



Full wwPDB EM Validation Report ⓘ

Oct 13, 2025 – 12:06 PM JST

PDB ID : 8Z4T / pdb_00008z4t
EMDB ID : EMD-39769
Title : MERS-CoV S ectodomain trimer in complex with receptor DPP4-750E
Authors : Wang, X.; Wang, Z.
Deposited on : 2024-04-17
Resolution : 3.93 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:

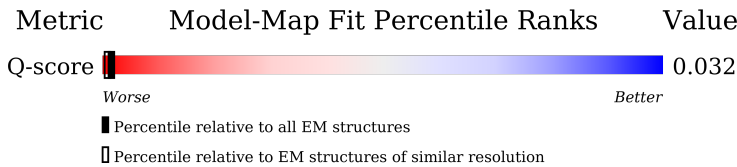
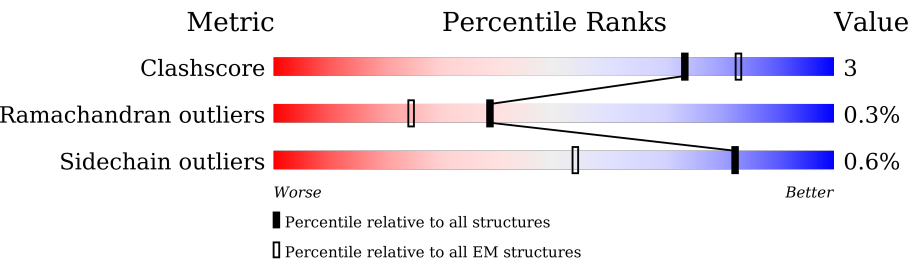
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.93 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	7811 (3.43 - 4.43)

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	1206	<div><div></div><div>71%7%22%</div></div>
1	B	1206	<div><div></div><div>84%10%5%</div></div>
1	C	1206	<div><div></div><div>83%11%5%</div></div>
2	D	728	<div><div>17%</div><div>88%12%</div></div>

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Mol	Chain	Length	Quality of chain
2	I	728	<div><div></div><div>28%</div><div>86%</div><div>13%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 36433 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	941	Total	C	N	O	S	0	0
			7249	4604	1208	1399	38		
1	B	1146	Total	C	N	O	S	0	0
			8785	5580	1457	1699	49		
1	C	1144	Total	C	N	O	S	0	0
			8790	5581	1455	1705	49		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	506	LEU	PHE	conflict	UNP K9N5Q8
A	748	SER	ARG	conflict	UNP K9N5Q8
A	751	GLY	ARG	conflict	UNP K9N5Q8
A	1020	GLN	HIS	conflict	UNP K9N5Q8
A	1060	PRO	VAL	conflict	UNP K9N5Q8
A	1061	PRO	LEU	conflict	UNP K9N5Q8
B	506	LEU	PHE	conflict	UNP K9N5Q8
B	748	SER	ARG	conflict	UNP K9N5Q8
B	751	GLY	ARG	conflict	UNP K9N5Q8
B	1020	GLN	HIS	conflict	UNP K9N5Q8
B	1060	PRO	VAL	conflict	UNP K9N5Q8
B	1061	PRO	LEU	conflict	UNP K9N5Q8
C	506	LEU	PHE	conflict	UNP K9N5Q8
C	748	SER	ARG	conflict	UNP K9N5Q8
C	751	GLY	ARG	conflict	UNP K9N5Q8
C	1020	GLN	HIS	conflict	UNP K9N5Q8
C	1060	PRO	VAL	conflict	UNP K9N5Q8
C	1061	PRO	LEU	conflict	UNP K9N5Q8

- Molecule 2 is a protein called Dipeptidyl peptidase 4 soluble form.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	728	Total	C	N	O	S	0	0
			5795	3708	956	1106	25		
2	I	728	Total	C	N	O	S	0	0
			5814	3725	957	1107	25		

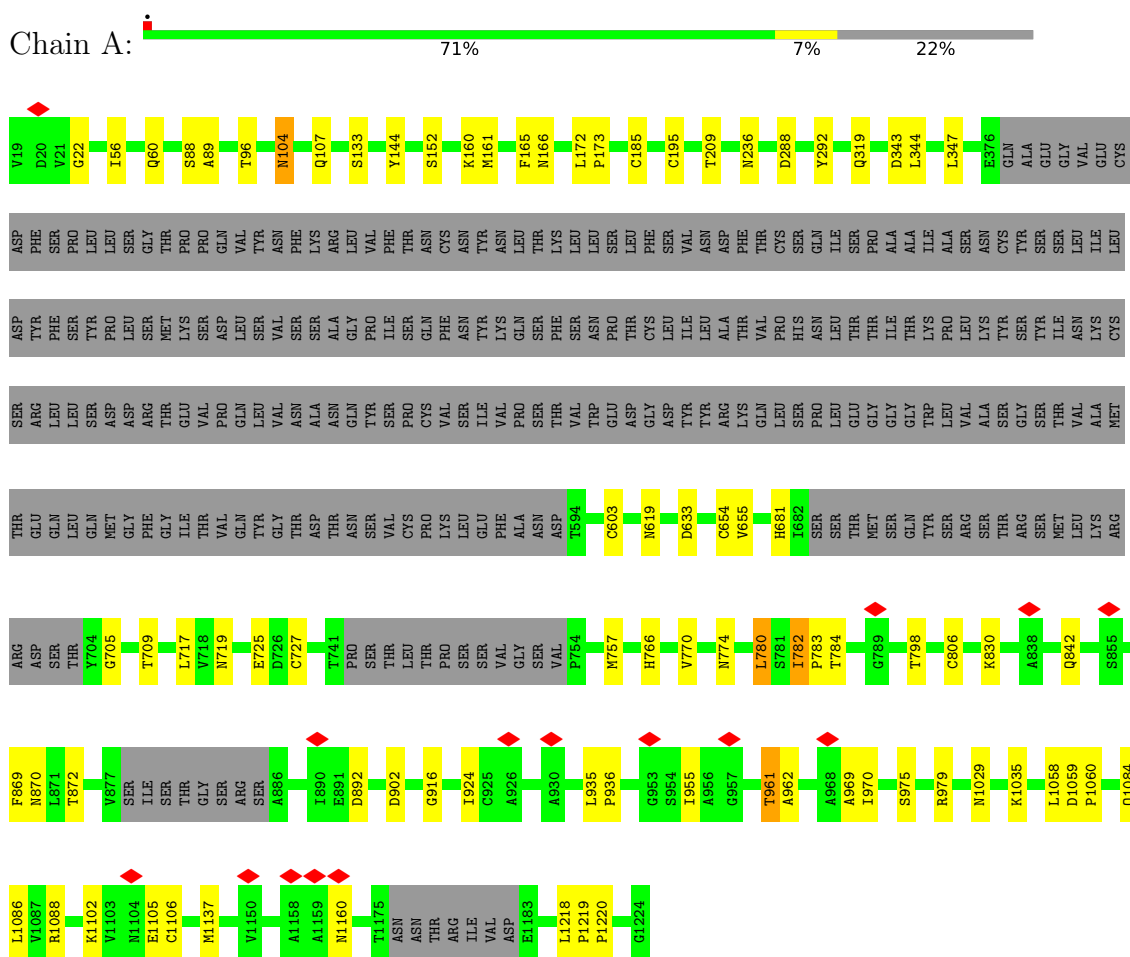
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	750	GLU	HIS	variant	UNP P27487
I	750	GLU	HIS	variant	UNP P27487

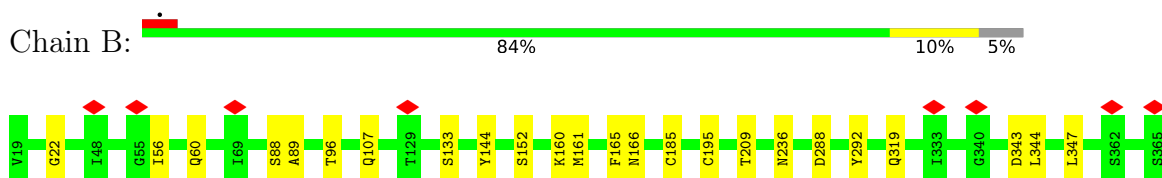
3 Residue-property plots

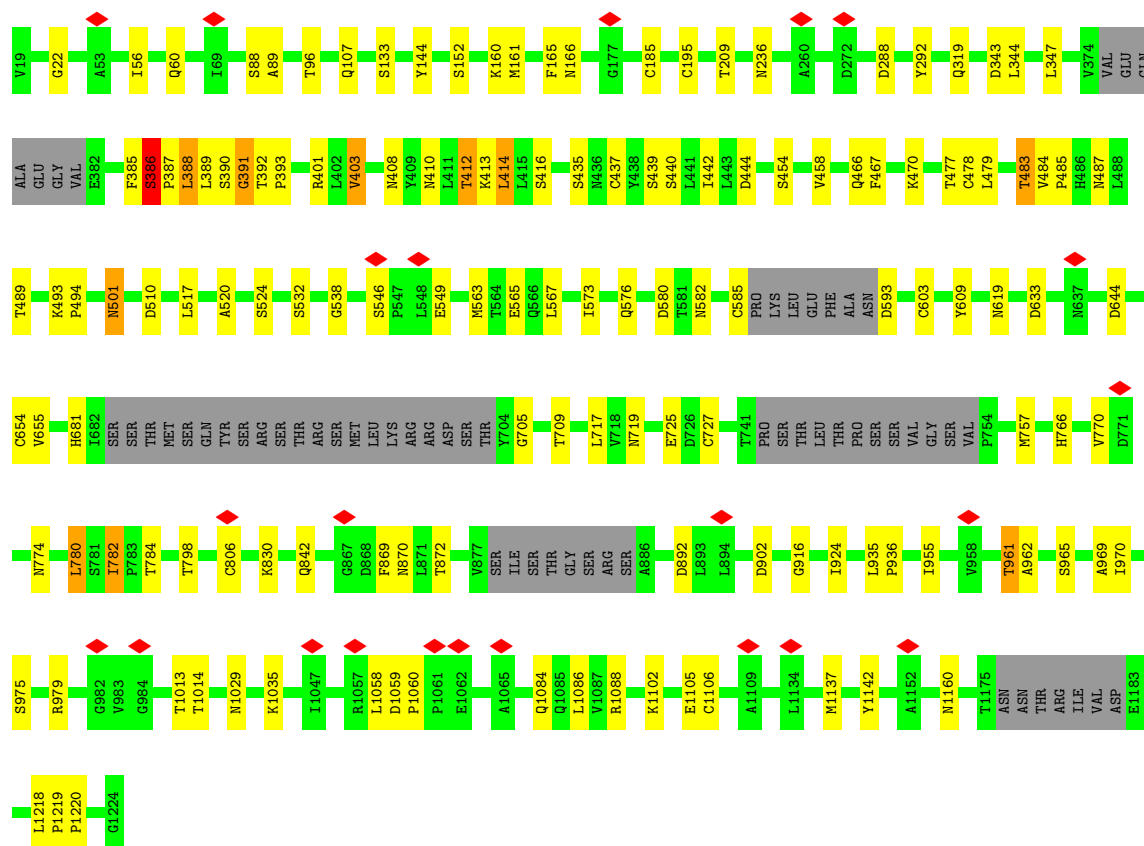
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein

