



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 03:38 PM UTC

PDB ID : 7FEJ / pdb_00007fej
EMDB ID : EMD-31556
Title : Complex of FMDV A/AF/72 and bovine neutralizing scFv antibody R55
Authors : He, Y.; Li, K.; Lou, Z.
Deposited on : 2021-07-20
Resolution : 3.91 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

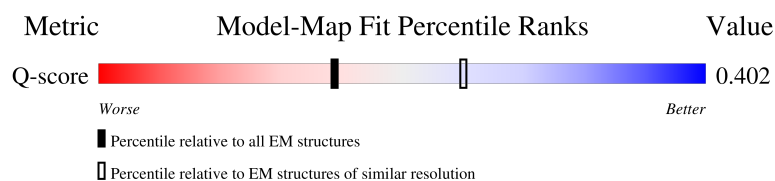
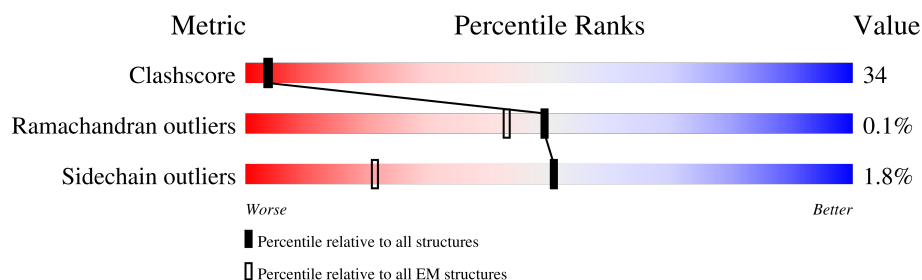
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.91 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	7920 (3.41 - 4.41)

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	1	212	
2	2	218	
3	3	221	
4	4	85	

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Mol	Chain	Length	Quality of chain
5	H	126	42% 33% • 22%
6	L	123	42% 42% • • 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6691 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 A/AF/72 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	189	Total	C	N	O	S	0	0
			1484	935	272	273	4		

- Molecule 2 is a protein called A/AF/72 VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	205	Total	C	N	O	S	0	0
			1625	1038	281	301	5		

- Molecule 3 is a protein called A/AF/72 VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	220	Total	C	N	O	S	0	0
			1689	1078	273	328	10		

- Molecule 4 is a protein called Capsid protein VP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	45	Total	C	N	O	S	0	0
			348	220	56	70	2		

- Molecule 5 is a protein called IG HEAVY CHAIN VARIABLE REGION.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	98	Total	C	N	O	S	0	0
			750	472	120	155	3		

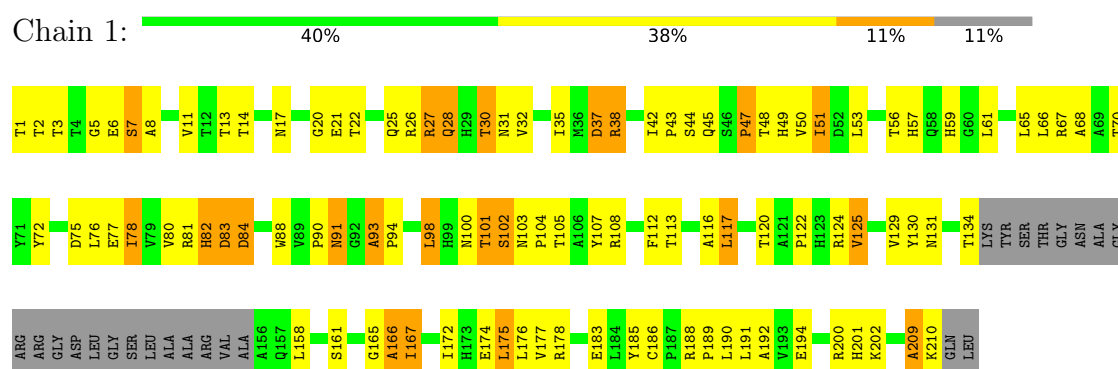
- Molecule 6 is a protein called IG LAMDA CHAIN VARIABLE REGION.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	109	Total	C	N	O	S	0	0
			795	486	138	169	2		

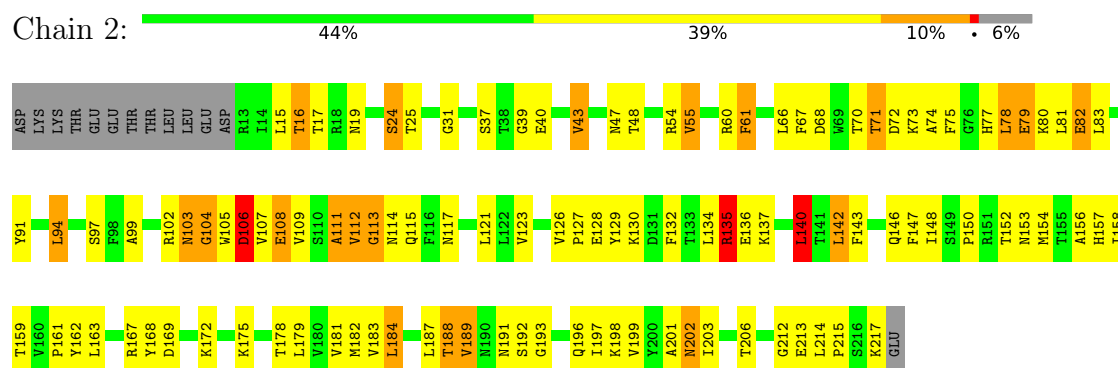
3 Residue-property plots

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: A/AF/72 VP1



• Molecule 2: A/AF/72 VP2

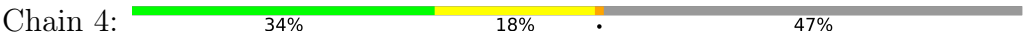


• Molecule 3: A/AF/72 VP3





• Molecule 4: Capsid protein VP0



• Molecule 5: IG HEAVY CHAIN VARIABLE REGION



• Molecule 6: IG LAMDA CHAIN VARIABLE REGION



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25317	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-16 (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0032	Depositor
Map size ($\text{\AA}$)	446.4, 446.4, 446.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.93, 0.93, 0.93	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	1	0.52	1/1519 (0.1%)	1.56	48/2074 (2.3%)
2	2	0.52	0/1670	1.37	44/2273 (1.9%)
3	3	0.41	0/1738	1.25	46/2379 (1.9%)
4	4	0.30	0/354	1.05	7/476 (1.5%)
5	H	0.46	0/765	1.27	9/1039 (0.9%)
6	L	0.65	0/808	1.55	19/1098 (1.7%)
All	All	0.50	1/6854 (0.0%)	1.38	173/9339 (1.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	82	HIS	C-N	-6.41	1.25	1.33

