



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:10 AM UTC

PDB ID : 7V5J / pdb_00007v5j
EMDB ID : EMD-31725
Title : MERS S ectodomain trimer in complex with neutralizing antibody 0722(state 2)
Authors : Wang, X.; Zhao, J.; Wang, Z.; Zeng, J.; Zhang, S.; Wang, Y.
Deposited on : 2021-08-17
Resolution : 2.80 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:

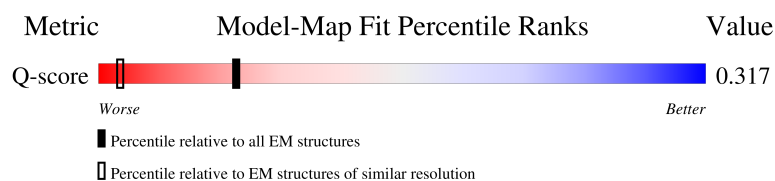
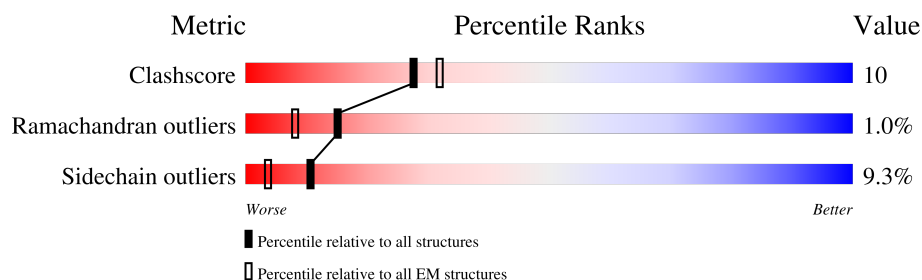
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.



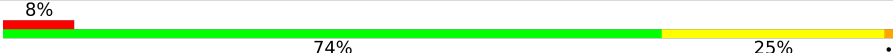
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	A	1189	
1	B	1189	
1	C	1189	
2	D	212	

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Mol	Chain	Length	Quality of chain
2	F	212	 8%74%25%
2	H	212	 5%74%24%
3	E	222	 9%78%21%
3	G	222	 6%78%20%
3	I	222	 7%73%24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36189 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1133	Total	C	N	O	S	0	0
			8770	5579	1448	1692	51		
1	B	1137	Total	C	N	O	S	0	0
			8796	5589	1455	1701	51		
1	C	1135	Total	C	N	O	S	1	0
			8794	5587	1454	1703	50		

- Molecule 2 is a protein called 0722 L.

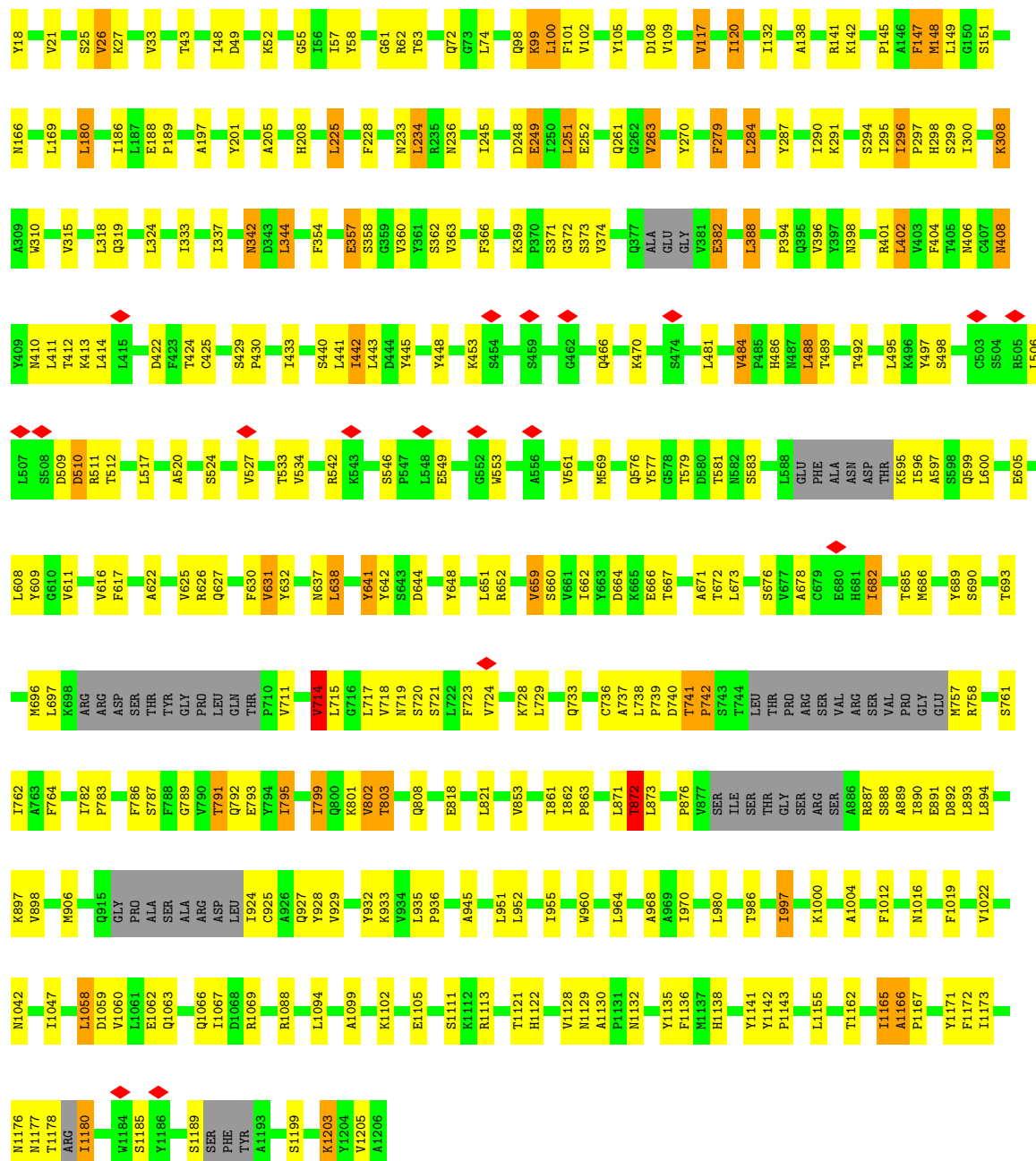
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	212	Total	C	N	O	S	0	0
			1591	997	262	326	6		
2	F	212	Total	C	N	O	S	0	0
			1615	1012	265	332	6		
2	H	212	Total	C	N	O	S	0	0
			1619	1015	266	332	6		

- Molecule 3 is a protein called 0722 H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	222	Total	C	N	O	S	0	0
			1668	1057	275	329	7		
3	G	222	Total	C	N	O	S	0	0
			1668	1057	275	329	7		
3	I	222	Total	C	N	O	S	0	0
			1668	1057	275	329	7		

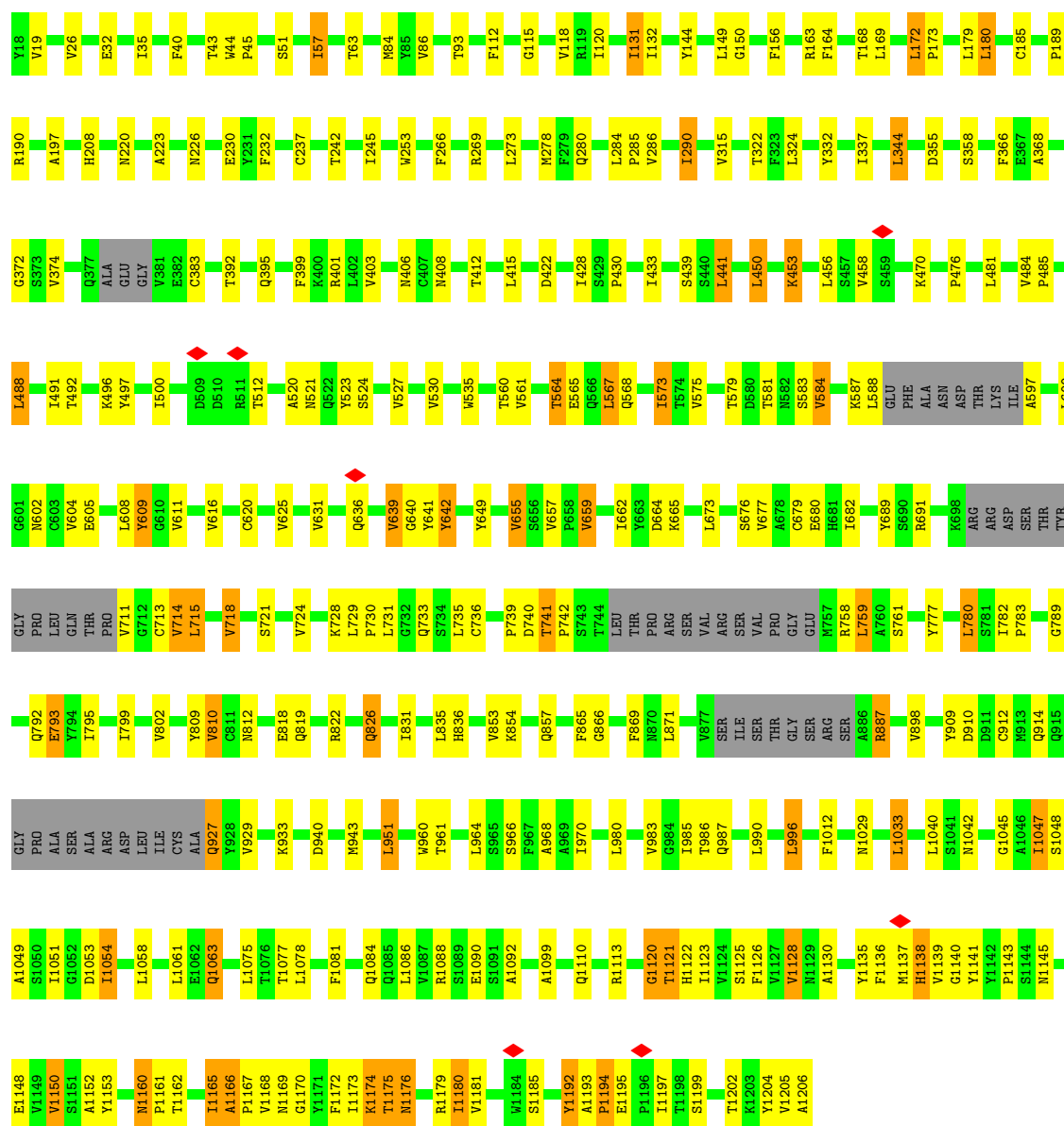


• Molecule 1: Spike glycoprotein

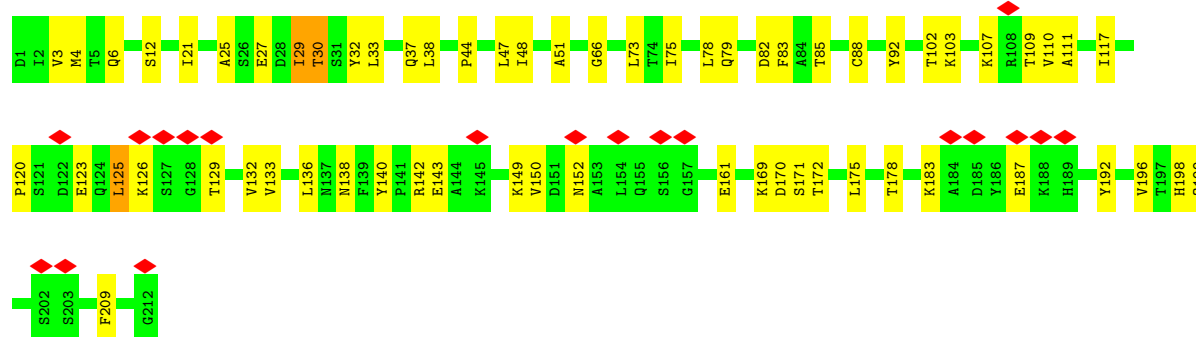
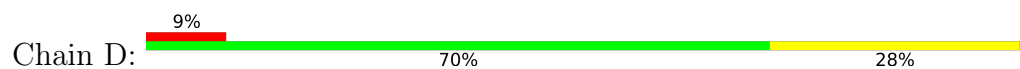