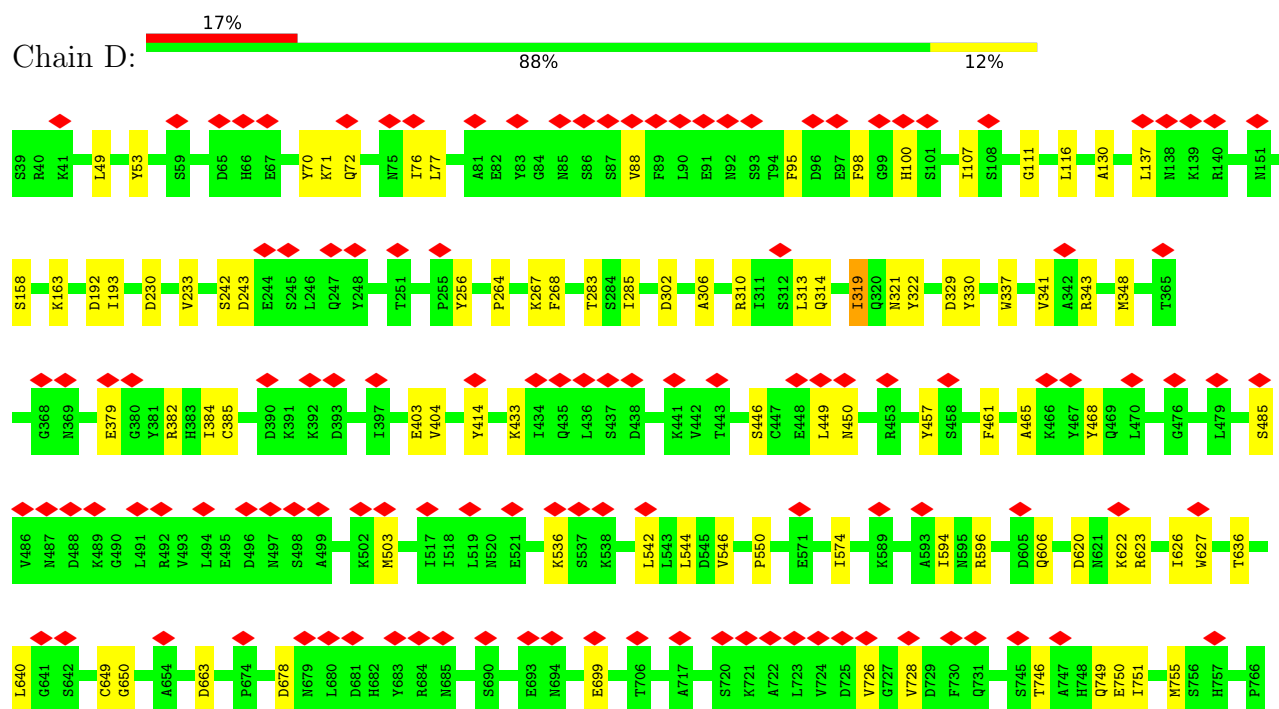


• Molecule 1: Spike glycoprotein

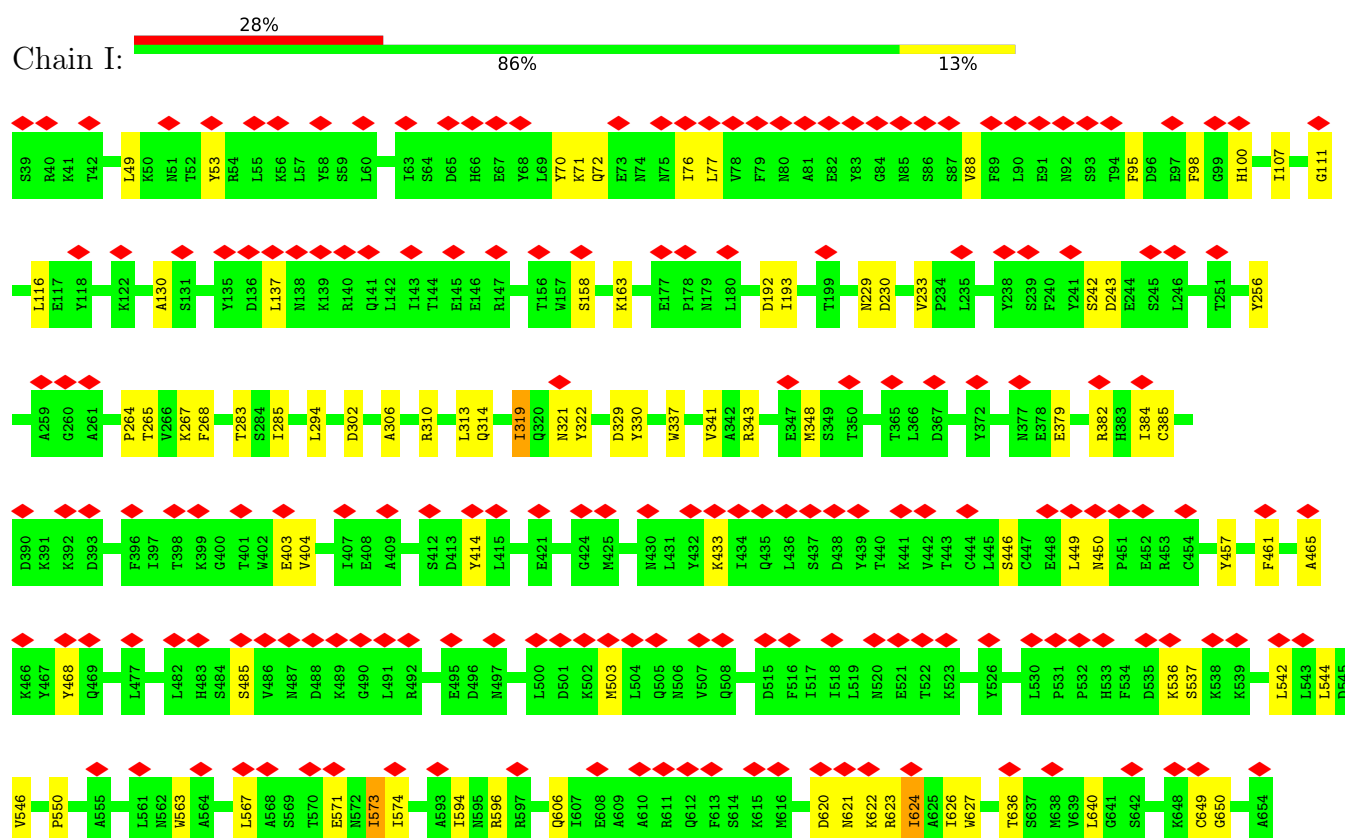




- Molecule 2: Dipeptidyl peptidase 4 soluble form



- Molecule 2: Dipeptidyl peptidase 4 soluble form





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	397140	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)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.519	Depositor
Minimum map value	-0.857	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.001	Depositor
Map size (Å)	329.80002, 329.80002, 329.80002	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	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	1.32	30/7418 (0.4%)	1.31	74/10086 (0.7%)
1	B	1.22	29/8992 (0.3%)	1.26	78/12239 (0.6%)
1	C	1.22	29/8997 (0.3%)	1.26	80/12247 (0.7%)
2	D	0.60	0/5963	0.90	6/8128 (0.1%)
2	I	0.60	0/5984	0.91	6/8157 (0.1%)
All	All	1.08	88/37354 (0.2%)	1.17	244/50857 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	870	ASN	C-O	13.50	1.41	1.24
1	C	870	ASN	C-O	13.46	1.41	1.24
1	A	870	ASN	C-O	13.45	1.41	1.24
1	B	1106	CYS	C-N	12.83	1.45	1.33
1	C	1106	CYS	C-N	12.63	1.45	1.33
1	A	1106	CYS	C-N	12.60	1.45	1.33
1	C	1106	CYS	C-O	-10.45	1.11	1.23
1	B	1106	CYS	C-O	-10.43	1.11	1.23
1	B	774	ASN	C-O	10.41	1.36	1.23
1	C	774	ASN	C-O	10.40	1.36	1.23
1	A	774	ASN	C-O	10.39	1.36	1.23
1	A	1106	CYS	C-O	-10.36	1.11	1.23
1	C	166	ASN	C-O	-10.35	1.10	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	ASN	C-O	-10.25	1.11	1.24
1	A	166	ASN	C-O	-10.16	1.11	1.24
1	C	1106	CYS	N-CA	-9.43	1.34	1.46
1	B	1106	CYS	N-CA	-9.35	1.34	1.46
1	A	1106	CYS	N-CA	-9.31	1.34	1.46
1	B	870	ASN	C-N	-9.04	1.22	1.33
1	C	870	ASN	C-N	-8.98	1.22	1.33
1	A	870	ASN	C-N	-8.98	1.22	1.33
1	A	681	HIS	CB-CG	-8.72	1.38	1.50
1	C	681	HIS	CB-CG	-8.70	1.38	1.50
1	B	681	HIS	CB-CG	-8.67	1.38	1.50
1	B	603	CYS	C-O	-8.27	1.13	1.24
1	A	603	CYS	C-O	-8.23	1.14	1.24
1	C	603	CYS	C-O	-8.16	1.14	1.24
1	A	655	VAL	CA-C	-7.87	1.43	1.52
1	C	655	VAL	CA-C	-7.79	1.43	1.52
1	B	655	VAL	CA-C	-7.64	1.43	1.52
1	A	185	CYS	C-O	-7.49	1.15	1.23
1	C	185	CYS	C-O	-7.47	1.15	1.23
1	B	185	CYS	C-O	-7.40	1.15	1.23
1	A	727	CYS	C-O	-7.37	1.15	1.24
1	C	1086	LEU	CB-CG	7.35	1.68	1.53
1	A	1086	LEU	CB-CG	7.34	1.68	1.53
1	C	727	CYS	C-O	-7.33	1.15	1.24
1	B	1086	LEU	CB-CG	7.32	1.68	1.53
1	C	870	ASN	CA-CB	-7.29	1.41	1.53
1	B	727	CYS	C-O	-7.27	1.15	1.24
1	B	870	ASN	CA-CB	-7.18	1.41	1.53
1	A	870	ASN	CA-CB	-7.17	1.41	1.53
1	A	806	CYS	C-O	6.84	1.32	1.24
1	B	806	CYS	C-O	6.81	1.32	1.24
1	C	806	CYS	C-O	6.75	1.32	1.24
1	A	236	ASN	CA-C	-6.67	1.44	1.53
1	C	619	ASN	C-O	6.58	1.31	1.24
1	B	236	ASN	CA-C	-6.54	1.44	1.53
1	C	236	ASN	CA-C	-6.53	1.44	1.53
1	B	619	ASN	C-O	6.53	1.31	1.24
1	A	619	ASN	C-O	6.52	1.31	1.24
1	A	719	ASN	C-O	-6.47	1.16	1.23
1	C	719	ASN	C-O	-6.46	1.16	1.23
1	B	719	ASN	C-O	-6.44	1.16	1.23
1	A	236	ASN	C-O	6.39	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	236	ASN	C-O	6.36	1.31	1.23
1	C	236	ASN	C-O	6.24	1.31	1.23
1	C	1137	MET	CB-CG	-6.19	1.33	1.52
1	A	1137	MET	CB-CG	-6.16	1.33	1.52
1	B	1137	MET	CB-CG	-6.12	1.34	1.52
1	B	774	ASN	CA-C	-6.10	1.46	1.53
1	A	774	ASN	CA-C	-6.04	1.46	1.53
1	C	774	ASN	CA-C	-6.02	1.46	1.53
1	C	869	PHE	C-N	-5.83	1.25	1.33
1	B	869	PHE	C-N	-5.74	1.25	1.33
1	B	166	ASN	CA-CB	-5.72	1.43	1.53
1	A	869	PHE	C-N	-5.71	1.25	1.33
1	C	166	ASN	CA-CB	-5.64	1.44	1.53
1	A	166	ASN	CA-CB	-5.64	1.44	1.53
1	C	774	ASN	CA-CB	-5.64	1.46	1.52
1	A	774	ASN	CA-CB	-5.57	1.46	1.52
1	C	774	ASN	C-N	-5.46	1.26	1.33
1	A	774	ASN	C-N	-5.41	1.26	1.33
1	B	774	ASN	CA-CB	-5.40	1.46	1.52
1	B	774	ASN	C-N	-5.39	1.26	1.33
1	B	806	CYS	C-N	-5.35	1.26	1.33
1	A	806	CYS	C-N	-5.30	1.26	1.33
1	C	806	CYS	C-N	-5.28	1.27	1.33
1	B	780	LEU	CG-CD2	-5.26	1.35	1.52
1	C	780	LEU	CG-CD2	-5.24	1.35	1.52
1	A	780	LEU	CG-CD2	-5.23	1.35	1.52
1	B	1218	LEU	CG-CD2	-5.16	1.35	1.52
1	B	292	TYR	CB-CG	-5.16	1.40	1.51
1	A	104	ASN	C-O	5.15	1.29	1.23
1	C	1218	LEU	CG-CD2	-5.14	1.35	1.52
1	C	292	TYR	CB-CG	-5.13	1.40	1.51
1	A	292	TYR	CB-CG	-5.12	1.40	1.51
1	A	1218	LEU	CG-CD2	-5.11	1.35	1.52