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	7	SER	N-CA-C	-26.06	75.36	110.55
5	H	48	LEU	N-CA-C	-18.91	82.72	109.95
6	L	107	THR	N-CA-C	-16.67	81.54	108.55
3	3	219	ARG	N-CA-C	-15.18	84.26	109.46
1	1	31	ASN	N-CA-C	-14.58	86.90	109.07
1	1	83	ASP	N-CA-C	14.35	130.57	112.92
6	L	7	THR	N-CA-C	-13.97	87.74	109.95
6	L	86	GLU	N-CA-C	-13.68	84.60	108.13
5	H	49	GLY	N-CA-C	13.14	134.37	112.30
6	L	8	GLN	N-CA-C	-12.77	93.44	108.25
1	1	77	GLU	N-CA-C	-12.74	87.97	109.24
1	1	27	ARG	N-CA-C	-12.46	81.58	107.37
5	H	63	LEU	N-CA-C	-12.37	87.05	108.20
2	2	188	THR	N-CA-C	-12.15	89.52	109.07
2	2	112	VAL	N-CA-C	-12.07	91.09	108.36
2	2	105	TRP	CB-CA-C	-12.04	93.04	110.62
3	3	73	LEU	N-CA-C	-11.94	86.83	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	106	ASP	N-CA-CB	-11.79	90.96	110.53
6	L	7	THR	CB-CA-C	11.66	130.71	109.37
1	1	102	SER	N-CA-C	-11.60	99.25	113.41
2	2	81	LEU	N-CA-C	-11.46	91.00	108.99
3	3	18	ASP	N-CA-CB	11.34	130.55	110.37
1	1	26	ARG	N-CA-C	-11.23	90.10	108.41
1	1	83	ASP	CB-CA-C	-11.17	91.69	110.56
5	H	64	LYS	N-CA-C	-11.16	91.13	108.76
1	1	30	THR	N-CA-C	-11.04	88.56	107.99
2	2	15	LEU	N-CA-C	-11.02	91.44	109.40
6	L	108	THR	N-CA-C	-10.87	90.22	108.26
1	1	38	ARG	N-CA-C	10.73	124.94	110.35
4	4	75	ALA	N-CA-C	-10.65	92.27	108.99
6	L	24	CYS	N-CA-C	-10.59	91.56	109.24
1	1	8	ALA	N-CA-C	-10.30	94.02	108.54
3	3	219	ARG	CB-CA-C	9.94	126.10	109.80
2	2	82	GLU	N-CA-C	-9.72	94.16	109.72
1	1	116	ALA	N-CA-C	-9.57	92.59	108.76
1	1	93	ALA	N-CA-C	9.46	121.56	109.65
2	2	188	THR	CB-CA-C	9.43	126.03	109.72
3	3	154	SER	N-CA-C	9.42	125.09	113.50
3	3	71	GLN	CB-CA-C	9.34	126.13	110.43
6	L	86	GLU	N-CA-CB	9.32	125.96	110.59
2	2	79	GLU	N-CA-C	-9.26	93.32	108.41
3	3	25	ILE	CB-CA-C	-9.25	101.93	110.63
1	1	209	ALA	N-CA-C	9.21	121.31	111.28
5	H	64	LYS	N-CA-CB	9.20	127.48	111.39
3	3	18	ASP	N-CA-C	-9.18	89.53	109.81
2	2	112	VAL	CB-CA-C	9.09	123.20	110.84
3	3	73	LEU	N-CA-CB	9.05	124.56	110.71
3	3	131	GLU	N-CA-C	8.96	123.31	112.38
6	L	107	THR	CB-CA-C	8.80	125.70	109.86
3	3	17	THR	N-CA-C	-8.71	94.21	108.41
2	2	15	LEU	CB-CA-C	8.52	125.64	109.37
6	L	48	ARG	N-CA-C	-8.52	96.12	109.07
1	1	91	ASN	N-CA-C	8.48	122.89	112.54
6	L	85	ASP	N-CA-C	-8.45	92.10	107.98
4	4	74	SER	N-CA-C	-8.44	95.59	108.67
2	2	81	LEU	CB-CA-C	8.41	127.85	109.94
3	3	82	ALA	N-CA-C	-8.41	92.11	107.75
2	2	111	ALA	N-CA-C	-8.37	93.42	108.48
3	3	108	HIS	CB-CA-C	8.30	124.18	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	8	GLN	N-CA-CB	8.20	122.81	111.25
3	3	200	LEU	CB-CA-C	8.07	124.14	109.37
1	1	77	GLU	CB-CA-C	8.03	125.26	109.35
3	3	100	GLN	CB-CA-C	7.97	126.80	111.17
1	1	8	ALA	N-CA-CB	-7.95	96.30	110.60
2	2	189	VAL	N-CA-C	-7.86	96.40	107.80
6	L	24	CYS	CB-CA-C	7.72	124.63	109.35
1	1	84	ASP	N-CA-C	-7.64	98.20	108.74
3	3	218	PRO	N-CA-C	-7.59	96.83	112.47
3	3	192	HIS	CB-CA-C	7.58	122.91	109.65
2	2	43	VAL	CB-CA-C	-7.47	99.04	111.29
4	4	31	GLN	N-CA-C	7.42	120.42	111.82
6	L	108	THR	N-CA-CB	7.42	122.86	110.77
3	3	109	PHE	N-CA-C	-7.34	96.99	109.24
1	1	166	ALA	N-CA-C	-7.32	96.24	108.75
1	1	91	ASN	CB-CA-C	-7.30	95.04	110.31
2	2	78	LEU	N-CA-C	-7.30	97.35	108.96
1	1	21	GLU	CB-CA-C	7.30	124.20	110.62
3	3	199	THR	CB-CA-C	-7.30	97.75	109.80
3	3	108	HIS	N-CA-C	-7.30	95.78	108.69
2	2	71	THR	CB-CA-C	7.24	124.03	110.63
1	1	116	ALA	CB-CA-C	7.22	122.78	109.70
3	3	142	HIS	N-CA-C	7.20	119.12	111.28
1	1	176	LEU	N-CA-C	-7.15	98.28	109.72
2	2	172	LYS	N-CA-C	7.08	121.01	112.38
2	2	111	ALA	CB-CA-C	7.05	121.78	109.80
4	4	75	ALA	CB-CA-C	7.03	124.92	109.94
2	2	104	GLY	N-CA-C	-6.95	99.46	112.10
6	L	48	ARG	CB-CA-C	6.94	125.37	110.45
3	3	130	MET	CB-CA-C	-6.90	96.74	109.37
1	1	21	GLU	N-CA-C	-6.88	98.26	108.79
5	H	94	TYR	CB-CA-C	-6.86	95.33	109.94
3	3	76	LYS	N-CA-C	-6.85	98.90	109.52
2	2	79	GLU	CB-CA-C	6.79	121.43	110.16
3	3	201	VAL	N-CA-C	-6.79	97.84	107.75
6	L	49	THR	N-CA-C	-6.78	98.15	109.07
1	1	166	ALA	CB-CA-C	6.73	123.00	109.68
1	1	167	ILE	N-CA-C	-6.72	98.44	108.12
3	3	75	ALA	CB-CA-C	6.72	124.25	109.94
2	2	105	TRP	N-CA-C	-6.70	96.20	107.80
1	1	175	LEU	N-CA-C	-6.69	97.68	109.06
1	1	78	ILE	N-CA-C	-6.67	97.94	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	161	SER	N-CA-C	6.65	121.41	113.16
1	1	175	LEU	CB-CA-C	6.60	122.78	109.38
1	1	117	LEU	N-CA-CB	6.55	122.04	110.37
1	1	84	ASP	N-CA-CB	6.53	122.12	111.21
3	3	154	SER	CB-CA-C	-6.50	97.45	109.29
1	1	98	LEU	N-CA-C	6.49	120.29	112.38
2	2	113	GLY	N-CA-C	-6.39	98.04	113.18
4	4	31	GLN	CB-CA-C	-6.38	98.43	110.67
3	3	83	ALA	N-CA-CB	6.27	122.13	111.66
2	2	60	ARG	CB-CA-C	6.22	123.83	110.45
3	3	26	TYR	N-CA-C	-6.22	100.02	109.85
2	2	184	LEU	N-CA-C	6.21	120.58	112.89
2	2	135	ARG	N-CA-C	-6.16	105.90	113.41
2	2	184	LEU	CB-CA-C	-6.15	97.15	109.99
2	2	80	LYS	N-CA-C	-6.14	101.11	110.14
3	3	155	LYS	N-CA-CB	6.14	120.23	110.65
3	3	146	ALA	CB-CA-C	6.12	122.33	109.79
4	4	76	PHE	N-CA-C	-6.11	98.78	108.73
1	1	82	HIS	O-C-N	-6.09	116.14	123.03
3	3	172	ALA	N-CA-C	-6.07	100.39	110.17
1	1	78	ILE	N-CA-CB	6.07	122.64	112.44
3	3	83	ALA	N-CA-C	-6.06	99.86	109.07
1	1	66	LEU	N-CA-C	6.05	117.55	111.07
1	1	37	ASP	CB-CA-C	6.02	122.23	110.67
1	1	26	ARG	CB-CA-C	5.87	119.90	110.16
3	3	192	HIS	N-CA-C	-5.82	98.39	108.69
3	3	16	THR	CB-CA-C	5.81	120.56	110.68
2	2	61	PHE	N-CA-C	-5.78	100.28	109.76
6	L	25	SER	N-CA-C	-5.76	98.35	108.20
2	2	153	ASN	N-CA-CB	5.74	120.06	110.59
2	2	103	ASN	CB-CA-C	5.70	122.34	111.17
1	1	201	HIS	N-CA-C	5.68	117.48	111.28
2	2	152	THR	CB-CA-C	-5.67	99.05	109.15
2	2	16	THR	N-CA-CB	5.67	120.10	110.87
2	2	94	LEU	N-CA-C	5.66	117.52	111.36
1	1	82	HIS	CB-CA-C	-5.62	100.53	109.80
2	2	16	THR	N-CA-C	-5.61	95.98	107.70
2	2	152	THR	N-CA-C	5.60	120.99	114.04
3	3	200	LEU	N-CA-CB	-5.60	101.89	110.85
2	2	54	ARG	CB-CA-C	5.57	118.20	109.84
3	3	201	VAL	N-CA-CB	5.52	118.82	111.64
2	2	140	LEU	N-CA-C	-5.47	106.66	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	121	TYR	CB-CA-C	-5.45	99.90	109.71
3	3	101	TYR	N-CA-CB	5.45	120.30	111.21
1	1	117	LEU	N-CA-C	-5.43	97.81	109.81
5	H	111	GLN	N-CA-C	5.40	117.16	111.28
3	3	218	PRO	N-CA-CB	5.39	108.91	103.25
2	2	82	GLU	N-CA-CB	5.36	120.25	111.08
1	1	47	PRO	N-CA-CB	-5.30	97.69	103.25
4	4	75	ALA	N-CA-CB	5.29	121.36	111.52
1	1	167	ILE	N-CA-CB	5.29	119.24	111.52
2	2	108	GLU	CB-CA-C	5.28	120.13	109.68
3	3	72	ARG	CB-CA-C	-5.27	99.93	110.42
1	1	101	THR	CB-CA-C	-5.26	102.79	111.36
1	1	125	VAL	N-CA-CB	5.15	118.14	111.19
2	2	108	GLU	N-CA-C	-5.15	99.95	108.75
3	3	193	GLY	N-CA-C	-5.11	101.08	113.18
3	3	147	GLU	N-CA-CB	5.11	119.09	110.77
5	H	68	SER	CB-CA-C	5.09	119.75	109.68
2	2	106	ASP	N-CA-C	-5.07	97.73	107.57
1	1	20	GLY	N-CA-C	-5.07	106.71	112.79
5	H	68	SER	N-CA-C	-5.07	100.08	108.75
3	3	20	LYS	CB-CA-C	5.07	120.04	110.62
1	1	209	ALA	CB-CA-C	-5.06	102.39	110.79
2	2	24	SER	N-CA-C	-5.06	100.03	108.32
3	3	171	THR	CB-CA-C	-5.05	99.52	109.67
2	2	55	VAL	N-CA-C	-5.02	101.25	108.53
3	3	75	ALA	N-CA-C	-5.02	101.11	108.99
6	L	36	VAL	CA-C-N	5.02	125.47	121.61
6	L	36	VAL	C-N-CA	5.02	125.47	121.61
1	1	28	GLN	N-CA-C	-5.01	107.15	114.12
3	3	26	TYR	N-CA-CB	5.01	119.32	111.20

There are no chirality outliers.

There are no planarity outliers.

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	1	1484	0	1481	131	0
2	2	1625	0	1589	162	0
3	3	1689	0	1616	146	0
4	4	348	0	321	9	0
5	H	750	0	724	69	0
6	L	795	0	761	76	0
All	All	6691	0	6492	450	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 34.

