



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:13 AM UTC

PDB ID : 3J7X / pdb_00003j7x
EMDB ID : EMD-6037
Title : Capsid Expansion Mechanism Of Bacteriophage T7 Revealed By Multi-State Atomic Models Derived From Cryo-EM Reconstructions
Authors : Guo, F.; Liu, Z.; Fang, P.A.; Zhang, Q.; Wright, E.T.; Wu, W.; Zhang, C.; Vago, F.; Ren, Y.; Jakata, J.; Chiu, W.; Serwer, P.; Jiang, W.
Deposited on : 2014-08-12
Resolution : 3.60 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

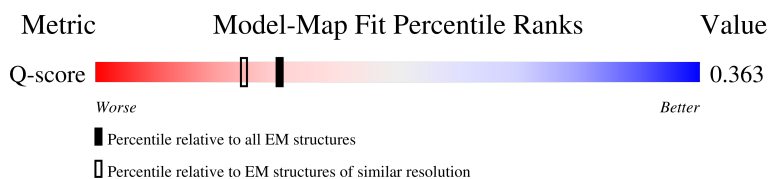
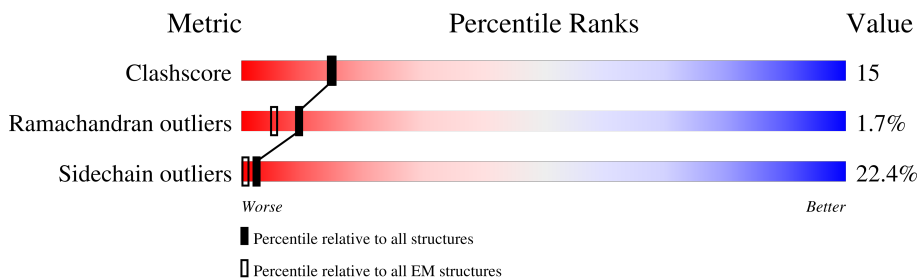
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	345	
1	B	345	
1	C	345	
1	D	345	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	345	16% 58% 31% 9% ..
1	F	345	16% 58% 33% 8% .
1	G	345	33% 58% 32% 10% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17829 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.

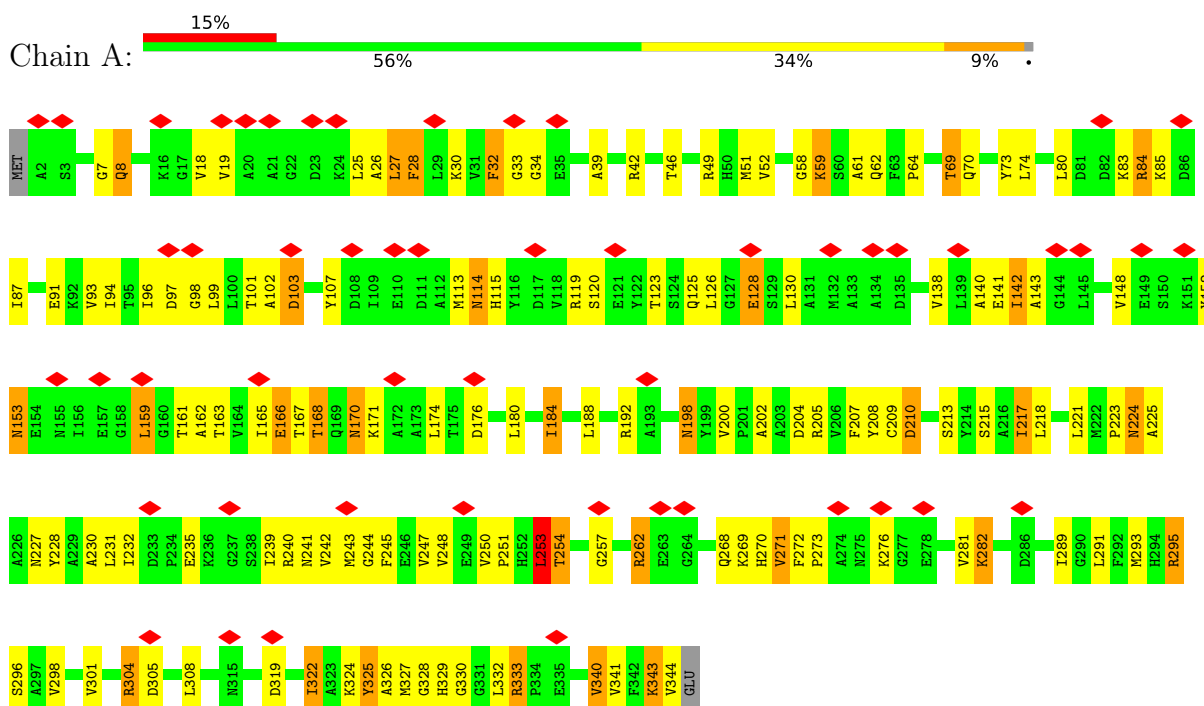
- Molecule 1 is a protein called Major capsid protein 10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	B	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	C	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	D	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	E	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	F	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	G	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		

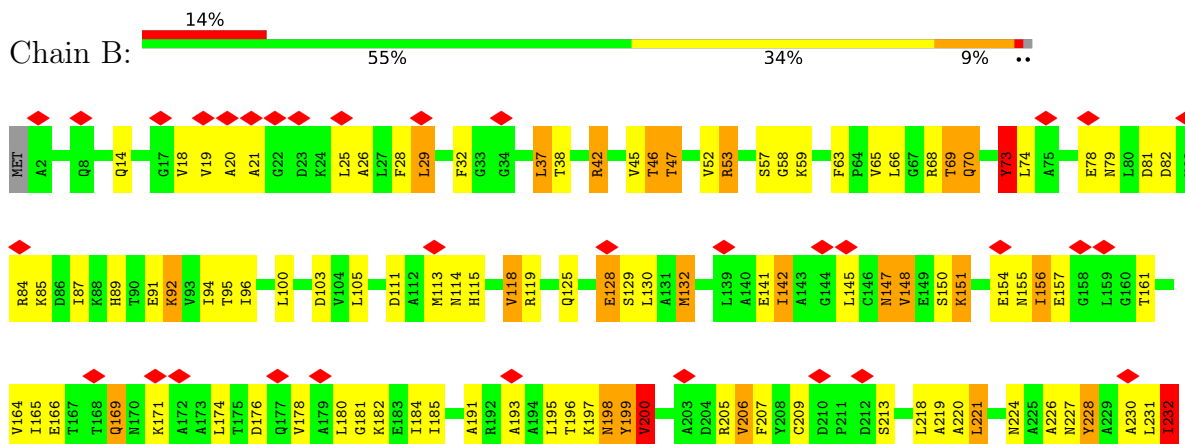
3 Residue-property plots

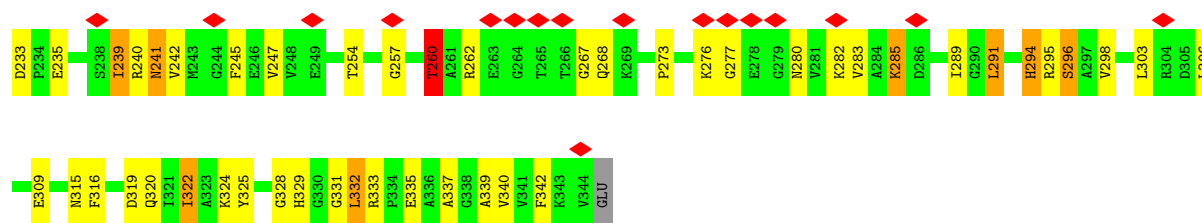
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Major capsid protein 10A