All (244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1106	CYS	CA-C-O	11.40	134.57	120.31
1	A	1106	CYS	CA-C-O	11.33	134.48	120.31
1	C	1106	CYS	CA-C-O	11.32	134.46	120.31
1	C	725	GLU	N-CA-C	-9.42	102.36	114.04
1	A	725	GLU	N-CA-C	-9.31	102.49	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1218	LEU	CD1-CG-CD2	9.31	131.28	110.80
1	B	725	GLU	N-CA-C	-9.30	102.50	114.04
1	A	1218	LEU	CD1-CG-CD2	9.29	131.24	110.80
1	C	1218	LEU	CD1-CG-CD2	9.28	131.21	110.80
1	A	1160	ASN	CA-C-N	9.10	128.74	119.82
1	A	1160	ASN	C-N-CA	9.10	128.74	119.82
1	C	1160	ASN	CA-C-N	9.04	128.69	119.82
1	C	1160	ASN	C-N-CA	9.04	128.69	119.82
1	B	1160	ASN	CA-C-N	9.03	128.67	119.82
1	B	1160	ASN	C-N-CA	9.03	128.67	119.82
1	A	60	GLN	N-CA-C	8.98	122.74	111.69
1	C	60	GLN	N-CA-C	8.95	122.70	111.69
1	B	60	GLN	N-CA-C	8.89	122.63	111.69
1	C	654	CYS	N-CA-C	-8.46	97.50	110.10
1	B	654	CYS	N-CA-C	-8.42	97.33	109.96
1	A	654	CYS	N-CA-C	-8.30	97.51	109.96
1	A	780	LEU	CD1-CG-CD2	8.28	129.01	110.80
1	C	780	LEU	CD1-CG-CD2	8.27	128.99	110.80
1	B	780	LEU	CD1-CG-CD2	8.26	128.97	110.80
1	B	936	PRO	CA-C-N	8.00	127.95	120.03
1	B	936	PRO	C-N-CA	8.00	127.95	120.03
1	A	936	PRO	CA-C-N	7.99	127.94	120.03
1	A	936	PRO	C-N-CA	7.99	127.94	120.03
1	C	936	PRO	CA-C-N	7.93	127.89	120.03
1	C	936	PRO	C-N-CA	7.93	127.89	120.03
1	A	1060	PRO	N-CA-C	7.11	119.37	110.70
1	C	1060	PRO	N-CA-C	7.10	119.36	110.70
1	B	709	THR	CA-C-N	7.06	126.76	119.56
1	B	709	THR	C-N-CA	7.06	126.76	119.56
1	B	1060	PRO	N-CA-C	7.06	119.31	110.70
1	A	709	THR	CA-C-N	7.00	126.70	119.56
1	A	709	THR	C-N-CA	7.00	126.70	119.56
1	C	709	THR	CA-C-N	6.94	126.64	119.56
1	C	709	THR	C-N-CA	6.94	126.64	119.56
1	C	935	LEU	CA-C-N	6.90	124.63	119.66
1	C	935	LEU	C-N-CA	6.90	124.63	119.66
1	B	935	LEU	CA-C-N	6.88	124.62	119.66
1	B	935	LEU	C-N-CA	6.88	124.62	119.66
1	A	935	LEU	CA-C-N	6.81	124.56	119.66
1	A	935	LEU	C-N-CA	6.81	124.56	119.66
1	C	96	THR	CA-C-N	6.77	126.75	119.78
1	C	96	THR	C-N-CA	6.77	126.75	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	THR	CA-C-N	6.72	126.70	119.78
1	B	96	THR	C-N-CA	6.72	126.70	119.78
1	C	1106	CYS	CA-C-N	-6.71	114.43	122.35
1	C	1106	CYS	C-N-CA	-6.71	114.43	122.35
1	B	1106	CYS	CA-C-N	-6.71	114.44	122.35
1	B	1106	CYS	C-N-CA	-6.71	114.44	122.35
1	A	96	THR	CA-C-N	6.69	126.67	119.78
1	A	96	THR	C-N-CA	6.69	126.67	119.78
1	A	1106	CYS	CA-C-N	-6.65	114.51	122.35
1	A	1106	CYS	C-N-CA	-6.65	114.51	122.35
1	A	56	ILE	N-CA-C	6.62	118.11	108.58
1	C	1059	ASP	CA-C-N	6.61	127.19	120.38
1	C	1059	ASP	C-N-CA	6.61	127.19	120.38
1	A	133	SER	CA-C-N	6.59	127.11	119.47
1	A	133	SER	C-N-CA	6.59	127.11	119.47
1	B	133	SER	CA-C-N	6.59	127.11	119.47
1	B	133	SER	C-N-CA	6.59	127.11	119.47
1	A	22	GLY	CA-C-N	6.58	126.54	120.03
1	A	22	GLY	C-N-CA	6.58	126.54	120.03
1	B	56	ILE	N-CA-C	6.57	118.04	108.58
1	A	1059	ASP	CA-C-N	6.57	127.14	120.38
1	A	1059	ASP	C-N-CA	6.57	127.14	120.38
1	C	56	ILE	N-CA-C	6.56	118.03	108.58
1	B	1059	ASP	CA-C-N	6.56	127.14	120.38
1	B	1059	ASP	C-N-CA	6.56	127.14	120.38
1	B	870	ASN	CA-C-O	-6.56	111.13	120.51
1	C	133	SER	CA-C-N	6.54	127.06	119.47
1	C	133	SER	C-N-CA	6.54	127.06	119.47
1	C	22	GLY	CA-C-N	6.53	126.50	120.03
1	C	22	GLY	C-N-CA	6.53	126.50	120.03
1	B	22	GLY	CA-C-N	6.51	126.47	120.03
1	B	22	GLY	C-N-CA	6.51	126.47	120.03
1	A	870	ASN	CA-C-O	-6.50	111.21	120.51
1	C	386	SER	CA-C-N	6.50	127.97	119.84
1	C	386	SER	C-N-CA	6.50	127.97	119.84
1	C	870	ASN	CA-C-O	-6.49	111.22	120.51
1	B	386	SER	CA-C-N	6.49	127.95	119.84
1	B	386	SER	C-N-CA	6.49	127.95	119.84
1	C	1220	PRO	N-CA-C	6.48	118.61	110.70
1	A	1220	PRO	N-CA-C	6.46	118.58	110.70
1	B	1220	PRO	N-CA-C	6.44	118.55	110.70
1	A	144	TYR	CA-C-N	6.39	126.30	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	TYR	C-N-CA	6.39	126.30	119.85
1	C	144	TYR	CA-C-N	6.36	126.27	119.85
1	C	144	TYR	C-N-CA	6.36	126.27	119.85
1	B	144	TYR	CA-C-N	6.34	126.26	119.85
1	B	144	TYR	C-N-CA	6.34	126.26	119.85
1	C	766	HIS	CA-C-N	6.29	126.26	120.03
1	C	766	HIS	C-N-CA	6.29	126.26	120.03
2	I	450	ASN	CA-C-N	6.27	125.76	119.24
2	I	450	ASN	C-N-CA	6.27	125.76	119.24
2	D	450	ASN	CA-C-N	6.26	125.75	119.24
2	D	450	ASN	C-N-CA	6.26	125.75	119.24
1	B	766	HIS	CA-C-N	6.24	126.21	120.03
1	B	766	HIS	C-N-CA	6.24	126.21	120.03
1	A	766	HIS	CA-C-N	6.13	126.10	120.03
1	A	766	HIS	C-N-CA	6.13	126.10	120.03
1	B	924	ILE	N-CA-C	-6.08	105.13	111.58
1	A	1106	CYS	N-CA-CB	6.07	119.60	110.19
1	C	166	ASN	CA-C-N	-6.07	112.82	121.50
1	C	166	ASN	C-N-CA	-6.07	112.82	121.50
1	C	1106	CYS	N-CA-CB	6.06	119.58	110.19
1	B	1106	CYS	N-CA-CB	6.04	119.55	110.19
1	C	924	ILE	N-CA-C	-6.03	105.19	111.58
1	C	782	ILE	CA-C-N	6.02	125.98	119.78
1	C	782	ILE	C-N-CA	6.02	125.98	119.78
1	B	166	ASN	CA-C-N	-6.02	112.89	121.50
1	B	166	ASN	C-N-CA	-6.02	112.89	121.50
1	A	924	ILE	N-CA-C	-6.02	105.20	111.58
1	B	916	GLY	CA-C-N	5.98	125.92	119.76
1	B	916	GLY	C-N-CA	5.98	125.92	119.76
1	A	782	ILE	CA-C-N	5.98	125.94	119.78
1	A	782	ILE	C-N-CA	5.98	125.94	119.78
1	A	166	ASN	CA-C-N	-5.97	112.96	121.50
1	A	166	ASN	C-N-CA	-5.97	112.96	121.50
1	B	782	ILE	CA-C-N	5.97	125.93	119.78
1	B	782	ILE	C-N-CA	5.97	125.93	119.78
1	C	902	ASP	CA-C-N	5.96	125.58	119.56
1	C	902	ASP	C-N-CA	5.96	125.58	119.56
1	A	902	ASP	CA-C-N	5.95	125.57	119.56
1	A	902	ASP	C-N-CA	5.95	125.57	119.56
1	C	195	CYS	CA-C-N	5.94	125.62	119.56
1	C	195	CYS	C-N-CA	5.94	125.62	119.56
1	C	916	GLY	CA-C-N	5.92	125.86	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	916	GLY	C-N-CA	5.92	125.86	119.76
1	B	195	CYS	CA-C-N	5.91	125.59	119.56
1	B	195	CYS	C-N-CA	5.91	125.59	119.56
1	A	195	CYS	CA-C-N	5.90	125.58	119.56
1	A	195	CYS	C-N-CA	5.90	125.58	119.56
1	A	288	ASP	N-CA-C	-5.88	102.77	110.53
1	A	916	GLY	CA-C-N	5.87	125.81	119.76
1	A	916	GLY	C-N-CA	5.87	125.81	119.76
1	B	288	ASP	N-CA-C	-5.87	102.78	110.53
1	C	970	ILE	CA-C-N	5.85	125.81	119.78
1	C	970	ILE	C-N-CA	5.85	125.81	119.78
1	C	288	ASP	N-CA-C	-5.85	102.81	110.53
2	I	233	VAL	CA-C-N	5.84	125.85	119.89
2	I	233	VAL	C-N-CA	5.84	125.85	119.89
1	B	902	ASP	CA-C-N	5.83	125.45	119.56
1	B	902	ASP	C-N-CA	5.83	125.45	119.56
1	A	872	THR	CA-C-N	5.82	128.08	120.28
1	A	872	THR	C-N-CA	5.82	128.08	120.28
1	B	1106	CYS	N-CA-C	5.82	120.42	112.04
1	C	412	THR	N-CA-C	-5.80	104.96	111.28
1	A	970	ILE	CA-C-N	5.80	125.75	119.78
1	A	970	ILE	C-N-CA	5.80	125.75	119.78
1	B	412	THR	N-CA-C	-5.80	104.96	111.28
2	D	233	VAL	CA-C-N	5.80	125.80	119.89
2	D	233	VAL	C-N-CA	5.80	125.80	119.89
1	C	872	THR	CA-C-N	5.79	128.03	120.28
1	C	872	THR	C-N-CA	5.79	128.03	120.28
1	A	1106	CYS	N-CA-C	5.78	120.37	112.04
1	C	1106	CYS	N-CA-C	5.77	120.35	112.04
1	A	1218	LEU	CA-C-N	5.77	123.81	119.66
1	A	1218	LEU	C-N-CA	5.77	123.81	119.66
1	B	970	ILE	CA-C-N	5.76	125.71	119.78
1	B	970	ILE	C-N-CA	5.76	125.71	119.78
1	B	872	THR	CA-C-N	5.75	127.98	120.28
1	B	872	THR	C-N-CA	5.75	127.98	120.28
1	C	209	THR	CA-C-N	5.75	125.87	119.32
1	C	209	THR	C-N-CA	5.75	125.87	119.32
1	B	1218	LEU	CA-C-N	5.74	123.80	119.66
1	B	1218	LEU	C-N-CA	5.74	123.80	119.66
1	A	955	ILE	N-CA-C	5.74	115.93	110.42
1	C	705	GLY	CA-C-N	5.72	125.48	119.76
1	C	705	GLY	C-N-CA	5.72	125.48	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1219	PRO	CA-C-N	5.71	126.26	120.38
1	C	1219	PRO	C-N-CA	5.71	126.26	120.38
1	B	1219	PRO	CA-C-N	5.69	126.24	120.38
1	B	1219	PRO	C-N-CA	5.69	126.24	120.38
1	A	1219	PRO	CA-C-N	5.68	126.23	120.38
1	A	1219	PRO	C-N-CA	5.68	126.23	120.38
1	C	955	ILE	N-CA-C	5.68	115.88	110.42
1	B	955	ILE	N-CA-C	5.68	115.88	110.42
1	A	705	GLY	CA-C-N	5.67	125.44	119.76
1	A	705	GLY	C-N-CA	5.67	125.44	119.76
1	B	1105	GLU	CA-C-N	5.67	134.05	121.80
1	B	1105	GLU	C-N-CA	5.67	134.05	121.80
1	C	1105	GLU	CA-C-N	5.67	134.05	121.80
1	C	1105	GLU	C-N-CA	5.67	134.05	121.80
1	A	209	THR	CA-C-N	5.67	125.78	119.32
1	A	209	THR	C-N-CA	5.67	125.78	119.32
1	C	1218	LEU	CA-C-N	5.67	123.74	119.66
1	C	1218	LEU	C-N-CA	5.67	123.74	119.66
1	A	1105	GLU	CA-C-N	5.66	134.03	121.80
1	A	1105	GLU	C-N-CA	5.66	134.03	121.80
1	B	705	GLY	CA-C-N	5.64	125.40	119.76
1	B	705	GLY	C-N-CA	5.64	125.40	119.76
1	B	209	THR	CA-C-N	5.64	125.75	119.32
1	B	209	THR	C-N-CA	5.64	125.75	119.32
1	B	1029	ASN	CA-CB-CG	5.58	118.18	112.60
1	C	1029	ASN	CA-CB-CG	5.56	118.16	112.60
1	B	892	ASP	CA-CB-CG	5.56	118.16	112.60
2	D	130	ALA	N-CA-C	5.56	116.41	108.74
2	I	130	ALA	N-CA-C	5.55	116.41	108.74
1	A	1029	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	892	ASP	CA-CB-CG	5.48	118.08	112.60
1	C	892	ASP	CA-CB-CG	5.45	118.05	112.60
2	I	319	ILE	CB-CA-C	-5.44	106.03	111.80
2	D	319	ILE	CB-CA-C	-5.43	106.05	111.80
1	A	319	GLN	CA-C-N	5.34	126.52	119.84
1	A	319	GLN	C-N-CA	5.34	126.52	119.84
1	C	961	THR	N-CA-C	5.31	115.30	108.34
1	B	774	ASN	CA-C-O	-5.29	115.34	122.44
1	C	319	GLN	CA-C-N	5.29	126.46	119.84
1	C	319	GLN	C-N-CA	5.29	126.46	119.84
1	A	784	THR	N-CA-C	-5.29	106.76	114.12
1	C	774	ASN	CA-C-O	-5.29	115.35	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	784	THR	N-CA-C	-5.29	106.77	114.12
1	B	319	GLN	CA-C-N	5.29	126.45	119.84
1	B	319	GLN	C-N-CA	5.29	126.45	119.84
1	A	774	ASN	CA-C-O	-5.24	115.41	122.44
1	B	961	THR	N-CA-C	5.24	115.21	108.34
1	A	961	THR	N-CA-C	5.24	115.20	108.34
1	C	784	THR	N-CA-C	-5.22	106.86	114.12
1	A	344	LEU	CB-CG-CD2	5.20	126.30	110.70
1	B	344	LEU	CB-CG-CD2	5.18	126.23	110.70
1	C	1102	LYS	CA-C-N	-5.17	114.05	120.56
1	C	1102	LYS	C-N-CA	-5.17	114.05	120.56
1	A	725	GLU	CA-C-O	5.16	125.51	119.06
1	A	1102	LYS	CA-C-N	-5.16	114.06	120.56
1	A	1102	LYS	C-N-CA	-5.16	114.06	120.56
1	C	344	LEU	CB-CG-CD2	5.16	126.19	110.70
1	C	347	LEU	CD1-CG-CD2	-5.16	99.46	110.80
1	B	1102	LYS	CA-C-N	-5.13	114.09	120.56
1	B	1102	LYS	C-N-CA	-5.13	114.09	120.56
1	B	725	GLU	CA-C-O	5.12	125.47	119.06
1	A	347	LEU	CD1-CG-CD2	-5.12	99.54	110.80
1	B	347	LEU	CD1-CG-CD2	-5.11	99.55	110.80
1	C	1142	TYR	CA-C-N	5.07	125.05	120.03
1	C	1142	TYR	C-N-CA	5.07	125.05	120.03
1	C	725	GLU	CA-C-O	5.07	125.39	119.06
1	C	965	SER	N-CA-C	5.05	119.49	113.23
1	A	1058	LEU	N-CA-C	5.04	117.78	109.72
1	B	965	SER	N-CA-C	5.01	119.44	113.23
1	B	1058	LEU	N-CA-C	5.01	117.73	109.72
1	C	1058	LEU	N-CA-C	5.00	117.72	109.72