• Molecule 1: Spike glycoprotein

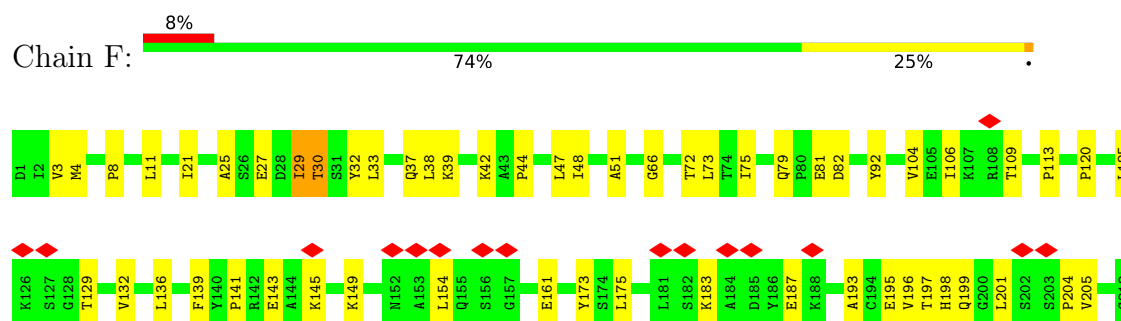




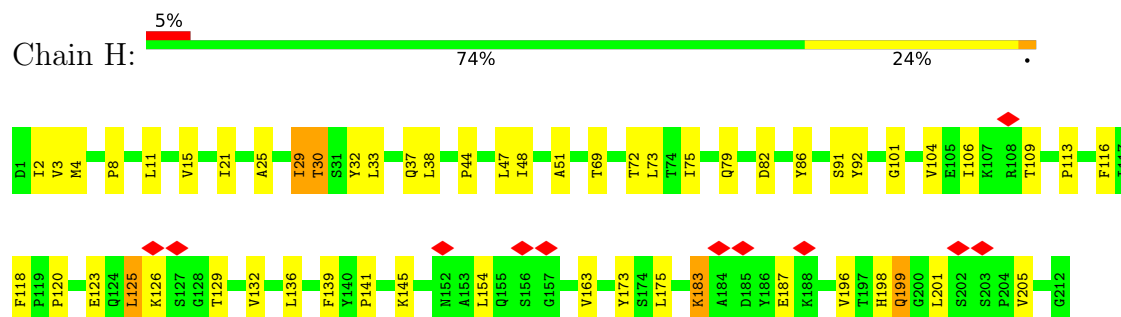
• Molecule 2: 0722 L



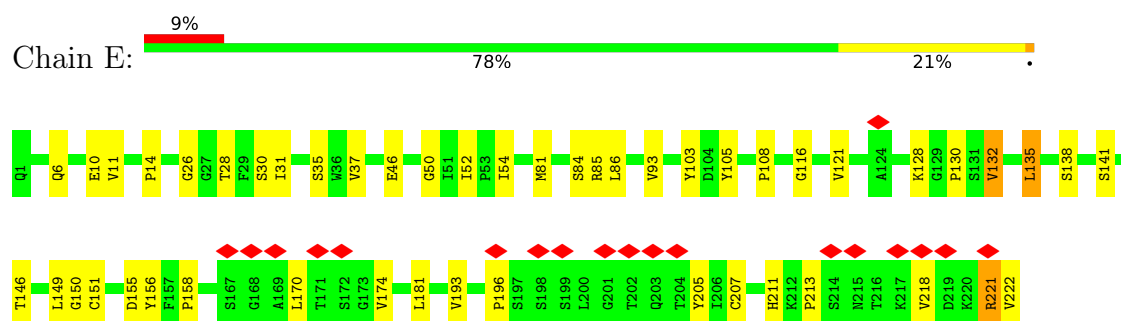
• Molecule 2: 0722 L



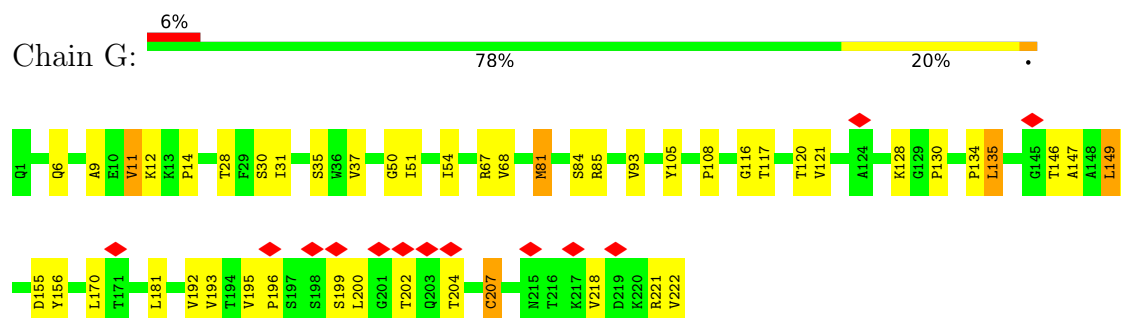
- Molecule 2: 0722 L



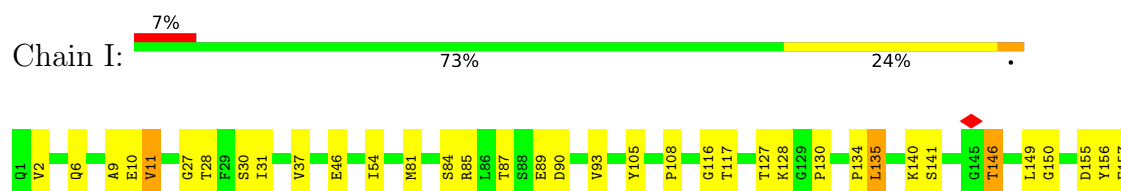
- Molecule 3: 0722 H



- Molecule 3: 0722 H



- Molecule 3: 0722 H





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1463548	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	346.4, 346.4, 346.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.99	0/8969	1.20	9/12189 (0.1%)
1	B	0.99	0/8992	1.20	5/12220 (0.0%)
1	C	1.00	0/8992	1.19	13/12223 (0.1%)
2	D	1.02	0/1626	1.16	1/2212 (0.0%)
2	F	1.02	0/1651	1.15	1/2245 (0.0%)
2	H	1.03	0/1655	1.18	0/2249
3	E	1.03	0/1711	1.17	2/2336 (0.1%)
3	G	1.03	0/1711	1.17	1/2336 (0.0%)
3	I	1.01	0/1711	1.20	4/2336 (0.2%)
All	All	1.00	0/37018	1.19	36/50346 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	158	PRO	CA-N-CD	-10.55	97.23	112.00
1	A	606	TYR	CB-CA-C	-9.97	95.15	110.90
1	A	1205	VAL	N-CA-C	-9.05	102.51	110.74
1	A	931	GLY	N-CA-C	-8.63	102.38	112.73
1	A	639	VAL	N-CA-C	-8.59	102.84	111.77
1	C	1138	HIS	CB-CA-C	-8.32	95.14	110.62
3	I	158	PRO	CB-CA-C	7.92	124.63	111.56
1	C	741	THR	CB-CA-C	7.26	117.54	110.71
1	C	1167	PRO	N-CA-C	-7.19	103.54	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1203	LYS	CB-CA-C	6.86	116.62	109.83
1	A	600	LEU	N-CA-C	-6.82	104.70	113.16
1	C	1175	THR	N-CA-C	-6.65	105.20	113.38
3	E	105	TYR	CB-CA-C	-6.35	100.25	110.79
1	C	715	LEU	N-CA-C	-5.99	105.93	113.18
1	C	639	VAL	N-CA-C	-5.99	105.53	111.88
1	C	1138	HIS	N-CA-C	5.90	117.81	108.79
1	B	929	VAL	N-CA-C	-5.89	104.61	110.62
2	D	66	GLY	CA-C-O	-5.83	118.21	122.23
1	B	693	THR	N-CA-C	-5.82	105.76	112.92
2	F	66	GLY	CA-C-O	-5.78	118.24	122.23
1	C	1120	GLY	CA-C-O	-5.71	117.67	122.29
3	I	105	TYR	CB-CA-C	-5.63	101.44	110.79
1	A	790	VAL	CA-C-O	-5.60	115.78	121.67
1	C	996	LEU	N-CA-C	-5.53	106.12	112.92
1	C	1160	ASN	CB-CA-C	5.41	115.79	110.71
1	C	809	TYR	CA-C-O	-5.34	114.59	120.36
1	A	643	SER	N-CA-C	-5.30	105.50	111.28
1	A	712	GLY	CA-C-O	-5.27	116.26	120.79
1	B	791	THR	CA-C-O	-5.18	115.55	120.94
3	I	158	PRO	N-CA-C	5.17	123.13	112.47
1	B	685	THR	CB-CA-C	5.15	119.33	111.80
3	E	26	GLY	CA-C-O	-5.11	118.15	122.29
1	C	144	TYR	CB-CA-C	5.09	115.57	109.31
1	C	453	LYS	N-CA-C	-5.08	107.76	114.31
3	G	105	TYR	CB-CA-C	-5.07	102.38	110.79
1	B	872	THR	CB-CA-C	5.01	119.03	110.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	51[A]	SER	Mainchain
1	C	51[B]	SER	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8770	0	8501	185	0
1	B	8796	0	8526	192	0
1	C	8794	0	8514	176	0
2	D	1591	0	1529	42	0
2	F	1615	0	1560	33	0
2	H	1619	0	1571	26	0
3	E	1668	0	1624	20	0
3	G	1668	0	1624	24	0
3	I	1668	0	1624	28	0
All	All	36189	0	35073	693	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 (693) 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:D:109:THR:HG21	2:D:169:LYS:C	1.64	1.20
2:F:39:LYS:CB	2:F:42:LYS:NZ	2.08	1.15
2:D:109:THR:HG21	2:D:170:ASP:N	1.57	1.14
2:F:39:LYS:CB	2:F:42:LYS:HZ3	1.66	1.09
1:A:906:MET:SD	1:C:713:CYS:SG	2.53	1.05
1:C:793:GLU:OE1	1:C:793:GLU:C	2.00	1.03
2:F:79:GLN:CB	2:F:81:GLU:OE2	2.11	0.99
2:D:109:THR:HG22	2:D:169:LYS:O	1.63	0.98
2:D:109:THR:CG2	2:D:169:LYS:C	2.37	0.98
1:B:872:THR:HB	1:B:890:ILE:HD11	1.46	0.94
2:D:109:THR:CG2	2:D:169:LYS:O	2.15	0.94
1:C:1179:ARG:HD3	1:C:1185:SER:HA	1.48	0.92
3:G:11:VAL:HG23	3:G:120:THR:O	1.69	0.92
1:A:579:THR:HA	1:B:61:GLY:HA2	1.51	0.92
1:A:328:SER:HB2	1:A:330:ASP:OD1	1.70	0.91
1:C:793:GLU:OE1	1:C:793:GLU:O	1.87	0.91
1:C:795:ILE:HG21	1:C:1099:ALA:HB2	1.55	0.89
2:F:79:GLN:HB2	2:F:81:GLU:OE2	1.72	0.88
2:F:39:LYS:CB	2:F:42:LYS:HZ2	1.82	0.88
1:A:185:CYS:HB3	1:A:237:CYS:HA	1.54	0.86
1:A:906:MET:HE1	1:C:713:CYS:SG	2.14	0.86
2:F:81:GLU:OE1	2:F:81:GLU:N	2.09	0.84
1:B:876:PRO:HD3	1:B:888:SER:HA	1.60	0.83
2:D:143:GLU:OE1	2:D:143:GLU:N	2.12	0.82
2:F:79:GLN:HB3	2:F:81:GLU:OE2	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:986:THR:HA	1:C:1180:ILE:HD13	1.63	0.80
1:C:792:GLN:NE2	1:C:1138:HIS:HB2	1.97	0.80
1:A:906:MET:CE	1:C:713:CYS:SG	2.72	0.78
1:C:731:LEU:HD22	1:C:742:PRO:HA	1.66	0.78
1:B:736:CYS:HB3	1:B:739:PRO:HD2	1.65	0.77
1:A:164:PHE:HB3	1:A:168:THR:HG21	1.68	0.77
1:C:866:GLY:HA3	1:C:869:PHE:HB2	1.65	0.76
1:C:1128:VAL:HB	1:C:1137:MET:HE1	1.68	0.76
1:B:889:ALA:O	1:B:892:ASP:HB2	1.86	0.75
1:C:450:LEU:HA	1:C:453:LYS:HE2	1.68	0.75
1:B:308:LYS:HB2	1:B:310:TRP:CZ2	2.22	0.74
1:A:425:CYS:HB2	1:B:1058:LEU:HD13	1.70	0.74
1:B:733:GLN:HB3	1:B:741:THR:HB	1.69	0.74
1:B:484:VAL:HG21	1:B:488:LEU:HB2	1.70	0.73
1:A:393:PRO:HD3	1:A:491:ILE:HG23	1.69	0.73
2:D:109:THR:OG1	2:D:171:SER:HB3	1.87	0.72
3:I:170:LEU:HD21	3:I:193:VAL:HG11	1.72	0.72
1:A:694:ARG:HD3	1:A:697:LEU:HB3	1.71	0.71
1:B:98:GLN:O	1:B:99:LYS:CB	2.37	0.71
3:G:170:LEU:HD21	3:G:193:VAL:HG11	1.73	0.71
1:A:21:VAL:HB	1:A:240:MET:HG3	1.73	0.71
1:C:792:GLN:HE21	1:C:1137:MET:C	1.98	0.71
1:C:1042:ASN:HA	1:C:1049:ALA:HB1	1.72	0.70
1:B:1178:THR:HG21	1:B:1189:SER:HB3	1.73	0.70
2:F:143:GLU:HB2	2:F:199:GLN:HE22	1.57	0.70
2:D:85:THR:OG1	2:D:103:LYS:NZ	2.20	0.70
3:E:170:LEU:HD21	3:E:193:VAL:HG11	1.74	0.70
1:B:120:ILE:HB	1:B:251:LEU:HG	1.73	0.69
1:B:887:ARG:H	1:B:945:ALA:HB1	1.56	0.69
1:B:1166:ALA:HB1	1:B:1167:PRO:HD2	1.75	0.69
1:A:1053:ASP:HA	1:A:1057:ARG:HB2	1.74	0.68
2:D:109:THR:OG1	2:D:171:SER:CB	2.32	0.68
1:B:149:LEU:HB3	1:B:290:ILE:HG21	1.74	0.68
1:C:1199:SER:HB3	1:C:1205:VAL:HA	1.76	0.68
3:I:179:ALA:HB1	3:I:187:TYR:HB3	1.76	0.67
1:B:742:PRO:HG2	1:B:758:ARG:HB3	1.77	0.66
1:B:801:LYS:HB2	1:B:935:LEU:HB2	1.77	0.66
1:C:57:ILE:HA	1:C:278:MET:HB3	1.77	0.66
1:C:1110:GLN:HA	1:C:1122:HIS:HD2	1.61	0.66
1:B:497:TYR:HB2	1:B:561:VAL:HB	1.77	0.66
2:D:85:THR:HA	2:D:102:THR:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:11:VAL:HG11	3:I:158:PRO:HG3	1.76	0.66
1:A:1130:ALA:HB2	1:A:1135:TYR:HB2	1.77	0.66
1:C:736:CYS:HB2	1:C:739:PRO:HD2	1.78	0.66
1:C:1122:HIS:HE1	1:C:1125:SER:HB2	1.61	0.65
1:C:500:ILE:HD11	1:C:530:VAL:HG11	1.78	0.65
1:B:887:ARG:HG2	1:B:892:ASP:OD1	1.96	0.65
1:B:678:ALA:HB3	1:B:717:LEU:HB2	1.79	0.65
1:C:172:LEU:HD22	1:C:173:PRO:HD2	1.78	0.65
1:C:600:LEU:HG	1:C:602:ASN:HB2	1.78	0.64
1:B:873:LEU:HD23	1:B:952:LEU:HD13	1.79	0.64
1:A:666:GLU:HG2	1:A:667:THR:N	2.11	0.64
1:B:960:TRP:HB2	1:B:970:ILE:HD13	1.79	0.64
2:F:141:PRO:HD2	2:F:198:HIS:HE1	1.63	0.64
1:B:897:LYS:HZ1	1:B:1012:PHE:H	1.46	0.64
1:A:388:LEU:HD12	1:A:443:LEU:HD21	1.80	0.63
3:G:6:GLN:HG3	3:G:116:GLY:H	1.63	0.63
1:A:865:PHE:HB3	1:A:871:LEU:HD12	1.79	0.63
1:C:657:VAL:HG13	1:C:677:VAL:HG21	1.79	0.63
1:C:987:GLN:HG3	1:C:990:LEU:HB2	1.79	0.63
1:B:509:ASP:O	1:B:510:ASP:HB2	1.98	0.63
1:C:792:GLN:HG3	1:C:1136:PHE:O	1.98	0.63
1:A:631:VAL:H	1:A:640:GLY:HA2	1.64	0.63
1:A:728:LYS:HD3	1:A:740:ASP:HA	1.78	0.63
1:B:509:ASP:OD1	1:B:510:ASP:N	2.32	0.63
1:A:742:PRO:HA	1:A:757:MET:HB3	1.81	0.63
1:A:1051:ILE:HG22	1:A:1054:ILE:HG22	1.80	0.63
1:B:799:ILE:HD13	1:B:1088:ARG:HG3	1.80	0.63
2:H:201:LEU:HD21	2:H:205:VAL:HG12	1.81	0.63
1:C:1168:VAL:HG22	1:C:1170:GLY:H	1.64	0.62
1:C:324:LEU:HB3	1:C:337:ILE:HB	1.81	0.62
1:B:595:LYS:HG3	1:B:597:ALA:H	1.64	0.62
1:C:1029:ASN:HA	1:C:1088:ARG:HH12	1.64	0.62
1:C:1040:LEU:HD13	1:C:1077:THR:HB	1.82	0.62
1:A:807:LYS:HG3	1:A:821:LEU:HD23	1.80	0.62
1:B:366:PHE:HB3	1:B:689:TYR:HB3	1.82	0.62
1:C:485:PRO:HG2	1:C:488:LEU:HB2	1.80	0.62
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.81	0.61
2:H:29:ILE:HG22	2:H:32:TYR:HB2	1.82	0.61
1:A:269:ARG:HA	1:A:273:LEU:HB3	1.83	0.61
3:I:150:GLY:HA3	3:I:192:VAL:HA	1.82	0.61
1:B:662:ILE:HB	1:B:671:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:THR:HG22	1:C:492:THR:HB	1.82	0.61
3:E:205:TYR:H	3:E:221:ARG:HH21	1.49	0.61
1:B:542:ARG:HB3	1:B:553:TRP:HE1	1.66	0.60
1:A:63:THR:HG22	1:C:631:VAL:HG23	1.83	0.60
1:A:524:SER:HB3	1:A:527:VAL:HG23	1.83	0.60
1:B:1016:ASN:HB3	1:B:1019:PHE:HB2	1.83	0.60
3:I:130:PRO:HB3	3:I:156:TYR:HB3	1.83	0.60
1:C:659:VAL:HG11	1:C:691:ARG:HH12	1.66	0.60
2:H:33:LEU:HB3	2:H:51:ALA:HB2	1.82	0.60
1:A:397:TYR:HB3	1:A:468:ASN:HD22	1.66	0.60
1:A:631:VAL:HG12	1:A:640:GLY:HA2	1.84	0.60
3:G:130:PRO:HB3	3:G:156:TYR:HB3	1.83	0.60
2:H:141:PRO:HD2	2:H:198:HIS:CE1	2.37	0.60
1:C:1051:ILE:HG13	1:C:1053:ASP:H	1.65	0.60
1:A:606:TYR:CE1	1:A:615:GLY:HA3	2.38	0.59
1:B:109:VAL:HG22	1:B:294:SER:HB3	1.85	0.59
1:B:1105:GLU:HB3	1:B:1113:ARG:HH22	1.65	0.59
3:I:6:GLN:HG3	3:I:116:GLY:H	1.67	0.59
