



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 02:52 AM UTC

PDB ID : 3J04 / pdb_00003j04
EMDB ID : EMD-5257
Title : EM structure of the heavy meromyosin subfragment of Chick smooth muscle
Myosin with regulatory light chain in phosphorylated state
Authors : Baumann, B.A.J.; Taylor, D.; Huang, Z.; Tama, F.; Fagnant, P.M.; Trybus,
K.; Taylor, K.
Deposited on : 2011-02-18
Resolution : 20.00 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:

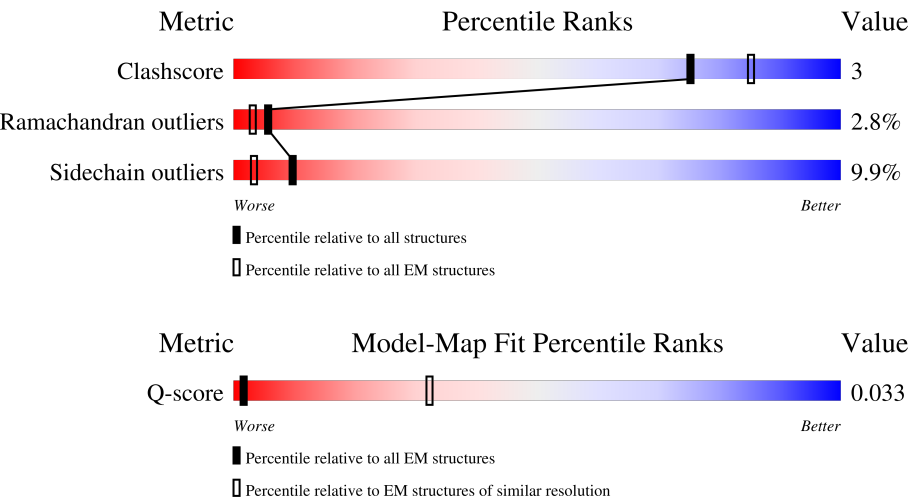
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 20.00 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	28 (19.50 - 20.50)

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	909	28% 79% 15% • •
1	D	909	29% 80% 14% • • •
2	B	143	72% 70% 22% • •
2	E	143	65% 67% 22% 8% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	148	53% 78% 19%
3	F	148	39% 78% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19065 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 Myosin-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	903	Total	C	N	O	S	0	0
			7214	4585	1228	1365	36		
1	D	903	Total	C	N	O	S	0	0
			7231	4596	1233	1366	36		

- Molecule 2 is a protein called Myosin regulatory light chain 2, smooth muscle major isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	143	Total	C	N	O	S	0	0
			1160	727	189	234	10		
2	E	143	Total	C	N	O	S	0	0
			1160	727	189	234	10		

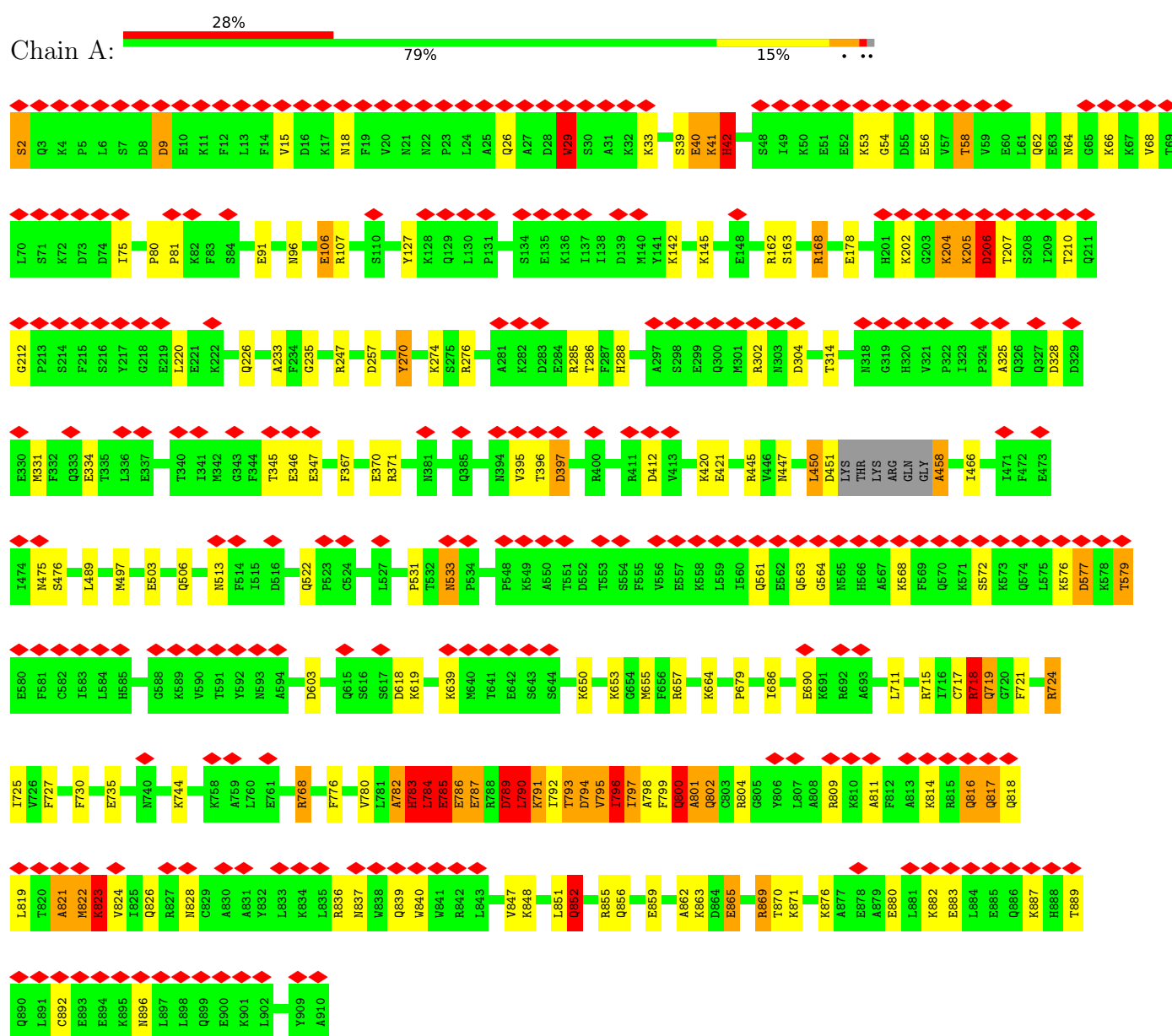
- Molecule 3 is a protein called Myosin light polypeptide 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	148	Total	C	N	O	S	0	0
			1150	716	189	234	11		
3	F	148	Total	C	N	O	S	0	0
			1150	716	189	234	11		

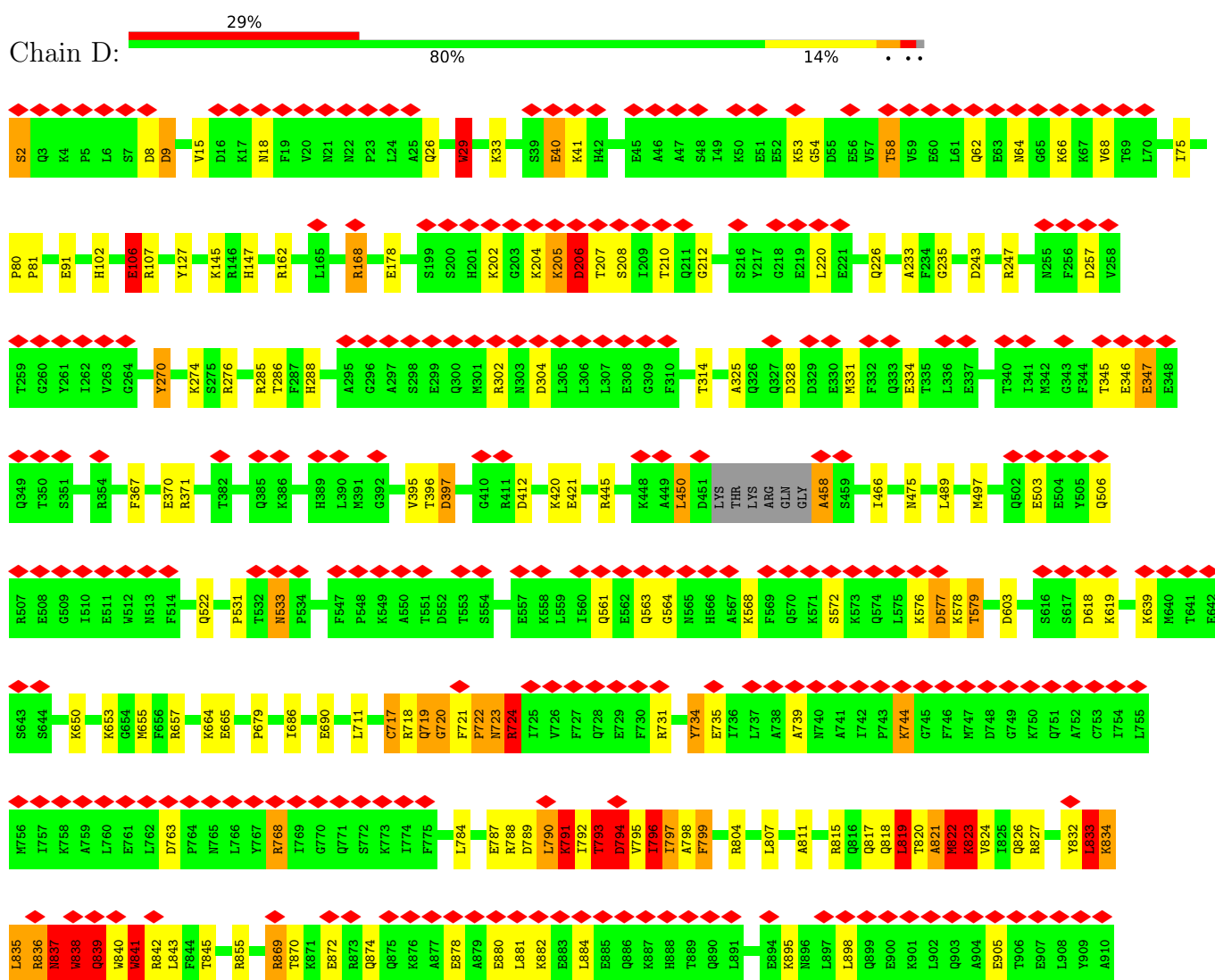
3 Residue-property plots

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.