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	386	SER	Peptide
1	C	386	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7249	0	6953	24	0
1	B	8785	0	8367	48	0
1	C	8790	0	8410	55	0
2	D	5795	0	5310	48	0
2	I	5814	0	5348	52	0
All	All	36433	0	34388	216	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 (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLN:HE21	1:B:160:LYS:HB3	1.42	0.84
1:A:107:GLN:HE21	1:A:160:LYS:HB3	1.42	0.83
1:C:107:GLN:HE21	1:C:160:LYS:HB3	1.42	0.83
2:D:596:ARG:NH2	2:D:678:ASP:OD1	2.12	0.83
2:I:596:ARG:NH2	2:I:678:ASP:OD1	2.12	0.82
2:I:621:ASN:HA	2:I:624:ILE:HD11	1.69	0.74
1:C:107:GLN:NE2	1:C:160:LYS:HB3	2.06	0.71
2:I:746:THR:O	2:I:750:GLU:HG3	1.91	0.70
1:B:107:GLN:NE2	1:B:160:LYS:HB3	2.06	0.70
1:A:107:GLN:NE2	1:A:160:LYS:HB3	2.06	0.69
2:D:640:LEU:HD11	2:D:650:GLY:HA3	1.74	0.69
2:I:329:ASP:OD1	2:I:343:ARG:NH1	2.25	0.69
2:D:329:ASP:OD1	2:D:343:ARG:NH1	2.25	0.68
2:I:640:LEU:HD11	2:I:650:GLY:HA3	1.74	0.68
2:D:746:THR:O	2:D:750:GLU:HG3	1.95	0.67
2:D:242:SER:OG	2:D:243:ASP:N	2.27	0.67
2:I:242:SER:OG	2:I:243:ASP:N	2.27	0.65
2:D:302:ASP:HB3	2:D:314:GLN:HB2	1.78	0.65
1:B:493:LYS:NZ	1:B:565:GLU:O	2.31	0.64
1:C:493:LYS:NZ	1:C:565:GLU:O	2.31	0.64
2:I:302:ASP:HB3	2:I:314:GLN:HB2	1.78	0.64
1:B:538:GLY:HA3	2:D:267:LYS:HD3	1.82	0.61
1:C:538:GLY:HA3	2:I:267:LYS:HD3	1.81	0.60
2:I:751:ILE:HG12	2:I:755:MET:HE2	1.84	0.60
1:B:107:GLN:NE2	1:B:160:LYS:HD3	2.17	0.60
2:D:751:ILE:HG12	2:D:755:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:384:ILE:HG13	2:I:404:VAL:HG21	1.84	0.59
1:A:107:GLN:NE2	1:A:160:LYS:HD3	2.17	0.59
1:C:343:ASP:N	1:C:343:ASP:OD1	2.35	0.59
2:D:384:ILE:HG13	2:D:404:VAL:HG21	1.84	0.59
1:C:107:GLN:NE2	1:C:160:LYS:HD3	2.17	0.58
1:A:107:GLN:HE22	1:A:160:LYS:HD3	1.68	0.58
1:B:410:ASN:HB3	1:B:413:LYS:HB2	1.85	0.58
1:C:410:ASN:HB3	1:C:413:LYS:HB2	1.85	0.58
1:C:107:GLN:HE22	1:C:160:LYS:HD3	1.69	0.57
1:A:830:LYS:HD2	1:C:1035:LYS:HE3	1.87	0.57
2:I:158:SER:HB3	2:I:163:LYS:HB2	1.86	0.57
1:B:107:GLN:HE22	1:B:160:LYS:HD3	1.68	0.57
1:C:390:SER:OG	1:C:391:GLY:N	2.38	0.57
1:A:1035:LYS:HE3	1:B:830:LYS:HD2	1.87	0.56
1:A:343:ASP:N	1:A:343:ASP:OD1	2.35	0.56
1:B:1035:LYS:HE3	1:C:830:LYS:HD2	1.87	0.56
2:D:158:SER:HB3	2:D:163:LYS:HB2	1.86	0.56
1:C:386:SER:OG	1:C:388:LEU:HB3	2.06	0.56
2:D:465:ALA:O	2:D:485:SER:OG	2.23	0.56
2:I:465:ALA:O	2:I:485:SER:OG	2.23	0.55
1:B:343:ASP:OD1	1:B:343:ASP:N	2.35	0.55
1:B:798:THR:HA	1:B:842:GLN:OE1	2.07	0.55
2:D:49:LEU:HD22	2:D:749:GLN:HA	1.89	0.55
2:I:310:ARG:NH1	2:I:329:ASP:OD2	2.40	0.55
2:I:49:LEU:HD22	2:I:749:GLN:HA	1.89	0.54
2:D:310:ARG:NH1	2:D:329:ASP:OD2	2.40	0.54
1:C:388:LEU:HD23	1:C:389:LEU:HD13	1.90	0.54
1:A:798:THR:HA	1:A:842:GLN:OE1	2.07	0.54
1:C:798:THR:HA	1:C:842:GLN:OE1	2.07	0.54
2:D:620:ASP:OD2	2:D:623:ARG:HD3	2.08	0.53
2:I:620:ASP:OD2	2:I:623:ARG:HD3	2.08	0.53
1:B:390:SER:OG	1:B:391:GLY:N	2.38	0.53
2:I:567:LEU:HB3	2:I:573:ILE:HG23	1.91	0.52
1:B:1035:LYS:HE3	1:C:830:LYS:CD	2.41	0.51
1:C:501:ASN:HD22	1:C:501:ASN:C	2.19	0.51
1:A:830:LYS:CD	1:C:1035:LYS:HE3	2.41	0.51
1:B:408:ASN:HB2	1:B:585:CYS:O	2.11	0.51
1:C:107:GLN:HG2	1:C:161:MET:O	2.11	0.51
2:I:98:PHE:CD2	2:I:100:HIS:HB2	2.46	0.50
1:A:1035:LYS:HE3	1:B:830:LYS:CD	2.41	0.50
2:D:98:PHE:CD2	2:D:100:HIS:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLN:HG2	1:B:161:MET:O	2.11	0.50
2:I:626:ILE:HG23	2:I:636:THR:HG23	1.94	0.50
1:C:408:ASN:HB2	1:C:585:CYS:O	2.11	0.50
1:A:107:GLN:HG2	1:A:161:MET:O	2.12	0.50
1:C:401:ARG:HD2	1:C:442:ILE:HG23	1.93	0.50
2:D:626:ILE:HG23	2:D:636:THR:HG23	1.94	0.49
1:B:440:SER:HB3	1:B:576:GLN:HB3	1.94	0.49
2:D:726:VAL:HG23	2:D:728:VAL:HG23	1.95	0.49
1:C:440:SER:HB3	1:C:576:GLN:HB3	1.94	0.49
1:B:401:ARG:HD2	1:B:442:ILE:HG23	1.93	0.49
1:C:483:THR:O	1:C:485:PRO:HD3	2.13	0.49
2:I:95:PHE:CE1	2:I:116:LEU:HD11	2.48	0.49
1:B:385:PHE:HB2	1:B:386:SER:HB2	1.95	0.48
1:B:483:THR:O	1:B:485:PRO:HD3	2.13	0.48
1:B:780:LEU:HG	1:B:782:ILE:HB	1.95	0.48
2:D:95:PHE:CE1	2:D:116:LEU:HD11	2.48	0.48
1:B:961:THR:OG1	1:B:962:ALA:N	2.46	0.48
1:C:385:PHE:HB2	1:C:386:SER:HB2	1.95	0.48
1:C:386:SER:HB3	1:C:388:LEU:HD22	1.94	0.48
2:I:76:ILE:HD13	2:I:107:ILE:HD11	1.96	0.48
2:I:726:VAL:HG23	2:I:728:VAL:HG23	1.95	0.48
2:D:76:ILE:HD13	2:D:107:ILE:HD11	1.96	0.48
1:A:780:LEU:HG	1:A:782:ILE:HB	1.95	0.47
2:D:322:TYR:HD2	2:D:348:MET:HE3	1.79	0.47
1:C:780:LEU:HG	1:C:782:ILE:HB	1.95	0.47
2:I:322:TYR:HD2	2:I:348:MET:HE3	1.80	0.47
2:I:77:LEU:HD23	2:I:88:VAL:HA	1.97	0.47
2:I:571:GLU:HB2	2:I:573:ILE:HG22	1.96	0.47
1:C:88:SER:OG	1:C:89:ALA:N	2.48	0.47
1:C:470:LYS:O	1:C:520:ALA:HA	2.15	0.47
2:D:77:LEU:HD23	2:D:88:VAL:HA	1.97	0.47
2:D:192:ASP:O	2:D:193:ILE:HD13	2.16	0.46
2:I:192:ASP:O	2:I:193:ILE:HD13	2.16	0.46
2:D:72:GLN:HB3	2:D:77:LEU:HD12	1.97	0.46
1:C:466:GLN:HG2	1:C:517:LEU:HD22	1.97	0.46
1:A:961:THR:OG1	1:A:962:ALA:N	2.46	0.46
1:B:470:LYS:O	1:B:520:ALA:HA	2.15	0.46
1:B:975:SER:OG	1:B:979:ARG:NH1	2.48	0.46
2:D:382:ARG:H	2:D:403:GLU:HG2	1.81	0.46
2:I:72:GLN:HB3	2:I:77:LEU:HD12	1.97	0.46
1:A:975:SER:OG	1:A:979:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:PRO:HD2	1:B:563:MET:HE3	1.97	0.46
2:I:53:TYR:HD1	2:I:503:MET:HE2	1.81	0.46
1:C:386:SER:HG	1:C:388:LEU:HB3	1.81	0.46
1:C:975:SER:OG	1:C:979:ARG:NH1	2.48	0.46
1:A:770:VAL:HG12	1:B:969:ALA:HB2	1.98	0.45
1:B:467:PHE:O	1:B:524:SER:HB2	2.16	0.45
1:B:770:VAL:HG12	1:C:969:ALA:HB2	1.98	0.45
1:C:410:ASN:HB3	1:C:413:LYS:CB	2.46	0.45
2:I:546:VAL:HG12	2:I:627:TRP:O	2.16	0.45
1:B:466:GLN:HG2	1:B:517:LEU:HD22	1.97	0.45
2:I:414:TYR:CD1	2:I:433:LYS:HD2	2.51	0.45
2:I:550:PRO:HG3	2:I:594:ILE:HD11	1.98	0.45
1:A:969:ALA:HB2	1:C:770:VAL:HG12	1.98	0.45
1:B:88:SER:OG	1:B:89:ALA:N	2.48	0.45
1:B:410:ASN:HB3	1:B:413:LYS:CB	2.46	0.45
2:D:53:TYR:HD1	2:D:503:MET:HE2	1.81	0.45
2:D:550:PRO:HG3	2:D:594:ILE:HD11	1.98	0.45
2:I:649:CYS:HB3	2:I:699:GLU:HB2	1.98	0.45
1:B:385:PHE:HA	1:B:386:SER:HA	1.55	0.45
1:C:467:PHE:O	1:C:524:SER:HB2	2.16	0.45
2:D:546:VAL:HG12	2:D:627:TRP:O	2.16	0.45
1:C:546:SER:OG	1:C:549:GLU:HB2	2.17	0.45
2:D:649:CYS:HB3	2:D:699:GLU:HB2	1.98	0.45
1:A:88:SER:OG	1:A:89:ALA:N	2.48	0.45
1:B:401:ARG:HD3	1:B:444:ASP:OD1	2.17	0.45
1:C:385:PHE:HA	1:C:386:SER:HA	1.55	0.45
1:B:546:SER:HG	1:B:549:GLU:HB2	1.81	0.44
1:C:478:CYS:HB2	1:C:573:ILE:HB	1.99	0.44
2:D:414:TYR:CD1	2:D:433:LYS:HD2	2.51	0.44
1:B:152:SER:OG	1:B:165:PHE:HB2	2.18	0.44
1:C:494:PRO:HD2	1:C:563:MET:HE3	1.97	0.44
2:I:382:ARG:H	2:I:403:GLU:HG2	1.81	0.44
1:A:152:SER:OG	1:A:165:PHE:HB2	2.18	0.44
1:C:401:ARG:HD3	1:C:444:ASP:OD1	2.17	0.44
1:A:633:ASP:OD1	1:A:633:ASP:C	2.61	0.44
1:C:401:ARG:NH1	1:C:444:ASP:OD1	2.49	0.44
1:B:546:SER:OG	1:B:549:GLU:HB2	2.17	0.44
1:C:403:VAL:HG13	1:C:442:ILE:HD11	2.00	0.44
1:C:152:SER:OG	1:C:165:PHE:HB2	2.18	0.44
1:A:782:ILE:HA	1:A:783:PRO:HD3	1.91	0.43
1:B:1084:GLN:HE21	1:B:1088:ARG:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:633:ASP:OD1	1:C:633:ASP:C	2.61	0.43
1:B:478:CYS:HB2	1:B:573:ILE:HB	1.99	0.43
2:D:283:THR:HG22	2:D:285:ILE:HD12	2.00	0.43
2:I:542:LEU:HD12	2:I:574:ILE:O	2.18	0.43
2:D:306:ALA:HB3	2:D:310:ARG:HB3	2.00	0.43
2:D:542:LEU:HD12	2:D:574:ILE:O	2.19	0.43
1:B:479:LEU:HD12	1:B:479:LEU:HA	1.90	0.43
1:B:717:LEU:HD23	1:B:757:MET:HB2	2.01	0.43
1:A:1084:GLN:HE21	1:A:1088:ARG:HD2	1.83	0.43
1:C:1084:GLN:HE21	1:C:1088:ARG:HD2	1.83	0.43
1:C:392:THR:HA	1:C:393:PRO:HD2	1.84	0.42
2:I:306:ALA:HB3	2:I:310:ARG:HB3	2.00	0.42
1:C:1013:THR:OG1	1:C:1014:THR:N	2.51	0.42
2:D:446:SER:HB2	2:D:457:TYR:CE2	2.54	0.42
2:D:379:GLU:OE2	2:D:379:GLU:N	2.53	0.42
2:I:230:ASP:OD1	2:I:264:PRO:HB3	2.19	0.42
2:I:341:VAL:C	2:I:343:ARG:H	2.28	0.42
2:I:283:THR:HG22	2:I:285:ILE:HD12	2.00	0.42
1:B:1013:THR:OG1	1:B:1014:THR:N	2.51	0.42
1:C:609:TYR:OH	1:C:644:ASP:OD2	2.38	0.42
2:I:70:TYR:CG	2:I:71:LYS:N	2.87	0.42
1:A:172:LEU:HA	1:A:173:PRO:HD2	1.95	0.42
2:D:70:TYR:CG	2:D:71:LYS:N	2.87	0.42
1:B:609:TYR:OH	1:B:644:ASP:OD2	2.38	0.42
2:D:268:PHE:CE2	2:D:313:LEU:HD21	2.55	0.42
2:D:544:LEU:HD21	2:D:606:GLN:HG3	2.02	0.42
2:D:622:LYS:O	2:D:623:ARG:HG3	2.20	0.42
2:I:446:SER:HB2	2:I:457:TYR:CE2	2.54	0.42
1:C:961:THR:OG1	1:C:962:ALA:N	2.46	0.42
2:D:461:PHE:CD1	2:D:468:TYR:HB3	2.55	0.42
2:I:158:SER:CB	2:I:163:LYS:HB2	2.49	0.42
2:I:379:GLU:OE2	2:I:379:GLU:N	2.52	0.42
2:I:461:PHE:CD1	2:I:468:TYR:HB3	2.55	0.42
1:A:717:LEU:HD23	1:A:757:MET:HB2	2.01	0.42
1:B:386:SER:CB	1:B:388:LEU:H	2.33	0.42
1:B:401:ARG:NH1	1:B:444:ASP:OD1	2.49	0.42
1:C:593:ASP:N	1:C:593:ASP:OD1	2.51	0.42
2:D:158:SER:CB	2:D:163:LYS:HB2	2.49	0.41
2:D:544:LEU:HD12	2:D:544:LEU:HA	1.74	0.41
2:I:449:LEU:HD23	2:I:449:LEU:HA	1.87	0.41
1:B:386:SER:C	1:B:388:LEU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ASP:OD1	1:B:633:ASP:C	2.61	0.41
1:C:717:LEU:HD23	1:C:757:MET:HB2	2.01	0.41
2:D:341:VAL:C	2:D:343:ARG:H	2.28	0.41
1:C:386:SER:CB	1:C:388:LEU:H	2.32	0.41
2:D:111:GLY:O	2:D:137:LEU:HD12	2.20	0.41
2:I:256:TYR:CZ	2:I:663:ASP:HB3	2.56	0.41
2:I:622:LYS:O	2:I:623:ARG:HG3	2.20	0.41
2:D:256:TYR:CZ	2:D:663:ASP:HB3	2.56	0.41
2:D:230:ASP:OD1	2:D:264:PRO:HB3	2.19	0.41
1:C:386:SER:C	1:C:388:LEU:H	2.28	0.41
1:C:388:LEU:HD22	1:C:414:LEU:HD21	2.03	0.41
2:I:544:LEU:HD21	2:I:606:GLN:HG3	2.02	0.41
2:I:111:GLY:O	2:I:137:LEU:HD12	2.21	0.41
1:B:593:ASP:N	1:B:593:ASP:OD1	2.51	0.41
2:I:268:PHE:CE2	2:I:313:LEU:HD21	2.55	0.41
2:I:319:ILE:C	2:I:321:ASN:H	2.28	0.41
2:D:319:ILE:C	2:D:321:ASN:H	2.28	0.41
1:A:104:ASN:O	1:A:104:ASN:CG	2.64	0.40
2:I:294:LEU:HD23	2:I:294:LEU:HA	1.78	0.40
2:I:330:TYR:HB2	2:I:337:TRP:CH2	2.56	0.40
1:B:502:LYS:NZ	1:B:513:GLU:OE2	2.51	0.40
1:C:479:LEU:HD12	1:C:479:LEU:HA	1.90	0.40
2:D:330:TYR:HB2	2:D:337:TRP:CH2	2.56	0.40
2:I:229:ASN:HB3	2:I:265:THR:OG1	2.22	0.40
1:C:501:ASN:C	1:C:501:ASN:ND2	2.79	0.40
2:D:449:LEU:HD23	2:D:449:LEU:HA	1.87	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	929/1206 (77%)	912 (98%)	17 (2%)	0	100	100
1	B	1132/1206 (94%)	1092 (96%)	33 (3%)	7 (1%)	22	57
1	C	1130/1206 (94%)	1090 (96%)	33 (3%)	7 (1%)	22	57
2	D	726/728 (100%)	676 (93%)	49 (7%)	1 (0%)	48	81
2	I	726/728 (100%)	676 (93%)	49 (7%)	1 (0%)	48	81
All	All	4643/5074 (92%)	4446 (96%)	181 (4%)	16 (0%)	38	70

