



# Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 06:21 AM JST

PDB ID : 7V6N  
EMDB ID : EMD-31743  
Title : MERS S ectodomain trimer in complex with neutralizing antibody 111 state1  
Authors : Wang, X.; Zhao, J.; Wang, Z.; Zeng, J.; Zhang, S.; Wang, Y.  
Deposited on : 2021-08-20  
Resolution : 3.99 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

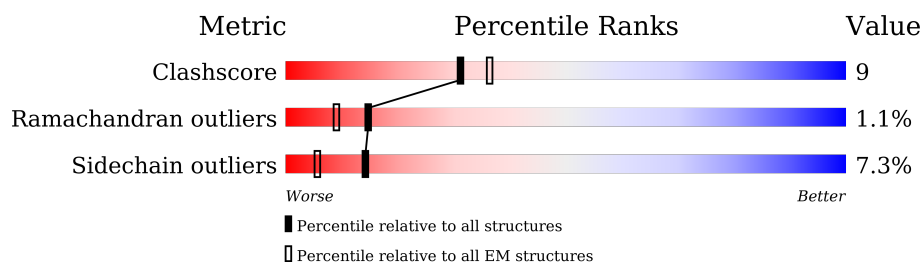
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.99 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 73% 20% • 5%
1	B	1189	 71% 20% • 7%
1	C	1189	 73% 18% • 8%
2	D	216	 28% 83% 15% •
2	F	216	 25% 75% 23% •
2	H	216	 30% 78% 20% •
3	E	227	 16% 77% 21% •
3	G	227	 18% 81% 17% •

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Mol	Chain	Length	Quality of chain
3	I	227	<div><div></div><div>14%</div><div>78%</div><div>21%</div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34448 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	1135	Total	C	N	O	S	0	0
			8343	5254	1399	1643	47		
1	B	1102	Total	C	N	O	S	1	0
			8184	5184	1364	1591	45		
1	C	1097	Total	C	N	O	S	1	0
			8029	5066	1338	1576	49		

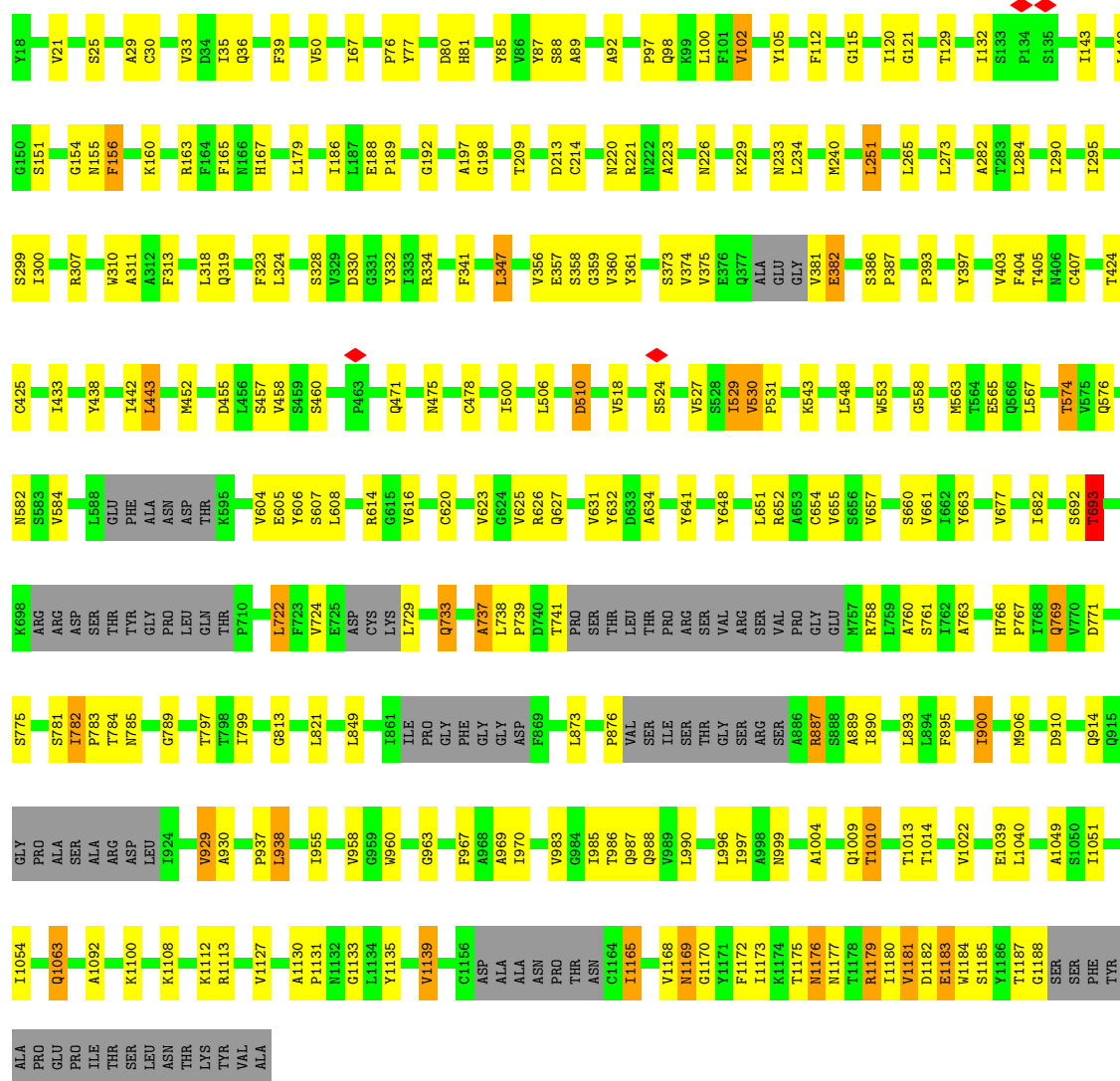
- Molecule 2 is a protein called 111 L.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	216	Total	C	N	O	S	0	0
			1623	1014	274	327	8		
2	F	216	Total	C	N	O	S	0	0
			1637	1019	275	335	8		
2	H	216	Total	C	N	O	S	0	0
			1622	1008	274	332	8		

- Molecule 3 is a protein called 111 H.

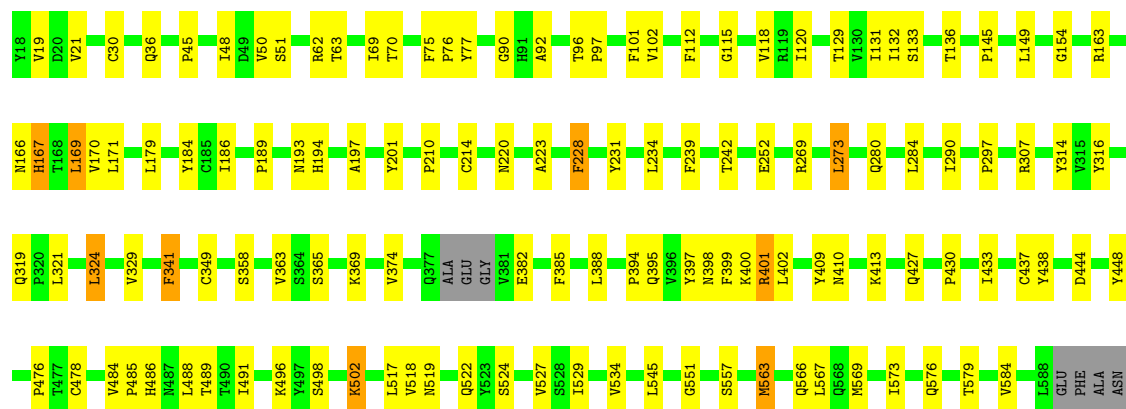
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	227	Total	C	N	O	S	0	0
			1658	1042	278	332	6		
3	G	227	Total	C	N	O	S	0	0
			1700	1077	283	334	6		
3	I	227	Total	C	N	O	S	0	0
			1652	1036	282	328	6		

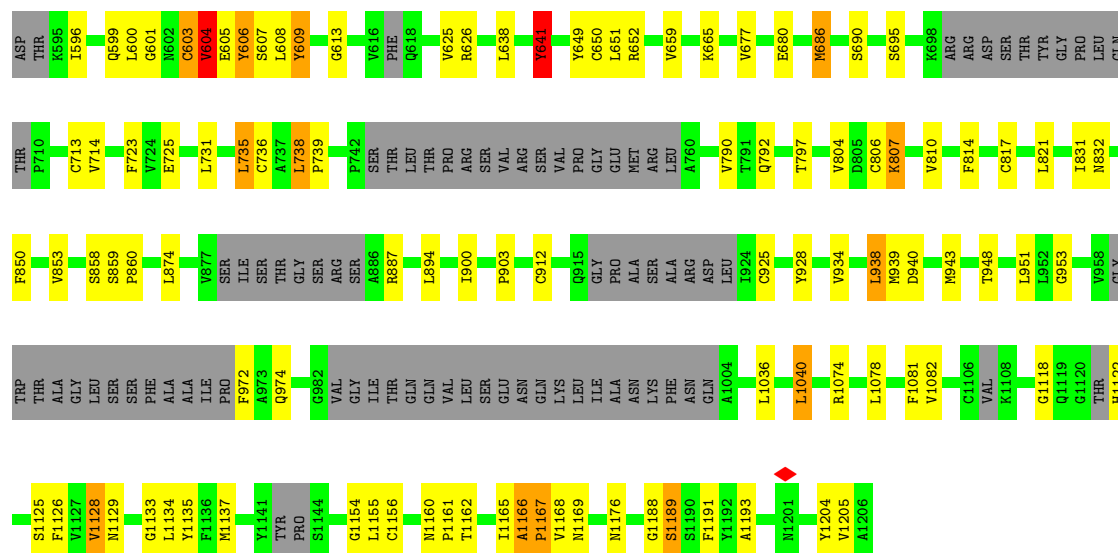




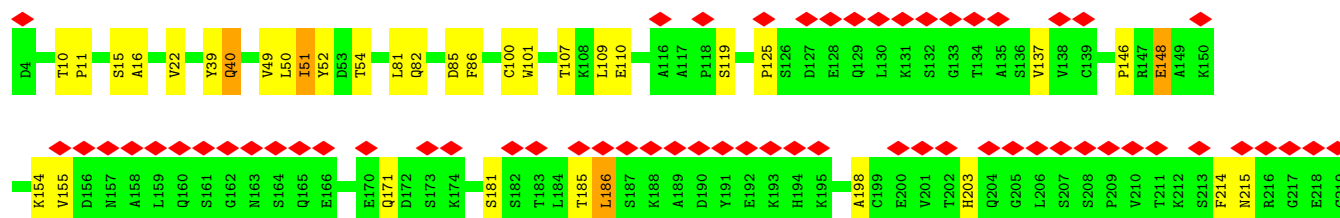
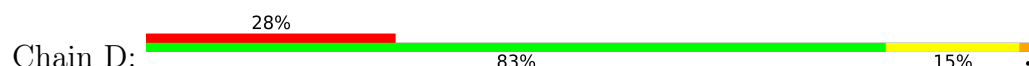
• Molecule 1: Spike glycoprotein

Chain C: 73% 18% 8%

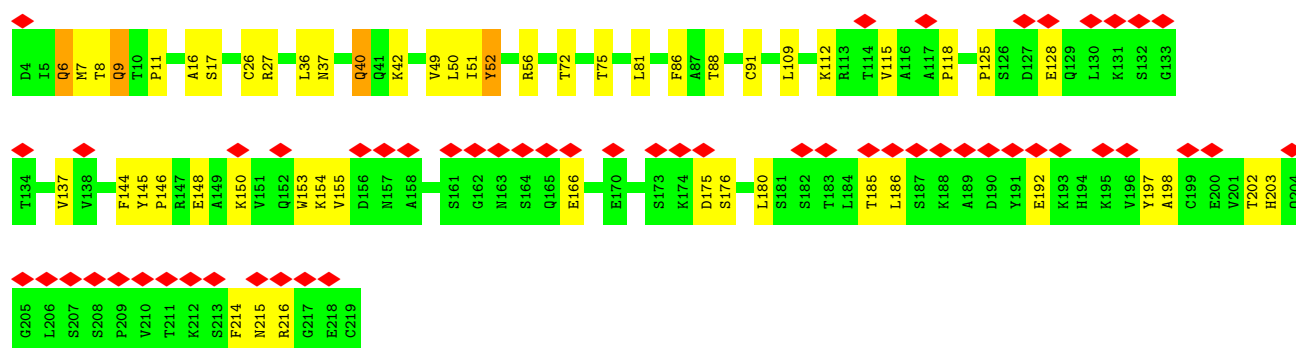
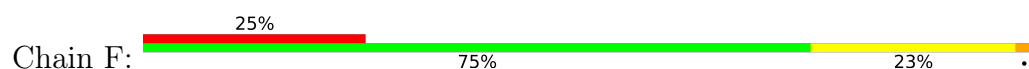