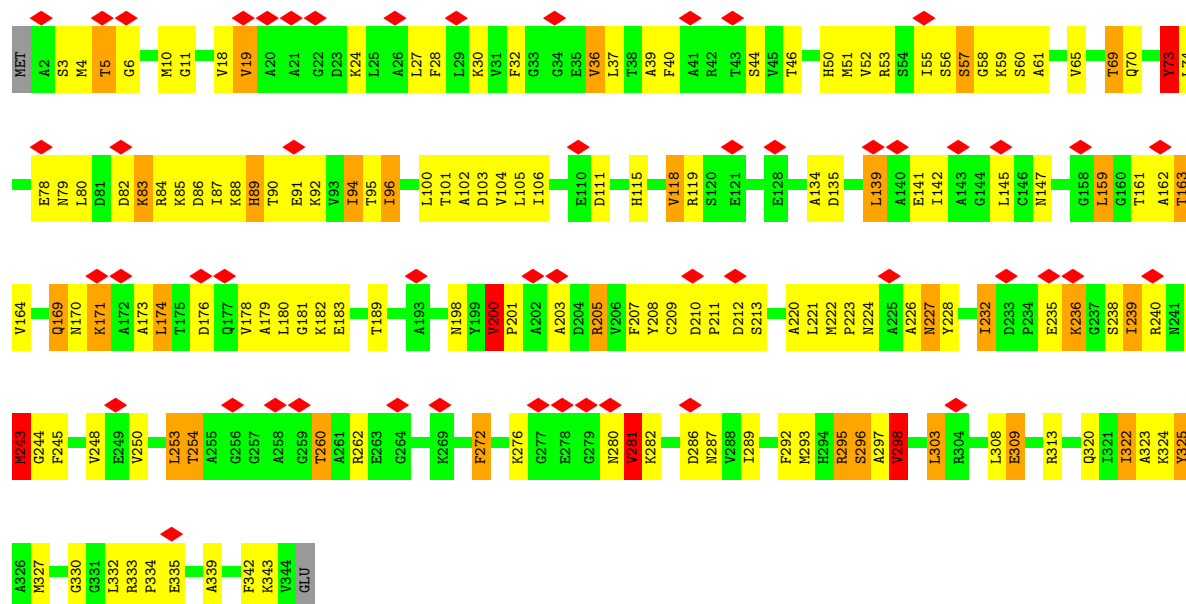


• Molecule 1: Major capsid protein 10A



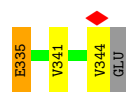


• Molecule 1: Major capsid protein 10A

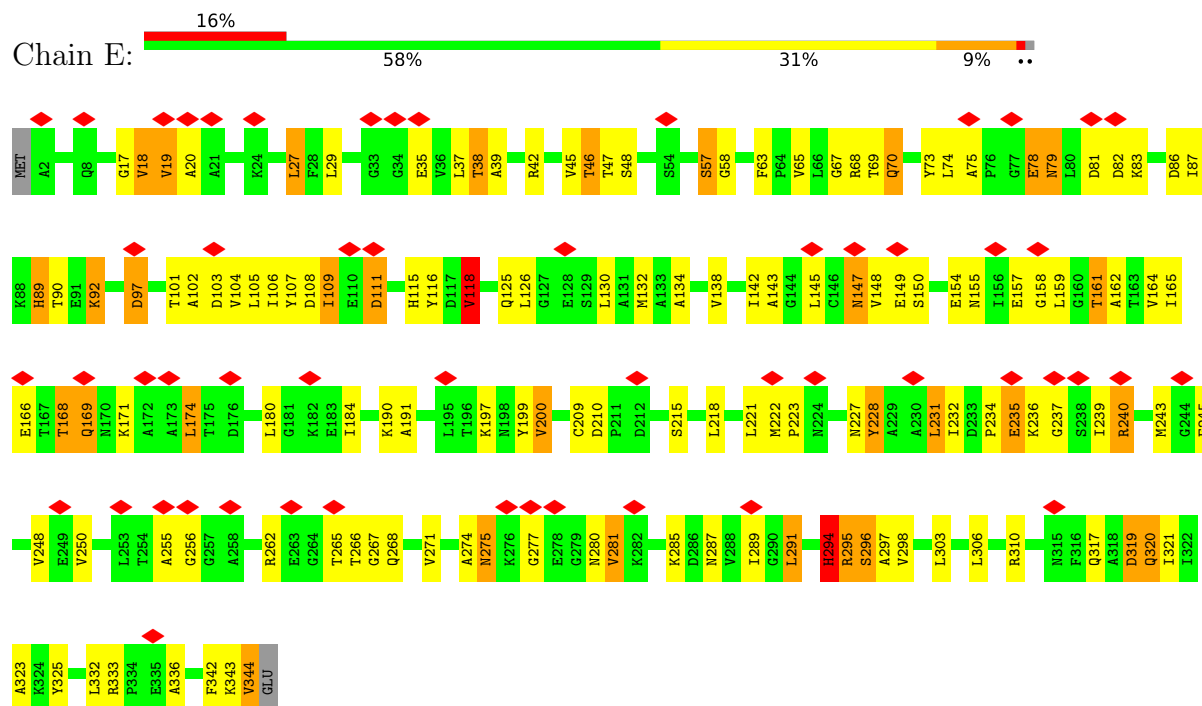


• Molecule 1: Major capsid protein 10A

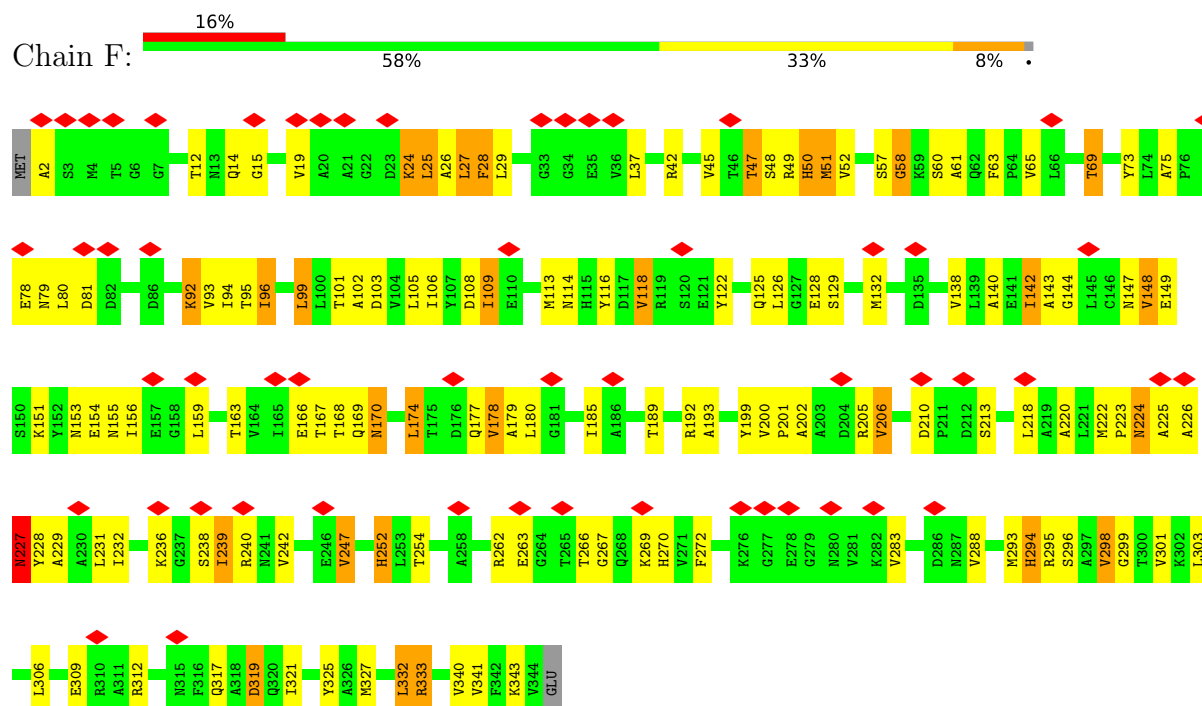




• Molecule 1: Major capsid protein 10A

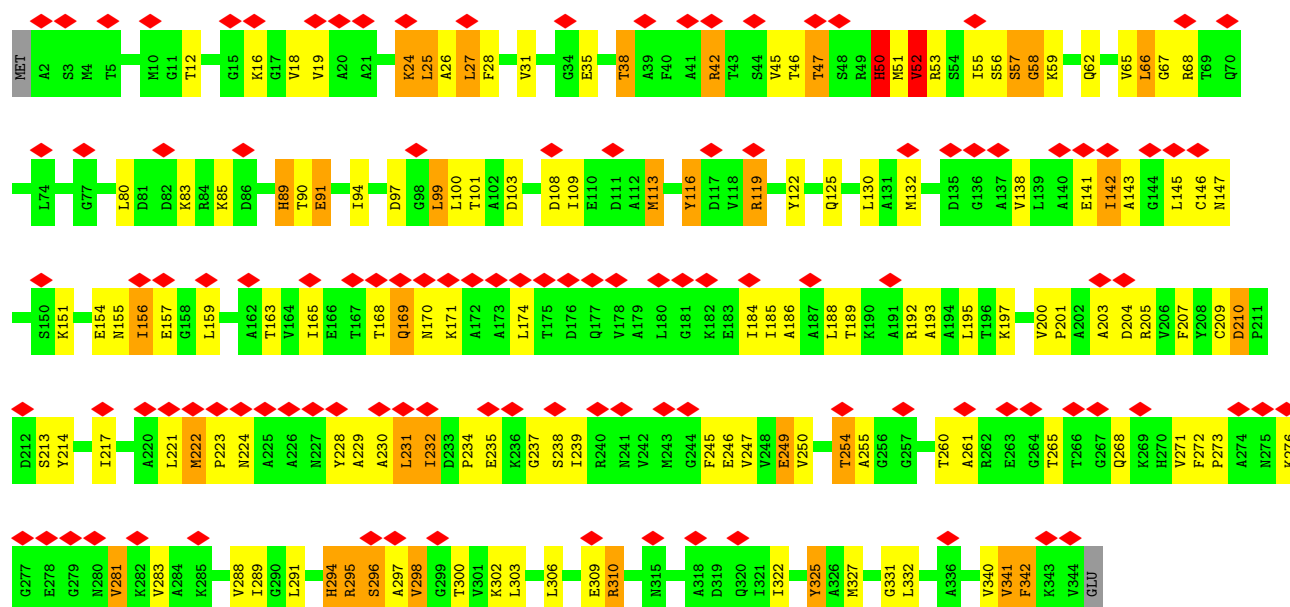


• Molecule 1: Major capsid protein 10A



• Molecule 1: Major capsid protein 10A

Chain G: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	33952	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	57727	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	28.700	Depositor
Minimum map value	-18.852	Depositor
Average map value	0.120	Depositor
Map value standard deviation	1.198	Depositor
Recommended contour level	4.6	Depositor
Map size ($\text{\AA}$)	880.0, 880.0, 880.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	0.37	0/2582	0.91	9/3491 (0.3%)
1	B	0.38	0/2582	0.98	10/3491 (0.3%)
1	C	0.37	0/2582	0.94	10/3491 (0.3%)
1	D	0.38	0/2582	0.96	15/3491 (0.4%)
1	E	0.38	0/2582	0.93	6/3491 (0.2%)
1	F	0.39	0/2582	0.90	5/3491 (0.1%)
1	G	0.38	0/2582	0.98	13/3491 (0.4%)
All	All	0.38	0/18074	0.94	68/24437 (0.3%)

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	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	2
All	All	0	9

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	VAL	CA-C-N	-8.89	110.56	119.90
1	B	200	VAL	C-N-CA	-8.89	110.56	119.90
1	G	296	SER	N-CA-C	7.59	122.49	113.23
1	D	176	ASP	N-CA-C	-7.08	104.25	113.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	27	LEU	N-CA-C	-6.86	104.94	113.38
1	D	40	PHE	N-CA-C	6.74	117.98	108.00
1	A	176	ASP	N-CA-C	-6.64	105.18	113.28
1	D	67	GLY	N-CA-C	6.61	121.05	110.87
1	G	67	GLY	N-CA-C	6.50	120.89	110.87
1	C	200	VAL	CA-C-N	6.37	127.81	119.84
1	C	200	VAL	C-N-CA	6.37	127.81	119.84
1	G	99	LEU	CB-CA-C	-6.25	108.35	115.79
1	C	260	THR	CB-CA-C	-6.20	109.41	116.54
1	G	58	GLY	N-CA-C	6.19	120.54	112.25
1	D	175	THR	N-CA-C	6.18	118.37	108.41
1	E	115	HIS	N-CA-C	6.13	118.88	111.40
1	B	227	ASN	N-CA-C	6.08	118.08	108.79
1	F	238	SER	N-CA-C	-6.03	105.50	112.92
1	C	58	GLY	N-CA-C	6.03	120.33	112.25
1	D	43	THR	CB-CA-C	-5.95	109.70	116.54
1	F	58	GLY	N-CA-C	5.90	120.15	112.25
1	F	147	ASN	N-CA-C	5.87	120.56	113.17
1	F	227	ASN	N-CA-C	5.86	118.27	110.53
1	E	27	LEU	N-CA-C	-5.76	106.29	113.38
1	D	260	THR	CB-CA-C	-5.71	109.46	117.23
1	C	250	VAL	N-CA-C	5.70	113.19	107.55
1	G	50	HIS	N-CA-C	5.69	117.57	108.41
1	D	58	GLY	N-CA-C	5.68	119.87	112.25
1	B	169	GLN	N-CA-C	5.68	115.60	108.45
1	A	168	THR	CB-CA-C	-5.64	110.08	116.63
1	E	57	SER	CB-CA-C	-5.64	109.56	117.23
1	D	49	ARG	N-CA-C	-5.63	105.91	112.89
1	D	68	ARG	CB-CA-C	-5.63	109.09	115.79
1	G	276	LYS	N-CA-C	5.62	117.21	111.14
1	A	254	THR	CB-CA-C	-5.62	110.08	116.54
1	G	68	ARG	CB-CA-C	-5.62	109.11	115.79
1	C	296	SER	CA-C-N	5.59	131.77	121.70
1	C	296	SER	C-N-CA	5.59	131.77	121.70
1	G	57	SER	CB-CA-C	-5.57	109.66	117.23
1	E	256	GLY	N-CA-C	-5.55	105.97	115.08
1	B	14	GLN	CB-CA-C	-5.55	110.19	116.63
1	G	254	THR	CB-CA-C	-5.53	110.22	116.63
1	C	57	SER	CB-CA-C	-5.53	109.71	117.23
1	B	235	GLU	N-CA-C	-5.50	106.61	113.38
1	A	58	GLY	N-CA-C	5.45	118.33	112.33
1	D	117	ASP	CA-C-N	5.43	131.48	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	ASP	C-N-CA	5.43	131.48	121.70
1	G	250	VAL	CA-C-N	5.43	125.05	119.56
1	G	250	VAL	C-N-CA	5.43	125.05	119.56
1	A	253	LEU	N-CA-C	-5.43	102.13	109.95
1	B	228	TYR	N-CA-C	5.39	119.24	109.32
1	B	73	TYR	N-CA-C	5.39	119.02	112.23
1	D	34	GLY	N-CA-C	-5.38	108.20	115.36
1	A	271	VAL	N-CA-C	5.37	116.10	108.42
1	E	168	THR	CB-CA-C	-5.34	109.97	117.23
1	B	260	THR	CB-CA-C	-5.32	110.00	117.23
1	F	52	VAL	N-CA-C	5.30	116.25	109.30
1	D	46	THR	CB-CA-C	-5.21	110.54	116.54
1	C	73	TYR	N-CA-C	5.19	115.91	108.74
1	G	116	TYR	N-CA-C	5.18	117.25	108.02
1	B	230	ALA	CB-CA-C	-5.17	110.59	116.54
1	A	230	ALA	N-CA-C	5.17	115.65	108.00
1	C	295	ARG	N-CA-C	-5.16	99.81	110.80
1	A	250	VAL	CA-C-N	5.12	125.41	119.47
1	A	250	VAL	C-N-CA	5.12	125.41	119.47
1	D	222	MET	CA-C-N	-5.11	113.45	119.84
1	D	222	MET	C-N-CA	-5.11	113.45	119.84
1	E	228	TYR	N-CA-C	5.08	117.56	109.02

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	GLN	Peptide
1	B	294	HIS	Peptide
1	C	238	SER	Peptide
1	C	243	MET	Peptide
1	D	294	HIS	Peptide
1	E	294	HIS	Peptide
1	F	294	HIS	Peptide
1	G	116	TYR	Peptide
1	G	294	HIS	Peptide

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	2547	0	2573	90	0
1	B	2547	0	2573	93	0
1	C	2547	0	2573	93	0
1	D	2547	0	2573	79	0
1	E	2547	0	2573	86	0
1	F	2547	0	2573	92	0
1	G	2547	0	2573	79	0
All	All	17829	0	18011	538	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 15.