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	582	ASN
1	C	582	ASN
1	B	414	LEU
1	B	580	ASP
1	C	414	LEU
1	C	580	ASP
1	B	567	LEU
1	C	567	LEU
2	D	536	LYS
2	I	536	LYS
1	B	487	ASN
1	C	487	ASN
1	B	387	PRO
1	C	387	PRO
1	B	391	GLY
1	C	391	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	788/1037 (76%)	788 (100%)	0	100	100
1	B	954/1037 (92%)	953 (100%)	1 (0%)	92	95
1	C	965/1037 (93%)	949 (98%)	16 (2%)	56	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	603/653 (92%)	602 (100%)	1 (0%)	92	93
2	I	608/653 (93%)	602 (99%)	6 (1%)	73	81
All	All	3918/4417 (89%)	3894 (99%)	24 (1%)	82	87

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	437	CYS
1	C	388	LEU
1	C	403	VAL
1	C	412	THR
1	C	416	SER
1	C	435	SER
1	C	437	CYS
1	C	439	SER
1	C	454	SER
1	C	458	VAL
1	C	477	THR
1	C	483	THR
1	C	484	VAL
1	C	489	THR
1	C	501	ASN
1	C	510	ASP
1	C	532	SER
2	D	385	CYS
2	I	385	CYS
2	I	537	SER
2	I	563	TRP
2	I	573	ILE
2	I	624	ILE
2	I	673	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	A	194	HIS
1	A	280	GLN
1	A	599	GLN
1	A	619	ASN

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Mol	Chain	Res	Type
1	A	636	GLN
1	A	733	GLN
1	A	848	ASN
1	A	981	ASN
1	A	987	GLN
1	A	1009	GLN
1	A	1072	ASN
1	A	1097	GLN
1	A	1208	GLN
1	B	107	GLN
1	B	125	ASN
1	B	280	GLN
1	B	421	ASN
1	B	466	GLN
1	B	475	ASN
1	B	519	ASN
1	B	619	ASN
1	B	636	GLN
1	B	848	ASN
1	B	907	GLN
1	B	981	ASN
1	B	987	GLN
1	B	1009	GLN
1	B	1072	ASN
1	B	1084	GLN
1	B	1097	GLN
1	B	1208	GLN
1	C	107	GLN
1	C	125	ASN
1	C	280	GLN
1	C	466	GLN
1	C	501	ASN
1	C	619	ASN
1	C	636	GLN
1	C	733	GLN
1	C	848	ASN
1	C	981	ASN
1	C	987	GLN
1	C	1072	ASN
1	C	1084	GLN
1	C	1097	GLN
1	C	1208	GLN

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Mol	Chain	Res	Type
2	D	72	GLN
2	D	100	HIS
2	D	345	HIS
2	I	72	GLN
2	I	100	HIS
2	I	345	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

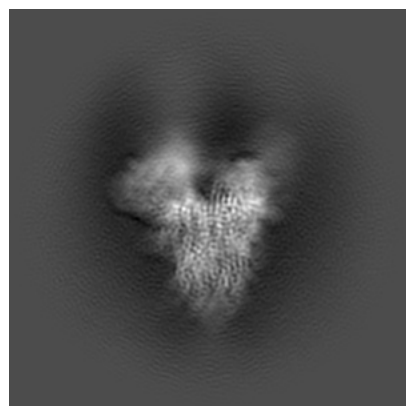
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39769. These allow visual inspection of the internal detail of the map and identification of artifacts.

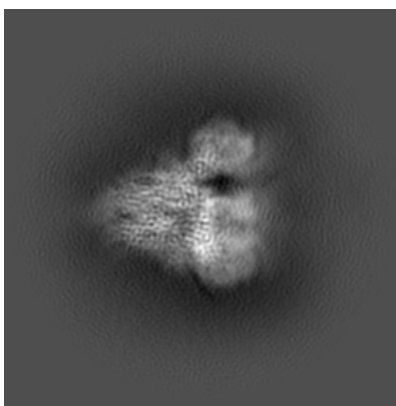
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