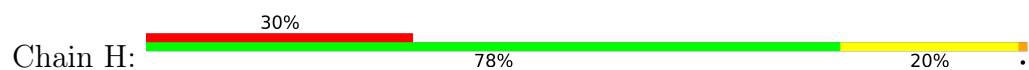
• Molecule 2: 111 L

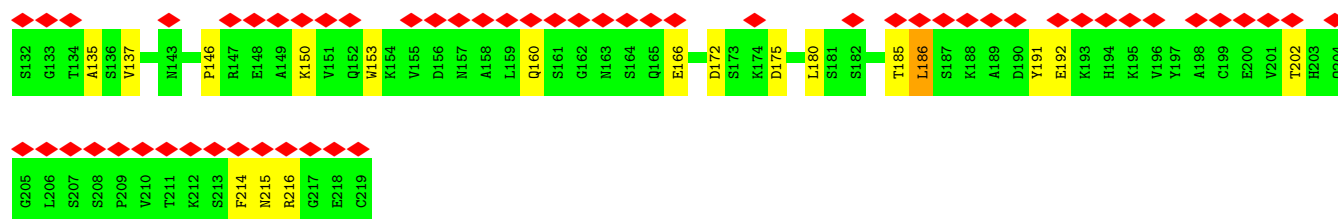


• Molecule 2: 111 L

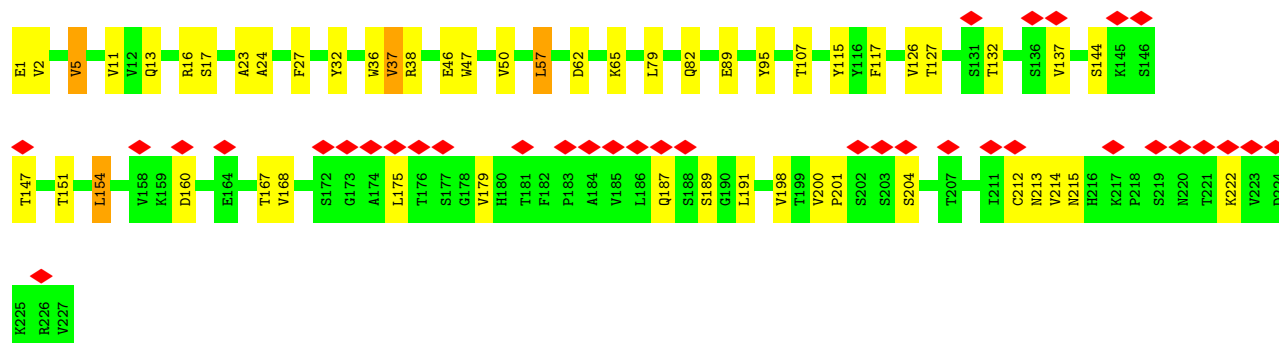
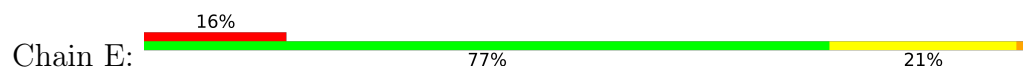


• Molecule 2: 111 L

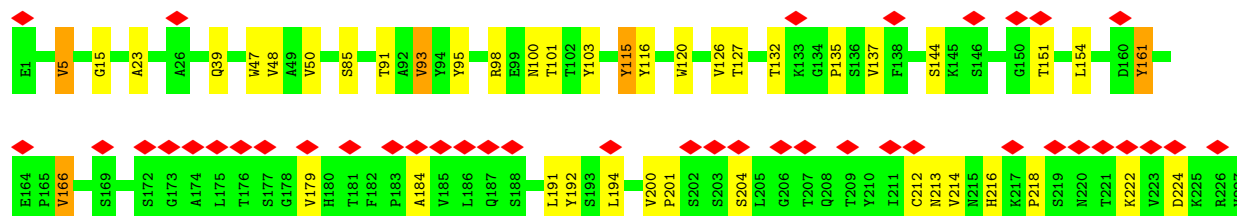
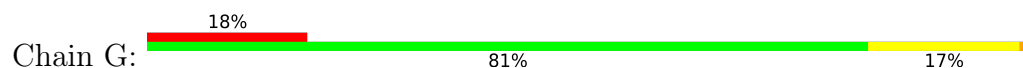




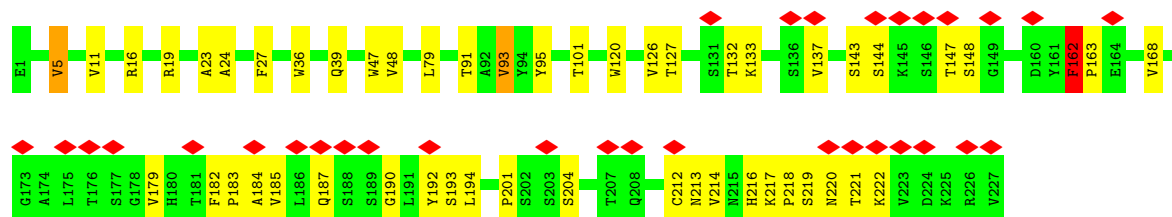
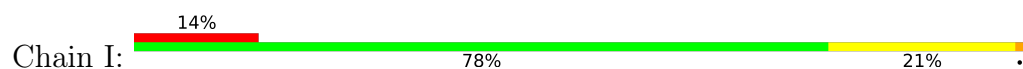
• Molecule 3: 111 H



• Molecule 3: 111 H



• Molecule 3: 111 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	0.061	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size ( $\text{\AA}$ )	351.328, 351.328, 351.328	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0979, 1.0979, 1.0979	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.66	0/8508	0.66	0/11597
1	B	0.66	0/8350	0.66	1/11378 (0.0%)
1	C	0.66	0/8184	0.66	0/11155
2	D	0.64	0/1656	0.63	0/2252
2	F	0.64	0/1670	0.63	0/2270
2	H	0.64	0/1654	0.64	0/2251
3	E	0.66	0/1698	0.63	0/2321
3	G	0.65	0/1746	0.63	0/2383
3	I	0.66	0/1691	0.64	0/2307
All	All	0.66	0/35157	0.65	1/47914 (0.0%)

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	B	0	2
1	C	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	930	ALA	N-CA-C	-5.38	96.48	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	50	VAL	Mainchain

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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	8343	0	7804	149	0
1	B	8184	0	7710	156	0
1	C	8029	0	7450	119	0
2	D	1623	0	1558	20	0
2	F	1637	0	1570	29	0
2	H	1622	0	1545	33	0
3	E	1658	0	1557	24	0
3	G	1700	0	1609	21	0
3	I	1652	0	1551	48	0
All	All	34448	0	32354	571	0