All (538) 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:C:296:SER:HA	1:C:298:VAL:H	1.46	0.80
1:C:32:PHE:HA	1:D:62:GLN:H	1.45	0.79
1:C:147:ASN:HD21	1:C:282:LYS:HB2	1.49	0.77
1:C:163:THR:HB	1:C:339:ALA:H	1.49	0.77
1:A:184:ILE:HD11	1:A:289:ILE:HG21	1.66	0.76
1:E:67:GLY:H	1:E:87:ILE:HG22	1.52	0.74
1:B:100:LEU:HA	1:C:73:TYR:HB3	1.69	0.74
1:G:205:ARG:HB2	1:G:245:PHE:HB3	1.70	0.73
1:C:170:ASN:HB3	1:C:173:ALA:HB2	1.69	0.73
1:E:75:ALA:HB3	1:E:78:GLU:HG2	1.71	0.73
1:G:154:GLU:HG3	1:G:155:ASN:HD22	1.54	0.72
1:E:158:GLY:HA2	1:E:159:LEU:HB2	1.72	0.71
1:F:239:ILE:HD12	1:F:247:VAL:HG21	1.73	0.71
1:C:276:LYS:HG3	1:C:287:ASN:HD21	1.55	0.71
1:G:295:ARG:C	1:G:297:ALA:HA	2.16	0.70
1:A:243:MET:HE2	1:F:218:LEU:HD11	1.74	0.70
1:B:205:ARG:HA	1:B:294:HIS:HA	1.73	0.70
1:D:233:ASP:OD1	1:D:233:ASP:N	2.25	0.70
1:F:42:ARG:NH2	1:F:132:MET:SD	2.65	0.69
1:B:231:LEU:HG	1:B:232:ILE:HG23	1.74	0.69
1:E:227:ASN:H	1:F:227:ASN:HD22	1.39	0.69
1:C:198:ASN:ND2	1:C:335:GLU:O	2.25	0.69
1:G:42:ARG:NH2	1:G:132:MET:SD	2.61	0.69
1:A:244:GLY:H	1:F:236:LYS:H	1.41	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:ARG:HH11	1:G:42:ARG:H	1.40	0.68
1:A:99:LEU:HD11	1:A:324:LYS:HB2	1.75	0.68
1:G:119:ARG:H	1:G:119:ARG:HH11	1.42	0.68
1:E:102:ALA:HB1	1:E:126:LEU:HD22	1.75	0.67
1:E:215:SER:HB3	1:F:193:ALA:HB2	1.75	0.67
1:D:45:VAL:HG13	1:D:46:THR:HG23	1.77	0.67
1:F:47:THR:OG1	1:F:48:SER:N	2.27	0.67
1:A:119:ARG:NH2	1:A:319:ASP:OD1	2.27	0.67
1:E:274:ALA:HA	1:E:285:LYS:HB3	1.77	0.67
1:E:221:LEU:HD23	1:E:232:ILE:HB	1.77	0.66
1:C:103:ASP:OD1	1:D:84:ARG:NH2	2.28	0.66
1:E:275:ASN:ND2	1:E:277:GLY:O	2.28	0.66
1:F:96:ILE:HG22	1:F:301:VAL:HG21	1.76	0.66
1:B:141:GLU:OE2	1:B:331:GLY:N	2.29	0.65
1:C:88:LYS:O	1:C:89:HIS:ND1	2.30	0.65
1:A:224:ASN:N	1:A:224:ASN:OD1	2.29	0.65
1:D:253:LEU:C	1:D:254:THR:HG1	2.04	0.64
1:D:253:LEU:O	1:D:285:LYS:NZ	2.29	0.64
1:G:209:CYS:SG	1:G:213:SER:OG	2.55	0.64
1:G:51:MET:HB2	1:G:297:ALA:HB3	1.78	0.64
1:B:57:SER:OG	1:B:58:GLY:N	2.31	0.64
1:E:79:ASN:HD21	1:E:81:ASP:HB3	1.63	0.64
1:A:159:LEU:HD13	1:A:198:ASN:HA	1.78	0.63
1:A:241:ASN:ND2	1:A:245:PHE:O	2.30	0.63
1:E:171:LYS:HA	1:E:174:LEU:HD22	1.79	0.63
1:F:224:ASN:N	1:F:224:ASN:OD1	2.31	0.63
1:A:171:LYS:HA	1:A:174:LEU:HB2	1.81	0.63
1:C:254:THR:HA	1:C:272:PHE:HD2	1.64	0.63
1:C:169:GLN:HB3	1:C:343:LYS:HE2	1.80	0.63
1:C:295:ARG:C	1:C:297:ALA:HB3	2.24	0.63
1:D:42:ARG:NE	1:E:199:TYR:OH	2.25	0.63
1:B:37:LEU:HB2	1:C:65:VAL:HG12	1.81	0.63
1:G:209:CYS:SG	1:G:210:ASP:N	2.71	0.63
1:E:102:ALA:HB3	1:E:323:ALA:HB3	1.81	0.62
1:A:209:CYS:SG	1:A:210:ASP:N	2.72	0.62
1:C:39:ALA:HB2	1:D:67:GLY:HA2	1.80	0.62
1:C:181:GLY:HA3	1:C:220:ALA:HB2	1.81	0.62
1:D:250:VAL:HG23	1:D:253:LEU:HD23	1.82	0.62
1:A:227:ASN:ND2	1:F:223:PRO:O	2.31	0.62
1:C:243:MET:O	1:C:245:PHE:N	2.32	0.62
1:C:161:THR:OG1	1:C:162:ALA:N	2.25	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:HA	1:B:228:TYR:HE2	1.65	0.61
1:F:178:VAL:HG23	1:F:220:ALA:HA	1.82	0.61
1:A:113:MET:O	1:A:114:ASN:ND2	2.32	0.61
1:F:114:ASN:HD22	1:F:116:TYR:H	1.48	0.61
1:A:103:ASP:HB2	1:A:322:ILE:HG22	1.82	0.60
1:B:69:THR:OG1	1:B:70:GLN:N	2.33	0.60
1:E:296:SER:OG	1:E:333:ARG:NH2	2.34	0.60
1:A:96:ILE:HA	1:A:328:GLY:HA3	1.83	0.60
1:D:302:LYS:NZ	1:D:305:ASP:OD2	2.34	0.60
1:E:125:GLN:OE1	1:F:69:THR:OG1	2.19	0.60
1:D:117:ASP:OD2	1:D:117:ASP:N	2.34	0.60
1:C:203:ALA:HA	1:C:205:ARG:HD2	1.82	0.60
1:B:294:HIS:O	1:B:295:ARG:HG2	2.02	0.60
1:C:51:MET:HG2	1:C:296:SER:HB3	1.83	0.60
1:G:38:THR:OG1	1:G:125:GLN:NE2	2.35	0.59
1:D:88:LYS:O	1:D:89:HIS:ND1	2.35	0.59
1:F:201:PRO:O	1:F:205:ARG:NH1	2.35	0.59
1:D:235:GLU:OE2	1:E:240:ARG:NH1	2.36	0.59
1:B:18:VAL:HB	1:B:21:ALA:HB2	1.84	0.59
1:F:178:VAL:O	1:F:180:LEU:N	2.35	0.59
1:G:232:ILE:HA	1:G:239:ILE:H	1.66	0.59
1:A:125:GLN:HG3	1:B:69:THR:HG22	1.83	0.59
1:A:184:ILE:HG21	1:A:217:ILE:HG12	1.83	0.59
1:D:229:ALA:HB2	1:E:228:TYR:CZ	2.38	0.59
1:E:103:ASP:OD1	1:E:262:ARG:NH2	2.36	0.59
1:B:125:GLN:NE2	1:B:128:GLU:OE1	2.35	0.59
1:D:37:LEU:HD12	1:E:65:VAL:HG12	1.85	0.58
1:G:25:LEU:HD13	1:G:25:LEU:H	1.68	0.58
1:D:117:ASP:HA	1:D:118:VAL:HG12	1.85	0.58
1:E:148:VAL:HG22	1:E:281:VAL:HG23	1.85	0.58
1:G:42:ARG:H	1:G:42:ARG:NH1	2.02	0.58
1:A:168:THR:O	1:A:343:LYS:NZ	2.35	0.58
1:D:181:GLY:O	1:D:185:ILE:HG12	2.04	0.58
1:B:161:THR:OG1	1:B:337:ALA:O	2.21	0.57
1:E:143:ALA:O	1:E:147:ASN:ND2	2.38	0.57
1:B:309:GLU:HG2	1:B:322:ILE:HG12	1.87	0.57
1:C:289:ILE:HD11	1:C:342:PHE:CZ	2.39	0.57
1:A:153:ASN:N	1:A:153:ASN:OD1	2.37	0.57
1:D:181:GLY:HA3	1:D:220:ALA:HB2	1.86	0.57
1:F:202:ALA:O	1:F:205:ARG:NH1	2.38	0.57
1:A:39:ALA:HB1	1:B:68:ARG:HH21	1.67	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ILE:HD12	1:B:291:LEU:HD13	1.88	0.56
1:B:218:LEU:HD11	1:B:232:ILE:HD13	1.88	0.56
1:D:144:GLY:O	1:D:148:VAL:HG23	2.06	0.56
1:F:178:VAL:C	1:F:180:LEU:H	2.13	0.56
1:F:92:LYS:NZ	1:F:93:VAL:O	2.38	0.56
1:E:319:ASP:OD2	1:E:319:ASP:N	2.38	0.56
1:F:294:HIS:O	1:F:294:HIS:ND1	2.39	0.56
1:B:81:ASP:OD1	1:B:82:ASP:N	2.39	0.56
1:E:266:THR:OG1	1:E:267:GLY:N	2.38	0.56
1:F:288:VAL:HA	1:F:341:VAL:HG12	1.88	0.56
1:E:42:ARG:HG2	1:F:199:TYR:CZ	2.41	0.56
1:B:276:LYS:NZ	1:B:277:GLY:O	2.38	0.55
1:D:165:ILE:HG12	1:D:166:GLU:H	1.71	0.55
1:E:150:SER:OG	1:E:280:ASN:ND2	2.40	0.55
1:F:102:ALA:HB1	1:F:126:LEU:HD22	1.88	0.55
1:G:46:THR:HB	1:G:47:THR:HA	1.87	0.55
1:G:50:HIS:O	1:G:50:HIS:ND1	2.39	0.55
1:C:208:TYR:HE2	1:C:293:MET:HE2	1.70	0.55
1:C:86:ASP:OD1	1:C:87:ILE:N	2.40	0.55
1:A:273:PRO:HG2	1:A:281:VAL:HG21	1.89	0.55
1:G:119:ARG:HA	1:G:122:TYR:HB2	1.89	0.55
1:E:104:VAL:O	1:E:320:GLN:HB2	2.07	0.54
1:G:25:LEU:HB2	1:G:26:ALA:HA	1.89	0.54
1:G:342:PHE:HD1	1:G:342:PHE:H	1.53	0.54
1:D:45:VAL:HG22	1:D:46:THR:H	1.73	0.54
1:E:235:GLU:O	1:E:237:GLY:N	2.35	0.54
1:F:142:ILE:HD12	1:F:293:MET:HE2	1.89	0.54
1:B:28:PHE:CD2	1:C:59:LYS:HB2	2.42	0.54
1:D:147:ASN:HB2	1:D:283:VAL:HG11	1.90	0.54
1:B:125:GLN:HG3	1:C:87:ILE:HD11	1.90	0.54
1:C:171:LYS:NZ	1:C:286:ASP:O	2.40	0.54
1:E:143:ALA:HB2	1:E:291:LEU:HD13	1.88	0.54
1:G:138:VAL:O	1:G:142:ILE:HG22	2.07	0.54
1:G:169:GLN:OE1	1:G:170:ASN:N	2.39	0.54
1:C:69:THR:OG1	1:C:70:GLN:N	2.41	0.54
1:G:203:ALA:O	1:G:205:ARG:N	2.41	0.53
1:B:129:SER:HB3	1:C:69:THR:HG23	1.91	0.53
1:C:235:GLU:N	1:D:242:VAL:O	2.36	0.53
1:A:223:PRO:HB3	1:B:226:ALA:HB1	1.91	0.53
1:B:180:LEU:O	1:B:184:ILE:HG12	2.08	0.53
1:G:273:PRO:HG2	1:G:281:VAL:HG21	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ALA:H	1:C:333:ARG:HG3	1.74	0.53
1:C:111:ASP:OD1	1:C:119:ARG:NH2	2.41	0.53
1:D:333:ARG:O	1:D:335:GLU:N	2.37	0.53
1:B:65:VAL:HG22	1:B:91:GLU:HA	1.91	0.53
1:D:79:ASN:N	1:D:79:ASN:OD1	2.43	0.52
1:G:56:SER:OG	1:G:57:SER:N	2.42	0.52
1:A:215:SER:HB2	1:B:193:ALA:HB2	1.91	0.52
1:C:226:ALA:O	1:C:227:ASN:ND2	2.42	0.52
1:B:262:ARG:HD3	1:C:85:LYS:HB2	1.91	0.52
1:B:79:ASN:ND2	1:F:2:ALA:O	2.43	0.52
1:D:159:LEU:HB3	1:D:335:GLU:HB2	1.92	0.52
1:E:78:GLU:OE2	1:E:83:LYS:NZ	2.43	0.52
1:C:262:ARG:O	1:D:70:GLN:NE2	2.43	0.52
1:D:101:THR:OG1	1:D:102:ALA:N	2.43	0.52
1:F:168:THR:OG1	1:F:169:GLN:N	2.42	0.52
1:A:273:PRO:HG2	1:A:281:VAL:HG11	1.92	0.52
1:E:174:LEU:HD21	1:E:180:LEU:HD13	1.92	0.52
1:A:61:ALA:HB3	1:A:301:VAL:HG21	1.90	0.52
1:D:231:LEU:HG	1:D:232:ILE:HG23	1.92	0.52
1:E:143:ALA:HB1	1:E:291:LEU:HD22	1.92	0.52
1:G:214:TYR:CG	1:G:249:GLU:HG2	2.44	0.52
1:A:205:ARG:HD2	1:A:244:GLY:O	2.10	0.51
1:C:296:SER:HA	1:C:298:VAL:N	2.21	0.51
1:D:327:MET:SD	1:D:329:HIS:NE2	2.83	0.51
1:F:252:HIS:H	1:F:252:HIS:CD2	2.28	0.51
1:A:174:LEU:HD13	1:A:180:LEU:HD13	1.92	0.51
1:F:50:HIS:HE1	1:F:298:VAL:HG22	1.75	0.51
1:G:201:PRO:HG2	1:G:294:HIS:NE2	2.26	0.51
1:A:202:ALA:HA	1:A:205:ARG:NH2	2.25	0.51
1:A:207:PHE:HD2	1:A:247:VAL:HG22	1.74	0.51
1:F:170:ASN:OD1	1:F:170:ASN:N	2.40	0.51
1:E:180:LEU:O	1:E:184:ILE:HG12	2.10	0.51
1:A:240:ARG:HA	1:A:240:ARG:HH11	1.75	0.51
1:D:100:LEU:HD23	1:D:325:TYR:HE2	1.75	0.51
1:F:79:ASN:OD1	1:F:80:LEU:N	2.44	0.51
1:F:103:ASP:OD2	1:F:103:ASP:N	2.44	0.51
1:B:155:ASN:ND2	1:B:156:ILE:H	2.09	0.51
1:E:287:ASN:HB2	1:E:342:PHE:HB2	1.91	0.51
1:F:294:HIS:O	1:F:295:ARG:HG2	2.11	0.50
1:G:223:PRO:HA	1:G:224:ASN:C	2.36	0.50
1:B:156:ILE:HG23	1:B:157:GLU:H	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:ASP:O	1:D:325:TYR:HB2	2.10	0.50
1:F:101:THR:OG1	1:F:102:ALA:N	2.44	0.50
1:A:170:ASN:OD1	1:A:170:ASN:N	2.43	0.50
1:A:305:ASP:O	1:A:325:TYR:HB2	2.11	0.50
1:D:174:LEU:HD21	1:D:180:LEU:HD12	1.93	0.50
1:E:108:ASP:HA	1:E:111:ASP:HB3	1.93	0.50
1:A:28:PHE:HB3	1:B:59:LYS:HB2	1.94	0.50
1:B:130:LEU:HD23	1:B:306:LEU:HD11	1.92	0.50
1:C:36:VAL:HG23	1:D:64:PRO:HG2	1.93	0.50
1:C:212:ASP:OD2	1:C:213:SER:N	2.44	0.50
1:E:343:LYS:HD3	1:E:344:VAL:HB	1.93	0.50
1:F:174:LEU:HD13	1:F:180:LEU:HB2	1.94	0.50
1:F:227:ASN:OD1	1:F:227:ASN:N	2.45	0.50
1:F:293:MET:HG3	1:F:295:ARG:H	1.77	0.50
1:F:319:ASP:OD2	1:F:319:ASP:N	2.43	0.50
1:F:27:LEU:HD12	1:G:91:GLU:HB3	1.94	0.50
1:B:114:ASN:O	1:B:115:HIS:ND1	2.44	0.50
1:D:315:ASN:OD1	1:D:315:ASN:N	2.41	0.50
1:G:25:LEU:HB2	1:G:26:ALA:CA	2.42	0.50
1:F:199:TYR:O	1:F:200:VAL:HB	2.11	0.50
1:E:166:GLU:HB3	1:E:343:LYS:HB2	1.93	0.49
1:A:74:LEU:HD11	1:F:99:LEU:HG	1.93	0.49
1:A:138:VAL:O	1:A:142:ILE:HG22	2.13	0.49
1:E:134:ALA:O	1:E:138:VAL:HG23	2.13	0.49
1:G:306:LEU:HA	1:G:325:TYR:HB2	1.95	0.49
1:D:253:LEU:O	1:D:254:THR:OG1	2.23	0.49
1:C:61:ALA:HB3	1:C:94:ILE:HD11	1.94	0.49
1:G:66:LEU:HD23	1:G:89:HIS:HE1	1.77	0.49
1:G:296:SER:N	1:G:297:ALA:HA	2.28	0.49
1:B:119:ARG:NH2	1:B:319:ASP:OD2	2.45	0.49
1:B:241:ASN:OD1	1:B:241:ASN:N	2.45	0.49
1:B:262:ARG:O	1:C:70:GLN:NE2	2.45	0.49
1:E:97:ASP:N	1:E:97:ASP:OD1	2.46	0.49
1:A:120:SER:O	1:A:123:THR:OG1	2.23	0.49
1:C:222:MET:HE3	1:C:223:PRO:HD2	1.94	0.49
1:D:3:SER:OG	1:D:4:MET:N	2.44	0.49
1:E:234:PRO:O	1:E:235:GLU:HG3	2.13	0.49
1:G:302:LYS:HB3	1:G:327:MET:HE3	1.94	0.49
1:E:165:ILE:HG12	1:E:166:GLU:H	1.78	0.49
1:C:3:SER:OG	1:C:4:MET:N	2.46	0.48
1:F:60:SER:OG	1:F:61:ALA:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:HD13	1:B:29:LEU:H	1.78	0.48
1:E:294:HIS:CE1	1:E:296:SER:HB3	2.48	0.48
1:G:24:LYS:HE3	1:G:24:LYS:H	1.77	0.48
1:G:51:MET:O	1:G:52:VAL:HG22	2.13	0.48
1:A:42:ARG:HE	1:A:128:GLU:CD	2.20	0.48
1:A:208:TYR:HE1	1:A:293:MET:HE2	1.79	0.48
1:A:327:MET:SD	1:A:329:HIS:NE2	2.75	0.48
1:A:224:ASN:HD22	1:B:182:LYS:NZ	2.11	0.48
1:G:12:THR:O	1:G:27:LEU:HB2	2.14	0.48
1:C:253:LEU:HD13	1:C:254:THR:H	1.79	0.48
1:E:223:PRO:HA	1:F:228:TYR:HE1	1.78	0.48
1:F:206:VAL:HG12	1:F:293:MET:H	1.78	0.48
1:G:143:ALA:O	1:G:147:ASN:HB3	2.14	0.48
1:G:186:ALA:O	1:G:189:THR:OG1	2.24	0.48
1:G:203:ALA:O	1:G:205:ARG:HG3	2.13	0.48
1:A:97:ASP:OD1	1:A:98:GLY:N	2.41	0.48
1:C:325:TYR:HE2	1:C:327:MET:HE3	1.79	0.48
1:D:99:LEU:HD23	1:E:74:LEU:HD23	1.96	0.48
1:F:15:GLY:N	1:G:90:THR:OG1	2.46	0.48
1:F:205:ARG:HA	1:F:294:HIS:HA	1.96	0.48
1:C:178:VAL:C	1:C:180:LEU:H	2.21	0.48
1:E:17:GLY:C	1:E:19:VAL:H	2.22	0.48
1:F:149:GLU:OE1	1:F:149:GLU:N	2.44	0.48
1:F:166:GLU:HB2	1:F:341:VAL:O	2.14	0.48
1:B:219:ALA:HB2	1:C:189:THR:HG21	1.96	0.47
1:A:142:ILE:HG23	1:A:143:ALA:H	1.78	0.47
1:D:86:ASP:O	1:D:88:LYS:N	2.47	0.47
1:D:262:ARG:O	1:E:70:GLN:NE2	2.34	0.47
1:G:51:MET:HB3	1:G:300:THR:OG1	2.14	0.47
1:G:309:GLU:OE2	1:G:310:ARG:N	2.45	0.47
1:A:244:GLY:H	1:F:236:LYS:N	2.09	0.47
1:A:253:LEU:HD22	1:A:254:THR:H	1.80	0.47
1:C:50:HIS:H	1:C:295:ARG:NH2	2.13	0.47
1:D:232:ILE:HG22	1:D:239:ILE:HG23	1.96	0.47
1:E:45:VAL:HG22	1:E:46:THR:H	1.79	0.47
1:E:231:LEU:HD13	1:E:232:ILE:H	1.80	0.47
1:A:167:THR:HG23	1:A:168:THR:HG23	1.96	0.47
1:A:101:THR:OG1	1:A:102:ALA:N	2.48	0.47
1:A:257:GLY:HA2	1:A:268:GLN:HB3	1.96	0.47
1:B:233:ASP:OD2	1:B:233:ASP:N	2.48	0.47
1:C:56:SER:OG	1:C:57:SER:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:SER:OG	1:C:94:ILE:O	2.25	0.47
1:C:86:ASP:C	1:C:88:LYS:H	2.23	0.47
1:F:205:ARG:HB3	1:F:206:VAL:H	1.54	0.47
1:A:119:ARG:O	1:A:123:THR:HG23	2.14	0.47