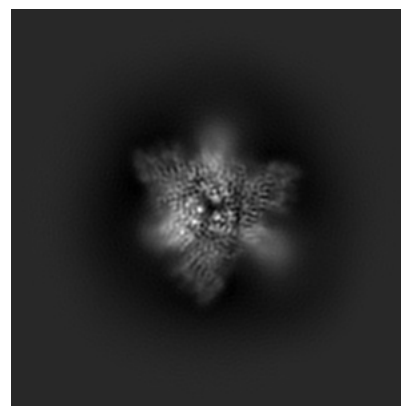
6.1.1 Primary map



X

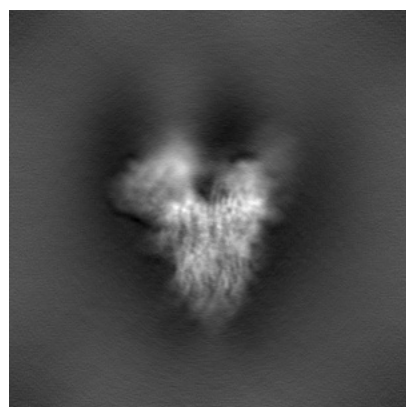


Y

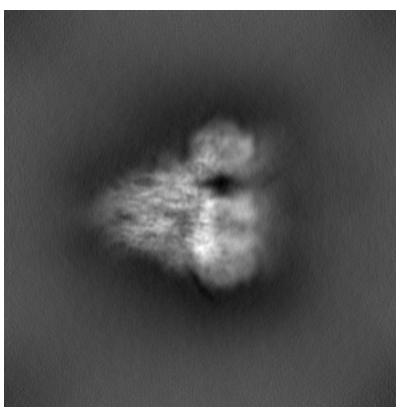


Z

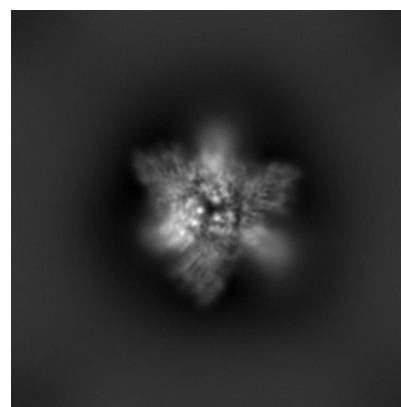
6.1.2 Raw map



X



Y

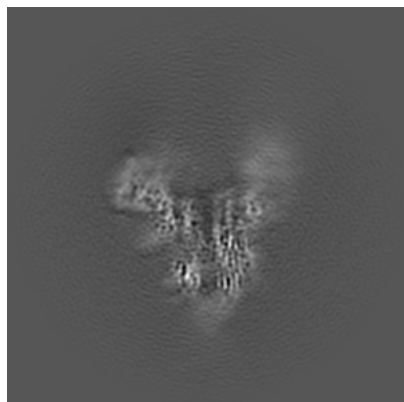


Z

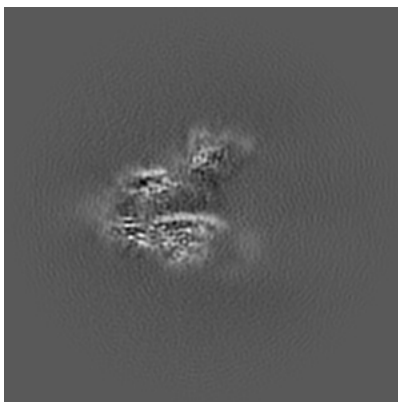
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

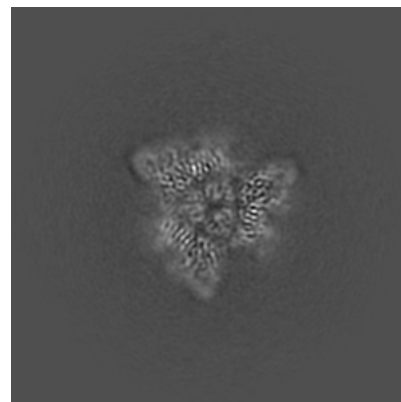
6.2.1 Primary map



X Index: 170

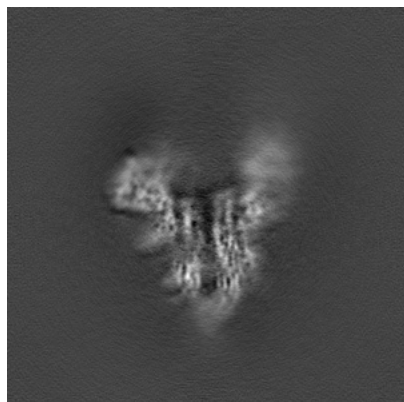


Y Index: 170

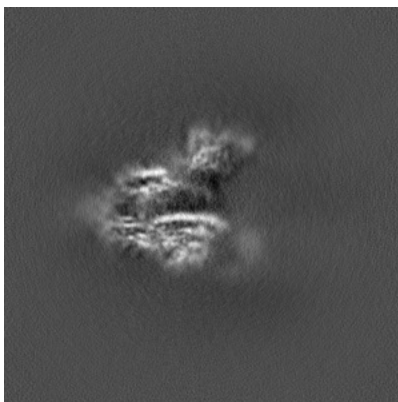


Z Index: 170

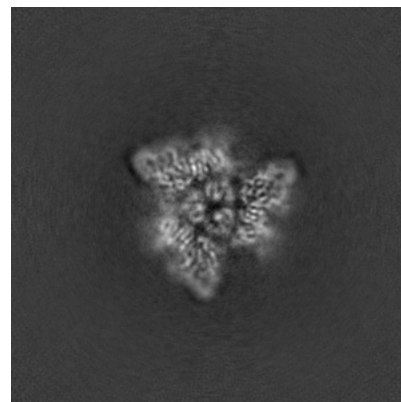
6.2.2 Raw map



X Index: 170



Y Index: 170

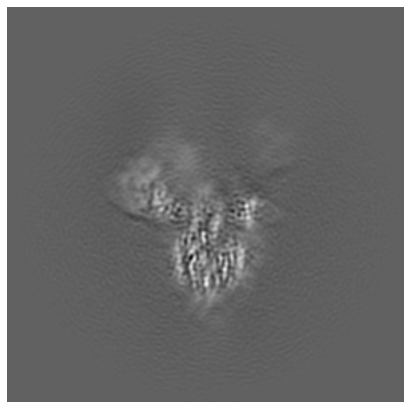


Z Index: 170

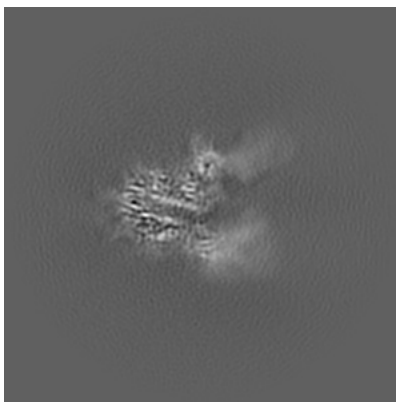
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

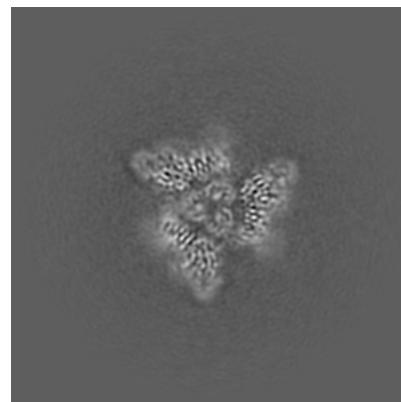
6.3.1 Primary map



X Index: 154

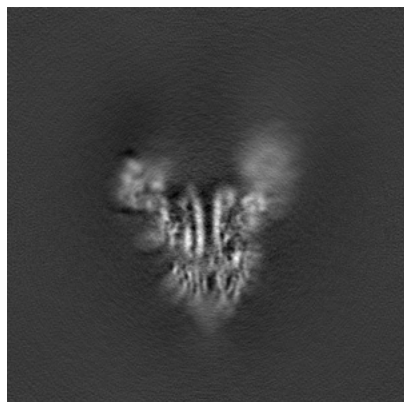


Y Index: 152

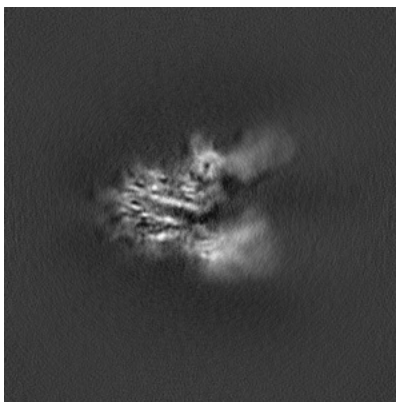


Z Index: 172

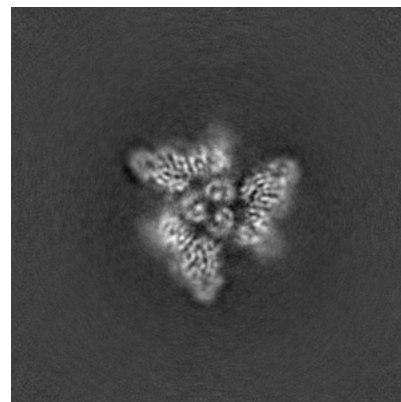
6.3.2 Raw map



X Index: 174



Y Index: 152

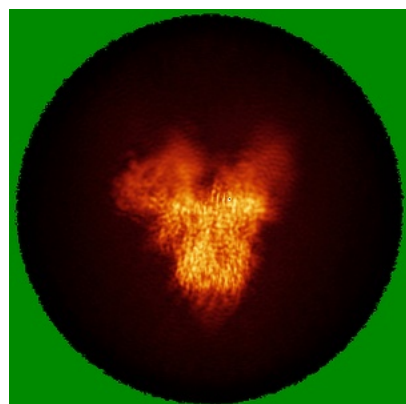


Z Index: 173

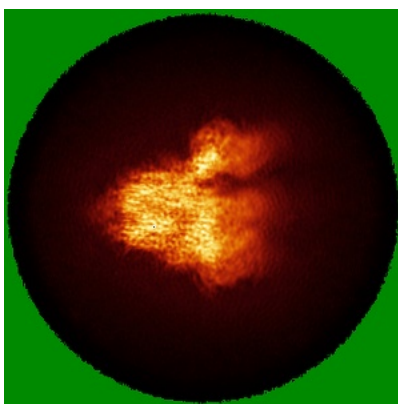
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

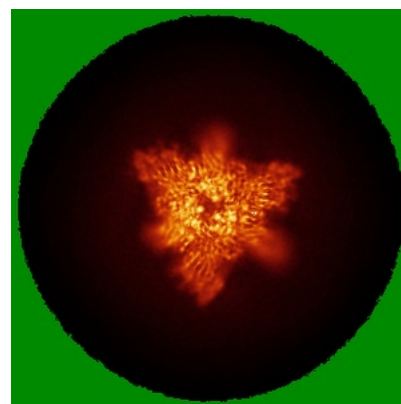
6.4.1 Primary map



X

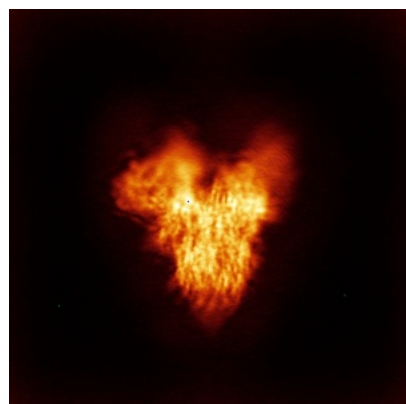


Y

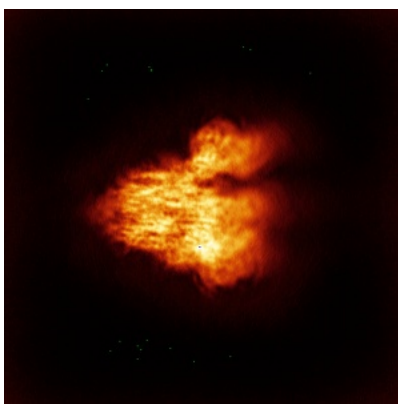


Z

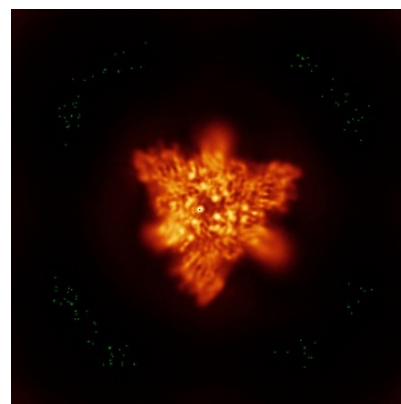
6.4.2 Raw map



X



Y

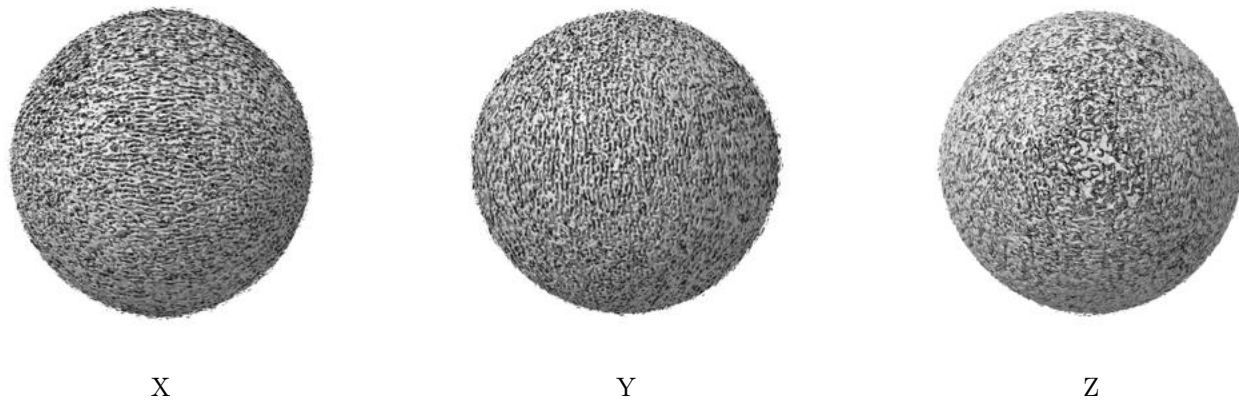


Z

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

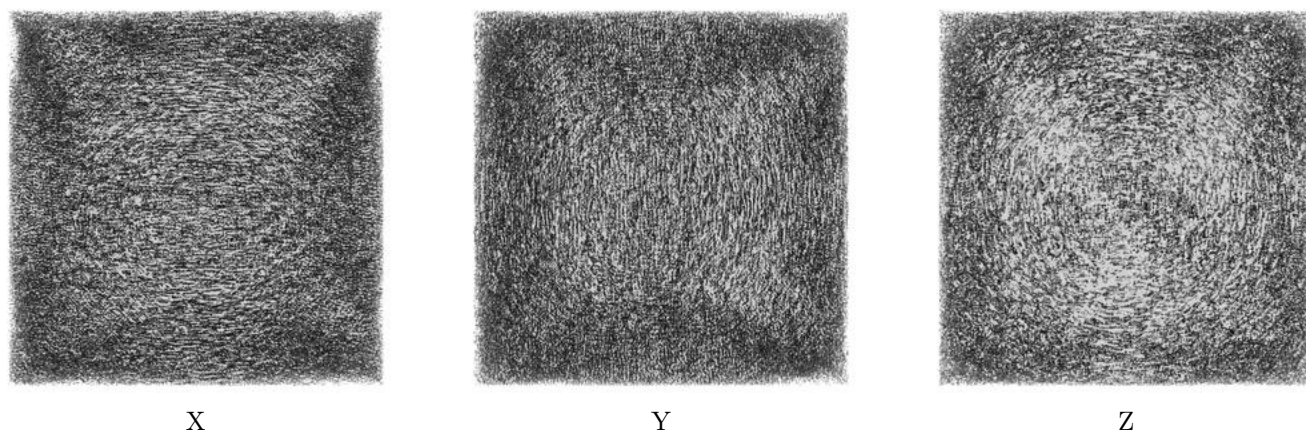
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.001. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