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

All (571) 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)
1:B:330:ASP:CG	1:B:334:ARG:HH22	1.08	1.54
3:I:216:HIS:CE1	3:I:218:PRO:CG	2.17	1.28
1:B:330:ASP:CG	1:B:334:ARG:NH2	1.91	1.23
1:A:36:GLN:HB3	1:A:39:PHE:CD1	1.77	1.17
1:B:359:GLY:O	1:B:361:TYR:CE2	1.97	1.16
1:B:330:ASP:OD2	1:B:334:ARG:NH2	1.79	1.14
3:I:216:HIS:CE1	3:I:218:PRO:HG2	1.80	1.11
2:F:112:LYS:HA	2:F:145:TYR:OH	1.51	1.10
3:I:216:HIS:HE1	3:I:218:PRO:CB	1.67	1.06
3:I:216:HIS:HE1	3:I:218:PRO:HB2	1.16	1.04
3:I:216:HIS:CE1	3:I:218:PRO:CD	2.39	1.04
3:I:216:HIS:CE1	3:I:218:PRO:HB2	1.91	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ASP:OD2	1:B:332:TYR:HD2	1.41	1.03
3:I:216:HIS:CE1	3:I:218:PRO:CB	2.39	1.03
3:I:216:HIS:CE1	3:I:218:PRO:HD2	1.93	1.03
1:B:328:SER:HB2	1:B:334:ARG:CZ	1.88	1.02
2:F:112:LYS:HA	2:F:145:TYR:HH	1.27	0.99
3:I:216:HIS:ND1	3:I:218:PRO:HD2	1.78	0.98
1:A:36:GLN:HB3	1:A:39:PHE:HD1	1.19	0.97
1:B:359:GLY:O	1:B:361:TYR:CD2	2.18	0.97
1:B:328:SER:CB	1:B:334:ARG:CZ	2.45	0.95
1:A:119:ARG:HG3	1:A:314:TYR:HD1	1.42	0.84
2:H:95:CYS:HB3	2:H:98:LEU:CG	2.08	0.84
1:A:898:VAL:HG21	1:A:1131:PRO:HG3	1.59	0.83
3:I:184:ALA:HB1	3:I:192:TYR:HB3	1.60	0.82
1:B:737:ALA:H	1:C:938:LEU:HA	1.45	0.81
1:B:29:ALA:HB2	1:B:192:GLY:HA3	1.64	0.80
1:B:330:ASP:OD2	1:B:332:TYR:CD2	2.31	0.80
2:H:95:CYS:HB3	2:H:98:LEU:HG	1.63	0.80
1:B:332:TYR:HB2	1:B:334:ARG:NH1	1.98	0.78
2:H:99:ARG:NE	2:H:99:ARG:HA	1.99	0.78
1:C:189:PRO:HB2	1:C:197:ALA:HB2	1.67	0.77
1:C:518:VAL:HG12	1:C:524:SER:HB2	1.67	0.77
1:A:1130:ALA:HB2	1:A:1135:TYR:HB2	1.65	0.77
2:H:99:ARG:HA	2:H:99:ARG:HE	1.49	0.77
2:F:17:SER:HB3	2:F:112:LYS:HB2	1.67	0.76
1:B:330:ASP:OD1	1:B:334:ARG:NH2	2.19	0.75
1:C:220:ASN:HB3	1:C:223:ALA:HB2	1.67	0.75
1:B:220:ASN:HB3	1:B:223:ALA:HB2	1.69	0.75
1:C:269:ARG:HA	1:C:273:LEU:HB3	1.69	0.75
2:H:95:CYS:SG	2:H:97:THR:OG1	2.37	0.75
3:G:184:ALA:HB1	3:G:192:TYR:HB3	1.68	0.74
1:B:332:TYR:HB2	1:B:334:ARG:HH12	1.50	0.74
1:C:545:LEU:O	1:C:551:GLY:HA2	1.88	0.74
1:B:330:ASP:CG	1:B:332:TYR:HD2	1.91	0.74
1:B:330:ASP:CG	1:B:332:TYR:CD2	2.61	0.73
3:I:216:HIS:CG	3:I:218:PRO:HD2	2.23	0.73
1:C:167:HIS:H	1:C:186:ILE:HA	1.53	0.73
1:C:193:ASN:HD22	3:I:101:THR:HB	1.54	0.72
1:B:1177:ASN:HA	1:B:1188:GLY:HA3	1.72	0.71
1:B:328:SER:CB	1:B:334:ARG:NE	2.53	0.71
1:B:330:ASP:OD2	1:B:334:ARG:CZ	2.38	0.71
1:C:70:THR:HA	1:C:324:LEU:HA	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:216:HIS:HB3	3:I:219:SER:OG	1.91	0.71
1:C:77:TYR:HB3	1:C:319:GLN:HE22	1.57	0.69
1:B:524:SER:HB3	1:B:527:VAL:HG23	1.75	0.69
1:A:210:PRO:HA	1:A:214:CYS:HB2	1.73	0.69
1:A:524:SER:HB3	1:A:527:VAL:HG23	1.74	0.69
1:B:729:LEU:N	1:B:761:SER:HG	1.91	0.69
3:I:163:PRO:HB2	3:I:216:HIS:HE2	1.58	0.69
1:A:741:THR:HG23	1:A:759:LEU:HB3	1.75	0.68
1:A:43:THR:N	1:A:44:TRP:CZ3	2.53	0.67
1:C:437:CYS:HB2	1:C:609:TYR:HA	1.76	0.67
3:I:216:HIS:NE2	3:I:218:PRO:HG2	2.10	0.66
1:C:797:THR:HB	1:C:1133:GLY:HA2	1.77	0.66
3:I:219:SER:O	3:I:221:THR:N	2.28	0.66
1:C:738:LEU:H	1:C:739:PRO:CD	2.06	0.66
2:F:16:ALA:HB1	2:F:81:LEU:HD13	1.77	0.66
1:A:522:GLN:HA	1:A:522:GLN:NE2	2.11	0.65
2:H:95:CYS:HB3	2:H:98:LEU:CD1	2.26	0.65
1:A:990:LEU:HD21	1:A:1184:TRP:HB2	1.78	0.65
1:C:120:ILE:HB	1:C:252:GLU:HG3	1.79	0.65
2:F:52:TYR:HB2	2:F:56:ARG:HE	1.62	0.65
1:C:1036:LEU:HD13	1:C:1081:PHE:HD1	1.61	0.64
1:B:77:TYR:HB3	1:B:80:ASP:HB2	1.79	0.64
2:H:99:ARG:HE	2:H:99:ARG:CA	2.11	0.64
1:B:1177:ASN:HA	1:B:1188:GLY:CA	2.27	0.64
2:H:16:ALA:HB1	2:H:81:LEU:HD13	1.79	0.64
3:I:219:SER:C	3:I:221:THR:N	2.52	0.63
1:A:522:GLN:HA	1:A:522:GLN:HE21	1.63	0.63
1:C:48:ILE:HD13	1:C:76:PRO:HB2	1.79	0.63
1:B:775:SER:HA	1:C:972:PHE:HE2	1.64	0.63
1:C:166:ASN:HB2	1:C:186:ILE:HG23	1.79	0.63
1:A:1171:TYR:HB3	1:A:1177:ASN:H	1.63	0.62
1:B:625:VAL:HG23	1:B:627:GLN:H	1.63	0.62
3:I:36:TRP:HE1	3:I:79:LEU:HD22	1.64	0.62
1:B:330:ASP:CG	1:B:334:ARG:CZ	2.67	0.62
1:B:330:ASP:OD1	1:B:334:ARG:NH1	2.32	0.62
2:H:52:TYR:HB2	2:H:56:ARG:HE	1.65	0.62
2:H:95:CYS:HB3	2:H:98:LEU:HD12	1.80	0.62
3:I:219:SER:C	3:I:221:THR:H	2.03	0.61
1:B:92:ALA:HB1	1:B:97:PRO:HA	1.82	0.61
1:C:524:SER:HB3	1:C:527:VAL:HG23	1.83	0.61
1:A:506:LEU:HB3	1:A:553:TRP:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLN:HB3	1:A:39:PHE:CE1	2.36	0.60
1:A:629:ARG:HB3	1:A:643:SER:HA	1.83	0.60
3:I:216:HIS:ND1	3:I:218:PRO:CD	2.53	0.60
1:A:42:LYS:C	1:A:44:TRP:CE3	2.59	0.60
1:B:1180:ILE:HG22	1:B:1182:ASP:H	1.67	0.60
2:F:49:VAL:HG13	3:G:120:TRP:HZ2	1.66	0.60
1:B:458:VAL:HA	1:B:471:GLN:HB3	1.84	0.60
1:A:43:THR:N	1:A:44:TRP:CE3	2.69	0.59
1:A:929:VAL:HG13	1:A:931:GLY:H	1.67	0.59
1:A:395:GLN:HG2	1:A:498:SER:HB2	1.83	0.59
3:E:160:ASP:HA	3:E:191:LEU:HB3	1.84	0.59
1:A:783:PRO:HB3	1:A:1143:PRO:HB3	1.85	0.59
1:B:330:ASP:OD1	1:B:334:ARG:CZ	2.51	0.59
1:B:425:CYS:HA	1:B:478:CYS:HA	1.84	0.59
3:I:133:LYS:H	3:I:162:PHE:HB3	1.66	0.59
1:B:733:GLN:HG2	1:B:741:THR:HG23	1.85	0.59
1:C:738:LEU:H	1:C:739:PRO:HD3	1.66	0.59
1:A:631:VAL:H	1:A:640:GLY:HA2	1.69	0.58
1:A:983:VAL:HG21	1:A:1123:ILE:HG12	1.84	0.58
2:F:56:ARG:HD2	3:G:115:TYR:HD1	1.68	0.58
2:F:154:LYS:HB2	2:F:198:ALA:HB3	1.85	0.58
1:A:962:ALA:HA	1:C:1168:VAL:HA	1.86	0.58
1:B:92:ALA:H	1:B:307:ARG:HH11	1.49	0.58
2:H:125:PRO:HD3	2:H:137:VAL:HG22	1.86	0.58
1:B:1130:ALA:HB2	1:B:1135:TYR:HB2	1.86	0.58
3:E:154:LEU:HD23	3:E:200:VAL:HG21	1.86	0.58
1:A:61:GLY:HA2	1:C:579:THR:HA	1.85	0.58
3:I:187:GLN:HG3	3:I:190:GLY:H	1.69	0.57
3:G:166:VAL:HG22	3:G:216:HIS:CD2	2.39	0.57
3:I:213:ASN:HB3	3:I:222:LYS:HE2	1.84	0.57
1:A:963:GLY:H	1:C:1168:VAL:HG22	1.68	0.57
1:B:634:ALA:HB2	1:C:69:ILE:HG21	1.85	0.57
2:H:40:GLN:HB2	2:H:50:LEU:HD11	1.87	0.57
3:I:201:PRO:HG2	3:I:204:SER:HB2	1.87	0.57
1:B:506:LEU:HB3	1:B:553:TRP:HB3	1.87	0.57
2:H:192:GLU:HA	2:H:216:ARG:HH12	1.68	0.57
1:C:149:LEU:HB3	1:C:290:ILE:HG21	1.87	0.57
1:C:314:TYR:HB3	1:C:316:TYR:CZ	2.40	0.57
1:C:369:LYS:HE3	1:C:690:SER:HA	1.85	0.57
2:D:39:TYR:CE1	2:D:49:VAL:HG12	2.40	0.56
1:B:605:GLU:HA	1:B:614:ARG:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:VAL:HG22	2:D:81:LEU:HD11	1.87	0.56
3:E:115:TYR:HB2	3:E:117:PHE:CE2	2.40	0.56
3:E:201:PRO:HG2	3:E:204:SER:HB2	1.86	0.56
1:A:85:TYR:O	1:A:312:ALA:HB1	2.05	0.56
1:B:328:SER:HB2	1:B:334:ARG:NH1	2.20	0.56
1:B:876:PRO:HD3	1:B:889:ALA:HB2	1.86	0.56
1:B:1172:PHE:CZ	1:B:1181:VAL:HG13	2.41	0.56
1:B:500:ILE:HA	1:B:558:GLY:HA2	1.87	0.56
1:A:1173:ILE:H	1:A:1177:ASN:HB2	1.70	0.56
1:B:657:VAL:HG13	1:B:677:VAL:HG21	1.86	0.56
1:A:84:MET:HA	1:A:314:TYR:HD2	1.71	0.56
3:E:175:LEU:HB3	3:E:198:VAL:HG21	1.87	0.56
3:G:39:GLN:HB3	3:G:93:VAL:HG13	1.88	0.56
2:H:82:GLN:H	2:H:85:ASP:HB2	1.71	0.55
3:E:187:GLN:HE21	3:E:189:SER:HB3	1.72	0.55
2:H:99:ARG:NE	2:H:99:ARG:CA	2.69	0.55
1:C:374:VAL:H	1:C:606:TYR:HA	1.72	0.55
3:E:36:TRP:HE1	3:E:79:LEU:HD22	1.71	0.55
1:B:33:VAL:HG22	1:B:100:LEU:HD12	1.89	0.55
2:D:214:PHE:HD2	2:D:215:ASN:O	1.90	0.55
3:I:5:VAL:HG13	3:I:23:ALA:HB3	1.89	0.55
1:C:170:VAL:HG11	1:C:228:PHE:HE2	1.71	0.55
3:E:144:SER:HB2	3:E:147:THR:HG23	1.88	0.55
2:H:214:PHE:HD2	2:H:215:ASN:O	1.90	0.55
1:B:625:VAL:HG22	1:C:63:THR:HG22	1.89	0.55
2:F:214:PHE:HD2	2:F:215:ASN:O	1.90	0.55
1:B:1165:ILE:HD12	1:B:1170:GLY:H	1.72	0.54
3:I:91:THR:HG23	3:I:127:THR:HA	1.88	0.54
1:A:831:ILE:HG23	1:A:1082:VAL:HG21	1.89	0.54
1:A:936:PRO:HD2	1:C:736:CYS:HB3	1.89	0.54
1:A:1036:LEU:HD13	1:A:1081:PHE:HD1	1.72	0.54
1:A:1172:PHE:HD2	1:A:1179:ARG:HG3	1.73	0.54
1:C:925:CYS:HB3	1:C:928:TYR:HB2	1.88	0.54
1:B:729:LEU:HA	1:B:763:ALA:HB3	1.88	0.54
1:C:1128:VAL:HG23	1:C:1135:TYR:HB3	1.89	0.54
1:A:956:ALA:HB2	1:A:973:ALA:HA	1.90	0.54
2:H:95:CYS:CB	2:H:98:LEU:HG	2.34	0.54
3:I:216:HIS:HE1	3:I:218:PRO:CG	1.81	0.54
3:I:39:GLN:HB3	3:I:93:VAL:HG13	1.89	0.53
1:A:662:ILE:HD13	1:A:735:LEU:HD13	1.90	0.53
1:A:1152:ALA:O	1:A:1154:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:2:VAL:HG13	3:E:27:PHE:HB2	1.89	0.53
2:H:17:SER:HB3	2:H:112:LYS:HB2	1.90	0.53
1:B:328:SER:HB2	1:B:330:ASP:OD1	2.09	0.53
2:H:49:VAL:HG13	3:I:120:TRP:HZ2	1.72	0.53
2:D:101:TRP:HB2	3:E:47:TRP:HB3	1.89	0.53
1:A:1151:SER:HB2	1:A:1170:GLY:HA3	1.90	0.53
1:A:497:TYR:HB2	1:A:561:VAL:HB	1.91	0.53
1:A:722:LEU:HD13	1:A:758:ARG:HG3	1.91	0.53
3:G:39:GLN:HB2	3:G:95:TYR:HE1	1.74	0.53
2:H:95:CYS:CB	2:H:98:LEU:HD12	2.38	0.53
1:B:359:GLY:O	1:B:361:TYR:HE2	1.78	0.53
1:B:375:VAL:HG22	1:B:607:SER:HB3	1.91	0.53
1:C:625:VAL:O	1:C:626:ARG:HB2	2.09	0.53
3:G:166:VAL:HG22	3:G:216:HIS:HD2	1.74	0.53
1:A:258:GLN:HG2	1:A:263:VAL:HG22	1.91	0.52
3:G:100:ASN:HB2	3:G:116:TYR:HB2	1.91	0.52
