



Full wwPDB EM Validation Report ⓘ

Aug 12, 2025 – 12:13 PM JST

PDB ID : 9ITH / pdb_00009ith
EMDB ID : EMD-60865
Title : Nav1.5 in complex with TTX
Authors : Yan, N.; Li, Z.; Wu, T.
Deposited on : 2024-07-20
Resolution : 3.40 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.dev126
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

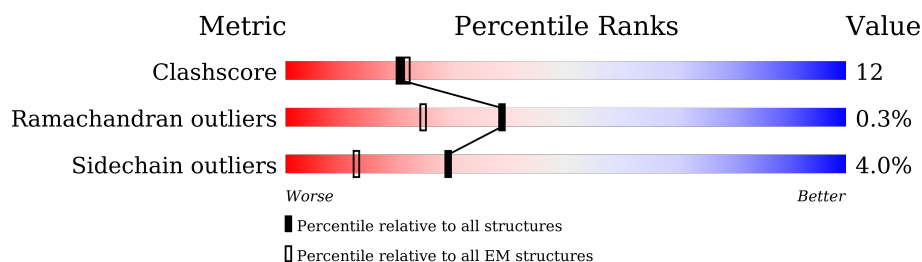
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	2059	 <div> <div>34%</div> <div>18%</div> <div>.</div> <div>44%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9424 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 Sodium channel protein type 5 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1151	9237	6115	1458	1591	73	0	0

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP Q14524
A	-41	ALA	-	expression tag	UNP Q14524
A	-40	SER	-	expression tag	UNP Q14524
A	-39	TRP	-	expression tag	UNP Q14524
A	-38	SER	-	expression tag	UNP Q14524
A	-37	HIS	-	expression tag	UNP Q14524
A	-36	PRO	-	expression tag	UNP Q14524
A	-35	GLN	-	expression tag	UNP Q14524
A	-34	PHE	-	expression tag	UNP Q14524
A	-33	GLU	-	expression tag	UNP Q14524
A	-32	LYS	-	expression tag	UNP Q14524
A	-31	GLY	-	expression tag	UNP Q14524
A	-30	GLY	-	expression tag	UNP Q14524
A	-29	GLY	-	expression tag	UNP Q14524
A	-28	ALA	-	expression tag	UNP Q14524
A	-27	ARG	-	expression tag	UNP Q14524
A	-26	GLY	-	expression tag	UNP Q14524
A	-25	GLY	-	expression tag	UNP Q14524
A	-24	SER	-	expression tag	UNP Q14524
A	-23	GLY	-	expression tag	UNP Q14524
A	-22	GLY	-	expression tag	UNP Q14524
A	-21	GLY	-	expression tag	UNP Q14524
A	-20	SER	-	expression tag	UNP Q14524
A	-19	TRP	-	expression tag	UNP Q14524
A	-18	SER	-	expression tag	UNP Q14524
A	-17	HIS	-	expression tag	UNP Q14524
A	-16	PRO	-	expression tag	UNP Q14524
A	-15	GLN	-	expression tag	UNP Q14524

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP Q14524
A	-13	GLU	-	expression tag	UNP Q14524
A	-12	LYS	-	expression tag	UNP Q14524
A	-11	GLY	-	expression tag	UNP Q14524
A	-10	PHE	-	expression tag	UNP Q14524
A	-9	ASP	-	expression tag	UNP Q14524
A	-8	TYR	-	expression tag	UNP Q14524
A	-7	LYS	-	expression tag	UNP Q14524
A	-6	ASP	-	expression tag	UNP Q14524
A	-5	ASP	-	expression tag	UNP Q14524
A	-4	ASP	-	expression tag	UNP Q14524
A	-3	ASP	-	expression tag	UNP Q14524
A	-2	LYS	-	expression tag	UNP Q14524
A	-1	GLY	-	expression tag	UNP Q14524
A	0	THR	-	expression tag	UNP Q14524

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



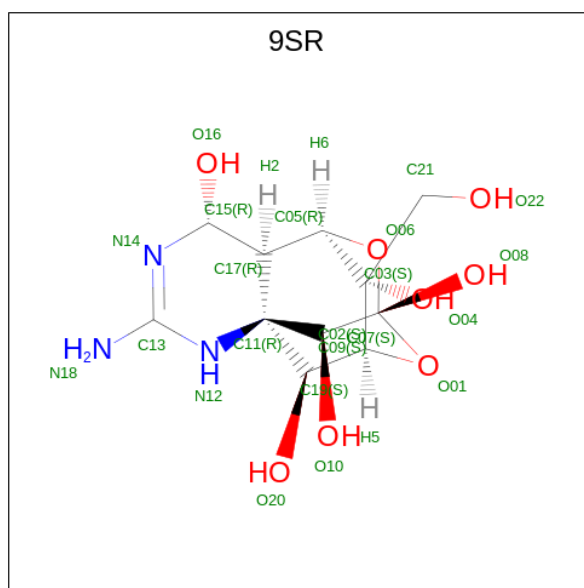
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is (1R,5R,6R,7R,9S,11S,12S,13S,14S)-3-amino-14-(hydroxymethyl)-8,10-dioxo-2,4-diazatetracyclo[7.3.1.1.7,11.0.1,6]tetradec-3-ene-5,9,12,13,14-pentol (non-preferred name) (CCD ID: 9SR) (formula: C₁₁H₁₇N₃O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			22	11	3	8	

- Molecule 4 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: C₃₄H₅₆O₅).

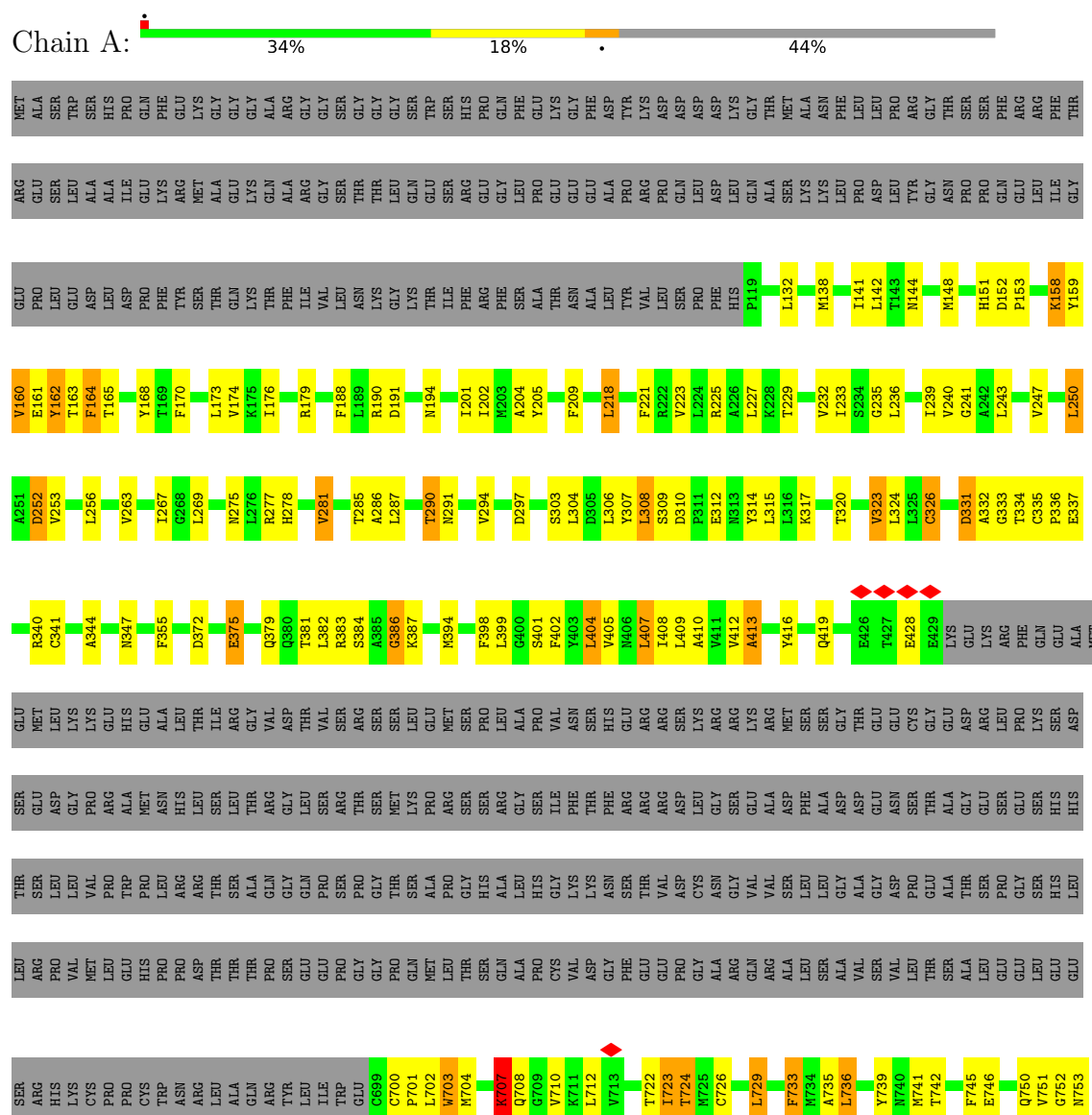


Total	C	O
39	34	5

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: Sodium channel protein type 5 subunit alpha





ALA
ASP
PHE
PRO
PRO
SER
PRO
ASP
ARG
ASP
ARG
GLU
SER
ILE
VAL

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145139	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.172	Depositor
Minimum map value	-0.115	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0171	Depositor
Map size (\AA)	261.84, 261.84, 261.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.091, 1.091, 1.091	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 9Z9, 9SR

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	1.48	127/9462 (1.3%)	1.34	154/12835 (1.2%)