1:B:181:GLY:O	1:B:185:ILE:HG12	2.15	0.47
1:C:224:ASN:HD21	1:D:182:LYS:HE2	1.80	0.47
1:E:310:ARG:HB3	1:E:321:ILE:HG13	1.96	0.47
1:A:7:GLY:O	1:A:8:GLN:HB3	2.15	0.47
1:A:204:ASP:OD2	1:A:295:ARG:HB3	2.15	0.47
1:D:89:HIS:O	1:D:90:THR:OG1	2.32	0.47
1:E:89:HIS:CD2	1:E:89:HIS:H	2.32	0.47
1:A:333:ARG:HH11	1:A:333:ARG:HB2	1.78	0.47
1:E:38:THR:OG1	1:E:39:ALA:N	2.48	0.47
1:F:210:ASP:OD1	1:F:210:ASP:N	2.46	0.47
1:G:141:GLU:O	1:G:145:LEU:HB2	2.15	0.47
1:C:239:ILE:HG22	1:C:240:ARG:H	1.79	0.46
1:F:210:ASP:OD1	1:F:213:SER:OG	2.32	0.46
1:B:147:ASN:OD1	1:B:147:ASN:N	2.47	0.46
1:E:97:ASP:HB3	1:F:73:TYR:CE2	2.50	0.46
1:G:156:ILE:HG13	1:G:157:GLU:H	1.79	0.46
1:B:150:SER:O	1:B:151:LYS:HG3	2.16	0.46
1:B:213:SER:HB2	1:B:289:ILE:HG23	1.97	0.46
1:C:235:GLU:HG3	1:D:241:ASN:HB2	1.96	0.46
1:C:101:THR:OG1	1:C:323:ALA:O	2.19	0.46
1:B:25:LEU:HA	1:B:26:ALA:HA	1.78	0.46
1:C:308:LEU:HA	1:C:323:ALA:HA	1.96	0.46
1:D:294:HIS:O	1:D:294:HIS:ND1	2.49	0.46
1:E:106:ILE:HG22	1:E:111:ASP:HB2	1.97	0.46
1:G:165:ILE:HD12	1:G:341:VAL:HG13	1.96	0.46
1:A:276:LYS:HA	1:A:281:VAL:HG23	1.98	0.46
1:C:159:LEU:HD22	1:C:159:LEU:H	1.81	0.46
1:E:228:TYR:HA	1:F:228:TYR:HB3	1.96	0.46
1:D:157:GLU:CD	1:D:159:LEU:HG	2.41	0.46
1:E:294:HIS:HE1	1:E:296:SER:HB3	1.81	0.46
1:A:59:LYS:HD2	1:F:28:PHE:HB3	1.98	0.46
1:F:24:LYS:O	1:F:25:LEU:HD22	2.16	0.46
1:G:254:THR:HG22	1:G:272:PHE:CE2	2.51	0.46
1:B:42:ARG:HH21	1:B:132:MET:HG2	1.81	0.46
1:B:198:ASN:HD22	1:B:335:GLU:CD	2.24	0.46
1:C:141:GLU:HG3	1:C:145:LEU:HD12	1.98	0.46
1:E:184:ILE:HD11	1:E:289:ILE:HG12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:OG1	1:A:70:GLN:N	2.48	0.45
1:A:223:PRO:HG2	1:B:221:LEU:HD12	1.97	0.45
1:B:291:LEU:HA	1:B:339:ALA:HA	1.99	0.45
1:C:161:THR:HG22	1:C:334:PRO:O	2.16	0.45
1:D:229:ALA:HB2	1:E:228:TYR:CE1	2.51	0.45
1:E:289:ILE:HD11	1:E:342:PHE:CD2	2.51	0.45
1:G:221:LEU:O	1:G:222:MET:HB2	2.15	0.45
1:A:209:CYS:SG	1:A:213:SER:HB2	2.56	0.45
1:A:224:ASN:ND2	1:B:182:LYS:HG2	2.32	0.45
1:A:251:PRO:HG3	1:B:199:TYR:CE1	2.51	0.45
1:E:47:THR:HA	1:E:48:SER:HA	1.56	0.45
1:D:269:LYS:HG3	1:E:73:TYR:CE2	2.50	0.45
1:G:100:LEU:HD21	1:G:325:TYR:CE1	2.51	0.45
1:G:192:ARG:HH11	1:G:193:ALA:HA	1.81	0.45
1:B:176:ASP:OD2	1:B:178:VAL:N	2.48	0.45
1:C:210:ASP:HB2	1:C:211:PRO:HD2	1.98	0.45
1:E:218:LEU:O	1:E:222:MET:HG3	2.16	0.45
1:F:301:VAL:O	1:F:327:MET:HB2	2.16	0.45
1:G:47:THR:O	1:G:47:THR:OG1	2.35	0.45
1:B:205:ARG:HB3	1:B:206:VAL:H	1.58	0.45
1:C:207:PHE:HD1	1:C:292:PHE:HB3	1.81	0.45
1:F:12:THR:O	1:F:27:LEU:HD22	2.16	0.45
1:F:269:LYS:HB3	1:F:270:HIS:CE1	2.52	0.45
1:C:174:LEU:H	1:C:174:LEU:HD22	1.81	0.45
1:C:94:ILE:HG22	1:C:330:GLY:HA3	1.98	0.45
1:C:176:ASP:C	1:C:178:VAL:H	2.25	0.45
1:C:309:GLU:HG3	1:C:322:ILE:HG23	1.99	0.45
1:D:100:LEU:HD13	1:E:73:TYR:HD1	1.82	0.45
1:D:138:VAL:O	1:D:142:ILE:HG22	2.16	0.45
1:G:50:HIS:CD2	1:G:138:VAL:HG11	2.52	0.45
1:A:126:LEU:HA	1:B:69:THR:HG21	1.98	0.45
1:C:96:ILE:HG13	1:C:303:LEU:HD11	1.98	0.45
1:B:52:VAL:O	1:B:53:ARG:HD2	2.17	0.45
1:E:154:GLU:OE1	1:E:155:ASN:N	2.47	0.45
1:E:235:GLU:C	1:E:237:GLY:H	2.24	0.45
1:B:315:ASN:OD1	1:B:316:PHE:N	2.48	0.45
1:C:262:ARG:HD2	1:D:72:ALA:HB2	1.99	0.45
1:D:198:ASN:HD22	1:D:335:GLU:HG3	1.82	0.45
1:E:164:VAL:HG21	1:E:191:ALA:HB2	1.99	0.45
1:A:224:ASN:HA	1:A:225:ALA:HA	1.54	0.44
1:B:295:ARG:HG3	1:B:296:SER:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:GLU:H	1:F:63:PHE:HE1	1.64	0.44
1:G:203:ALA:C	1:G:205:ARG:H	2.25	0.44
1:G:245:PHE:HB2	1:G:246:GLU:H	1.53	0.44
1:F:144:GLY:O	1:F:148:VAL:HB	2.16	0.44
1:F:225:ALA:HA	1:F:226:ALA:HA	1.62	0.44
1:C:209:CYS:SG	1:C:213:SER:HB2	2.57	0.44
1:D:117:ASP:HA	1:D:118:VAL:CB	2.48	0.44
1:F:154:GLU:OE2	1:F:155:ASN:N	2.51	0.44
1:F:200:VAL:HG13	1:F:294:HIS:CD2	2.52	0.44
1:A:184:ILE:O	1:A:188:LEU:HB2	2.18	0.44
1:B:224:ASN:HB3	1:C:182:LYS:HE2	1.98	0.44
1:C:134:ALA:HB2	1:C:325:TYR:OH	2.17	0.44
1:D:186:ALA:O	1:D:189:THR:OG1	2.30	0.44
1:F:25:LEU:N	1:F:26:ALA:HB3	2.32	0.44
1:G:230:ALA:HA	1:G:231:LEU:HA	1.63	0.44
1:G:254:THR:OG1	1:G:255:ALA:N	2.50	0.44
1:A:103:ASP:OD1	1:B:84:ARG:NH1	2.39	0.44
1:B:257:GLY:HA3	1:B:268:GLN:HB3	2.00	0.44
1:F:201:PRO:HD2	1:F:294:HIS:CD2	2.52	0.44
1:A:99:LEU:HA	1:A:326:ALA:HB2	2.00	0.44
1:C:50:HIS:HB3	1:C:52:VAL:HG23	1.98	0.44
1:E:45:VAL:C	1:E:47:THR:H	2.25	0.44
1:E:184:ILE:CD1	1:E:289:ILE:HG12	2.48	0.44
1:E:200:VAL:HG21	1:E:336:ALA:HB2	2.00	0.44
1:G:207:PHE:HB2	1:G:245:PHE:CE1	2.53	0.44
1:G:222:MET:HB3	1:G:223:PRO:CD	2.47	0.44
1:C:228:TYR:HA	1:D:228:TYR:HB3	1.99	0.44
1:D:104:VAL:HG11	1:D:122:TYR:HD2	1.83	0.44
1:G:296:SER:O	1:G:296:SER:OG	2.33	0.44
1:A:34:GLY:HA3	1:B:63:PHE:HE1	1.83	0.44
1:B:164:VAL:HG21	1:B:191:ALA:HB2	2.00	0.44
1:F:125:GLN:O	1:F:128:GLU:HG3	2.17	0.44
1:G:185:ILE:O	1:G:189:THR:HG23	2.17	0.44
1:G:265:THR:O	1:G:268:GLN:HG3	2.18	0.44
1:A:166:GLU:OE2	1:A:167:THR:N	2.51	0.43
1:B:294:HIS:ND1	1:B:296:SER:OG	2.50	0.43
1:D:29:LEU:HD12	1:D:29:LEU:H	1.83	0.43
1:G:174:LEU:HD23	1:G:174:LEU:HA	1.86	0.43
1:A:289:ILE:HD12	1:A:340:VAL:HG22	2.00	0.43
1:B:66:LEU:HD12	1:B:66:LEU:HA	1.82	0.43
1:B:89:HIS:O	1:B:89:HIS:ND1	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LYS:HB3	1:B:342:PHE:CD1	2.53	0.43
1:B:239:ILE:HG23	1:B:240:ARG:H	1.83	0.43
1:C:221:LEU:HG	1:C:232:ILE:HD11	2.00	0.43
1:E:161:THR:OG1	1:E:162:ALA:N	2.51	0.43
1:B:19:VAL:HA	1:B:20:ALA:HA	1.56	0.43
1:B:81:ASP:O	1:B:84:ARG:HG2	2.18	0.43
1:C:92:LYS:HD3	1:C:92:LYS:HA	1.81	0.43
1:D:50:HIS:HE1	1:D:300:THR:HG23	1.84	0.43
1:F:109:ILE:HG12	1:G:99:LEU:HG	1.99	0.43
1:B:70:GLN:HE21	1:B:70:GLN:HB3	1.60	0.43
1:B:92:LYS:HD3	1:B:332:LEU:HB3	2.00	0.43
1:A:148:VAL:HG11	1:A:281:VAL:HA	2.00	0.43
1:C:101:THR:OG1	1:C:102:ALA:N	2.52	0.43
1:E:57:SER:OG	1:E:58:GLY:N	2.48	0.43
1:A:51:MET:HG2	1:A:296:SER:HA	2.01	0.43
1:B:181:GLY:HA3	1:B:220:ALA:HB2	2.00	0.43
1:F:113:MET:SD	1:G:59:LYS:HA	2.59	0.43
1:F:185:ILE:O	1:F:189:THR:HG23	2.19	0.43
1:G:57:SER:OG	1:G:58:GLY:N	2.51	0.43
1:G:289:ILE:HB	1:G:340:VAL:HG23	2.01	0.43
1:A:141:GLU:HG2	1:A:330:GLY:HA2	2.01	0.43
1:A:165:ILE:HG12	1:A:166:GLU:H	1.83	0.43
1:B:273:PRO:O	1:B:285:LYS:HB3	2.19	0.43
1:D:35:GLU:HB2	1:E:63:PHE:CD1	2.53	0.43
1:E:69:THR:OG1	1:E:70:GLN:N	2.52	0.43
1:E:280:ASN:ND2	1:E:280:ASN:O	2.52	0.43
1:A:69:THR:HG23	1:F:129:SER:HB2	2.00	0.43
1:A:244:GLY:HA2	1:F:236:LYS:HB3	2.00	0.43
1:B:254:THR:HG21	1:B:285:LYS:HB2	2.01	0.43
1:C:200:VAL:HA	1:C:201:PRO:HD3	1.75	0.43
1:E:19:VAL:HB	1:E:20:ALA:H	1.60	0.43
1:F:151:LYS:HE3	1:F:151:LYS:HB3	1.77	0.43
1:G:294:HIS:O	1:G:294:HIS:CG	2.70	0.43
1:B:328:GLY:O	1:B:329:HIS:ND1	2.52	0.43
1:E:255:ALA:HB1	1:E:268:GLN:HE22	1.84	0.43
1:F:122:TYR:O	1:F:126:LEU:HG	2.19	0.43
1:G:109:ILE:O	1:G:113:MET:HB2	2.19	0.43
1:B:207:PHE:HD1	1:B:247:VAL:HG22	1.84	0.43
1:B:294:HIS:O	1:B:294:HIS:CG	2.71	0.43
1:B:306:LEU:HD12	1:B:325:TYR:CG	2.54	0.43
1:C:236:LYS:H	1:C:236:LYS:HG3	1.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:PRO:O	1:D:225:ALA:N	2.51	0.43
1:A:25:LEU:HA	1:A:26:ALA:HA	1.85	0.42
1:G:103:ASP:OD2	1:G:103:ASP:N	2.51	0.42
1:A:148:VAL:HG22	1:A:282:LYS:H	1.85	0.42
1:E:109:ILE:HD13	1:E:109:ILE:HA	1.88	0.42
1:E:295:ARG:C	1:E:297:ALA:N	2.75	0.42
1:F:51:MET:HB3	1:F:299:GLY:HA2	2.01	0.42
1:G:260:THR:OG1	1:G:261:ALA:N	2.51	0.42
1:C:106:ILE:HG21	1:C:119:ARG:HH21	1.82	0.42
1:D:149:GLU:HB2	1:D:151:LYS:O	2.19	0.42
1:D:255:ALA:HB1	1:D:268:GLN:OE1	2.20	0.42
1:E:243:MET:C	1:E:245:PHE:H	2.27	0.42
1:G:154:GLU:O	1:G:155:ASN:ND2	2.52	0.42
1:B:28:PHE:CE2	1:C:59:LYS:HB2	2.54	0.42
1:C:51:MET:SD	1:C:53:ARG:NH2	2.93	0.42
1:F:75:ALA:HB3	1:F:78:GLU:HG3	2.00	0.42
1:B:232:ILE:HG13	1:B:233:ASP:N	2.35	0.42
1:G:222:MET:SD	1:G:229:ALA:HA	2.59	0.42
1:C:83:LYS:NZ	1:C:83:LYS:H	2.17	0.42
1:D:81:ASP:HA	1:D:84:ARG:NH1	2.33	0.42
1:G:142:ILE:HB	1:G:298:VAL:HG21	2.02	0.42
1:B:322:ILE:HD11	1:B:324:LYS:HE3	2.02	0.42
1:D:96:ILE:HA	1:D:328:GLY:HA3	2.01	0.42
1:D:204:ASP:OD1	1:D:204:ASP:N	2.51	0.42
1:A:84:ARG:HA	1:F:262:ARG:HD3	2.01	0.42
1:B:103:ASP:N	1:B:103:ASP:OD1	2.53	0.42
1:C:5:THR:HG22	1:C:6:GLY:H	1.85	0.42
1:G:146:CYS:HB2	1:G:331:GLY:HA3	2.02	0.42
1:F:266:THR:OG1	1:F:267:GLY:N	2.53	0.42
1:C:232:ILE:H	1:C:232:ILE:HG12	1.62	0.41
1:A:224:ASN:HD22	1:B:182:LYS:HZ2	1.68	0.41
1:C:104:VAL:HG22	1:C:105:LEU:H	1.84	0.41
1:E:92:LYS:HE2	1:E:332:LEU:HA	2.02	0.41
1:F:14:GLN:HB2	1:G:89:HIS:O	2.20	0.41
1:F:24:LYS:HE3	1:F:24:LYS:HB3	1.89	0.41
1:F:239:ILE:HG22	1:F:240:ARG:H	1.85	0.41
1:A:27:LEU:HD13	1:A:27:LEU:O	2.19	0.41
1:D:294:HIS:O	1:D:294:HIS:CG	2.72	0.41
1:F:138:VAL:O	1:F:142:ILE:HG22	2.20	0.41
1:F:333:ARG:HH11	1:F:333:ARG:HB2	1.85	0.41
1:A:207:PHE:CD2	1:A:247:VAL:HG22	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:THR:OG1	1:B:47:THR:N	2.53	0.41
1:B:174:LEU:HD11	1:B:180:LEU:HD13	2.02	0.41
1:B:198:ASN:N	1:B:198:ASN:OD1	2.51	0.41
1:B:260:THR:OG1	1:B:267:GLY:O	2.34	0.41
1:D:42:ARG:HH22	1:D:132:MET:HE3	1.84	0.41
1:E:295:ARG:HD2	1:E:296:SER:H	1.86	0.41
1:A:140:ALA:HA	1:A:272:PHE:CZ	2.56	0.41
1:C:207:PHE:HE2	1:C:209:CYS:HB2	1.85	0.41
1:A:32:PHE:CG	1:A:33:GLY:N	2.87	0.41
1:C:50:HIS:CE1	1:C:298:VAL:HB	2.55	0.41
1:D:294:HIS:O	1:D:295:ARG:HG2	2.20	0.41
1:E:37:LEU:O	1:F:65:VAL:HA	2.20	0.41
1:E:168:THR:OG1	1:E:169:GLN:N	2.53	0.41
1:E:294:HIS:O	1:E:294:HIS:CG	2.73	0.41
1:G:184:ILE:HB	1:G:217:ILE:HD11	2.02	0.41
1:B:218:LEU:HD12	1:B:218:LEU:HA	1.86	0.41
1:B:232:ILE:CG2	1:B:239:ILE:HA	2.51	0.41
1:B:276:LYS:HE2	1:B:276:LYS:HB2	1.92	0.41
1:A:85:LYS:NZ	1:F:263:GLU:OE1	2.32	0.41
1:A:304:ARG:HA	1:A:304:ARG:NE	2.35	0.41
1:B:148:VAL:HG12	1:B:282:LYS:H	1.86	0.41
1:D:100:LEU:HD23	1:D:325:TYR:CE2	2.53	0.41
1:D:107:TYR:HB2	1:D:110:GLU:HB2	2.03	0.41
1:F:94:ILE:HD11	1:F:332:LEU:HD12	2.01	0.41
1:G:26:ALA:HB1	1:G:28:PHE:H	1.86	0.41
1:A:62:GLN:NE2	1:A:91:GLU:OE1	2.54	0.41
1:A:269:LYS:O	1:A:270:HIS:ND1	2.53	0.41
1:C:11:GLY:HA3	1:C:28:PHE:CE1	2.56	0.41
1:C:79:ASN:OD1	1:C:82:ASP:N	2.54	0.41
1:C:83:LYS:H	1:C:83:LYS:HZ3	1.68	0.41
1:D:59:LYS:HB3	1:D:59:LYS:HE2	1.90	0.41
1:D:99:LEU:HD11	1:D:324:LYS:HD3	2.02	0.41
1:D:125:GLN:OE1	1:E:68:ARG:HG3	2.20	0.41
1:E:199:TYR:O	1:E:200:VAL:HB	2.21	0.41
1:F:57:SER:OG	1:F:58:GLY:N	2.52	0.41
1:F:143:ALA:HB3	1:F:272:PHE:HZ	1.86	0.41
1:F:222:MET:SD	1:F:223:PRO:HD2	2.61	0.41
1:G:100:LEU:HD11	1:G:130:LEU:HG	2.03	0.41
1:A:269:LYS:HG2	1:B:73:TYR:HE1	1.86	0.41
1:C:139:LEU:HD13	1:C:139:LEU:HA	1.90	0.41
1:C:313:ARG:HB2	1:C:320:GLN:OE1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ILE:HD11	1:D:301:VAL:HG22	2.02	0.41
1:D:222:MET:HB3	1:D:223:PRO:HD3	2.02	0.41
1:E:116:TYR:CE1	1:E:118:VAL:HG22	2.56	0.41
1:A:161:THR:OG1	1:A:162:ALA:N	2.54	0.40
1:C:44:SER:OG	1:C:135:ASP:OD2	2.36	0.40
1:D:117:ASP:HA	1:D:118:VAL:CG1	2.49	0.40
1:F:25:LEU:HB3	1:F:28:PHE:HD1	1.86	0.40
1:G:237:GLY:HA3	1:G:238:SER:HA	1.68	0.40
1:A:73:TYR:OH	1:F:269:LYS:NZ	2.53	0.40
1:A:167:THR:OG1	1:A:168:THR:N	2.54	0.40
1:F:228:TYR:CG	1:F:229:ALA:N	2.89	0.40
1:A:64:PRO:O	1:F:37:LEU:HB3	2.21	0.40
1:D:231:LEU:HD13	1:D:242:VAL:HG13	2.02	0.40
1:G:214:TYR:CD1	1:G:249:GLU:HG2	2.56	0.40
1:A:262:ARG:HG3	1:B:85:LYS:HB2	2.04	0.40
1:C:276:LYS:O	1:C:281:VAL:HG12	2.22	0.40
1:F:140:ALA:HA	1:F:272:PHE:CZ	2.57	0.40
1:C:96:ILE:HG13	1:C:303:LEU:HD21	2.04	0.40
1:C:178:VAL:HG22	1:C:179:ALA:H	1.86	0.40
1:D:31:VAL:HG22	1:D:32:PHE:H	1.87	0.40
1:D:184:ILE:HD12	1:D:184:ILE:HA	1.89	0.40
1:G:16:LYS:HA	1:G:16:LYS:HD2	1.95	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	341/345 (99%)	282 (83%)	58 (17%)	1 (0%)	36	65
1	B	341/345 (99%)	279 (82%)	53 (16%)	9 (3%)	4	27
1	C	341/345 (99%)	251 (74%)	84 (25%)	6 (2%)	6	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	341/345 (99%)	275 (81%)	63 (18%)	3 (1%)	14	46
1	E	341/345 (99%)	281 (82%)	53 (16%)	7 (2%)	5	31
1	F	341/345 (99%)	276 (81%)	57 (17%)	8 (2%)	5	30
1	G	341/345 (99%)	276 (81%)	59 (17%)	6 (2%)	6	34
All	All	2387/2415 (99%)	1920 (80%)	427 (18%)	40 (2%)	9	35