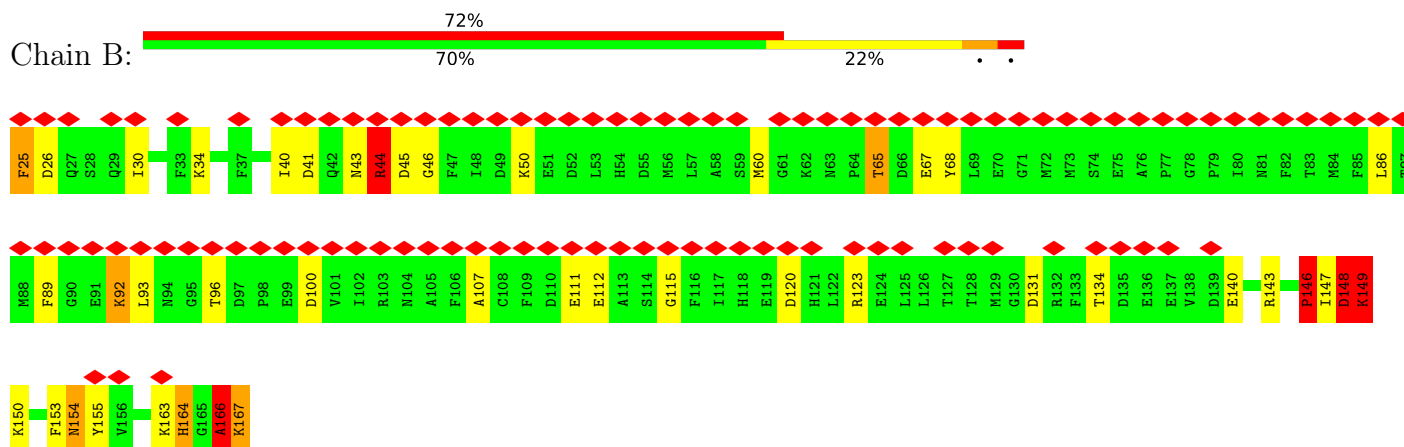
• Molecule 1: Myosin-11



• Molecule 1: Myosin-11

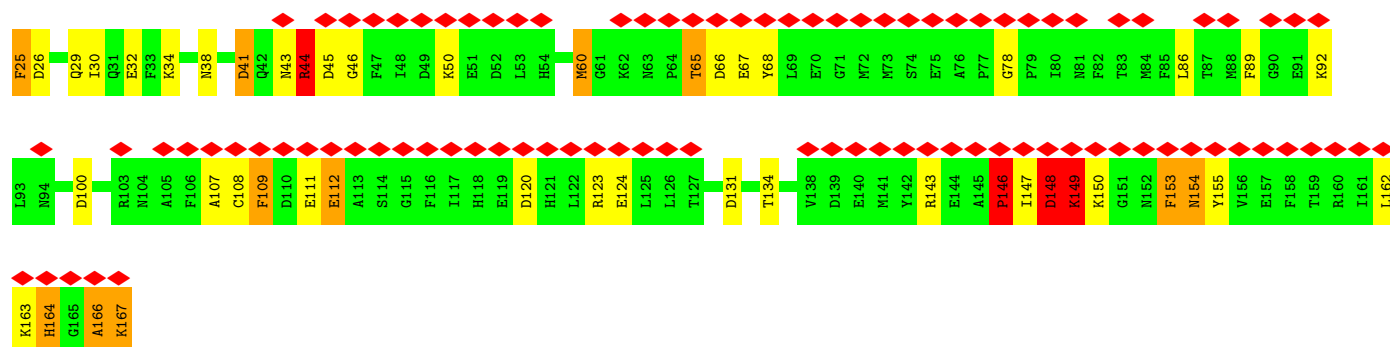


- Molecule 2: Myosin regulatory light chain 2, smooth muscle major isoform

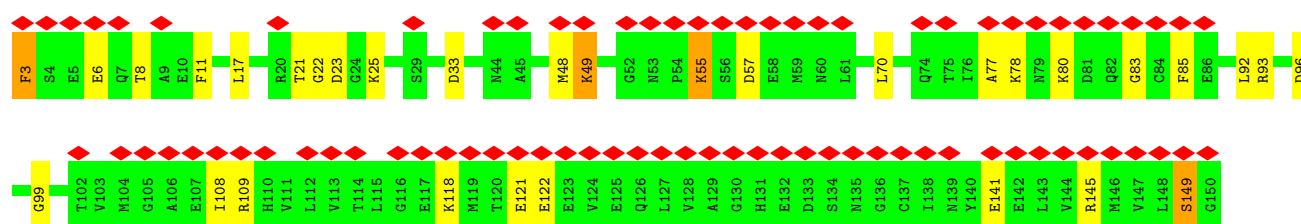
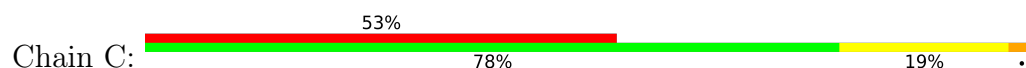


- Molecule 2: Myosin regulatory light chain 2, smooth muscle major isoform

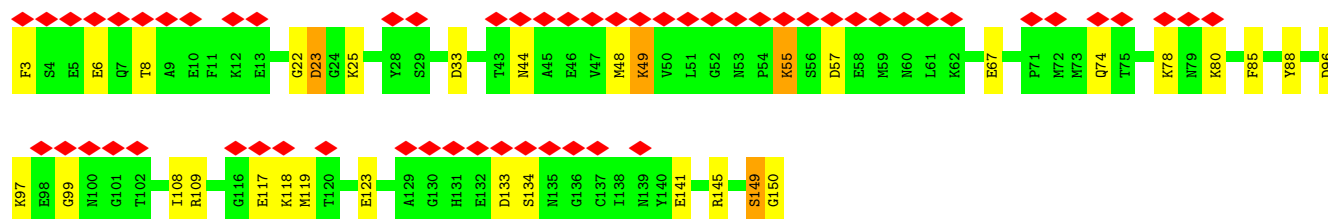
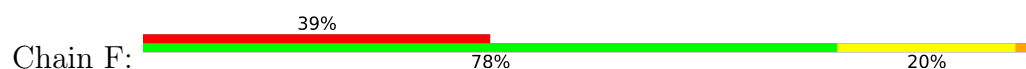




• Molecule 3: Myosin light polypeptide 6



• Molecule 3: Myosin light polypeptide 6



4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	2D CRYSTAL, a =Not provided Å, b =Not provided Å, c =Not provided Å, γ =Not provided°, space group=Not provided	Depositor
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	determined using ICE and corrected with CTFAPPLY	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	Not provided	
Magnification	24000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	4.404	Depositor
Minimum map value	-4.670	Depositor
Average map value	-0.034	Depositor
Map value standard deviation	1.010	Depositor
Recommended contour level	0.609	Depositor
Map size (Å)	419.0693, 428.995, 85.9985	wwPDB
Map dimensions	169, 81, 35	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.4797, 2.4514, 2.4571	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	1.01	10/7333 (0.1%)	2.50	178/9877 (1.8%)
1	D	0.96	7/7351 (0.1%)	2.31	144/9902 (1.5%)
2	B	1.04	3/1184 (0.3%)	2.19	29/1589 (1.8%)
2	E	1.02	1/1184 (0.1%)	2.06	36/1589 (2.3%)
3	C	1.01	4/1163 (0.3%)	1.92	13/1559 (0.8%)
3	F	1.00	1/1163 (0.1%)	1.73	17/1559 (1.1%)
All	All	0.99	26/19378 (0.1%)	2.31	417/26075 (1.6%)

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	46
1	D	0	48
2	B	0	11
2	E	0	13
3	C	0	5
3	F	0	5
All	All	0	128

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	SER	C-O	-12.60	0.98	1.23
1	D	2	SER	C-O	-12.42	0.98	1.23
3	C	83	GLY	C-N	-8.25	1.22	1.33
2	B	111	GLU	C-N	7.44	1.44	1.33
1	D	895	LYS	C-N	7.28	1.43	1.33
3	C	23	ASP	C-N	7.27	1.42	1.33
1	A	730	PHE	C-N	6.98	1.43	1.33
1	A	856	GLN	C-N	6.95	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	859	GLU	C-N	6.78	1.42	1.33
2	B	93	LEU	C-N	6.78	1.43	1.33
1	A	847	VAL	C-N	6.65	1.42	1.33
1	A	2	SER	N-CA	-6.52	1.33	1.46
1	D	603	ASP	CA-CB	6.34	1.57	1.52
1	D	811	ALA	C-N	6.12	1.41	1.33
2	E	111	GLU	C-N	6.06	1.41	1.33
1	D	874	GLN	C-N	6.00	1.41	1.33
1	A	603	ASP	CA-CB	5.97	1.56	1.52
3	F	44	ASN	C-N	-5.49	1.26	1.33
2	B	96	THR	C-N	-5.42	1.25	1.33
1	D	898	LEU	C-N	5.39	1.41	1.33
1	A	727	PHE	C-N	5.35	1.40	1.33
1	A	142	LYS	C-N	5.25	1.40	1.33
1	D	2	SER	CA-C	-5.18	1.42	1.52
3	C	92	LEU	C-N	5.09	1.41	1.33
1	A	862	ALA	C-N	5.07	1.40	1.33
3	C	77	ALA	C-N	5.06	1.41	1.33