1:A:605:GLU:HA	1:A:614:ARG:HA	1.83	0.59
1:C:1168:VAL:HG11	1:C:1180:ILE:HA	1.85	0.59
2:D:33:LEU:HB3	2:D:51:ALA:HB2	1.85	0.59
1:B:429:SER:HB2	1:C:1058:LEU:C	2.28	0.59
1:C:780:LEU:HD21	1:C:1170:GLY:HA2	1.85	0.59
2:H:21:ILE:HD12	2:H:73:LEU:HD23	1.85	0.59
1:C:441:LEU:HG	1:C:573:ILE:HD11	1.85	0.58
1:A:779:LYS:HA	1:A:1150:VAL:HA	1.84	0.58
1:C:985:ILE:HG13	1:C:1168:VAL:HB	1.85	0.58
2:D:78:LEU:HD13	2:D:83:PHE:HE1	1.67	0.58
1:C:631:VAL:HG12	1:C:640:GLY:HA2	1.85	0.58
2:D:109:THR:C	2:D:170:ASP:O	2.44	0.58
1:C:401:ARG:NH1	1:C:521:ASN:OD1	2.36	0.58
1:C:1047:ILE:HG23	1:C:1048:SER:H	1.68	0.58
1:A:504:SER:HA	1:A:515:PRO:HA	1.84	0.58
1:B:791:THR:HA	1:B:1138:HIS:HB3	1.84	0.58
1:A:220:ASN:HB3	1:A:223:ALA:HB2	1.86	0.58
3:E:6:GLN:HG3	3:E:116:GLY:H	1.68	0.58
1:B:138:ALA:HB1	1:B:141:ARG:HH21	1.69	0.57
1:B:721:SER:C	1:B:723:PHE:H	2.12	0.57
2:F:33:LEU:HB3	2:F:51:ALA:HB2	1.87	0.57
1:A:542:ARG:HG2	1:A:555:VAL:HG22	1.86	0.57
1:C:777:TYR:HB3	1:C:1150:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:VAL:HG13	1:A:639:VAL:HG13	1.87	0.57
1:C:910:ASP:O	1:C:914:GLN:HG2	2.04	0.57
2:H:29:ILE:HG23	2:H:92:TYR:HB2	1.86	0.57
1:B:401:ARG:HD2	1:B:442:ILE:HG23	1.87	0.57
1:A:626:ARG:HD3	1:A:648:TYR:HD2	1.69	0.56
1:A:906:MET:H	1:C:676:SER:HA	1.69	0.56
1:C:1192:TYR:HB2	1:C:1194:PRO:HG3	1.86	0.56
2:D:21:ILE:HD12	2:D:73:LEU:HD23	1.86	0.56
2:H:38:LEU:HD13	2:H:44:PRO:HG3	1.87	0.56
1:A:187:LEU:HD23	1:A:187:LEU:H	1.70	0.56
1:B:98:GLN:O	1:B:99:LYS:HB3	2.04	0.56
2:F:141:PRO:HD2	2:F:198:HIS:CE1	2.40	0.56
1:B:616:VAL:HB	1:B:652:ARG:HB2	1.87	0.56
1:C:163:ARG:HH22	1:C:189:PRO:HD3	1.69	0.56
3:I:157:PHE:CG	3:I:158:PRO:HD2	2.41	0.56
1:A:210:PRO:HG2	1:A:302:SER:HB3	1.87	0.56
1:A:869:PHE:HE2	1:A:973:ALA:HB2	1.70	0.56
1:C:792:GLN:NE2	1:C:1137:MET:C	2.64	0.56
1:B:889:ALA:O	1:B:893:LEU:HD23	2.05	0.55
1:B:872:THR:O	1:B:889:ALA:HB3	2.06	0.55
1:C:1126:PHE:HB2	1:C:1137:MET:HB2	1.88	0.55
1:B:736:CYS:SG	1:B:737:ALA:N	2.79	0.55
1:B:897:LYS:NZ	1:B:1012:PHE:H	2.04	0.55
1:A:430:PRO:HD3	1:B:1058:LEU:HD12	1.88	0.55
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.89	0.55
2:H:141:PRO:HD2	2:H:198:HIS:HE1	1.71	0.55
1:B:366:PHE:HE1	1:B:659:VAL:HB	1.70	0.55
1:C:724:VAL:HB	1:C:758:ARG:HG2	1.88	0.55
1:C:792:GLN:HG3	1:C:1136:PHE:C	2.31	0.55
2:H:37:GLN:HB2	2:H:47:LEU:HD11	1.87	0.55
1:C:484:VAL:HB	1:C:567:LEU:HB3	1.89	0.55
3:I:127:THR:HG21	3:I:213:PRO:HB2	1.89	0.55
1:B:783:PRO:HB3	1:B:1143:PRO:HB3	1.89	0.55
3:E:205:TYR:H	3:E:221:ARG:NH2	2.05	0.55
2:F:4:MET:HE1	2:F:25:ALA:HB2	1.88	0.55
1:B:388:LEU:HD12	1:B:445:TYR:HB3	1.89	0.54
1:C:1152:ALA:HB2	1:C:1173:ILE:HG22	1.89	0.54
2:F:29:ILE:HG23	2:F:92:TYR:HB2	1.89	0.54
1:A:441:LEU:HB2	1:A:584:VAL:HG21	1.88	0.54
1:A:261:GLN:HG2	1:C:403:VAL:HG11	1.88	0.54
1:B:142:LYS:HG3	1:B:251:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:30:SER:HB2	3:E:54:ILE:HB	1.88	0.54
2:F:38:LEU:HD13	2:F:44:PRO:HG3	1.89	0.54
2:F:201:LEU:HD21	2:F:205:VAL:HG12	1.88	0.54
1:B:888:SER:OG	1:B:891:GLU:HG3	2.07	0.54
1:C:679:CYS:HB3	1:C:713:CYS:HB2	1.90	0.54
2:H:29:ILE:O	2:H:30:THR:C	2.51	0.54
1:A:468:ASN:HD21	1:A:500:ILE:H	1.56	0.54
1:B:374:VAL:HA	1:B:597:ALA:HA	1.89	0.54
2:D:110:VAL:HA	2:D:140:TYR:HD1	1.73	0.54
1:B:498:SER:HB3	1:B:534:VAL:HG23	1.90	0.54
1:B:795:ILE:HG21	1:B:1099:ALA:HB2	1.89	0.54
1:B:889:ALA:HA	1:B:892:ASP:OD2	2.08	0.54
1:A:369:LYS:HE2	1:A:690:SER:HB3	1.89	0.54
1:A:437:CYS:HB3	1:A:610:GLY:HA2	1.89	0.53
1:A:397:TYR:HD2	1:A:527:VAL:HG13	1.72	0.53
1:A:440:SER:HB3	1:A:576:GLN:HB3	1.90	0.53
1:A:820:LEU:HD13	1:A:1067:ILE:HD13	1.91	0.53
1:A:994:GLN:HB3	1:A:997:ILE:HD11	1.90	0.53
1:C:731:LEU:H	1:C:740:ASP:HB3	1.72	0.53
1:B:189:PRO:HB2	1:B:197:ALA:HB2	1.90	0.53
1:B:862:ILE:HB	1:B:863:PRO:HD2	1.90	0.53
1:A:1165:ILE:HG23	1:A:1167:PRO:HD3	1.91	0.53
1:A:784:THR:H	1:A:1145:ASN:HB2	1.73	0.53
1:C:1172:PHE:HB2	1:C:1185:SER:HB3	1.90	0.53
2:F:161:GLU:HB3	2:F:175:LEU:HD11	1.90	0.53
3:I:204:THR:HA	3:I:221:ARG:HH21	1.73	0.53
1:B:105:TYR:HA	1:B:108:ASP:OD2	2.09	0.53
3:G:135:LEU:HB2	3:G:150:GLY:H	1.73	0.53
2:H:25:ALA:HB3	2:H:69:THR:HA	1.89	0.53
1:B:410:ASN:HB2	1:B:413:LYS:HE3	1.91	0.53
1:A:986:THR:HA	1:A:990:LEU:HD23	1.90	0.52
2:D:29:ILE:HG22	2:D:32:TYR:HB2	1.90	0.52
1:A:898:VAL:HA	1:A:1023:GLN:HE22	1.73	0.52
3:I:30:SER:HB2	3:I:54:ILE:HB	1.91	0.52
1:A:112:PHE:CE1	1:A:115:GLY:HA2	2.45	0.52
1:A:1152:ALA:O	1:A:1153:TYR:HB2	2.08	0.52
1:B:1173:ILE:HD12	1:B:1177:ASN:HB2	1.90	0.52
1:A:611:VAL:HB	1:A:638:LEU:HD22	1.89	0.52
1:A:1191:PHE:CD1	1:C:1195:GLU:HB2	2.44	0.52
3:I:127:THR:HA	3:I:157:PHE:HB3	1.91	0.52
2:D:110:VAL:HA	2:D:140:TYR:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:887:ARG:HA	1:B:891:GLU:OE1	2.09	0.52
1:C:799:ILE:HG23	1:C:1092:ALA:HB2	1.91	0.52
2:F:29:ILE:O	2:F:30:THR:C	2.53	0.52
1:B:404:PHE:HB2	1:B:441:LEU:HB3	1.92	0.52
1:B:98:GLN:O	1:B:99:LYS:HB2	2.08	0.52
1:B:151:SER:HB2	1:B:166:ASN:HD22	1.74	0.52
2:D:109:THR:O	2:D:170:ASP:O	2.27	0.52
1:A:401:ARG:HD3	1:B:261:GLN:HA	1.92	0.52
1:C:789:GLY:H	1:C:1140:GLY:H	1.57	0.52
2:F:21:ILE:HD12	2:F:73:LEU:HD23	1.92	0.52
1:A:412:THR:HB	1:A:434:ALA:HB1	1.92	0.51
1:A:780:LEU:HG	1:B:968:ALA:HA	1.90	0.51
1:B:1060:VAL:O	1:B:1063:GLN:HG3	2.10	0.51
1:C:673:LEU:HD22	1:C:735:LEU:HD11	1.91	0.51
1:C:659:VAL:HG11	1:C:691:ARG:NH1	2.25	0.51
1:C:724:VAL:HG22	1:C:728:LYS:HG3	1.92	0.51
3:G:30:SER:HB2	3:G:54:ILE:HB	1.93	0.51
1:B:786:PHE:HA	1:B:1141:TYR:CE1	2.45	0.51
2:F:149:LYS:HG3	2:F:193:ALA:HB3	1.92	0.51
2:H:113:PRO:HB3	2:H:139:PHE:HB3	1.93	0.51
1:A:1043:THR:HB	1:C:636:GLN:HB2	1.92	0.51
1:C:1205:VAL:O	1:C:1206:ALA:C	2.53	0.51
2:D:170:ASP:O	2:D:172:THR:HG23	2.09	0.51
1:A:50:VAL:HG22	1:A:78:GLN:HG3	1.92	0.51
1:B:102:VAL:HG11	1:B:205:ALA:HB3	1.93	0.51
1:C:406:ASN:H	1:C:584:VAL:HG12	1.75	0.51
1:C:641:TYR:HA	1:C:649:TYR:O	2.10	0.51
1:B:74:LEU:HD12	1:B:318:LEU:HB3	1.91	0.51
1:C:399:PHE:O	1:C:523:TYR:CE1	2.64	0.51
1:A:718:VAL:HG12	1:A:720:SER:H	1.76	0.51
1:B:980:LEU:HD22	1:B:997:ILE:HD12	1.93	0.51
2:D:29:ILE:O	2:D:30:THR:C	2.53	0.51
1:A:418:PHE:HA	1:A:484:VAL:HG13	1.93	0.51
1:A:605:GLU:H	1:A:615:GLY:H	1.57	0.51
1:A:496:LYS:HD3	1:A:560:THR:HB	1.93	0.51
1:A:1128:VAL:HG23	1:A:1135:TYR:HB3	1.91	0.51
3:E:132:VAL:HG12	3:E:151:CYS:HB2	1.92	0.50
1:A:715:LEU:HD11	1:A:735:LEU:HB3	1.94	0.50
1:A:1158:ALA:HB2	1:A:1203:LYS:HE2	1.93	0.50
1:B:151:SER:HA	1:B:291:LYS:H	1.76	0.50
1:B:509:ASP:O	1:B:510:ASP:CB	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LEU:HB3	1:C:290:ILE:HG21	1.92	0.50
1:C:662:ILE:HG12	1:C:735:LEU:HD13	1.93	0.50
1:C:1160:ASN:N	1:C:1161:PRO:HD3	2.26	0.50
1:A:411:LEU:HB3	1:A:434:ALA:HA	1.92	0.50
1:A:1163:ASN:O	1:A:1196:PRO:HD2	2.10	0.50
1:C:366:PHE:HB2	1:C:691:ARG:HA	1.93	0.50
1:B:117:VAL:HG22	1:B:318:LEU:HG	1.93	0.50
3:E:146:THR:HA	3:E:196:PRO:HA	1.94	0.50
2:H:139:PHE:HB2	2:H:198:HIS:CE1	2.47	0.50
1:A:601:GLY:C	1:A:603:CYS:H	2.19	0.50
1:B:342:ASN:HB3	1:B:344:LEU:HG	1.92	0.50
1:B:366:PHE:CE1	1:B:659:VAL:HB	2.47	0.50
1:A:328:SER:CB	1:A:330:ASP:OD1	2.53	0.50
2:D:4:MET:HE1	2:D:25:ALA:HB2	1.92	0.50
1:B:372:GLY:HA2	1:B:596:ILE:HD11	1.93	0.50
1:B:728:LYS:HB3	1:B:761:SER:H	1.76	0.50
1:C:284:LEU:HG	1:C:286:VAL:HG23	1.94	0.50
1:B:622:ALA:HA	1:B:648:TYR:CD2	2.47	0.49
1:B:676:SER:HB2	1:C:927:GLN:HE22	1.77	0.49
1:A:925:CYS:HB3	1:A:928:TYR:HB2	1.95	0.49
1:C:1130:ALA:HB2	1:C:1135:TYR:HB2	1.93	0.49
1:A:734:SER:HA	1:A:739:PRO:HD2	1.93	0.49
1:C:718:VAL:HB	1:C:721:SER:HB3	1.94	0.49
1:A:987:GLN:O	1:A:988:GLN:C	2.54	0.49
2:D:136:LEU:HD11	2:D:196:VAL:HG11	1.95	0.49
2:F:81:GLU:H	2:F:81:GLU:CD	2.10	0.49
1:B:48:ILE:HD11	1:B:55:GLY:HA3	1.95	0.49
1:C:990:LEU:HD13	1:C:1180:ILE:HD11	1.94	0.49
3:I:177:PHE:HE2	3:I:192:VAL:HG22	1.77	0.49
1:A:795:ILE:O	1:A:1095:SER:HB3	2.13	0.49
2:H:4:MET:HE1	2:H:25:ALA:HB2	1.94	0.49
1:A:965:SER:HA	1:C:1143:PRO:HG3	1.95	0.49
1:B:853:VAL:HG13	1:B:951:LEU:HD22	1.94	0.49
1:C:358:SER:HB2	1:C:733:GLN:HE22	1.76	0.49
1:A:576:GLN:HG2	1:A:578:GLY:H	1.78	0.49
1:A:596:ILE:HG13	1:A:597:ALA:N	2.28	0.49
1:B:440:SER:HB3	1:B:576:GLN:HG3	1.95	0.49
1:C:792:GLN:HA	1:C:792:GLN:OE1	2.13	0.49
3:G:150:GLY:HA3	3:G:192:VAL:HG12	1.95	0.49
1:B:448:TYR:CZ	1:B:481:LEU:HB3	2.48	0.49
1:C:980:LEU:HD23	1:C:1123:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:ILE:HG22	2:F:32:TYR:HB2	1.95	0.49
1:A:875:GLU:N	1:A:875:GLU:OE1	2.46	0.48
1:A:267:SER:HB3	1:A:270:TYR:HD2	1.79	0.48
1:A:364:SER:HB3	1:A:693:THR:HG21	1.95	0.48
1:A:457:SER:HB3	1:A:460:SER:HB3	1.95	0.48
1:A:498:SER:HB3	1:A:534:VAL:HG23	1.94	0.48
1:A:1154:GLY:HA3	1:A:1205:VAL:H	1.78	0.48
