



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 04:31 AM UTC

PDB ID : 6WGF / pdb_00006wgf
EMDB ID : EMD-21664
Title : Atomic model of mutant Mcm2-7 hexamer with Mcm6 WHD truncation
Authors : Yuan, Z.; Schneider, S.; Dodd, T.; Riera, A.; Bai, L.; Yan, C.; Magdalou, I.;
Ivanov, I.; Stillman, B.; Li, H.; Speck, C.
Deposited on : 2020-04-05
Resolution : 7.70 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

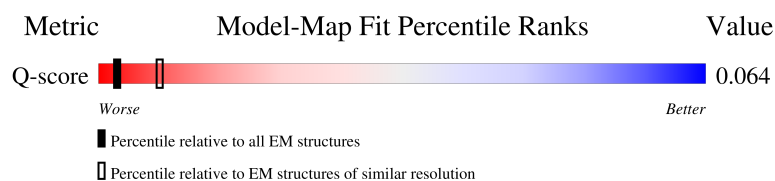
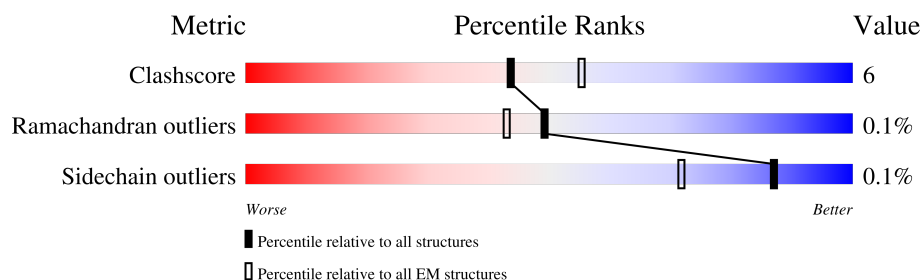
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.70 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	384 (7.20 - 8.20)

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	2	868	44% 50% 9% 41%
2	7	845	46% 55% 12% 33%
3	6	1017	41% 48% 7% 45%
4	5	775	63% 65% 11% 23%

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Mol	Chain	Length	Quality of chain
5	4	933	51% 53% 14% 32%
6	3	971	43% 48% 11% 42%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26076 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 DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	508	Total	C	N	O	S	0	0
			3946	2490	692	747	17		

- Molecule 2 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	563	Total	C	N	O	S	0	0
			4311	2709	748	828	26		

- Molecule 3 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	564	Total	C	N	O	S	0	0
			4401	2783	763	832	23		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

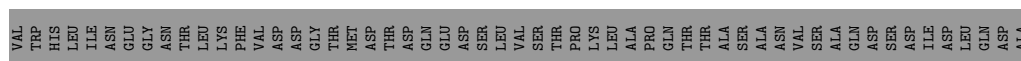
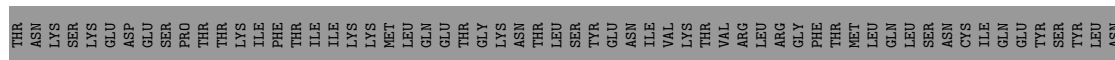
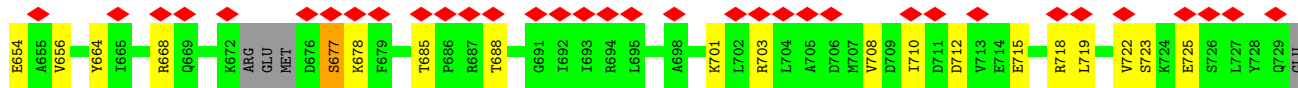
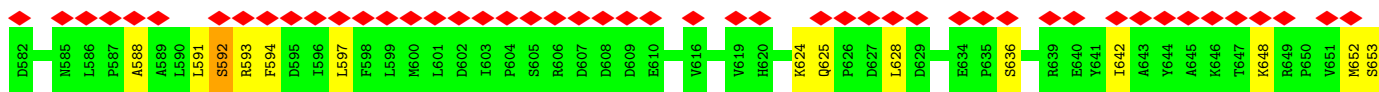
Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	598	Total	C	N	O	S	0	0
			4314	2707	742	846	19		

- Molecule 5 is a protein called DNA replication licensing factor MCM4.

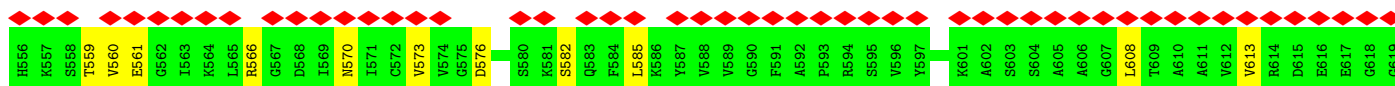
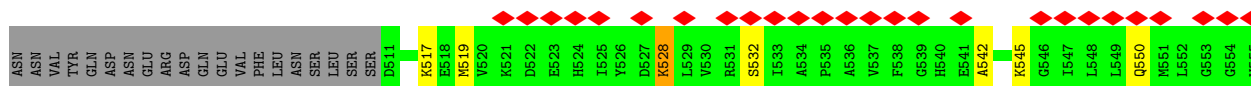
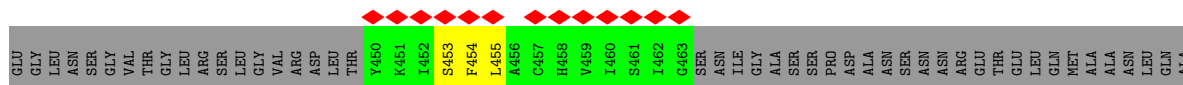
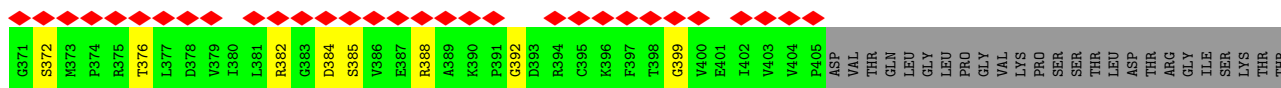
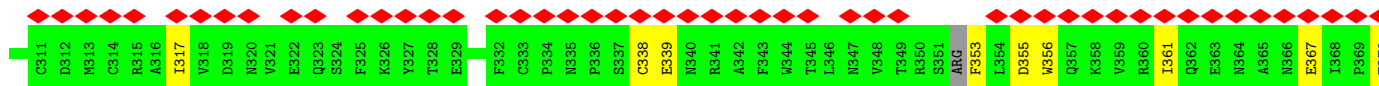
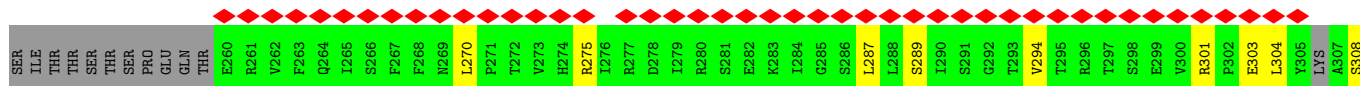
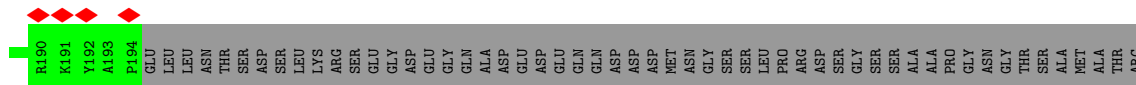
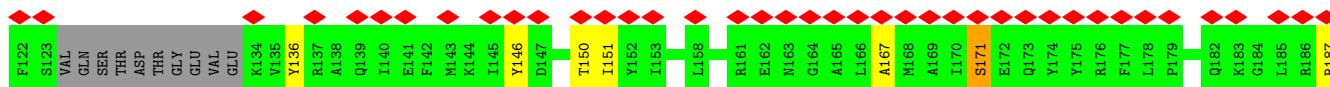
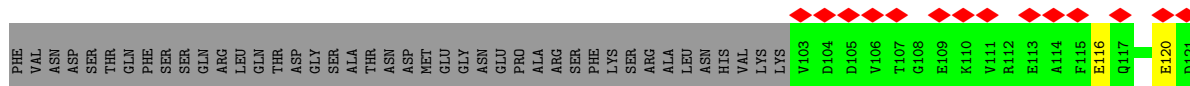
Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	636	Total	C	N	O	S	0	0
			4790	3000	838	926	26		

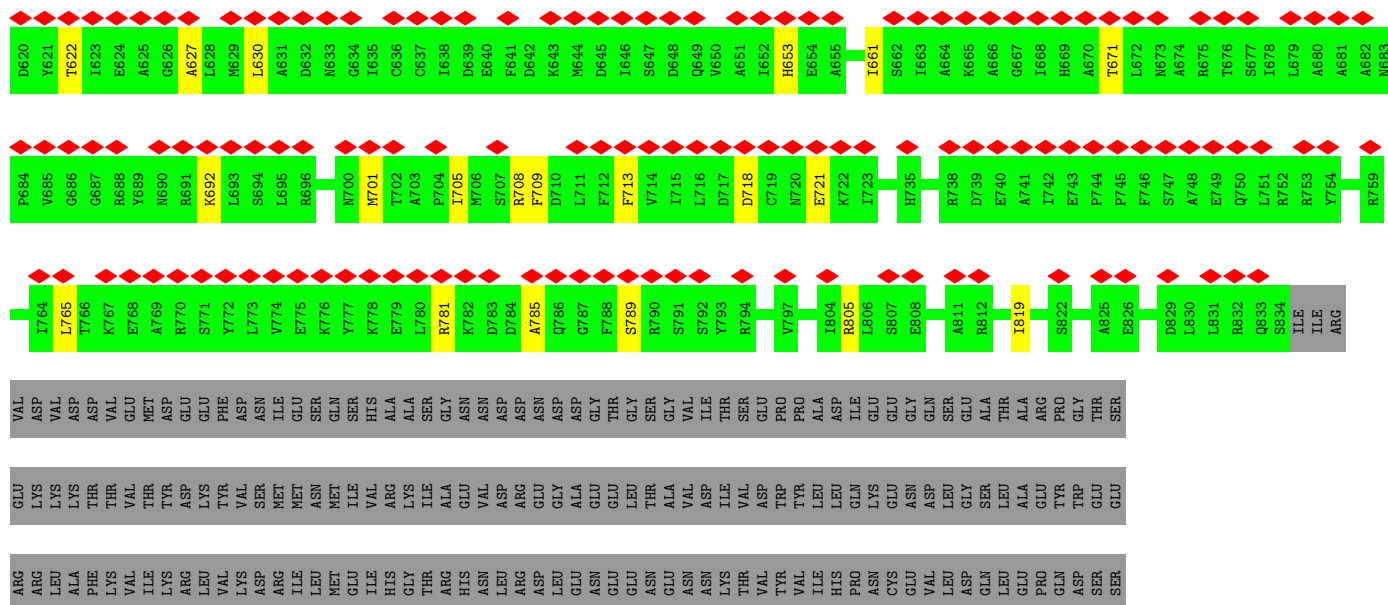
- Molecule 6 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	566	Total	C	N	O	S	0	0
			4314	2720	756	827	11		