All (417) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	719	GLN	O-C-N	-67.64	31.43	122.06
1	D	837	ASN	O-C-N	-58.84	44.33	122.59
1	A	796	ILE	CA-C-O	-54.31	52.90	120.78
1	A	42	HIS	O-C-N	-50.11	61.01	122.65
1	A	794	ASP	O-C-N	-47.11	64.92	122.87
1	D	720	GLY	O-C-N	42.27	161.38	122.92
1	D	841	TRP	O-C-N	-41.94	64.80	122.68
3	C	149	SER	O-C-N	-40.64	68.95	122.19
1	D	793	THR	O-C-N	-38.49	71.39	122.59
1	A	205	LYS	O-C-N	35.14	169.33	122.59
1	D	205	LYS	O-C-N	34.63	168.65	122.59
2	B	166	ALA	O-C-N	-33.94	77.45	122.59
1	D	723	ASN	O-C-N	-33.26	78.36	122.59
1	A	206	ASP	O-C-N	-32.88	78.86	122.59
1	D	837	ASN	CA-C-O	-32.50	74.03	120.51
1	A	796	ILE	O-C-N	-31.99	82.58	122.57
1	D	817	GLN	O-C-N	31.84	158.45	122.15
1	D	206	ASP	O-C-N	-31.38	80.86	122.59
1	A	786	GLU	O-C-N	30.78	163.53	122.59
1	A	719	GLN	N-CA-C	30.72	145.53	112.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	723	ASN	CA-C-N	-28.45	67.19	121.54
1	D	723	ASN	C-N-CA	-28.45	67.19	121.54
1	A	785	GLU	CA-C-O	-28.29	80.06	120.51
1	A	817	GLN	O-C-N	-28.20	92.81	121.85
1	A	785	GLU	O-C-N	28.02	159.86	122.59
1	A	42	HIS	CA-C-O	-27.91	89.84	121.94
1	A	782	ALA	O-C-N	-27.90	85.96	122.23
1	D	822	MET	O-C-N	-27.79	85.63	122.59
1	A	42	HIS	N-CA-C	-27.41	75.18	110.53
1	A	784	LEU	O-C-N	-27.25	86.34	122.59
1	D	820	THR	O-C-N	27.07	158.59	122.59
1	D	839	GLN	O-C-N	-26.87	86.85	122.59
2	B	153	PHE	O-C-N	26.39	153.99	122.86
1	D	822	MET	CA-C-O	25.93	157.59	120.51
2	E	153	PHE	O-C-N	25.62	153.10	122.86
1	A	823	LYS	CA-C-N	-25.23	81.72	120.82
1	A	823	LYS	C-N-CA	-25.23	81.72	120.82
1	D	790	LEU	O-C-N	24.61	155.32	122.59
1	D	717	CYS	O-C-N	-23.58	91.74	122.39
1	A	42	HIS	CA-C-N	22.86	166.22	121.41
1	A	42	HIS	C-N-CA	22.86	166.22	121.41
1	D	819	LEU	CA-C-N	22.14	163.82	121.54
1	D	819	LEU	C-N-CA	22.14	163.82	121.54
1	D	819	LEU	O-C-N	-21.55	93.93	122.59
1	D	797	ILE	CA-C-N	-21.32	89.45	122.49
1	D	797	ILE	C-N-CA	-21.32	89.45	122.49
1	A	787	GLU	O-C-N	-21.05	98.16	122.15
1	A	783	HIS	CA-C-N	20.06	159.85	121.54
1	A	783	HIS	C-N-CA	20.06	159.85	121.54
1	D	797	ILE	CA-C-O	-19.35	97.93	120.96
1	A	818	GLN	CA-C-N	-19.17	94.56	120.63
1	A	818	GLN	C-N-CA	-19.17	94.56	120.63
3	F	149	SER	O-C-N	-19.09	96.91	122.49
1	A	817	GLN	CA-C-N	18.88	152.85	122.65
1	A	817	GLN	C-N-CA	18.88	152.85	122.65
1	A	787	GLU	CA-C-O	18.58	140.12	120.42
1	D	819	LEU	CA-C-O	18.46	146.91	120.51
1	D	821	ALA	O-C-N	-18.20	102.64	121.93
1	A	852	GLN	CA-C-N	17.52	141.74	123.16
1	A	852	GLN	C-N-CA	17.52	141.74	123.16
1	D	723	ASN	CA-C-O	-17.45	95.55	120.51
1	D	822	MET	CA-C-N	17.43	154.82	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	822	MET	C-N-CA	17.43	154.82	121.54
1	A	821	ALA	CA-C-N	-17.32	88.46	121.54
1	A	821	ALA	C-N-CA	-17.32	88.46	121.54
1	A	799	PHE	CA-C-N	-17.11	96.03	122.37
1	A	799	PHE	C-N-CA	-17.11	96.03	122.37
2	E	154	ASN	O-C-N	-16.89	100.26	122.72
1	A	787	GLU	CA-C-N	16.57	153.18	121.54
1	A	787	GLU	C-N-CA	16.57	153.18	121.54
1	A	783	HIS	CA-C-O	-16.53	96.87	120.51
1	A	822	MET	CA-C-N	-16.20	90.61	121.54
1	A	822	MET	C-N-CA	-16.20	90.61	121.54
2	B	154	ASN	O-C-N	-16.08	101.20	122.59
1	D	717	CYS	CA-C-O	16.03	138.88	119.49
1	A	783	HIS	O-C-N	15.77	143.56	122.59
1	A	822	MET	CA-C-O	-15.67	98.11	120.51
1	A	458	ALA	O-C-N	-15.41	98.34	123.00
1	D	717	CYS	CA-C-N	15.32	150.80	121.54
1	D	717	CYS	C-N-CA	15.32	150.80	121.54
1	D	458	ALA	O-C-N	-15.07	98.88	123.00
1	D	724	ARG	N-CA-C	-14.88	79.11	110.80
1	D	837	ASN	N-CA-C	-14.87	79.12	110.80
1	D	793	THR	CA-C-O	-14.78	99.37	120.51
1	A	796	ILE	CA-C-N	-14.76	95.41	121.97
1	A	796	ILE	C-N-CA	-14.76	95.41	121.97
1	A	817	GLN	CA-C-O	14.20	134.13	118.52
1	A	852	GLN	O-C-N	13.80	140.94	122.59
1	A	785	GLU	CA-C-N	13.39	147.12	121.54
1	A	785	GLU	C-N-CA	13.39	147.12	121.54
1	A	818	GLN	O-C-N	13.25	138.24	122.34
1	D	2	SER	O-C-N	-13.22	101.85	123.00
1	D	797	ILE	N-CA-C	-12.74	98.46	110.82
1	D	839	GLN	N-CA-C	12.30	136.99	110.80
1	A	718	ARG	O-C-N	-12.27	106.27	122.59
1	D	821	ALA	CA-C-N	12.14	144.74	121.54
1	D	821	ALA	C-N-CA	12.14	144.74	121.54
1	A	791	LYS	CA-C-O	12.12	133.72	120.63
2	E	166	ALA	O-C-N	-12.11	108.95	122.88
2	E	149	LYS	N-CA-C	12.00	136.36	110.80
2	B	149	LYS	N-CA-C	11.96	136.27	110.80
1	A	719	GLN	CA-C-O	-11.66	104.18	119.80
1	A	821	ALA	O-C-N	-11.09	107.19	122.06
1	D	791	LYS	CA-C-O	-10.95	104.84	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	799	PHE	N-CA-C	-10.77	87.86	110.80
1	A	811	ALA	CA-C-N	10.67	135.00	120.38
1	A	811	ALA	C-N-CA	10.67	135.00	120.38
1	D	817	GLN	CA-C-N	10.49	136.25	120.31
1	D	817	GLN	C-N-CA	10.49	136.25	120.31
1	A	791	LYS	N-CA-C	10.44	123.96	111.33
1	A	816	GLN	O-C-N	-10.42	108.74	122.59
1	A	822	MET	N-CA-C	-10.25	88.96	110.80
1	A	791	LYS	O-C-N	-9.93	111.60	122.12
1	D	818	GLN	CA-C-N	9.80	140.25	121.54
1	D	818	GLN	C-N-CA	9.80	140.25	121.54
3	F	150	GLY	CA-C-O	-9.52	100.80	120.80
1	D	721	PHE	CA-C-O	-9.50	107.15	120.16
1	A	791	LYS	CA-C-N	9.35	135.49	121.65
1	A	791	LYS	C-N-CA	9.35	135.49	121.65
1	A	789	ASP	CA-C-N	9.19	132.78	120.65
1	A	789	ASP	C-N-CA	9.19	132.78	120.65
1	A	799	PHE	O-C-N	9.18	134.80	122.59
1	A	786	GLU	CA-C-N	9.12	133.25	120.29
1	A	786	GLU	C-N-CA	9.12	133.25	120.29
2	E	109	PHE	CA-C-N	9.09	133.77	120.87
2	E	109	PHE	C-N-CA	9.09	133.77	120.87
1	D	450	LEU	O-C-N	-8.80	108.91	123.00
2	E	148	ASP	CA-CB-CG	8.81	121.41	112.60
2	B	153	PHE	CA-C-N	8.80	138.34	121.54
2	B	153	PHE	C-N-CA	8.80	138.34	121.54
2	E	153	PHE	CA-C-N	8.79	140.15	123.09
2	E	153	PHE	C-N-CA	8.79	140.15	123.09
2	B	148	ASP	CA-CB-CG	8.68	121.28	112.60
1	D	818	GLN	O-C-N	-8.57	111.72	122.27
1	A	823	LYS	O-C-N	8.48	133.86	122.59
1	D	839	GLN	CB-CA-C	-8.44	93.62	110.42
1	D	820	THR	CA-C-N	8.43	136.84	121.41
1	D	820	THR	C-N-CA	8.43	136.84	121.41
1	D	842	ARG	N-CA-C	-8.36	102.86	113.72
2	E	41	ASP	CA-CB-CG	8.31	120.91	112.60
1	A	206	ASP	CA-C-N	8.27	136.54	121.41
1	A	206	ASP	C-N-CA	8.27	136.54	121.41
2	E	149	LYS	CB-CA-C	-8.25	94.00	110.42
2	B	149	LYS	CB-CA-C	-8.22	94.06	110.42
1	A	811	ALA	O-C-N	-8.19	113.44	122.12
1	A	717	CYS	O-C-N	-8.16	113.61	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	823	LYS	O-C-N	-8.14	111.76	122.59
2	B	44	ARG	N-CA-C	8.13	120.66	108.31
2	E	120	ASP	CA-CB-CG	-8.07	104.53	112.60
1	A	715	ARG	CA-C-N	8.05	130.77	120.70
1	A	715	ARG	C-N-CA	8.05	130.77	120.70
2	B	100	ASP	CA-CB-CG	-7.94	104.66	112.60
2	E	100	ASP	CA-CB-CG	-7.83	104.77	112.60
1	A	784	LEU	CA-C-N	7.78	136.40	121.54
1	A	784	LEU	C-N-CA	7.78	136.40	121.54
1	D	206	ASP	CA-C-N	7.77	135.63	121.41
1	D	206	ASP	C-N-CA	7.77	135.63	121.41
2	B	65	THR	CA-C-N	7.74	130.64	120.28
2	B	65	THR	C-N-CA	7.74	130.64	120.28
1	A	795	VAL	O-C-N	-7.69	112.71	122.17
1	A	823	LYS	CA-C-O	-7.68	109.53	120.51
3	F	99	GLY	CA-C-N	7.67	131.32	120.28
3	F	99	GLY	C-N-CA	7.67	131.32	120.28
1	D	724	ARG	O-C-N	-7.65	112.42	122.59
3	C	85	PHE	CA-C-N	7.64	130.52	120.28
3	C	85	PHE	C-N-CA	7.64	130.52	120.28
1	A	824	VAL	CA-C-N	7.61	130.74	120.77
1	A	824	VAL	C-N-CA	7.61	130.74	120.77
1	D	796	ILE	O-C-N	-7.60	113.07	122.57
1	D	838	TRP	O-C-N	-7.60	112.48	122.59
1	A	450	LEU	O-C-N	-7.56	110.90	123.00
1	D	790	LEU	CA-C-N	7.51	135.89	121.54
1	D	790	LEU	C-N-CA	7.51	135.89	121.54
1	A	822	MET	O-C-N	-7.51	110.98	123.00
3	F	85	PHE	CA-C-N	7.44	130.25	120.28
3	F	85	PHE	C-N-CA	7.44	130.25	120.28
3	F	23	ASP	CB-CA-C	7.43	123.42	110.64
1	A	304	ASP	CA-CB-CG	7.42	120.02	112.60
1	D	722	PRO	O-C-N	-7.42	110.20	122.36
1	D	817	GLN	N-CA-C	7.40	119.43	111.36
3	F	33	ASP	CA-CB-CG	-7.40	105.20	112.60
1	D	304	ASP	CA-CB-CG	7.38	119.98	112.60
2	E	65	THR	CA-C-N	7.31	130.08	120.28
2	E	65	THR	C-N-CA	7.31	130.08	120.28
1	A	798	ALA	N-CA-C	7.29	120.76	109.60
2	B	148	ASP	N-CA-C	7.29	121.28	112.38
3	C	33	ASP	CA-CB-CG	-7.28	105.32	112.60
2	B	148	ASP	CA-C-N	7.26	135.40	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	148	ASP	C-N-CA	7.26	135.40	121.54
1	D	822	MET	N-CA-C	-7.23	95.40	110.80
2	B	67	GLU	N-CA-CB	-7.21	98.30	110.49
1	D	818	GLN	CA-C-O	7.17	128.21	119.97
1	A	787	GLU	N-CA-C	7.16	119.17	111.36
1	D	412	ASP	CA-CB-CG	-7.14	105.46	112.60
2	E	148	ASP	CA-C-N	7.12	135.13	121.54
2	E	148	ASP	C-N-CA	7.12	135.13	121.54
2	E	148	ASP	N-CA-C	7.04	120.97	112.38
1	D	794	ASP	O-C-N	-7.01	113.26	122.59
1	A	823	LYS	N-CA-C	6.99	125.69	110.80
1	D	9	ASP	CA-CB-CG	6.99	119.59	112.60
1	A	797	ILE	N-CA-C	6.93	123.75	109.34
1	A	412	ASP	CA-CB-CG	-6.90	105.70	112.60
1	A	790	LEU	CA-C-N	6.88	129.81	120.38
1	A	790	LEU	C-N-CA	6.88	129.81	120.38
1	A	9	ASP	CA-CB-CG	6.88	119.48	112.60
1	D	54	GLY	CA-C-N	6.87	129.48	120.28
1	D	54	GLY	C-N-CA	6.87	129.48	120.28
1	D	270	TYR	CA-C-O	6.84	121.91	117.94
1	D	869	ARG	CD-NE-CZ	-6.84	114.82	124.40