1:C:1166:ALA:HA	1:C:1192:TYR:HB3	1.95	0.48
1:C:180:LEU:HB3	1:C:245:ILE:HD11	1.95	0.48
3:G:149:LEU:HD21	3:G:200:LEU:HD22	1.95	0.48
3:G:204:THR:HA	3:G:221:ARG:HH21	1.78	0.48
1:C:1202:THR:C	1:C:1204:TYR:H	2.21	0.48
1:B:422:ASP:HB3	1:B:481:LEU:HD12	1.96	0.48
1:B:510:ASP:O	1:B:511:ARG:HB3	2.14	0.48
1:C:496:LYS:HE3	1:C:560:THR:HB	1.96	0.48
1:B:887:ARG:N	1:B:945:ALA:HB1	2.26	0.48
1:B:49:ASP:HB3	1:B:52:LYS:HG2	1.96	0.48
2:D:161:GLU:HB3	2:D:175:LEU:HD11	1.96	0.48
1:A:691:ARG:HG2	1:A:693:THR:HG23	1.96	0.48
1:B:625:VAL:O	1:B:626:ARG:HB2	2.14	0.48
1:B:1059:ASP:HB3	1:B:1062:GLU:HB2	1.95	0.48
2:H:136:LEU:HD11	2:H:196:VAL:HG11	1.96	0.48
1:C:802:VAL:HG21	1:C:1033:LEU:HD11	1.96	0.48
1:A:185:CYS:HB3	1:A:237:CYS:CA	2.35	0.47
1:B:263:VAL:HG23	1:B:284:LEU:HB3	1.96	0.47
1:C:439:SER:HA	1:C:583:SER:HA	1.95	0.47
1:B:100:LEU:HD11	1:B:299:SER:HB3	1.96	0.47
1:C:521:ASN:OD1	1:C:521:ASN:O	2.32	0.47
3:G:204:THR:HG23	3:G:221:ARG:HE	1.79	0.47
3:I:134:PRO:HB3	3:I:222:VAL:HG22	1.95	0.47
1:B:406:ASN:HA	1:B:583:SER:HB2	1.95	0.47
1:C:1175:THR:O	1:C:1176:ASN:HB2	2.12	0.47
1:C:1193:ALA:N	1:C:1194:PRO:HD3	2.28	0.47
3:I:197:SER:HA	3:I:200:LEU:HD12	1.96	0.47
1:A:739:PRO:HA	1:A:759:LEU:O	2.14	0.47
1:B:625:VAL:HG23	1:C:332:TYR:HE1	1.79	0.47
1:B:638:LEU:H	1:B:638:LEU:HD22	1.79	0.47
2:F:113:PRO:HB3	2:F:139:PHE:HB3	1.96	0.47
1:A:580:ASP:HB2	1:A:630:PHE:HB2	1.96	0.47
1:B:251:LEU:HD12	1:B:252:GLU:H	1.80	0.47
1:B:1165:ILE:HG21	1:C:960:TRP:HZ2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:ASN:O	1:C:230:GLU:HG3	2.14	0.47
1:A:714:VAL:HG21	1:A:737:ALA:CB	2.45	0.47
2:H:123:GLU:HA	2:H:126:LYS:HG2	1.96	0.47
1:B:609:TYR:HB3	1:B:630:PHE:HZ	1.80	0.47
1:B:802:VAL:HG23	1:B:932:TYR:HB2	1.94	0.47
2:D:111:ALA:HB1	2:D:138:ASN:HB2	1.96	0.47
3:E:158:PRO:HD2	3:E:211:HIS:CE1	2.49	0.47
3:I:205:TYR:H	3:I:221:ARG:NH2	2.11	0.47
1:A:33:VAL:HG11	1:A:203:SER:HB3	1.97	0.47
1:B:524:SER:HB3	1:B:527:VAL:HG23	1.97	0.47
1:B:660:SER:HB2	1:B:673:LEU:HB3	1.95	0.47
1:B:793:GLU:HB3	1:B:1136:PHE:HB2	1.96	0.47
2:D:123:GLU:HA	2:D:126:LYS:HG2	1.96	0.47
1:B:608:LEU:HB3	1:B:611:VAL:O	2.15	0.47
2:F:79:GLN:CB	2:F:81:GLU:CD	2.87	0.47
1:B:18:TYR:HD1	1:B:236:ASN:HA	1.80	0.47
1:B:1016:ASN:HB3	1:B:1019:PHE:CB	2.45	0.47
2:D:143:GLU:H	2:D:143:GLU:CD	2.23	0.46
1:A:789:GLY:HA2	1:A:1139:VAL:HG13	1.96	0.46
1:A:937:PRO:O	1:A:939:MET:N	2.48	0.46
1:B:1066:GLN:O	1:B:1069:ARG:HG3	2.15	0.46
1:C:1075:LEU:HD12	1:C:1078:LEU:HD11	1.96	0.46
1:C:782:ILE:HG13	1:C:1172:PHE:CE1	2.50	0.46
1:C:1081:PHE:O	1:C:1084:GLN:HG3	2.14	0.46
3:I:127:THR:HG23	3:I:211:HIS:HE1	1.79	0.46
1:A:273:LEU:HD23	1:A:273:LEU:H	1.81	0.46
1:C:118:VAL:HG12	1:C:315:VAL:HG22	1.97	0.46
1:C:374:VAL:HA	1:C:597:ALA:HA	1.97	0.46
2:H:79:GLN:H	2:H:82:ASP:HB2	1.81	0.46
1:B:626:ARG:HA	1:B:641:TYR:OH	2.15	0.46
1:C:1110:GLN:HA	1:C:1122:HIS:CD2	2.45	0.46
3:G:14:PRO:HG3	3:G:121:VAL:HB	1.97	0.46
1:C:156:PHE:HE1	1:C:232:PHE:HZ	1.64	0.46
1:C:780:LEU:O	1:C:1148:GLU:HA	2.16	0.46
1:A:790:VAL:O	1:A:791:THR:HB	2.16	0.46
1:B:147:PHE:HB3	1:B:295:ILE:HD13	1.98	0.46
1:B:789:GLY:CA	1:B:1004:ALA:HB1	2.46	0.46
3:E:130:PRO:HB3	3:E:156:TYR:HB3	1.97	0.46
2:H:32:TYR:HB3	2:H:91:SER:HB3	1.98	0.46
1:A:666:GLU:HG2	1:A:667:THR:H	1.81	0.46
1:B:1111:SER:H	1:B:1122:HIS:HD1	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:SER:HB2	2:D:107:LYS:HD3	1.98	0.46
1:A:189:PRO:HB3	1:A:196:PRO:HB2	1.98	0.46
1:B:641:TYR:HB2	1:B:648:TYR:CE2	2.50	0.46
1:C:40:PHE:HA	1:C:131:ILE:HD11	1.98	0.46
1:C:835:LEU:HD12	1:C:835:LEU:HA	1.78	0.46
1:C:1192:TYR:HD1	1:C:1194:PRO:HD3	1.80	0.46
3:E:84:SER:O	3:E:85:ARG:HG2	2.16	0.46
2:F:136:LEU:HD11	2:F:196:VAL:HG11	1.97	0.46
1:B:208:HIS:HB3	1:B:300:ILE:HG23	1.98	0.46
1:B:448:TYR:HE2	1:B:453:LYS:HB2	1.81	0.46
1:C:220:ASN:HB3	1:C:223:ALA:HB2	1.97	0.46
3:G:207:CYS:HB3	3:G:222:VAL:HG21	1.98	0.46
1:B:897:LYS:HZ1	1:B:1012:PHE:N	2.13	0.45
1:A:734:SER:HB3	1:A:738:LEU:HB3	1.98	0.45
2:F:120:PRO:HD3	2:F:132:VAL:HG12	1.98	0.45
1:A:399:PHE:HB3	1:A:446:PHE:HB3	1.97	0.45
1:A:408:ASN:HD22	1:A:408:ASN:HA	1.60	0.45
1:A:985:ILE:HB	1:A:1180:ILE:N	2.31	0.45
3:I:135:LEU:HB2	3:I:150:GLY:H	1.81	0.45
3:G:84:SER:O	3:G:85:ARG:HG2	2.17	0.45
3:G:146:THR:HA	3:G:196:PRO:HA	1.98	0.45
1:A:1152:ALA:HB3	1:A:1172:PHE:HB2	1.98	0.45
1:B:382:GLU:HA	1:B:408:ASN:O	2.17	0.45
2:D:117:ILE:HG12	2:D:209:PHE:HD2	1.81	0.45
1:B:576:GLN:O	1:B:577:TYR:HB2	2.17	0.45
1:C:741:THR:HA	1:C:759:LEU:HA	1.99	0.45
1:C:951:LEU:HD12	1:C:951:LEU:HA	1.76	0.45
3:G:9:ALA:HA	3:G:117:THR:HG23	1.98	0.45
1:B:324:LEU:HB3	1:B:337:ILE:HB	1.98	0.45
1:B:388:LEU:HD13	1:B:443:LEU:HD21	1.98	0.45
1:C:600:LEU:CG	1:C:602:ASN:HB2	2.46	0.45
1:C:826:GLN:H	1:C:826:GLN:HG3	1.49	0.45
1:B:506:LEU:HB3	1:B:553:TRP:H	1.82	0.45
1:B:632:TYR:CE1	1:B:638:LEU:HB3	2.52	0.45
1:B:803:THR:O	1:B:932:TYR:HA	2.17	0.45
1:C:430:PRO:O	1:C:433:ILE:HG22	2.17	0.45
1:A:112:PHE:HE2	1:A:258:GLN:HB2	1.82	0.45
1:A:359:GLY:HA2	1:A:733:GLN:HG2	1.99	0.45
1:C:887:ARG:HA	1:C:887:ARG:HD3	1.72	0.45
1:A:234:LEU:H	1:A:234:LEU:HG	1.46	0.45
1:B:26:VAL:HG22	1:B:27:LYS:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:LEU:HD21	2:D:88:CYS:HB2	1.99	0.45
2:F:79:GLN:HB2	2:F:81:GLU:CD	2.38	0.45
1:B:1102:LYS:HB3	1:B:1102:LYS:HE2	1.81	0.44
1:C:1033:LEU:HD23	1:C:1033:LEU:HA	1.86	0.44
3:E:35:SER:HA	3:E:50:GLY:HA2	1.99	0.44
1:B:357:GLU:H	1:B:357:GLU:HG3	1.55	0.44
2:F:139:PHE:HB2	2:F:198:HIS:CE1	2.52	0.44
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.83	0.44
1:C:983:VAL:HG11	1:C:1123:ILE:HD13	1.98	0.44
3:I:181:LEU:HD13	3:I:181:LEU:HA	1.88	0.44
1:A:718:VAL:HG12	1:A:719:ASN:N	2.33	0.44
1:B:180:LEU:HB3	1:B:245:ILE:HD11	1.98	0.44
1:A:909:TYR:O	1:A:912:CYS:HB2	2.18	0.44
1:B:205:ALA:HB1	1:B:297:PRO:O	2.17	0.44
1:C:724:VAL:HG11	1:C:761:SER:HB2	1.99	0.44
1:C:780:LEU:CD2	1:C:1170:GLY:HA2	2.46	0.44
1:A:821:LEU:HD12	1:A:821:LEU:HA	1.82	0.44
1:A:835:LEU:HD12	1:A:835:LEU:HA	1.83	0.44
3:I:9:ALA:HA	3:I:117:THR:HG23	1.99	0.44
3:I:84:SER:O	3:I:85:ARG:HG2	2.17	0.44
1:A:715:LEU:CD2	1:B:936:PRO:HG2	2.47	0.44
1:A:804:VAL:HG12	1:A:835:LEU:HD22	1.98	0.44
1:B:894:LEU:HB2	1:B:1019:PHE:CE1	2.53	0.44
1:A:383:CYS:N	1:A:407:CYS:HB2	2.33	0.44
1:A:679:CYS:HA	1:A:717:LEU:HD23	1.99	0.44
1:A:1051:ILE:HD12	1:A:1051:ILE:HA	1.85	0.44
1:B:369:LYS:HZ2	1:B:690:SER:HA	1.83	0.44
1:B:625:VAL:HG13	1:B:627:GLN:H	1.83	0.44
1:C:476:PRO:HG2	1:C:575:VAL:HG23	2.00	0.44
2:D:142:ARG:HB2	2:D:143:GLU:OE1	2.18	0.44
3:E:174:VAL:HA	3:E:193:VAL:HG22	2.00	0.44
1:A:968:ALA:HB2	1:C:1169:ASN:HD22	1.83	0.44
1:B:631:VAL:HG23	1:C:63:THR:HG23	2.00	0.44
1:C:368:ALA:HA	1:C:689:TYR:HD1	1.82	0.44
1:A:455:ASP:HA	1:A:462:GLY:HA3	2.00	0.43
1:A:893:LEU:O	1:A:897:LYS:HG2	2.18	0.43
1:B:714:VAL:HB	1:B:715:LEU:H	1.64	0.43
2:H:125:LEU:HD12	2:H:183:LYS:HE3	2.00	0.43
2:H:163:VAL:HB	2:H:175:LEU:HD12	1.99	0.43
1:A:806:CYS:O	1:A:807:LYS:HB2	2.18	0.43
1:C:344:LEU:HD13	1:C:344:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:68:VAL:HG21	3:G:81:MET:HE2	2.00	0.43
1:A:149:LEU:HB3	1:A:290:ILE:HD13	2.00	0.43
1:A:831:ILE:HG23	1:A:1082:VAL:HG21	1.98	0.43
1:B:786:PHE:HB2	1:B:1000:LYS:HE3	2.01	0.43
1:B:789:GLY:HA2	1:B:1004:ALA:HB1	2.00	0.43
1:B:897:LYS:HG3	1:B:1012:PHE:HB2	1.99	0.43
2:D:120:PRO:HD3	2:D:132:VAL:HG12	2.00	0.43
1:A:102:VAL:HG12	1:A:299:SER:HB2	2.00	0.43
1:A:428:ILE:HG23	1:A:478:CYS:SG	2.59	0.43
1:A:595:LYS:HD2	1:A:600:LEU:HB2	2.00	0.43
1:B:787:SER:HB2	1:B:1142:TYR:O	2.18	0.43
1:C:1054:ILE:HA	1:C:1063:GLN:HG3	1.99	0.43
1:B:599:GLN:HB2	1:B:644:ASP:HB2	2.00	0.43
1:B:720:SER:HA	1:B:757:MET:SD	2.58	0.43
1:C:657:VAL:HG11	1:C:682:ILE:HD11	2.01	0.43
3:I:146:THR:HA	3:I:196:PRO:HA	2.00	0.43
1:A:56:ILE:HG23	1:A:75:PHE:CE1	2.53	0.43
1:A:714:VAL:HG21	1:A:737:ALA:HB3	2.00	0.43
1:A:900:ILE:HG22	1:A:902:ASP:H	1.84	0.43
1:C:497:TYR:HE2	1:C:564:THR:HG22	1.82	0.43
3:G:147:ALA:HB3	3:G:200:LEU:HD11	2.01	0.43
1:A:324:LEU:HG	1:A:354:PHE:CE1	2.54	0.43
1:A:608:LEU:HA	1:A:608:LEU:HD23	1.87	0.43
1:B:342:ASN:HD22	1:B:342:ASN:HA	1.58	0.43
1:C:179:LEU:HD11	1:C:242:THR:HB	2.01	0.43
1:C:1045:GLY:HA3	1:C:1049:ALA:HA	2.01	0.43
3:G:12:LYS:O	3:G:121:VAL:HA	2.18	0.43
3:G:199:SER:HA	3:G:202:THR:HG22	2.00	0.43
1:A:424:THR:HG23	1:A:479:LEU:HB3	2.00	0.43
1:A:951:LEU:O	1:A:955:ILE:HG13	2.18	0.43
2:D:38:LEU:HD13	2:D:44:PRO:HG3	2.00	0.43
3:G:207:CYS:HB3	3:G:222:VAL:CG2	2.49	0.43
1:A:61:GLY:HA2	1:C:581:THR:HG23	2.00	0.43
1:B:100:LEU:HD22	1:B:100:LEU:HA	1.85	0.43
1:B:358:SER:HB3	1:B:664:ASP:HA	2.00	0.43
1:C:189:PRO:HB2	1:C:197:ALA:HB2	2.00	0.43