All (450) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:215:PRO:HD3	3:3:143:CYS:SG	1.46	1.56
5:H:110:MET:SD	6:L:103:PHE:HZ	1.44	1.39
2:2:215:PRO:HG2	3:3:130:MET:CE	1.53	1.38
2:2:214:LEU:HD23	3:3:130:MET:CE	1.52	1.37
2:2:215:PRO:O	3:3:130:MET:CE	1.77	1.33
1:1:105:THR:CG2	3:3:16:THR:HB	1.59	1.31
2:2:215:PRO:CG	3:3:130:MET:CE	2.07	1.30
2:2:217:LYS:NZ	3:3:130:MET:SD	2.04	1.28
2:2:215:PRO:CD	3:3:143:CYS:SG	2.21	1.28
5:H:110:MET:SD	6:L:103:PHE:CZ	2.27	1.26
2:2:215:PRO:CD	3:3:130:MET:HE3	1.66	1.26
5:H:30:SER:HA	5:H:53:THR:OG1	1.33	1.25
1:1:105:THR:HG22	3:3:16:THR:CB	1.68	1.22
2:2:215:PRO:CG	3:3:130:MET:HE1	1.68	1.22
2:2:214:LEU:HD21	3:3:130:MET:CG	1.71	1.21
2:2:215:PRO:CB	3:3:130:MET:HE1	1.71	1.20
2:2:214:LEU:CD2	3:3:130:MET:HE2	1.70	1.20
1:1:5:GLY:O	1:1:7:SER:O	1.60	1.19
2:2:215:PRO:CA	3:3:130:MET:HE1	1.72	1.18
1:1:130:TYR:CE2	1:1:134:THR:HG22	1.81	1.15
6:L:36:VAL:HG12	6:L:93:THR:HB	1.15	1.13
5:H:60:ASN:O	5:H:63:LEU:O	1.65	1.12
5:H:61:PRO:HG2	6:L:99:SER:CB	1.80	1.11
6:L:42:ILE:HG22	6:L:43:PRO:HD2	1.27	1.11
6:L:51:ILE:CG2	6:L:54:SER:O	2.00	1.10
6:L:51:ILE:HG21	6:L:54:SER:O	1.52	1.09
1:1:130:TYR:HE2	1:1:134:THR:HG22	1.01	1.09
2:2:214:LEU:CD2	3:3:130:MET:CE	2.28	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:103:ASN:O	2:2:162:TYR:HB2	1.52	1.07
2:2:215:PRO:C	3:3:130:MET:HE1	1.78	1.07
1:1:105:THR:HG22	3:3:16:THR:CG2	1.85	1.06
1:1:105:THR:HG22	3:3:16:THR:HB	1.10	1.06
5:H:29:LEU:HD22	5:H:29:LEU:H	1.21	1.06
2:2:215:PRO:C	3:3:130:MET:CE	2.30	1.04
5:H:24:VAL:HG13	5:H:27:PHE:CZ	1.92	1.04
2:2:214:LEU:HD21	3:3:130:MET:HG2	1.35	1.04
1:1:130:TYR:CE2	1:1:134:THR:CG2	2.40	1.03
5:H:105:PHE:HB2	5:H:108:THR:OG1	1.57	1.03
2:2:111:ALA:O	2:2:154:MET:HB2	1.60	1.01
1:1:130:TYR:HE2	1:1:134:THR:CG2	1.72	1.01
2:2:215:PRO:O	3:3:130:MET:HE1	1.52	1.01
2:2:215:PRO:CD	3:3:130:MET:CE	2.35	1.01
2:2:215:PRO:O	3:3:130:MET:HE2	1.59	1.00
2:2:48:THR:HA	3:3:163:VAL:HG12	1.42	1.00
3:3:17:THR:HG23	3:3:17:THR:O	1.58	1.00
2:2:215:PRO:HG2	3:3:130:MET:SD	2.02	0.99
1:1:101:THR:O	1:1:101:THR:HG22	1.60	0.98
6:L:26:GLY:HA3	6:L:31:ILE:HD12	1.46	0.98
1:1:107:TYR:CE1	3:3:14:LEU:HD11	1.99	0.97
2:2:215:PRO:N	3:3:130:MET:CE	2.26	0.97
5:H:107:TYR:HB3	6:L:99:SER:O	1.64	0.96
6:L:5:VAL:HB	6:L:102:VAL:CG1	1.93	0.96
5:H:110:MET:CG	6:L:103:PHE:CZ	2.48	0.96
2:2:214:LEU:HD23	3:3:130:MET:HE2	0.96	0.95
2:2:215:PRO:CA	3:3:130:MET:CE	2.44	0.94
2:2:215:PRO:HD2	3:3:130:MET:HE3	1.46	0.94
5:H:30:SER:CA	5:H:53:THR:OG1	2.14	0.94
2:2:215:PRO:CG	3:3:130:MET:HE3	1.87	0.93
1:1:105:THR:H	3:3:16:THR:HG22	1.29	0.93
1:1:120:THR:HB	3:3:214:LEU:HD11	1.49	0.93
1:1:192:ALA:O	2:2:135:ARG:NH1	2.01	0.92
6:L:42:ILE:HG22	6:L:43:PRO:CD	1.98	0.92
1:1:91:ASN:OD1	1:1:91:ASN:O	1.88	0.92
1:1:30:THR:CG2	1:1:30:THR:O	2.18	0.92
5:H:61:PRO:HG2	6:L:99:SER:HB2	1.49	0.91
3:3:72:ARG:CZ	3:3:137:PRO:HG3	2.01	0.91
1:1:102:SER:HB3	3:3:217:ASP:OD2	1.71	0.90
6:L:36:VAL:HG12	6:L:93:THR:CB	2.02	0.89
1:1:105:THR:N	3:3:16:THR:HG22	1.86	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:214:LEU:HD23	3:3:130:MET:HE3	1.53	0.89
2:2:112:VAL:O	2:2:197:ILE:CD1	2.20	0.89
1:1:30:THR:O	1:1:30:THR:HG23	1.70	0.89
3:3:17:THR:O	3:3:17:THR:CG2	2.22	0.88
1:1:130:TYR:OH	1:1:134:THR:HG21	1.75	0.86
3:3:136:THR:HB	3:3:139:GLU:HB2	1.57	0.86
1:1:105:THR:O	3:3:15:VAL:HG13	1.76	0.86
1:1:90:PRO:HD2	3:3:216:ILE:HG21	1.56	0.86
6:L:6:LEU:H	6:L:102:VAL:CG1	1.89	0.85
1:1:104:PRO:HA	3:3:16:THR:CG2	2.06	0.85
2:2:47:ASN:ND2	3:3:167:ASP:OD1	2.09	0.84
6:L:5:VAL:HB	6:L:102:VAL:HG11	1.58	0.84
1:1:90:PRO:HD2	3:3:216:ILE:CG2	2.07	0.84
5:H:29:LEU:HB3	5:H:71:LYS:HD2	1.59	0.84
2:2:215:PRO:N	3:3:143:CYS:SG	2.50	0.83
3:3:72:ARG:CZ	3:3:137:PRO:CG	2.56	0.83
5:H:30:SER:HA	5:H:53:THR:HG1	1.42	0.83
2:2:107:VAL:HG23	2:2:203:ILE:HG12	1.61	0.82
5:H:61:PRO:HG2	6:L:99:SER:HB3	1.59	0.82
1:1:102:SER:CB	3:3:217:ASP:OD2	2.28	0.82
2:2:72:ASP:HB2	5:H:108:THR:CG2	2.10	0.81
2:2:215:PRO:CD	3:3:143:CYS:HG	1.77	0.81
1:1:103:ASN:O	3:3:16:THR:HG21	1.81	0.80
2:2:214:LEU:HD21	3:3:130:MET:HG3	1.61	0.80
2:2:215:PRO:HG2	3:3:130:MET:HE3	1.54	0.79
5:H:110:MET:HG2	6:L:103:PHE:CZ	2.17	0.79
1:1:82:HIS:O	1:1:108:ARG:NH2	2.16	0.78
3:3:72:ARG:NE	3:3:137:PRO:HG3	1.99	0.77
1:1:45:GLN:HB2	1:1:49:HIS:HB2	1.66	0.77
1:1:5:GLY:C	1:1:7:SER:O	2.27	0.77
2:2:91:TYR:OH	2:2:103:ASN:ND2	2.18	0.77
2:2:215:PRO:C	3:3:130:MET:HE2	2.04	0.76
6:L:30:ASN:HB3	6:L:95:ASP:HB2	1.66	0.76
1:1:13:THR:OG1	1:1:17:ASN:ND2	2.19	0.76
1:1:42:ILE:HD12	1:1:177:VAL:HG21	1.68	0.76
2:2:72:ASP:OD2	6:L:34:TYR:HD2	1.69	0.76
2:2:72:ASP:HB2	5:H:108:THR:HG21	1.67	0.75
5:H:29:LEU:H	5:H:29:LEU:CD2	1.97	0.75
1:1:90:PRO:CD	3:3:216:ILE:HG22	2.16	0.75
1:1:104:PRO:HA	3:3:16:THR:HG22	1.67	0.75
1:1:120:THR:HB	3:3:214:LEU:CD1	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:215:PRO:N	3:3:130:MET:HE3	1.98	0.74
1:1:107:TYR:HE1	3:3:14:LEU:HD11	1.49	0.74
1:1:28:GLN:O	1:1:28:GLN:HG2	1.88	0.74
2:2:215:PRO:HD3	3:3:143:CYS:HG	0.83	0.74
2:2:70:THR:CG2	6:L:33:ARG:O	2.35	0.74
2:2:214:LEU:HD12	3:3:129:GLY:HA3	1.70	0.74
1:1:37:ASP:O	1:1:178:ARG:HD2	1.88	0.74
1:1:101:THR:O	1:1:101:THR:CG2	2.32	0.74
2:2:112:VAL:O	2:2:197:ILE:HD12	1.89	0.73
1:1:90:PRO:CD	3:3:216:ILE:CG2	2.66	0.73
6:L:8:GLN:HE21	6:L:106:GLY:N	1.87	0.73
6:L:5:VAL:HB	6:L:102:VAL:HG13	1.69	0.72
5:H:29:LEU:HD22	5:H:29:LEU:N	2.01	0.72
1:1:113:THR:HA	3:3:10:GLY:O	1.90	0.72
2:2:140:LEU:C	2:2:140:LEU:HD23	2.15	0.72
2:2:109:VAL:HA	2:2:201:ALA:HA	1.72	0.71
1:1:37:ASP:O	1:1:178:ARG:HG3	1.90	0.71
1:1:100:ASN:HD21	3:3:219:ARG:HB2	1.54	0.71
5:H:24:VAL:HG13	5:H:27:PHE:CE2	2.26	0.71
6:L:6:LEU:HD23	6:L:91:CYS:HB3	1.72	0.71
5:H:86:THR:HG23	5:H:88:GLU:H	1.56	0.71
2:2:146:GLN:OE1	2:2:157:HIS:N	2.22	0.71
2:2:214:LEU:CD1	3:3:129:GLY:HA3	2.20	0.71
5:H:47:PHE:CD1	5:H:48:LEU:O	2.44	0.70
6:L:6:LEU:H	6:L:102:VAL:HG11	1.56	0.70
1:1:6:GLU:C	1:1:7:SER:O	2.16	0.70
2:2:37:SER:HB3	2:2:161:PRO:HG3	1.73	0.70
1:1:107:TYR:CE1	3:3:14:LEU:CD1	2.75	0.70
6:L:8:GLN:HE21	6:L:106:GLY:H	1.40	0.70
1:1:37:ASP:O	1:1:178:ARG:CD	2.40	0.69
3:3:63:TYR:HA	3:3:200:LEU:O	1.93	0.69
2:2:103:ASN:O	2:2:162:TYR:CB	2.38	0.69
2:2:215:PRO:HG2	3:3:130:MET:HE1	1.43	0.69
2:2:16:THR:HG23	2:2:25:THR:HG22	1.76	0.68
1:1:51:ILE:CD1	1:1:78:ILE:HG21	2.24	0.68
2:2:31:GLY:O	2:2:146:GLN:NE2	2.26	0.67
2:2:74:ALA:HB3	5:H:100:HIS:HB3	1.74	0.67
2:2:78:LEU:HD12	2:2:137:LYS:HE2	1.76	0.66
2:2:140:LEU:HD23	2:2:140:LEU:O	1.96	0.66
2:2:83:LEU:HD21	2:2:203:ILE:HD13	1.76	0.66
2:2:70:THR:HG23	6:L:33:ARG:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:83:ASP:O	1:1:84:ASP:OD1	2.13	0.66
1:1:27:ARG:HB3	1:1:30:THR:HG22	1.77	0.66
2:2:215:PRO:HG3	3:3:126:VAL:CG1	2.26	0.65
6:L:28:SER:HA	6:L:32:GLY:HA3	1.79	0.65