1	A	64	ASN	CA-CB-CG	6.78	119.38	112.60
2	B	120	ASP	CA-CB-CG	-6.75	105.85	112.60
1	D	717	CYS	N-CA-C	6.73	120.59	112.38
1	A	54	GLY	CA-C-N	6.72	129.28	120.28
1	A	54	GLY	C-N-CA	6.72	129.28	120.28
1	A	618	ASP	CA-C-N	6.66	129.20	120.28
1	A	618	ASP	C-N-CA	6.66	129.20	120.28
1	D	618	ASP	CA-C-N	6.66	129.20	120.28
1	D	618	ASP	C-N-CA	6.66	129.20	120.28
2	B	164	HIS	N-CA-CB	6.62	121.67	110.49
1	A	270	TYR	CA-C-O	6.60	121.77	117.94
2	E	164	HIS	N-CA-CB	6.58	121.61	110.49
1	A	797	ILE	CB-CA-C	-6.55	100.55	111.29
1	D	503	GLU	CB-CA-C	-6.54	99.94	110.79
1	D	798	ALA	N-CA-C	-6.53	104.54	113.30
2	E	67	GLU	N-CA-CB	-6.53	99.13	109.78
2	E	120	ASP	CB-CA-C	6.53	123.42	110.42
1	A	790	LEU	O-C-N	-6.53	115.24	122.03
1	A	397	ASP	CA-CB-CG	-6.49	106.11	112.60
1	A	795	VAL	CA-C-N	6.46	133.59	121.97
1	A	795	VAL	C-N-CA	6.46	133.59	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	328	ASP	CA-C-N	6.46	128.83	120.44
1	D	328	ASP	C-N-CA	6.46	128.83	120.44
1	D	64	ASN	CA-CB-CG	6.44	119.04	112.60
1	A	420	LYS	CA-C-N	6.43	128.89	120.28
1	A	420	LYS	C-N-CA	6.43	128.89	120.28
3	F	48	MET	CA-C-N	6.43	128.89	120.28
3	F	48	MET	C-N-CA	6.43	128.89	120.28
1	D	420	LYS	CA-C-N	6.40	128.86	120.28
1	D	420	LYS	C-N-CA	6.40	128.86	120.28
2	E	112	GLU	N-CA-C	-6.40	99.58	109.24
1	A	797	ILE	O-C-N	-6.38	114.59	122.57
1	A	839	GLN	N-CA-C	6.38	118.03	111.14
1	D	397	ASP	CA-CB-CG	-6.37	106.23	112.60
2	E	41	ASP	N-CA-CB	-6.37	99.73	110.49
1	A	664	LYS	CA-C-N	6.35	128.79	120.28
1	A	664	LYS	C-N-CA	6.35	128.79	120.28
1	A	328	ASP	CA-C-N	6.24	128.56	120.44
1	A	328	ASP	C-N-CA	6.24	128.56	120.44
1	A	62	GLN	CA-C-N	6.20	128.59	120.28
1	A	62	GLN	C-N-CA	6.20	128.59	120.28
1	D	664	LYS	CA-C-N	6.20	128.59	120.28
1	D	664	LYS	C-N-CA	6.20	128.59	120.28
1	A	889	THR	CA-C-N	6.16	128.44	120.44
1	A	889	THR	C-N-CA	6.16	128.44	120.44
1	A	202	LYS	N-CA-CB	-6.14	102.40	110.88
1	A	533	ASN	CA-C-O	-6.11	111.78	120.16
1	D	62	GLN	CA-C-N	6.11	128.46	120.28
1	D	62	GLN	C-N-CA	6.11	128.46	120.28
3	C	48	MET	CA-C-N	6.08	128.43	120.28
3	C	48	MET	C-N-CA	6.08	128.43	120.28
1	A	80	PRO	N-CA-C	6.08	118.12	110.70
1	D	106	GLU	CB-CG-CD	6.04	122.87	112.60
1	D	799	PHE	CA-C-N	6.03	133.04	122.79
1	D	799	PHE	C-N-CA	6.03	133.04	122.79
1	A	106	GLU	CB-CG-CD	6.01	122.82	112.60
1	A	42	HIS	CB-CA-C	6.00	122.83	110.40
2	B	143	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	2	SER	O-C-N	-5.99	113.42	123.00
2	E	143	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	A	837	ASN	CA-CB-CG	-5.92	106.67	112.60
3	F	6	GLU	N-CA-CB	-5.88	100.55	110.49
1	D	804	ARG	CA-C-N	5.88	126.63	119.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	804	ARG	C-N-CA	5.88	126.63	119.99
1	D	145	LYS	N-CA-C	5.87	118.12	110.43
1	D	799	PHE	O-C-N	-5.87	113.27	121.72
1	A	799	PHE	CA-C-O	-5.86	112.12	120.51
1	A	824	VAL	CA-C-O	5.86	126.07	119.92
1	D	2	SER	CA-C-O	5.85	130.74	120.80
1	D	744	LYS	CA-C-N	5.85	128.51	121.38
1	D	744	LYS	C-N-CA	5.85	128.51	121.38
1	A	395	VAL	N-CA-C	5.84	116.03	110.42
1	D	395	VAL	N-CA-C	5.84	116.03	110.42
1	A	826	GLN	N-CA-C	5.84	118.12	111.11
1	A	721	PHE	CA-C-N	5.82	126.58	120.12
1	A	721	PHE	C-N-CA	5.82	126.58	120.12
2	B	123	ARG	NE-CZ-NH2	5.82	124.44	119.20
2	E	123	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	D	832	TYR	N-CA-C	-5.76	105.58	113.30
1	A	367	PHE	CA-CB-CG	-5.75	108.05	113.80
3	F	117	GLU	CA-C-N	5.74	132.49	121.54
3	F	117	GLU	C-N-CA	5.74	132.49	121.54
2	B	92	LYS	N-CA-CB	-5.72	102.17	110.47
1	A	851	LEU	CA-C-N	5.72	132.46	121.54
1	A	851	LEU	C-N-CA	5.72	132.46	121.54
1	D	202	LYS	N-CA-CB	-5.70	102.30	110.80
1	D	836	ARG	N-CA-C	5.70	117.65	110.24
1	D	80	PRO	N-CA-C	5.70	117.66	110.70
1	D	835	LEU	N-CA-CB	5.70	120.12	110.49
1	D	837	ASN	CB-CA-C	5.69	121.74	110.42
1	D	724	ARG	CB-CA-C	5.69	121.74	110.42
1	D	711	LEU	CA-C-N	5.67	127.88	120.28
1	D	711	LEU	C-N-CA	5.67	127.88	120.28
1	A	717	CYS	CA-C-N	5.66	132.36	121.54
1	A	717	CYS	C-N-CA	5.66	132.36	121.54
2	E	107	ALA	CA-C-N	5.64	132.31	121.54
2	E	107	ALA	C-N-CA	5.64	132.31	121.54
1	A	791	LYS	CB-CA-C	-5.64	101.10	110.68
1	A	800	GLN	N-CA-CB	-5.64	101.68	110.98
2	E	38	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	711	LEU	CA-C-N	5.62	127.81	120.28
1	A	711	LEU	C-N-CA	5.62	127.81	120.28
1	D	533	ASN	CA-C-O	-5.61	112.47	120.16
1	A	744	LYS	CA-C-N	5.58	128.19	121.38
1	A	744	LYS	C-N-CA	5.58	128.19	121.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	892	CYS	CA-C-N	5.58	127.75	120.28
1	A	892	CYS	C-N-CA	5.58	127.75	120.28
1	D	220	LEU	CA-C-N	5.56	128.29	120.28
1	D	220	LEU	C-N-CA	5.56	128.29	120.28
3	C	49	LYS	N-CA-CB	-5.56	101.95	110.12
2	E	32	GLU	CB-CA-C	-5.52	102.21	110.88
1	D	768	ARG	CD-NE-CZ	-5.50	116.70	124.40
3	C	96	ASP	CA-C-N	5.49	129.06	120.82
3	C	96	ASP	C-N-CA	5.49	129.06	120.82
1	D	367	PHE	CA-CB-CG	-5.46	108.34	113.80
1	D	884	LEU	CA-C-N	5.46	127.60	120.28
1	D	884	LEU	C-N-CA	5.46	127.60	120.28
1	A	15	VAL	N-CA-C	5.46	116.75	109.37
1	A	814	LYS	N-CA-C	-5.46	106.57	113.18
2	B	89	PHE	CA-C-N	5.46	126.01	120.00
2	B	89	PHE	C-N-CA	5.46	126.01	120.00
1	A	577	ASP	CA-C-N	5.46	128.04	120.29
1	A	577	ASP	C-N-CA	5.46	128.04	120.29
2	B	134	THR	CA-C-N	5.46	127.59	120.28
2	B	134	THR	C-N-CA	5.46	127.59	120.28
1	D	64	ASN	N-CA-CB	-5.45	103.10	110.95
1	A	727	PHE	CA-C-N	5.45	127.53	120.44
1	A	727	PHE	C-N-CA	5.45	127.53	120.44
3	C	6	GLU	N-CA-CB	-5.44	101.30	110.49
1	A	9	ASP	CA-C-N	5.42	127.55	120.28
1	A	9	ASP	C-N-CA	5.42	127.55	120.28
2	E	66	ASP	CA-C-N	5.42	128.95	120.82
2	E	66	ASP	C-N-CA	5.42	128.95	120.82
3	C	85	PHE	N-CA-C	-5.42	106.72	113.55
1	A	475	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	793	THR	O-C-N	-5.38	116.28	122.09
1	D	833	LEU	O-C-N	-5.35	115.71	122.19
1	A	204	LYS	N-CA-C	5.35	117.63	110.35
1	A	768	ARG	CD-NE-CZ	-5.35	116.91	124.40
3	C	99	GLY	CA-C-N	5.35	127.88	120.29
3	C	99	GLY	C-N-CA	5.35	127.88	120.29
1	A	503	GLU	CB-CA-C	-5.34	101.92	110.79
1	D	81	PRO	CA-C-N	5.33	127.42	120.28
1	D	81	PRO	C-N-CA	5.33	127.42	120.28
1	D	15	VAL	N-CA-C	5.33	116.56	109.37
2	B	107	ALA	CA-C-N	5.32	128.35	120.17
2	B	107	ALA	C-N-CA	5.32	128.35	120.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	49	LYS	N-CA-CB	-5.31	102.31	110.12
1	A	717	CYS	CA-C-O	5.30	126.57	120.90
1	A	603	ASP	CB-CA-C	5.29	115.60	111.00
1	D	75	ILE	N-CA-C	5.29	115.20	108.12
1	A	793	THR	N-CA-C	-5.28	105.44	111.14
1	D	739	ALA	N-CA-C	5.26	119.19	112.87
1	A	64	ASN	N-CA-CB	-5.24	103.40	110.95
1	D	842	ARG	CA-C-N	5.24	127.56	120.65
1	D	842	ARG	C-N-CA	5.24	127.56	120.65
2	E	60	MET	CG-SD-CE	-5.23	89.39	100.90
1	D	823	LYS	CA-C-O	-5.23	113.04	120.51
1	D	233	ALA	N-CA-C	5.22	116.66	111.07
2	E	78	GLY	CA-C-N	5.22	125.22	119.90
2	E	78	GLY	C-N-CA	5.22	125.22	119.90
1	D	578	LYS	N-CA-CB	-5.22	102.44	110.16
1	D	880	GLU	CA-C-N	5.22	127.27	120.28
1	D	880	GLU	C-N-CA	5.22	127.27	120.28
2	B	112	GLU	N-CA-C	-5.21	101.26	109.50
1	D	29	TRP	CA-C-N	5.21	127.78	120.28
1	D	29	TRP	C-N-CA	5.21	127.78	120.28
1	A	717	CYS	N-CA-C	5.21	117.36	111.11
1	A	205	LYS	CA-C-N	5.21	131.48	121.54
1	A	205	LYS	C-N-CA	5.21	131.48	121.54
1	A	802	GLN	N-CA-CB	5.19	117.81	110.13
1	A	96	ASN	CA-C-N	5.19	127.19	120.44
1	A	96	ASN	C-N-CA	5.19	127.19	120.44
1	A	823	LYS	CB-CA-C	-5.17	100.13	110.42
1	D	577	ASP	CA-C-N	5.17	127.63	120.29
1	D	577	ASP	C-N-CA	5.17	127.63	120.29
1	A	856	GLN	CA-C-N	5.15	127.19	120.28
1	A	856	GLN	C-N-CA	5.15	127.19	120.28
1	A	81	PRO	CA-C-N	5.15	127.18	120.28
1	A	81	PRO	C-N-CA	5.15	127.18	120.28
1	D	58	THR	N-CA-CB	5.14	118.65	110.16
1	A	58	THR	N-CA-CB	5.14	118.63	110.16
1	A	75	ILE	N-CA-C	5.14	115.00	108.12
1	D	347	GLU	CA-C-N	5.13	127.16	120.28
1	D	347	GLU	C-N-CA	5.13	127.16	120.28
1	A	29	TRP	CA-C-N	5.13	127.67	120.28
1	A	29	TRP	C-N-CA	5.13	127.67	120.28
1	A	690	GLU	N-CA-CB	-5.12	102.42	110.46
1	D	208	SER	N-CA-C	5.10	118.71	109.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	120	ASP	CB-CA-C	5.10	120.57	110.42
1	A	476	SER	CA-C-N	5.10	127.11	120.28
1	A	476	SER	C-N-CA	5.10	127.11	120.28
2	E	134	THR	CA-C-N	5.08	127.09	120.28
2	E	134	THR	C-N-CA	5.08	127.09	120.28
1	A	220	LEU	CA-C-N	5.08	127.60	120.28
1	A	220	LEU	C-N-CA	5.08	127.60	120.28
1	D	243	ASP	CA-CB-CG	-5.07	107.53	112.60
1	D	690	GLU	N-CA-CB	-5.07	102.51	110.46
1	D	205	LYS	CA-C-N	5.06	131.21	121.54
1	D	205	LYS	C-N-CA	5.06	131.21	121.54
3	F	97	LYS	N-CA-C	5.05	116.79	111.28
1	D	790	LEU	N-CA-C	5.05	121.56	110.80
1	D	475	ASN	CA-CB-CG	-5.03	107.57	112.60
1	D	819	LEU	N-CA-C	-5.03	100.09	110.80
3	F	96	ASP	CA-C-N	5.02	127.00	120.28
3	F	96	ASP	C-N-CA	5.02	127.00	120.28
1	D	823	LYS	N-CA-C	5.01	121.47	110.80
1	A	233	ALA	N-CA-C	5.00	116.42	111.07