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	118	VAL
1	D	118	VAL
1	E	18	VAL
1	F	118	VAL
1	G	52	VAL
1	B	206	VAL
1	B	232	ILE
1	E	19	VAL
1	E	236	LYS
1	E	296	SER
1	F	178	VAL
1	F	206	VAL
1	F	239	ILE
1	G	232	ILE
1	B	239	ILE
1	C	118	VAL
1	C	239	ILE
1	C	281	VAL
1	D	296	SER
1	E	239	ILE
1	G	156	ILE
1	A	19	VAL
1	B	45	VAL
1	B	199	TYR
1	C	19	VAL
1	C	244	GLY
1	C	298	VAL
1	E	118	VAL
1	F	19	VAL
1	F	179	ALA
1	G	204	ASP
1	G	298	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	200	VAL
1	E	235	GLU
1	B	296	SER
1	F	296	SER
1	B	242	VAL
1	F	247	VAL
1	D	142	ILE
1	G	234	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	259/261 (99%)	197 (76%)	62 (24%)	1	5
1	B	259/261 (99%)	203 (78%)	56 (22%)	1	7
1	C	259/261 (99%)	201 (78%)	58 (22%)	1	6
1	D	259/261 (99%)	194 (75%)	65 (25%)	0	4
1	E	259/261 (99%)	205 (79%)	54 (21%)	1	7
1	F	259/261 (99%)	206 (80%)	53 (20%)	1	8
1	G	259/261 (99%)	200 (77%)	59 (23%)	1	6
All	All	1813/1827 (99%)	1406 (78%)	407 (22%)	2	6