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	ALA	CA-C	-9.87	1.40	1.52
1	A	341	CYS	CA-C	-9.80	1.40	1.52
1	A	1721	LEU	CA-C	-9.14	1.40	1.52
1	A	735	ALA	CA-C	-8.89	1.43	1.53
1	A	153	PRO	CA-C	-8.88	1.47	1.51
1	A	1711	ALA	CA-C	-8.84	1.41	1.52
1	A	333	GLY	CA-C	-8.05	1.45	1.52
1	A	900	ILE	CA-C	-7.93	1.42	1.52
1	A	1742	CYS	CA-C	-7.62	1.43	1.52
1	A	334	THR	CA-C	-7.61	1.43	1.52
1	A	900	ILE	C-O	-7.56	1.15	1.24
1	A	901	GLU	CA-C	-7.19	1.42	1.52
1	A	1446	MET	CA-C	-7.11	1.42	1.52
1	A	1718	SER	CA-C	-7.03	1.44	1.52
1	A	1218	SER	CA-C	-7.00	1.43	1.52
1	A	1414	GLN	N-CA	-7.00	1.38	1.46
1	A	394	MET	CA-C	-6.98	1.43	1.52
1	A	1689	ASP	CA-C	-6.96	1.43	1.52
1	A	1718	SER	C-O	-6.95	1.18	1.24
1	A	1318	GLU	CA-C	-6.79	1.44	1.52
1	A	1415	VAL	C-O	-6.78	1.16	1.24
1	A	1472	ASN	CA-C	-6.74	1.44	1.52
1	A	1411	ALA	CA-C	-6.70	1.44	1.52
1	A	1711	ALA	C-O	-6.68	1.16	1.24
1	A	880	HIS	CA-C	-6.64	1.44	1.52
1	A	1411	ALA	C-O	-6.62	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	LEU	CA-C	-6.56	1.44	1.52
1	A	159	TYR	CA-C	-6.55	1.45	1.52
1	A	1341	CYS	CA-C	-6.43	1.44	1.52
1	A	1449	TYR	CA-C	-6.36	1.44	1.52
1	A	1210	PHE	CA-C	-6.33	1.44	1.52
1	A	402	PHE	CA-C	-6.32	1.46	1.53
1	A	703	TRP	CA-C	-6.32	1.44	1.52
1	A	887	ALA	CA-C	-6.25	1.44	1.52
1	A	310	ASP	CA-C	-6.23	1.46	1.53
1	A	315	LEU	CA-C	-6.17	1.45	1.52
1	A	1711	ALA	N-CA	-6.16	1.38	1.46
1	A	317	LYS	CA-C	-6.15	1.45	1.52
1	A	401	SER	CA-C	-6.14	1.44	1.52
1	A	252	ASP	CA-C	-6.12	1.44	1.52
1	A	409	LEU	C-O	-6.11	1.17	1.24
1	A	1226	ASP	CA-C	-6.09	1.44	1.52
1	A	340	ARG	CA-C	-6.08	1.45	1.52
1	A	1221	ALA	CA-C	-6.06	1.44	1.52
1	A	347	ASN	CA-C	6.04	1.60	1.52
1	A	399	LEU	CA-C	-6.04	1.45	1.52
1	A	878	ARG	CA-C	-6.03	1.44	1.52
1	A	281	VAL	CA-C	-6.02	1.45	1.52
1	A	1411	ALA	N-CA	-6.01	1.39	1.46
1	A	869	ARG	CA-C	-6.00	1.44	1.52
1	A	1657	LEU	CA-C	-5.96	1.45	1.52
1	A	1728	CYS	CA-C	-5.90	1.45	1.53
1	A	1492	LYS	CA-C	-5.87	1.45	1.52
1	A	1771	ILE	CA-C	-5.82	1.45	1.52
1	A	382	LEU	C-O	-5.80	1.16	1.24
1	A	1666	LEU	CA-C	-5.77	1.45	1.52
1	A	1693	ASN	CA-C	-5.75	1.45	1.52
1	A	1710	SER	CA-C	-5.75	1.45	1.53
1	A	935	LEU	CA-C	-5.75	1.45	1.52
1	A	332	ALA	CA-CB	-5.74	1.44	1.53
1	A	1374	ASN	CA-C	-5.74	1.45	1.52
1	A	1753	THR	CA-C	-5.73	1.45	1.52
1	A	1416	ALA	CA-C	-5.72	1.44	1.52
1	A	1758	ILE	CA-C	-5.68	1.45	1.52
1	A	1320	MET	N-CA	-5.67	1.39	1.46
1	A	878	ARG	N-CA	-5.65	1.38	1.46
1	A	1712	GLY	CA-C	-5.65	1.45	1.51
1	A	240	VAL	CA-C	-5.64	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1686	ALA	CA-C	-5.63	1.48	1.53
1	A	912	GLN	CA-C	-5.63	1.45	1.52
1	A	919	PHE	CA-C	-5.62	1.45	1.52
1	A	1419	LYS	CA-C	-5.59	1.46	1.52
1	A	910	SER	CA-C	-5.58	1.45	1.52
1	A	1238	LEU	CA-C	-5.56	1.45	1.52
1	A	324	LEU	CA-C	-5.54	1.45	1.52
1	A	782	ASN	CA-C	-5.53	1.44	1.52
1	A	1419	LYS	C-O	-5.52	1.17	1.24
1	A	1411	ALA	C-N	-5.49	1.26	1.33
1	A	893	ARG	C-O	-5.48	1.17	1.24
1	A	881	MET	CA-C	-5.48	1.46	1.52
1	A	384	SER	CA-C	-5.48	1.44	1.52
1	A	1714	ASP	CA-C	-5.47	1.45	1.52
1	A	375	GLU	CA-C	-5.46	1.45	1.52
1	A	793	LEU	CA-C	-5.45	1.45	1.52
1	A	335	CYS	N-CA	-5.44	1.37	1.45
1	A	885	PHE	CA-C	-5.44	1.46	1.52
1	A	413	ALA	CA-C	-5.43	1.45	1.52
1	A	736	LEU	CA-C	-5.43	1.47	1.52
1	A	722	THR	CA-C	-5.41	1.45	1.52
1	A	900	ILE	C-N	-5.40	1.26	1.33
1	A	1711	ALA	CA-CB	-5.38	1.45	1.53
1	A	247	VAL	N-CA	-5.38	1.40	1.46
1	A	1713	TRP	CA-C	-5.37	1.45	1.52
1	A	817	LYS	CA-C	-5.33	1.45	1.52
1	A	1683	LYS	CA-C	-5.33	1.45	1.52
1	A	830	LYS	C-O	-5.32	1.18	1.24
1	A	830	LYS	N-CA	-5.31	1.40	1.46
1	A	814	ARG	CA-C	-5.31	1.45	1.52
1	A	1443	ASN	CA-C	-5.29	1.47	1.53
1	A	379	GLN	N-CA	-5.28	1.40	1.46
1	A	277	ARG	CA-C	-5.28	1.45	1.52
1	A	1411	ALA	CA-CB	-5.27	1.45	1.53
1	A	402	PHE	C-O	-5.25	1.17	1.23
1	A	903	MET	CA-C	-5.24	1.46	1.52
1	A	811	ARG	CA-C	-5.23	1.45	1.52
1	A	1322	VAL	CA-CB	-5.23	1.48	1.54
1	A	1495	TYR	CA-C	-5.22	1.46	1.52
1	A	790	ILE	N-CA	-5.19	1.40	1.46
1	A	1412	LEU	C-O	-5.18	1.17	1.24
1	A	1760	PHE	CA-C	-5.18	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1685	GLU	CA-C	-5.17	1.46	1.52
1	A	204	ALA	CA-C	-5.17	1.46	1.52
1	A	398	PHE	CA-C	-5.17	1.46	1.52
1	A	1368	GLU	CA-C	-5.16	1.46	1.52
1	A	1628	ALA	CA-C	-5.14	1.45	1.52
1	A	930	VAL	C-O	-5.14	1.18	1.24
1	A	708	GLN	CA-C	-5.13	1.46	1.52
1	A	903	MET	C-O	-5.11	1.18	1.24
1	A	863	LYS	CA-C	-5.11	1.46	1.52
1	A	1669	PHE	CA-C	-5.09	1.46	1.52
1	A	1307	ALA	CA-C	-5.08	1.45	1.52
1	A	904	TRP	C-O	-5.07	1.17	1.24
1	A	1322	VAL	CA-C	-5.07	1.46	1.52
1	A	930	VAL	CA-CB	-5.05	1.48	1.54
1	A	1291	LEU	CA-C	-5.03	1.46	1.52
1	A	375	GLU	C-O	-5.03	1.18	1.24
1	A	394	MET	C-O	-5.02	1.18	1.24

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	900	ILE	N-CA-C	13.61	124.46	110.72
1	A	903	MET	N-CA-C	-12.13	98.06	111.28
1	A	703	TRP	N-CA-C	-12.05	98.14	111.28
1	A	1440	TRP	N-CA-C	11.68	123.57	111.07
1	A	1591	TRP	N-CA-C	-10.32	99.45	113.18
1	A	704	MET	N-CA-C	10.15	122.43	111.36
1	A	912	GLN	N-CA-C	9.78	122.96	111.71
1	A	1437	GLN	CA-C-N	-9.70	110.80	120.31
1	A	1437	GLN	C-N-CA	-9.70	110.80	120.31
1	A	839	LEU	N-CA-C	-9.62	99.64	112.72
1	A	151	HIS	N-CA-C	9.52	121.73	111.36
1	A	1587	PHE	N-CA-C	9.51	121.73	111.36
1	A	708	GLN	N-CA-C	-9.49	100.94	111.28
1	A	1369	GLY	N-CA-C	9.48	123.30	110.69
1	A	386	GLY	N-CA-C	9.07	123.61	111.72
1	A	1690	ASP	N-CA-C	8.99	123.26	111.75
1	A	1595	ASP	N-CA-C	8.83	120.90	111.28
1	A	312	GLU	N-CA-C	-8.82	102.06	112.92
1	A	707	LYS	N-CA-C	-8.81	101.60	111.82
1	A	782	ASN	N-CA-C	-8.66	103.30	114.04
1	A	1210	PHE	N-CA-C	-8.65	101.85	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	888	PHE	N-CA-C	-8.65	101.86	111.28
1	A	306	LEU	N-CA-C	-8.56	102.03	111.36
1	A	1233	LYS	N-CA-C	8.40	120.06	111.07
1	A	1241	TYR	N-CA-C	-8.32	102.17	111.07
1	A	746	GLU	N-CA-C	8.30	120.10	111.14
1	A	878	ARG	N-CA-C	-8.27	103.19	113.28
1	A	1446	MET	N-CA-C	-8.17	103.32	113.20
1	A	227	LEU	N-CA-C	-8.08	102.98	112.92
1	A	739	TYR	N-CA-C	8.06	120.07	111.28
1	A	291	ASN	N-CA-C	7.95	119.95	111.28
1	A	309	SER	N-CA-C	7.89	121.39	111.69
1	A	307	TYR	N-CA-C	7.74	119.50	111.14
1	A	1320	MET	N-CA-C	-7.55	103.05	111.28
1	A	408	ILE	CB-CA-C	-7.43	102.46	111.97
1	A	1609	SER	N-CA-C	7.41	119.36	111.28
1	A	1313	ALA	N-CA-C	7.36	121.36	112.38
1	A	1586	TYR	N-CA-C	-7.36	103.19	111.14
1	A	1775	PHE	N-CA-C	-7.36	104.04	113.16
1	A	308	LEU	N-CA-C	-7.36	103.57	112.54
1	A	1293	PHE	N-CA-C	-7.32	101.85	111.74
1	A	158	LYS	N-CA-C	-7.28	104.55	113.50
1	A	1304	THR	N-CA-C	-7.18	104.51	113.20
1	A	286	ALA	N-CA-C	7.14	122.00	113.28
1	A	893	ARG	N-CA-C	-7.11	102.58	111.11
1	A	1770	ILE	CB-CA-C	-7.09	102.73	112.02
1	A	1306	ARG	N-CA-C	-7.08	104.63	113.20
1	A	337	GLU	N-CA-C	7.07	118.99	111.28
1	A	1601	LEU	N-CA-C	-7.07	103.58	111.28
1	A	331	ASP	CB-CA-C	-7.06	101.93	111.88
1	A	920	LEU	N-CA-C	-7.02	104.99	113.97
1	A	802	SER	N-CA-C	6.97	120.27	111.69
1	A	243	LEU	N-CA-C	-6.97	103.68	111.28
1	A	800	ARG	N-CA-C	-6.95	104.37	112.92
1	A	787	ILE	CB-CA-C	-6.94	103.09	111.97
1	A	164	PHE	N-CA-C	-6.93	103.65	111.07
1	A	723	ILE	N-CA-C	6.92	117.03	110.53
1	A	1312	ARG	N-CA-C	-6.89	103.79	111.71
1	A	161	GLU	N-CA-C	-6.87	103.79	111.28
1	A	819	ALA	N-CA-C	6.86	118.76	111.28
1	A	1744	SER	CA-C-N	-6.85	111.93	119.19
1	A	1744	SER	C-N-CA	-6.85	111.93	119.19
1	A	1318	GLU	N-CA-C	6.82	118.72	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1774	ASN	N-CA-C	-6.77	104.28	112.54
1	A	416	TYR	N-CA-C	-6.75	103.93	111.28
1	A	240	VAL	N-CA-C	-6.74	104.24	113.00
1	A	160	VAL	N-CA-C	6.72	116.85	110.53
1	A	153	PRO	O-C-N	6.72	124.40	121.31
1	A	1568	VAL	N-CA-C	-6.69	103.80	110.62
1	A	1472	ASN	N-CA-C	-6.68	104.00	111.28
1	A	404	LEU	N-CA-C	6.68	118.45	111.03
1	A	795	GLU	N-CA-C	6.65	118.53	111.28
1	A	1260	ALA	N-CA-C	6.62	118.58	111.36
1	A	1622	PHE	N-CA-C	6.60	118.14	111.07
1	A	804	LEU	N-CA-C	6.59	118.54	111.36
1	A	906	CYS	N-CA-C	-6.56	105.81	113.88
1	A	805	SER	N-CA-C	6.53	120.87	112.12
1	A	899	TRP	N-CA-C	6.42	120.33	112.23
1	A	1316	ARG	N-CA-C	6.39	118.25	111.28
1	A	871	SER	N-CA-C	-6.33	105.56	113.28
1	A	1738	SER	N-CA-C	6.32	118.31	110.91
1	A	428	GLU	N-CA-C	-6.19	104.53	111.28
1	A	1724	GLY	N-CA-C	6.18	124.94	112.34
1	A	736	LEU	N-CA-C	-6.17	103.32	113.50
1	A	1481	GLY	N-CA-C	6.09	118.49	111.36
1	A	326	CYS	N-CA-C	6.08	119.18	107.44
1	A	783	ILE	N-CA-C	-6.08	104.58	110.72
1	A	724	THR	N-CA-C	-6.06	104.67	111.28
1	A	1756	ILE	N-CA-C	-6.01	104.65	110.42
1	A	152	ASP	CA-C-N	-5.99	115.28	119.66
1	A	152	ASP	C-N-CA	-5.99	115.28	119.66
1	A	937	LEU	N-CA-C	-5.99	104.67	111.07
1	A	209	PHE	N-CA-C	5.96	117.65	111.03
1	A	1206	TRP	N-CA-C	5.95	117.76	111.28
1	A	1252	LEU	N-CA-C	-5.93	104.82	111.28
1	A	1621	LEU	N-CA-C	-5.91	104.42	111.69
1	A	923	MET	N-CA-C	5.90	117.40	110.97
1	A	204	ALA	CA-C-N	-5.88	111.94	120.29
1	A	204	ALA	C-N-CA	-5.88	111.94	120.29
1	A	1444	LEU	N-CA-C	5.87	119.26	111.75
1	A	898	GLU	N-CA-C	5.86	118.83	110.68
1	A	383	ARG	N-CA-C	-5.79	106.31	113.19
1	A	285	THR	N-CA-C	-5.78	100.57	109.52
1	A	1693	ASN	N-CA-C	-5.78	100.71	108.86
1	A	1741	ASP	CA-C-N	-5.77	114.87	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1741	ASP	C-N-CA	-5.77	114.87	123.00
1	A	1637	ILE	N-CA-C	5.75	121.31	109.34
1	A	897	GLY	N-CA-C	5.75	121.53	114.69
1	A	910	SER	N-CA-C	5.74	121.18	113.72
1	A	304	LEU	N-CA-C	-5.74	104.95	111.14
1	A	797	GLY	N-CA-C	5.72	119.60	112.73
1	A	886	HIS	N-CA-C	-5.71	105.06	111.28
1	A	870	ASP	N-CA-C	-5.71	100.52	109.25
1	A	1650	LEU	N-CA-C	-5.67	105.10	111.28
1	A	1238	LEU	N-CA-C	-5.65	105.13	111.28
1	A	818	LEU	N-CA-C	-5.64	106.38	113.20
1	A	1457	GLY	N-CA-C	5.64	119.98	112.77
1	A	1666	LEU	N-CA-C	-5.63	105.14	111.28
1	A	864	ASN	N-CA-C	5.63	117.42	111.28
1	A	1459	PHE	N-CA-C	5.61	118.25	111.40
1	A	1731	THR	N-CA-C	5.61	121.65	113.40
1	A	821	SER	N-CA-C	5.59	117.45	111.36
1	A	1503	SER	N-CA-C	-5.58	105.59	112.90
1	A	1558	ASN	N-CA-C	5.58	117.04	111.07
1	A	323	VAL	N-CA-C	-5.50	100.37	108.85
1	A	1576	ILE	N-CA-C	5.48	115.68	110.42
1	A	1241	TYR	CB-CA-C	-5.47	102.30	110.88
1	A	162	TYR	N-CA-C	5.46	117.31	111.36
1	A	347	ASN	N-CA-C	5.45	121.86	109.81
1	A	1259	VAL	N-CA-C	5.42	115.63	110.42
1	A	1726	PRO	CA-C-O	-5.40	115.31	121.96
1	A	1258	TRP	N-CA-C	-5.39	105.40	111.28
1	A	1295	GLU	N-CA-C	-5.39	105.41	112.41
1	A	1688	ILE	N-CA-C	-5.36	99.43	107.37
1	A	812	LEU	N-CA-C	5.36	117.88	111.71
1	A	913	SER	N-CA-C	5.36	117.12	111.28
1	A	381	THR	CB-CA-C	-5.35	102.48	110.88
1	A	218	LEU	N-CA-C	-5.32	106.38	112.92
1	A	1485	ILE	N-CA-C	-5.29	98.34	109.34
1	A	287	LEU	N-CA-C	5.28	122.04	110.80
1	A	807	LEU	N-CA-C	-5.26	105.45	111.07
1	A	1443	ASN	N-CA-C	5.26	117.27	110.65
1	A	806	VAL	N-CA-C	-5.25	103.92	111.17
1	A	868	LEU	N-CA-C	-5.25	106.57	112.87
1	A	1597	VAL	CB-CA-C	-5.24	105.17	112.04
1	A	1736	ASN	N-CA-C	5.19	116.62	111.07
1	A	1741	ASP	N-CA-C	-5.17	105.69	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1259	VAL	CB-CA-C	-5.14	105.40	111.97
1	A	733	PHE	N-CA-C	-5.13	105.77	111.36
1	A	1618	SER	N-CA-C	5.11	120.41	113.16
1	A	1686	ALA	CB-CA-C	-5.05	110.74	116.54
1	A	1568	VAL	CB-CA-C	-5.03	105.36	112.14
1	A	250	LEU	CB-CA-C	-5.02	103.81	111.83
1	A	1237	VAL	CB-CA-C	-5.00	105.31	112.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9237	0	9413	227	0
2	A	126	0	117	0	0
3	A	22	0	0	1	0
4	A	39	0	0	1	0
All	All	9424	0	9530	227	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 12.