2:D:78:LEU:HD23	2:D:78:LEU:HA	1.76	0.43
1:A:526:CYS:HB2	1:A:556:ALA:HB2	2.00	0.43
1:B:148:MET:HG2	1:B:296:ILE:HG12	2.01	0.43
1:B:1130:ALA:HB2	1:B:1135:TYR:HB2	2.01	0.43
1:C:43:THR:HG22	1:C:45:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:793:GLU:C	1:C:793:GLU:CD	2.83	0.43
2:D:111:ALA:HB3	2:D:172:THR:HG21	2.00	0.43
3:E:158:PRO:HB2	3:E:213:PRO:HG2	2.00	0.43
1:A:389:LEU:H	1:A:389:LEU:HG	1.71	0.42
1:A:740:ASP:HB2	1:A:760:ALA:HB2	2.01	0.42
1:A:1056:GLN:HE21	1:A:1056:GLN:HB2	1.58	0.42
1:B:270:TYR:HB2	1:B:279:PHE:HE1	1.84	0.42
1:B:1165:ILE:HG22	1:B:1172:PHE:H	1.84	0.42
3:E:135:LEU:HB2	3:E:150:GLY:H	1.84	0.42
2:H:120:PRO:HD3	2:H:132:VAL:HG12	2.01	0.42
1:A:149:LEU:HB2	1:A:169:LEU:HB3	2.01	0.42
1:A:738:LEU:H	1:A:738:LEU:HG	1.53	0.42
1:A:1078:LEU:HD12	1:A:1078:LEU:HA	1.83	0.42
1:A:1156:CYS:SG	1:A:1163:ASN:HB3	2.58	0.42
1:B:25:SER:HB2	1:B:233:ASN:HD21	1.84	0.42
1:B:951:LEU:O	1:B:955:ILE:HG13	2.19	0.42
2:F:79:GLN:H	2:F:82:ASP:HB2	1.83	0.42
1:A:1126:PHE:HB2	1:A:1137:MET:HE3	2.00	0.42
1:B:924:ILE:HG23	1:B:925:CYS:N	2.34	0.42
1:C:968:ALA:HB1	1:C:970:ILE:HG23	2.01	0.42
3:E:52:ILE:HD11	3:E:103:TYR:HA	2.01	0.42
1:B:248:ASP:O	1:B:249:GLU:HB2	2.19	0.42
1:C:1173:ILE:O	1:C:1174:LYS:C	2.62	0.42
2:F:37:GLN:HE22	2:F:82:ASP:HA	1.84	0.42
1:A:1053:ASP:HB2	1:A:1063:GLN:HG2	2.02	0.42
1:C:44:TRP:HD1	1:C:84:MET:HE1	1.83	0.42
2:F:197:THR:HG23	2:F:204:PRO:HG3	2.01	0.42
3:G:35:SER:HA	3:G:50:GLY:HA2	2.00	0.42
1:A:987:GLN:H	1:A:990:LEU:HB3	1.85	0.42
1:A:1156:CYS:CB	1:A:1163:ASN:HB3	2.50	0.42
1:A:1191:PHE:HD1	1:C:1195:GLU:HB2	1.83	0.42
1:B:362:SER:H	1:C:836:HIS:CE1	2.37	0.42
1:B:369:LYS:NZ	1:B:690:SER:HA	2.34	0.42
1:B:764:PHE:HB2	1:C:943:MET:HG3	2.01	0.42
1:C:604:VAL:HG12	1:C:605:GLU:N	2.35	0.42
1:C:631:VAL:H	1:C:640:GLY:HA2	1.84	0.42
3:E:151:CYS:HB3	3:E:222:VAL:HG21	2.02	0.42
1:A:99:LYS:H	1:A:99:LYS:HG3	1.71	0.42
1:A:663:TYR:CE2	1:A:665:LYS:HB2	2.55	0.42
1:A:937:PRO:C	1:A:939:MET:H	2.28	0.42
1:B:546:SER:HB3	1:B:549:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:680:GLU:H	1:C:680:GLU:HG3	1.66	0.42
1:C:783:PRO:HA	1:C:1145:ASN:O	2.19	0.42
3:G:67:ARG:HE	3:G:67:ARG:HB3	1.59	0.42
1:A:601:GLY:C	1:A:603:CYS:N	2.77	0.42
1:A:673:LEU:HD12	1:A:718:VAL:HG22	2.01	0.42
1:A:909:TYR:CE1	1:C:655:VAL:HG22	2.55	0.42
1:B:740:ASP:HB2	1:B:762:ILE:HG12	2.01	0.42
1:B:951:LEU:HD12	1:B:951:LEU:HA	1.88	0.42
1:C:149:LEU:HB2	1:C:169:LEU:HB3	2.02	0.42
1:C:266:PHE:HA	1:C:280:GLN:HA	2.02	0.42
1:C:269:ARG:HA	1:C:273:LEU:HB3	2.01	0.42
2:H:199:GLN:HE21	2:H:199:GLN:HB3	1.71	0.42
1:B:366:PHE:CD2	1:B:689:TYR:HB3	2.54	0.42
1:B:466:GLN:HB3	1:B:517:LEU:HD22	2.02	0.42
1:C:399:PHE:O	1:C:523:TYR:CZ	2.73	0.42
1:C:1047:ILE:HG21	1:C:1058:LEU:HD11	2.02	0.42
1:A:580:ASP:HB3	1:B:62:ARG:HA	2.00	0.42
1:B:510:ASP:O	1:B:511:ARG:CB	2.68	0.42
1:B:641:TYR:HD2	1:B:648:TYR:CE2	2.38	0.42
1:B:721:SER:C	1:B:723:PHE:N	2.76	0.42
1:B:1199:SER:HB2	1:B:1205:VAL:HG23	2.02	0.42
1:A:580:ASP:HB3	1:B:62:ARG:H	1.85	0.41
1:C:1165:ILE:O	1:C:1166:ALA:HB2	2.20	0.41
3:G:134:PRO:HB3	3:G:222:VAL:HG22	2.02	0.41
1:A:1005:LEU:O	1:A:1009:GLN:HG2	2.20	0.41
1:B:678:ALA:HB1	1:B:682:ILE:HG12	2.02	0.41
1:B:737:ALA:HB1	1:C:940:ASP:HB3	2.02	0.41
1:C:266:PHE:HB3	1:C:278:MET:HG3	2.01	0.41
1:C:470:LYS:HB3	1:C:520:ALA:HA	2.01	0.41
1:C:608:LEU:HB3	1:C:609:TYR:H	1.77	0.41
2:D:79:GLN:H	2:D:82:ASP:HB2	1.84	0.41
3:I:199:SER:HA	3:I:202:THR:HG22	2.01	0.41
1:B:631:VAL:HB	1:B:641:TYR:HB3	2.01	0.41
1:C:428:ILE:HG21	1:C:433:ILE:HD13	2.01	0.41
1:C:780:LEU:HD23	1:C:782:ILE:HD11	2.02	0.41
1:A:715:LEU:HD22	1:B:936:PRO:HG2	2.02	0.41
1:A:901:ALA:O	1:A:902:ASP:C	2.63	0.41
1:B:394:PRO:HB2	1:B:398:ASN:O	2.20	0.41
1:B:625:VAL:HG23	1:C:332:TYR:CE1	2.56	0.41
1:C:631:VAL:HG13	1:C:639:VAL:HG13	2.02	0.41
2:D:111:ALA:H	2:D:140:TYR:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2:VAL:HG22	3:I:27:GLY:HA3	2.03	0.41
3:I:156:TYR:HB2	3:I:211:HIS:CD2	2.56	0.41
1:A:518:VAL:HG23	1:A:524:SER:HB2	2.02	0.41
1:A:604:VAL:O	1:A:605:GLU:HB2	2.20	0.41
1:B:208:HIS:HB2	1:B:298:HIS:NE2	2.36	0.41
1:B:373:SER:HB3	1:B:605:GLU:CD	2.45	0.41
1:B:728:LYS:HD3	1:B:728:LYS:HA	1.94	0.41
1:B:964:LEU:HD12	1:B:964:LEU:HA	1.93	0.41
1:C:524:SER:HB3	1:C:527:VAL:HB	2.03	0.41
2:D:149:LYS:HD2	2:D:152:ASN:HA	2.03	0.41
1:A:397:TYR:HB3	1:A:468:ASN:ND2	2.34	0.41
1:A:404:PHE:HB2	1:A:441:LEU:HB3	2.02	0.41
1:A:1184:TRP:HB2	1:A:1185:SER:H	1.68	0.41
1:B:337:ILE:HG12	1:B:354:PHE:CE1	2.55	0.41
1:B:1180:ILE:HG22	1:B:1185:SER:OG	2.20	0.41
1:C:355:ASP:HB2	1:C:665:LYS:HE3	2.03	0.41
1:C:422:ASP:HB2	1:C:481:LEU:HD23	2.01	0.41
1:A:344:LEU:HD22	1:A:663:TYR:HD1	1.86	0.41
1:A:676:SER:HA	1:B:906:MET:HA	2.03	0.41
1:A:1043:THR:HA	1:A:1048:SER:HB2	2.03	0.41
1:A:1044:PHE:CE1	1:A:1073:GLY:HA3	2.55	0.41
1:B:234:LEU:H	1:B:234:LEU:HG	1.72	0.41
1:B:360:VAL:HG22	1:B:662:ILE:HG23	2.02	0.41
1:B:715:LEU:HD13	1:B:736:CYS:HB2	2.02	0.41
1:B:894:LEU:HB2	1:B:1019:PHE:HE1	1.86	0.41
1:C:408:ASN:HB3	1:C:587:LYS:HB3	2.03	0.41
1:C:782:ILE:HG13	1:C:1172:PHE:HE1	1.86	0.41
1:B:927:GLN:HE21	1:B:933:LYS:HE2	1.85	0.41
1:C:112:PHE:CE1	1:C:115:GLY:HA2	2.55	0.41
1:C:1113:ARG:HA	1:C:1113:ARG:HD2	1.82	0.41
2:H:199:GLN:H	2:H:199:GLN:HG2	1.55	0.41
1:A:87:TYR:HB2	1:A:143:ILE:HD13	2.03	0.41
1:A:150:GLY:HA3	1:A:164:PHE:HD2	1.86	0.41
1:A:470:LYS:HE3	1:A:470:LYS:HB3	1.95	0.41
1:A:718:VAL:HG12	1:A:719:ASN:H	1.86	0.41
1:B:120:ILE:HG21	1:B:145:PRO:HD3	2.03	0.41
1:B:430:PRO:O	1:B:433:ILE:HG12	2.21	0.41
1:B:672:THR:H	1:B:719:ASN:HB2	1.86	0.41
1:C:284:LEU:HA	1:C:285:PRO:HD3	1.92	0.41
1:C:871:LEU:HD12	1:C:871:LEU:HA	1.92	0.41
1:C:909:TYR:O	1:C:912:CYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1174:LYS:HB3	1:C:1175:THR:H	1.63	0.41
2:D:125:LEU:HD12	2:D:183:LYS:HE3	2.03	0.41
3:E:128:LYS:HE3	3:E:155:ASP:HB3	2.02	0.41
1:A:180:LEU:HB2	1:A:245:ILE:HD11	2.03	0.41
1:A:989:VAL:O	1:A:992:GLU:HG2	2.21	0.41
1:B:898:VAL:HG13	1:B:1019:PHE:CE2	2.56	0.41
1:C:1179:ARG:HA	1:C:1179:ARG:HD2	1.44	0.41
2:H:2:ILE:HG21	2:H:29:ILE:HD11	2.03	0.41
2:H:86:TYR:O	2:H:101:GLY:HA2	2.21	0.41
1:A:493:LYS:HA	1:A:567:LEU:HD11	2.02	0.40
1:A:788:PHE:HB3	1:A:1141:TYR:HA	2.03	0.40
1:B:21:VAL:HG23	1:B:225:LEU:HD11	2.02	0.40
1:B:188:GLU:HG2	1:B:189:PRO:HD2	2.02	0.40
1:B:1165:ILE:O	1:B:1166:ALA:HB3	2.21	0.40
1:C:150:GLY:HA3	1:C:164:PHE:CG	2.56	0.40
1:C:1113:ARG:HD3	1:C:1120:GLY:O	2.21	0.40
1:C:1153:TYR:HB3	1:C:1205:VAL:H	1.86	0.40
3:E:14:PRO:HA	3:E:86:LEU:HB2	2.04	0.40
2:F:198:HIS:HB3	2:F:201:LEU:HB2	2.03	0.40
3:I:87:THR:H	3:I:90:ASP:HB2	1.87	0.40
1:A:154:GLY:O	1:A:163:ARG:HB3	2.20	0.40
1:A:496:LYS:HE2	1:A:496:LYS:HB3	1.92	0.40
1:A:664:ASP:HB3	1:A:669:THR:O	2.21	0.40
1:A:936:PRO:HA	1:A:937:PRO:HD3	1.85	0.40
1:B:411:LEU:HD12	1:B:411:LEU:HA	1.84	0.40
3:E:138:SER:H	3:E:141:SER:HB2	1.85	0.40
3:G:128:LYS:HE3	3:G:155:ASP:HB3	2.03	0.40
3:I:128:LYS:CE	3:I:155:ASP:HB3	2.51	0.40
1:A:368:ALA:HB3	1:A:654:CYS:SG	2.61	0.40
1:A:617:PHE:HB3	1:A:651:LEU:HG	2.02	0.40
1:A:964:LEU:HD13	1:A:964:LEU:HA	1.88	0.40
1:A:1110:GLN:HA	1:A:1122:HIS:CE1	2.56	0.40
1:B:371:SER:N	1:B:605:GLU:HB2	2.36	0.40
1:C:642:TYR:H	1:C:649:TYR:H	1.69	0.40
1:C:819:GLN:HA	1:C:822:ARG:HD3	2.02	0.40
2:D:29:ILE:HG23	2:D:92:TYR:HB2	2.04	0.40
2:D:133:VAL:HG22	2:D:178:THR:HG22	2.04	0.40
3:E:14:PRO:HG3	3:E:121:VAL:HB	2.03	0.40
1:A:213:ASP:O	1:A:219:TYR:HA	2.22	0.40
1:A:343:ASP:HA	1:A:694:ARG:NH2	2.36	0.40
1:A:1054:ILE:HG13	1:A:1055:ILE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:LYS:HB3	1:B:520:ALA:HA	2.03	0.40
1:C:253:TRP:HB3	1:C:278:MET:HE1	2.03	0.40
1:C:729:LEU:HA	1:C:730:PRO:HD3	1.95	0.40
2:H:118:PHE:HD1	3:I:141:SER:HA	1.87	0.40
1:A:1166:ALA:HB1	1:A:1169:ASN:HB2	2.02	0.40
1:A:1167:PRO:HA	1:A:1171:TYR:CE1	2.57	0.40
1:B:402:LEU:HD13	1:B:445:TYR:HE1	1.86	0.40
1:C:190:ARG:HG3	1:C:230:GLU:O	2.22	0.40
1:C:1121:THR:OG1	1:C:1141:TYR:HB3	2.21	0.40
2:D:150:VAL:HG22	2:D:192:TYR:HA	2.03	0.40
2:F:149:LYS:HG2	2:F:195:GLU:OE1	2.21	0.40
3:I:204:THR:HG23	3:I:221:ARG:HE	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	1117/1189 (94%)	1034 (93%)	72 (6%)	11 (1%)	12	38
1	B	1119/1189 (94%)	1042 (93%)	62 (6%)	15 (1%)	9	31
1	C	1122/1189 (94%)	1051 (94%)	60 (5%)	11 (1%)	12	38
2	D	210/212 (99%)	201 (96%)	8 (4%)	1 (0%)	24	55
2	F	210/212 (99%)	203 (97%)	5 (2%)	2 (1%)	12	38
2	H	210/212 (99%)	204 (97%)	4 (2%)	2 (1%)	12	38
3	E	220/222 (99%)	218 (99%)	1 (0%)	1 (0%)	24	55
3	G	220/222 (99%)	218 (99%)	1 (0%)	1 (0%)	24	55
3	I	220/222 (99%)	214 (97%)	3 (1%)	3 (1%)	9	30
All	All	4648/4869 (96%)	4385 (94%)	216 (5%)	47 (1%)	15	38