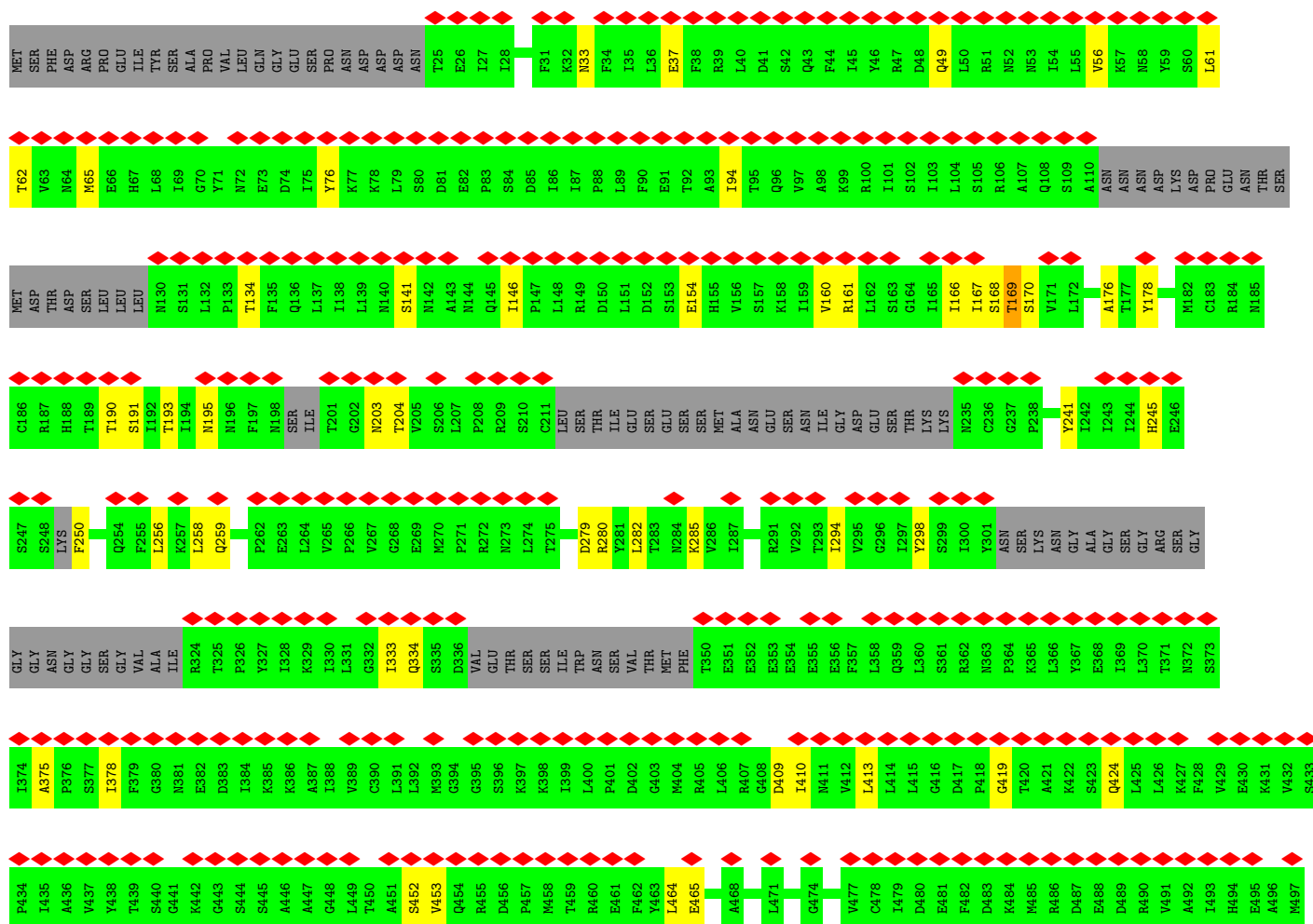


● Molecule 3: DNA replication licensing factor MCM6

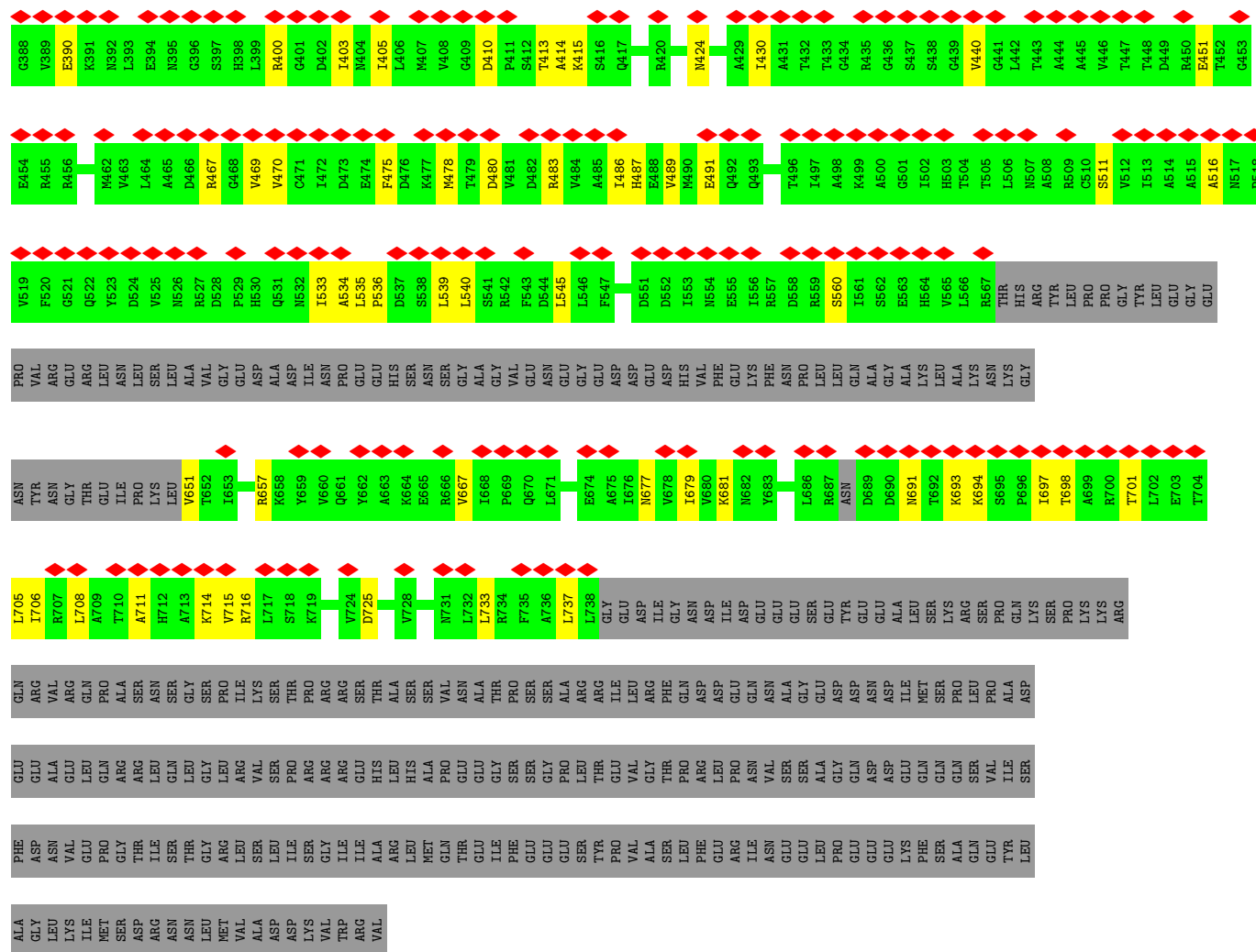




• Molecule 4: Minichromosome maintenance protein 5







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24072	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	262.0, 262.0, 262.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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	2	0.39	0/4010	1.04	23/5417 (0.4%)
2	7	0.39	0/4368	1.00	20/5903 (0.3%)
3	6	0.39	0/4473	1.06	17/6039 (0.3%)
4	5	0.41	0/4359	1.04	26/5920 (0.4%)
5	4	0.51	5/4845 (0.1%)	1.12	44/6553 (0.7%)
6	3	0.40	0/4382	1.01	21/5956 (0.4%)
All	All	0.42	5/26437 (0.0%)	1.05	151/35788 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	919	LEU	CA-C	8.16	1.62	1.52
5	4	696	PRO	C-N	7.55	1.43	1.34
5	4	918	VAL	N-CA	7.25	1.54	1.46
5	4	918	VAL	CA-C	7.20	1.61	1.52
5	4	919	LEU	N-CA	6.91	1.54	1.46