All (227) 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:A:700:CYS:SG	1:A:701:PRO:HD3	1.91	1.11
1:A:1337:VAL:HG21	1:A:1468:VAL:HG21	1.34	1.10
1:A:1608:LEU:CD2	1:A:1625:ILE:HD13	1.82	1.07
1:A:1608:LEU:HD21	1:A:1625:ILE:HD13	1.36	1.06
1:A:1213:PHE:CZ	1:A:1217:LEU:HD11	1.94	1.01
1:A:372:ASP:OD2	1:A:900:ILE:HG22	1.67	0.94
1:A:1612:ILE:CD1	1:A:1621:LEU:HD23	1.99	0.92
1:A:160:VAL:CG1	1:A:164:PHE:CE2	2.55	0.88
1:A:1608:LEU:HD23	1:A:1625:ILE:HG21	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1608:LEU:HD23	1:A:1625:ILE:HD13	1.62	0.81
1:A:1744:SER:OG	1:A:1747:VAL:HG12	1.83	0.77
1:A:387:LYS:HG2	1:A:1691:MET:HE3	1.67	0.77
1:A:372:ASP:CG	1:A:900:ILE:HG22	2.11	0.74
1:A:1734:ASN:HB2	1:A:1739:ARG:H	1.51	0.74
1:A:331:ASP:O	1:A:386:GLY:HA2	1.88	0.73
1:A:1612:ILE:HD13	1:A:1621:LEU:HD23	1.69	0.73
1:A:160:VAL:HG13	1:A:164:PHE:CE2	2.23	0.73
1:A:1684:TRP:HD1	1:A:1688:ILE:HG22	1.53	0.72
1:A:900:ILE:HD11	1:A:904:TRP:CE2	2.26	0.71
1:A:900:ILE:HD11	1:A:904:TRP:NE1	2.06	0.71
1:A:1413:LEU:HD23	1:A:1713:TRP:CH2	2.25	0.70
1:A:798:LEU:C	1:A:800:ARG:H	2.00	0.69
1:A:141:ILE:HG21	1:A:229:THR:HG22	1.74	0.69
1:A:900:ILE:HD11	1:A:904:TRP:CZ2	2.28	0.68
1:A:1650:LEU:O	1:A:1654:LEU:HG	1.93	0.68
1:A:160:VAL:HA	1:A:163:THR:HG22	1.75	0.67
1:A:387:LYS:HE2	1:A:1691:MET:HG3	1.77	0.66
1:A:1608:LEU:HD21	1:A:1625:ILE:CD1	2.22	0.66
1:A:1672:SER:O	1:A:1676:MET:HG3	1.95	0.66
1:A:1338:LEU:O	1:A:1342:LEU:HG	1.96	0.66
1:A:808:ARG:HA	1:A:811:ARG:HH21	1.61	0.66
1:A:893:ARG:HG2	1:A:898:GLU:HB2	1.79	0.65
1:A:1379:ASN:HB2	1:A:1432:ARG:HH12	1.60	0.65
1:A:700:CYS:HG	1:A:701:PRO:HD3	1.62	0.64
1:A:1590:SER:HA	1:A:1593:ILE:HG22	1.80	0.64
1:A:1608:LEU:CD2	1:A:1625:ILE:HG21	2.27	0.64
1:A:160:VAL:HG12	1:A:164:PHE:CE2	2.31	0.64
1:A:838:ALA:C	1:A:840:GLY:H	2.06	0.63
1:A:707:LYS:O	1:A:710:VAL:HG12	1.99	0.63
1:A:218:LEU:HG	1:A:221:PHE:CE2	2.33	0.62
1:A:164:PHE:HB3	1:A:168:TYR:HE2	1.63	0.62
1:A:1720:ILE:HG21	1:A:1748:GLY:HA3	1.82	0.62
1:A:138:MET:O	1:A:142:LEU:HD13	1.99	0.62
1:A:867:GLU:HG3	1:A:909:VAL:HG12	1.81	0.61
1:A:256:LEU:HD13	1:A:1643:ILE:HG23	1.81	0.61
1:A:190:ARG:O	1:A:190:ARG:NH1	2.32	0.61
1:A:256:LEU:HB2	1:A:1643:ILE:HD12	1.82	0.61
1:A:900:ILE:CD1	1:A:904:TRP:CZ2	2.84	0.61
1:A:801:MET:HG2	1:A:807:LEU:HD11	1.83	0.61
1:A:867:GLU:C	1:A:869:ARG:N	2.59	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1440:TRP:O	1:A:1441:GLU:HG2	2.02	0.59
1:A:1518:GLN:HA	1:A:1521:ILE:HG12	1.84	0.59
1:A:1308:LEU:HB3	1:A:1311:LEU:HD12	1.85	0.59
1:A:1729:ASP:HB3	1:A:1732:LEU:HD11	1.82	0.59
1:A:1534:ILE:O	1:A:1538:ILE:HG13	2.03	0.59
1:A:1525:VAL:HG21	1:A:1578:LYS:HA	1.85	0.58
1:A:726:CYS:SG	1:A:756:PHE:CD1	2.95	0.58
1:A:1214:MET:HE1	1:A:1246:PHE:HD1	1.68	0.58
1:A:1542:MET:HG2	1:A:1546:MET:HE3	1.84	0.58
1:A:1726:PRO:O	1:A:1727:TYR:HB2	2.02	0.58
1:A:1518:GLN:N	1:A:1518:GLN:OE1	2.37	0.57
1:A:250:LEU:HD11	1:A:412:VAL:HG22	1.86	0.57
1:A:869:ARG:HD3	1:A:876:LEU:HB3	1.87	0.57
1:A:1650:LEU:HG	1:A:1654:LEU:HD21	1.86	0.57
1:A:218:LEU:HG	1:A:221:PHE:HE2	1.67	0.57
1:A:235:GLY:HA3	1:A:841:ASN:ND2	2.20	0.57
1:A:1200:HIS:O	1:A:1204:HIS:N	2.38	0.55
1:A:236:LEU:HD22	1:A:845:VAL:HG23	1.88	0.55
1:A:867:GLU:C	1:A:869:ARG:H	2.13	0.55
1:A:1729:ASP:HB3	1:A:1732:LEU:CD1	2.37	0.55
1:A:290:THR:HB	1:A:294:VAL:HG21	1.89	0.55
1:A:1529:ALA:O	1:A:1533:THR:HG22	2.07	0.55
1:A:900:ILE:C	1:A:902:THR:N	2.60	0.54
1:A:1365:ASN:HA	1:A:1393:LEU:HD23	1.90	0.54
1:A:710:VAL:CG1	1:A:770:ALA:HA	2.39	0.53
1:A:798:LEU:C	1:A:800:ARG:N	2.66	0.53
1:A:164:PHE:HB3	1:A:168:TYR:CE2	2.44	0.53
1:A:275:ASN:OD1	1:A:278:HIS:NE2	2.41	0.53
1:A:900:ILE:CD1	1:A:904:TRP:CE2	2.92	0.52
1:A:1389:LEU:HD12	1:A:1389:LEU:H	1.73	0.52
1:A:1429:VAL:HG21	1:A:1447:TYR:CE2	2.45	0.52
1:A:173:LEU:HD23	1:A:176:ILE:HD11	1.91	0.52
1:A:900:ILE:HG12	1:A:904:TRP:CE2	2.45	0.52
1:A:736:LEU:HB3	1:A:745:PHE:HE1	1.75	0.51
1:A:876:LEU:HB2	1:A:877:PRO:HD2	1.92	0.51
1:A:1213:PHE:CZ	1:A:1217:LEU:CD1	2.82	0.51
1:A:1415:VAL:HA	1:A:1421:TRP:HB3	1.92	0.51
1:A:1413:LEU:HD23	1:A:1713:TRP:CZ2	2.46	0.51
1:A:900:ILE:HD11	1:A:904:TRP:HE1	1.72	0.51
1:A:1696:THR:OG1	1:A:1697:PHE:N	2.42	0.51
1:A:736:LEU:HB3	1:A:745:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1335:MET:HE3	1:A:1335:MET:HA	1.93	0.50
1:A:1235:ILE:O	1:A:1236:LYS:C	2.54	0.50
1:A:160:VAL:CG1	1:A:164:PHE:HE2	2.17	0.50
1:A:158:LYS:O	1:A:162:TYR:HD2	1.95	0.50
1:A:1220:GLY:C	1:A:1222:LEU:N	2.70	0.50
1:A:900:ILE:O	1:A:902:THR:N	2.45	0.50
1:A:900:ILE:C	1:A:902:THR:H	2.18	0.49
1:A:914:LEU:O	1:A:915:CYS:C	2.54	0.49
1:A:404:LEU:O	1:A:405:VAL:C	2.54	0.49
1:A:879:TRP:HE3	1:A:890:ILE:HG12	1.77	0.49
1:A:900:ILE:CG1	1:A:904:TRP:CE2	2.95	0.49
1:A:1455:ILE:O	1:A:1459:PHE:HB3	2.11	0.49
1:A:1274:LEU:O	1:A:1278:ILE:HG13	2.13	0.49
1:A:1346:LEU:O	1:A:1350:ILE:HG13	2.12	0.49
1:A:1553:SER:O	1:A:1557:ILE:HG13	2.13	0.49
1:A:700:CYS:SG	1:A:701:PRO:CD	2.83	0.48
1:A:812:LEU:O	1:A:815:VAL:HG23	2.12	0.48
1:A:1273:TRP:O	1:A:1277:LEU:HD12	2.14	0.48
1:A:191:ASP:HB3	1:A:194:ASN:OD1	2.14	0.48
1:A:413:ALA:HB2	1:A:935:LEU:HD11	1.95	0.48
1:A:1732:LEU:HD22	1:A:1741:ASP:CG	2.39	0.48
1:A:170:PHE:O	1:A:174:VAL:HG23	2.14	0.47
1:A:232:VAL:O	1:A:233:ILE:C	2.56	0.47
1:A:726:CYS:SG	1:A:756:PHE:HD1	2.35	0.47
1:A:1528:GLN:O	1:A:1532:VAL:HG22	2.14	0.47
1:A:805:SER:C	1:A:807:LEU:N	2.69	0.47
1:A:868:LEU:HG	1:A:909:VAL:CG1	2.44	0.47
1:A:902:THR:O	1:A:903:MET:C	2.55	0.47
1:A:1374:ASN:HB3	1:A:1377:ILE:HG13	1.95	0.47
1:A:233:ILE:HB	1:A:236:LEU:HG	1.97	0.46
1:A:703:TRP:O	1:A:707:LYS:HB2	2.15	0.46
1:A:835:SER:HB3	1:A:937:LEU:HD21	1.95	0.46
1:A:1199:TYR:HE1	1:A:1261:TYR:CE1	2.33	0.46
1:A:1499:LYS:HB3	1:A:1499:LYS:HE3	1.67	0.46
1:A:1572:THR:HA	1:A:1599:VAL:HG11	1.97	0.46
1:A:710:VAL:HG13	1:A:770:ALA:HA	1.98	0.46
1:A:726:CYS:SG	1:A:756:PHE:CE1	3.09	0.46
1:A:239:ILE:HD13	1:A:842:LEU:HG	1.96	0.46
1:A:935:LEU:HD23	1:A:939:LEU:HD13	1.97	0.46
1:A:1229:LEU:O	1:A:1230:GLU:C	2.57	0.46
1:A:1720:ILE:C	1:A:1722:ASN:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:O	1:A:221:PHE:HD2	1.99	0.45
1:A:162:TYR:HA	1:A:165:THR:OG1	2.16	0.45
1:A:876:LEU:HD13	1:A:882:MET:HE2	1.99	0.45
1:A:239:ILE:C	1:A:241:GLY:N	2.75	0.45
1:A:838:ALA:C	1:A:840:GLY:N	2.70	0.45
1:A:1214:MET:HE3	1:A:1214:MET:HB3	1.74	0.45
1:A:1552:GLN:HG3	1:A:1557:ILE:HG12	1.99	0.45
1:A:1703:CYS:O	1:A:1706:GLN:HG3	2.17	0.45
1:A:1541:ASN:O	1:A:1544:THR:HG22	2.17	0.45
1:A:1773:GLU:C	1:A:1776:SER:H	2.23	0.45
1:A:767:LYS:HB3	1:A:776:TYR:HE1	1.81	0.45
1:A:1214:MET:HE1	1:A:1246:PHE:CD1	2.51	0.45
1:A:1422:MET:HB2	3:A:2110:9SR:O08	2.17	0.45
1:A:1437:GLN:HG3	1:A:1438:PRO:HD2	2.00	0.44
1:A:1625:ILE:H	1:A:1625:ILE:HG13	1.47	0.44
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.80	0.44
1:A:793:LEU:HD23	1:A:793:LEU:HA	1.72	0.44
1:A:1559:ILE:O	1:A:1563:ILE:HG12	2.17	0.44
1:A:1596:PHE:O	1:A:1597:VAL:C	2.60	0.44
1:A:790:ILE:HD13	1:A:790:ILE:HA	1.74	0.44
1:A:1471:ASP:O	1:A:1472:ASN:C	2.55	0.44
1:A:1365:ASN:HB2	1:A:1373:LEU:HD11	1.99	0.44
1:A:148:MET:SD	1:A:223:VAL:HA	2.58	0.44
1:A:1488:THR:HG22	1:A:1489:GLU:H	1.82	0.44
1:A:702:LEU:O	1:A:703:TRP:C	2.59	0.43
1:A:1612:ILE:HD12	1:A:1621:LEU:HD23	1.91	0.43
1:A:1744:SER:OG	1:A:1747:VAL:CG1	2.61	0.43
1:A:1776:SER:O	1:A:1780:GLU:HB2	2.19	0.43
1:A:201:ILE:HD13	1:A:201:ILE:HA	1.67	0.43
1:A:892:PHE:O	1:A:893:ARG:C	2.61	0.43
1:A:1775:PHE:O	1:A:1779:THR:HB	2.17	0.43
1:A:1207:PHE:HE2	1:A:1253:GLU:HG2	1.82	0.43
1:A:1750:LEU:O	1:A:1754:THR:HG22	2.18	0.43
1:A:188:PHE:C	1:A:190:ARG:H	2.26	0.43
1:A:144:ASN:HD21	1:A:225:ARG:HD2	1.83	0.43
1:A:308:LEU:HB3	1:A:344:ALA:CB	2.49	0.43
1:A:407:LEU:HD12	1:A:407:LEU:HA	1.49	0.43
1:A:868:LEU:HG	1:A:909:VAL:HG11	1.99	0.43
1:A:710:VAL:HG11	1:A:770:ALA:HA	2.00	0.43
1:A:726:CYS:HG	1:A:756:PHE:HD1	1.60	0.43
1:A:795:GLU:HB3	1:A:807:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:MET:HE3	1:A:741:MET:HB2	1.78	0.42
1:A:179:ARG:O	1:A:188:PHE:HB2	2.19	0.42
1:A:910:SER:O	1:A:910:SER:OG	2.31	0.42
1:A:1590:SER:HA	1:A:1593:ILE:CG2	2.47	0.42
1:A:834:ASN:HD22	1:A:838:ALA:HB3	1.84	0.42
1:A:851:PHE:O	1:A:855:VAL:HG23	2.19	0.42
1:A:1564:ASN:O	1:A:1568:VAL:HG23	2.18	0.42
1:A:750:GLN:C	1:A:752:GLY:N	2.75	0.42
1:A:805:SER:O	1:A:808:ARG:N	2.53	0.42
1:A:1630:ILE:O	1:A:1633:ILE:HB	2.20	0.42
1:A:1258:TRP:HZ2	1:A:1276:PHE:HE2	1.67	0.42
1:A:806:VAL:O	1:A:807:LEU:C	2.60	0.42
1:A:1319:GLY:O	1:A:1320:MET:C	2.59	0.42
1:A:934:PHE:O	1:A:935:LEU:C	2.61	0.42
1:A:1530:PHE:O	1:A:1534:ILE:HG12	2.20	0.42
1:A:1542:MET:O	1:A:1546:MET:HG3	2.20	0.42
1:A:1491:GLN:O	1:A:1492:LYS:C	2.61	0.42
1:A:1545:MET:SD	1:A:1633:ILE:HD11	2.60	0.42
1:A:1725:PRO:HB2	1:A:1726:PRO:HD3	2.02	0.42
1:A:751:VAL:O	1:A:751:VAL:HG12	2.20	0.42
1:A:1388:ASN:OD1	1:A:1393:LEU:HB2	2.19	0.41
1:A:1542:MET:HG3	1:A:1633:ILE:HD12	2.02	0.41
1:A:1722:ASN:OD1	1:A:1727:TYR:HB3	2.20	0.41
1:A:218:LEU:HA	1:A:221:PHE:CE2	2.56	0.41
1:A:1240:GLU:O	1:A:1241:TYR:C	2.63	0.41
1:A:903:MET:O	1:A:904:TRP:C	2.62	0.41
1:A:1194:LEU:O	1:A:1197:THR:HG22	2.20	0.41
1:A:1220:GLY:C	1:A:1222:LEU:H	2.27	0.41
1:A:1717:LEU:HD13	1:A:1752:PHE:CD2	2.55	0.41
1:A:848:ILE:HD13	1:A:848:ILE:HA	1.83	0.41
1:A:1453:PHE:O	1:A:1457:GLY:N	2.44	0.41
1:A:1578:LYS:HD3	1:A:1592:ASN:HD21	1.85	0.41
1:A:729:LEU:HB3	1:A:756:PHE:CZ	2.56	0.41
1:A:1595:ASP:O	1:A:1596:PHE:C	2.58	0.41
1:A:164:PHE:O	1:A:165:THR:C	2.61	0.41
1:A:252:ASP:O	1:A:253:VAL:C	2.62	0.41
1:A:263:VAL:O	1:A:267:ILE:HG13	2.21	0.41
1:A:269:LEU:HD12	1:A:355:PHE:O	2.21	0.41
1:A:753:ASN:O	1:A:754:LEU:C	2.63	0.41
1:A:880:HIS:NE2	1:A:886:HIS:CD2	2.89	0.41
1:A:900:ILE:O	1:A:901:GLU:C	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ALA:HB1	1:A:1775:PHE:HE1	1.86	0.40
1:A:1590:SER:CA	1:A:1593:ILE:HG22	2.51	0.40
1:A:281:VAL:HG12	1:A:314:TYR:HD1	1.85	0.40
1:A:723:ILE:O	1:A:724:THR:C	2.60	0.40
1:A:1245:MET:HE3	1:A:1245:MET:HB3	1.90	0.40
1:A:1330:ALA:O	1:A:1334:ILE:HG12	2.21	0.40
1:A:805:SER:O	1:A:806:VAL:C	2.62	0.40
1:A:813:LEU:C	1:A:815:VAL:N	2.77	0.40
1:A:218:LEU:HA	1:A:221:PHE:CD2	2.57	0.40
1:A:707:LYS:HE2	1:A:707:LYS:HB3	1.98	0.40
1:A:1429:VAL:HG13	1:A:1444:LEU:HA	2.03	0.40
1:A:1704:LEU:HD23	1:A:1704:LEU:HA	1.87	0.40
1:A:1771:ILE:HG21	4:A:2111:9Z9:C14	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1145/2059 (56%)	1073 (94%)	68 (6%)	4 (0%)	37 66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1735	SER
1	A	303	SER
1	A	297	ASP
1	A	1366	GLN