1:1:90:PRO:HB3	3:3:214:LEU:HD13	1.77	0.65
2:2:146:GLN:HB3	2:2:156:ALA:HB1	1.77	0.65
6:L:42:ILE:CG2	6:L:43:PRO:HD2	2.17	0.65
2:2:104:GLY:C	2:2:206:THR:HG22	2.22	0.65
1:1:200:ARG:O	1:1:202:LYS:HG2	1.96	0.64
1:1:51:ILE:HD12	1:1:78:ILE:HG21	1.80	0.64
1:1:130:TYR:CZ	1:1:134:THR:CG2	2.81	0.64
3:3:72:ARG:NH2	3:3:137:PRO:HG2	2.12	0.64
5:H:111:GLN:HE21	6:L:94:GLY:N	1.95	0.64
1:1:130:TYR:CZ	1:1:134:THR:HG21	2.33	0.63
6:L:42:ILE:CG2	6:L:43:PRO:CD	2.73	0.63
2:2:83:LEU:HD11	2:2:203:ILE:CD1	2.28	0.63
5:H:110:MET:HE2	5:H:110:MET:HA	1.80	0.63
1:1:130:TYR:CE2	1:1:134:THR:HG21	2.32	0.63
2:2:112:VAL:O	2:2:197:ILE:HD11	1.99	0.63
2:2:215:PRO:O	3:3:130:MET:SD	2.57	0.63
2:2:72:ASP:HB2	5:H:108:THR:HG23	1.80	0.62
6:L:48:ARG:HH12	6:L:61:VAL:HG22	1.63	0.62
6:L:6:LEU:N	6:L:102:VAL:HG11	2.14	0.62
2:2:113:GLY:HA3	2:2:150:PRO:HB3	1.81	0.62
2:2:47:ASN:OD1	3:3:164:SER:O	2.18	0.62
5:H:110:MET:SD	6:L:103:PHE:CE1	2.91	0.62
6:L:22:ILE:HG21	6:L:107:THR:HG21	1.81	0.62
5:H:111:GLN:NE2	6:L:94:GLY:N	2.48	0.62
6:L:80:SER:O	6:L:82:GLN:NE2	2.31	0.62
1:1:70:THR:HG22	1:1:188:ARG:HE	1.65	0.61
2:2:47:ASN:OD1	3:3:166:ALA:O	2.18	0.61
1:1:91:ASN:OD1	1:1:91:ASN:C	2.44	0.61
1:1:107:TYR:HE1	3:3:14:LEU:CD1	2.12	0.61
1:1:209:ALA:O	1:1:210:LYS:HB2	2.01	0.61
3:3:72:ARG:NH2	3:3:137:PRO:CG	2.63	0.61
6:L:22:ILE:CG2	6:L:107:THR:HG21	2.30	0.60
3:3:119:ALA:O	3:3:150:THR:OG1	2.13	0.60
6:L:26:GLY:CA	6:L:31:ILE:HD12	2.26	0.60
2:2:47:ASN:HD22	2:2:167:ARG:HG3	1.66	0.59
3:3:15:VAL:HB	3:3:18:ASP:HB2	1.82	0.59
1:1:102:SER:OG	3:3:217:ASP:OD2	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:83:LEU:HD11	2:2:203:ILE:HD13	1.83	0.59
5:H:39:GLN:HE22	6:L:41:GLN:HE22	1.51	0.59
5:H:47:PHE:CD1	5:H:110:MET:CE	2.85	0.59
2:2:109:VAL:HG11	2:2:123:VAL:HG11	1.84	0.59
5:H:34:VAL:HG21	5:H:78:VAL:HG11	1.85	0.58
6:L:5:VAL:CB	6:L:102:VAL:HG13	2.34	0.58
1:1:48:THR:HG22	1:1:48:THR:O	2.02	0.58
6:L:36:VAL:HA	6:L:92:ALA:O	2.03	0.58
1:1:42:ILE:CD1	1:1:177:VAL:HG21	2.32	0.58
2:2:97:SER:O	2:2:97:SER:OG	2.19	0.58
3:3:63:TYR:CB	3:3:200:LEU:O	2.52	0.58
6:L:8:GLN:NE2	6:L:106:GLY:N	2.52	0.58
1:1:37:ASP:O	1:1:178:ARG:CG	2.51	0.58
2:2:214:LEU:CD2	3:3:130:MET:CG	2.64	0.58
2:2:43:VAL:HG12	2:2:43:VAL:O	2.03	0.58
2:2:127:PRO:HD2	2:2:143:PHE:CD1	2.38	0.58
2:2:123:VAL:HG23	2:2:158:ILE:HD11	1.86	0.58
2:2:214:LEU:HD11	3:3:129:GLY:C	2.29	0.58
3:3:100:GLN:NE2	3:3:213:ARG:HH21	2.02	0.58
5:H:110:MET:HG2	6:L:103:PHE:CE2	2.38	0.58
2:2:129:TYR:HB2	2:2:178:THR:OG1	2.04	0.57
1:1:105:THR:N	3:3:16:THR:CG2	2.65	0.57
3:3:72:ARG:CZ	3:3:137:PRO:HG2	2.34	0.57
6:L:50:ILE:HG22	6:L:51:ILE:HG12	1.86	0.57
3:3:135:ASP:OD1	3:3:135:ASP:N	2.32	0.56
2:2:72:ASP:OD2	6:L:34:TYR:CD2	2.57	0.56
1:1:107:TYR:CD1	3:3:14:LEU:HD11	2.40	0.56
2:2:134:LEU:HD12	2:2:134:LEU:O	2.06	0.56
1:1:104:PRO:HG3	3:3:17:THR:HG21	1.88	0.56
6:L:80:SER:OG	6:L:82:GLN:NE2	2.39	0.56
5:H:67:LEU:HB3	5:H:82:LEU:HD12	1.88	0.55
1:1:104:PRO:CA	3:3:16:THR:CG2	2.82	0.55
2:2:146:GLN:OE1	2:2:156:ALA:CA	2.55	0.55
1:1:183:GLU:OE1	1:1:185:TYR:OH	2.24	0.55
3:3:63:TYR:CA	3:3:200:LEU:O	2.53	0.55
2:2:40:GLU:N	2:2:40:GLU:OE1	2.39	0.55
2:2:214:LEU:CD2	3:3:130:MET:HE3	2.24	0.55
3:3:181:VAL:HG23	3:3:182:GLN:HG2	1.88	0.55
5:H:29:LEU:CB	5:H:71:LYS:HD2	2.35	0.55
2:2:77:HIS:ND1	5:H:100:HIS:CE1	2.74	0.55
2:2:137:LYS:HB3	2:2:182:MET:SD	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:26:GLY:HA3	6:L:31:ILE:CD1	2.30	0.54
1:1:88:TRP:HE1	1:1:165:GLY:HA3	1.73	0.54
2:2:99:ALA:CB	2:2:212:GLY:O	2.56	0.54
2:2:68:ASP:OD2	6:L:69:ARG:NH1	2.41	0.54
5:H:24:VAL:CG1	5:H:27:PHE:CE2	2.91	0.54
1:1:80:VAL:HG22	1:1:175:LEU:HD13	1.89	0.53
2:2:146:GLN:OE1	2:2:156:ALA:HA	2.08	0.53
2:2:73:LYS:HD3	2:2:77:HIS:CD2	2.43	0.53
2:2:215:PRO:HG3	3:3:126:VAL:HG12	1.91	0.53
4:4:79:LEU:HD13	4:4:83:LEU:HD12	1.90	0.53
6:L:37:GLY:N	6:L:92:ALA:O	2.42	0.53
1:1:81:ARG:HG2	1:1:174:GLU:HG2	1.90	0.53
3:3:66:THR:HG22	3:3:189:GLN:HE22	1.73	0.53
1:1:68:ALA:O	1:1:188:ARG:N	2.41	0.53
5:H:24:VAL:CG1	5:H:27:PHE:CZ	2.82	0.53
1:1:56:THR:O	1:1:67:ARG:NH2	2.42	0.53
6:L:88:ASP:HA	6:L:107:THR:O	2.09	0.53
1:1:167:ILE:HD11	1:1:175:LEU:HD22	1.91	0.53
2:2:134:LEU:HD23	5:H:31:ASP:O	2.09	0.53
5:H:47:PHE:CD1	5:H:110:MET:HE3	2.44	0.52
2:2:106:ASP:HA	2:2:159:THR:HA	1.91	0.52
1:1:93:ALA:HB2	3:3:216:ILE:HD13	1.90	0.52
2:2:99:ALA:HB3	2:2:212:GLY:HA3	1.91	0.52
3:3:58:ASP:N	3:3:58:ASP:OD1	2.42	0.52
1:1:112:PHE:O	3:3:10:GLY:HA2	2.10	0.52
2:2:55:VAL:HG11	2:2:94:LEU:HD21	1.91	0.52
3:3:78:ASP:OD2	3:3:180:ASN:HB2	2.10	0.52
2:2:102:ARG:HD2	2:2:168:TYR:HE1	1.74	0.52
5:H:111:GLN:NE2	6:L:94:GLY:H	2.07	0.52
1:1:124:ARG:O	1:1:125:VAL:HG13	2.09	0.52
6:L:13:SER:HB3	6:L:112:LEU:HD11	1.92	0.52
6:L:9:PRO:O	6:L:107:THR:HG23	2.10	0.51
1:1:42:ILE:HG23	1:1:43:PRO:HD2	1.92	0.51
2:2:129:TYR:CE1	2:2:132:PHE:HE1	2.29	0.51
2:2:213:GLU:O	3:3:127:PRO:CG	2.58	0.51
3:3:117:SER:O	3:3:117:SER:OG	2.28	0.51
2:2:37:SER:OG	2:2:39:GLY:O	2.26	0.51
3:3:134:PRO:O	3:3:188:TYR:OH	2.21	0.51
3:3:159:SER:O	3:3:159:SER:OG	2.29	0.51
5:H:47:PHE:CE1	5:H:48:LEU:O	2.63	0.51
2:2:109:VAL:HG13	2:2:148:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:115:GLN:O	2:2:115:GLN:HG3	2.11	0.50
1:1:104:PRO:CA	3:3:16:THR:HG22	2.40	0.50
1:1:105:THR:HG22	3:3:16:THR:HG22	1.87	0.50
2:2:47:ASN:O	2:2:48:THR:OG1	2.24	0.50
1:1:50:VAL:HA	1:1:166:ALA:HA	1.93	0.50
1:1:30:THR:O	1:1:30:THR:HG22	2.10	0.50
2:2:169:ASP:OD1	2:2:169:ASP:N	2.41	0.50
3:3:109:PHE:HB3	3:3:200:LEU:HD11	1.94	0.50
1:1:65:LEU:O	1:1:68:ALA:HB3	2.12	0.50
1:1:51:ILE:CD1	1:1:78:ILE:CG2	2.90	0.50
1:1:112:PHE:O	1:1:112:PHE:CD1	2.64	0.50
3:3:149:ASP:OD1	3:3:150:THR:N	2.45	0.49
5:H:39:GLN:HE22	6:L:41:GLN:NE2	2.09	0.49
2:2:187:LEU:HD22	2:2:197:ILE:HG22	1.93	0.49
2:2:214:LEU:HD21	3:3:130:MET:SD	2.52	0.49
1:1:90:PRO:HG2	3:3:216:ILE:CG2	2.42	0.49
2:2:214:LEU:HD23	2:2:214:LEU:C	2.38	0.49
3:3:72:ARG:NH2	3:3:137:PRO:HG3	2.28	0.49
6:L:39:TYR:O	6:L:89:TYR:HA	2.13	0.49
2:2:142:LEU:CD1	2:2:142:LEU:N	2.76	0.49
1:1:49:HIS:O	1:1:167:ILE:O	2.31	0.49
1:1:107:TYR:CD1	3:3:14:LEU:CD1	2.96	0.48
1:1:131:ASN:ND2	2:2:175:LYS:O	2.44	0.48
4:4:15:SER:OG	4:4:16:GLY:N	2.46	0.48
5:H:99:ILE:HG13	5:H:100:HIS:CD2	2.48	0.48
5:H:109:TYR:CD1	5:H:109:TYR:C	2.92	0.48
1:1:25:GLN:HG3	1:1:27:ARG:NH1	2.29	0.48
1:1:129:VAL:HG21	2:2:130:LYS:HB2	1.94	0.48
3:3:136:THR:HG22	3:3:138:GLU:HG3	1.94	0.48
5:H:27:PHE:HB2	5:H:97:LYS:HD2	1.95	0.48
2:2:83:LEU:HD21	2:2:203:ILE:HG21	1.96	0.48
4:4:31:GLN:O	4:4:31:GLN:HG3	2.14	0.48
4:4:35:ASP:OD1	4:4:36:THR:N	2.46	0.48
1:1:105:THR:O	3:3:15:VAL:CG1	2.56	0.48
2:2:191:ASN:OD1	2:2:192:SER:N	2.46	0.48
5:H:86:THR:H	5:H:89:ASP:HB2	1.78	0.48
6:L:8:GLN:NE2	6:L:106:GLY:H	2.09	0.48
1:1:122:PRO:HG3	3:3:170:TYR:HE1	1.78	0.48