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	919	LEU	N-CA-C	11.31	125.11	108.60
3	6	136	TYR	N-CA-C	9.56	121.70	111.28
4	5	245	HIS	N-CA-C	9.14	121.24	111.28
1	2	413	ASP	N-CA-C	8.91	121.33	110.91
3	6	304	LEU	N-CA-C	8.85	120.62	110.97
3	6	550	GLN	CA-C-N	8.19	132.33	120.38
3	6	550	GLN	C-N-CA	8.19	132.33	120.38
2	7	228	ARG	N-CA-C	-7.81	103.55	113.23
2	7	406	THR	N-CA-C	7.76	122.19	112.87
5	4	920	GLY	CA-C-N	-7.69	106.85	121.54
5	4	920	GLY	C-N-CA	-7.69	106.85	121.54
5	4	918	VAL	N-CA-C	7.63	121.57	108.90
1	2	688	ASP	CA-C-N	7.50	131.08	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	688	ASP	C-N-CA	7.50	131.08	120.28
2	7	101	ASP	N-CA-C	7.49	121.35	110.42
3	6	721	GLU	N-CA-C	7.43	120.32	111.33
1	2	493	ILE	N-CA-C	7.38	122.13	112.76
6	3	281	ASP	N-CA-C	7.29	119.86	111.11
5	4	893	HIS	N-CA-C	-7.09	99.66	110.30
5	4	208	ILE	N-CA-C	7.02	119.91	113.10
6	3	197	ILE	N-CA-C	-6.96	106.44	113.47
5	4	811	MET	CA-C-N	6.95	132.75	122.74
5	4	811	MET	C-N-CA	6.95	132.75	122.74
1	2	417	VAL	N-CA-C	-6.93	105.87	113.43
5	4	592	SER	CA-C-N	6.89	134.91	121.41
5	4	592	SER	C-N-CA	6.89	134.91	121.41
3	6	388	ARG	N-CA-C	-6.87	105.18	113.97
5	4	712	VAL	N-CA-C	6.67	118.04	109.30
5	4	728	TYR	N-CA-C	-6.66	105.18	113.38
6	3	667	VAL	N-CA-C	6.62	118.11	108.58
2	7	319	SER	N-CA-C	6.58	118.53	111.36
1	2	414	LEU	N-CA-C	-6.57	102.81	113.19
5	4	777	MET	N-CA-C	-6.56	105.28	113.28
4	5	609	LYS	N-CA-C	6.55	118.30	111.03
6	3	440	VAL	N-CA-C	-6.53	105.19	113.22
4	5	168	SER	N-CA-C	6.43	119.74	108.75
2	7	121	ILE	N-CA-C	-6.38	104.05	111.00
5	4	573	SER	N-CA-C	6.38	124.39	110.80
1	2	490	ASP	N-CA-C	6.36	120.20	109.76
4	5	203	ASN	CA-C-N	6.36	129.12	120.54
4	5	203	ASN	C-N-CA	6.36	129.12	120.54
4	5	758	HIS	N-CA-C	-6.34	105.60	113.15
1	2	206	THR	N-CA-C	-6.33	105.60	113.38
5	4	533	LEU	CA-C-N	6.31	130.29	120.82
5	4	533	LEU	C-N-CA	6.31	130.29	120.82
2	7	677	SER	CA-C-N	6.30	130.27	120.82
2	7	677	SER	C-N-CA	6.30	130.27	120.82
2	7	515	LEU	N-CA-C	-6.28	105.44	113.23
5	4	352	CYS	N-CA-C	6.24	120.21	112.47
6	3	487	HIS	N-CA-C	-6.15	104.13	111.69
6	3	715	VAL	N-CA-C	-6.12	103.24	111.44
5	4	187	ILE	N-CA-C	6.12	116.17	110.42
6	3	360	PHE	N-CA-C	6.06	117.88	111.28
5	4	463	VAL	N-CA-C	6.03	117.51	109.37
1	2	365	THR	N-CA-C	5.96	120.03	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	789	SER	N-CA-C	-5.92	98.20	110.80
6	3	94	HIS	N-CA-C	5.90	123.37	110.80
4	5	76	TYR	N-CA-C	5.89	117.71	111.28
1	2	491	ARG	N-CA-C	5.87	118.36	111.02
4	5	512	VAL	N-CA-C	-5.86	99.98	108.89
1	2	760	GLN	N-CA-C	5.83	117.64	111.28
5	4	193	ASN	CA-CB-CG	5.83	118.43	112.60
1	2	329	GLY	N-CA-C	5.83	119.64	110.96
2	7	338	THR	N-CA-C	5.81	119.84	112.87
4	5	280	ARG	N-CA-C	5.79	123.13	110.80
4	5	760	THR	N-CA-C	-5.75	100.86	109.15
3	6	171	SER	N-CA-C	5.74	119.38	112.38
5	4	426	SER	N-CA-C	-5.72	106.65	113.97
6	3	694	LYS	N-CA-C	5.70	121.94	114.75
5	4	668	ARG	N-CA-C	5.70	119.71	112.87
5	4	696	PRO	N-CA-C	5.68	117.63	110.70
4	5	518	SER	N-CA-C	-5.67	101.34	110.14
6	3	706	ILE	N-CA-C	-5.67	106.78	113.42
5	4	630	CYS	N-CA-C	5.67	117.97	108.73
4	5	169	THR	N-CA-C	-5.66	96.31	107.69
4	5	170	SER	N-CA-C	5.65	120.21	111.56
4	5	279	ASP	CA-C-N	5.63	132.30	121.54
4	5	279	ASP	C-N-CA	5.63	132.30	121.54
1	2	673	ILE	N-CA-C	-5.62	104.79	113.16
6	3	280	ASP	CA-C-N	5.61	128.12	120.54
6	3	280	ASP	C-N-CA	5.61	128.12	120.54
1	2	339	PHE	N-CA-C	5.61	117.57	108.26
2	7	544	GLN	N-CA-C	5.57	119.77	112.92
5	4	518	LEU	CA-C-N	5.55	128.27	120.28
5	4	518	LEU	C-N-CA	5.55	128.27	120.28
2	7	624	LYS	CA-C-N	5.54	132.78	121.48
2	7	624	LYS	C-N-CA	5.54	132.78	121.48
1	2	354	ASP	N-CA-C	-5.53	100.78	109.25
3	6	151	ILE	N-CA-C	5.52	118.37	110.09
2	7	628	LEU	N-CA-C	-5.51	102.03	110.14
3	6	146	TYR	N-CA-C	5.50	119.71	112.89
5	4	320	ASN	N-CA-C	-5.49	106.63	113.38
5	4	827	ARG	N-CA-C	-5.49	105.30	111.28
6	3	233	THR	N-CA-C	-5.49	106.25	113.17
4	5	419	GLY	N-CA-C	-5.49	106.02	111.56
1	2	671	GLU	N-CA-C	5.47	121.90	109.81
5	4	545	PHE	N-CA-C	-5.47	105.34	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	692	LYS	N-CA-C	5.46	122.44	110.80
6	3	451	GLU	CA-C-N	5.46	127.91	120.54
6	3	451	GLU	C-N-CA	5.46	127.91	120.54
6	3	540	LEU	N-CA-C	-5.46	105.36	112.23
5	4	693	ASP	N-CA-C	5.41	118.71	111.24
4	5	546	ILE	N-CA-C	-5.41	106.42	111.45
6	3	693	LYS	N-CA-C	5.37	119.52	111.96
4	5	154	GLU	CA-C-N	5.35	129.72	122.07
4	5	154	GLU	C-N-CA	5.35	129.72	122.07
3	6	785	ALA	CA-C-N	5.34	129.71	122.07
3	6	785	ALA	C-N-CA	5.34	129.71	122.07
4	5	424	GLN	N-CA-C	-5.32	107.33	113.88
2	7	592	SER	N-CA-C	-5.32	105.53	112.23
2	7	112	HIS	N-CA-C	-5.30	105.96	112.90
3	6	528	LYS	N-CA-C	-5.29	106.67	113.23
4	5	204	THR	N-CA-C	5.29	117.46	111.11
2	7	424	GLY	CA-C-N	5.29	129.91	122.46
2	7	424	GLY	C-N-CA	5.29	129.91	122.46
4	5	610	CYS	N-CA-C	5.28	118.33	110.52
1	2	601	LYS	N-CA-C	-5.27	107.22	113.97
4	5	241	TYR	N-CA-C	5.24	118.76	109.96
5	4	251	TYR	CA-C-N	5.23	127.82	120.28
5	4	251	TYR	C-N-CA	5.23	127.82	120.28
2	7	488	SER	CA-C-N	5.23	128.02	120.38
2	7	488	SER	C-N-CA	5.23	128.02	120.38
6	3	677	ASN	N-CA-C	5.21	116.96	111.28
5	4	428	ARG	CA-C-N	5.21	128.50	121.05
5	4	428	ARG	C-N-CA	5.21	128.50	121.05
3	6	630	LEU	N-CA-C	-5.20	101.79	110.17
5	4	374	ILE	N-CA-C	-5.19	104.60	111.09
6	3	560	SER	N-CA-C	5.19	119.71	113.17
5	4	203	TYR	N-CA-C	5.19	118.36	111.30
6	3	359	ILE	N-CA-C	5.18	115.40	110.53
4	5	759	GLU	CA-C-N	-5.17	113.60	121.66
4	5	759	GLU	C-N-CA	-5.17	113.60	121.66
6	3	123	PRO	CA-N-CD	-5.17	104.77	112.00
2	7	456	VAL	N-CA-C	5.16	115.40	108.17
1	2	415	VAL	CA-C-N	5.16	129.66	122.08
1	2	415	VAL	C-N-CA	5.16	129.66	122.08
5	4	914	ASP	N-CA-C	-5.16	106.57	112.86
1	2	207	ILE	CA-C-N	5.15	127.49	120.54
1	2	207	ILE	C-N-CA	5.15	127.49	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	700	SER	N-CA-C	-5.14	105.75	112.23
3	6	385	SER	N-CA-C	-5.14	107.01	113.28
1	2	355	SER	N-CA-C	5.13	119.17	113.01
5	4	520	SER	N-CA-C	-5.11	107.60	113.88
1	2	617	ARG	N-CA-C	-5.09	105.38	112.45
5	4	582	HIS	N-CA-C	-5.07	106.36	112.54
4	5	56	VAL	N-CA-C	-5.06	108.04	112.90
5	4	421	ASP	CA-C-N	5.05	132.75	124.31
5	4	421	ASP	C-N-CA	5.05	132.75	124.31
3	6	356	TRP	CA-CB-CG	5.04	123.17	113.60
5	4	711	LYS	CA-C-N	5.00	128.00	120.69
5	4	711	LYS	C-N-CA	5.00	128.00	120.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	3946	0	3931	49	0
2	7	4311	0	4316	58	0
3	6	4401	0	4348	41	0
4	5	4314	0	4080	63	0
5	4	4790	0	4612	75	0
6	3	4314	0	4268	64	0
All	All	26076	0	25555	333	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 6.