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	1013/1794 (56%)	972 (96%)	41 (4%)	27 52

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	202	ILE
1	A	205	TYR
1	A	290	THR
1	A	320	THR
1	A	323	VAL
1	A	326	CYS
1	A	336	PRO
1	A	375	GLU
1	A	407	LEU
1	A	419	GLN
1	A	707	LYS
1	A	712	LEU
1	A	729	LEU
1	A	733	PHE
1	A	742	THR
1	A	764	MET
1	A	790	ILE
1	A	804	LEU
1	A	806	VAL
1	A	811	ARG
1	A	848	ILE
1	A	881	MET
1	A	906	CYS
1	A	909	VAL
1	A	931	LEU
1	A	937	LEU
1	A	1206	TRP
1	A	1212	ILE
1	A	1239	LEU

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Mol	Chain	Res	Type
1	A	1247	THR
1	A	1286	LEU
1	A	1308	LEU
1	A	1328	VAL
1	A	1465	PHE
1	A	1485	ILE
1	A	1625	ILE
1	A	1720	ILE
1	A	1750	LEU
1	A	1758	ILE
1	A	1777	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	ASN
1	A	350	HIS
1	A	834	ASN
1	A	886	HIS
1	A	1507	GLN
1	A	1558	ASN
1	A	1774	ASN