2:2:123:VAL:HG12	2:2:181:VAL:HG22	1.95	0.48
5:H:111:GLN:HE21	6:L:94:GLY:CA	2.26	0.48
2:2:214:LEU:CD2	3:3:130:MET:HG3	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:122:PRO:HG3	3:3:170:TYR:CE1	2.48	0.48
2:2:107:VAL:HG21	2:2:179:LEU:HD22	1.95	0.47
5:H:66:ARG:O	5:H:83:SER:N	2.47	0.47
2:2:47:ASN:ND2	2:2:167:ARG:HG3	2.29	0.47
2:2:111:ALA:HB2	2:2:199:VAL:HG12	1.96	0.47
1:1:189:PRO:HG2	2:2:136:GLU:OE1	2.14	0.47
2:2:66:LEU:HB2	2:2:199:VAL:HG23	1.96	0.47
2:2:196:GLN:NE2	2:2:198:LYS:HZ3	2.13	0.47
6:L:9:PRO:O	6:L:107:THR:CG2	2.63	0.47
2:2:48:THR:CA	3:3:163:VAL:HG12	2.29	0.47
3:3:112:THR:OG1	3:3:199:THR:OG1	2.33	0.47
1:1:27:ARG:HB3	1:1:30:THR:CG2	2.43	0.47
3:3:63:TYR:HB2	3:3:199:THR:HB	1.96	0.47
1:1:35:ILE:HD11	1:1:61:LEU:HD21	1.96	0.47
1:1:104:PRO:HA	3:3:16:THR:HG23	1.94	0.47
2:2:117:ASN:HB2	2:2:188:THR:O	2.15	0.47
2:2:82:GLU:HA	2:2:178:THR:HG22	1.97	0.46
3:3:72:ARG:O	3:3:188:TYR:HD1	1.97	0.46
5:H:33:ALA:HB1	5:H:51:ILE:O	2.15	0.46
1:1:57:HIS:HE1	1:1:59:HIS:HD2	1.63	0.46
2:2:126:VAL:HG23	2:2:143:PHE:CE1	2.50	0.46
5:H:30:SER:C	5:H:53:THR:OG1	2.59	0.46
1:1:14:THR:HB	1:1:22:THR:HG21	1.96	0.46
1:1:105:THR:CG2	3:3:16:THR:CB	2.45	0.46
1:1:51:ILE:HD11	1:1:78:ILE:CG2	2.46	0.46
2:2:214:LEU:HD11	3:3:129:GLY:CA	2.46	0.46
1:1:42:ILE:CG2	1:1:43:PRO:HD2	2.46	0.46
2:2:66:LEU:HB2	2:2:199:VAL:O	2.15	0.46
3:3:71:GLN:O	3:3:72:ARG:HG3	2.16	0.46
5:H:39:GLN:HA	5:H:45:LEU:HD23	1.98	0.46
2:2:108:GLU:O	2:2:202:ASN:N	2.49	0.46
2:2:75:PHE:HA	2:2:183:VAL:O	2.17	0.45
1:1:105:THR:HG21	3:3:16:THR:HB	1.77	0.45
2:2:99:ALA:HB2	2:2:212:GLY:O	2.16	0.45
3:3:67:ARG:NH2	3:3:74:LEU:O	2.49	0.45
1:1:57:HIS:CE1	1:1:59:HIS:HD2	2.34	0.45
2:2:214:LEU:CD1	3:3:129:GLY:CA	2.94	0.45
1:1:70:THR:HG22	1:1:188:ARG:NE	2.30	0.45
6:L:36:VAL:HG21	6:L:74:ALA:CB	2.47	0.45
1:1:48:THR:HG23	1:1:98:LEU:CD1	2.47	0.45
1:1:91:ASN:O	1:1:91:ASN:CG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:60:ASN:O	5:H:63:LEU:C	2.53	0.45
2:2:19:ASN:HB2	2:2:61:PHE:CE1	2.52	0.45
2:2:74:ALA:HB1	5:H:102:TYR:CE1	2.51	0.45
1:1:130:TYR:OH	1:1:134:THR:CG2	2.55	0.45
2:2:126:VAL:HG23	2:2:143:PHE:CD1	2.52	0.45
4:4:21:ILE:HG13	4:4:21:ILE:O	2.17	0.45
5:H:110:MET:HG2	6:L:101:SER:OG	2.17	0.45
1:1:93:ALA:CB	3:3:216:ILE:CD1	2.95	0.44
2:2:103:ASN:N	2:2:103:ASN:OD1	2.50	0.44
6:L:15:SER:H	6:L:18:GLN:HE22	1.64	0.44
1:1:93:ALA:HA	1:1:94:PRO:HD3	1.95	0.44
3:3:63:TYR:HB2	3:3:200:LEU:O	2.16	0.44
3:3:70:GLY:O	3:3:71:GLN:HB2	2.18	0.44
2:2:104:GLY:O	2:2:206:THR:N	2.37	0.44
3:3:34:ARG:O	3:3:34:ARG:HG2	2.18	0.44
1:1:42:ILE:HG12	1:1:56:THR:HG22	1.99	0.44
2:2:72:ASP:HA	5:H:104:VAL:HG11	2.00	0.44
2:2:189:VAL:HG23	2:2:193:GLY:O	2.18	0.44
2:2:196:GLN:NE2	2:2:198:LYS:NZ	2.65	0.44
6:L:15:SER:N	6:L:18:GLN:HE22	2.16	0.44
1:1:51:ILE:HD11	1:1:76:LEU:HD23	2.00	0.44
1:1:44:SER:HB2	1:1:172:ILE:HG22	2.00	0.43
4:4:83:LEU:HD23	4:4:84:LEU:N	2.32	0.43
2:2:202:ASN:N	2:2:202:ASN:OD1	2.50	0.43
3:3:64:VAL:HG23	3:3:64:VAL:O	2.18	0.43
6:L:6:LEU:N	6:L:102:VAL:CG1	2.67	0.43
5:H:39:GLN:NE2	6:L:41:GLN:HE22	2.16	0.43
2:2:43:VAL:O	2:2:43:VAL:CG1	2.65	0.43
2:2:121:LEU:HB3	2:2:148:ILE:HB	2.01	0.43
5:H:98:SER:HB3	5:H:109:TYR:CE2	2.53	0.43
6:L:51:ILE:HG22	6:L:54:SER:O	2.05	0.43
2:2:79:GLU:OE2	2:2:79:GLU:HA	2.18	0.43
5:H:109:TYR:O	5:H:110:MET:C	2.62	0.43
1:1:32:VAL:HA	1:1:35:ILE:HG22	2.01	0.43
1:1:90:PRO:CG	3:3:216:ILE:CG2	2.96	0.43
2:2:72:ASP:CB	5:H:108:THR:HG23	2.49	0.43
5:H:111:GLN:OE1	6:L:35:ASP:O	2.37	0.43
6:L:33:ARG:HG3	6:L:34:TYR:CD1	2.54	0.43
1:1:68:ALA:HB2	1:1:190:LEU:HD13	2.01	0.42
3:3:120:ARG:HD3	3:3:190:ILE:HD11	2.01	0.42
1:1:45:GLN:HB2	1:1:49:HIS:CB	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:214:LEU:HD23	2:2:215:PRO:N	2.34	0.42
1:1:53:LEU:HD12	1:1:72:TYR:CE2	2.55	0.42
1:1:188:ARG:NH2	2:2:128:GLU:O	2.52	0.42
2:2:74:ALA:HB1	5:H:102:TYR:CZ	2.54	0.42
1:1:1:THR:O	1:1:2:THR:OG1	2.31	0.42
1:1:130:TYR:HB2	1:1:158:LEU:HD13	2.01	0.42
3:3:194:LYS:HG3	3:3:196:GLU:HG2	2.00	0.42
5:H:111:GLN:HE21	6:L:94:GLY:HA3	1.84	0.42
2:2:112:VAL:O	2:2:197:ILE:CG1	2.67	0.42
3:3:122:MET:HE1	3:3:141:ALA:HA	2.02	0.42
6:L:6:LEU:H	6:L:102:VAL:HG12	1.79	0.42
1:1:70:THR:HG23	1:1:186:CYS:O	2.20	0.42
1:1:88:TRP:NE1	1:1:165:GLY:HA3	2.34	0.42
2:2:147:PHE:HE2	2:2:184:LEU:HD11	1.85	0.42
6:L:12:VAL:HG13	6:L:109:LEU:HD23	2.02	0.42
1:1:3:THR:HG21	1:1:11:VAL:HG11	2.02	0.42
5:H:61:PRO:CG	6:L:99:SER:HB3	2.38	0.42
1:1:93:ALA:CB	3:3:216:ILE:HD13	2.49	0.41
1:1:100:ASN:N	1:1:100:ASN:HD22	2.17	0.41
2:2:67:PHE:HA	6:L:55:LYS:HD3	2.01	0.41
2:2:67:PHE:O	2:2:199:VAL:HG22	2.19	0.41
2:2:70:THR:HG22	2:2:71:THR:N	2.35	0.41
3:3:67:ARG:NH1	3:3:71:GLN:HG2	2.35	0.41
1:1:75:ASP:OD1	1:1:75:ASP:N	2.51	0.41
2:2:114:ASN:HD22	2:2:193:GLY:HA2	1.85	0.41
3:3:148:TRP:HD1	3:3:149:ASP:O	2.03	0.41
3:3:157:THR:O	3:3:157:THR:OG1	2.35	0.41
1:1:83:ASP:C	1:1:84:ASP:OD1	2.63	0.41
4:4:22:ILE:HD12	4:4:22:ILE:HA	1.91	0.41
1:1:38:ARG:HD2	1:1:61:LEU:HD23	2.02	0.41
6:L:89:TYR:HE1	6:L:109:LEU:HD12	1.86	0.41
3:3:90:TYR:O	3:3:94:ILE:HG22	2.20	0.41
3:3:219:ARG:HD3	3:3:219:ARG:HA	1.77	0.41
2:2:17:THR:OG1	2:2:24:SER:O	2.38	0.41
4:4:27:MET:HE2	4:4:27:MET:HB3	1.76	0.41
5:H:24:VAL:HB	5:H:76:ASN:OD1	2.21	0.41
5:H:51:ILE:HA	5:H:57:THR:HA	2.03	0.41
1:1:194:GLU:HA	2:2:135:ARG:NH2	2.36	0.41
2:2:140:LEU:C	2:2:140:LEU:CD2	2.87	0.41
3:3:67:ARG:HA	3:3:67:ARG:HD3	1.84	0.41
5:H:40:ALA:HB1	5:H:41:PRO:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:189:VAL:HG23	2:2:193:GLY:C	2.46	0.40
3:3:133:PRO:HA	3:3:134:PRO:HD3	1.92	0.40
5:H:111:GLN:HG2	6:L:93:THR:HA	2.03	0.40
1:1:104:PRO:C	3:3:16:THR:HG22	2.44	0.40
6:L:52:TYR:HE2	6:L:58:PRO:HB3	1.86	0.40
2:2:107:VAL:HG22	2:2:108:GLU:N	2.37	0.40
2:2:142:LEU:H	2:2:142:LEU:HD13	1.85	0.40
2:2:163:LEU:HD12	2:2:163:LEU:O	2.20	0.40
3:3:43:ASN:O	3:3:46:ASP:HB3	2.22	0.40
5:H:27:PHE:CD2	5:H:27:PHE:O	2.73	0.40
2:2:146:GLN:OE1	2:2:156:ALA:HB1	2.22	0.40
4:4:77:THR:OG1	4:4:78:GLY:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	185/212 (87%)	169 (91%)	15 (8%)	1 (0%)	24	59
2	2	203/218 (93%)	192 (95%)	11 (5%)	0	100	100
3	3	218/221 (99%)	202 (93%)	16 (7%)	0	100	100
4	4	41/85 (48%)	39 (95%)	2 (5%)	0	100	100
5	H	96/126 (76%)	92 (96%)	4 (4%)	0	100	100
6	L	107/123 (87%)	104 (97%)	3 (3%)	0	100	100
All	All	850/985 (86%)	798 (94%)	51 (6%)	1 (0%)	49	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	47	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	1	161/176 (92%)	158 (98%)	3 (2%)	50	66
2	2	178/191 (93%)	173 (97%)	5 (3%)	38	59
3	3	181/182 (100%)	179 (99%)	2 (1%)	65	74
4	4	37/67 (55%)	37 (100%)	0	100	100
5	H	86/110 (78%)	85 (99%)	1 (1%)	63	73
6	L	90/100 (90%)	88 (98%)	2 (2%)	45	64
All	All	733/826 (89%)	720 (98%)	13 (2%)	51	67