All (333) 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)
4:5:758:HIS:HA	6:3:534:ALA:CB	1.39	1.48
4:5:758:HIS:HA	6:3:534:ALA:HB1	1.22	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:211:LEU:HD11	1:2:274:VAL:HG11	1.17	1.13
4:5:758:HIS:CA	6:3:534:ALA:CB	2.30	1.10
4:5:758:HIS:CA	6:3:534:ALA:HB1	1.81	1.10
2:7:540:VAL:CG1	2:7:546:ILE:HD11	1.81	1.09
1:2:211:LEU:CD1	1:2:274:VAL:HG11	1.86	1.06
4:5:758:HIS:HA	6:3:534:ALA:HB2	1.12	1.05
4:5:757:LYS:O	6:3:534:ALA:HB1	1.63	0.97
5:4:918:VAL:CB	5:4:925:ARG:O	2.13	0.96
2:7:540:VAL:HG11	2:7:546:ILE:HD11	1.50	0.93
4:5:178:TYR:HD1	4:5:193:THR:HG22	1.36	0.91
5:4:203:TYR:HH	5:4:221:ASP:N	1.70	0.90
2:7:540:VAL:CG1	2:7:546:ILE:CD1	2.51	0.88
4:5:33:ASN:O	4:5:37:GLU:HB2	1.77	0.84
2:7:426:LEU:O	2:7:430:LYS:HB2	1.78	0.84
5:4:916:VAL:HA	5:4:927:VAL:CB	2.09	0.83
4:5:734:ARG:O	4:5:738:VAL:CB	2.29	0.81
1:2:333:GLN:CB	1:2:385:TYR:HD2	1.93	0.81
2:7:251:VAL:HG12	2:7:340:VAL:HG22	1.62	0.80
4:5:167:ILE:HD11	4:5:259:GLN:HG2	1.63	0.79
1:2:330:VAL:HG12	1:2:330:VAL:O	1.82	0.77
1:2:331:PHE:O	1:2:385:TYR:HB2	1.84	0.76
5:4:881:MET:O	5:4:924:ARG:O	2.02	0.76
4:5:134:THR:HG21	4:5:195:ASN:OD1	1.86	0.75
1:2:333:GLN:CB	1:2:385:TYR:CD2	2.70	0.74
4:5:757:LYS:O	6:3:534:ALA:CB	2.35	0.74
1:2:578:ALA:HA	1:2:592:GLU:O	1.86	0.74
1:2:328:THR:HG22	1:2:590:THR:HG21	1.68	0.73
1:2:386:GLN:HB3	1:2:410:LEU:CB	2.19	0.72
3:6:303:GLU:O	3:6:353:PHE:HA	1.89	0.72
4:5:622:LEU:HD12	4:5:677:VAL:HG11	1.70	0.71
1:2:332:PRO:HA	1:2:383:ARG:O	1.89	0.71
1:2:332:PRO:O	1:2:382:TYR:HB3	1.91	0.71
5:4:647:GLU:O	5:4:651:GLN:HB2	1.90	0.71
4:5:282:LEU:HD12	4:5:333:ILE:HD13	1.71	0.70
2:7:588:ALA:O	2:7:592:SER:HB3	1.92	0.70
4:5:729:SER:O	4:5:732:THR:N	2.24	0.69
6:3:475:PHE:CD2	6:3:535:LEU:HD21	2.28	0.69
5:4:334:ARG:CZ	5:4:615:VAL:HG23	2.23	0.68
5:4:881:MET:H	5:4:926:SER:CB	2.06	0.68
4:5:758:HIS:CA	6:3:534:ALA:HB2	2.06	0.68
1:2:386:GLN:HA	1:2:386:GLN:OE1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:475:PHE:HD2	6:3:535:LEU:HD21	1.61	0.66
4:5:622:LEU:CD1	4:5:677:VAL:HG11	2.26	0.65
1:2:332:PRO:HB2	1:2:382:TYR:HB2	1.78	0.65
4:5:770:ILE:O	4:5:774:GLY:N	2.31	0.62
2:7:540:VAL:HG12	2:7:546:ILE:CD1	2.30	0.62
3:6:399:GLY:HA3	3:6:455:LEU:O	1.99	0.62
4:5:282:LEU:CD1	4:5:333:ILE:HD13	2.29	0.61
5:4:913:GLU:C	5:4:915:LYS:H	2.06	0.61
6:3:386:MET:HE1	6:3:714:LYS:HB3	1.82	0.61
4:5:757:LYS:C	6:3:534:ALA:HB1	2.24	0.61
5:4:662:ILE:O	5:4:662:ILE:HG13	2.00	0.61
3:6:582:SER:O	3:6:585:LEU:HB3	2.01	0.61
4:5:178:TYR:CD1	4:5:193:THR:HG22	2.26	0.60
4:5:660:THR:HG21	4:5:677:VAL:HG22	1.84	0.60
5:4:882:SER:HA	5:4:924:ARG:O	2.02	0.59
5:4:891:ASN:O	5:4:894:SER:HA	2.03	0.59
1:2:332:PRO:HB2	1:2:382:TYR:CB	2.31	0.59
1:2:335:LYS:HD2	1:2:383:ARG:HB3	1.85	0.58
1:2:386:GLN:CB	1:2:410:LEU:CB	2.81	0.58
5:4:911:GLN:HA	5:4:916:VAL:O	2.04	0.57
2:7:436:LEU:CD1	2:7:642:ILE:HD13	2.34	0.57
2:7:722:VAL:HA	2:7:725:GLU:HB2	1.88	0.55
4:5:65:MET:SD	4:5:161:ARG:NH2	2.78	0.55
2:7:260:TYR:HB3	2:7:298:LEU:HD12	1.88	0.55
2:7:495:ALA:HA	2:7:509:GLU:O	2.07	0.55
5:4:645:LEU:HA	5:4:648:VAL:HG22	1.88	0.55
5:4:654:ILE:O	5:4:664:THR:HA	2.07	0.54
4:5:729:SER:O	4:5:731:GLN:N	2.40	0.54
6:3:405:ILE:HG12	6:3:545:LEU:HB2	1.89	0.54
1:2:332:PRO:C	1:2:382:TYR:HB3	2.32	0.54
5:4:534:GLU:O	5:4:538:LYS:HB2	2.07	0.54
2:7:540:VAL:HG12	2:7:546:ILE:HD11	1.79	0.54
4:5:282:LEU:CD1	4:5:333:ILE:HG21	2.38	0.54
4:5:758:HIS:C	6:3:534:ALA:HB1	2.31	0.54
5:4:561:ASP:H	5:4:803:ARG:HD2	1.73	0.54
5:4:811:MET:HG2	5:4:812:LYS:HG3	1.90	0.54
1:2:764:MET:HA	1:2:767:ILE:HD12	1.89	0.53
4:5:729:SER:H	4:5:775:VAL:C	2.17	0.53
5:4:564:ILE:HG22	5:4:704:LEU:HB3	1.91	0.53
4:5:757:LYS:C	4:5:759:GLU:H	2.14	0.53
6:3:733:LEU:O	6:3:737:LEU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:683:ASN:H	5:4:691:ASN:HD21	1.56	0.53
1:2:544:ASP:O	1:2:549:LYS:NZ	2.38	0.53
1:2:588:GLU:OE1	1:2:590:THR:HG23	2.08	0.53
1:2:386:GLN:CG	1:2:410:LEU:CB	2.87	0.53
2:7:118:CYS:SG	2:7:198:ARG:NH2	2.82	0.53
1:2:286:TYR:HE2	1:2:293:ILE:HD11	1.74	0.53
6:3:32:LEU:HD13	6:3:132:LEU:HD22	1.90	0.53
2:7:540:VAL:HG13	2:7:546:ILE:CD1	2.38	0.53
4:5:166:ILE:HD12	4:5:256:LEU:HD23	1.90	0.52
3:6:382:ARG:HH11	3:6:455:LEU:HD21	1.74	0.52
3:6:167:ALA:O	3:6:171:SER:HB3	2.09	0.52
5:4:543:GLN:NE2	5:4:670:SER:OG	2.42	0.52
5:4:701:ARG:HG2	5:4:796:ARG:HE	1.74	0.52
2:7:463:GLY:HA2	6:3:698:THR:HA	1.91	0.52
1:2:286:TYR:CE2	1:2:293:ILE:HD11	2.46	0.52
4:5:717:GLU:O	4:5:721:ARG:CB	2.58	0.52
4:5:753:TYR:O	4:5:757:LYS:CB	2.58	0.52
6:3:469:VAL:HG12	6:3:511:SER:HB3	1.91	0.51
1:2:386:GLN:CD	1:2:415:VAL:HG23	2.36	0.51
1:2:626:GLN:NE2	1:2:628:SER:O	2.43	0.51
5:4:371:CYS:SG	5:4:373:ARG:NH2	2.83	0.51
1:2:330:VAL:O	1:2:330:VAL:CG1	2.52	0.51
4:5:453:VAL:HA	4:5:464:LEU:HA	1.93	0.51
3:6:275:ARG:NH1	3:6:367:GLU:O	2.44	0.50
4:5:190:THR:OG1	4:5:191:SER:N	2.43	0.50
4:5:736:GLU:O	4:5:740:THR:N	2.44	0.50
6:3:27:ARG:NH2	6:3:109:SER:OG	2.43	0.50
2:7:122:ASP:OD2	2:7:198:ARG:NH2	2.44	0.50
5:4:606:THR:OG1	5:4:607:ARG:N	2.43	0.50
5:4:888:LYS:O	5:4:892:GLU:CB	2.59	0.50
6:3:410:ASP:O	6:3:415:LYS:NZ	2.40	0.50
3:6:370:THR:O	5:4:428:ARG:NH2	2.44	0.50
2:7:648:LYS:HB2	2:7:701:LYS:HG2	1.92	0.50
1:2:386:GLN:HG2	1:2:410:LEU:CB	2.42	0.50
6:3:43:ARG:NH1	6:3:136:MET:O	2.45	0.50
6:3:172:THR:OG1	6:3:173:ALA:N	2.44	0.50
6:3:400:ARG:HD3	6:3:491:GLU:HA	1.94	0.49
2:7:543:GLN:NE2	2:7:545:THR:O	2.44	0.49
5:4:335:SER:OG	5:4:395:GLN:NE2	2.45	0.49
4:5:258:LEU:HD22	4:5:294:ILE:HD12	1.93	0.49
4:5:649:THR:OG1	4:5:650:ILE:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:390:GLU:HG2	6:3:467:ARG:HH22	1.77	0.49
1:2:603:VAL:HG22	1:2:645:SER:HB3	1.95	0.49
2:7:208:SER:OG	2:7:209:GLN:N	2.45	0.49
2:7:436:LEU:HD23	2:7:473:ILE:HD12	1.94	0.49
2:7:664:TYR:OH	2:7:668:ARG:NH1	2.45	0.49
4:5:649:THR:HG23	4:5:652:GLN:H	1.76	0.49
5:4:909:ARG:O	5:4:913:GLU:N	2.40	0.49
6:3:478:MET:O	6:3:483:ARG:NH2	2.45	0.49
6:3:679:ILE:HD11	6:3:705:LEU:HD12	1.94	0.49
4:5:134:THR:HG21	4:5:195:ASN:CG	2.37	0.49
2:7:436:LEU:HD13	2:7:642:ILE:HD13	1.94	0.49
1:2:670:THR:OG1	1:2:671:GLU:N	2.46	0.49
2:7:420:PRO:O	2:7:625:GLN:NE2	2.46	0.49
3:6:570:ASN:ND2	3:6:708:ARG:O	2.46	0.49
2:7:653:SER:OG	2:7:654:GLU:N	2.46	0.49
4:5:176:ALA:HA	4:5:250:PHE:HA	1.95	0.49
5:4:184:ASN:O	5:4:260:GLN:NE2	2.46	0.49
5:4:916:VAL:CA	5:4:927:VAL:CB	2.85	0.49
6:3:424:ASN:O	6:3:657:ARG:NH1	2.44	0.49
2:7:251:VAL:HG12	2:7:340:VAL:CG2	2.38	0.48
6:3:367:LEU:HD21	6:3:378:LYS:HB2	1.95	0.48
2:7:656:VAL:HG23	2:7:710:ILE:HD12	1.95	0.48
5:4:543:GLN:HE22	5:4:628:VAL:HG12	1.78	0.48
5:4:631:ILE:O	5:4:673:ALA:HA	2.13	0.48
6:3:253:HIS:HA	6:3:278:LEU:O	2.13	0.48
4:5:285:LYS:HD3	4:5:333:ILE:HD11	1.95	0.48
2:7:436:LEU:CD1	2:7:642:ILE:CD1	2.91	0.48
5:4:587:ARG:HG2	5:4:624:SER:HA	1.95	0.48
1:2:558:LYS:NZ	3:6:561:GLU:OE2	2.46	0.48
6:3:119:ALA:HB1	6:3:222:THR:HG22	1.95	0.48
6:3:348:ARG:NH2	6:3:349:ASN:OD1	2.47	0.48
4:5:61:LEU:HD21	4:5:94:ILE:HD13	1.95	0.48
5:4:573:SER:O	5:4:576:GLN:HB2	2.14	0.48
6:3:533:ILE:HG22	6:3:535:LEU:HD13	1.96	0.48
1:2:536:ASP:O	1:2:815:ARG:NH1	2.47	0.48
2:7:436:LEU:HD11	2:7:642:ILE:HD11	1.95	0.48
5:4:632:ASP:OD1	5:4:632:ASP:N	2.47	0.48
5:4:713:ASP:OD1	5:4:713:ASP:N	2.47	0.48
2:7:715:GLU:OE2	2:7:718:ARG:NH1	2.46	0.47
6:3:294:VAL:HG12	6:3:326:VAL:HG22	1.96	0.47
6:3:486:ILE:HA	6:3:489:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:639:ASP:OD1	5:4:642:ARG:NH1	2.48	0.47
4:5:282:LEU:HD12	4:5:333:ILE:HG21	1.96	0.47
2:7:400:ARG:NH1	2:7:636:SER:OG	2.48	0.47
2:7:546:ILE:HB	2:7:557:LEU:HB3	1.97	0.47
1:2:686:LEU:O	3:6:781:ARG:NH1	2.47	0.47