1:A:1172:PHE:HZ	1:A:1180:ILE:HG23	1.73	0.52
1:A:36:GLN:OE1	1:A:39:PHE:CE1	2.63	0.52
1:B:530:VAL:HG22	1:B:531:PRO:HD2	1.91	0.52
1:A:457:SER:HB3	1:A:460:SER:HB3	1.92	0.52
1:B:393:PRO:HG2	1:B:567:LEU:HD21	1.92	0.52
1:C:735:LEU:HB3	1:C:739:PRO:HD2	1.92	0.52
1:C:484:VAL:HG11	1:C:491:ILE:HG21	1.91	0.52
2:F:40:GLN:HB2	2:F:50:LEU:HD11	1.91	0.52
1:B:358:SER:CB	1:B:663:TYR:HB3	2.39	0.52
1:B:529:ILE:HB	1:B:543:LYS:HG3	1.91	0.52
1:B:737:ALA:N	1:C:938:LEU:HA	2.20	0.52
1:C:900:ILE:HG12	1:C:903:PRO:HD3	1.92	0.51
3:I:219:SER:HB2	3:I:221:THR:OG1	2.11	0.51
1:B:1172:PHE:HB2	1:B:1177:ASN:HB2	1.93	0.51
1:C:358:SER:HB3	1:C:665:LYS:H	1.74	0.51
3:I:185:VAL:HG22	3:I:193:SER:H	1.75	0.51
3:I:39:GLN:HB2	3:I:95:TYR:HE1	1.75	0.51
1:B:738:LEU:HD21	1:C:940:ASP:H	1.75	0.51
3:G:91:THR:HG23	3:G:127:THR:HA	1.93	0.51
3:G:213:ASN:HB3	3:G:222:LYS:HE2	1.93	0.51
1:A:741:THR:HA	1:A:759:LEU:HA	1.93	0.51
1:A:358:SER:HB3	1:A:665:LYS:H	1.75	0.51
1:B:1054:ILE:HG22	1:B:1063:GLN:HG3	1.93	0.51
1:C:853:VAL:HG13	1:C:951:LEU:HG	1.91	0.51
3:E:24:ALA:HB1	3:E:27:PHE:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:SER:HB2	1:B:334:ARG:NH2	2.24	0.51
1:C:194:HIS:HA	1:C:201:TYR:HA	1.93	0.51
1:C:496:LYS:HA	1:C:563:MET:HG3	1.93	0.51
3:E:5:VAL:HG13	3:E:23:ALA:HB3	1.92	0.51
3:G:201:PRO:HG2	3:G:204:SER:HB2	1.92	0.51
1:A:664:ASP:HB2	1:A:669:THR:O	2.11	0.50
1:A:893:LEU:O	1:A:897:LYS:HG2	2.11	0.50
1:A:924:ILE:HG13	1:A:925:CYS:N	2.26	0.50
1:B:397:TYR:HB2	1:B:527:VAL:HG22	1.93	0.50
1:B:937:PRO:O	1:B:938:LEU:HB3	2.10	0.50
1:B:1187:THR:O	1:B:1188:GLY:C	2.49	0.50
3:E:47:TRP:HZ2	3:E:50:VAL:HG12	1.77	0.50
1:B:890:ILE:HA	1:B:893:LEU:HD12	1.92	0.50
1:C:102:VAL:HB	1:C:297:PRO:HB2	1.93	0.50
1:C:1040:LEU:HD21	1:C:1078:LEU:HG	1.94	0.50
1:B:154:GLY:O	1:B:163:ARG:HB3	2.12	0.50
1:C:394:PRO:HB2	1:C:398:ASN:O	2.11	0.50
2:H:166:GLU:HB3	2:H:180:LEU:HD11	1.93	0.50
1:A:360:VAL:HG22	1:A:662:ILE:HG22	1.94	0.50
1:A:875:GLU:OE2	1:A:887:ARG:N	2.44	0.50
3:E:62:ASP:HA	3:E:65:LYS:HE3	1.93	0.50
1:B:149:LEU:HB3	1:B:290:ILE:HD13	1.94	0.50
1:C:1188:GLY:O	1:C:1189:SER:HB2	2.12	0.50
2:D:119:SER:HB3	3:E:151:THR:HG21	1.93	0.50
2:F:86:PHE:HB3	2:F:109:LEU:HB2	1.93	0.50
1:C:606:TYR:O	1:C:608:LEU:N	2.43	0.49
2:D:154:LYS:HG3	2:D:198:ALA:HB3	1.94	0.49
1:A:120:ILE:HG21	1:A:145:PRO:HD3	1.92	0.49
1:B:799:ILE:HG23	1:B:1092:ALA:HB2	1.93	0.49
1:C:395:GLN:HG3	1:C:498:SER:HB2	1.94	0.49
1:B:771:ASP:HA	1:C:860:PRO:HD3	1.94	0.49
1:C:112:PHE:CE2	1:C:115:GLY:HA2	2.48	0.49
1:C:154:GLY:O	1:C:163:ARG:HB3	2.12	0.49
3:G:154:LEU:HD23	3:G:200:VAL:HG21	1.94	0.49
1:A:773:LEU:HD11	1:A:779:LYS:HG3	1.93	0.49
2:F:150:LYS:HB2	2:F:202:THR:HB	1.94	0.49
1:B:188:GLU:HB3	1:B:233:ASN:HB2	1.94	0.49
3:I:133:LYS:H	3:I:162:PHE:CB	2.25	0.49
1:B:112:PHE:CZ	1:B:115:GLY:HA2	2.48	0.49
1:B:189:PRO:HB2	1:B:197:ALA:HB2	1.95	0.49
3:I:163:PRO:CB	3:I:216:HIS:HE2	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:GLY:O	1:A:718:VAL:HG23	2.13	0.49
1:B:88:SER:HA	1:B:310:TRP:HD1	1.77	0.49
1:B:404:PHE:HE2	1:B:443:LEU:HB2	1.77	0.49
1:B:724:VAL:HG12	1:B:760:ALA:HB3	1.95	0.49
1:A:312:ALA:HB3	1:A:314:TYR:OH	2.13	0.48
2:D:146:PRO:HD2	2:D:203:HIS:CE1	2.48	0.48
1:A:408:ASN:HA	1:A:585:CYS:O	2.13	0.48
3:E:37:VAL:HG23	3:E:95:TYR:HB2	1.95	0.48
1:B:29:ALA:HB3	3:G:103:TYR:CD2	2.49	0.48
1:B:85:TYR:HB2	1:B:313:PHE:CE2	2.48	0.48
1:B:769:GLN:HG3	1:C:858:SER:HB3	1.94	0.48
1:C:903:PRO:HA	1:C:934:VAL:HG21	1.95	0.48
3:I:11:VAL:HG12	3:I:127:THR:HB	1.95	0.48
1:A:676:SER:HA	1:B:906:MET:H	1.78	0.48
1:B:209:THR:H	1:B:213:ASP:HB2	1.77	0.48
1:C:486:HIS:HB3	1:C:566:GLN:HE22	1.77	0.48
2:D:40:GLN:HB2	2:D:50:LEU:HD11	1.96	0.48
3:I:132:THR:OG1	3:I:162:PHE:HB3	2.13	0.48
1:A:165:PHE:HA	1:A:187:LEU:HB2	1.95	0.48
1:B:797:THR:H	1:B:1133:GLY:HA2	1.78	0.48
1:B:1168:VAL:O	1:B:1169:ASN:C	2.52	0.48
1:A:122:ALA:HB2	1:A:251:LEU:HD13	1.95	0.48
1:A:192:GLY:H	1:A:198:GLY:HA3	1.79	0.48
1:A:985:ILE:H	1:A:985:ILE:HG12	1.47	0.48
1:C:519:ASN:HB2	1:C:522:GLN:HB2	1.94	0.48
2:F:8:THR:HG22	2:F:27:ARG:HG2	1.95	0.48
1:A:496:LYS:HE2	1:A:560:THR:HG21	1.96	0.48
1:A:599:GLN:O	1:A:600:LEU:HB2	2.14	0.48
3:G:137:VAL:HG21	3:G:214:VAL:HG11	1.95	0.48
1:A:712:GLY:O	1:A:717:LEU:HA	2.14	0.48
1:A:971:PRO:HD2	1:A:975:SER:H	1.79	0.48
1:B:374:VAL:H	1:B:606:TYR:HA	1.79	0.48
1:A:74:LEU:HB3	1:A:318:LEU:HB3	1.95	0.47
1:A:425:CYS:HA	1:A:478:CYS:HA	1.96	0.47
1:A:496:LYS:HA	1:A:563:MET:HG2	1.96	0.47
1:B:616:VAL:H	1:B:652:ARG:H	1.61	0.47
1:A:780:LEU:O	1:A:1148:GLU:HA	2.14	0.47
1:A:43:THR:C	1:A:44:TRP:CE3	2.88	0.47
1:C:409:TYR:HD1	1:C:584:VAL:HG12	1.80	0.47
2:H:39:TYR:CE1	2:H:49:VAL:HG12	2.50	0.47
1:A:138:ALA:HB3	1:A:309:ALA:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASP:HB2	1:A:354:PHE:CE1	2.50	0.47
1:A:369:LYS:HE2	1:A:690:SER:HB3	1.96	0.47
1:A:500:ILE:HA	1:A:558:GLY:HA2	1.95	0.47
1:A:1172:PHE:CZ	1:A:1180:ILE:HG23	2.49	0.47
1:B:1175:THR:O	1:B:1176:ASN:HB2	2.14	0.47
1:B:452:MET:HB2	1:B:455:ASP:HB2	1.95	0.47
1:C:478:CYS:HB2	1:C:573:ILE:HB	1.96	0.47
2:F:7:MET:SD	2:F:26:CYS:HB2	2.55	0.47
1:A:397:TYR:HB2	1:A:527:VAL:HG22	1.95	0.47
1:A:522:GLN:HE21	1:A:522:GLN:CA	2.25	0.47
1:B:92:ALA:HA	1:B:98:GLN:HB2	1.96	0.47
2:F:146:PRO:HD2	2:F:203:HIS:CE1	2.48	0.47
3:I:217:LYS:N	3:I:218:PRO:CD	2.77	0.47
1:A:538:GLY:H	1:A:559:SER:HA	1.80	0.47
1:B:100:LEU:HB3	1:B:299:SER:HB3	1.97	0.47
1:A:142:LYS:HA	1:A:311:ALA:HB3	1.97	0.47
1:A:296:ILE:N	1:A:297:PRO:HD3	2.30	0.47
1:A:442:ILE:HB	1:A:574:THR:HB	1.96	0.47
1:C:273:LEU:HD23	1:C:273:LEU:H	1.80	0.47
1:C:399:PHE:HB2	1:C:401:ARG:HH21	1.80	0.47
1:B:457:SER:HB3	1:B:460:SER:HB3	1.97	0.46
1:B:789:GLY:HA3	1:B:1004:ALA:HB1	1.96	0.46
2:F:125:PRO:HD3	2:F:137:VAL:HG22	1.97	0.46
1:B:102:VAL:HG13	1:B:299:SER:HB2	1.96	0.46
1:B:506:LEU:HD22	1:B:553:TRP:HE3	1.79	0.46
1:C:427:GLN:HE21	1:C:476:PRO:HA	1.80	0.46
2:D:86:PHE:HA	2:D:109:LEU:HD12	1.97	0.46
2:F:115:VAL:HA	2:F:145:TYR:HB3	1.95	0.46
1:B:782:ILE:N	1:B:783:PRO:HD3	2.30	0.46
1:C:385:PHE:HE2	1:C:410:ASN:H	1.63	0.46
1:C:399:PHE:HB2	1:C:401:ARG:NH2	2.31	0.46
1:C:545:LEU:HB2	1:C:551:GLY:O	2.16	0.46
1:A:448:TYR:CZ	1:A:456:LEU:HB2	2.51	0.46
1:A:783:PRO:O	1:A:1182:ASP:HA	2.14	0.46
1:B:330:ASP:OD2	1:B:334:ARG:NH1	2.48	0.46
1:B:1009:GLN:O	1:B:1010:THR:C	2.54	0.46
1:C:831:ILE:HG23	1:C:1082:VAL:HG21	1.98	0.46
1:A:780:LEU:HD12	1:A:1172:PHE:CE1	2.51	0.46
1:A:33:VAL:HG11	1:A:203:SER:HB3	1.98	0.46
1:A:77:TYR:HB3	1:A:319:GLN:HE22	1.81	0.46
1:A:83:ASP:O	1:A:314:TYR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:175:ASP:O	2:F:176:SER:OG	2.28	0.46
1:C:807:LYS:HA	1:C:821:LEU:HD13	1.97	0.46
1:C:1154:GLY:HA3	1:C:1205:VAL:HB	1.98	0.46
2:D:125:PRO:HD3	2:D:137:VAL:HG22	1.98	0.46
1:A:116:PHE:HB2	1:A:315:VAL:HG13	1.98	0.46
1:B:692:SER:O	1:B:693:THR:HB	2.15	0.46
1:B:789:GLY:HA2	1:B:1139:VAL:O	2.16	0.46
1:A:952:LEU:O	1:A:955:ILE:HG12	2.15	0.46
1:B:105:TYR:HB3	1:B:295:ILE:HG23	1.98	0.45
1:C:912:CYS:HB3	1:C:928:TYR:HE2	1.81	0.45
1:C:1165:ILE:HA	1:C:1169:ASN:CB	2.46	0.45
2:H:150:LYS:HB2	2:H:202:THR:HB	1.97	0.45
1:B:963:GLY:H	1:B:967:PHE:HE2	1.63	0.45
1:C:686:MET:H	1:C:686:MET:HG2	1.48	0.45
2:H:22:VAL:HG22	2:H:81:LEU:HD11	1.98	0.45
3:I:144:SER:HB2	3:I:147:THR:HG23	1.99	0.45
1:B:25:SER:HB2	1:B:229:LYS:HG3	1.97	0.45
1:B:403:VAL:HG12	1:B:442:ILE:HG12	1.98	0.45
1:A:118:VAL:HA	1:A:314:TYR:O	2.16	0.45
3:E:137:VAL:HG11	3:E:214:VAL:HG21	1.98	0.45
1:A:385:PHE:HE1	1:A:410:ASN:H	1.65	0.45
1:C:1155:LEU:HA	1:C:1204:TYR:HA	1.97	0.45
1:A:119:ARG:HG3	1:A:314:TYR:CD1	2.34	0.45
1:C:75:PHE:HB2	1:C:321:LEU:HB2	1.97	0.45
1:C:605:GLU:HA	1:C:613:GLY:O	2.17	0.45
1:A:799:ILE:HG23	1:A:1092:ALA:HB2	1.98	0.45
1:A:913:MET:HA	1:C:652:ARG:HD2	1.99	0.45
1:A:1042:ASN:HD22	1:A:1042:ASN:HA	1.51	0.45
1:B:606:TYR:CZ	1:B:651:LEU:HD22	2.52	0.45
1:C:169:LEU:HB3	1:C:184:TYR:HD1	1.82	0.45
1:C:1126:PHE:HB2	1:C:1137:MET:HB3	1.99	0.45
1:C:341:PHE:HA	1:C:695:SER:HB2	1.98	0.45
2:H:160:GLN:HE22	2:H:186:LEU:HD11	1.82	0.45
1:A:433:ILE:HB	1:A:438:TYR:HE1	1.82	0.44
1:B:36:GLN:HB3	1:B:39:PHE:HD2	1.81	0.44
1:B:386:SER:N	1:B:387:PRO:HD2	2.32	0.44
1:A:333:ILE:HD11	1:A:336:ALA:HB2	1.98	0.44
1:A:970:ILE:N	1:A:971:PRO:HD3	2.31	0.44
1:B:265:LEU:HB2	1:B:282:ALA:HB3	1.99	0.44
1:C:485:PRO:HG2	1:C:488:LEU:HB2	1.98	0.44
3:E:13:GLN:HE21	3:E:13:GLN:HB3	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LEU:HA	1:A:481:LEU:HD21	2.00	0.44
1:B:151:SER:HA	1:B:290:ILE:HA	2.00	0.44
1:B:359:GLY:C	1:B:361:TYR:CE2	2.83	0.44
1:B:407:CYS:O	1:B:584:VAL:HG13	2.17	0.44
1:C:210:PRO:HA	1:C:214:CYS:HB2	1.99	0.44
1:C:502:LYS:HG3	1:C:557:SER:HB3	1.99	0.44
1:C:599:GLN:HG3	1:C:649:TYR:CZ	2.51	0.44