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	988	GLN
1	B	26	VAL
1	B	99	LYS
1	B	249	GLU
1	C	810	VAL
1	C	1176	ASN
2	D	30	THR
2	F	30	THR
2	H	30	THR
3	I	158	PRO
3	I	161	VAL
1	A	602	ASN
1	A	605	GLU
1	A	607	SER
1	A	791	THR
1	A	1059	ASP
1	A	1146	HIS
1	B	714	VAL
1	C	168	THR
1	C	372	GLY
1	A	382	GLU
1	A	785	ASN
1	B	382	GLU
1	B	792	GLN
1	C	929	VAL
1	A	1171	TYR
1	B	58	TYR
1	B	486	HIS
1	B	510	ASP
1	C	966	SER
1	C	1047	ILE
1	A	1119	GLN
1	B	43	THR
1	B	928	TYR
1	B	1166	ALA
1	B	1203	LYS
1	C	609	TYR
1	C	1166	ALA
1	C	1194	PRO
3	E	108	PRO
3	G	108	PRO
3	I	108	PRO

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Mol	Chain	Res	Type
1	B	742	PRO
1	B	738	LEU
1	C	714	VAL
2	F	8	PRO
2	H	8	PRO

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	A	975/1022 (95%)	888 (91%)	87 (9%)	9	29
1	B	979/1022 (96%)	877 (90%)	102 (10%)	7	22
1	C	978/1022 (96%)	889 (91%)	89 (9%)	9	28
2	D	180/186 (97%)	169 (94%)	11 (6%)	17	46
2	F	185/186 (100%)	168 (91%)	17 (9%)	8	27
2	H	186/186 (100%)	167 (90%)	19 (10%)	7	23
3	E	185/185 (100%)	170 (92%)	15 (8%)	11	33
3	G	185/185 (100%)	172 (93%)	13 (7%)	14	40
3	I	185/185 (100%)	164 (89%)	21 (11%)	5	19
All	All	4038/4179 (97%)	3664 (91%)	374 (9%)	11	27

All (374) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	26	VAL
1	A	62	ARG
1	A	63	THR
1	A	67	ILE
1	A	86	VAL
1	A	93	THR
1	A	99	LYS
1	A	140	ILE

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Mol	Chain	Res	Type
1	A	172	LEU
1	A	174	ASP
1	A	179	LEU
1	A	185	CYS
1	A	206	THR
1	A	208	HIS
1	A	214	CYS
1	A	234	LEU
1	A	237	CYS
1	A	263	VAL
1	A	333	ILE
1	A	337	ILE
1	A	363	VAL
1	A	366	PHE
1	A	367	GLU
1	A	389	LEU
1	A	401	ARG
1	A	402	LEU
1	A	405	THR
1	A	412	THR
1	A	427	GLN
1	A	428	ILE
1	A	436	ASN
1	A	452	MET
1	A	484	VAL
1	A	491	ILE
1	A	492	THR
1	A	514	VAL
1	A	517	LEU
1	A	522	GLN
1	A	523	TYR
1	A	529	ILE
1	A	554	LEU
1	A	575	VAL
1	A	599	GLN
1	A	600	LEU
1	A	617	PHE
1	A	620	CYS
1	A	623	VAL
1	A	625	VAL
1	A	629	ARG
1	A	642	TYR

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Mol	Chain	Res	Type
1	A	650	CYS
1	A	657	VAL
1	A	659	VAL
1	A	667	THR
1	A	693	THR
1	A	697	LEU
1	A	717	LEU
1	A	729	LEU
1	A	731	LEU
1	A	738	LEU
1	A	779	LYS
1	A	784	THR
1	A	795	ILE
1	A	854	LYS
1	A	893	LEU
1	A	961	THR
1	A	964	LEU
1	A	986	THR
1	A	987	GLN
1	A	1012	PHE
1	A	1013	THR
1	A	1015	THR
1	A	1022	VAL
1	A	1036	LEU
1	A	1040	LEU
1	A	1051	ILE
1	A	1056	GLN
1	A	1070	LEU
1	A	1117	CYS
1	A	1147	ILE
1	A	1163	ASN
1	A	1164	CYS
1	A	1168	VAL
1	A	1173	ILE
1	A	1180	ILE
1	A	1184	TRP
1	B	33	VAL
1	B	57	ILE
1	B	63	THR
1	B	72	GLN
1	B	100	LEU
1	B	101	PHE

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Mol	Chain	Res	Type
1	B	117	VAL
1	B	120	ILE
1	B	132	ILE
1	B	147	PHE
1	B	148	MET
1	B	169	LEU
1	B	180	LEU
1	B	186	ILE
1	B	201	TYR
1	B	225	LEU
1	B	228	PHE
1	B	234	LEU
1	B	251	LEU
1	B	263	VAL
1	B	279	PHE
1	B	284	LEU
1	B	287	TYR
1	B	296	ILE
1	B	308	LYS
1	B	315	VAL
1	B	319	GLN
1	B	333	ILE
1	B	342	ASN
1	B	344	LEU
1	B	357	GLU
1	B	363	VAL
1	B	388	LEU
1	B	396	VAL
1	B	402	LEU
1	B	408	ASN
1	B	412	THR
1	B	414	LEU
1	B	424	THR
1	B	425	CYS
1	B	442	ILE
1	B	484	VAL
1	B	488	LEU
1	B	489	THR
1	B	492	THR
1	B	495	LEU
1	B	512	THR
1	B	533	THR

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Mol	Chain	Res	Type
1	B	569	MET
1	B	579	THR
1	B	581	THR
1	B	600	LEU
1	B	617	PHE
1	B	631	VAL
1	B	637	ASN
1	B	638	LEU
1	B	641	TYR
1	B	642	TYR
1	B	651	LEU
1	B	659	VAL
1	B	666	GLU
1	B	667	THR
1	B	682	ILE
1	B	686	MET
1	B	696	MET
1	B	697	LEU
1	B	711	VAL
1	B	714	VAL
1	B	718	VAL
1	B	724	VAL
1	B	729	LEU
1	B	741	THR
1	B	782	ILE
1	B	795	ILE
1	B	799	ILE
1	B	802	VAL
1	B	803	THR
1	B	808	GLN
1	B	818	GLU
1	B	821	LEU
1	B	861	ILE
1	B	871	LEU
1	B	872	THR
1	B	986	THR
1	B	997	ILE
1	B	1022	VAL
1	B	1042	ASN
1	B	1047	ILE
1	B	1058	LEU
1	B	1067	ILE

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Mol	Chain	Res	Type
1	B	1094	LEU
1	B	1121	THR
1	B	1128	VAL
1	B	1129	ASN
1	B	1132	ASN
1	B	1155	LEU
1	B	1162	THR
1	B	1165	ILE
1	B	1171	TYR
1	B	1176	ASN
1	B	1180	ILE
1	B	1203	LYS
1	C	19	VAL
1	C	26	VAL
1	C	32	GLU
1	C	35	ILE
1	C	57	ILE
1	C	86	VAL
1	C	93	THR
1	C	120	ILE
1	C	131	ILE
1	C	132	ILE
1	C	172	LEU
1	C	180	LEU
1	C	185	CYS
1	C	208	HIS
1	C	237	CYS
1	C	290	ILE
1	C	322	THR
1	C	344	LEU
1	C	383	CYS
1	C	395	GLN
1	C	412	THR
1	C	415	LEU
1	C	441	LEU
1	C	450	LEU
1	C	456	LEU
1	C	458	VAL
1	C	488	LEU
1	C	491	ILE
1	C	512	THR
1	C	535	TRP

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Mol	Chain	Res	Type
1	C	561	VAL
1	C	564	THR
1	C	565	GLU
1	C	567	LEU
1	C	568	GLN
1	C	573	ILE
1	C	579	THR
1	C	584	VAL
1	C	588	LEU
1	C	611	VAL
1	C	616	VAL
1	C	620	CYS
1	C	625	VAL
1	C	642	TYR
1	C	655	VAL
1	C	659	VAL
1	C	664	ASP
1	C	711	VAL
1	C	714	VAL
1	C	715	LEU
1	C	718	VAL
1	C	759	LEU
1	C	780	LEU
1	C	793	GLU
1	C	810	VAL
1	C	812	ASN
1	C	818	GLU
1	C	826	GLN
1	C	831	ILE
1	C	853	VAL
1	C	854	LYS
1	C	857	GLN
1	C	865	PHE
1	C	887	ARG
1	C	898	VAL
1	C	927	GLN
1	C	933	LYS
1	C	951	LEU
1	C	961	THR
1	C	964	LEU
1	C	996	LEU
1	C	1012	PHE

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Mol	Chain	Res	Type
1	C	1033	LEU
1	C	1054	ILE
1	C	1061	LEU
1	C	1063	GLN
1	C	1086	LEU
1	C	1090	GLU
1	C	1121	THR
1	C	1128	VAL
1	C	1139	VAL
1	C	1150	VAL
1	C	1162	THR
1	C	1165	ILE
1	C	1174	LYS
1	C	1180	ILE
1	C	1181	VAL
1	C	1192	TYR
1	C	1197	ILE
2	D	3	VAL
2	D	6	GLN
2	D	27	GLU
2	D	29	ILE
2	D	48	ILE
2	D	75	ILE
2	D	125	LEU
2	D	129	THR
2	D	187	GLU
2	D	198	HIS
2	D	199	GLN
3	E	10	GLU
3	E	11	VAL
3	E	28	THR
3	E	31	ILE
3	E	37	VAL
3	E	46	GLU
3	E	81	MET
3	E	93	VAL
3	E	132	VAL
3	E	135	LEU
3	E	149	LEU
3	E	181	LEU
3	E	207	CYS
3	E	218	VAL

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Mol	Chain	Res	Type
3	E	221	ARG
2	F	3	VAL
2	F	11	LEU
2	F	27	GLU
2	F	29	ILE
2	F	48	ILE
2	F	72	THR
2	F	75	ILE
2	F	104	VAL
2	F	106	ILE
2	F	109	THR
2	F	125	LEU
2	F	129	THR
2	F	145	LYS
2	F	154	LEU
2	F	173	TYR
2	F	183	LYS
2	F	187	GLU
3	G	11	VAL
3	G	28	THR
3	G	31	ILE
3	G	37	VAL
3	G	51	ILE
3	G	81	MET
3	G	93	VAL
3	G	135	LEU
3	G	149	LEU
3	G	181	LEU
3	G	195	VAL
3	G	207	CYS
3	G	218	VAL
2	H	3	VAL
2	H	11	LEU
2	H	15	VAL
2	H	29	ILE
2	H	48	ILE
2	H	72	THR
2	H	75	ILE
2	H	104	VAL
2	H	106	ILE
2	H	109	THR
2	H	116	PHE