2:7:677:SER:OG	2:7:678:LYS:N	2.46	0.47
3:6:453:SER:OG	3:6:454:PHE:N	2.48	0.47
5:4:311:CYS:SG	5:4:312:LYS:N	2.87	0.47
6:3:266:PRO:O	6:3:269:GLN:NE2	2.47	0.47
5:4:339:ILE:HG13	5:4:394:LYS:HB3	1.97	0.47
5:4:535:ASP:OD1	5:4:535:ASP:N	2.48	0.47
5:4:763:THR:OG1	5:4:764:GLU:N	2.48	0.47
3:6:566:ARG:O	3:6:805:ARG:NH1	2.48	0.47
2:7:451:ARG:NH2	2:7:453:ASP:O	2.48	0.46
3:6:338:CYS:SG	3:6:339:GLU:N	2.88	0.46
5:4:209:LEU:HD12	5:4:250:ALA:HB2	1.97	0.46
5:4:419:VAL:HG12	5:4:463:VAL:HG11	1.97	0.46
6:3:708:LEU:O	6:3:711:ALA:HB3	2.15	0.46
5:4:589:VAL:HG21	5:4:620:ALA:HB1	1.96	0.46
6:3:716:ARG:NH2	6:3:725:ASP:OD1	2.49	0.46
1:2:324:VAL:HG23	1:2:420:PRO:HA	1.96	0.46
2:7:350:ASP:HB2	2:7:382:ARG:HG2	1.97	0.46
2:7:418:ILE:HG13	2:7:429:LYS:HD3	1.98	0.46
5:4:775:VAL:HA	5:4:778:ARG:HB2	1.97	0.46
4:5:622:LEU:CD1	4:5:677:VAL:CG1	2.93	0.46
6:3:297:VAL:O	6:3:321:ILE:HA	2.16	0.46
3:6:294:VAL:HG13	3:6:392:GLY:H	1.81	0.46
4:5:452:SER:O	4:5:465:GLU:N	2.48	0.46
2:7:591:LEU:HA	2:7:594:PHE:HB2	1.98	0.46
4:5:282:LEU:HB2	4:5:333:ILE:CD1	2.45	0.46
4:5:409:ASP:O	4:5:658:ARG:NH1	2.48	0.46
5:4:605:ILE:HD11	5:4:614:LEU:HB3	1.97	0.46
6:3:480:ASP:N	6:3:480:ASP:OD1	2.48	0.46
3:6:576:ASP:OD1	3:6:576:ASP:N	2.48	0.46
1:2:242:LEU:HB3	1:2:295:VAL:HG12	1.97	0.46
5:4:825:ALA:O	5:4:828:LEU:HB3	2.15	0.46
5:4:542:LEU:HA	5:4:545:PHE:HB2	1.97	0.45
1:2:495:ASP:OD1	1:2:509:ARG:NH1	2.46	0.45
2:7:597:LEU:O	2:7:723:SER:OG	2.34	0.45
4:5:160:VAL:HG11	4:5:298:TYR:HB2	1.99	0.45
5:4:913:GLU:C	5:4:915:LYS:N	2.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:378:LYS:HA	6:3:381:ILE:HB	1.97	0.45
3:6:287:LEU:HA	3:6:399:GLY:O	2.17	0.45
2:7:555:THR:OG1	2:7:556:THR:N	2.50	0.45
5:4:248:LEU:HD11	5:4:257:LEU:HD23	1.99	0.45
4:5:282:LEU:CD1	4:5:333:ILE:CG2	2.95	0.45
5:4:435:VAL:HG23	5:4:466:VAL:HG12	1.97	0.45
3:6:150:THR:HG21	3:6:384:ASP:HB2	1.98	0.45
6:3:475:PHE:HB3	6:3:516:ALA:HB2	1.99	0.45
1:2:367:CYS:SG	1:2:369:SER:OG	2.74	0.45
2:7:290:SER:OG	2:7:291:GLN:OE1	2.35	0.45
5:4:381:SER:O	5:4:381:SER:OG	2.35	0.45
6:3:430:ILE:HB	6:3:470:VAL:HG12	1.99	0.45
1:2:631:ILE:O	1:2:637:VAL:HA	2.16	0.44
4:5:146:ILE:HD11	4:5:160:VAL:HG23	2.00	0.44
2:7:685:THR:O	2:7:688:THR:OG1	2.35	0.44
2:7:436:LEU:HD11	2:7:642:ILE:CD1	2.48	0.44
5:4:334:ARG:NH1	5:4:615:VAL:HG23	2.32	0.44
2:7:542:GLU:HG3	2:7:593:ARG:HH21	1.82	0.44
5:4:910:LEU:O	5:4:915:LYS:N	2.51	0.44
4:5:708:LEU:O	4:5:712:ARG:CB	2.66	0.44
5:4:911:GLN:HA	5:4:916:VAL:C	2.42	0.44
6:3:536:PRO:HD2	6:3:539:LEU:HD12	1.99	0.44
4:5:141:SER:O	4:5:334:GLN:NE2	2.51	0.44
4:5:752:LEU:O	4:5:755:LEU:N	2.51	0.44
1:2:539:VAL:HG12	1:2:679:ILE:HB	1.99	0.44
3:6:361:ILE:O	3:6:376:THR:OG1	2.33	0.44
4:5:413:LEU:HD23	4:5:553:ILE:HG12	2.00	0.44
1:2:211:LEU:HD11	1:2:274:VAL:CG1	2.12	0.44
3:6:701:MET:HB2	3:6:705:ILE:HD11	2.00	0.44
4:5:166:ILE:HD11	4:5:294:ILE:HD11	1.98	0.44
5:4:921:GLU:C	5:4:923:VAL:H	2.26	0.44
6:3:413:THR:HB	6:3:414:ALA:H	1.66	0.44
2:7:415:ALA:O	2:7:429:LYS:NZ	2.45	0.43
6:3:346:ASP:HA	6:3:349:ASN:HD22	1.83	0.43
2:7:245:ILE:HD13	2:7:343:LEU:HD12	2.01	0.43
3:6:718:ASP:OD1	3:6:718:ASP:N	2.51	0.43
5:4:252:LYS:HB3	5:4:252:LYS:HE2	1.84	0.43
5:4:312:LYS:HB2	5:4:316:GLU:HB2	2.00	0.43
6:3:705:LEU:HD21	6:3:733:LEU:HD11	2.00	0.43
5:4:518:LEU:HA	5:4:521:LEU:HB3	1.99	0.43
6:3:430:ILE:O	6:3:470:VAL:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:431:ALA:HB2	2:7:719:LEU:HD11	1.99	0.43
6:3:350:ILE:O	6:3:354:SER:OG	2.35	0.43
3:6:559:THR:OG1	3:6:560:VAL:N	2.52	0.43
5:4:695:PRO:HA	5:4:696:PRO:HD3	1.88	0.43
4:5:660:THR:CG2	4:5:677:VAL:HG22	2.48	0.43
6:3:691:ASN:HD21	6:3:697:ILE:H	1.67	0.43
1:2:627:GLN:HB3	1:2:643:ARG:HG2	2.01	0.42
2:7:354:ILE:HG22	2:7:377:GLU:HB3	2.00	0.42
4:5:375:ALA:HB1	4:5:378:ILE:HB	2.01	0.42
3:6:608:LEU:O	3:6:627:ALA:N	2.52	0.42
2:7:275:SER:OG	2:7:277:THR:O	2.37	0.42
3:6:701:MET:HE3	3:6:705:ILE:HG13	2.02	0.42
3:6:765:LEU:HA	3:6:819:ILE:HG22	2.02	0.42
5:4:539:GLY:O	5:4:543:GLN:HB2	2.19	0.42
3:6:116:GLU:OE2	3:6:187:ARG:NH1	2.52	0.42
6:3:203:ALA:O	6:3:207:GLY:N	2.51	0.42
6:3:295:VAL:HB	6:3:325:THR:HB	2.00	0.42
6:3:366:SER:OG	6:3:651:VAL:O	2.37	0.42
1:2:211:LEU:HA	1:2:214:PHE:HB3	2.02	0.42
2:7:333:ILE:HD13	2:7:351:VAL:HG11	2.02	0.42
6:3:679:ILE:HD12	6:3:679:ILE:HA	1.92	0.42
1:2:331:PHE:O	1:2:385:TYR:CB	2.62	0.42
3:6:308:SER:HB3	3:6:317:ILE:HD11	2.02	0.42
3:6:372:SER:OG	5:4:428:ARG:NE	2.52	0.42
5:4:569:ASP:H	5:4:709:LEU:HA	1.84	0.42
1:2:357:GLU:OE1	3:6:301:ARG:HD3	2.19	0.42
2:7:205:LYS:HE3	2:7:205:LYS:HB2	1.93	0.42
2:7:318:LEU:HD23	2:7:320:GLN:H	1.85	0.42
2:7:540:VAL:CG1	2:7:546:ILE:HD13	2.48	0.42
3:6:542:ALA:HA	3:6:545:LYS:HE3	2.02	0.42
5:4:332:VAL:HG23	5:4:429:ALA:HA	2.02	0.42
6:3:375:ASP:HA	6:3:378:LYS:HZ2	1.85	0.42
2:7:330:SER:OG	2:7:331:LEU:N	2.52	0.41
3:6:613:VAL:HG12	3:6:622:THR:H	1.85	0.41
6:3:221:LEU:HD12	6:3:221:LEU:HA	1.95	0.41
1:2:343:LYS:HD3	1:2:343:LYS:HA	1.92	0.41
2:7:484:THR:OG1	2:7:485:GLY:N	2.53	0.41
4:5:631:LYS:HD2	4:5:631:LYS:HA	1.90	0.41
5:4:916:VAL:CB	5:4:927:VAL:CB	2.98	0.41
3:6:517:LYS:HA	3:6:517:LYS:HD2	1.87	0.41
4:5:285:LYS:HD3	4:5:333:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:518:LEU:HD12	5:4:521:LEU:HD23	2.02	0.41
5:4:715:LYS:HZ3	5:4:718:ARG:HH12	1.67	0.41
2:7:299:PHE:HB3	5:4:362:ARG:HD2	2.02	0.41
4:5:673:GLN:H	4:5:676:HIS:HD2	1.67	0.41
5:4:538:LYS:HE3	5:4:828:LEU:HD12	2.02	0.41
1:2:518:SER:HA	1:2:537:ILE:HB	2.02	0.41
2:7:652:MET:HA	2:7:708:VAL:HB	2.03	0.41
5:4:589:VAL:CG1	5:4:623:LEU:HD23	2.51	0.41
1:2:616:ASP:OD1	1:2:616:ASP:N	2.53	0.41
3:6:270:LEU:HD12	3:6:289:SER:HB3	2.01	0.41
1:2:326:ARG:HD3	1:2:389:THR:HG23	2.03	0.41
3:6:573:VAL:HG12	3:6:713:PHE:HB2	2.03	0.41
6:3:698:THR:O	6:3:701:THR:OG1	2.36	0.41
3:6:519:MET:HE3	3:6:519:MET:HB2	1.95	0.41
4:5:410:ILE:HD12	4:5:552:MET:HE1	2.03	0.41
5:4:428:ARG:NH1	5:4:431:ASP:OD2	2.53	0.41
6:3:475:PHE:HE2	6:3:535:LEU:HD23	1.85	0.41
1:2:538:ASN:HA	1:2:646:ILE:O	2.20	0.41
3:6:661:ILE:O	3:6:671:THR:HA	2.21	0.41
5:4:637:MET:HE1	5:4:645:LEU:HD21	2.03	0.41
3:6:566:ARG:HH22	3:6:708:ARG:HE	1.69	0.41
3:6:653:HIS:HB2	3:6:705:ILE:HG22	2.03	0.41
4:5:169:THR:O	4:5:169:THR:OG1	2.37	0.41
5:4:881:MET:O	5:4:924:ARG:C	2.64	0.41
6:3:384:MET:SD	6:3:511:SER:OG	2.71	0.41
3:6:570:ASN:HB2	3:6:709:PHE:HA	2.02	0.40
5:4:910:LEU:O	5:4:916:VAL:N	2.54	0.40
5:4:917:ILE:H	5:4:927:VAL:HA	1.86	0.40
6:3:183:GLU:HA	6:3:293:ASN:HA	2.02	0.40
6:3:681:LYS:HE2	6:3:681:LYS:HB3	1.94	0.40
1:2:334:LEU:HD12	1:2:337:VAL:HB	2.04	0.40
2:7:59:LYS:HB2	2:7:60:GLY:H	1.67	0.40
4:5:49:GLN:NE2	4:5:62:THR:OG1	2.47	0.40
4:5:754:ALA:O	4:5:758:HIS:N	2.51	0.40
6:3:366:SER:OG	6:3:366:SER:O	2.38	0.40
6:3:403:ILE:O	6:3:511:SER:OG	2.39	0.40
3:6:116:GLU:O	3:6:120:GLU:HB2	2.21	0.40
3:6:528:LYS:O	3:6:532:SER:HB3	2.22	0.40
2:7:339:LEU:O	2:7:342:SER:OG	2.38	0.40
2:7:703:ARG:NH1	2:7:712:ASP:OD1	2.47	0.40
3:6:355:ASP:OD1	3:6:355:ASP:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:551:THR:OG1	5:4:552:PHE:N	2.55	0.40
6:3:23:ASP:HA	6:3:26:ARG:HE	1.85	0.40
6:3:123:PRO:HA	6:3:126:GLU:HG2	2.01	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	2	494/868 (57%)	475 (96%)	19 (4%)	0	100	100
2	7	551/845 (65%)	533 (97%)	18 (3%)	0	100	100
3	6	550/1017 (54%)	527 (96%)	23 (4%)	0	100	100
4	5	576/775 (74%)	553 (96%)	23 (4%)	0	100	100
5	4	616/933 (66%)	580 (94%)	34 (6%)	2 (0%)	36	72
6	3	552/971 (57%)	532 (96%)	20 (4%)	0	100	100
All	All	3339/5409 (62%)	3200 (96%)	137 (4%)	2 (0%)	49	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	4	373	ARG
5	4	921	GLU