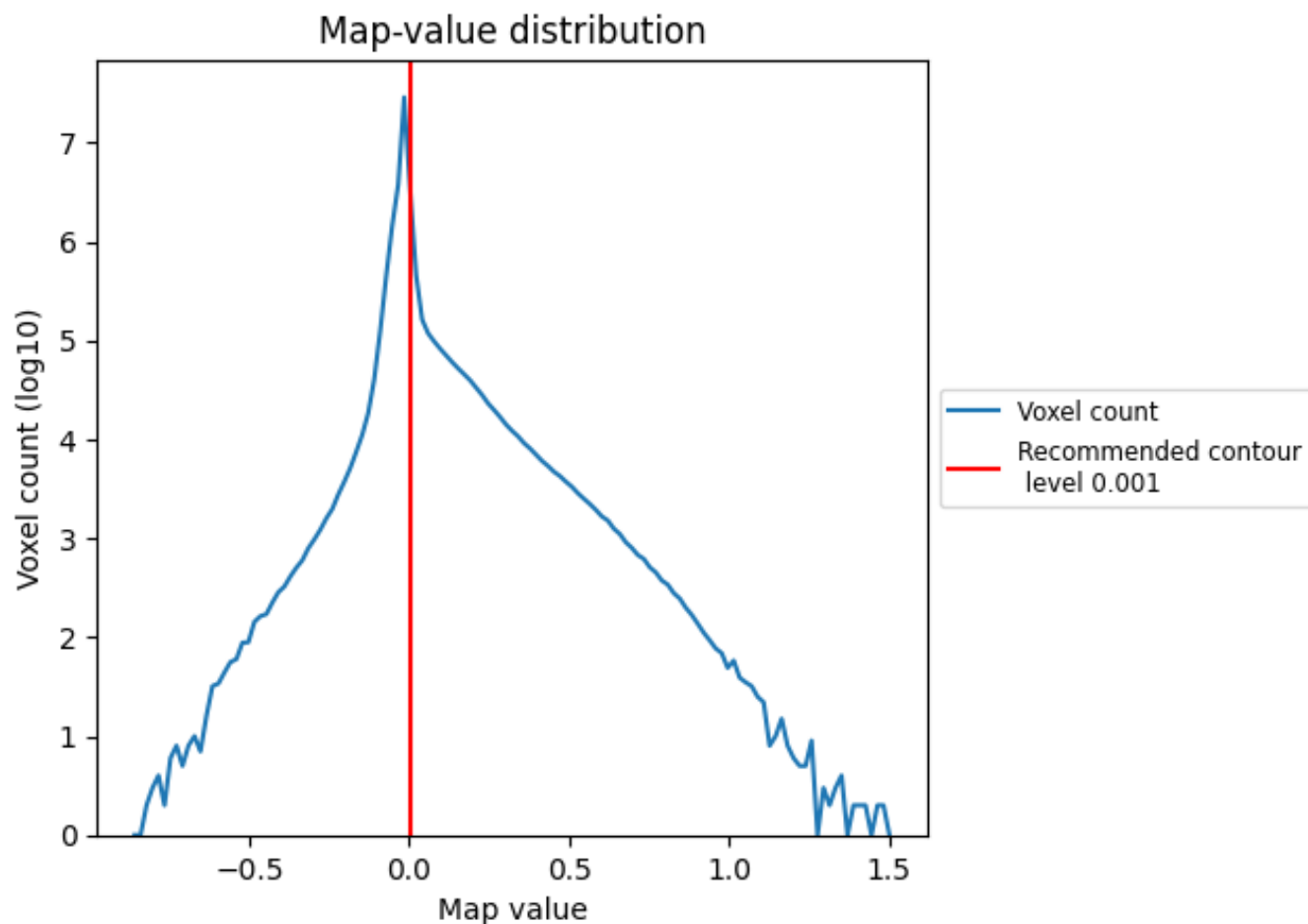
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

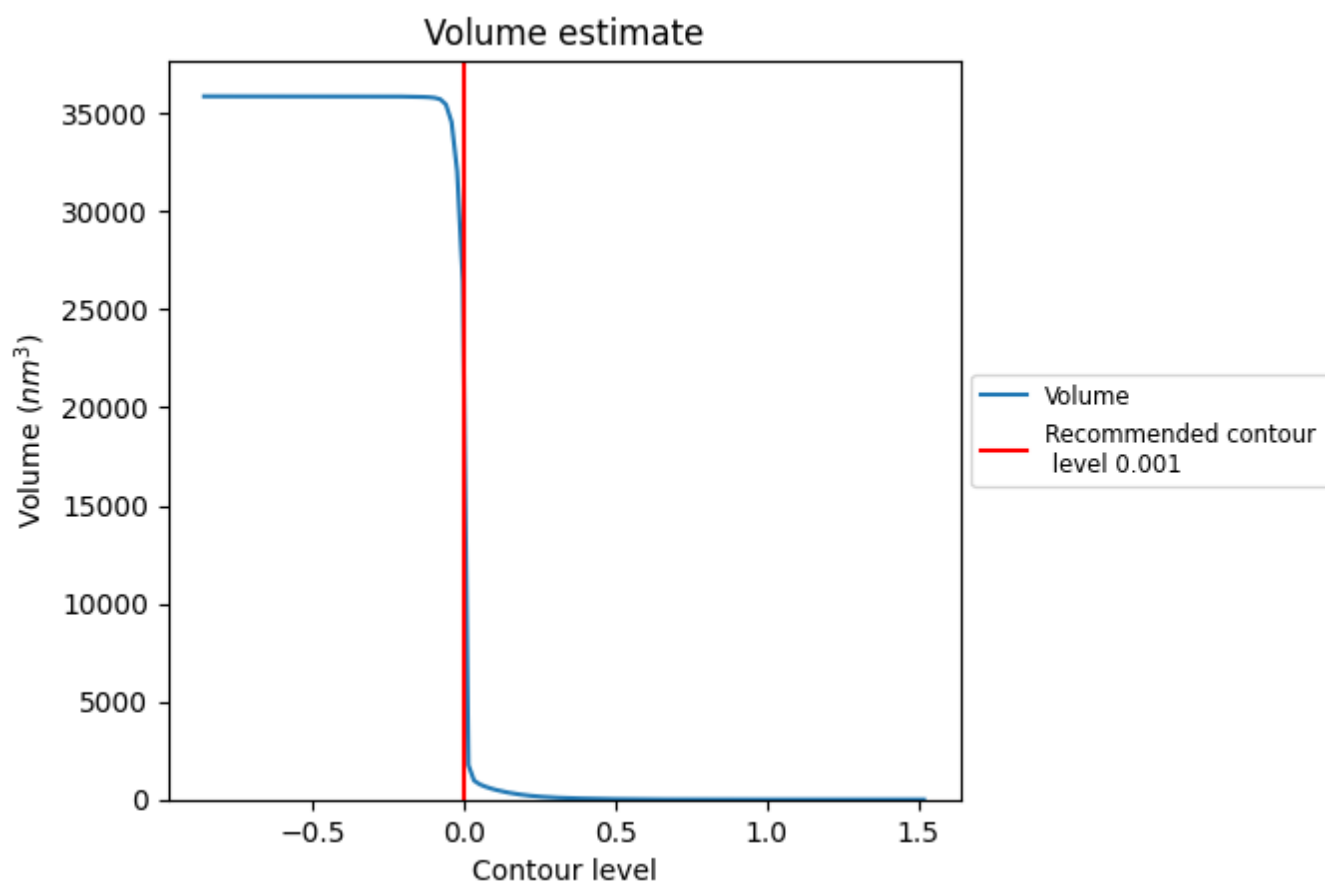
This section contains the results of statistical analysis of the map.

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.

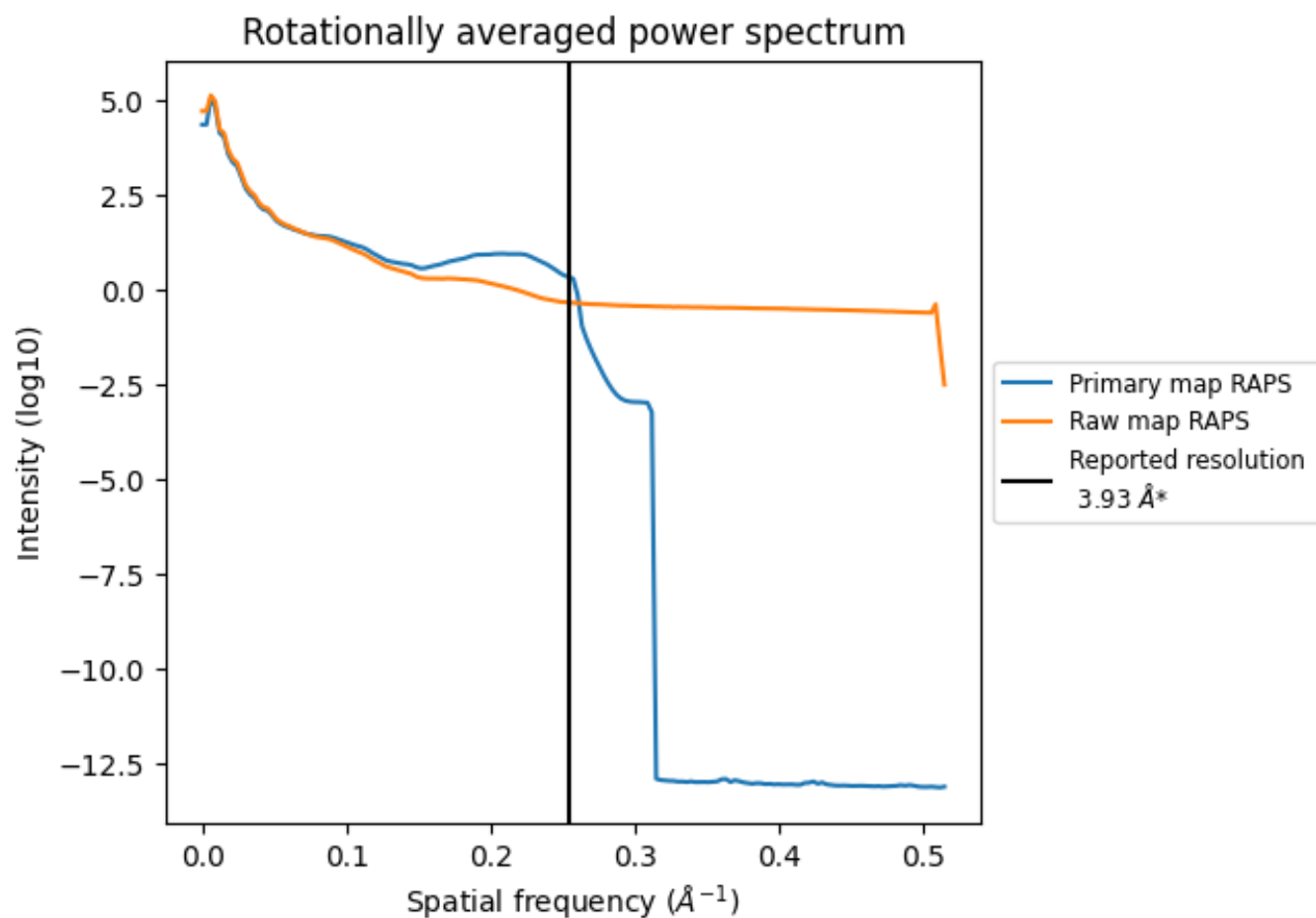
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 20703 nm^3 ; this corresponds to an approximate mass of 18702 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 ⓘ