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](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	A	2107	1	14,14,15	0.60	0	17,19,21	0.94	1 (5%)
2	NAG	A	2102	1	14,14,15	0.43	0	17,19,21	0.98	1 (5%)
2	NAG	A	2106	1	14,14,15	0.72	1 (7%)	17,19,21	1.51	2 (11%)
2	NAG	A	2108	1	14,14,15	0.55	0	17,19,21	1.48	2 (11%)
2	NAG	A	2101	1	14,14,15	0.62	0	17,19,21	1.19	2 (11%)
2	NAG	A	2103	1	14,14,15	0.47	0	17,19,21	1.15	2 (11%)
2	NAG	A	2105	1	14,14,15	0.62	0	17,19,21	1.38	3 (17%)
4	9Z9	A	2111	-	44,44,44	0.62	1 (2%)	66,68,68	1.03	4 (6%)
2	NAG	A	2109	1	14,14,15	0.62	0	17,19,21	1.78	3 (17%)
2	NAG	A	2104	1	14,14,15	0.44	0	17,19,21	1.27	3 (17%)
3	9SR	A	2110	-	16,25,25	2.72	6 (37%)	18,44,44	1.74	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	2107	1	-	4/6/23/26	0/1/1/1
2	NAG	A	2102	1	-	3/6/23/26	0/1/1/1
2	NAG	A	2106	1	-	2/6/23/26	0/1/1/1
2	NAG	A	2108	1	-	2/6/23/26	0/1/1/1
2	NAG	A	2101	1	-	1/6/23/26	0/1/1/1
2	NAG	A	2103	1	-	3/6/23/26	0/1/1/1
2	NAG	A	2105	1	-	2/6/23/26	0/1/1/1
4	9Z9	A	2111	-	-	8/12/100/100	0/6/6/6
2	NAG	A	2109	1	-	4/6/23/26	0/1/1/1
2	NAG	A	2104	1	-	3/6/23/26	0/1/1/1
3	9SR	A	2110	-	-	0/3/70/70	0/5/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2110	9SR	C21-C03	5.10	1.63	1.52
3	A	2110	9SR	C13-N18	4.55	1.45	1.34
3	A	2110	9SR	C03-C05	-4.26	1.45	1.53
3	A	2110	9SR	C03-C02	-4.06	1.45	1.53
3	A	2110	9SR	O20-C19	-3.74	1.35	1.42
3	A	2110	9SR	O04-C03	-2.76	1.39	1.43
4	A	2111	9Z9	O80-C79	-2.06	1.40	1.43
2	A	2106	NAG	C2-N2	-2.03	1.42	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2110	9SR	C17-C11-N12	5.63	114.33	108.12
4	A	2111	9Z9	O80-C73-C76	4.56	115.01	110.77
2	A	2109	NAG	C2-N2-C7	-4.47	116.54	122.90
2	A	2106	NAG	C2-N2-C7	-4.40	116.64	122.90
2	A	2108	NAG	C3-C4-C5	-4.18	102.78	110.24
2	A	2109	NAG	C4-C3-C2	-4.01	105.14	111.02
2	A	2104	NAG	C4-C3-C2	-3.19	106.34	111.02
4	A	2111	9Z9	C77-C78-C79	3.07	112.82	108.56
2	A	2101	NAG	C1-O5-C5	-2.81	108.39	112.19
2	A	2101	NAG	O5-C5-C4	-2.80	104.00	110.83
2	A	2105	NAG	C1-O5-C5	2.76	115.93	112.19
2	A	2106	NAG	C3-C4-C5	-2.76	105.32	110.24
2	A	2108	NAG	C4-C3-C2	-2.65	107.13	111.02
3	A	2110	9SR	C03-C02-C19	-2.57	110.35	114.38
2	A	2104	NAG	O5-C5-C6	2.57	111.23	107.20
2	A	2105	NAG	C6-C5-C4	-2.48	107.19	113.00
4	A	2111	9Z9	C79-O80-C73	2.39	118.24	113.72
2	A	2109	NAG	O5-C1-C2	-2.36	107.56	111.29
2	A	2103	NAG	C1-O5-C5	-2.32	109.04	112.19
2	A	2103	NAG	O5-C5-C6	2.30	110.82	107.20
2	A	2107	NAG	C1-C2-N2	2.25	114.33	110.49
2	A	2105	NAG	O5-C5-C6	-2.13	103.86	107.20
2	A	2102	NAG	O5-C5-C4	-2.11	105.70	110.83
2	A	2104	NAG	C3-C4-C5	-2.04	106.61	110.24
4	A	2111	9Z9	O80-C73-O72	-2.02	104.15	109.78

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2103	NAG	O7-C7-N2-C2
2	A	2105	NAG	C8-C7-N2-C2
2	A	2105	NAG	O7-C7-N2-C2
2	A	2107	NAG	C8-C7-N2-C2
2	A	2107	NAG	O7-C7-N2-C2
2	A	2108	NAG	O7-C7-N2-C2
4	A	2111	9Z9	C22-C21-O20-C17
4	A	2111	9Z9	C48-C23-C24-O25
4	A	2111	9Z9	C24-C23-C48-O49
2	A	2103	NAG	C8-C7-N2-C2
2	A	2108	NAG	C8-C7-N2-C2
2	A	2106	NAG	C8-C7-N2-C2
2	A	2106	NAG	O7-C7-N2-C2
2	A	2109	NAG	O5-C5-C6-O6
2	A	2102	NAG	C8-C7-N2-C2
2	A	2102	NAG	O7-C7-N2-C2
2	A	2107	NAG	O5-C5-C6-O6
4	A	2111	9Z9	C21-C22-C23-C24
4	A	2111	9Z9	O20-C21-C22-C23
4	A	2111	9Z9	C22-C23-C24-O25
4	A	2111	9Z9	C22-C23-C48-O49
2	A	2109	NAG	C4-C5-C6-O6
2	A	2101	NAG	O5-C5-C6-O6
2	A	2107	NAG	C4-C5-C6-O6
2	A	2102	NAG	O5-C5-C6-O6
2	A	2104	NAG	O5-C5-C6-O6
4	A	2111	9Z9	C23-C24-O25-C26
2	A	2109	NAG	C8-C7-N2-C2
2	A	2104	NAG	C8-C7-N2-C2
2	A	2104	NAG	O7-C7-N2-C2
2	A	2109	NAG	O7-C7-N2-C2
2	A	2103	NAG	C1-C2-N2-C7

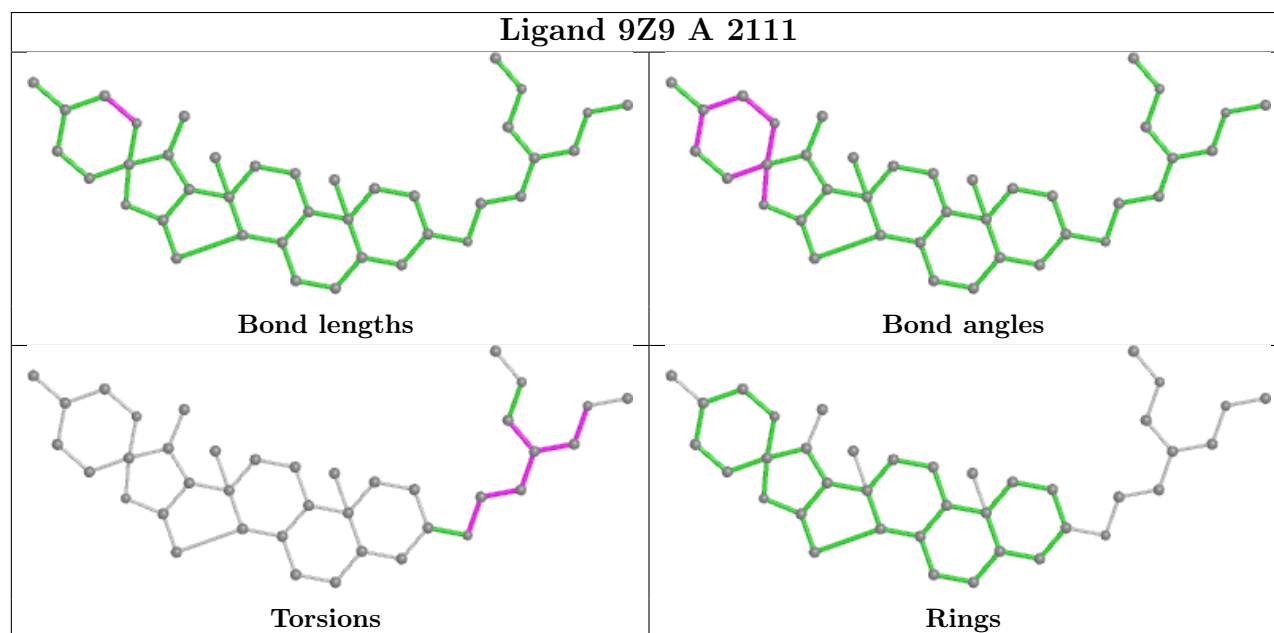
There are no ring outliers.

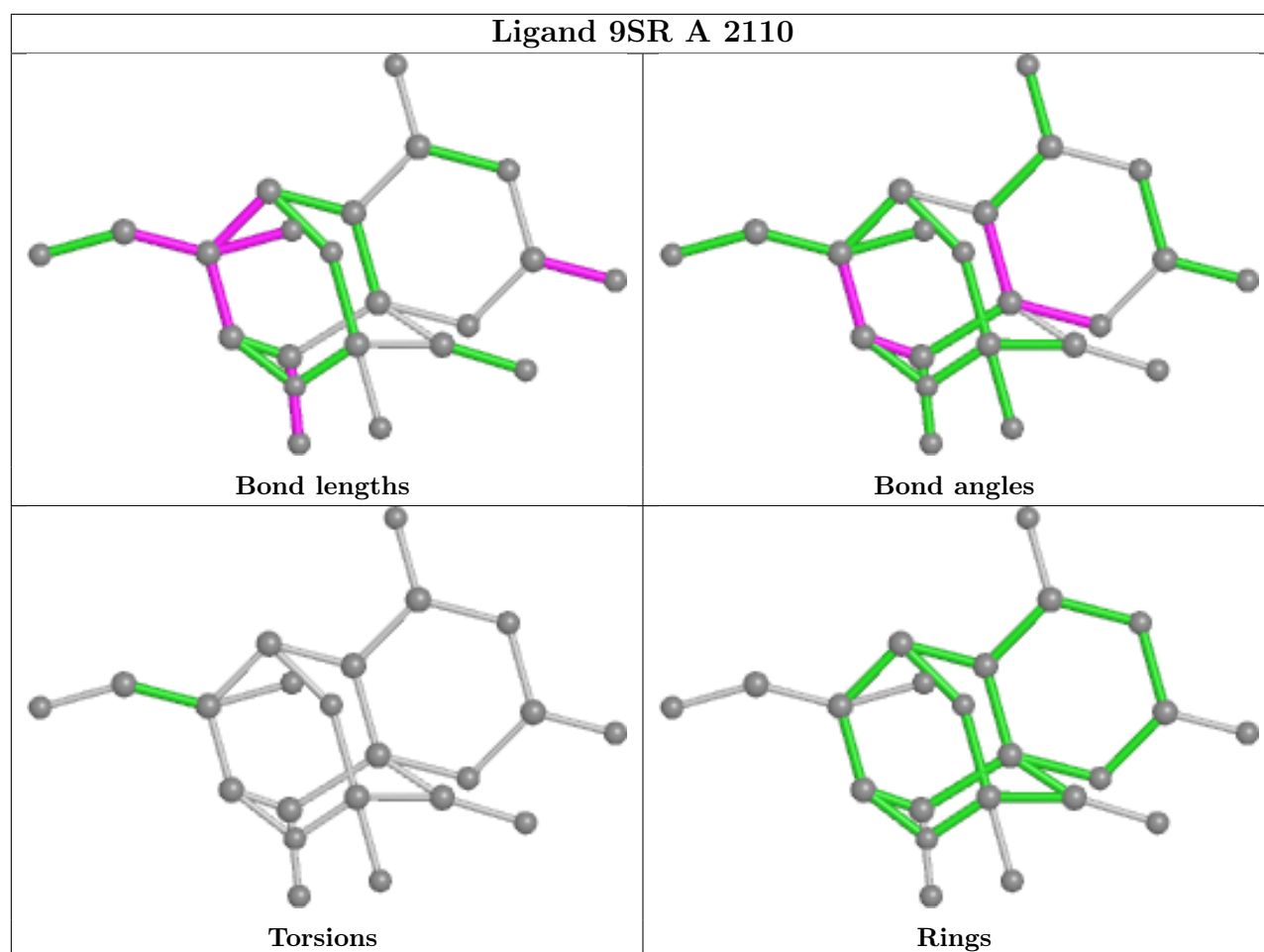
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2111	9Z9	1	0
3	A	2110	9SR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

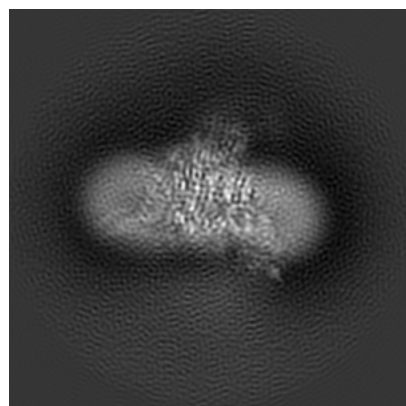
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60865. These allow visual inspection of the internal detail of the map and identification of artifacts.