5.3.2 Protein sidechains [i](#)

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	2	427/770 (56%)	426 (100%)	1 (0%)	87	87
2	7	470/753 (62%)	470 (100%)	0	100	100
3	6	470/886 (53%)	470 (100%)	0	100	100
4	5	434/688 (63%)	434 (100%)	0	100	100
5	4	497/848 (59%)	496 (100%)	1 (0%)	87	87
6	3	463/835 (55%)	463 (100%)	0	100	100
All	All	2761/4780 (58%)	2759 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	385	TYR
5	4	720	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	245	ASN
1	2	248	HIS
1	2	508	HIS
1	2	551	GLN
2	7	68	GLN
2	7	108	GLN
2	7	271	GLN
2	7	379	GLN
2	7	425	ASN
2	7	544	GLN
2	7	568	ASN
2	7	585	ASN
2	7	625	GLN
3	6	149	ASN
3	6	524	HIS
3	6	556	HIS
3	6	570	ASN
3	6	720	ASN
3	6	750	GLN
4	5	33	ASN
4	5	43	GLN

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Mol	Chain	Res	Type
4	5	49	GLN
4	5	67	HIS
4	5	145	GLN
4	5	411	ASN
4	5	499	GLN
4	5	625	ASN
4	5	676	HIS
5	4	193	ASN
5	4	247	ASN
5	4	253	GLN
5	4	395	GLN
5	4	543	GLN
5	4	579	GLN
5	4	646	HIS
5	4	652	GLN
5	4	691	ASN
5	4	808	HIS
5	4	815	ASN
6	3	46	GLN
6	3	269	GLN
6	3	293	ASN
6	3	324	ASN
6	3	395	ASN
6	3	517	ASN
6	3	691	ASN

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.

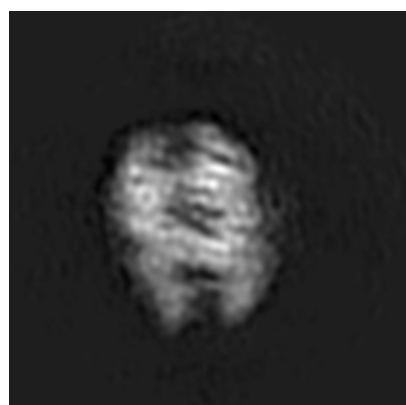
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21664. These allow visual inspection of the internal detail of the map and identification of artifacts.

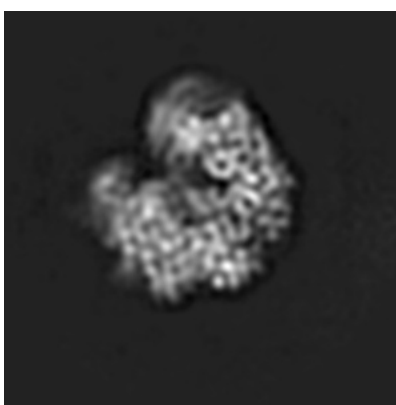
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

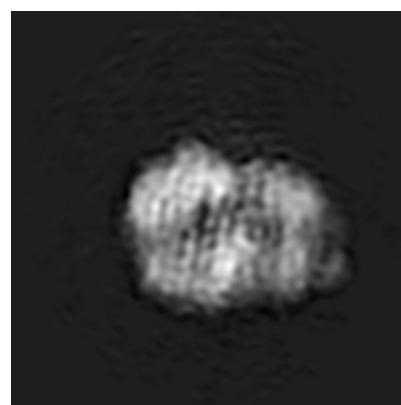
6.1.1 Primary map



X



Y

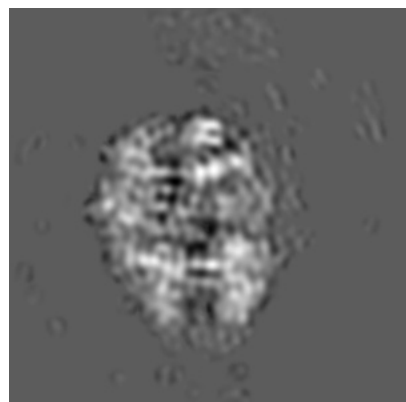


Z

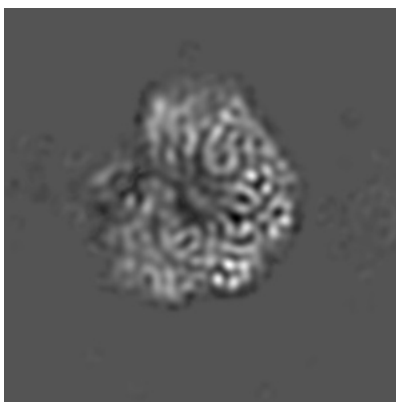
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

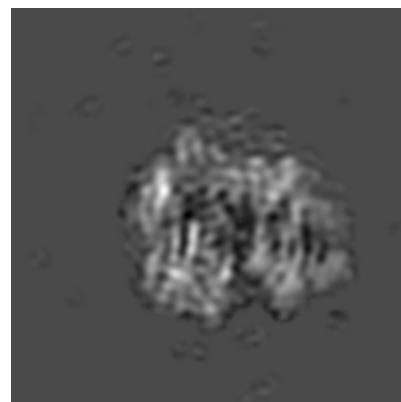
6.2.1 Primary map



X Index: 100



Y Index: 100

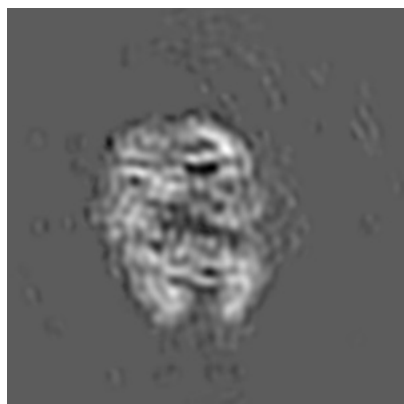


Z Index: 100

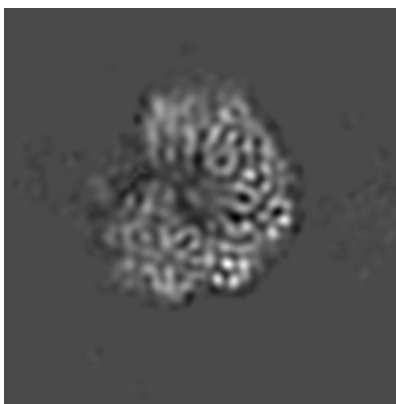
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

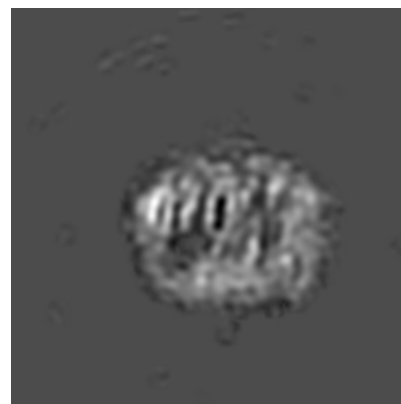
6.3.1 Primary map



X Index: 104



Y Index: 102

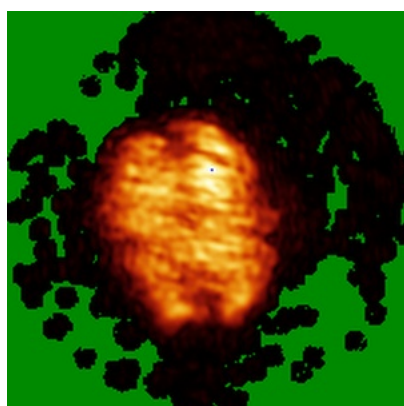


Z Index: 119

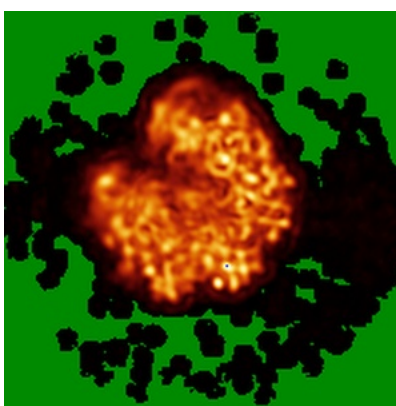
The images above show the largest variance slices of the map in three orthogonal directions.