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Mol	Chain	Res	Type
2	H	125	LEU
2	H	129	THR
2	H	145	LYS
2	H	154	LEU
2	H	173	TYR
2	H	183	LYS
2	H	187	GLU
2	H	199	GLN
3	I	10	GLU
3	I	11	VAL
3	I	28	THR
3	I	31	ILE
3	I	37	VAL
3	I	46	GLU
3	I	81	MET
3	I	89	GLU
3	I	93	VAL
3	I	135	LEU
3	I	140	LYS
3	I	146	THR
3	I	149	LEU
3	I	158	PRO
3	I	161	VAL
3	I	181	LEU
3	I	189	LEU
3	I	195	VAL
3	I	207	CYS
3	I	218	VAL
3	I	221	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	91	HIS
1	A	166	ASN
1	A	167	HIS
1	A	408	ASN
1	A	436	ASN
1	A	468	ASN
1	A	501	ASN
1	A	670	HIS

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Mol	Chain	Res	Type
1	A	765	ASN
1	A	766	HIS
1	A	848	ASN
1	A	974	GLN
1	A	987	GLN
1	A	1020	GLN
1	A	1023	GLN
1	A	1056	GLN
1	A	1084	GLN
1	A	1085	GLN
1	A	1129	ASN
1	A	1146	HIS
1	A	1160	ASN
1	A	1169	ASN
1	B	66	ASN
1	B	98	GLN
1	B	111	GLN
1	B	166	ASN
1	B	220	ASN
1	B	280	GLN
1	B	410	ASN
1	B	486	HIS
1	B	576	GLN
1	B	627	GLN
1	B	688	GLN
1	B	719	ASN
1	B	765	ASN
1	B	769	GLN
1	B	792	GLN
1	B	832	ASN
1	B	994	GLN
1	B	1029	ASN
1	B	1042	ASN
1	B	1097	GLN
1	B	1110	GLN
1	B	1132	ASN
1	B	1145	ASN
1	B	1146	HIS
1	B	1201	ASN
1	C	81	HIS
1	C	111	GLN
1	C	194	HIS

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Mol	Chain	Res	Type
1	C	208	HIS
1	C	258	GLN
1	C	280	GLN
1	C	319	GLN
1	C	348	HIS
1	C	408	ASN
1	C	421	ASN
1	C	436	ASN
1	C	466	GLN
1	C	475	ASN
1	C	501	ASN
1	C	576	GLN
1	C	582	ASN
1	C	670	HIS
1	C	681	HIS
1	C	733	GLN
1	C	769	GLN
1	C	792	GLN
1	C	808	GLN
1	C	832	ASN
1	C	836	HIS
1	C	857	GLN
1	C	927	GLN
1	C	987	GLN
1	C	1027	ASN
1	C	1056	GLN
1	C	1119	GLN
1	C	1122	HIS
1	C	1145	ASN
1	C	1160	ASN
1	C	1201	ASN
2	D	79	GLN
2	D	147	GLN
3	E	99	GLN
3	E	107	ASN
3	E	182	GLN
2	F	37	GLN
2	F	79	GLN
2	F	138	ASN
2	F	147	GLN
2	F	198	HIS
2	F	199	GLN

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Mol	Chain	Res	Type
3	G	107	ASN
3	G	182	GLN
2	H	34	ASN
2	H	79	GLN
2	H	138	ASN
2	H	147	GLN
2	H	198	HIS
2	H	199	GLN
3	I	107	ASN
3	I	175	HIS
3	I	182	GLN
3	I	210	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

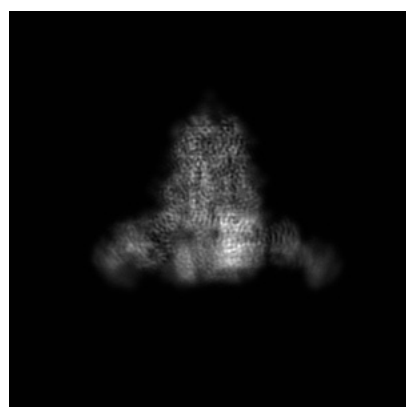
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31725. These allow visual inspection of the internal detail of the map and identification of artifacts.

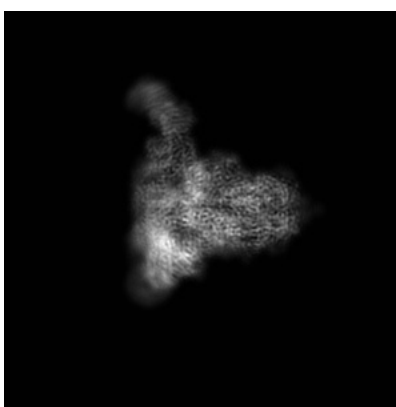
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

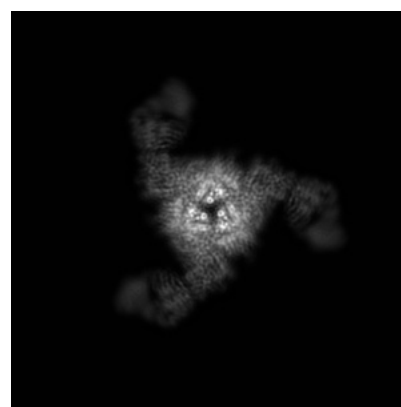
6.1.1 Primary map



X



Y

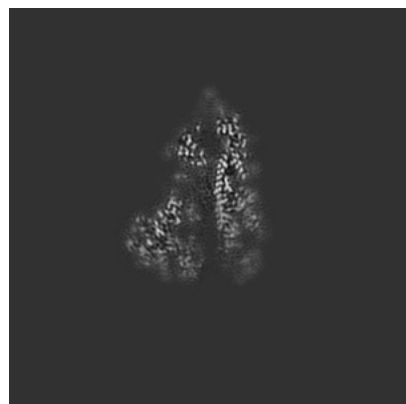


Z

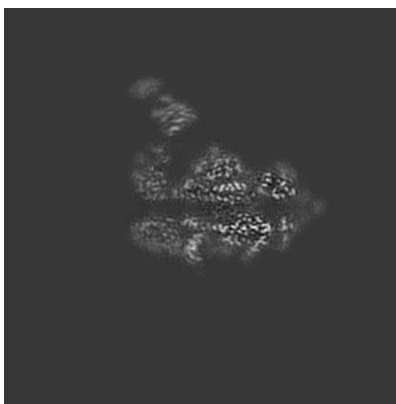
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

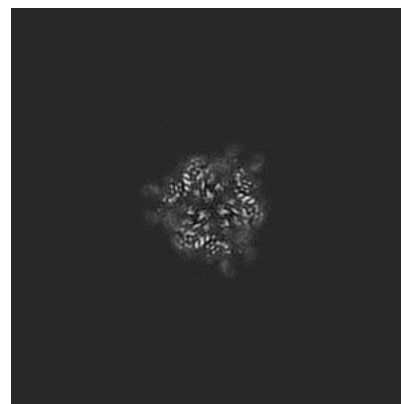
6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

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

6.3 Largest variance slices [i](#)

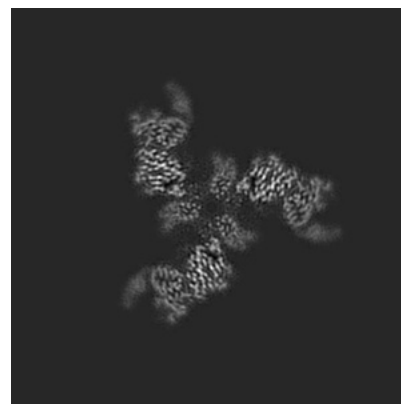
6.3.1 Primary map



X Index: 153



Y Index: 173

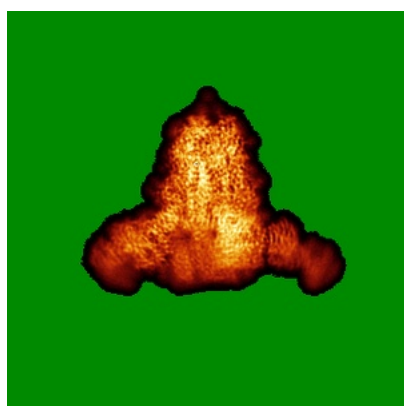


Z Index: 132

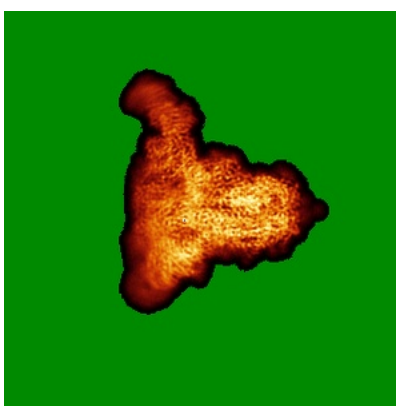
The images above show the largest variance slices of the map in three orthogonal directions.

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

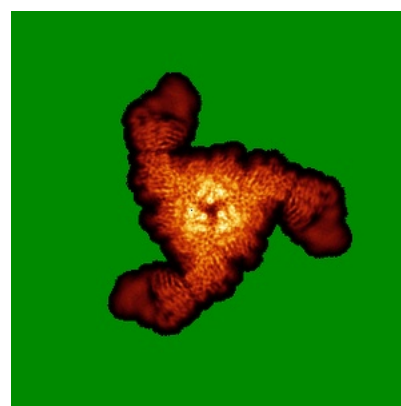
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

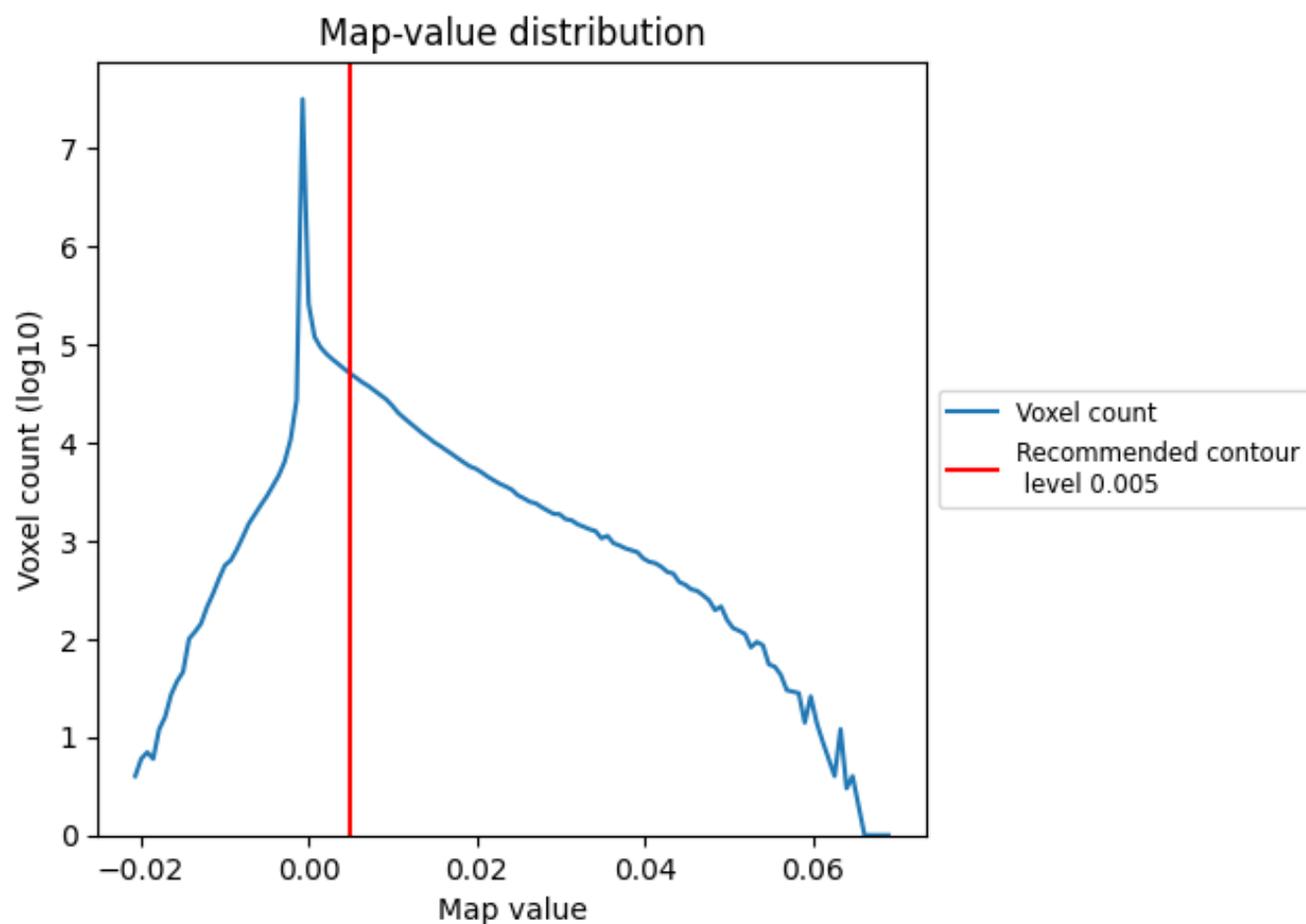
6.6 Mask visualisation

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

7 Map analysis [i](#)

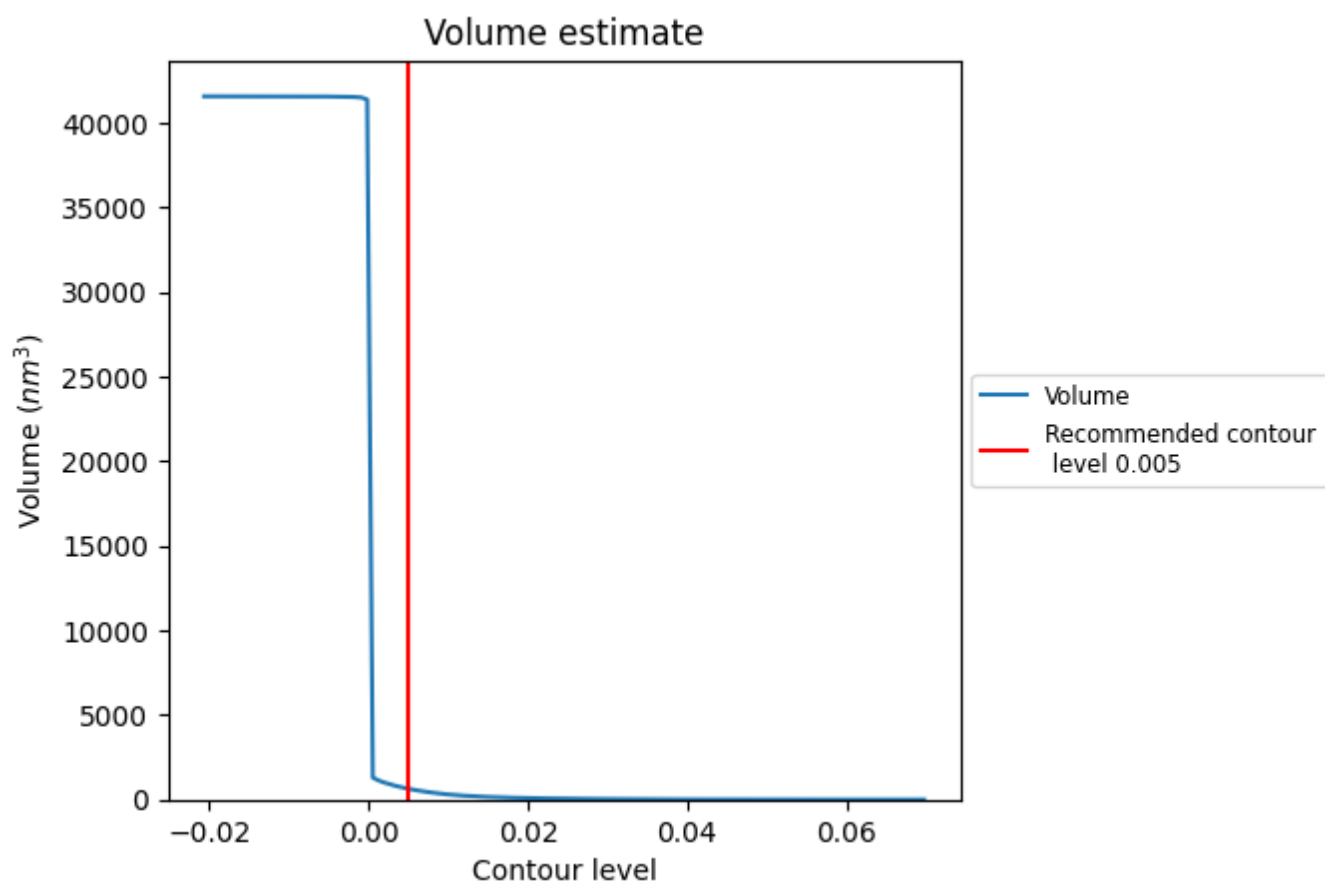
This section contains the results of statistical analysis of the map.