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	51	ILE
1	1	117	LEU
1	1	191	LEU
2	2	106	ASP
2	2	135	ARG
2	2	140	LEU
2	2	142	LEU
2	2	202	ASN
3	3	73	LEU
3	3	135	ASP
5	H	29	LEU
6	L	107	THR
6	L	108	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	17	ASN
1	1	23	GLN
1	1	45	GLN
1	1	57	HIS

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Mol	Chain	Res	Type
1	1	59	HIS
1	1	100	ASN
1	1	123	HIS
1	1	203	GLN
2	2	42	HIS
2	2	103	ASN
2	2	114	ASN
2	2	166	ASN
2	2	196	GLN
2	2	209	HIS
3	3	100	GLN
3	3	108	HIS
3	3	182	GLN
3	3	189	GLN
3	3	192	HIS
4	4	31	GLN
4	4	37	GLN
5	H	16	GLN
5	H	39	GLN
5	H	100	HIS
5	H	111	GLN
6	L	8	GLN
6	L	41	GLN
6	L	72	ASN
6	L	82	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 ⓘ

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.

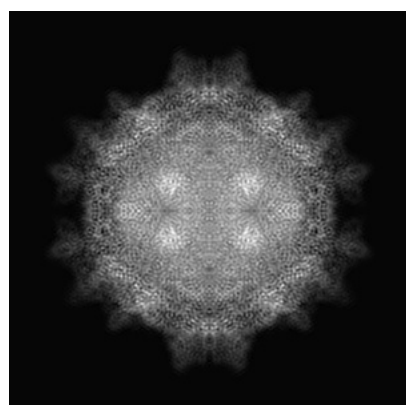
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31556. These allow visual inspection of the internal detail of the map and identification of artifacts.

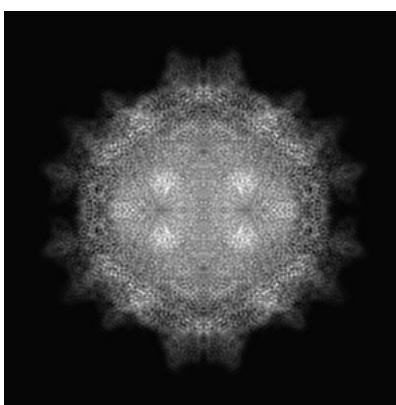
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

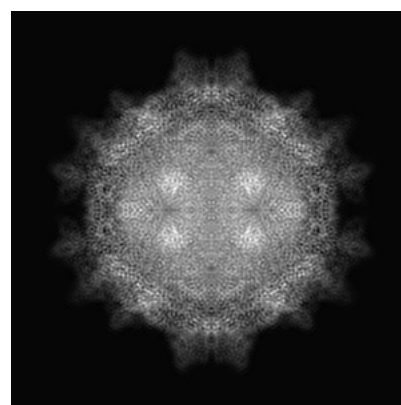
6.1.1 Primary map



X



Y

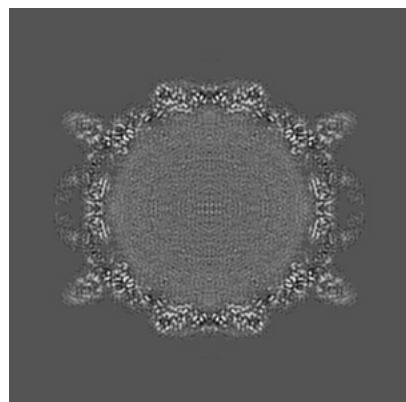


Z

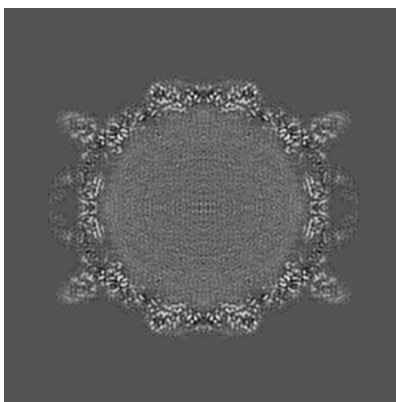
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

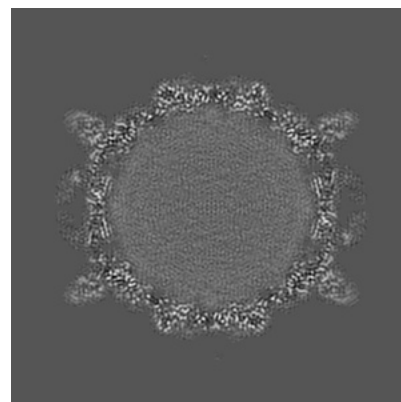
6.2.1 Primary map



X Index: 240



Y Index: 240

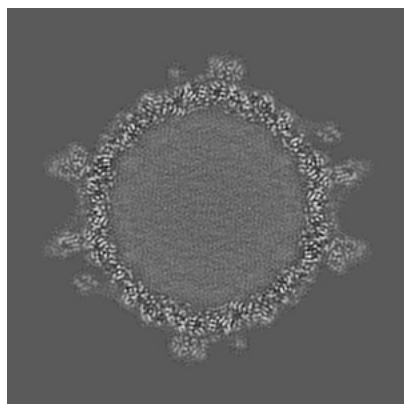


Z Index: 240

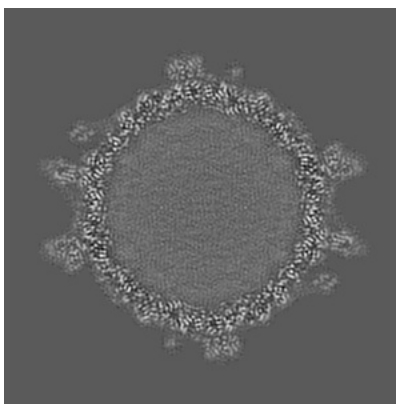
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

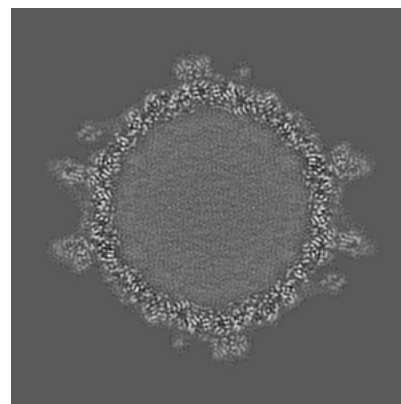
6.3.1 Primary map



X Index: 209



Y Index: 271

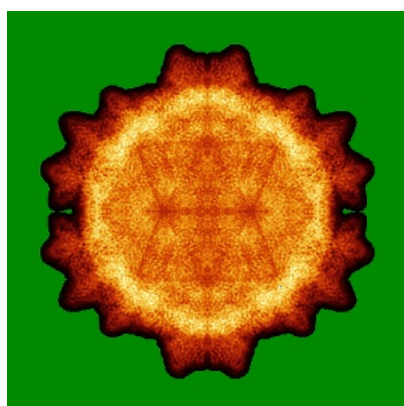


Z Index: 270

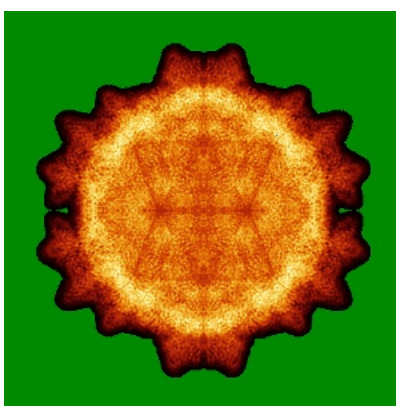
The images above show the largest variance slices of the map in three orthogonal directions.

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

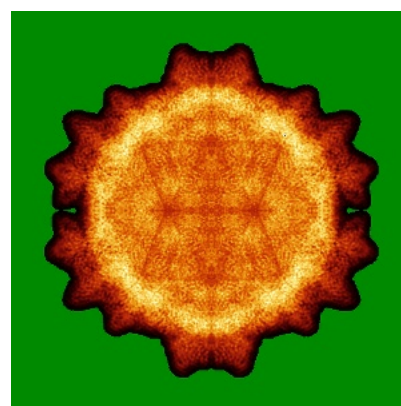
6.4.1 Primary map



X



Y

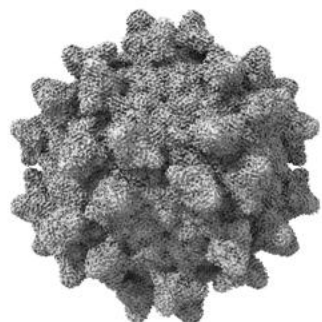


Z

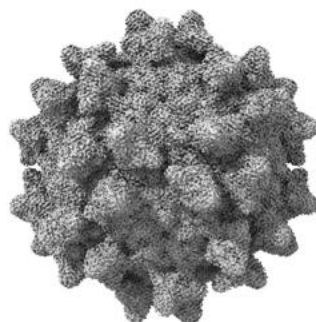
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

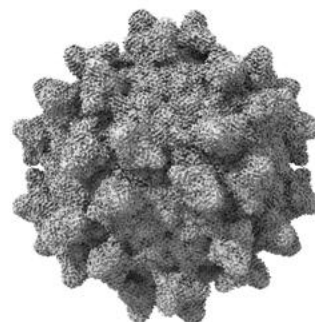
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