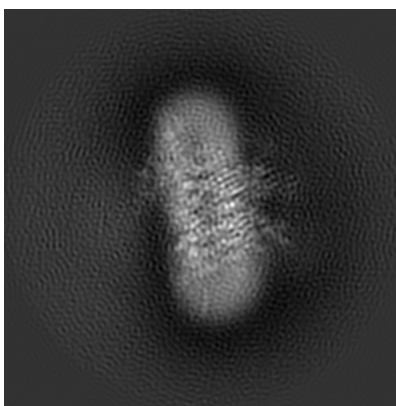
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

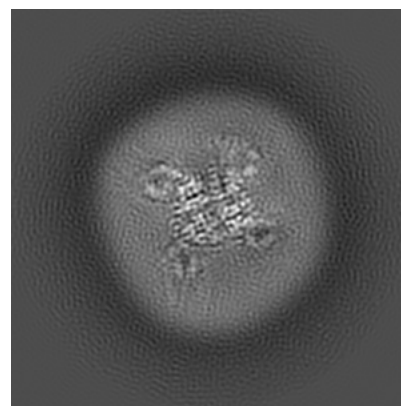
6.1.1 Primary map



X

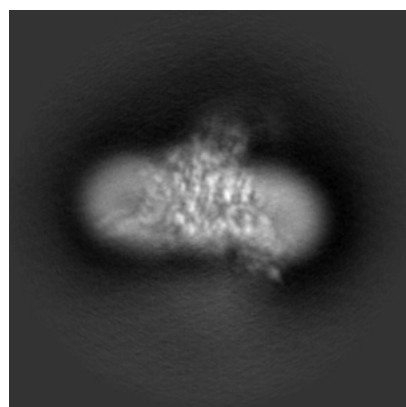


Y

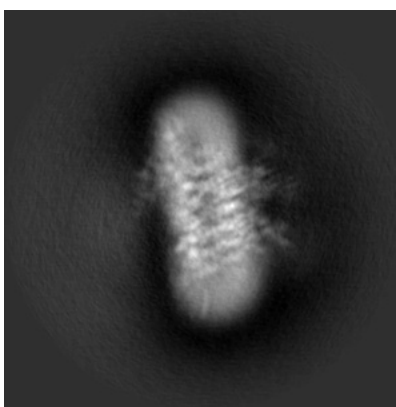


Z

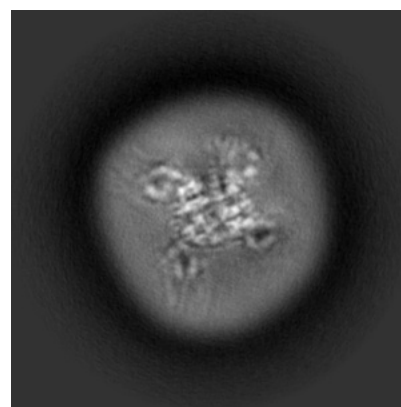
6.1.2 Raw map



X



Y

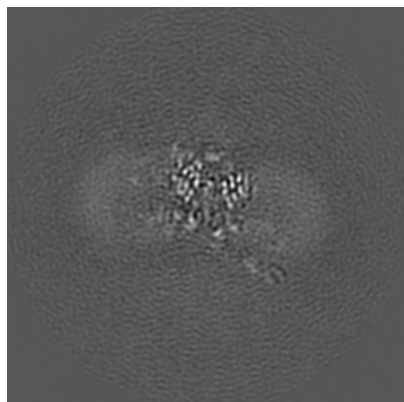


Z

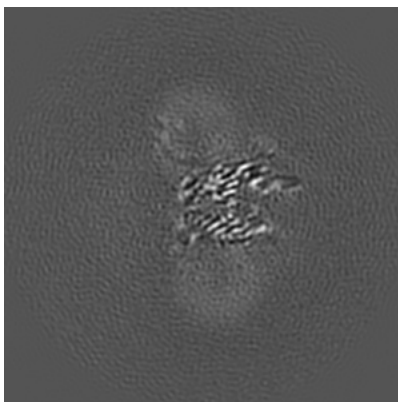
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

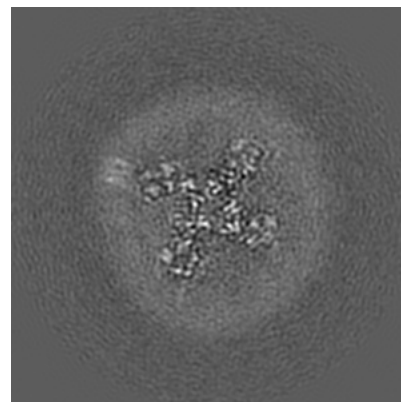
6.2.1 Primary map



X Index: 120

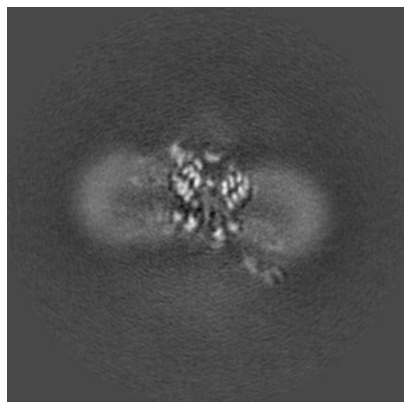


Y Index: 120

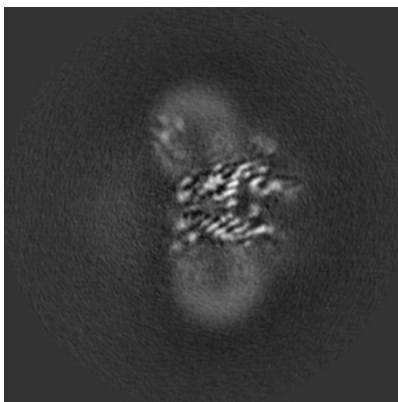


Z Index: 120

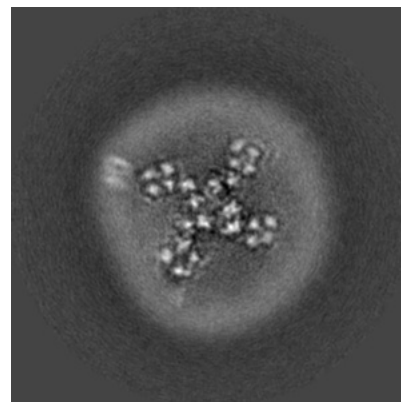
6.2.2 Raw map



X Index: 120



Y Index: 120

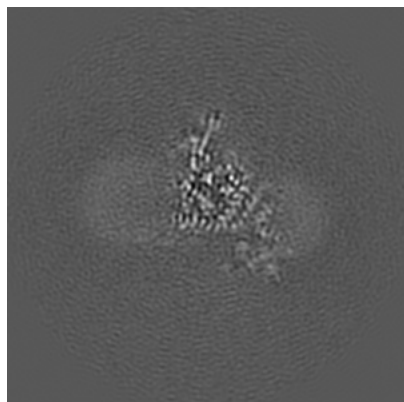


Z Index: 120

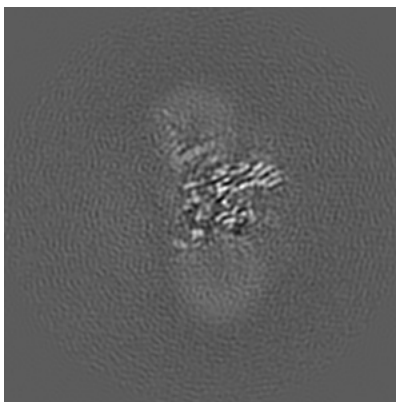
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

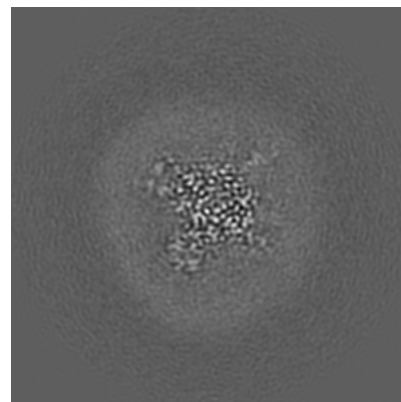
6.3.1 Primary map



X Index: 133

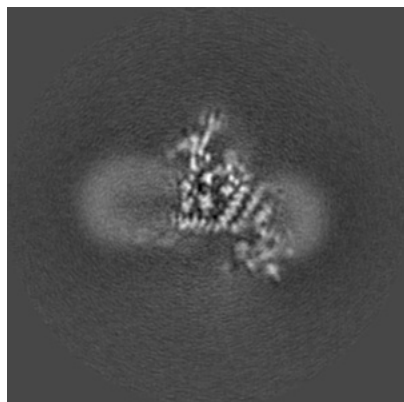


Y Index: 112

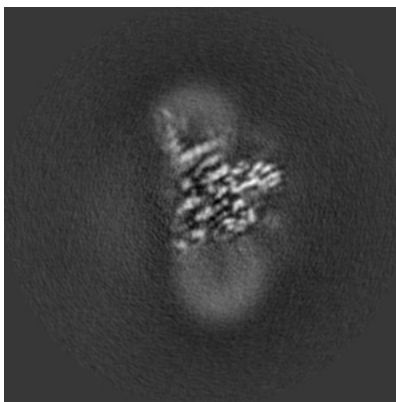


Z Index: 132

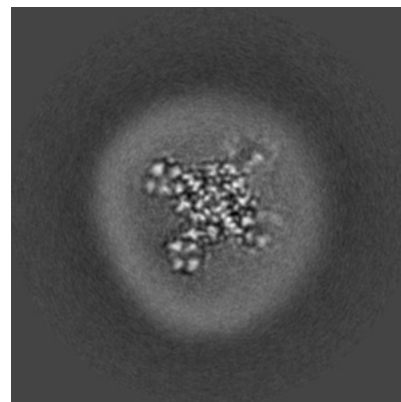
6.3.2 Raw map



X Index: 133



Y Index: 111

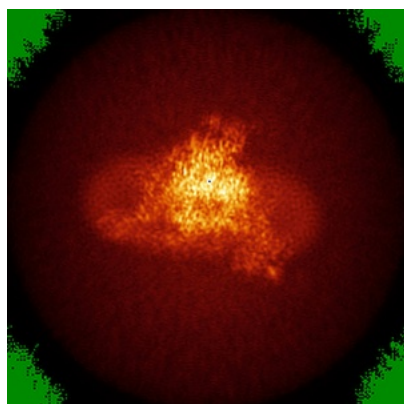


Z Index: 131

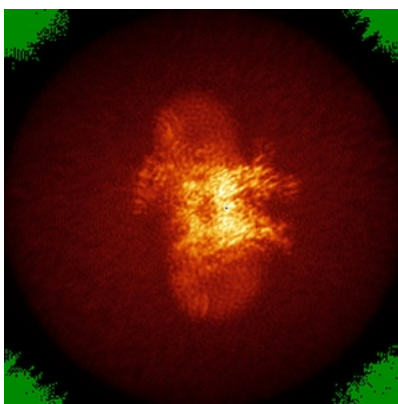
The images above show the largest variance slices of the map in three orthogonal directions.