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.

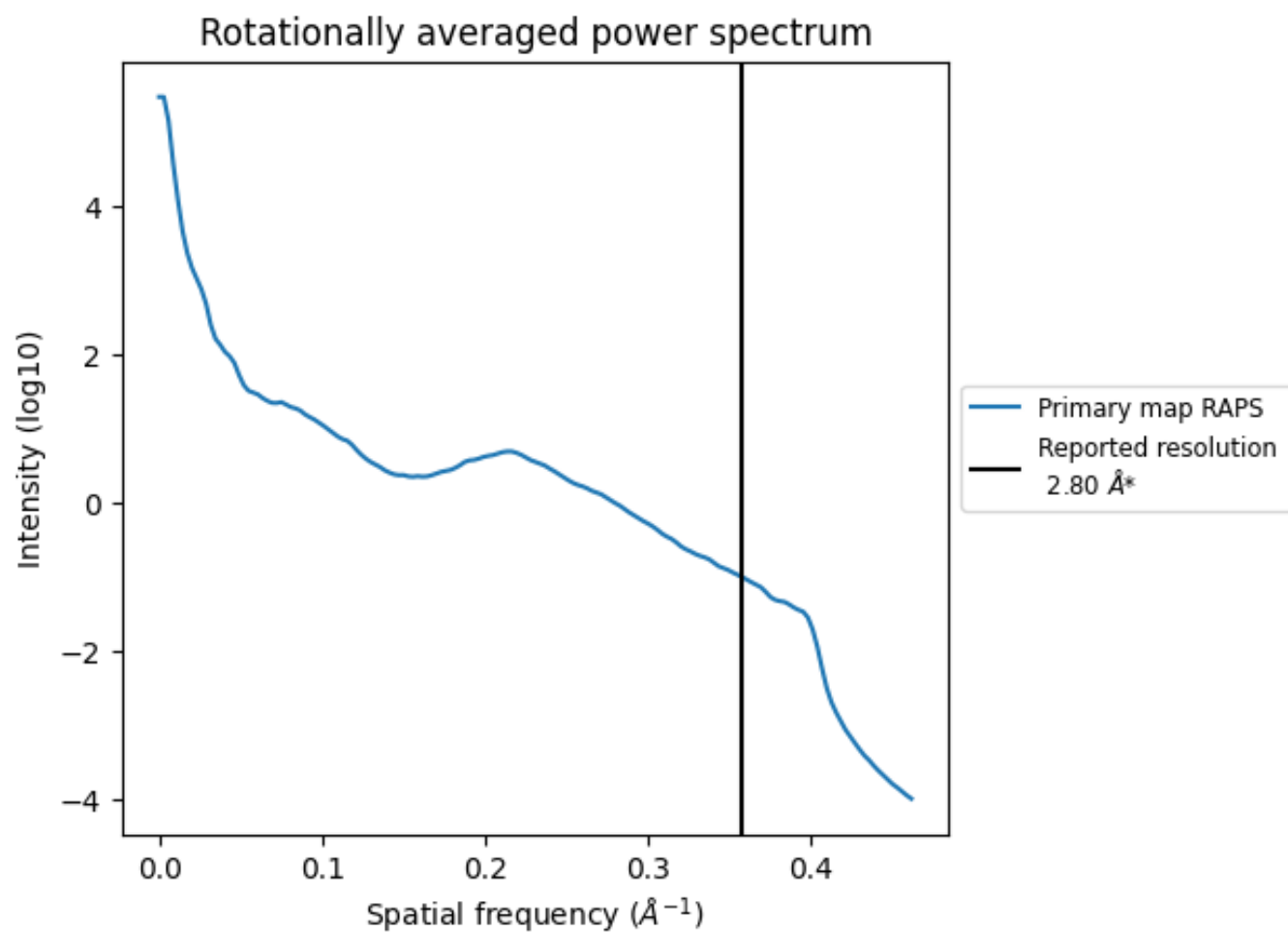
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 641 nm^3 ; this corresponds to an approximate mass of 579 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

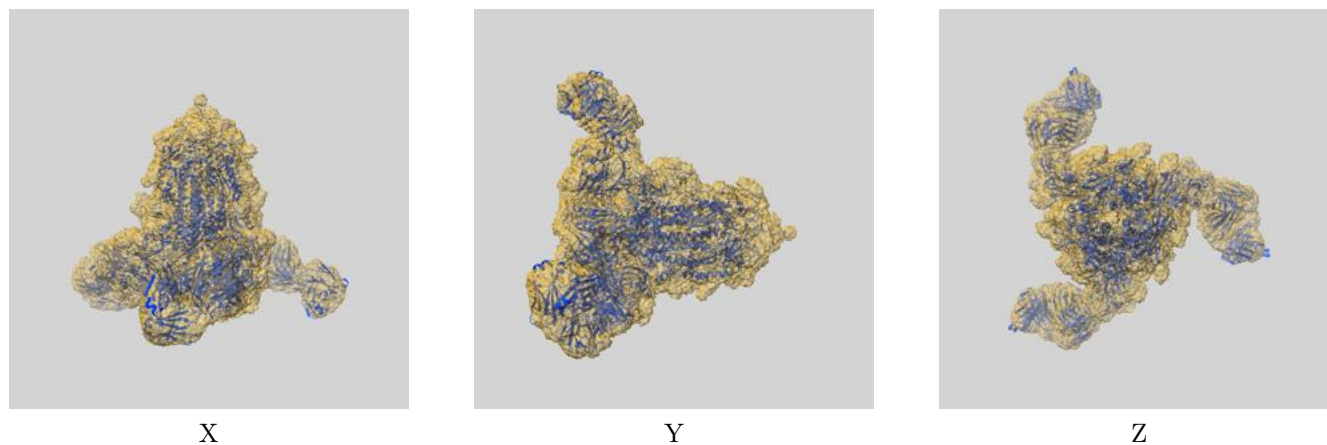
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

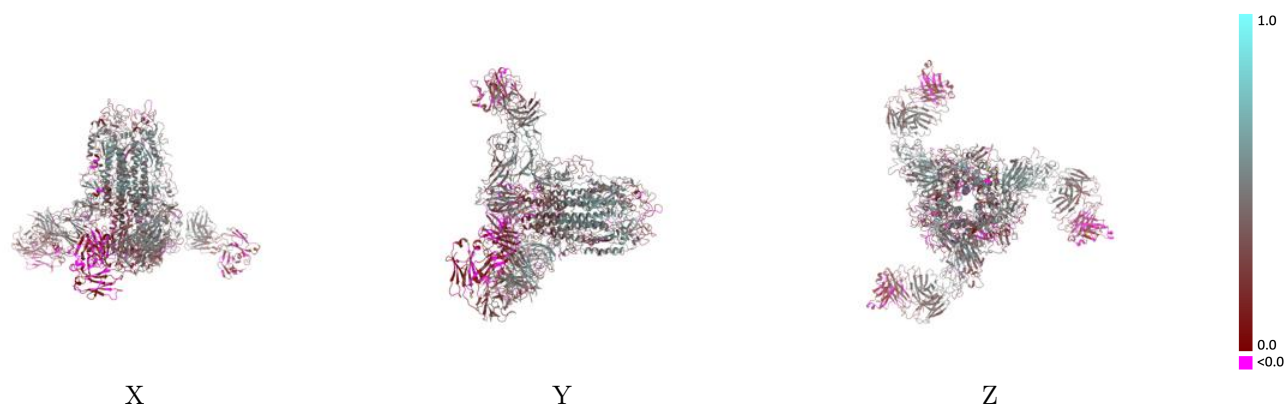
This section contains information regarding the fit between EMDB map EMD-31725 and PDB model 7V5J. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



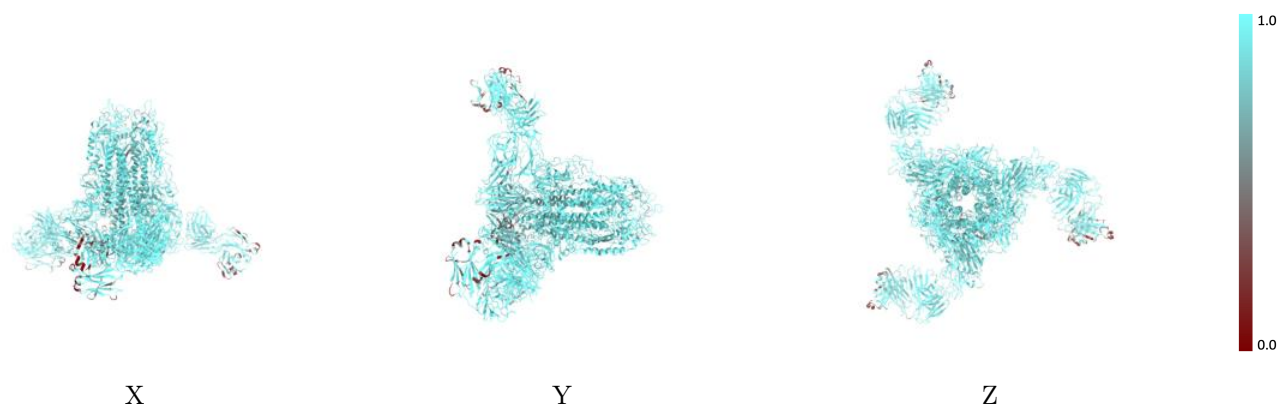
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



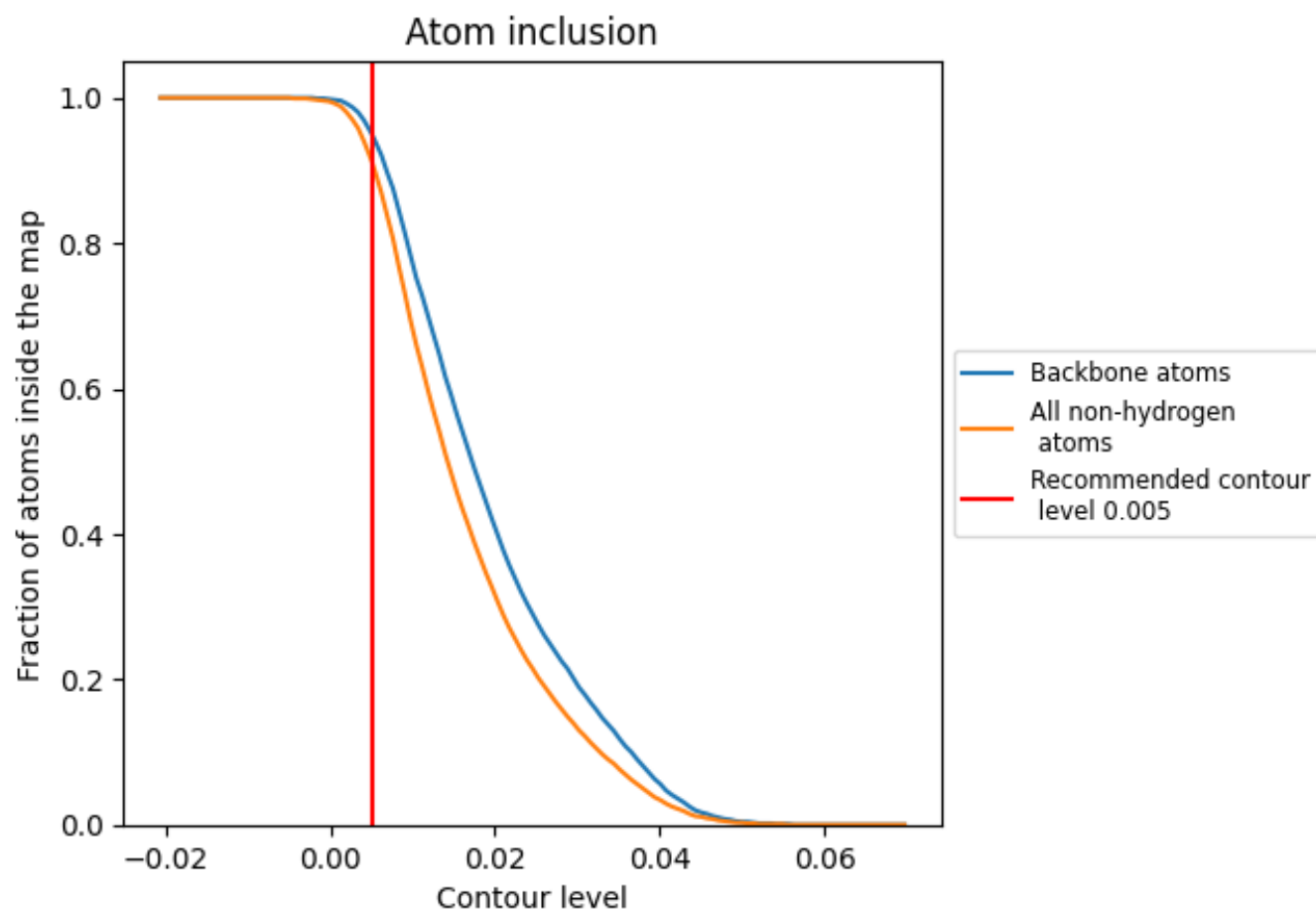
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9140	0.3170
A	0.9160	0.3440
B	0.9080	0.3040
C	0.9390	0.3830
D	0.8920	0.2160
E	0.8670	0.2470
F	0.8810	0.2200
G	0.9130	0.2880
H	0.9090	0.2260
I	0.9000	0.2760

1.0

0.0

<0.0