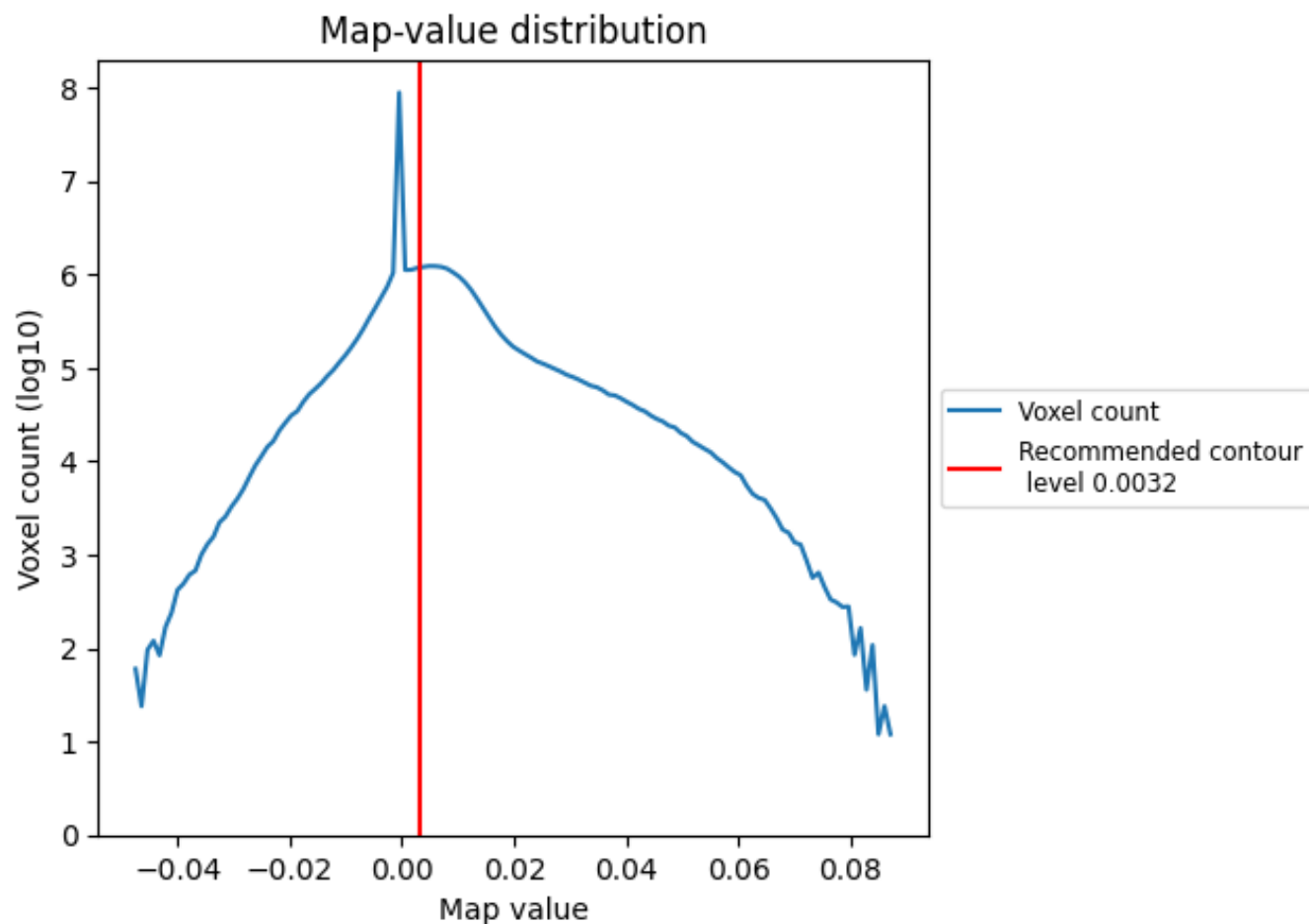
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

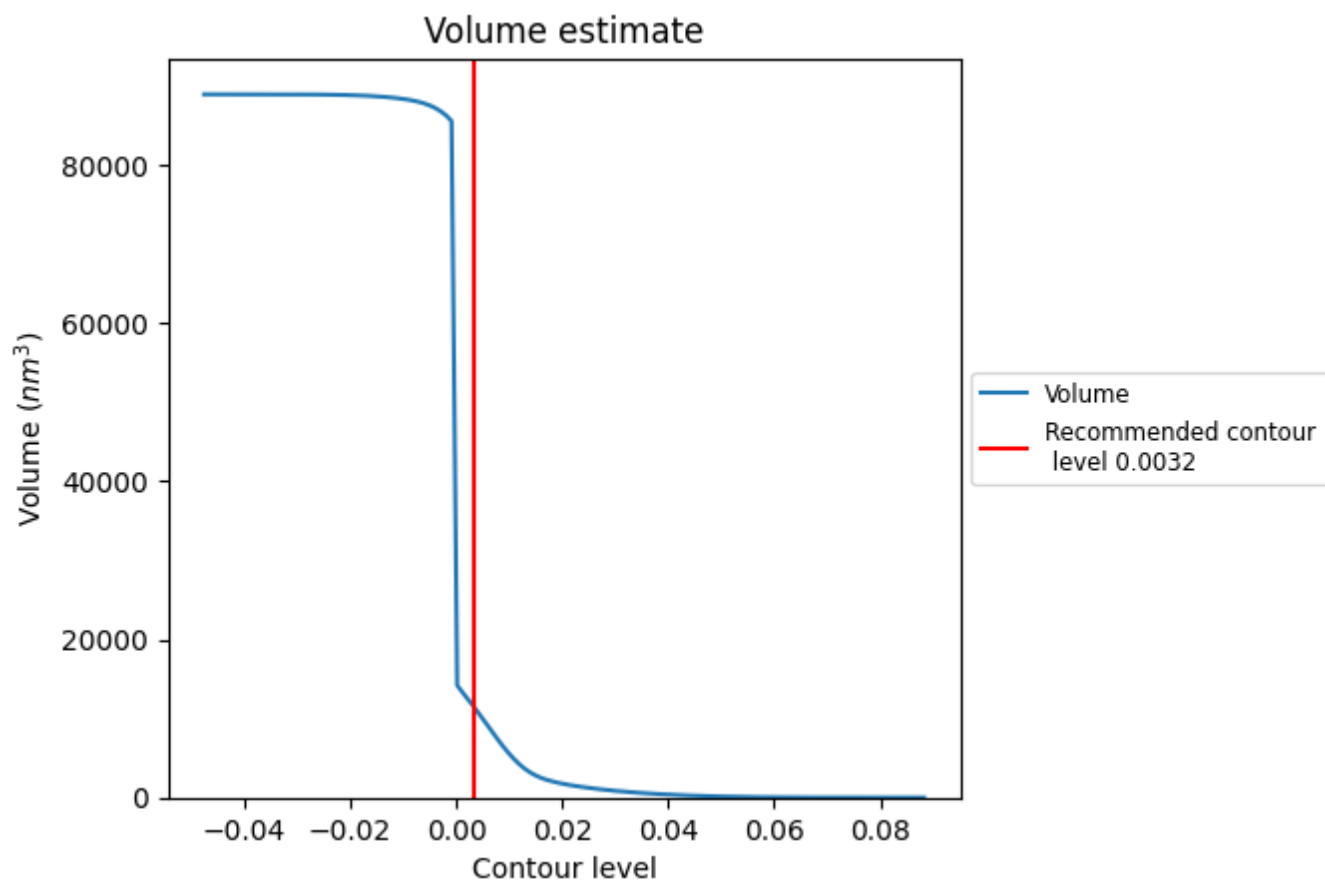
This section contains the results of statistical analysis of the map.

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.

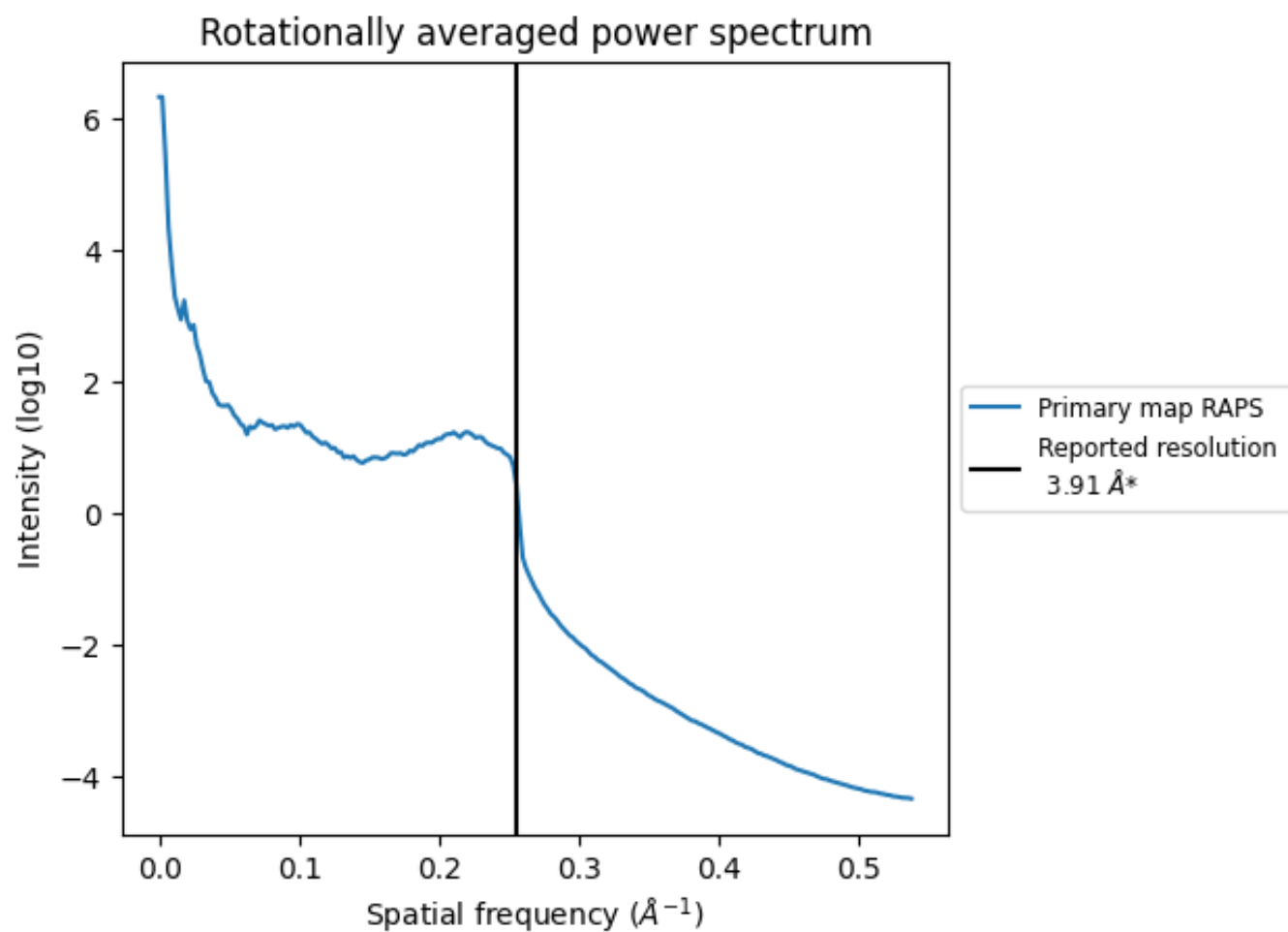
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11627 nm³; this corresponds to an approximate mass of 10503 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 0.256 Å⁻¹