All (407) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	VAL
1	A	27	LEU
1	A	28	PHE
1	A	30	LYS
1	A	32	PHE
1	A	46	THR
1	A	49	ARG
1	A	52	VAL
1	A	59	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	69	THR
1	A	80	LEU
1	A	83	LYS
1	A	84	ARG
1	A	87	ILE
1	A	93	VAL
1	A	94	ILE
1	A	103	ASP
1	A	107	TYR
1	A	114	ASN
1	A	115	HIS
1	A	128	GLU
1	A	130	LEU
1	A	142	ILE
1	A	152	TYR
1	A	153	ASN
1	A	159	LEU
1	A	163	THR
1	A	166	GLU
1	A	170	ASN
1	A	184	ILE
1	A	192	ARG
1	A	198	ASN
1	A	200	VAL
1	A	210	ASP
1	A	217	ILE
1	A	218	LEU
1	A	221	LEU
1	A	224	ASN
1	A	228	TYR
1	A	231	LEU
1	A	232	ILE
1	A	235	GLU
1	A	239	ILE
1	A	242	VAL
1	A	248	VAL
1	A	253	LEU
1	A	262	ARG
1	A	271	VAL
1	A	282	LYS
1	A	291	LEU
1	A	295	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	298	VAL
1	A	304	ARG
1	A	308	LEU
1	A	322	ILE
1	A	325	TYR
1	A	332	LEU
1	A	333	ARG
1	A	340	VAL
1	A	341	VAL
1	A	343	LYS
1	A	344	VAL
1	B	29	LEU
1	B	32	PHE
1	B	37	LEU
1	B	38	THR
1	B	42	ARG
1	B	46	THR
1	B	47	THR
1	B	53	ARG
1	B	69	THR
1	B	70	GLN
1	B	73	TYR
1	B	74	LEU
1	B	78	GLU
1	B	87	ILE
1	B	92	LYS
1	B	94	ILE
1	B	95	THR
1	B	96	ILE
1	B	105	LEU
1	B	111	ASP
1	B	113	MET
1	B	118	VAL
1	B	128	GLU
1	B	132	MET
1	B	142	ILE
1	B	145	LEU
1	B	147	ASN
1	B	148	VAL
1	B	151	LYS
1	B	154	GLU
1	B	156	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	165	ILE
1	B	166	GLU
1	B	169	GLN
1	B	195	LEU
1	B	196	THR
1	B	197	LYS
1	B	198	ASN
1	B	200	VAL
1	B	209	CYS
1	B	221	LEU
1	B	232	ILE
1	B	241	ASN
1	B	245	PHE
1	B	260	THR
1	B	280	ASN
1	B	283	VAL
1	B	285	LYS
1	B	291	LEU
1	B	298	VAL
1	B	303	LEU
1	B	320	GLN
1	B	322	ILE
1	B	332	LEU
1	B	333	ARG
1	B	340	VAL
1	C	5	THR
1	C	10	MET
1	C	18	VAL
1	C	19	VAL
1	C	24	LYS
1	C	27	LEU
1	C	30	LYS
1	C	36	VAL
1	C	37	LEU
1	C	40	PHE
1	C	46	THR
1	C	55	ILE
1	C	69	THR
1	C	73	TYR
1	C	74	LEU
1	C	78	GLU
1	C	80	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	83	LYS
1	C	84	ARG
1	C	89	HIS
1	C	90	THR
1	C	91	GLU
1	C	94	ILE
1	C	95	THR
1	C	96	ILE
1	C	100	LEU
1	C	115	HIS
1	C	118	VAL
1	C	139	LEU
1	C	142	ILE
1	C	159	LEU
1	C	163	THR
1	C	164	VAL
1	C	169	GLN
1	C	171	LYS
1	C	174	LEU
1	C	183	GLU
1	C	200	VAL
1	C	205	ARG
1	C	227	ASN
1	C	232	ILE
1	C	236	LYS
1	C	242	VAL
1	C	243	MET
1	C	248	VAL
1	C	253	LEU
1	C	254	THR
1	C	260	THR
1	C	272	PHE
1	C	280	ASN
1	C	281	VAL
1	C	298	VAL
1	C	303	LEU
1	C	309	GLU
1	C	322	ILE
1	C	324	LYS
1	C	325	TYR
1	C	332	LEU
1	D	3	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	19	VAL
1	D	27	LEU
1	D	28	PHE
1	D	29	LEU
1	D	38	THR
1	D	43	THR
1	D	50	HIS
1	D	51	MET
1	D	52	VAL
1	D	66	LEU
1	D	68	ARG
1	D	69	THR
1	D	78	GLU
1	D	79	ASN
1	D	80	LEU
1	D	81	ASP
1	D	84	ARG
1	D	85	LYS
1	D	86	ASP
1	D	91	GLU
1	D	92	LYS
1	D	94	ILE
1	D	105	LEU
1	D	110	GLU
1	D	114	ASN
1	D	115	HIS
1	D	117	ASP
1	D	118	VAL
1	D	126	LEU
1	D	139	LEU
1	D	142	ILE
1	D	149	GLU
1	D	154	GLU
1	D	157	GLU
1	D	163	THR
1	D	180	LEU
1	D	182	LYS
1	D	184	ILE
1	D	192	ARG
1	D	200	VAL
1	D	204	ASP
1	D	218	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	221	LEU
1	D	231	LEU
1	D	233	ASP
1	D	235	GLU
1	D	241	ASN
1	D	250	VAL
1	D	253	LEU
1	D	281	VAL
1	D	283	VAL
1	D	291	LEU
1	D	294	HIS
1	D	298	VAL
1	D	300	THR
1	D	306	LEU
1	D	309	GLU
1	D	315	ASN
1	D	317	GLN
1	D	325	TYR
1	D	332	LEU
1	D	335	GLU
1	D	341	VAL
1	D	344	VAL
1	E	18	VAL
1	E	27	LEU
1	E	29	LEU
1	E	38	THR
1	E	46	THR
1	E	70	GLN
1	E	78	GLU
1	E	79	ASN
1	E	82	ASP
1	E	86	ASP
1	E	89	HIS
1	E	90	THR
1	E	92	LYS
1	E	97	ASP
1	E	101	THR
1	E	105	LEU
1	E	107	TYR
1	E	109	ILE
1	E	111	ASP
1	E	118	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	130	LEU
1	E	132	MET
1	E	142	ILE
1	E	145	LEU
1	E	147	ASN
1	E	149	GLU
1	E	157	GLU
1	E	161	THR
1	E	169	GLN
1	E	174	LEU
1	E	190	LYS
1	E	197	LYS
1	E	200	VAL
1	E	209	CYS
1	E	210	ASP
1	E	231	LEU
1	E	240	ARG
1	E	248	VAL
1	E	250	VAL
1	E	265	THR
1	E	271	VAL
1	E	275	ASN
1	E	281	VAL
1	E	291	LEU
1	E	294	HIS
1	E	295	ARG
1	E	298	VAL
1	E	303	LEU
1	E	306	LEU
1	E	317	GLN
1	E	319	ASP
1	E	320	GLN
1	E	325	TYR
1	E	344	VAL
1	F	24	LYS
1	F	25	LEU
1	F	27	LEU
1	F	28	PHE
1	F	29	LEU
1	F	45	VAL
1	F	47	THR
1	F	49	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	50	HIS
1	F	51	MET
1	F	69	THR
1	F	81	ASP
1	F	92	LYS
1	F	95	THR
1	F	96	ILE
1	F	99	LEU
1	F	105	LEU
1	F	106	ILE
1	F	108	ASP
1	F	109	ILE
1	F	118	VAL
1	F	142	ILE
1	F	148	VAL
1	F	153	ASN
1	F	156	ILE
1	F	159	LEU
1	F	163	THR
1	F	167	THR
1	F	170	ASN
1	F	174	LEU
1	F	177	GLN
1	F	192	ARG
1	F	224	ASN
1	F	227	ASN
1	F	231	LEU
1	F	232	ILE
1	F	242	VAL
1	F	252	HIS
1	F	254	THR
1	F	283	VAL
1	F	298	VAL
1	F	303	LEU
1	F	306	LEU
1	F	309	GLU
1	F	312	ARG
1	F	317	GLN
1	F	319	ASP
1	F	321	ILE
1	F	325	TYR
1	F	332	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	333	ARG
1	F	340	VAL
1	F	343	LYS
1	G	18	VAL
1	G	19	VAL
1	G	24	LYS
1	G	25	LEU
1	G	31	VAL
1	G	35	GLU
1	G	38	THR
1	G	42	ARG
1	G	45	VAL
1	G	47	THR
1	G	50	HIS
1	G	52	VAL
1	G	53	ARG
1	G	55	ILE
1	G	62	GLN
1	G	65	VAL
1	G	66	LEU
1	G	80	LEU
1	G	83	LYS
1	G	85	LYS
1	G	89	HIS
1	G	91	GLU
1	G	94	ILE
1	G	97	ASP
1	G	101	THR
1	G	108	ASP
1	G	113	MET
1	G	119	ARG
1	G	142	ILE
1	G	151	LYS
1	G	159	LEU
1	G	163	THR
1	G	168	THR
1	G	169	GLN
1	G	171	LYS
1	G	188	LEU
1	G	195	LEU
1	G	197	LYS
1	G	200	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	210	ASP
1	G	222	MET
1	G	228	TYR
1	G	231	LEU
1	G	235	GLU
1	G	247	VAL
1	G	249	GLU
1	G	271	VAL
1	G	281	VAL
1	G	283	VAL
1	G	288	VAL
1	G	291	LEU
1	G	295	ARG
1	G	303	LEU
1	G	310	ARG
1	G	322	ILE
1	G	325	TYR
1	G	332	LEU
1	G	341	VAL
1	G	342	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	70	GLN
1	A	89	HIS
1	A	169	GLN
1	A	241	ASN
1	A	252	HIS
1	A	268	GLN
1	B	14	GLN
1	B	70	GLN
1	B	155	ASN
1	B	275	ASN
1	B	287	ASN
1	B	317	GLN
1	B	320	GLN
1	C	13	ASN
1	C	62	GLN
1	C	70	GLN
1	C	125	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	147	ASN
1	C	268	GLN
1	C	287	ASN
1	C	294	HIS
1	C	317	GLN
1	D	50	HIS
1	D	62	GLN
1	D	70	GLN
1	D	177	GLN
1	D	198	ASN
1	D	268	GLN
1	D	287	ASN
1	D	317	GLN
1	E	9	GLN
1	E	50	HIS
1	E	89	HIS
1	E	169	GLN
1	E	177	GLN
1	E	268	GLN
1	E	280	ASN
1	E	287	ASN
1	F	14	GLN
1	F	114	ASN
1	F	169	GLN
1	F	227	ASN
1	F	252	HIS
1	G	14	GLN
1	G	62	GLN
1	G	70	GLN
1	G	89	HIS
1	G	125	GLN
1	G	147	ASN
1	G	155	ASN
1	G	268	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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.