1:C:1129:ASN:HD22	1:C:1129:ASN:HA	1.66	0.44
2:D:40:GLN:HE21	2:D:40:GLN:HB3	1.60	0.44
2:F:118:PRO:HG3	2:F:144:PHE:HB3	1.99	0.44
3:G:15:GLY:HA2	3:G:85:SER:HA	1.99	0.44
1:A:1036:LEU:HD22	1:A:1081:PHE:HB2	2.00	0.44
1:B:77:TYR:CE1	1:B:341:PHE:HA	2.53	0.44
1:B:156:PHE:CD2	1:B:163:ARG:HB2	2.53	0.44
1:B:821:LEU:HD12	1:B:821:LEU:HA	1.78	0.44
1:C:641:TYR:HA	1:C:649:TYR:H	1.82	0.44
1:B:120:ILE:O	1:B:251:LEU:HB2	2.17	0.44
3:E:213:ASN:HB3	3:E:222:LYS:HE2	2.00	0.44
1:A:519:ASN:HB3	1:A:522:GLN:HG3	1.99	0.44
2:D:16:ALA:HB1	2:D:81:LEU:HD13	2.00	0.44
3:I:222:LYS:HD2	3:I:222:LYS:HA	1.82	0.44
1:A:366:PHE:HB3	1:A:689:TYR:CB	2.48	0.44
2:F:146:PRO:HD2	2:F:203:HIS:HE1	1.83	0.44
1:A:56:ILE:HG21	1:A:333:ILE:HD13	2.00	0.44
1:A:1150:VAL:O	1:A:1172:PHE:HA	2.18	0.44
1:C:92:ALA:HB1	1:C:97:PRO:HA	1.98	0.44
1:C:1122:HIS:HE2	1:C:1125:SER:HB3	1.82	0.44
1:C:1166:ALA:HB3	1:C:1167:PRO:HD3	2.00	0.44
3:I:216:HIS:ND1	3:I:219:SER:N	2.62	0.43
1:A:107:GLN:HG2	1:A:161:MET:H	1.83	0.43
1:A:1168:VAL:HA	1:B:967:PHE:HE1	1.83	0.43
1:B:910:ASP:O	1:B:914:GLN:HG2	2.18	0.43
1:B:1022:VAL:HG11	1:B:1131:PRO:HD2	2.01	0.43
1:A:43:THR:O	1:A:44:TRP:CD2	2.71	0.43
1:A:50:VAL:HG11	1:A:338:ASP:HB2	1.99	0.43
1:A:875:GLU:OE1	1:A:886:ALA:N	2.50	0.43
1:B:722:LEU:HG	1:B:758:ARG:HG2	2.00	0.43
1:C:394:PRO:HG2	1:C:400:LYS:HB2	2.00	0.43
1:A:1171:TYR:HB3	1:A:1177:ASN:N	2.30	0.43
1:B:330:ASP:CG	1:B:334:ARG:HH12	2.22	0.43
1:C:132:ILE:HG21	1:C:307:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:SER:HA	2:D:110:GLU:HG2	1.99	0.43
2:F:9:GLN:HE21	2:F:9:GLN:HB3	1.69	0.43
2:H:135:ALA:HB2	2:H:191:TYR:HB2	2.00	0.43
1:A:36:GLN:OE1	1:A:39:PHE:CD1	2.71	0.43
1:C:397:TYR:HB2	1:C:527:VAL:HG22	2.01	0.43
1:C:1156:CYS:HA	1:C:1162:THR:HB	2.00	0.43
3:E:11:VAL:HA	3:E:127:THR:O	2.18	0.43
2:F:6:GLN:H	2:F:6:GLN:HG3	1.68	0.43
1:A:1177:ASN:HD22	1:A:1177:ASN:HA	1.57	0.43
1:B:167:HIS:H	1:B:186:ILE:HG12	1.84	0.43
1:B:328:SER:CB	1:B:334:ARG:NH2	2.81	0.43
1:C:90:GLY:HA2	1:C:101:PHE:H	1.83	0.43
1:C:430:PRO:O	1:C:433:ILE:HG12	2.19	0.43
2:H:95:CYS:CB	2:H:98:LEU:CD1	2.95	0.43
1:A:405:THR:HB	1:A:582:ASN:HD21	1.84	0.43
1:A:634:ALA:HB2	1:B:67:ILE:HD13	2.00	0.43
1:B:67:ILE:H	1:B:67:ILE:HG13	1.56	0.43
1:B:330:ASP:CG	1:B:334:ARG:NH1	2.72	0.43
1:B:347:LEU:HD13	1:B:347:LEU:HA	1.88	0.43
1:B:192:GLY:O	1:B:198:GLY:HA3	2.19	0.43
2:D:148:GLU:H	2:D:148:GLU:HG3	1.51	0.43
1:A:312:ALA:HB3	1:A:314:TYR:CZ	2.54	0.43
1:A:498:SER:HB3	1:A:534:VAL:HG23	2.01	0.43
1:A:616:VAL:O	1:A:651:LEU:HA	2.19	0.43
1:A:781:SER:HB2	1:A:1146:HIS:HB3	2.01	0.43
1:A:1000:LYS:HE3	1:A:1000:LYS:HB3	1.79	0.43
1:B:360:VAL:HG13	1:B:660:SER:HB3	1.99	0.43
2:D:82:GLN:H	2:D:85:ASP:HB2	1.84	0.43
2:F:112:LYS:CA	2:F:145:TYR:OH	2.43	0.43
2:F:166:GLU:HB3	2:F:180:LEU:HD11	2.00	0.43
3:G:137:VAL:HG11	3:G:214:VAL:HG21	2.00	0.43
1:A:226:ASN:O	1:A:230:GLU:HG3	2.19	0.42
1:B:985:ILE:H	1:B:1183:GLU:HB3	1.83	0.42
1:C:118:VAL:HG11	1:C:145:PRO:HG3	2.00	0.42
2:F:40:GLN:HE21	2:F:40:GLN:HB3	1.54	0.42
1:A:36:GLN:CD	1:A:39:PHE:CE1	2.92	0.42
1:A:665:LYS:HE3	1:A:665:LYS:HB3	1.83	0.42
1:A:811:CYS:HB3	1:A:817:CYS:HB3	1.86	0.42
1:B:996:LEU:HB3	1:B:999:ASN:HB2	2.00	0.42
3:G:135:PRO:HB3	3:G:161:TYR:HB2	2.00	0.42
3:I:217:LYS:HB3	3:I:218:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:ALA:H	1:A:1171:TYR:N	2.17	0.42
1:B:381:VAL:O	1:B:382:GLU:C	2.57	0.42
2:F:37:ASN:O	2:F:91:CYS:HA	2.19	0.42
2:H:95:CYS:HB3	2:H:98:LEU:CB	2.48	0.42
2:H:172:ASP:HB2	2:H:175:ASP:HB2	2.01	0.42
1:A:780:LEU:HD12	1:A:1172:PHE:HE1	1.84	0.42
1:C:30:CYS:SG	1:C:231:TYR:HA	2.60	0.42
1:C:410:ASN:HB3	1:C:413:LYS:HD3	2.02	0.42
1:B:156:PHE:HB2	1:B:160:LYS:O	2.19	0.42
1:B:987:GLN:H	1:B:990:LEU:HB2	1.85	0.42
1:C:596:ILE:HD12	1:C:596:ILE:H	1.84	0.42
2:H:9:GLN:HG3	2:H:105:GLN:HB2	2.01	0.42
1:A:43:THR:C	1:A:44:TRP:CD2	2.93	0.42
1:B:506:LEU:HD21	1:B:510:ASP:HB2	2.01	0.42
1:B:641:TYR:HB2	1:B:648:TYR:CZ	2.55	0.42
1:C:92:ALA:H	1:C:307:ARG:HH11	1.68	0.42
3:I:162:PHE:H	3:I:163:PRO:CD	2.32	0.42
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.85	0.42
1:A:102:VAL:HG13	1:A:299:SER:HB3	2.02	0.42
1:A:324:LEU:HB3	1:A:337:ILE:HB	2.02	0.42
1:B:76:PRO:HD3	1:B:318:LEU:HD22	2.02	0.42
1:B:330:ASP:HB2	1:B:332:TYR:CE2	2.55	0.42
1:B:623:VAL:HG22	1:C:329:VAL:HG13	2.02	0.42
1:C:603:CYS:C	1:C:604:VAL:HG22	2.39	0.42
1:A:142:LYS:HE2	1:A:142:LYS:HB2	1.81	0.42
2:D:51:ILE:HG12	2:D:54:THR:HA	2.02	0.42
1:A:46:ARG:CZ	1:A:314:TYR:CZ	3.02	0.42
1:A:493:LYS:HA	1:A:567:LEU:HD22	2.02	0.42
1:A:146:ALA:HB3	1:A:297:PRO:HD2	2.02	0.42
1:A:606:TYR:HE1	1:A:608:LEU:HG	1.85	0.42
1:B:356:VAL:HG12	1:B:357:GLU:O	2.20	0.42
2:H:121:PHE:CE1	3:I:148:SER:HA	2.54	0.42
1:B:766:HIS:HA	1:B:767:PRO:HD3	1.93	0.41
3:E:57:LEU:HD12	3:E:57:LEU:HA	1.77	0.41
1:A:738:LEU:N	1:A:739:PRO:HD2	2.35	0.41
1:A:839:ASN:HD22	1:A:935:LEU:HD13	1.84	0.41
1:B:405:THR:HB	1:B:582:ASN:HD21	1.85	0.41
1:B:739:PRO:HA	1:B:760:ALA:HA	2.02	0.41
2:F:153:TRP:HZ3	2:F:197:TYR:HB3	1.85	0.41
3:G:5:VAL:HG13	3:G:23:ALA:HB3	2.02	0.41
1:B:1112:LYS:HE3	1:B:1112:LYS:HB3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:SER:HA	1:C:659:VAL:HG12	2.02	0.41
1:C:606:TYR:CZ	1:C:651:LEU:HD13	2.55	0.41
1:C:1176:ASN:HD22	1:C:1176:ASN:HA	1.67	0.41
1:B:87:TYR:HB2	1:B:143:ILE:HG21	2.02	0.41
1:B:1179:ARG:HB3	1:B:1185:SER:HA	2.03	0.41
1:C:36:GLN:HB2	1:C:101:PHE:CZ	2.55	0.41
1:C:133:SER:HB3	1:C:136:THR:HG22	2.02	0.41
2:F:42:LYS:HD3	2:F:42:LYS:HA	1.96	0.41
2:F:192:GLU:HA	2:F:216:ARG:HH12	1.86	0.41
3:G:216:HIS:CD2	3:G:218:PRO:HD2	2.54	0.41
3:G:224:ASP:OD1	3:G:224:ASP:N	2.53	0.41
3:I:137:VAL:HG11	3:I:214:VAL:HG21	2.01	0.41
1:A:807:LYS:H	1:A:810:VAL:HG23	1.85	0.41
1:B:442:ILE:HB	1:B:574:THR:HB	2.01	0.41
1:B:518:VAL:HG12	1:B:524:SER:HB2	2.03	0.41
1:B:958:VAL:HB	1:B:969:ALA:HA	2.02	0.41
1:B:1049:ALA:C	1:B:1051:ILE:H	2.23	0.41
3:I:24:ALA:HB1	3:I:27:PHE:HB3	2.01	0.41
1:B:614:ARG:HB2	1:B:654:CYS:HB2	2.02	0.41
1:B:887:ARG:HH11	1:B:895:PHE:HD2	1.68	0.41
1:C:388:LEU:HD21	1:C:402:LEU:HB2	2.03	0.41
1:C:814:PHE:HB2	1:C:817:CYS:SG	2.61	0.41
1:C:1160:ASN:N	1:C:1161:PRO:HD2	2.35	0.41
2:D:100:CYS:HA	3:E:47:TRP:CZ3	2.55	0.41
1:A:35:ILE:HD11	1:A:203:SER:HB2	2.03	0.41
1:A:604:VAL:HB	1:A:605:GLU:H	1.73	0.41
1:A:680:GLU:H	1:A:680:GLU:HG3	1.59	0.41
1:A:890:ILE:H	1:A:890:ILE:HG13	1.54	0.41
1:B:149:LEU:HD12	1:B:290:ILE:HG21	2.03	0.41
1:C:806:CYS:H	1:C:832:ASN:HD21	1.68	0.41
1:B:781:SER:C	1:B:783:PRO:HD3	2.41	0.41
1:B:988:GLN:HE21	1:B:988:GLN:HB3	1.69	0.41
1:C:859:SER:H	1:C:953:GLY:HA3	1.85	0.41
1:A:608:LEU:HD12	1:A:611:VAL:HB	2.03	0.41
1:A:808:GLN:HE22	1:C:365:SER:HB2	1.85	0.41
1:B:565:GLU:H	1:B:565:GLU:HG3	1.61	0.41
1:C:498:SER:HB3	1:C:534:VAL:HG23	2.03	0.41
1:C:606:TYR:CE2	1:C:651:LEU:HD22	2.56	0.41
1:C:792:GLN:HE22	1:C:1118:GLY:HA3	1.86	0.41
3:E:167:THR:HB	3:E:215:ASN:HB3	2.02	0.41
3:I:137:VAL:HG21	3:I:214:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LYS:HA	1:A:311:ALA:CB	2.51	0.41
1:A:804:VAL:H	1:A:835:LEU:HD13	1.85	0.41
1:B:226:ASN:HA	1:B:229:LYS:HG2	2.03	0.41
1:C:484:VAL:HB	1:C:569:MET:HE1	2.02	0.41
1:C:600:LEU:HD23	1:C:600:LEU:HA	1.87	0.41
2:D:186:LEU:HD13	2:D:186:LEU:HA	1.92	0.41
2:D:171:GLN:HE21	2:D:171:GLN:HB3	1.69	0.40
3:E:17:SER:HB3	3:E:82:GLN:HE21	1.85	0.40
1:A:381:VAL:O	1:A:382:GLU:C	2.59	0.40
1:A:985:ILE:HB	1:A:1192:TYR:OH	2.21	0.40
1:B:121:GLY:HA2	1:B:311:ALA:HB3	2.02	0.40
1:C:131:ILE:H	1:C:131:ILE:HD12	1.86	0.40
1:C:850:PHE:CD2	1:C:939:MET:HG3	2.55	0.40
2:H:16:ALA:O	2:H:111:ILE:HA	2.22	0.40
2:H:101:TRP:HB2	3:I:47:TRP:HB3	2.02	0.40
1:A:84:MET:HG3	1:A:314:TYR:HE2	1.87	0.40
1:A:409:TYR:CD2	1:A:584:VAL:HG12	2.56	0.40
1:B:849:LEU:HA	1:B:1100:LYS:HG3	2.03	0.40
3:I:182:PHE:HA	3:I:183:PRO:HD3	1.95	0.40
1:A:723:PHE:O	1:A:760:ALA:HB3	2.21	0.40
1:B:89:ALA:HA	1:B:300:ILE:HB	2.02	0.40
1:C:48:ILE:CD1	1:C:76:PRO:HB2	2.49	0.40
1:C:810:VAL:HG13	1:C:1074:ARG:HD2	2.03	0.40
2:D:10:THR:N	2:D:11:PRO:HD2	2.37	0.40
1:B:373:SER:HA	1:B:605:GLU:O	2.22	0.40
3:G:47:TRP:HE1	3:G:50:VAL:HB	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1119/1189 (94%)	1052 (94%)	51 (5%)	16 (1%)	9	40
1	B	1083/1189 (91%)	1015 (94%)	52 (5%)	16 (2%)	8	40
1	C	1072/1189 (90%)	1003 (94%)	54 (5%)	15 (1%)	9	40
2	D	214/216 (99%)	210 (98%)	4 (2%)	0	100	100
2	F	214/216 (99%)	211 (99%)	2 (1%)	1 (0%)	25	61
2	H	214/216 (99%)	209 (98%)	3 (1%)	2 (1%)	14	49
3	E	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
3	G	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
3	I	225/227 (99%)	217 (96%)	6 (3%)	2 (1%)	14	49
All	All	4591/4896 (94%)	4357 (95%)	182 (4%)	52 (1%)	15	45