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

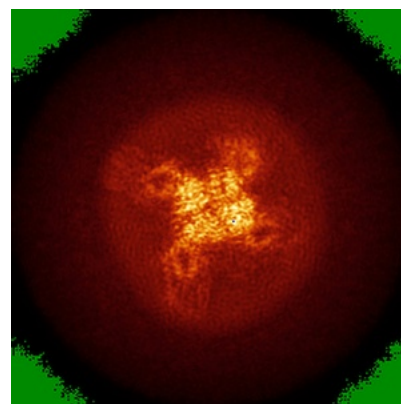
6.4.1 Primary map



X

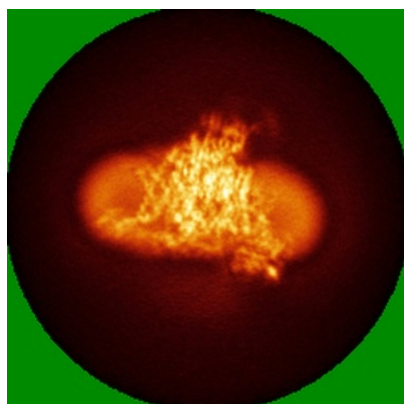


Y

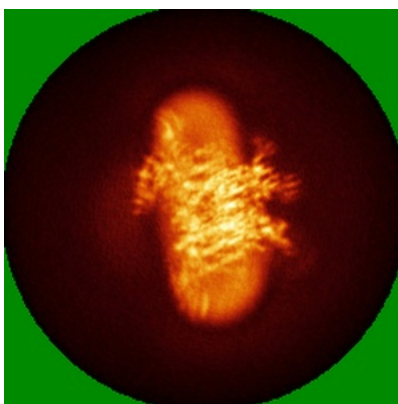


Z

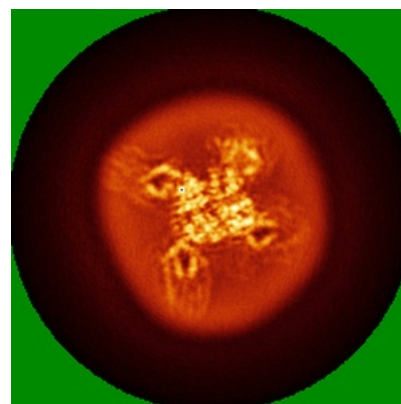
6.4.2 Raw map



X



Y

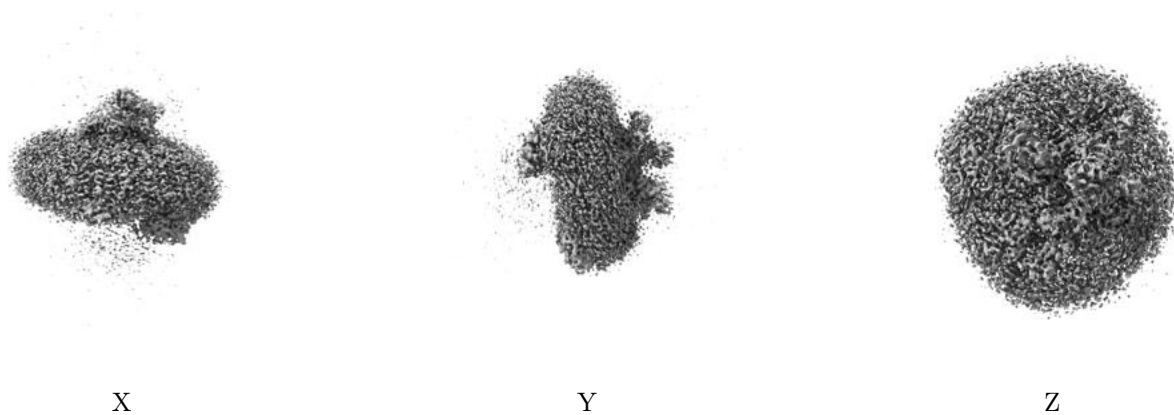


Z

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.

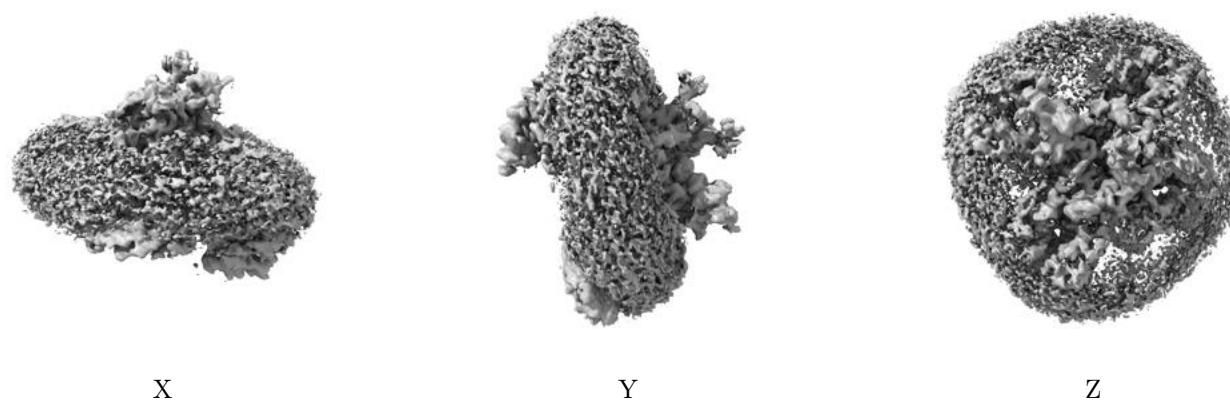
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0171. 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.

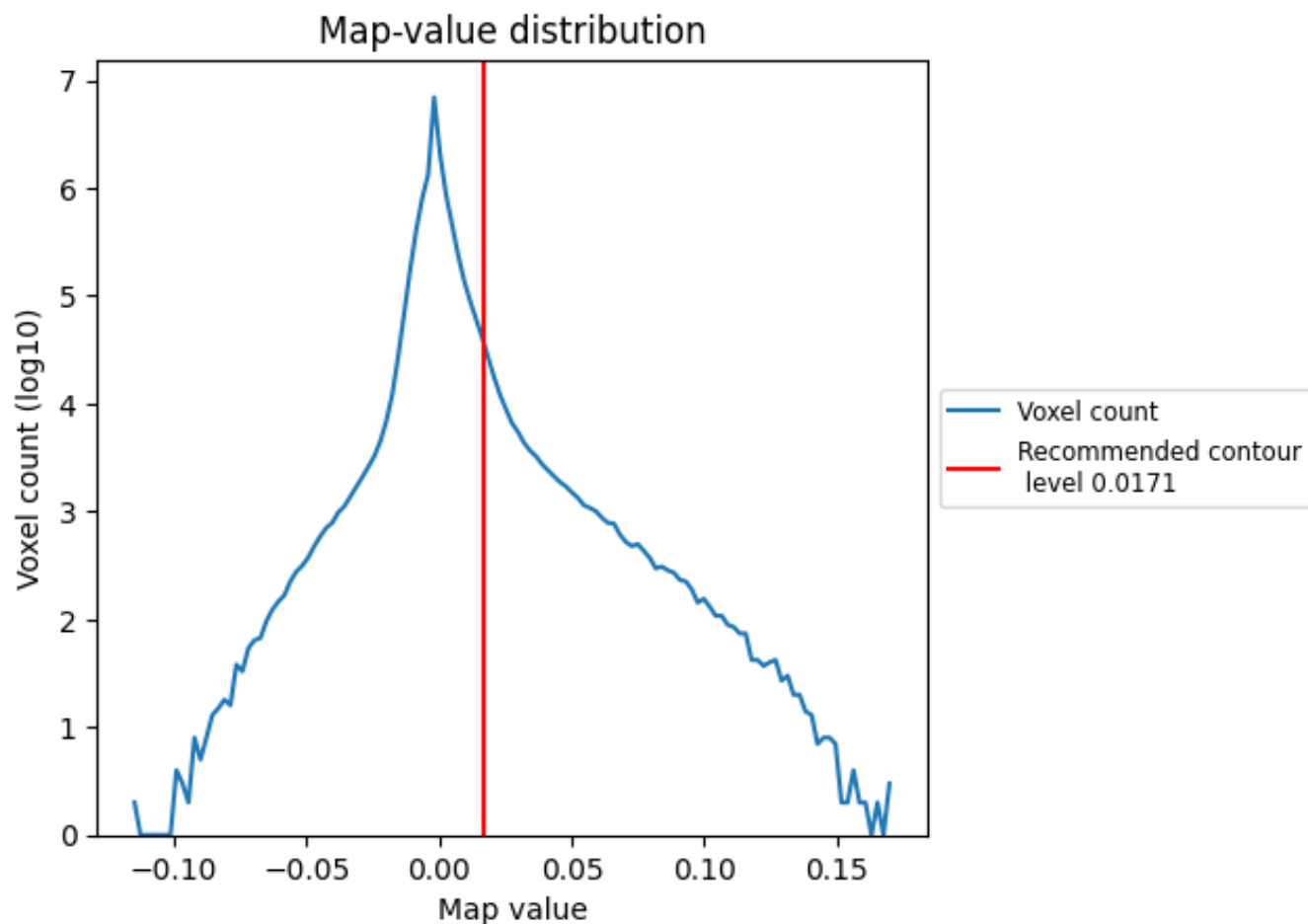
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

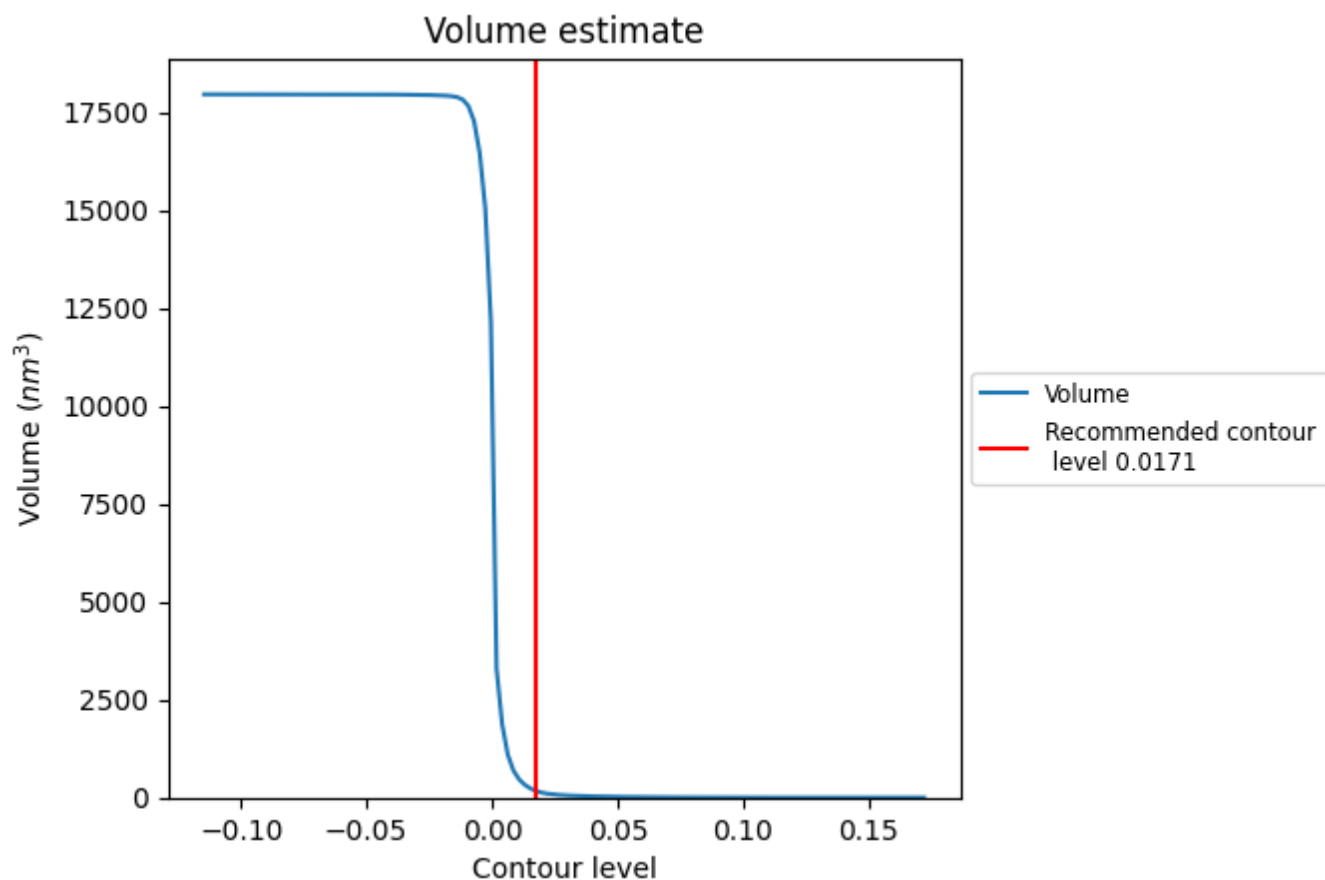
This section contains the results of statistical analysis of the map.

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.