8 Fourier-Shell correlation

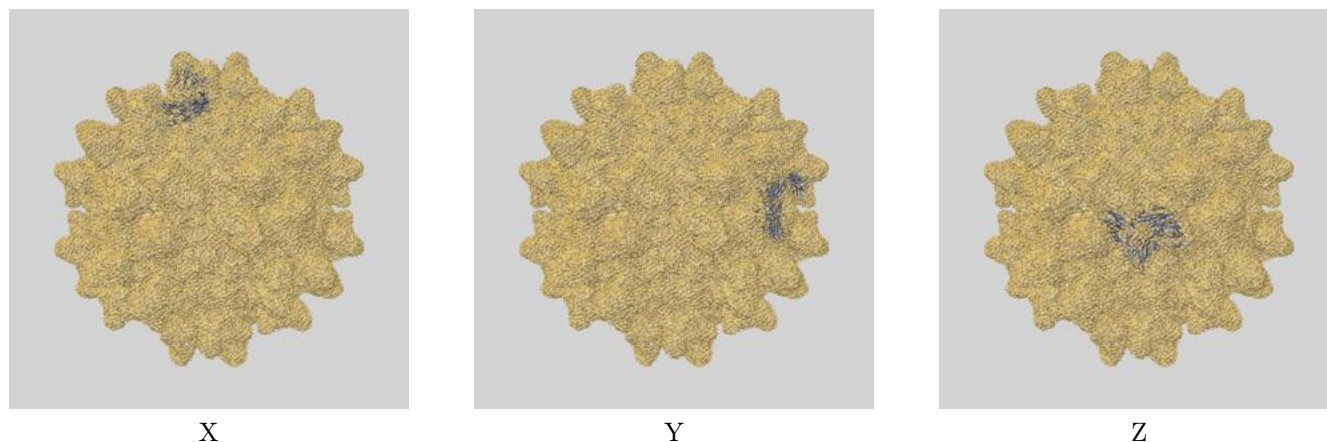
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

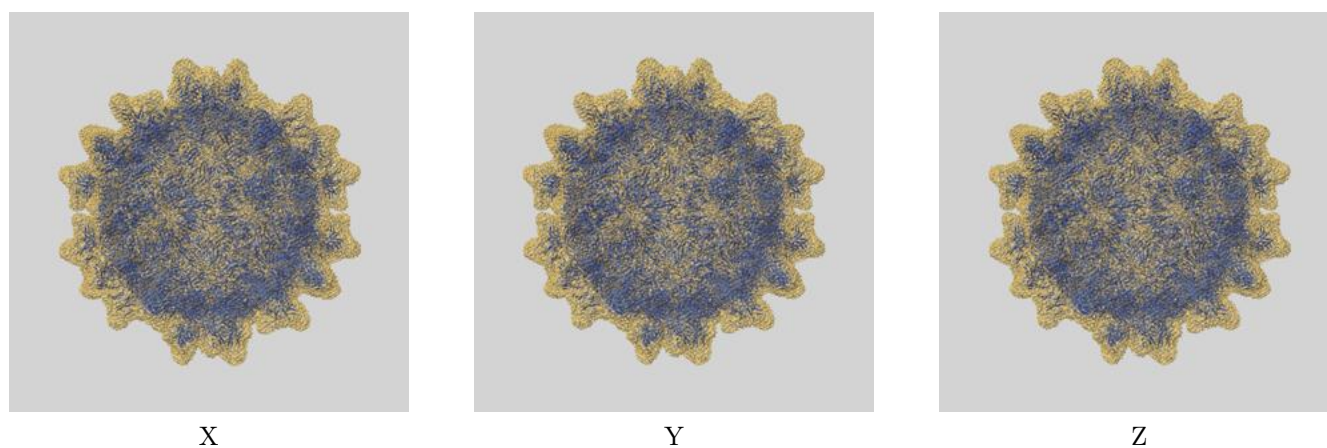
This section contains information regarding the fit between EMDB map EMD-31556 and PDB model 7FEJ. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

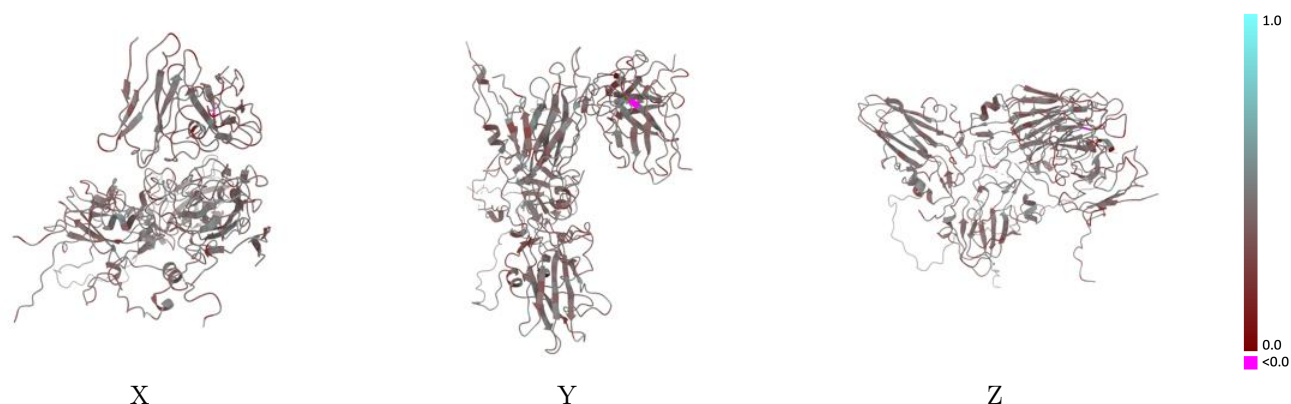


9.1.2 Map-model assembly overlay [i](#)



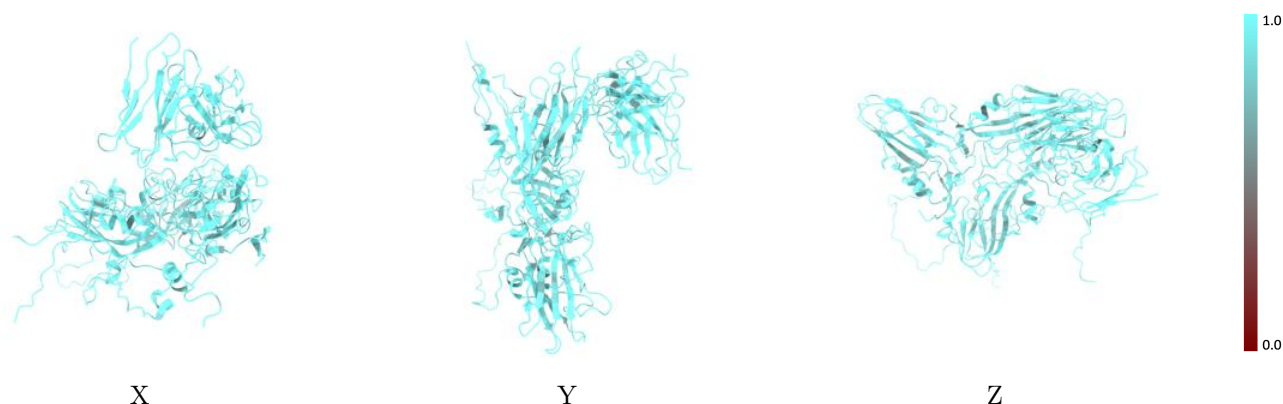
The images above show the 3D surface view of the map at the recommended contour level 0.0032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



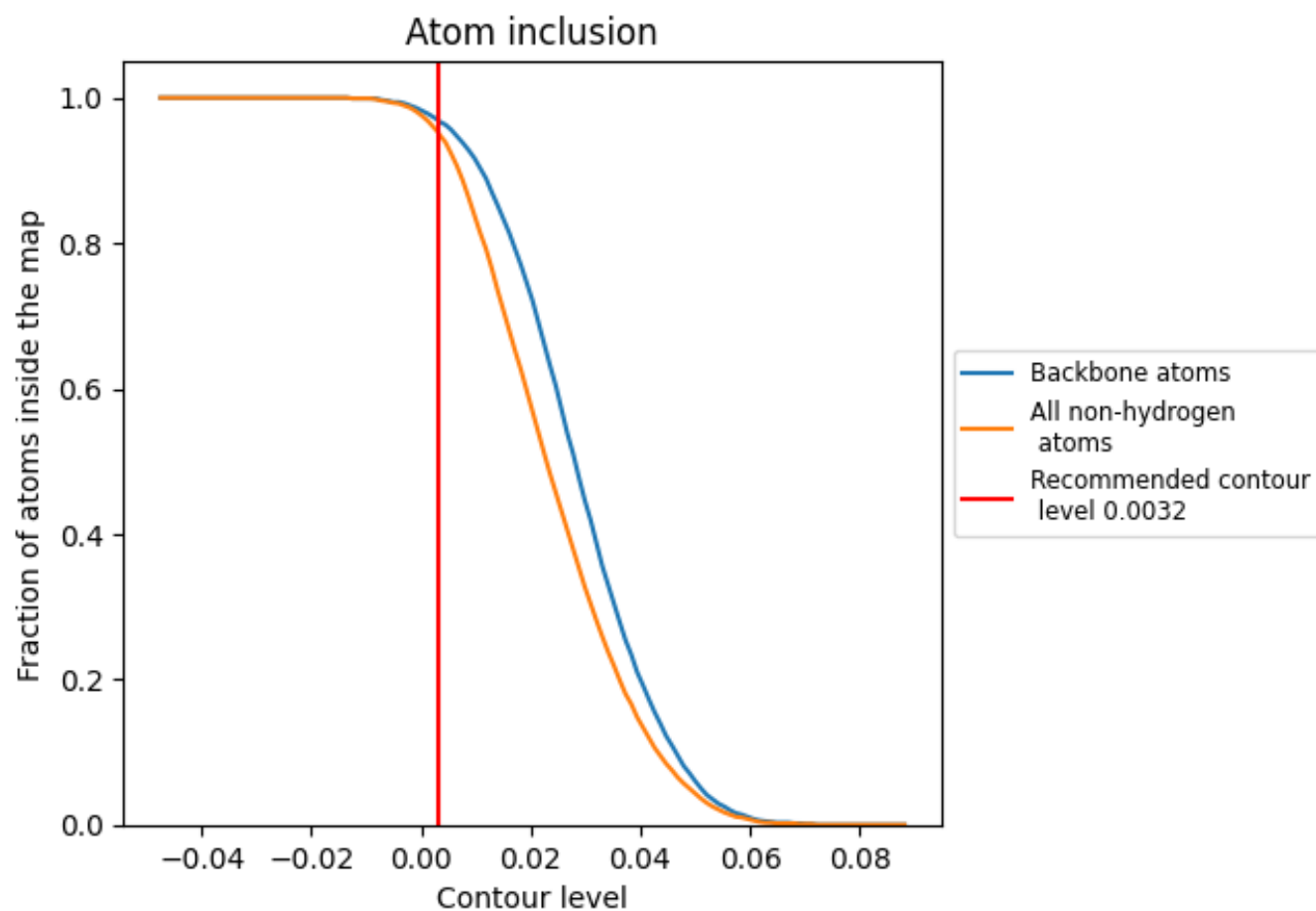
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.0032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.4020
1	0.9540	0.4080
2	0.9430	0.4160
3	0.9400	0.4040
4	0.9510	0.3940
H	0.9730	0.3880
L	0.9730	0.3730

1.0

0.0

<0.0