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	LEU
1	A	1153	TYR
1	B	733	GLN
1	B	782	ILE
1	B	1010	THR
1	B	1176	ASN
1	C	607	SER
1	C	738	LEU
1	C	1167	PRO
1	C	1189	SER
1	C	1191	PHE
3	I	220	ASN
1	B	1169	ASN
1	B	1173	ILE
1	B	1179	ARG
1	C	601	GLY
1	C	604	VAL
1	A	245	ILE
1	A	342	ASN
1	A	382	GLU
1	A	694	ARG
1	A	737	ALA
1	A	1042	ASN
1	A	1116	PHE
1	B	693	THR
1	B	737	ALA

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Mol	Chain	Res	Type
1	B	900	ILE
1	C	641	TYR
2	H	146	PRO
1	A	713	CYS
1	A	766	HIS
1	A	976	ILE
1	B	81	HIS
1	B	604	VAL
1	B	785	ASN
1	C	874	LEU
2	F	11	PRO
1	A	604	VAL
1	B	382	GLU
1	B	813	GLY
1	C	382	GLU
1	C	731	LEU
1	C	887	ARG
1	C	1166	ALA
2	H	11	PRO
1	C	45	PRO
3	I	162	PHE
1	A	45	PRO
1	A	739	PRO
1	A	1181	VAL
1	B	929	VAL
1	C	1193	ALA

### 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	875/1022 (86%)	813 (93%)	62 (7%)	12	35
1	B	865/1022 (85%)	796 (92%)	69 (8%)	10	32
1	C	832/1022 (81%)	774 (93%)	58 (7%)	12	35
2	D	181/192 (94%)	172 (95%)	9 (5%)	20	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	185/192 (96%)	171 (92%)	14 (8%)	11	33
2	H	181/192 (94%)	171 (94%)	10 (6%)	18	42
3	E	176/191 (92%)	160 (91%)	16 (9%)	7	26
3	G	183/191 (96%)	167 (91%)	16 (9%)	8	29
3	I	174/191 (91%)	162 (93%)	12 (7%)	13	36
All	All	3652/4215 (87%)	3386 (93%)	266 (7%)	14	34

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	71	TYR
1	A	101	PHE
1	A	102	VAL
1	A	142	LYS
1	A	171	LEU
1	A	172	LEU
1	A	179	LEU
1	A	204	PHE
1	A	208	HIS
1	A	221	ARG
1	A	227	SER
1	A	249	GLU
1	A	319	GLN
1	A	323	PHE
1	A	363	VAL
1	A	424	THR
1	A	427	GLN
1	A	450	LEU
1	A	510	ASP
1	A	555	VAL
1	A	563	MET
1	A	575	VAL
1	A	604	VAL
1	A	616	VAL
1	A	623	VAL
1	A	639	VAL
1	A	642	TYR
1	A	650	CYS
1	A	659	VAL

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Mol	Chain	Res	Type
1	A	673	LEU
1	A	680	GLU
1	A	697	LEU
1	A	713	CYS
1	A	795	ILE
1	A	802	VAL
1	A	809	TYR
1	A	810	VAL
1	A	890	ILE
1	A	897	LYS
1	A	899	THR
1	A	935	LEU
1	A	938	LEU
1	A	941	VAL
1	A	985	ILE
1	A	1000	LYS
1	A	1005	LEU
1	A	1012	PHE
1	A	1033	LEU
1	A	1042	ASN
1	A	1061	LEU
1	A	1070	LEU
1	A	1086	LEU
1	A	1116	PHE
1	A	1149	VAL
1	A	1157	ASP
1	A	1168	VAL
1	A	1175	THR
1	A	1177	ASN
1	A	1180	ILE
1	A	1181	VAL
1	A	1200	LEU
1	B	21	VAL
1	B	30	CYS
1	B	35	ILE
1	B	102	VAL
1	B	129	THR
1	B	132	ILE
1	B	155	ASN
1	B	156	PHE
1	B	165	PHE
1	B	179	LEU

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Mol	Chain	Res	Type
1	B	214	CYS
1	B	221	ARG
1	B	234	LEU
1	B	240	MET
1	B	251	LEU
1	B	273	LEU
1	B	284	LEU
1	B	319	GLN
1	B	323	PHE
1	B	324	LEU
1	B	347	LEU
1	B	424	THR
1	B	433	ILE
1	B	438	TYR
1	B	443	LEU
1	B	475	ASN
1	B	510	ASP
1	B	529	ILE
1	B	530	VAL
1	B	548	LEU
1	B	563	MET
1	B	574	THR
1	B	576	GLN
1	B	608	LEU
1	B	620	CYS
1	B	626	ARG
1	B	631	VAL
1	B	632	TYR
1	B	655	VAL
1	B	661	VAL
1	B	682	ILE
1	B	693	THR
1	B	722	LEU
1	B	769	GLN
1	B	784	THR
1	B	873	LEU
1	B	887	ARG
1	B	900	ILE
1	B	929	VAL
1	B	938	LEU
1	B	955	ILE
1	B	960	TRP

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Mol	Chain	Res	Type
1	B	970	ILE
1	B	983	VAL
1	B	986	THR
1	B	997	ILE
1	B	1013	THR
1	B	1014	THR
1	B	1039	GLU
1	B	1040	LEU
1	B	1063	GLN
1	B	1108	LYS
1	B	1113	ARG
1	B	1127	VAL
1	B	1139	VAL
1	B	1165	ILE
1	B	1181	VAL
1	B	1183	GLU
1	B	1184	TRP
1	C	19	VAL
1	C	21	VAL
1	C	50	VAL
1	C	62	ARG
1	C	96	THR
1	C	129	THR
1	C	167	HIS
1	C	169	LEU
1	C	171	LEU
1	C	179	LEU
1	C	228	PHE
1	C	234	LEU
1	C	239	PHE
1	C	242	THR
1	C	273	LEU
1	C	280	GLN
1	C	284	LEU
1	C	324	LEU
1	C	341	PHE
1	C	349	CYS
1	C	363	VAL
1	C	401	ARG
1	C	438	TYR
1	C	444	ASP
1	C	448	TYR

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Mol	Chain	Res	Type
1	C	489	THR
1	C	502	LYS
1	C	517	LEU
1	C	529	ILE
1	C	563	MET
1	C	567	LEU
1	C	576	GLN
1	C	603	CYS
1	C	604	VAL
1	C	606	TYR
1	C	609	TYR
1	C	638	LEU
1	C	641	TYR
1	C	650	CYS
1	C	677	VAL
1	C	680	GLU
1	C	686	MET
1	C	713	CYS
1	C	714	VAL
1	C	723	PHE
1	C	725	GLU
1	C	735	LEU
1	C	790	VAL
1	C	804	VAL
1	C	807	LYS
1	C	894	LEU
1	C	938	LEU
1	C	943	MET
1	C	948	THR
1	C	974	GLN
1	C	1040	LEU
1	C	1128	VAL
1	C	1134	LEU
2	D	40	GLN
2	D	51	ILE
2	D	52	TYR
2	D	107	THR
2	D	148	GLU
2	D	155	VAL
2	D	181	SER
2	D	185	THR
2	D	186	LEU

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Mol	Chain	Res	Type
3	E	1	GLU
3	E	5	VAL
3	E	16	ARG
3	E	32	TYR
3	E	37	VAL
3	E	38	ARG
3	E	46	GLU
3	E	57	LEU
3	E	89	GLU
3	E	107	THR
3	E	126	VAL
3	E	132	THR
3	E	154	LEU
3	E	168	VAL
3	E	179	VAL
3	E	212	CYS
2	F	6	GLN
2	F	9	GLN
2	F	36	LEU
2	F	40	GLN
2	F	51	ILE
2	F	52	TYR
2	F	72	THR
2	F	75	THR
2	F	88	THR
2	F	128	GLU
2	F	148	GLU
2	F	155	VAL
2	F	185	THR
2	F	186	LEU
3	G	5	VAL
3	G	48	VAL
3	G	93	VAL
3	G	98	ARG
3	G	101	THR
3	G	115	TYR
3	G	126	VAL
3	G	132	THR
3	G	144	SER
3	G	151	THR
3	G	161	TYR
3	G	166	VAL

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Mol	Chain	Res	Type
3	G	179	VAL
3	G	191	LEU
3	G	194	LEU
3	G	212	CYS
2	H	6	GLN
2	H	9	GLN
2	H	27	ARG
2	H	30	GLN
2	H	51	ILE
2	H	52	TYR
2	H	88	THR
2	H	153	TRP
2	H	185	THR
2	H	186	LEU
3	I	5	VAL
3	I	16	ARG
3	I	19	ARG
3	I	48	VAL
3	I	93	VAL
3	I	126	VAL
3	I	143	SER
3	I	162	PHE
3	I	168	VAL
3	I	179	VAL
3	I	194	LEU
3	I	212	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	A	280	GLN
1	A	398	ASN
1	A	427	GLN
1	A	436	ASN
1	A	516	GLN
1	A	522	GLN
1	A	627	GLN
1	A	792	GLN
1	A	800	GLN
1	A	1029	ASN
1	A	1042	ASN

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Mol	Chain	Res	Type
1	A	1084	GLN
1	A	1129	ASN
1	A	1132	ASN
1	A	1163	ASN
1	A	1177	ASN
1	B	155	ASN
1	B	194	HIS
1	B	576	GLN
1	B	769	GLN
1	B	812	ASN
1	B	833	GLN
1	B	988	GLN
1	B	1079	ASN
1	B	1110	GLN
1	B	1129	ASN
1	C	72	GLN
1	C	193	ASN
1	C	226	ASN
1	C	264	HIS
1	C	280	GLN
1	C	319	GLN
1	C	522	GLN
1	C	566	GLN
1	C	733	GLN
1	C	792	GLN
1	C	832	ASN
1	C	839	ASN
1	C	907	GLN
1	C	1027	ASN
1	C	1129	ASN
1	C	1176	ASN
2	D	40	GLN
2	D	82	GLN
2	D	93	GLN
2	D	160	GLN
2	D	171	GLN
3	E	13	GLN
3	E	187	GLN
2	F	40	GLN
2	F	165	GLN
2	F	171	GLN
3	G	13	GLN

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Mol	Chain	Res	Type
3	G	122	GLN
3	G	187	GLN
2	H	93	GLN
2	H	129	GLN
2	H	171	GLN
2	H	194	HIS
3	I	13	GLN
3	I	122	GLN
3	I	171	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.

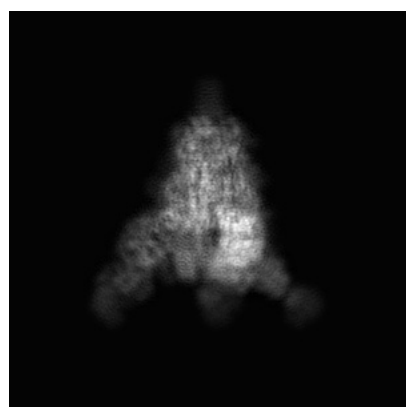
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31743. These allow visual inspection of the internal detail of the map and identification of artifacts.

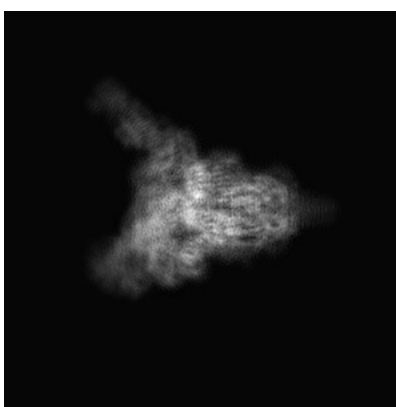
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

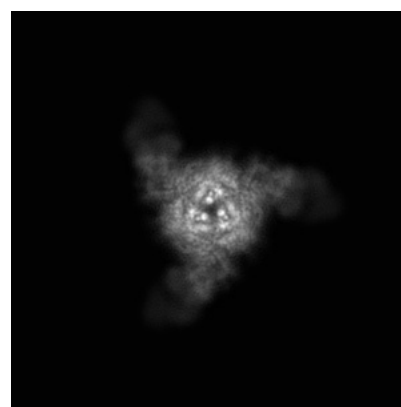
#### 6.1.1 Primary map



X



Y

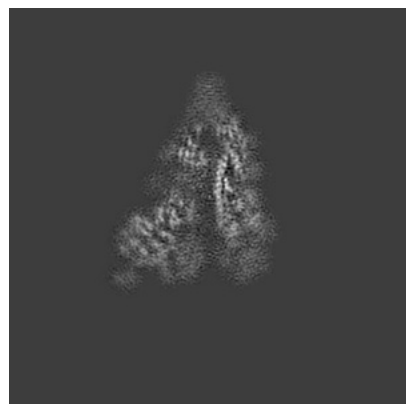


Z

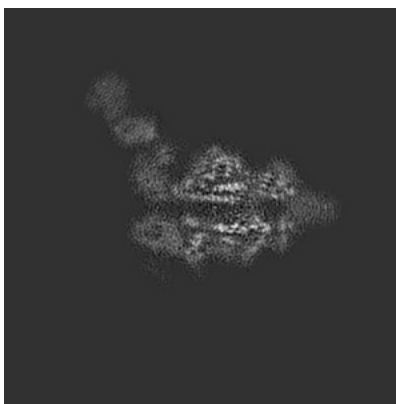
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