There are no chirality outliers.

All (128) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain
1	A	127	TYR	Sidechain
1	A	168	ARG	Sidechain
1	A	206	ASP	Peptide,Mainchain
1	A	212	GLY	Peptide
1	A	270	TYR	Sidechain
1	A	276	ARG	Sidechain
1	A	285	ARG	Sidechain
1	A	288	HIS	Mainchain
1	A	41	LYS	Mainchain
1	A	42	HIS	Peptide,Mainchain
1	A	450	LEU	Mainchain
1	A	458	ALA	Mainchain
1	A	657	ARG	Sidechain
1	A	718	ARG	Peptide,Mainchain
1	A	719	GLN	Mainchain
1	A	724	ARG	Mainchain
1	A	768	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	782	ALA	Peptide,Mainchain
1	A	783	HIS	Peptide
1	A	784	LEU	Peptide,Mainchain
1	A	785	GLU	Peptide
1	A	787	GLU	Mainchain
1	A	790	LEU	Mainchain
1	A	793	THR	Mainchain
1	A	794	ASP	Peptide,Mainchain
1	A	795	VAL	Peptide,Mainchain
1	A	796	ILE	Peptide,Mainchain
1	A	800	GLN	Peptide
1	A	816	GLN	Mainchain
1	A	817	GLN	Mainchain
1	A	821	ALA	Mainchain
1	A	822	MET	Mainchain
1	A	823	LYS	Mainchain
1	A	836	ARG	Sidechain
1	A	852	GLN	Peptide
1	A	855	ARG	Sidechain
1	A	869	ARG	Sidechain
2	B	131	ASP	Peptide
2	B	146	PRO	Peptide
2	B	147	ILE	Peptide
2	B	148	ASP	Peptide,Mainchain
2	B	154	ASN	Mainchain
2	B	166	ALA	Peptide,Mainchain
2	B	40	ILE	Peptide
2	B	44	ARG	Peptide
2	B	68	TYR	Sidechain
3	C	109	ARG	Sidechain
3	C	145	ARG	Sidechain
3	C	149	SER	Peptide,Mainchain
3	C	93	ARG	Sidechain
1	D	107	ARG	Sidechain
1	D	127	TYR	Sidechain
1	D	162	ARG	Sidechain
1	D	168	ARG	Sidechain
1	D	206	ASP	Peptide,Mainchain
1	D	212	GLY	Peptide
1	D	270	TYR	Sidechain
1	D	276	ARG	Sidechain
1	D	285	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	288	HIS	Mainchain
1	D	450	LEU	Mainchain
1	D	458	ALA	Mainchain
1	D	657	ARG	Sidechain
1	D	717	CYS	Peptide,Mainchain
1	D	719	GLN	Peptide
1	D	720	GLY	Peptide
1	D	722	PRO	Mainchain
1	D	723	ASN	Mainchain
1	D	724	ARG	Mainchain
1	D	731	ARG	Sidechain
1	D	734	TYR	Sidechain
1	D	768	ARG	Sidechain
1	D	788	ARG	Peptide
1	D	791	LYS	Mainchain
1	D	793	THR	Mainchain
1	D	794	ASP	Mainchain
1	D	796	ILE	Mainchain
1	D	797	ILE	Mainchain
1	D	799	PHE	Peptide,Mainchain
1	D	815	ARG	Sidechain
1	D	821	ALA	Peptide,Mainchain
1	D	822	MET	Peptide
1	D	823	LYS	Mainchain
1	D	827	ARG	Sidechain
1	D	833	LEU	Peptide
1	D	834	LYS	Peptide
1	D	836	ARG	Sidechain
1	D	837	ASN	Mainchain
1	D	839	GLN	Mainchain
1	D	840	TRP	Peptide
1	D	841	TRP	Peptide,Mainchain
1	D	855	ARG	Sidechain
1	D	869	ARG	Sidechain
2	E	109	PHE	Sidechain
2	E	131	ASP	Peptide
2	E	146	PRO	Peptide
2	E	147	ILE	Peptide
2	E	148	ASP	Peptide,Mainchain
2	E	153	PHE	Peptide
2	E	154	ASN	Mainchain
2	E	166	ALA	Peptide,Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	E	44	ARG	Peptide,Sidechain
2	E	68	TYR	Sidechain
3	F	109	ARG	Sidechain
3	F	145	ARG	Sidechain
3	F	149	SER	Peptide,Mainchain
3	F	88	TYR	Sidechain

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	A	7214	0	7239	17	0
1	D	7231	0	7264	12	0
2	B	1160	0	1076	32	0
2	E	1160	0	1076	35	0
3	C	1150	0	1116	17	0
3	F	1150	0	1114	5	0
All	All	19065	0	18885	115	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 3.

All (115) 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:E:25:PHE:CE2	2:E:86:LEU:HD11	1.15	1.63
3:C:3:PHE:CZ	3:C:70:LEU:HD11	1.15	1.61
2:E:25:PHE:CZ	2:E:30:ILE:HD11	1.34	1.60
2:B:25:PHE:CZ	2:B:30:ILE:HD11	1.29	1.59
2:E:25:PHE:CZ	2:E:86:LEU:HD11	1.36	1.59
2:B:25:PHE:HE2	2:B:86:LEU:CD1	1.09	1.58
2:E:25:PHE:CE2	2:E:86:LEU:CD1	1.84	1.55
2:B:25:PHE:CE2	2:B:86:LEU:CD1	1.80	1.54
2:B:25:PHE:CZ	2:B:86:LEU:HD11	1.43	1.51
2:B:25:PHE:CE2	2:B:86:LEU:HD11	1.01	1.50
2:E:25:PHE:HE2	2:E:86:LEU:CD1	1.17	1.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:PHE:HZ	3:C:70:LEU:CD1	1.20	1.50
2:B:25:PHE:CE1	2:B:30:ILE:HD11	1.53	1.42
2:B:25:PHE:CZ	2:B:30:ILE:CD1	2.06	1.36
2:E:25:PHE:CZ	2:E:30:ILE:CD1	2.13	1.29
2:E:25:PHE:CE1	2:E:30:ILE:HD11	1.67	1.28
2:E:167:LYS:HA	2:E:167:LYS:NZ	1.49	1.26
2:B:167:LYS:HA	2:B:167:LYS:NZ	1.58	1.18
2:E:167:LYS:HZ3	2:E:167:LYS:CA	1.55	1.17
2:B:167:LYS:HZ2	2:B:167:LYS:CA	1.61	1.12
3:C:3:PHE:CZ	3:C:70:LEU:CD1	2.06	1.12
1:A:780:VAL:O	1:A:783:HIS:O	1.71	1.09
2:E:167:LYS:C	2:E:167:LYS:HZ2	1.68	0.99
2:B:167:LYS:NZ	2:B:167:LYS:CA	2.24	0.97
2:B:167:LYS:HZ1	2:B:167:LYS:C	1.73	0.96
2:E:25:PHE:HE2	2:E:86:LEU:HD12	1.28	0.95
2:E:167:LYS:NZ	2:E:167:LYS:CA	2.17	0.95
2:B:25:PHE:HE2	2:B:86:LEU:HD12	1.31	0.95
3:C:3:PHE:CD2	3:C:11:PHE:HE2	1.85	0.95
2:B:167:LYS:HA	2:B:167:LYS:HZ2	0.77	0.94
2:B:167:LYS:NZ	2:B:167:LYS:C	2.30	0.90
1:D:2:SER:OG	1:D:18:ASN:OD1	1.90	0.90
2:E:167:LYS:NZ	2:E:167:LYS:C	2.31	0.89
2:E:25:PHE:CE2	2:E:86:LEU:HD12	2.05	0.86
2:E:25:PHE:CZ	2:E:86:LEU:CD1	2.30	0.85
2:B:25:PHE:HE2	2:B:86:LEU:HD13	1.38	0.85
2:B:25:PHE:CZ	2:B:86:LEU:CD1	2.34	0.85
2:E:25:PHE:HE2	2:E:86:LEU:HD13	1.40	0.82
2:B:25:PHE:CE1	2:B:30:ILE:CD1	2.44	0.82
2:E:25:PHE:HZ	2:E:30:ILE:HD11	1.35	0.81
2:B:25:PHE:HZ	2:B:30:ILE:HD11	1.42	0.81
2:B:25:PHE:HZ	2:B:86:LEU:HD21	1.46	0.79
3:C:3:PHE:CD2	3:C:11:PHE:CE2	2.71	0.78
2:E:25:PHE:CE1	2:E:30:ILE:CD1	2.54	0.77
2:E:167:LYS:HA	2:E:167:LYS:HZ3	0.67	0.77
2:B:25:PHE:CZ	2:B:30:ILE:HD13	2.17	0.76
2:E:25:PHE:CE2	2:E:86:LEU:HD13	2.16	0.75
3:C:3:PHE:CE1	3:C:8:THR:OG1	2.42	0.72
1:D:845:THR:HG22	2:E:167:LYS:HE2	1.70	0.72
2:E:25:PHE:CZ	2:E:30:ILE:HD13	2.23	0.71
3:C:3:PHE:CE2	3:C:11:PHE:CE2	2.79	0.71
1:D:2:SER:HG	1:D:18:ASN:CG	1.99	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:PHE:CE2	2:B:86:LEU:HD13	2.16	0.67
2:E:25:PHE:HZ	2:E:86:LEU:HD11	1.42	0.67
2:E:25:PHE:HD2	2:E:89:PHE:HE2	1.44	0.64
3:C:3:PHE:CE1	3:C:70:LEU:HD11	2.15	0.64
1:D:2:SER:CB	1:D:18:ASN:OD1	2.46	0.63
2:B:25:PHE:CE2	2:B:86:LEU:HD12	2.10	0.63
3:C:3:PHE:CD1	3:C:8:THR:OG1	2.51	0.62
1:A:39:SER:HB3	1:A:42:HIS:O	1.99	0.61
1:A:2:SER:HB2	1:A:18:ASN:OD1	1.99	0.61
3:C:3:PHE:HD1	3:C:3:PHE:O	1.84	0.60
2:B:25:PHE:CE2	2:B:30:ILE:HD13	2.37	0.60
2:B:25:PHE:CE2	2:B:30:ILE:CD1	2.78	0.60
2:B:25:PHE:HZ	2:B:86:LEU:CD2	2.15	0.60
3:C:3:PHE:CE2	3:C:11:PHE:CD2	2.89	0.59
3:C:3:PHE:CE2	3:C:11:PHE:HE2	2.16	0.59
2:B:25:PHE:CZ	2:B:86:LEU:HD21	2.34	0.59
2:E:25:PHE:HZ	2:E:86:LEU:HD21	1.67	0.59
1:D:845:THR:CG2	2:E:167:LYS:HE2	2.34	0.58
1:A:40:GLU:CD	1:A:41:LYS:HZ2	2.13	0.57
3:C:3:PHE:CE2	3:C:70:LEU:CD1	2.83	0.57
2:E:25:PHE:O	2:E:25:PHE:HD1	1.89	0.56
1:A:447:ASN:O	1:A:451:ASP:OD2	2.24	0.56
2:B:25:PHE:HD1	2:B:25:PHE:O	1.89	0.55
3:F:3:PHE:HD1	3:F:8:THR:HG1	1.54	0.55
1:A:883:GLU:OE1	1:A:887:LYS:NZ	2.40	0.55
3:C:3:PHE:HD2	3:C:11:PHE:HE2	1.46	0.55
1:A:780:VAL:O	1:A:783:HIS:C	2.47	0.55
1:D:40:GLU:CD	1:D:41:LYS:HZ2	2.15	0.54
2:E:25:PHE:CE2	2:E:30:ILE:CD1	2.86	0.54
1:A:876:LYS:NZ	1:A:880:GLU:OE2	2.38	0.52
2:E:25:PHE:HD2	2:E:89:PHE:CE2	2.24	0.52
1:A:883:GLU:OE2	1:A:887:LYS:NZ	2.40	0.51
2:E:25:PHE:CE2	2:E:30:ILE:HD13	2.46	0.51
1:A:145:LYS:HZ1	1:A:789:ASP:CG	2.19	0.50
3:C:55:LYS:HZ3	3:C:57:ASP:CG	2.20	0.49
1:D:421:GLU:CD	1:D:421:GLU:H	2.22	0.47
2:B:25:PHE:C	2:B:25:PHE:CD1	2.92	0.47
3:F:55:LYS:HZ3	3:F:57:ASP:CG	2.22	0.47
1:A:421:GLU:H	1:A:421:GLU:CD	2.22	0.47
1:A:876:LYS:NZ	1:A:880:GLU:OE1	2.46	0.46
3:F:3:PHE:N	3:F:3:PHE:CD2	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:25:PHE:C	2:E:25:PHE:CD1	2.93	0.45
1:D:2:SER:HB2	1:D:18:ASN:OD1	2.14	0.45
1:A:800:GLN:H	1:A:802:GLN:H	1.63	0.45
2:B:25:PHE:HD1	2:B:25:PHE:C	2.25	0.44
2:B:25:PHE:HZ	2:B:30:ILE:CD1	2.04	0.43
3:F:119:MET:HE2	3:F:123:GLU:HB3	2.01	0.43
1:A:883:GLU:CD	1:A:887:LYS:NZ	2.76	0.43
1:D:838:TRP:CD2	1:D:841:TRP:HB2	2.53	0.43
1:A:876:LYS:NZ	1:A:880:GLU:CD	2.77	0.43
3:C:3:PHE:CD1	3:C:3:PHE:N	2.84	0.42
1:A:865:GLU:OE1	1:A:869:ARG:NH2	2.53	0.42
1:D:789:ASP:HA	1:D:792:ILE:HG22	2.02	0.42
2:B:25:PHE:CZ	2:B:86:LEU:CD2	3.01	0.41
2:E:41:ASP:OD2	2:E:44:ARG:HA	2.20	0.41
2:E:25:PHE:HD1	2:E:25:PHE:C	2.26	0.41
1:D:843:LEU:CD1	2:E:60:MET:HE1	2.50	0.41
1:A:801:ALA:HA	1:A:804:ARG:HB2	2.02	0.41
2:B:25:PHE:CE1	2:B:30:ILE:CG1	3.03	0.41
3:C:3:PHE:CD1	3:C:3:PHE:C	2.97	0.41
3:F:3:PHE:CD2	3:F:74:GLN:HG2	2.56	0.41
2:E:25:PHE:CD2	2:E:89:PHE:HE2	2.31	0.41
1:D:102:HIS:O	1:D:106:GLU:HG2	2.21	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	899/909 (99%)	807 (90%)	69 (8%)	23 (3%)	4	25
1	D	899/909 (99%)	808 (90%)	65 (7%)	26 (3%)	3	23
2	B	141/143 (99%)	123 (87%)	11 (8%)	7 (5%)	1	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	141/143 (99%)	123 (87%)	12 (8%)	6 (4%)	2	17
3	C	146/148 (99%)	135 (92%)	9 (6%)	2 (1%)	9	40
3	F	146/148 (99%)	135 (92%)	8 (6%)	3 (2%)	5	30
All	All	2372/2400 (99%)	2131 (90%)	174 (7%)	67 (3%)	6	24

