	128	ALA	2.3
8	M	98	ALA	2.3
3	C	20	LEU	2.3
7	K	100	THR	2.3
9	N	211	LYS	2.3
8	M	32	TYR	2.3
7	K	65	GLY	2.3
5	J	624	ILE	2.3
9	N	137	SER	2.3
5	J	598	LEU	2.3
1	A	122	THR	2.3
1	A	1219	GLN	2.2
3	C	116	VAL	2.2
5	H	333	TYR	2.2
8	M	96	CYS	2.2
1	A	453	LEU	2.2
2	B	239	SER	2.2
1	A	494	ILE	2.2
5	G	65	VAL	2.2
5	H	479	ASN	2.2
5	H	512	VAL	2.2
8	M	35	GLN	2.2
8	M	37	VAL	2.2
10	L	187	HIS	2.2
5	D	188	GLU	2.2
5	H	557	LEU	2.2
1	A	1234	LYS	2.2
2	B	449	SER	2.2
9	N	178	THR	2.2
1	A	671	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	526	GLY	2.2
1	A	1251	GLY	2.2
5	H	416	GLY	2.2
1	A	59	LEU	2.2
5	H	606	LEU	2.2
8	M	63	LYS	2.2
9	N	145	LYS	2.2
7	K	99	GLY	2.2
4	F	2	GLN	2.2
5	J	295	PHE	2.2
5	H	466	ALA	2.2
1	A	422	LEU	2.2
5	H	568	LEU	2.2
8	M	103	SER	2.2
10	L	113	VAL	2.2
10	L	130	VAL	2.2
5	I	35	GLY	2.1
2	B	632	TYR	2.1
5	H	604	TYR	2.1
10	L	184	TYR	2.1
5	D	69	ALA	2.1
9	N	203	ALA	2.1
8	M	84	ILE	2.1
10	L	199	SER	2.1
9	N	215	ARG	2.1
7	K	21	LEU	2.1
8	M	47	TRP	2.1
5	J	352	VAL	2.1
5	D	93	THR	2.1
5	H	387	THR	2.1
7	K	14	THR	2.1
5	G	25	LEU	2.1
10	L	194	ALA	2.1
5	I	72	TYR	2.1
5	I	159	PRO	2.1
2	B	628	ILE	2.1
5	H	208	ARG	2.1
7	K	63	GLY	2.1
3	C	45	PHE	2.1
7	K	97	PHE	2.1
2	B	1132	LEU	2.1
6	E	206	THR	2.1

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Mol	Chain	Res	Type	RSRZ
5	J	207	GLN	2.1
5	J	390	SER	2.1
5	J	595	SER	2.1
2	B	1123	TYR	2.1
1	A	488	GLU	2.1
6	E	492	GLU	2.1
1	A	1231	ILE	2.1
7	K	3	VAL	2.1
1	A	8	PHE	2.1
10	L	207	PHE	2.1
1	A	1116	LEU	2.0
10	L	123	LEU	2.0
3	C	117	THR	2.0
5	H	488	SER	2.0
1	A	349	TYR	2.0
10	L	152	GLU	2.0
1	A	762	ILE	2.0
5	J	531	PRO	2.0
5	H	375	VAL	2.0
4	F	11	GLY	2.0
2	B	1089	LEU	2.0
5	J	504	LEU	2.0
7	K	33	LEU	2.0
6	E	567	THR	2.0
8	M	102	THR	2.0
9	N	167	THR	2.0
8	M	68	ALA	2.0
5	H	468	SER	2.0
5	H	397	ILE	2.0
2	B	1074	ASN	2.0
2	B	1170	LYS	2.0
5	J	556	ARG	2.0
7	K	76	ARG	2.0
2	B	897	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	MG	E	705	1/1	0.60	0.88	89,89,89,89	1
11	SO4	B	1204	5/5	0.68	0.14	75,77,108,134	0
11	SO4	A	1304	5/5	0.74	0.11	96,100,111,132	0
13	MG	A	1306	1/1	0.81	0.29	36,36,36,36	0
11	SO4	B	1203	5/5	0.82	0.14	55,70,82,87	0
11	SO4	E	701	5/5	0.83	0.23	66,67,86,90	0
11	SO4	D	701	5/5	0.86	0.10	64,66,79,88	0
13	MG	E	707	1/1	0.86	0.29	20,20,20,20	0
11	SO4	A	1303	5/5	0.87	0.12	67,69,84,106	0
13	MG	B	1205	1/1	0.87	0.22	40,40,40,40	0
11	SO4	B	1201	5/5	0.88	0.08	59,70,88,91	0
11	SO4	B	1202	5/5	0.88	0.10	45,57,60,69	0
11	SO4	A	1301	5/5	0.89	0.12	63,64,82,90	0
11	SO4	A	1302	5/5	0.89	0.13	63,66,73,79	0
13	MG	E	703	1/1	0.90	0.14	20,20,20,20	0
13	MG	E	704	1/1	0.93	0.25	30,30,30,30	0
13	MG	H	701	1/1	0.93	0.21	14,14,14,14	0
13	MG	E	702	1/1	0.94	0.17	24,24,24,24	0
13	MG	J	701	1/1	0.94	0.23	34,34,34,34	0
12	ZN	A	1305	1/1	0.96	0.04	129,129,129,129	0
13	MG	E	706	1/1	0.97	0.41	49,49,49,49	1

6.5 Other polymers ⓘ

There are no such residues in this entry.