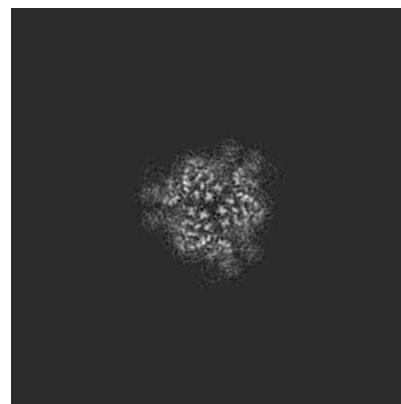
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

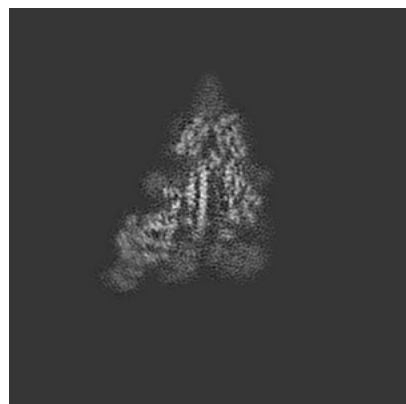


Z Index: 160

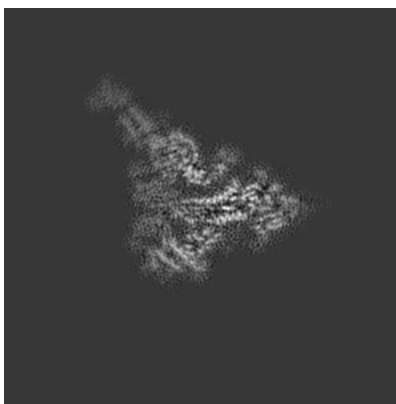
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

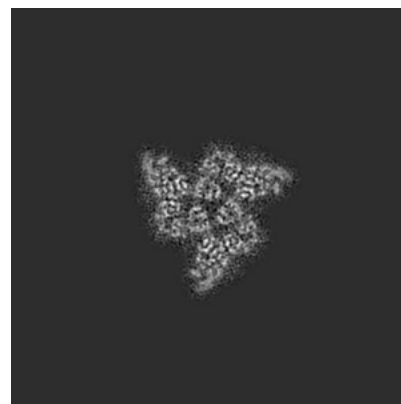
### 6.3.1 Primary map



X Index: 154



Y Index: 174

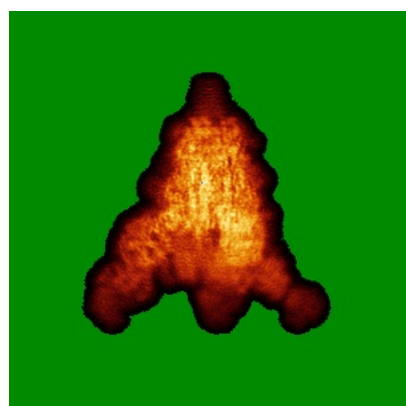


Z Index: 149

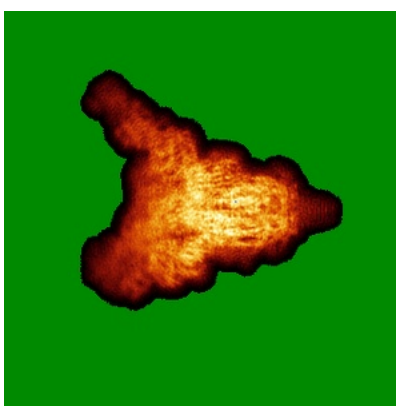
The images above show the largest variance slices of the map in three orthogonal directions.

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

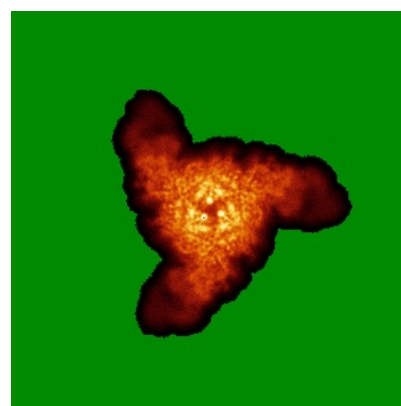
### 6.4.1 Primary map



X



Y

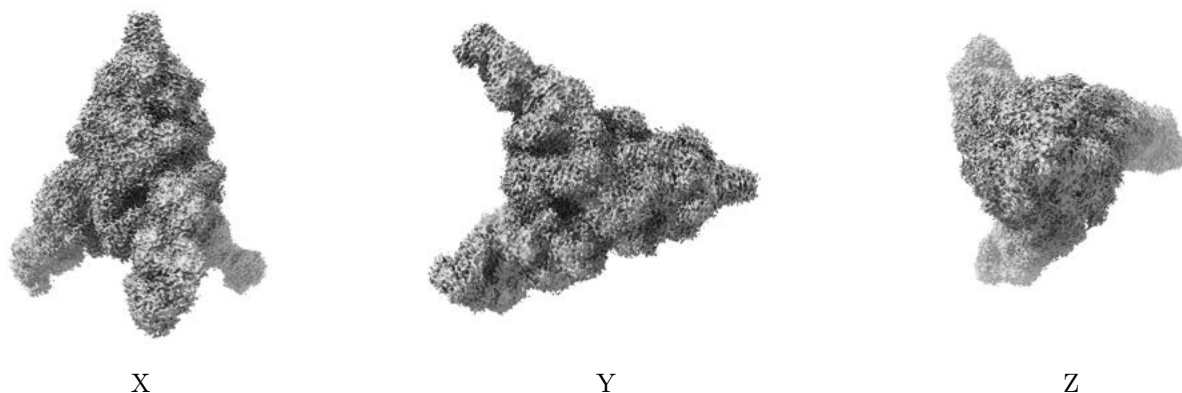


Z

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 [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

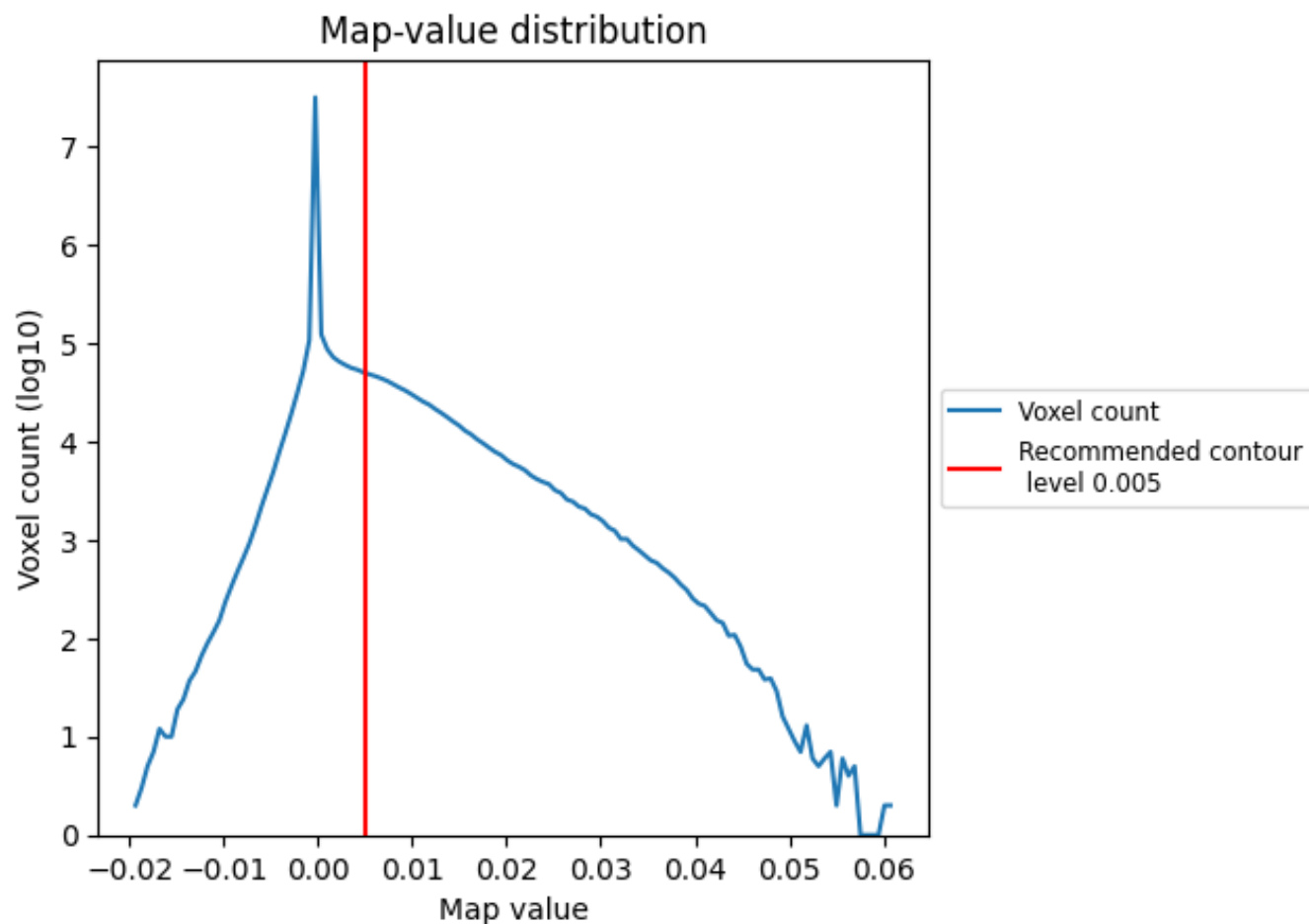
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

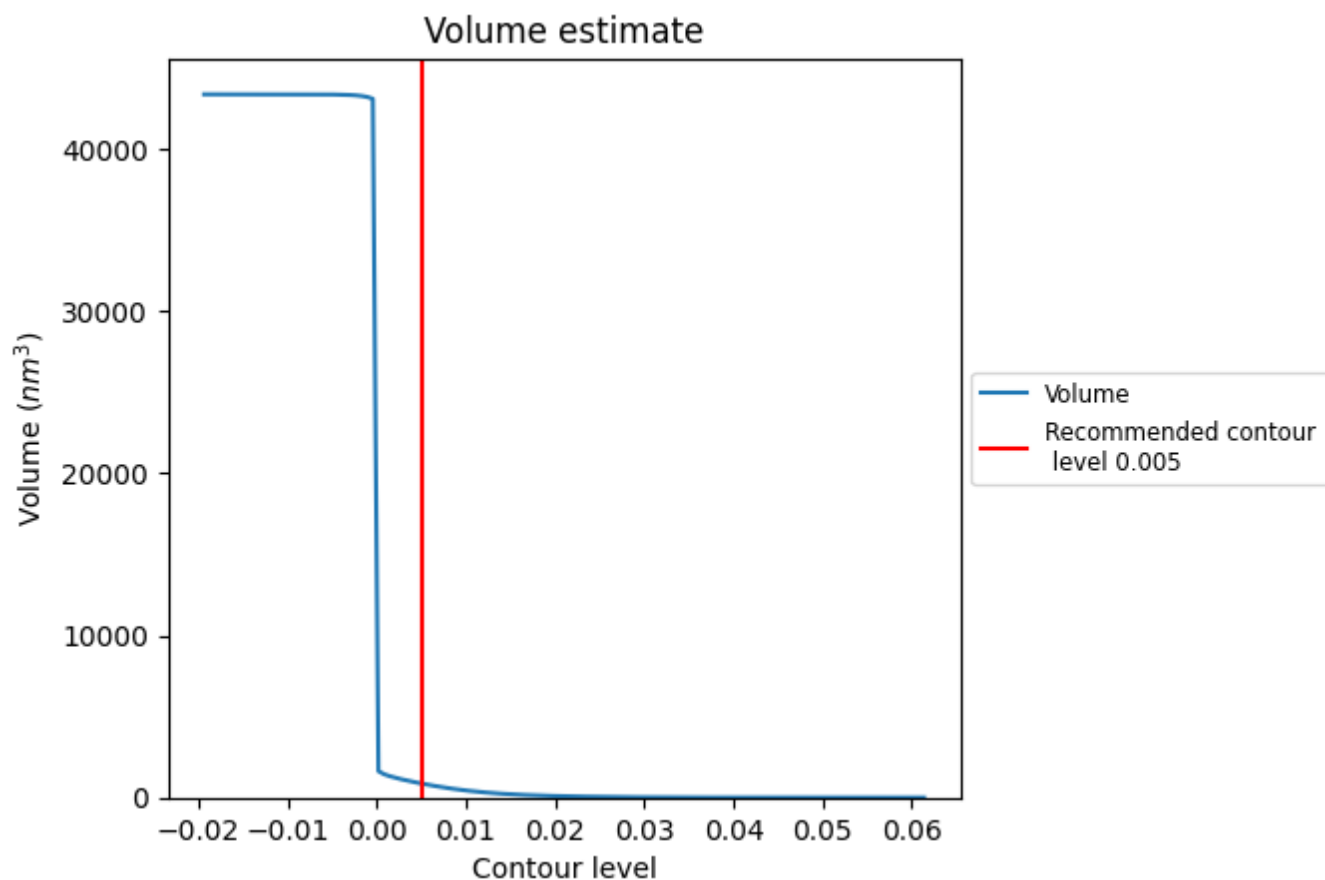
### 7.1 Map-value distribution [i](#)