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	ASN
1	A	564	GLY
1	A	679	PRO
1	A	724	ARG
1	A	785	GLU
1	A	786	GLU
1	A	801	ALA
1	A	823	LYS
1	A	852	GLN
2	B	149	LYS
2	B	164	HIS
1	D	168	ARG
1	D	533	ASN
1	D	564	GLY
1	D	679	PRO
1	D	724	ARG
1	D	790	LEU
1	D	793	THR
1	D	794	ASP
1	D	819	LEU
1	D	823	LYS
1	D	824	VAL
1	D	834	LYS
1	D	837	ASN
1	D	839	GLN
2	E	108	CYS
2	E	149	LYS
2	E	164	HIS
3	F	118	LYS
1	A	168	ARG
1	A	205	LYS
1	A	572	SER
1	A	796	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	118	LYS
1	D	205	LYS
1	D	572	SER
1	D	795	VAL
1	D	835	LEU
1	D	838	TRP
1	A	29	TRP
1	A	206	ASP
1	A	783	HIS
2	B	46	GLY
2	B	166	ALA
1	D	29	TRP
1	D	206	ASP
2	E	46	GLY
3	F	22	GLY
1	A	235	GLY
1	A	531	PRO
1	D	235	GLY
1	A	718	ARG
1	A	784	LEU
2	B	45	ASP
1	D	325	ALA
1	D	531	PRO
1	D	579	THR
3	F	133	ASP
1	A	325	ALA
1	A	579	THR
1	A	797	ILE
2	B	115	GLY
3	C	22	GLY
1	D	796	ILE
2	E	45	ASP
2	B	146	PRO
2	E	146	PRO

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	A	779/801 (97%)	707 (91%)	72 (9%)	8	27
1	D	782/801 (98%)	708 (90%)	74 (10%)	8	25
2	B	125/125 (100%)	107 (86%)	18 (14%)	3	13
2	E	125/125 (100%)	106 (85%)	19 (15%)	3	12
3	C	125/127 (98%)	113 (90%)	12 (10%)	8	25
3	F	125/127 (98%)	115 (92%)	10 (8%)	11	31
All	All	2061/2106 (98%)	1856 (90%)	205 (10%)	10	24

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	26	GLN
1	A	29	TRP
1	A	33	LYS
1	A	40	GLU
1	A	53	LYS
1	A	56	GLU
1	A	58	THR
1	A	66	LYS
1	A	68	VAL
1	A	91	GLU
1	A	106	GLU
1	A	162	ARG
1	A	163	SER
1	A	178	GLU
1	A	204	LYS
1	A	207	THR
1	A	210	THR
1	A	226	GLN
1	A	247	ARG
1	A	257	ASP
1	A	274	LYS
1	A	286	THR
1	A	302	ARG
1	A	314	THR
1	A	331	MET
1	A	334	GLU
1	A	345	THR
1	A	346	GLU
1	A	347	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	370	GLU
1	A	371	ARG
1	A	396	THR
1	A	397	ASP
1	A	445	ARG
1	A	466	ILE
1	A	489	LEU
1	A	497	MET
1	A	506	GLN
1	A	513	ASN
1	A	522	GLN
1	A	561	GLN
1	A	563	GLN
1	A	568	LYS
1	A	576	LYS
1	A	577	ASP
1	A	579	THR
1	A	619	LYS
1	A	639	LYS
1	A	650	LYS
1	A	653	LYS
1	A	655	MET
1	A	686	ILE
1	A	718	ARG
1	A	725	ILE
1	A	735	GLU
1	A	776	PHE
1	A	789	ASP
1	A	790	LEU
1	A	791	LYS
1	A	792	ILE
1	A	809	ARG
1	A	819	LEU
1	A	828	ASN
1	A	840	TRP
1	A	848	LYS
1	A	863	LYS
1	A	865	GLU
1	A	870	THR
1	A	871	LYS
1	A	882	LYS
1	A	896	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	25	PHE
2	B	26	ASP
2	B	34	LYS
2	B	41	ASP
2	B	43	ASN
2	B	44	ARG
2	B	50	LYS
2	B	60	MET
2	B	65	THR
2	B	92	LYS
2	B	140	GLU
2	B	146	PRO
2	B	148	ASP
2	B	149	LYS
2	B	150	LYS
2	B	155	TYR
2	B	163	LYS
2	B	167	LYS
3	C	3	PHE
3	C	17	LEU
3	C	21	THR
3	C	25	LYS
3	C	49	LYS
3	C	55	LYS
3	C	78	LYS
3	C	80	LYS
3	C	108	ILE
3	C	121	GLU
3	C	122	GLU
3	C	141	GLU
1	D	8	ASP
1	D	9	ASP
1	D	26	GLN
1	D	29	TRP
1	D	33	LYS
1	D	40	GLU
1	D	53	LYS
1	D	58	THR
1	D	66	LYS
1	D	68	VAL
1	D	91	GLU
1	D	106	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	147	HIS
1	D	178	GLU
1	D	204	LYS
1	D	207	THR
1	D	210	THR
1	D	226	GLN
1	D	247	ARG
1	D	257	ASP
1	D	274	LYS
1	D	286	THR
1	D	302	ARG
1	D	314	THR
1	D	331	MET
1	D	334	GLU
1	D	345	THR
1	D	346	GLU
1	D	347	GLU
1	D	370	GLU
1	D	371	ARG
1	D	396	THR
1	D	397	ASP
1	D	445	ARG
1	D	466	ILE
1	D	489	LEU
1	D	497	MET
1	D	506	GLN
1	D	522	GLN
1	D	561	GLN
1	D	563	GLN
1	D	568	LYS
1	D	576	LYS
1	D	577	ASP
1	D	579	THR
1	D	619	LYS
1	D	639	LYS
1	D	650	LYS
1	D	653	LYS
1	D	655	MET
1	D	665	GLU
1	D	686	ILE
1	D	718	ARG
1	D	719	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	734	TYR
1	D	735	GLU
1	D	744	LYS
1	D	763	ASP
1	D	784	LEU
1	D	787	GLU
1	D	791	LYS
1	D	794	ASP
1	D	807	LEU
1	D	819	LEU
1	D	822	MET
1	D	823	LYS
1	D	826	GLN
1	D	833	LEU
1	D	870	THR
1	D	872	GLU
1	D	878	GLU
1	D	881	LEU
1	D	882	LYS
1	D	905	GLU
2	E	25	PHE
2	E	26	ASP
2	E	29	GLN
2	E	34	LYS
2	E	43	ASN
2	E	44	ARG
2	E	50	LYS
2	E	65	THR
2	E	92	LYS
2	E	112	GLU
2	E	124	GLU
2	E	146	PRO
2	E	148	ASP
2	E	149	LYS
2	E	150	LYS
2	E	155	TYR
2	E	162	LEU
2	E	163	LYS
2	E	167	LYS
3	F	23	ASP
3	F	25	LYS
3	F	49	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	55	LYS
3	F	67	GLU
3	F	78	LYS
3	F	80	LYS
3	F	108	ILE
3	F	134	SER
3	F	141	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	A	565	ASN
1	A	661	GLN
1	A	666	GLN
1	A	676	ASN
1	A	751	GLN
1	A	765	ASN
3	C	16	GLN
1	D	42	HIS
1	D	186	ASN
1	D	415	GLN
1	D	418	GLN
1	D	533	ASN
1	D	565	ASN
1	D	661	GLN
1	D	666	GLN
1	D	751	GLN
1	D	886	GLN
1	D	890	GLN
3	F	60	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 [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.

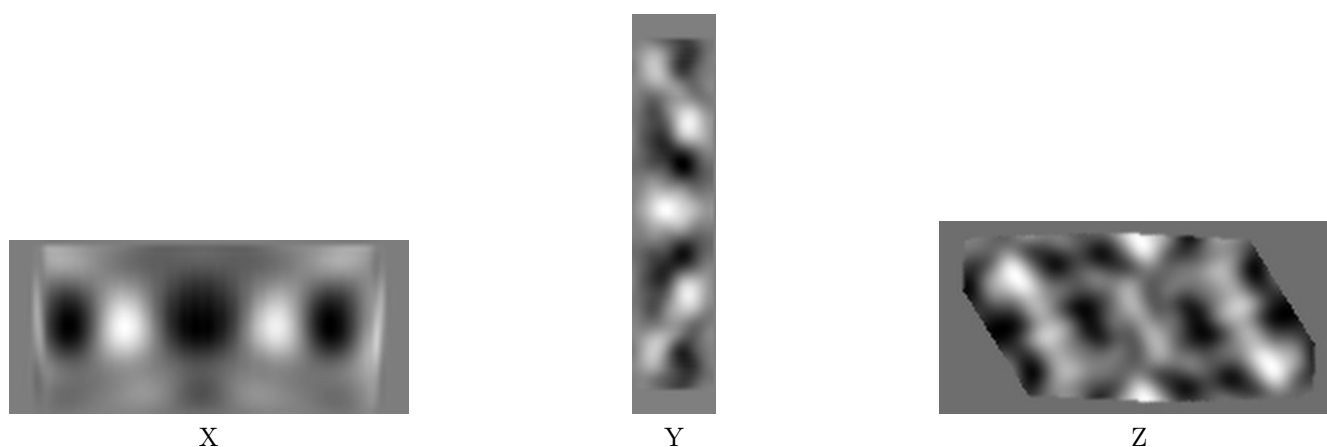
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5257. 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](#)