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

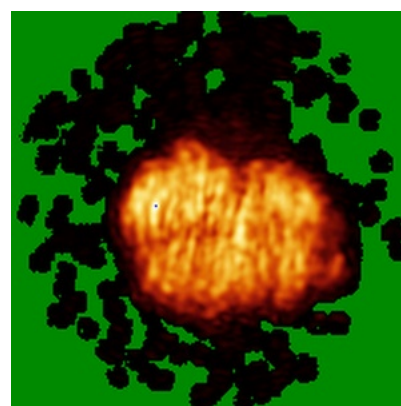
6.4.1 Primary map



X



Y

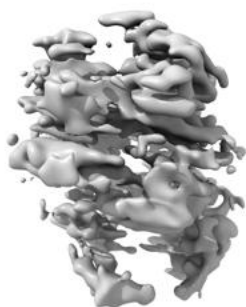


Z

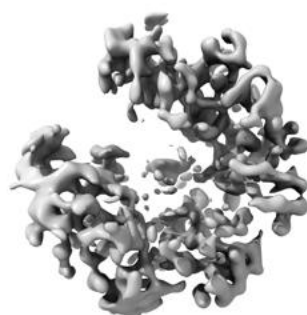
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

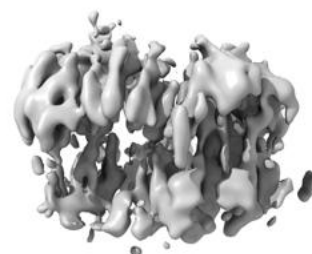
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

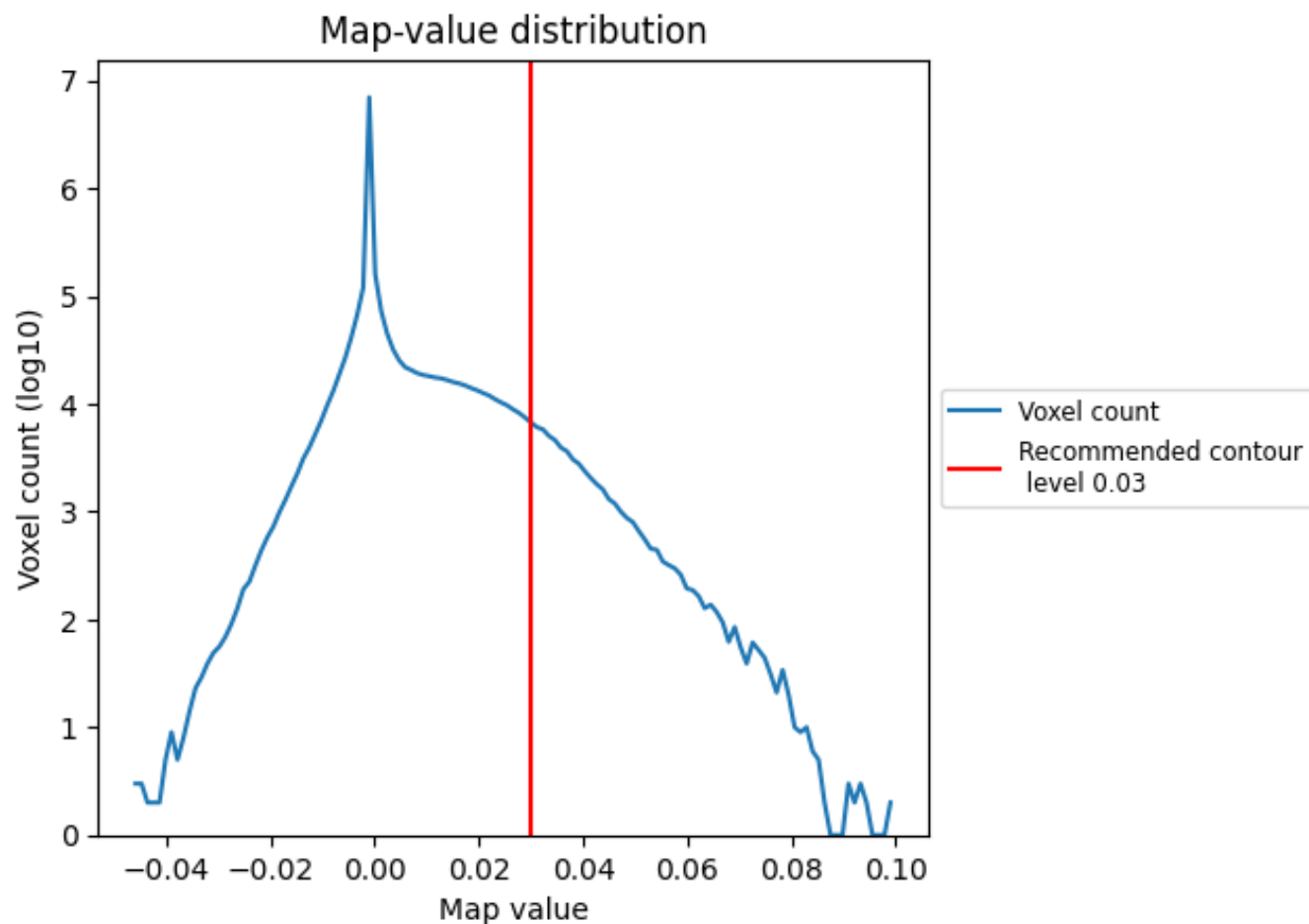
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

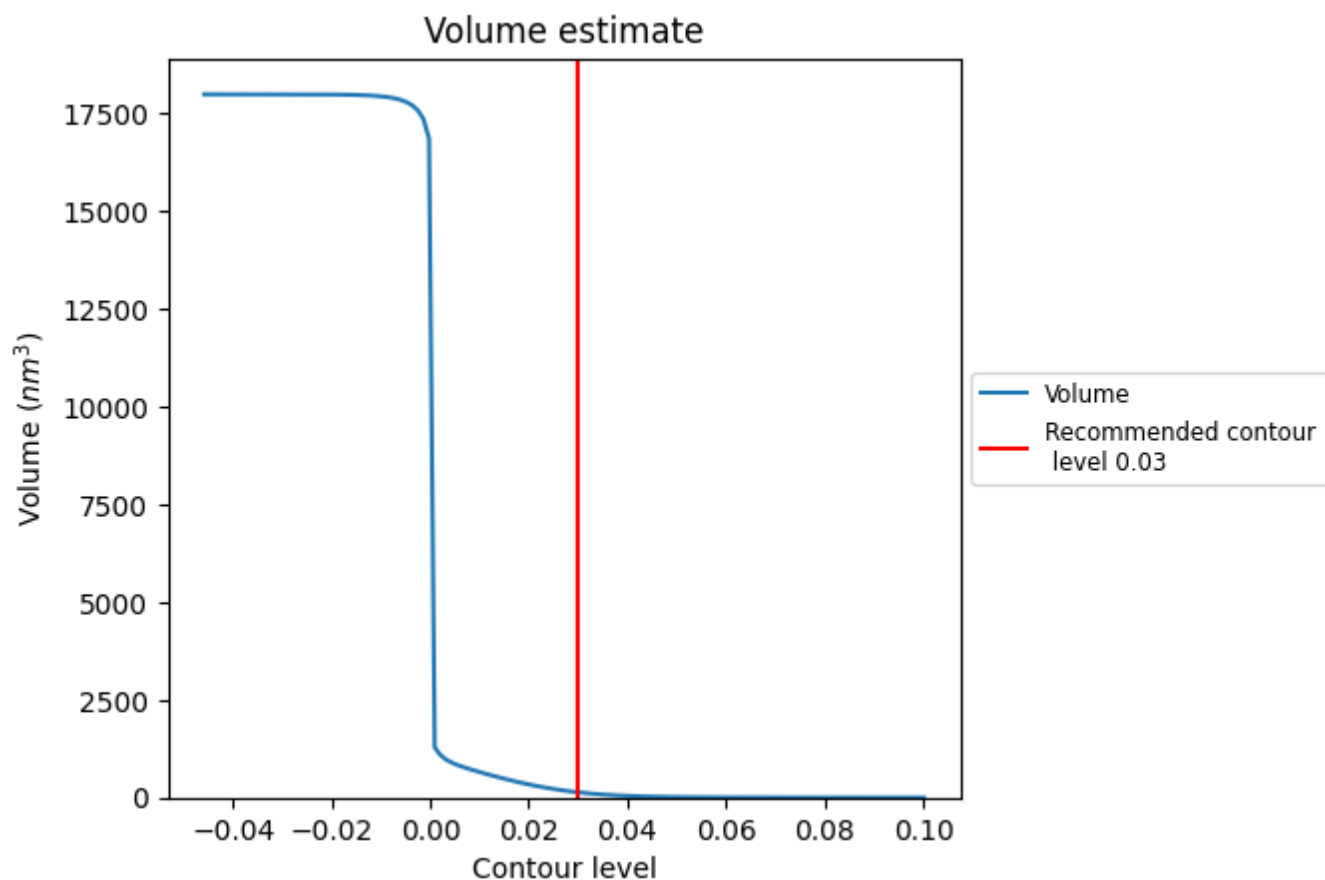
This section contains the results of statistical analysis of the map.

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.

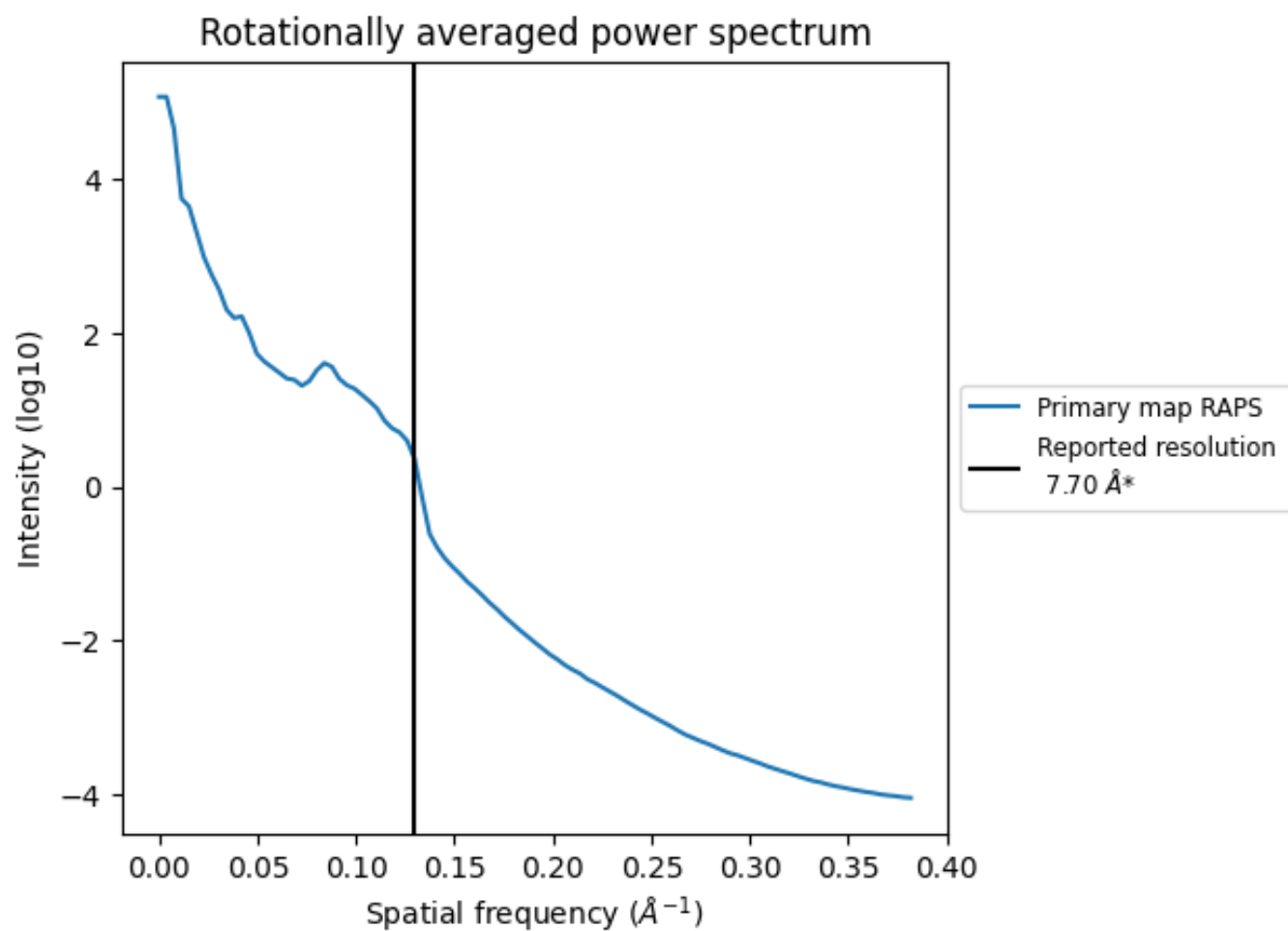
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm³; this corresponds to an approximate mass of 121 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 0.130 Å⁻¹