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



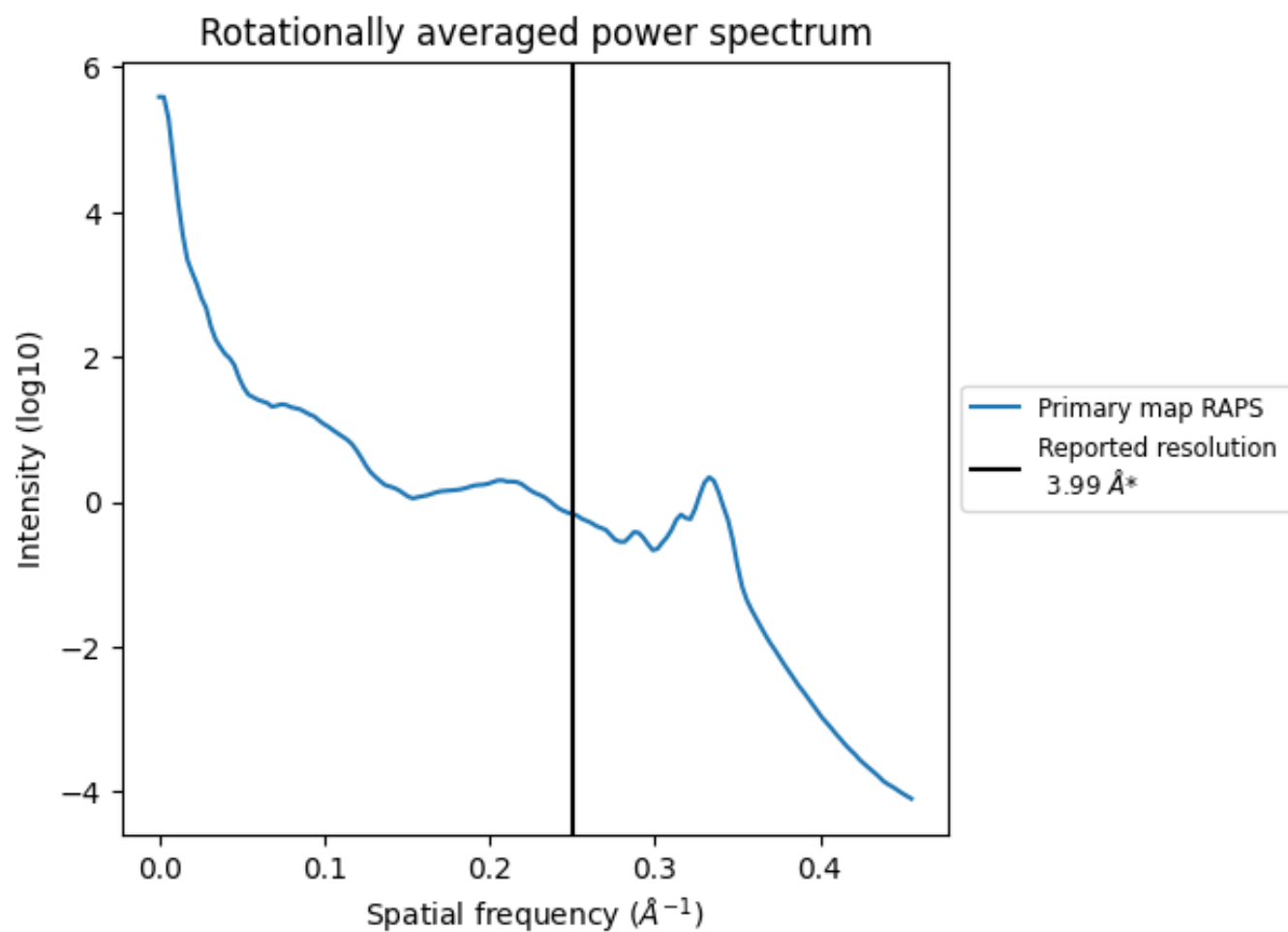
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 869 nm<sup>3</sup>; this corresponds to an approximate mass of 785 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.251 Å<sup>-1</sup>

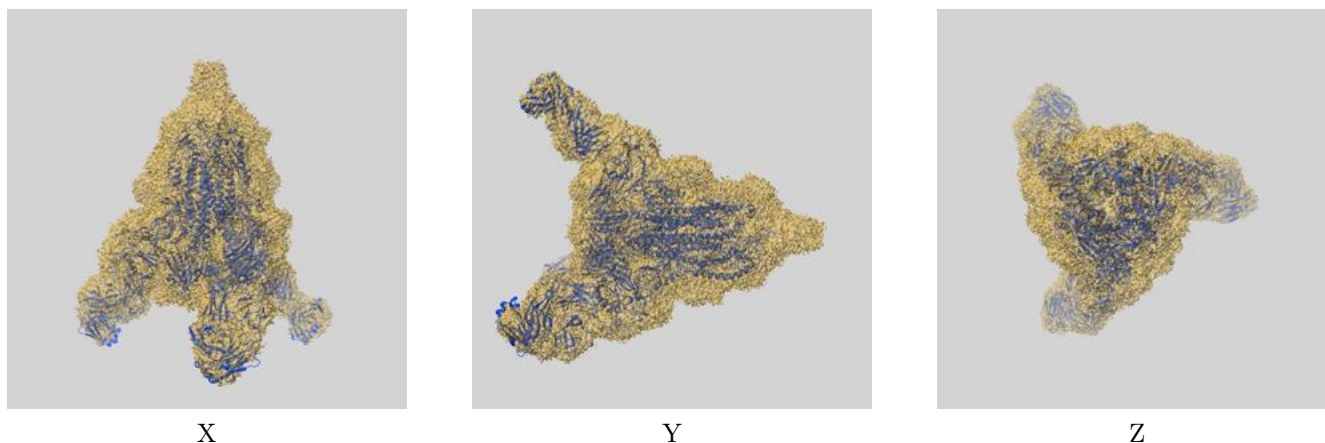
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

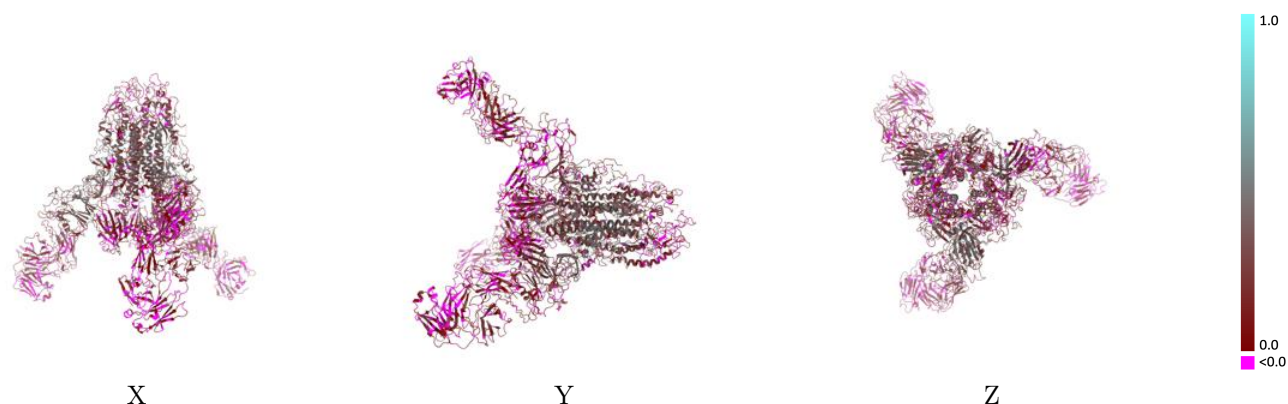
This section contains information regarding the fit between EMDB map EMD-31743 and PDB model 7V6N. Per-residue inclusion information can be found in section [3](#) on page [5](#).

### 9.1 Map-model overlay [i](#)



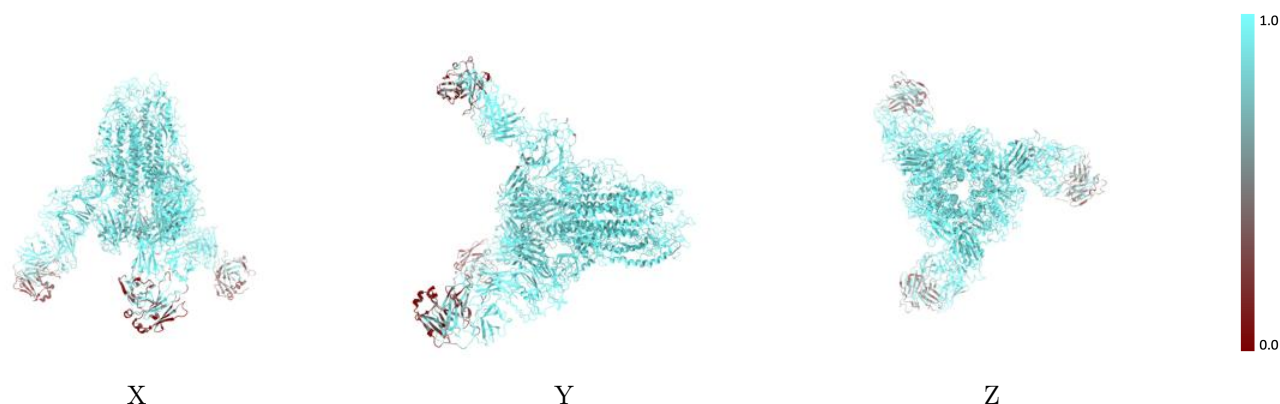
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



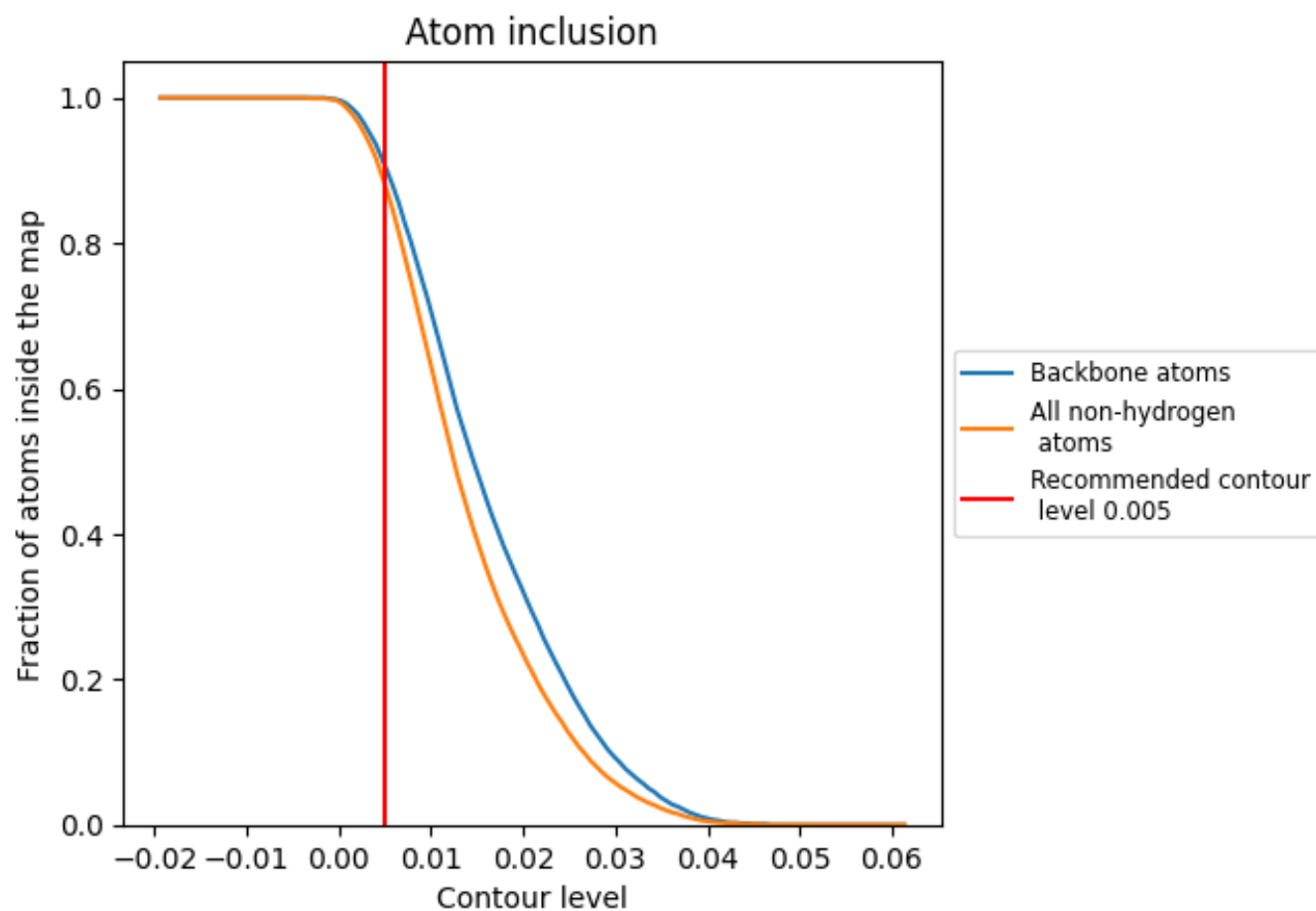
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 91% of all backbone atoms, 88% 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	<div></div> 0.8800	<div></div> 0.1680
A	<div></div> 0.9470	<div></div> 0.1990
B	<div></div> 0.9380	<div></div> 0.1770
C	<div></div> 0.9580	<div></div> 0.2290
D	<div></div> 0.6710	<div></div> 0.0950
E	<div></div> 0.7690	<div></div> 0.0910
F	<div></div> 0.6740	<div></div> 0.0840
G	<div></div> 0.7420	<div></div> 0.0780
H	<div></div> 0.6460	<div></div> 0.0760
I	<div></div> 0.7710	<div></div> 0.0940

1.0

0.0

<0.0