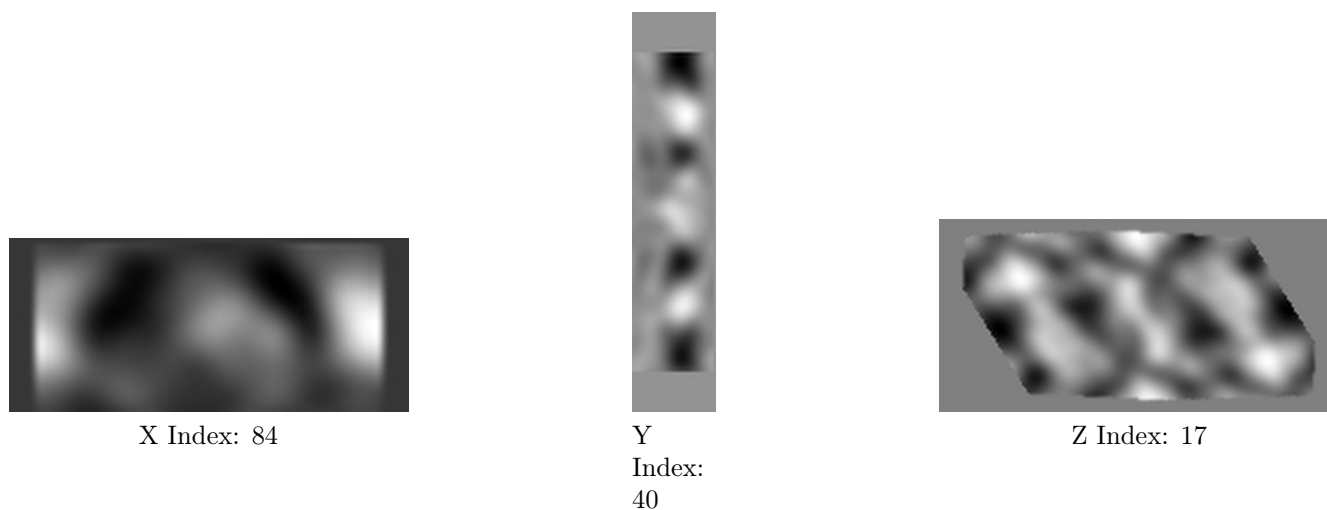
6.1.1 Primary map



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

6.2 Central slices [i](#)

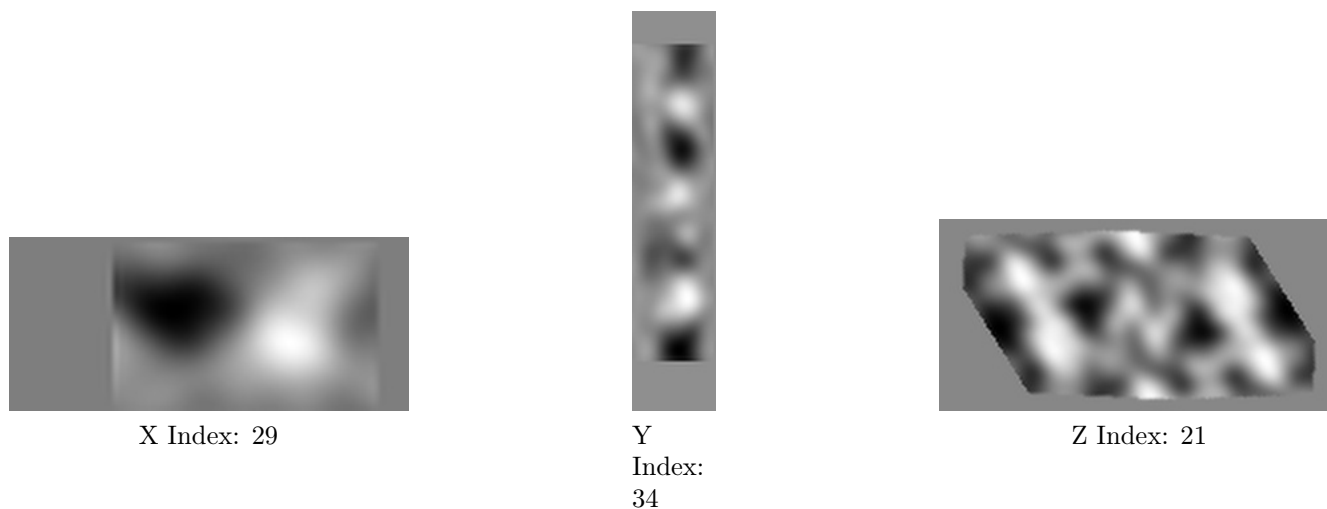
6.2.1 Primary map



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

6.3 Largest variance slices [i](#)

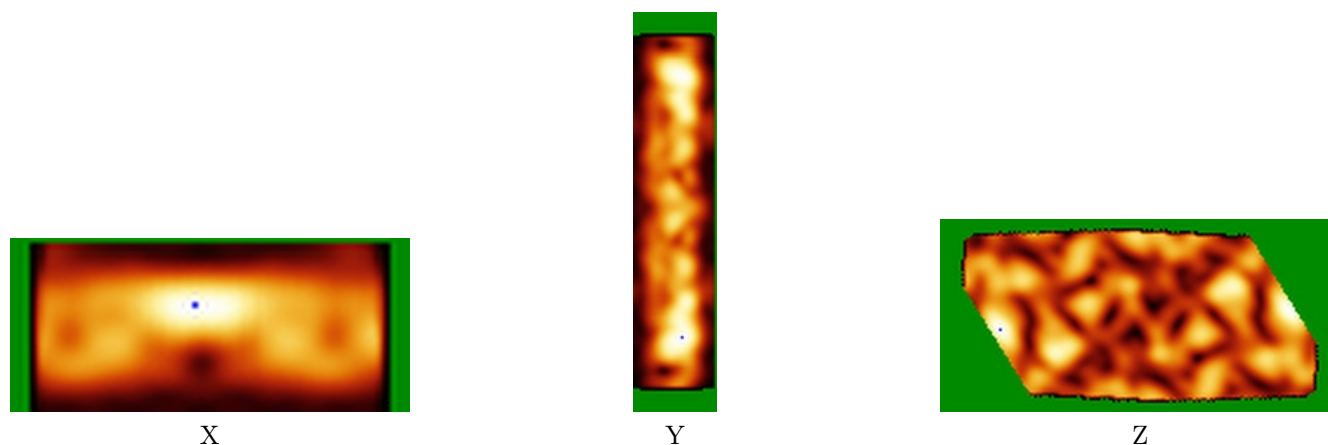
6.3.1 Primary map



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

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

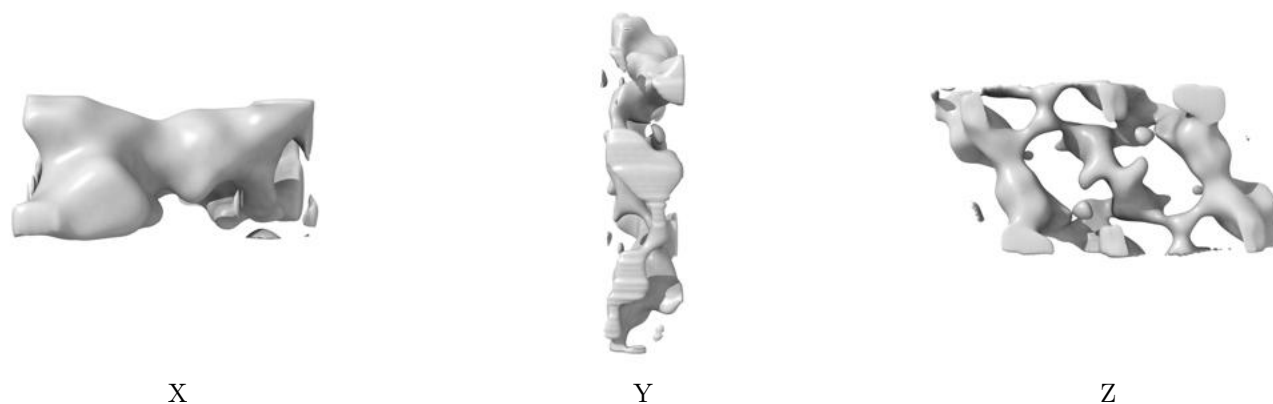
6.4.1 Primary map



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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.609. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