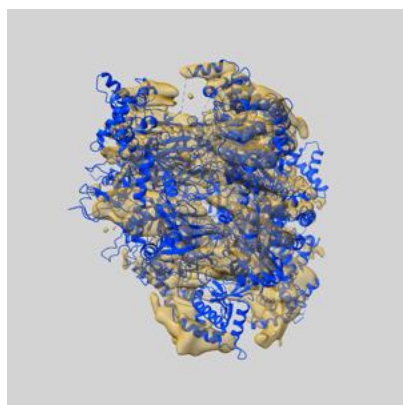
8 Fourier-Shell correlation

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

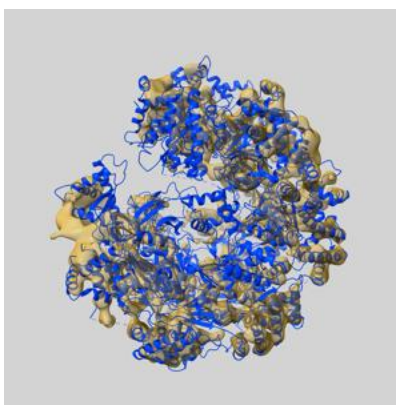
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21664 and PDB model 6WGF. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

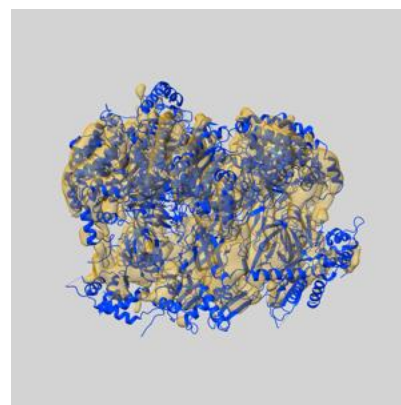
9.1 Map-model overlay [i](#)



X



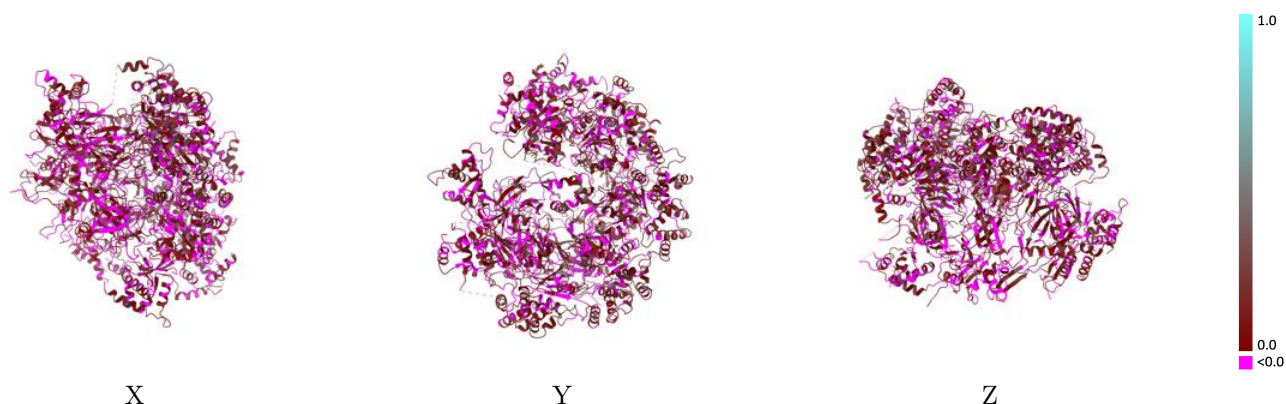
Y



Z

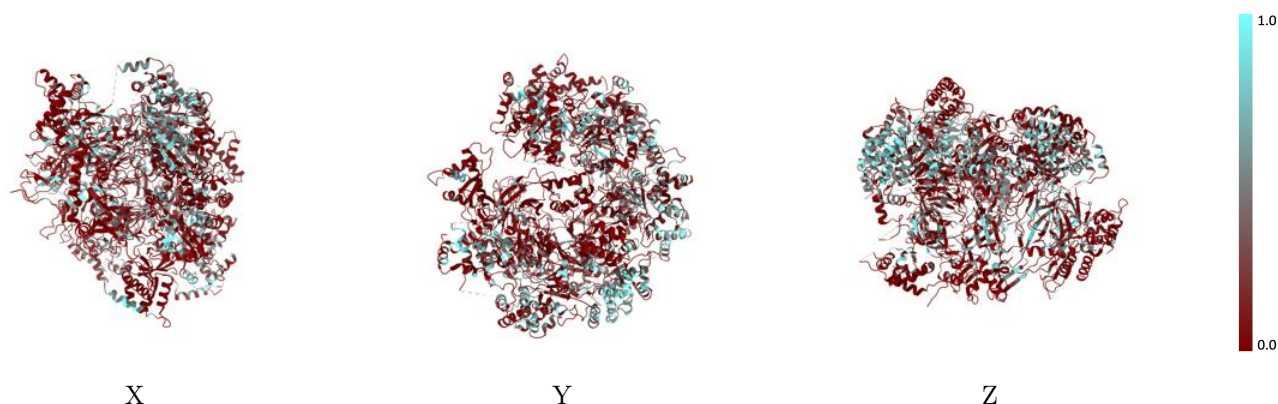
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



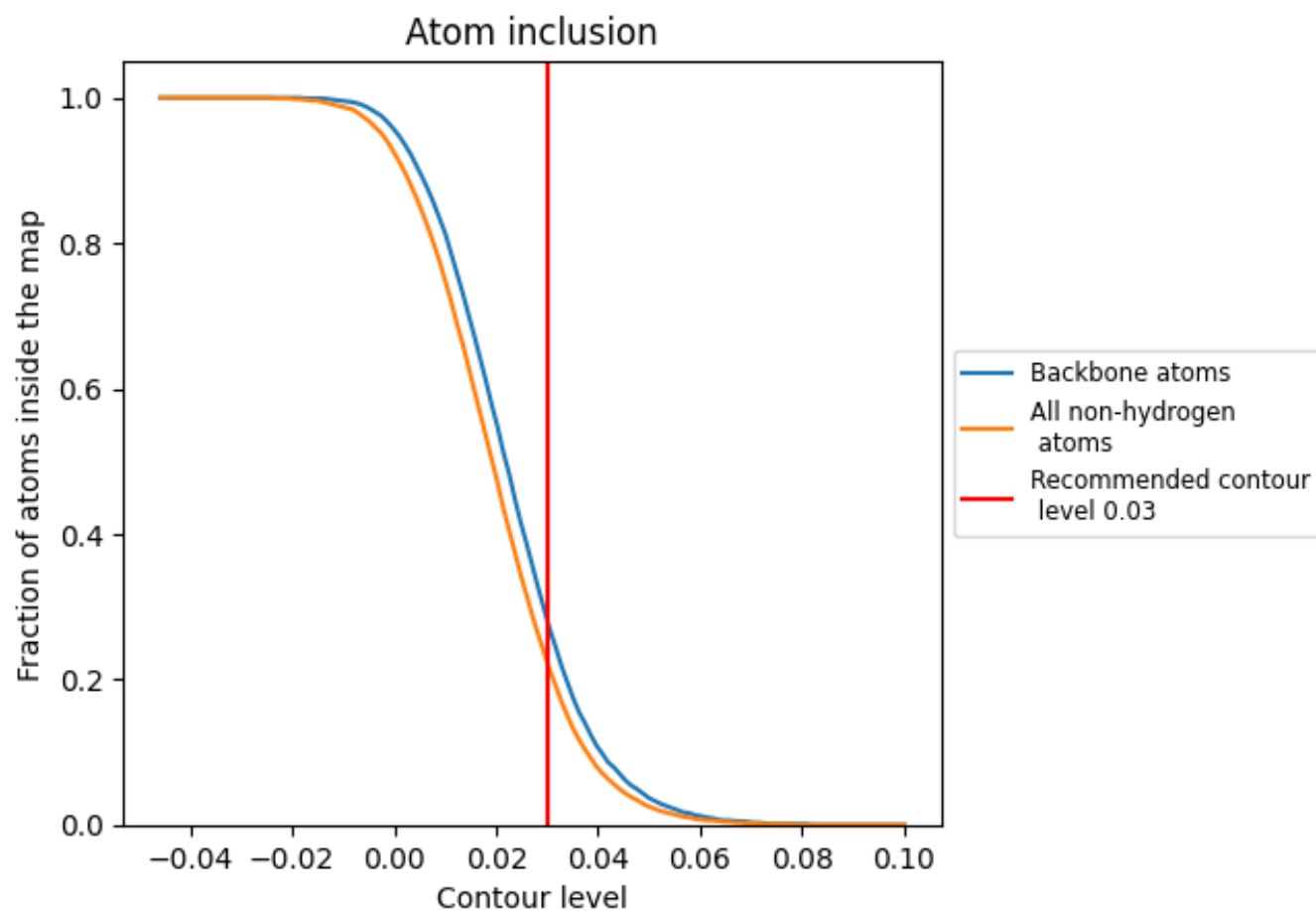
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 28% of all backbone atoms, 22% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2240	0.0640
2	0.2130	0.0560
3	0.2420	0.0760
4	0.2200	0.0640
5	0.1740	0.0530
6	0.2380	0.0640
7	0.2570	0.0700

1.0

0.0

<0.0