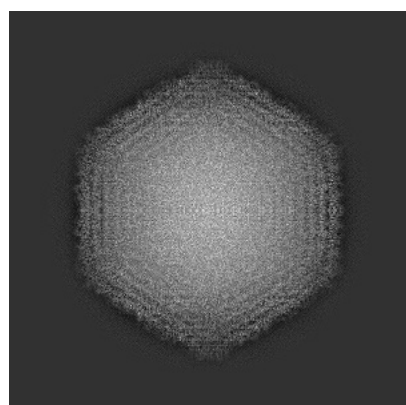
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6037. These allow visual inspection of the internal detail of the map and identification of artifacts.

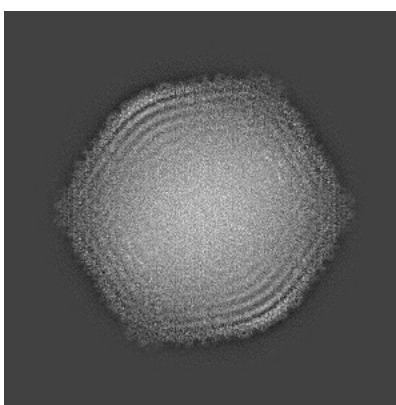
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

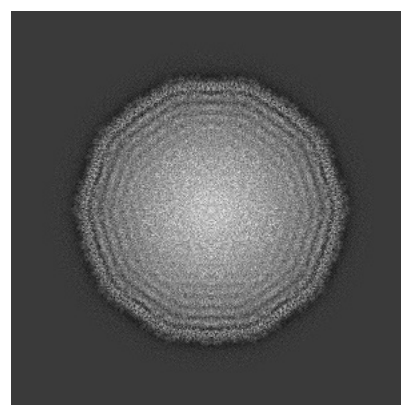
6.1.1 Primary map



X



Y

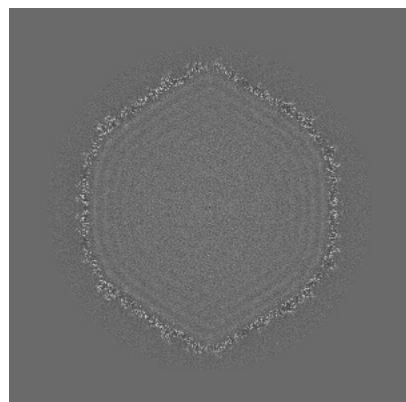


Z

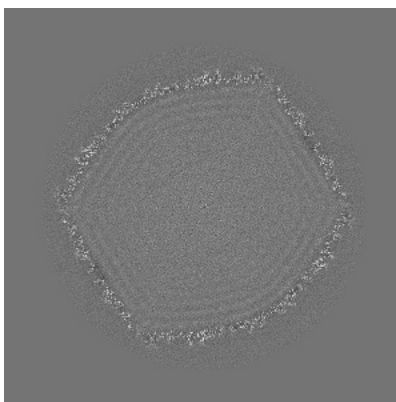
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

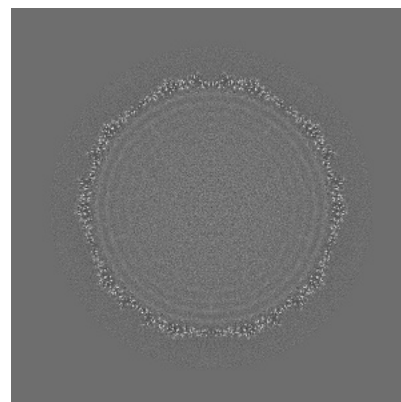
6.2.1 Primary map



X Index: 400



Y Index: 400

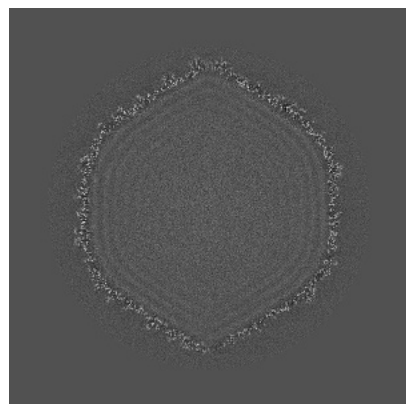


Z Index: 400

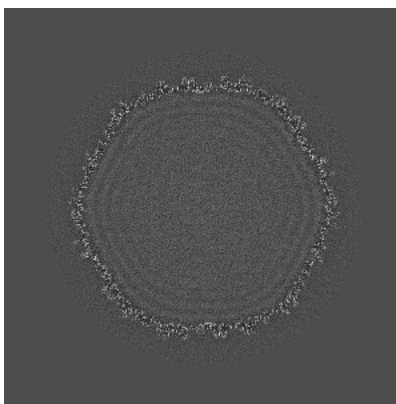
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

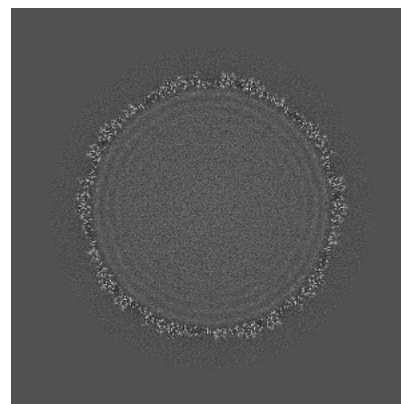
6.3.1 Primary map



X Index: 394



Y Index: 333

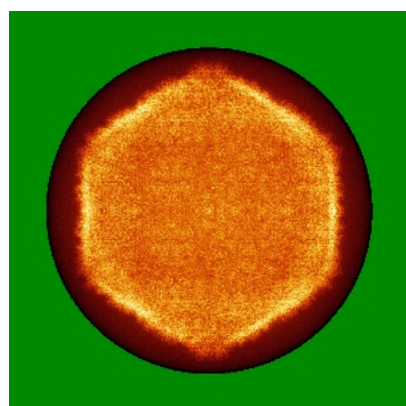


Z Index: 402

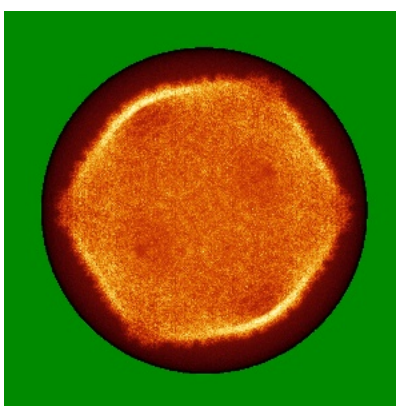
The images above show the largest variance slices of the map in three orthogonal directions.

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

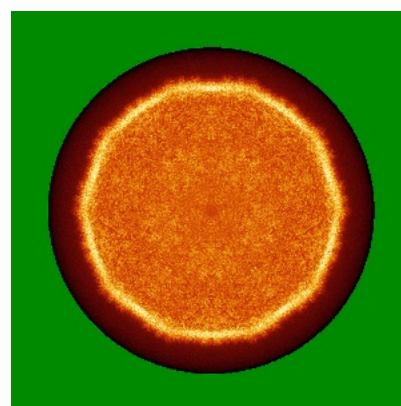
6.4.1 Primary map



X



Y

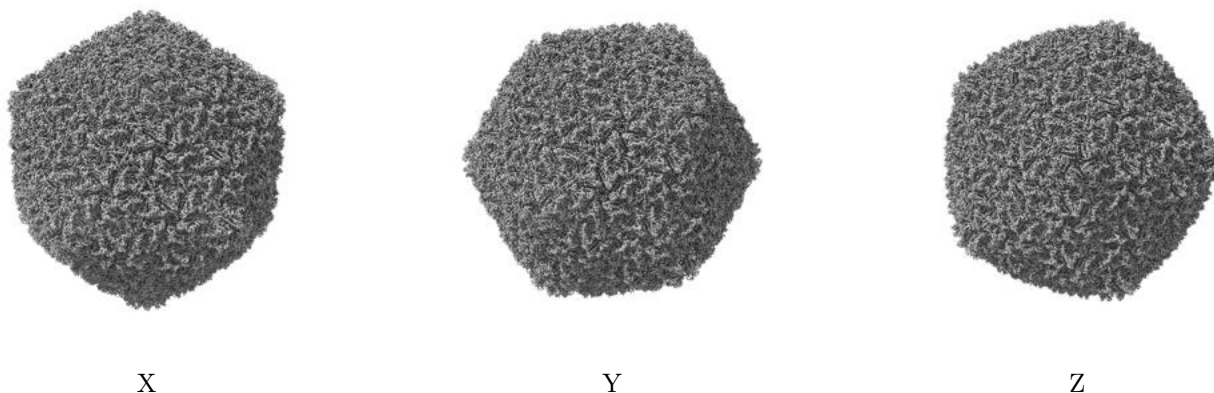


Z

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 4.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

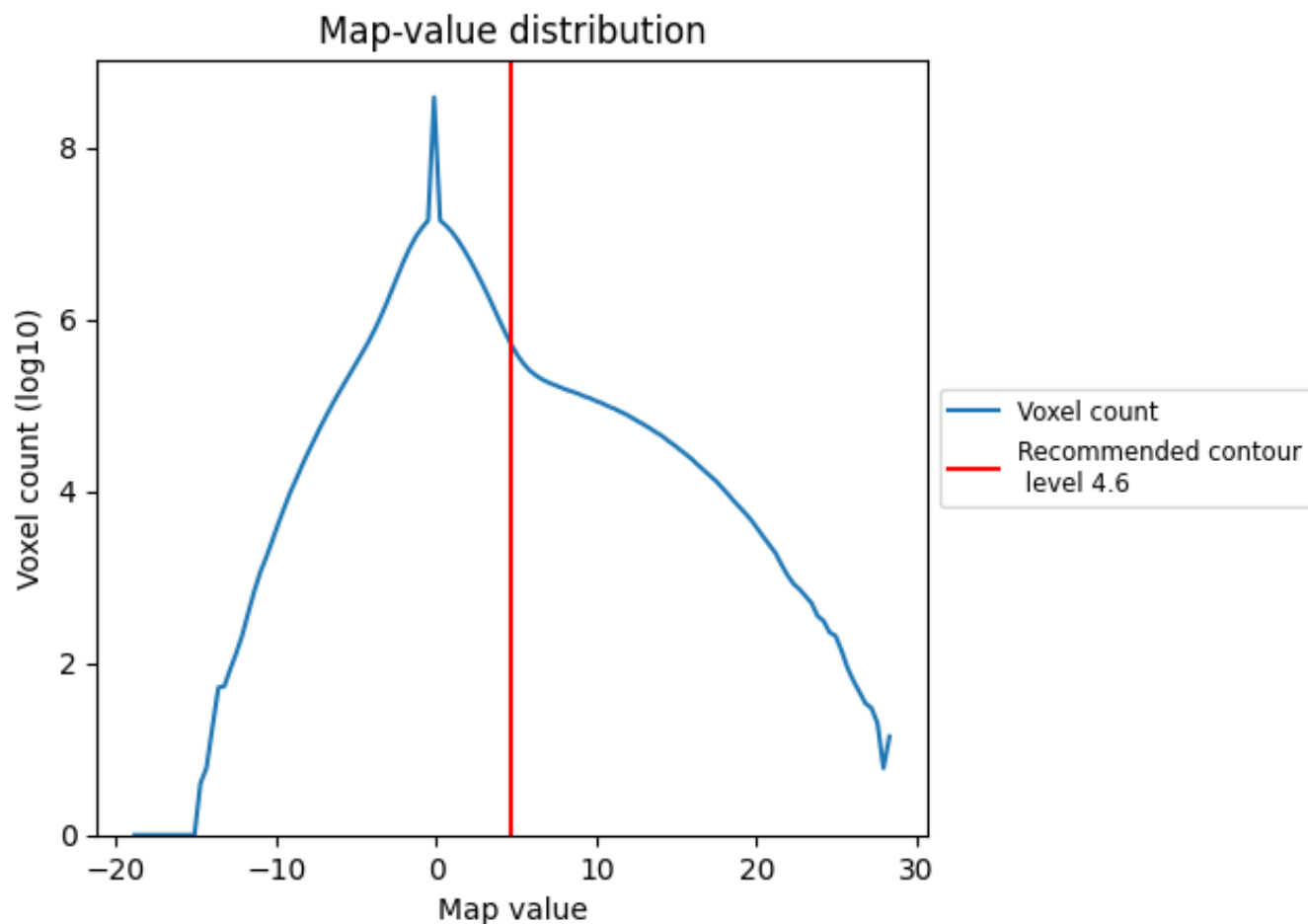
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

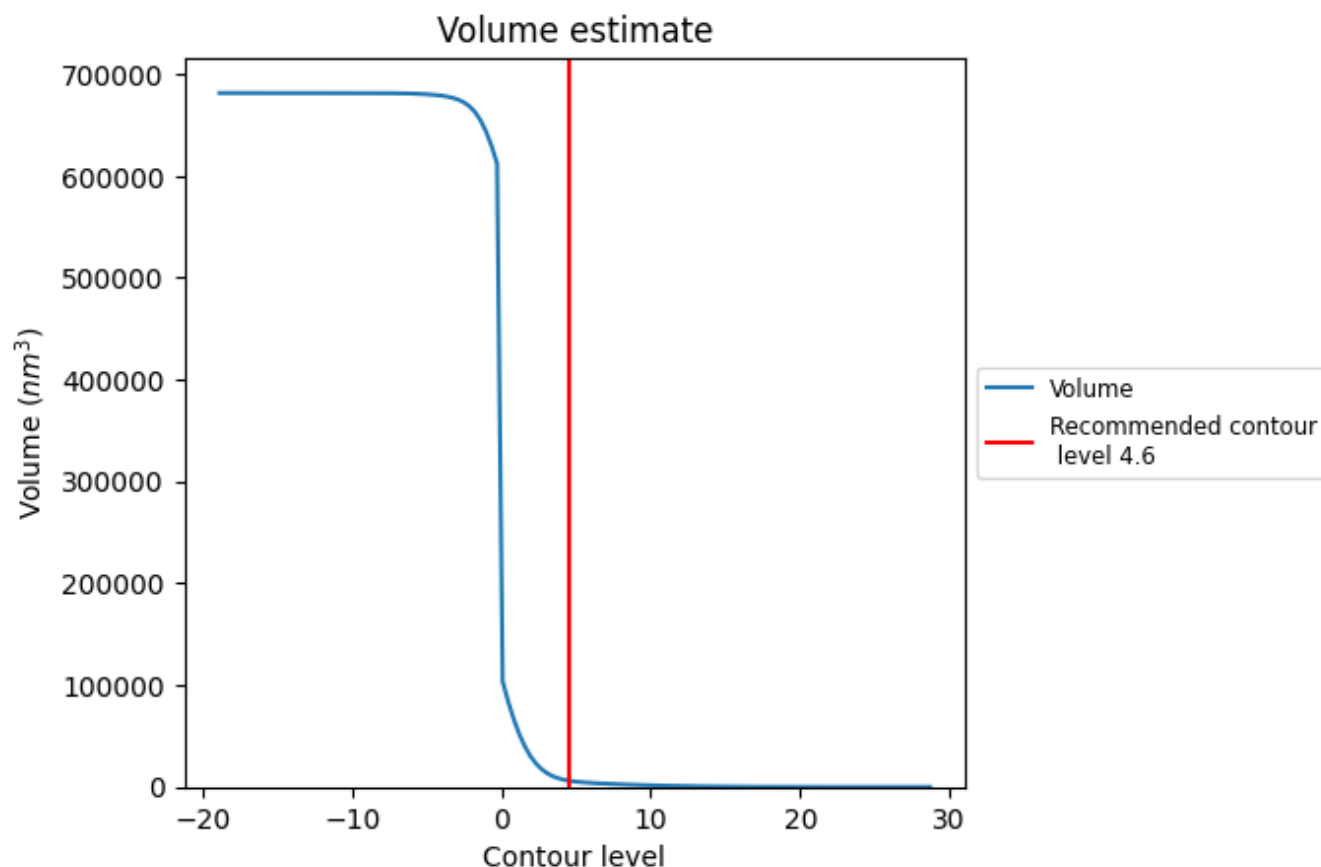
This section contains the results of statistical analysis of the map.