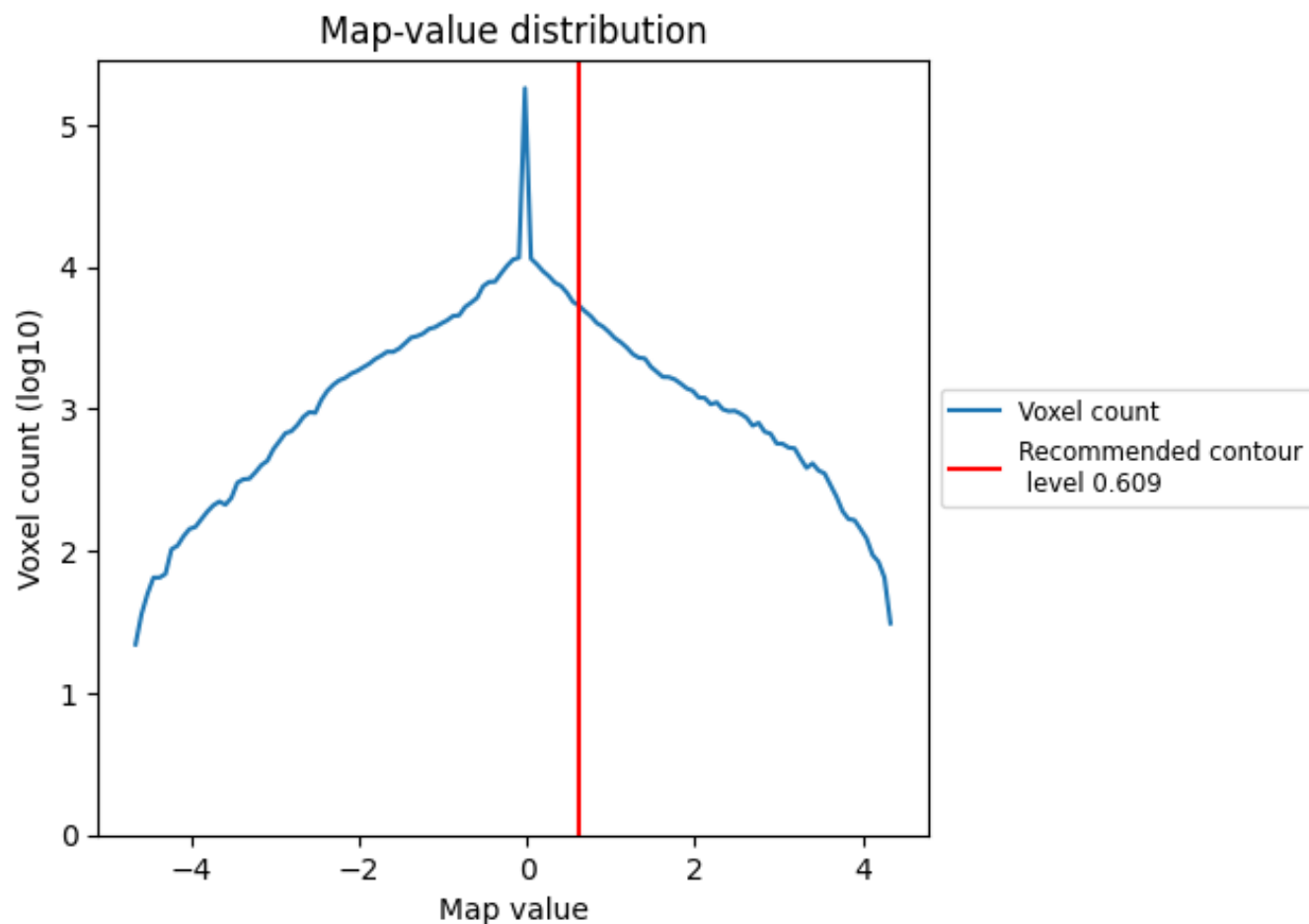
6.6 Mask visualisation

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

7 Map analysis [i](#)

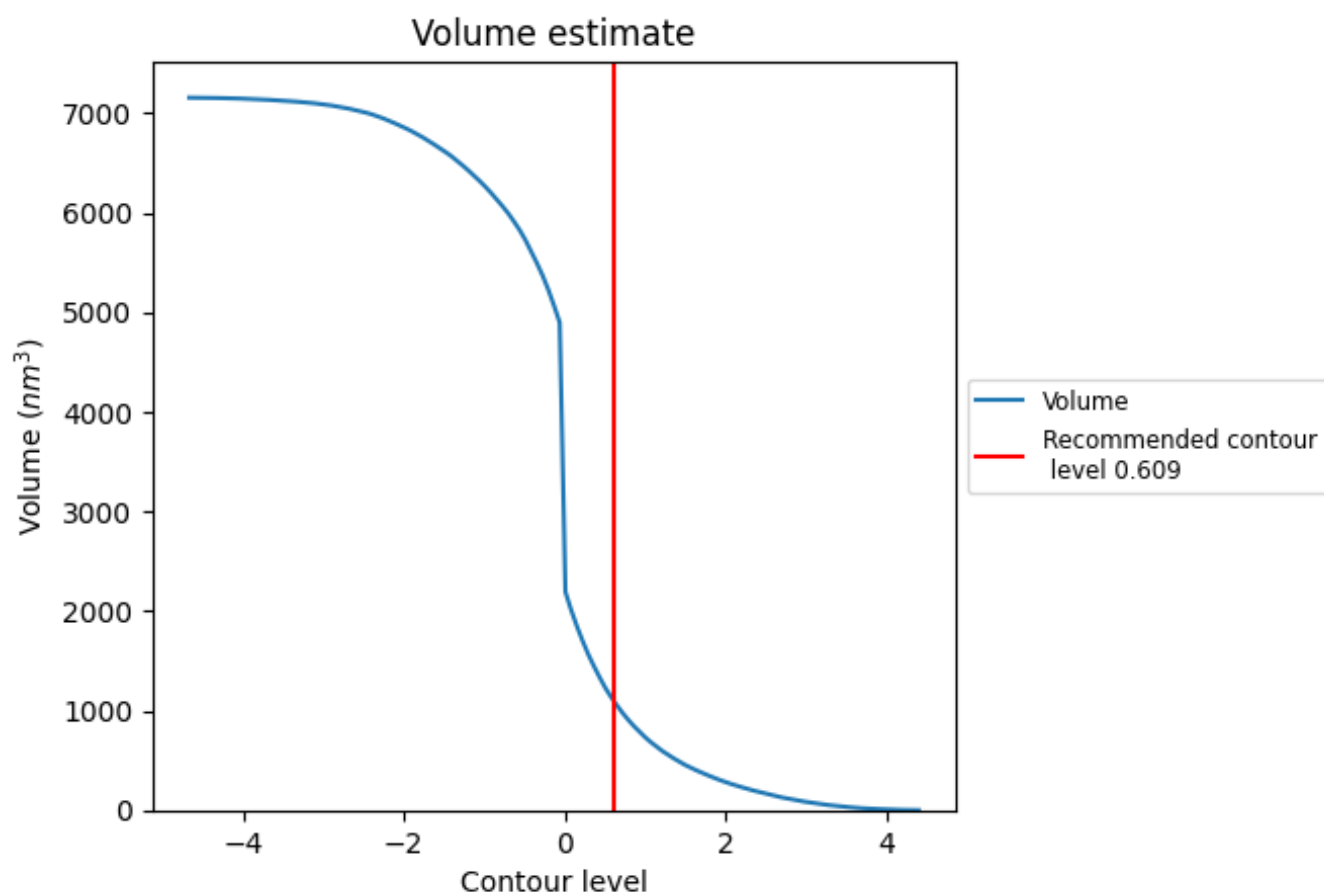
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1100 nm³; this corresponds to an approximate mass of 993 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

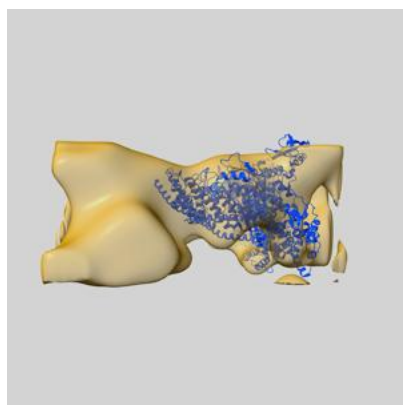
8 Fourier-Shell correlation ⓘ

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

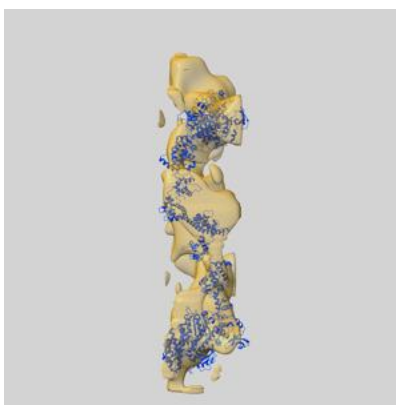
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5257 and PDB model 3J04. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

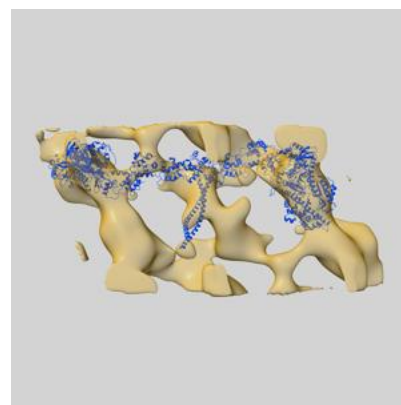
9.1 Map-model overlay [i](#)



X



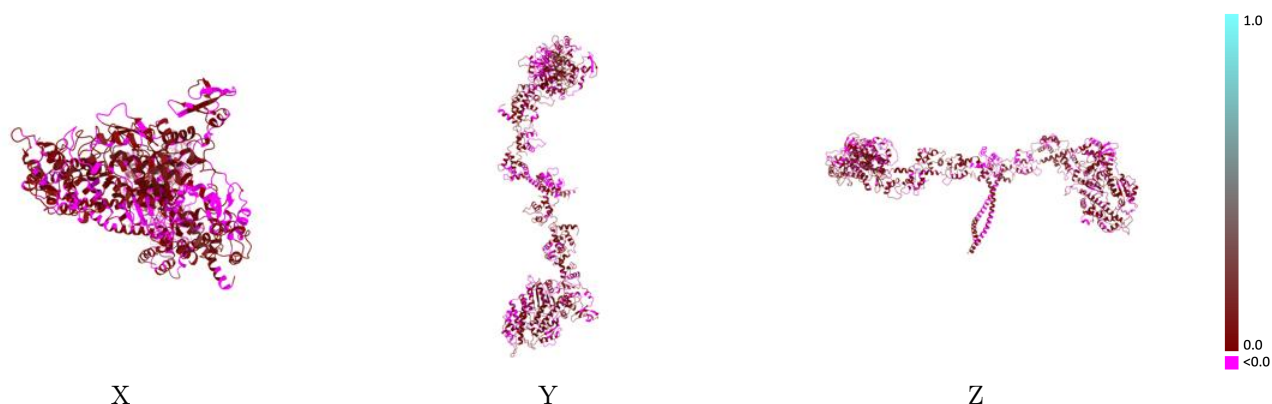
Y



Z

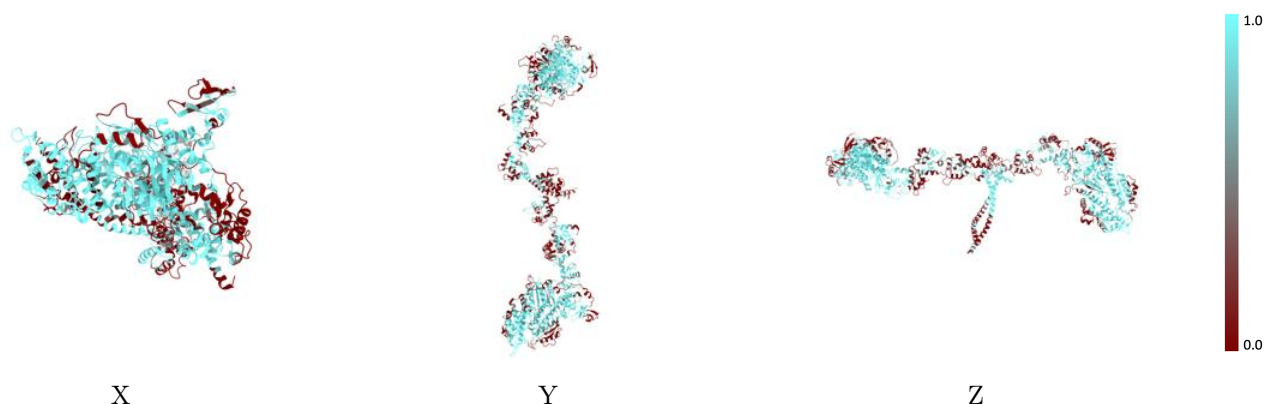
The images above show the 3D surface view of the map at the recommended contour level 0.609 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



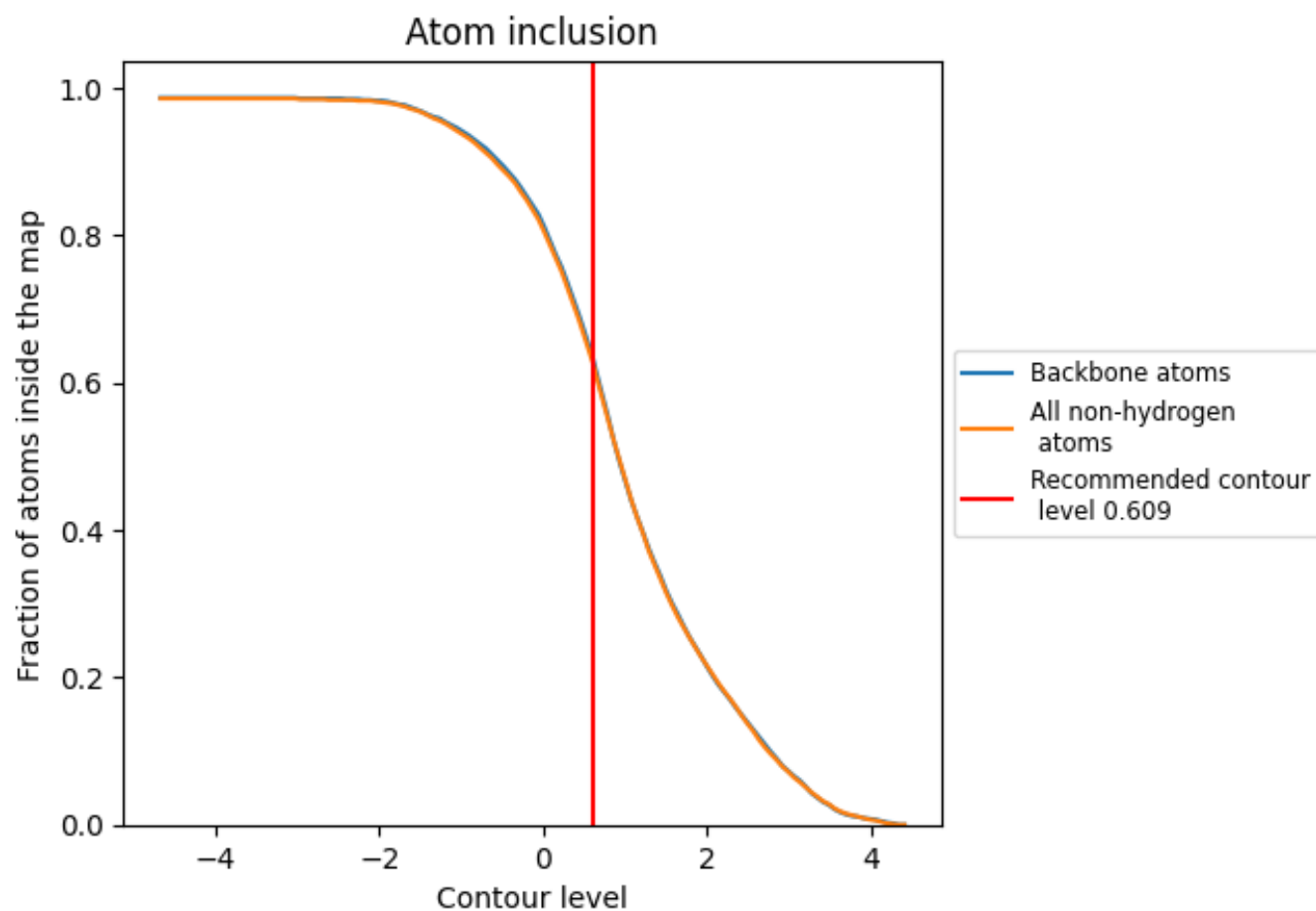
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.609).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 62% 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 (0.609) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6250	0.0330
A	0.7000	0.0360
B	0.2770	0.0070
C	0.4640	0.0460
D	0.6840	0.0320
E	0.3280	0.0040
F	0.6000	0.0560

1.0

0.0

<0.0