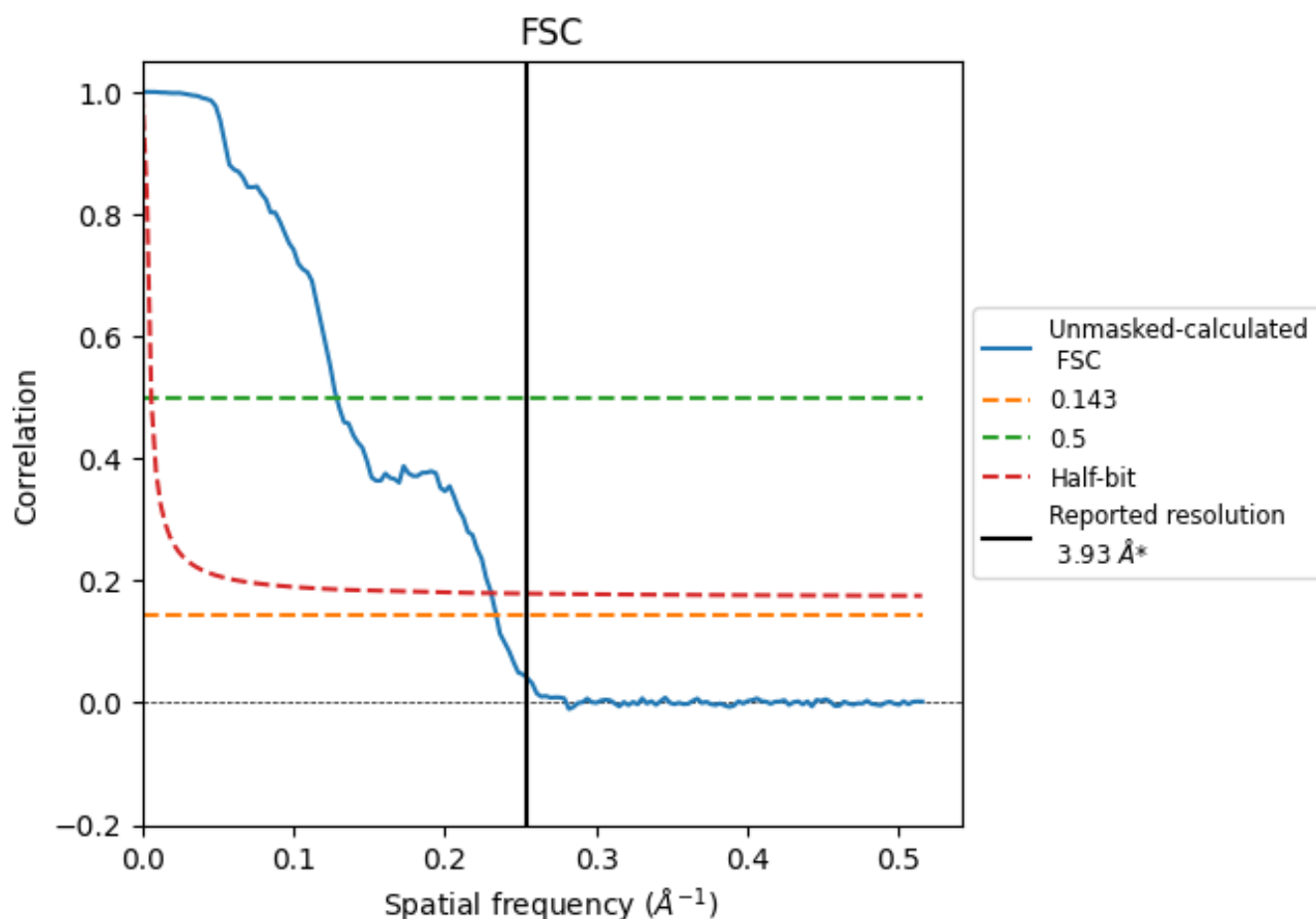


*Reported resolution corresponds to spatial frequency of 0.254 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.254 \AA^{-1}

8.2 Resolution estimates [i](#)

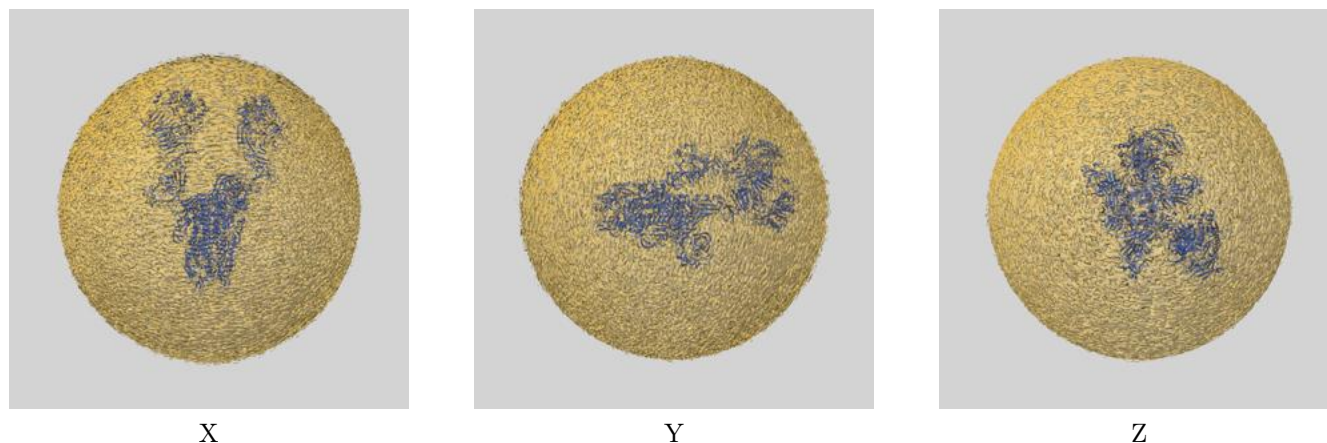
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.28	7.79	4.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

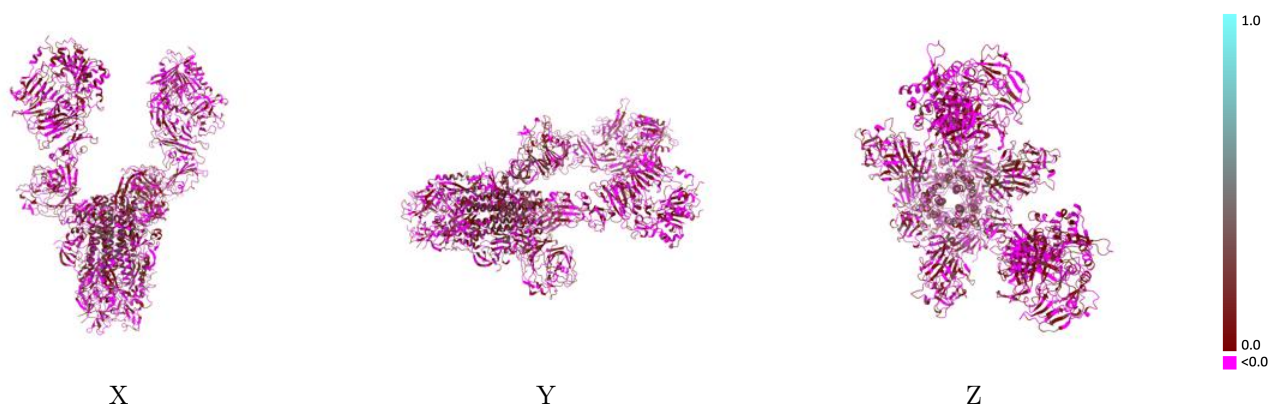
This section contains information regarding the fit between EMDB map EMD-39769 and PDB model 8Z4T. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



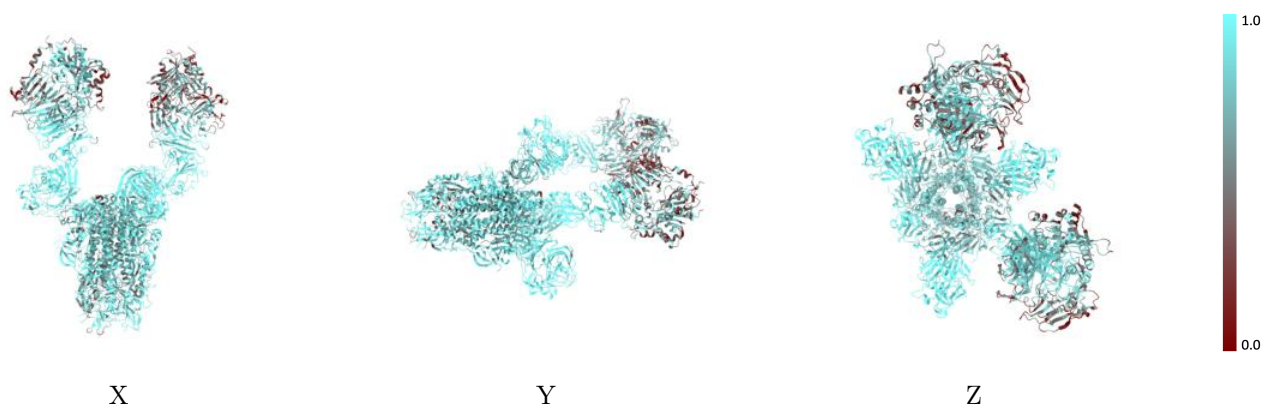
The images above show the 3D surface view of the map at the recommended contour level 0.001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



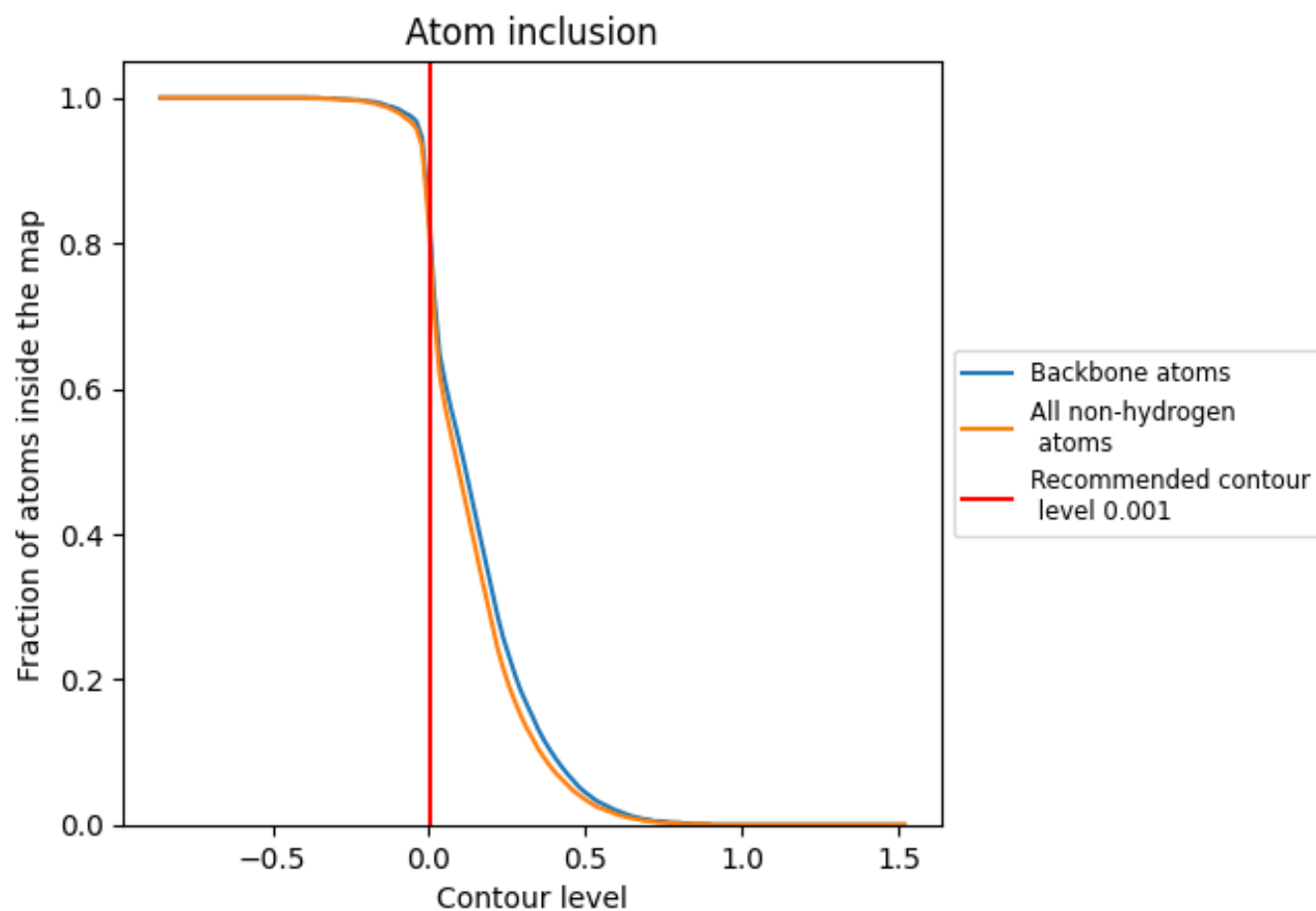
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.001).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8190	<div></div> 0.0320
A	<div></div> 0.9050	<div></div> 0.0550
B	<div></div> 0.8920	<div></div> 0.0270
C	<div></div> 0.9080	<div></div> 0.0590
D	<div></div> 0.6870	<div></div> 0.0110
I	<div></div> 0.5980	<div></div> -0.0090