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.

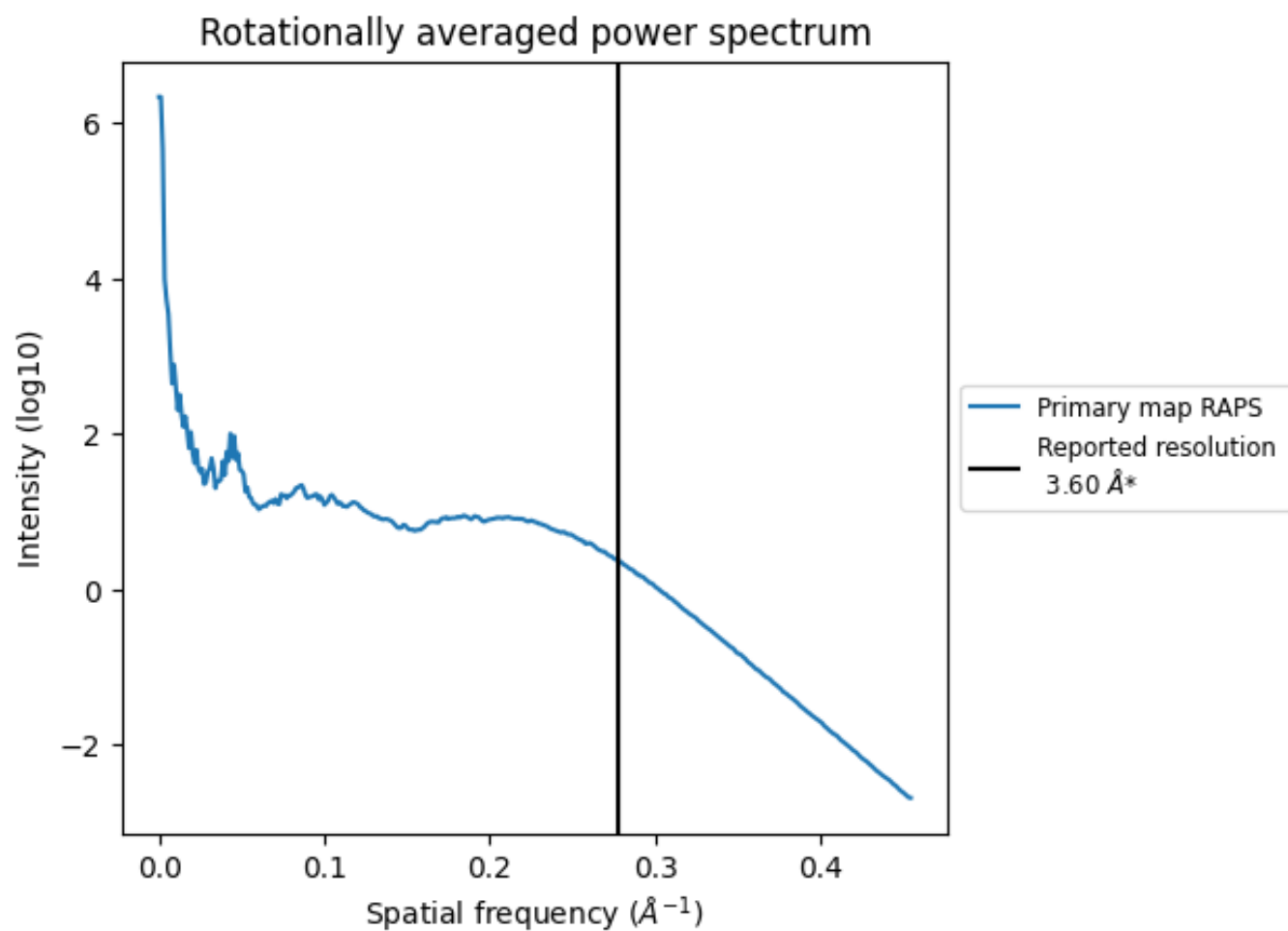
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5943 nm^3 ; this corresponds to an approximate mass of 5368 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 0.278 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

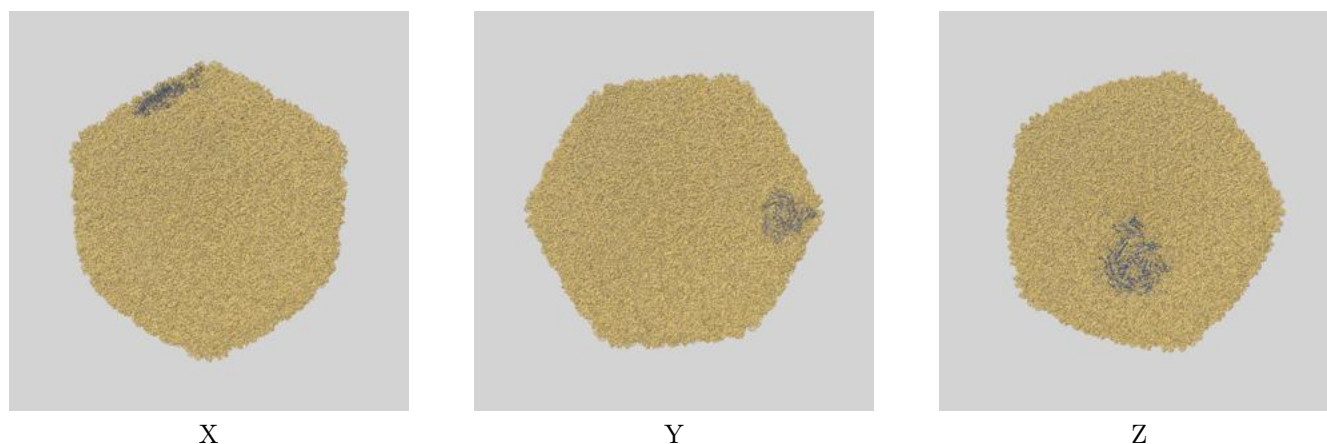
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

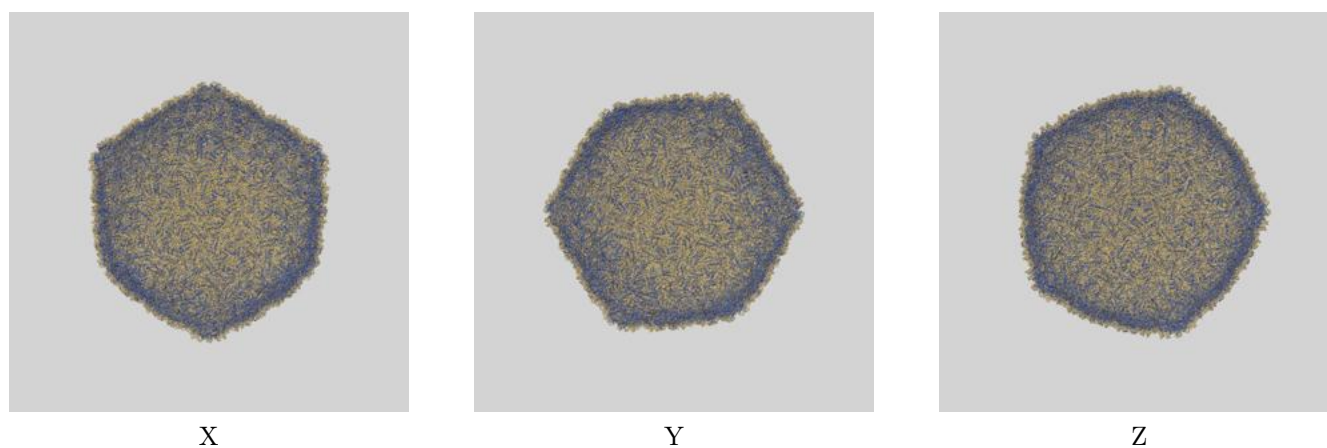
This section contains information regarding the fit between EMDB map EMD-6037 and PDB model 3J7X. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



9.1.2 Map-model assembly overlay [i](#)



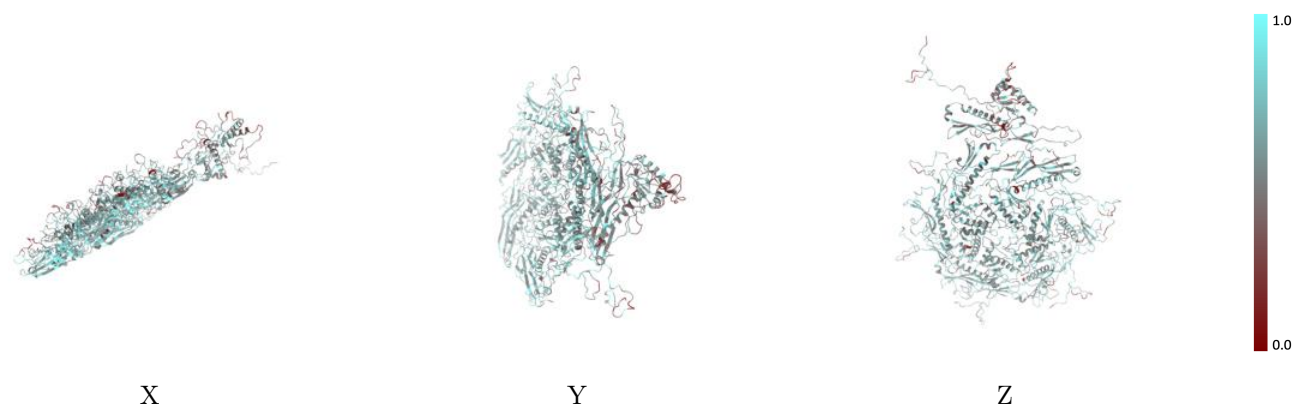
The images above show the 3D surface view of the map at the recommended contour level 4.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



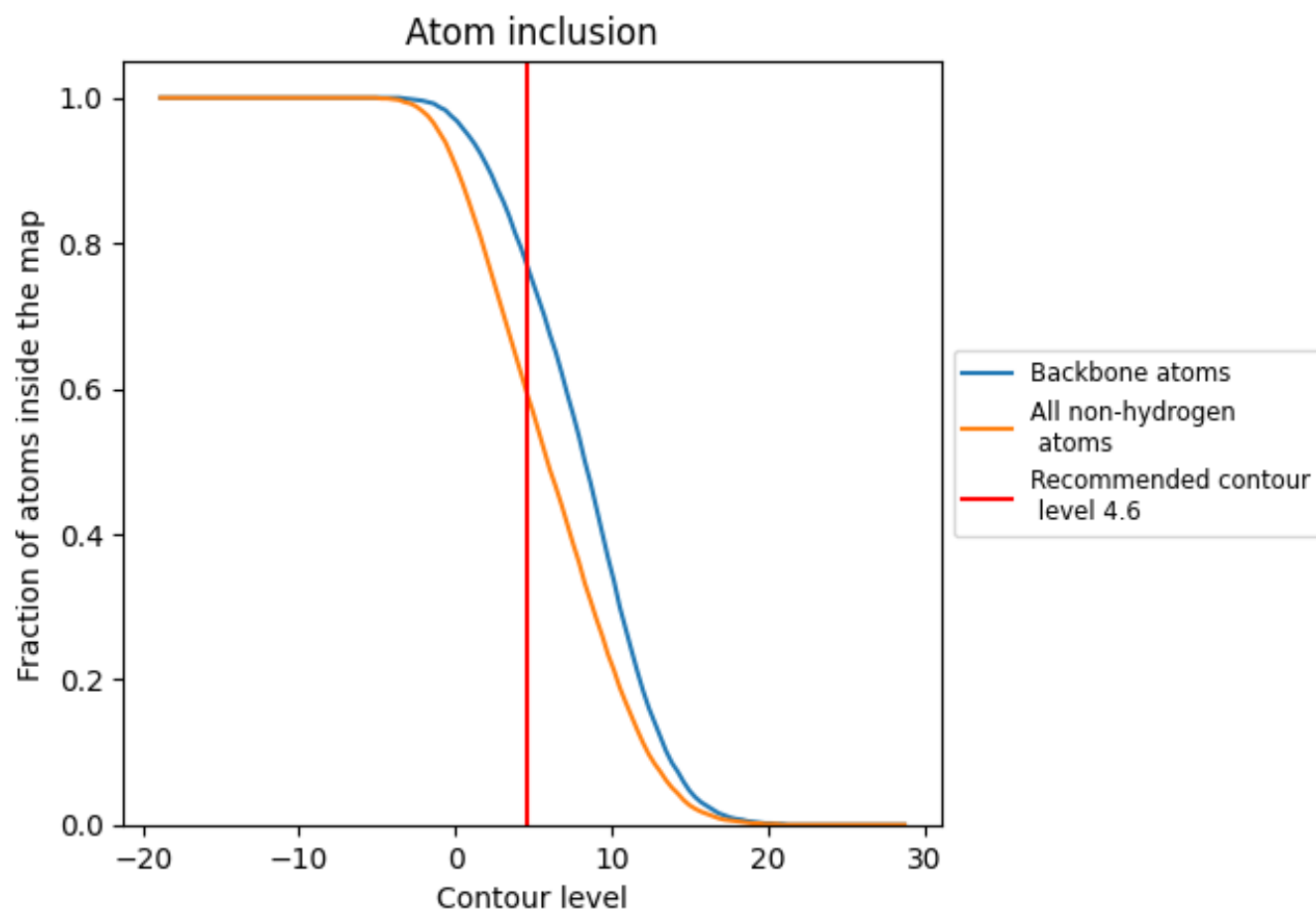
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 59% 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 (4.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5910	0.3630
A	0.5950	0.3660
B	0.6080	0.3700
C	0.6100	0.3690
D	0.6240	0.3720
E	0.6080	0.3680
F	0.6020	0.3730
G	0.4930	0.3240

1.0

0.0

<0.0