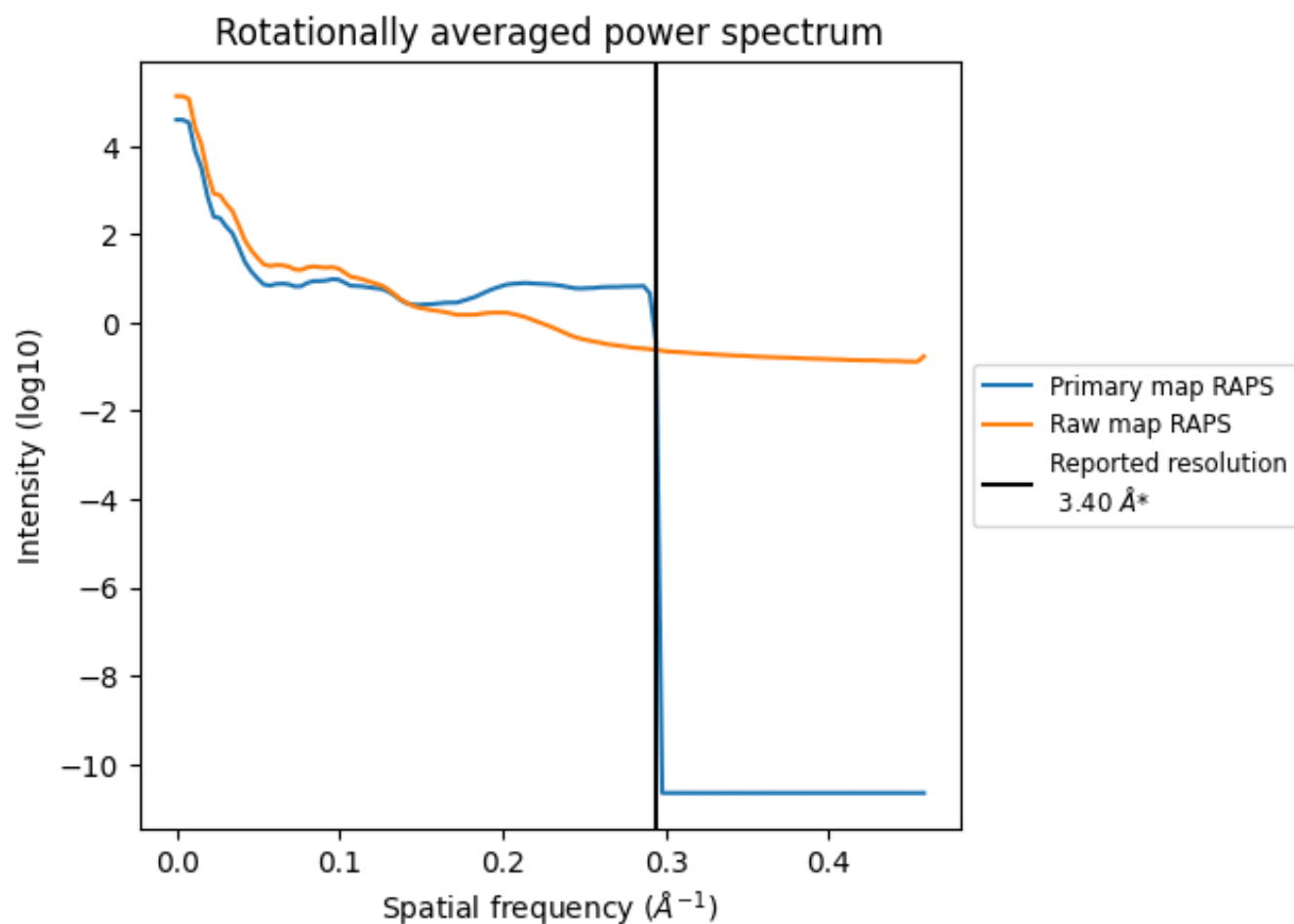
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 182 nm³; this corresponds to an approximate mass of 164 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 ⓘ

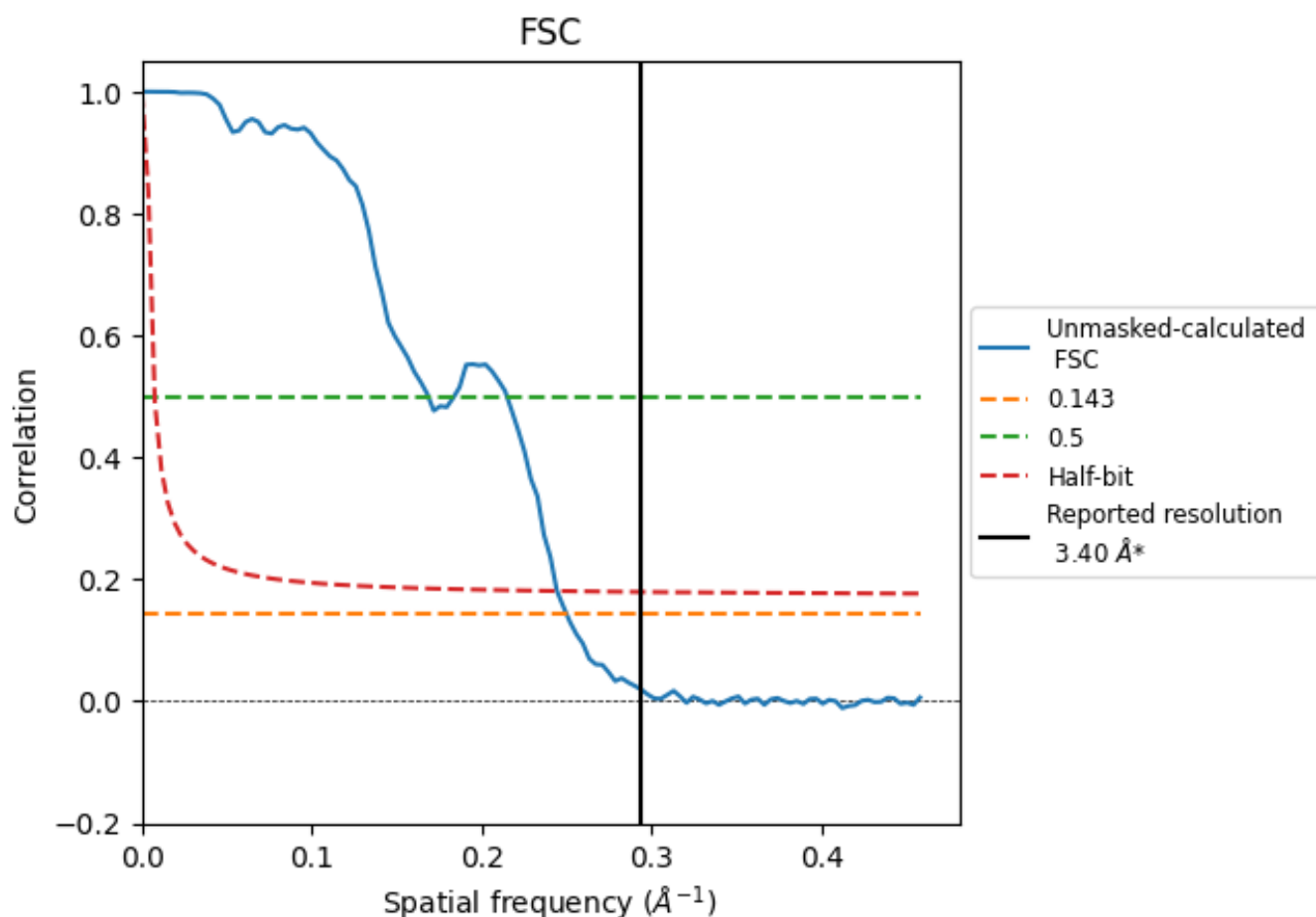


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

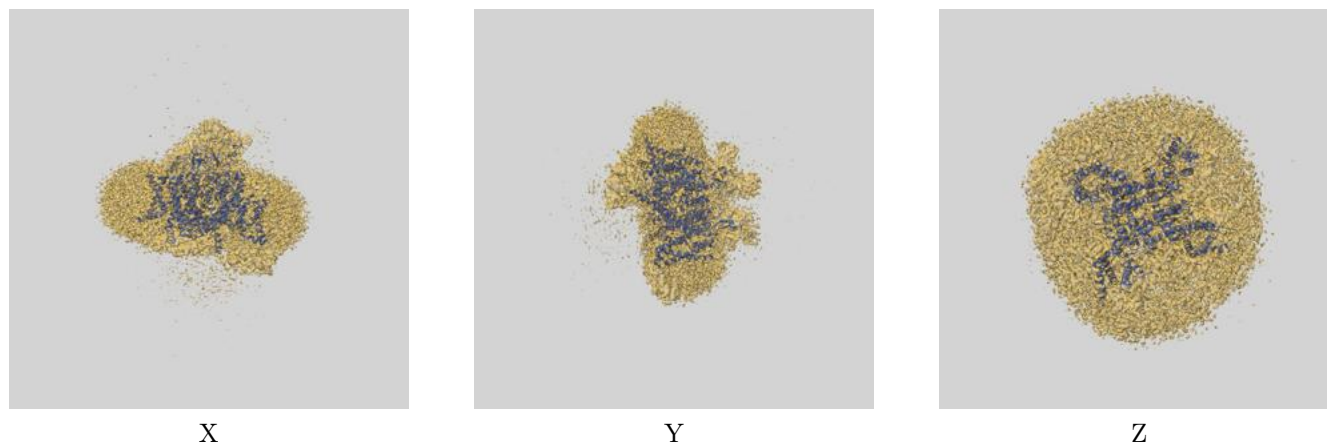
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.00	5.93	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.00 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

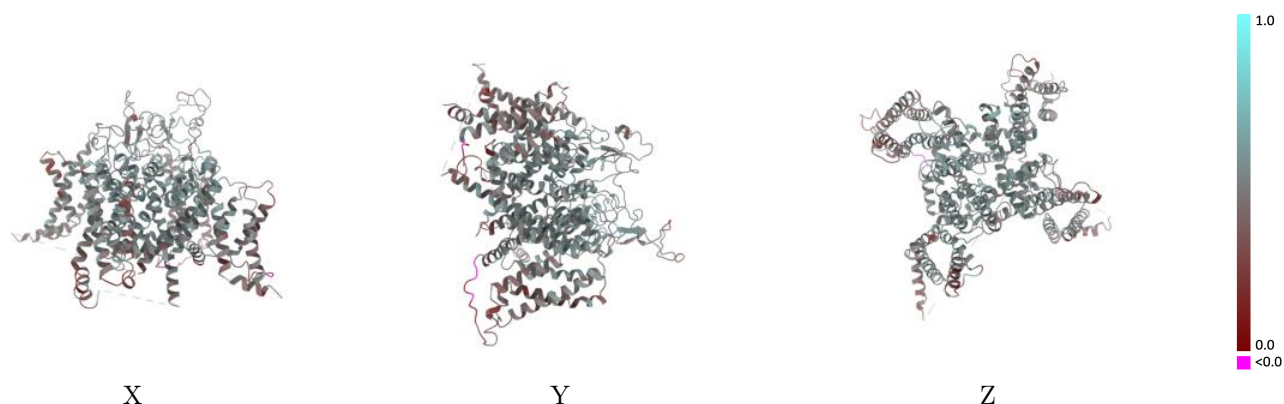
This section contains information regarding the fit between EMDB map EMD-60865 and PDB model 9ITH. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



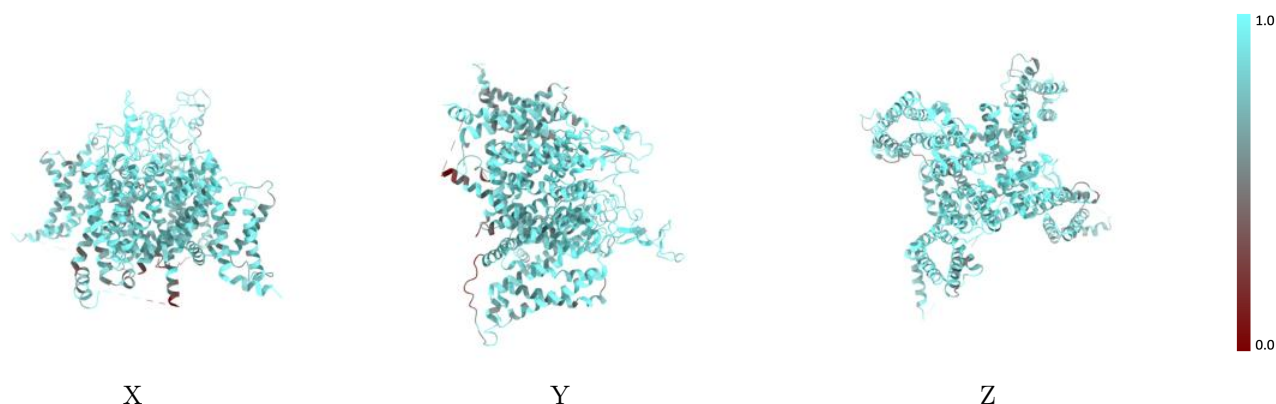
The images above show the 3D surface view of the map at the recommended contour level 0.0171 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



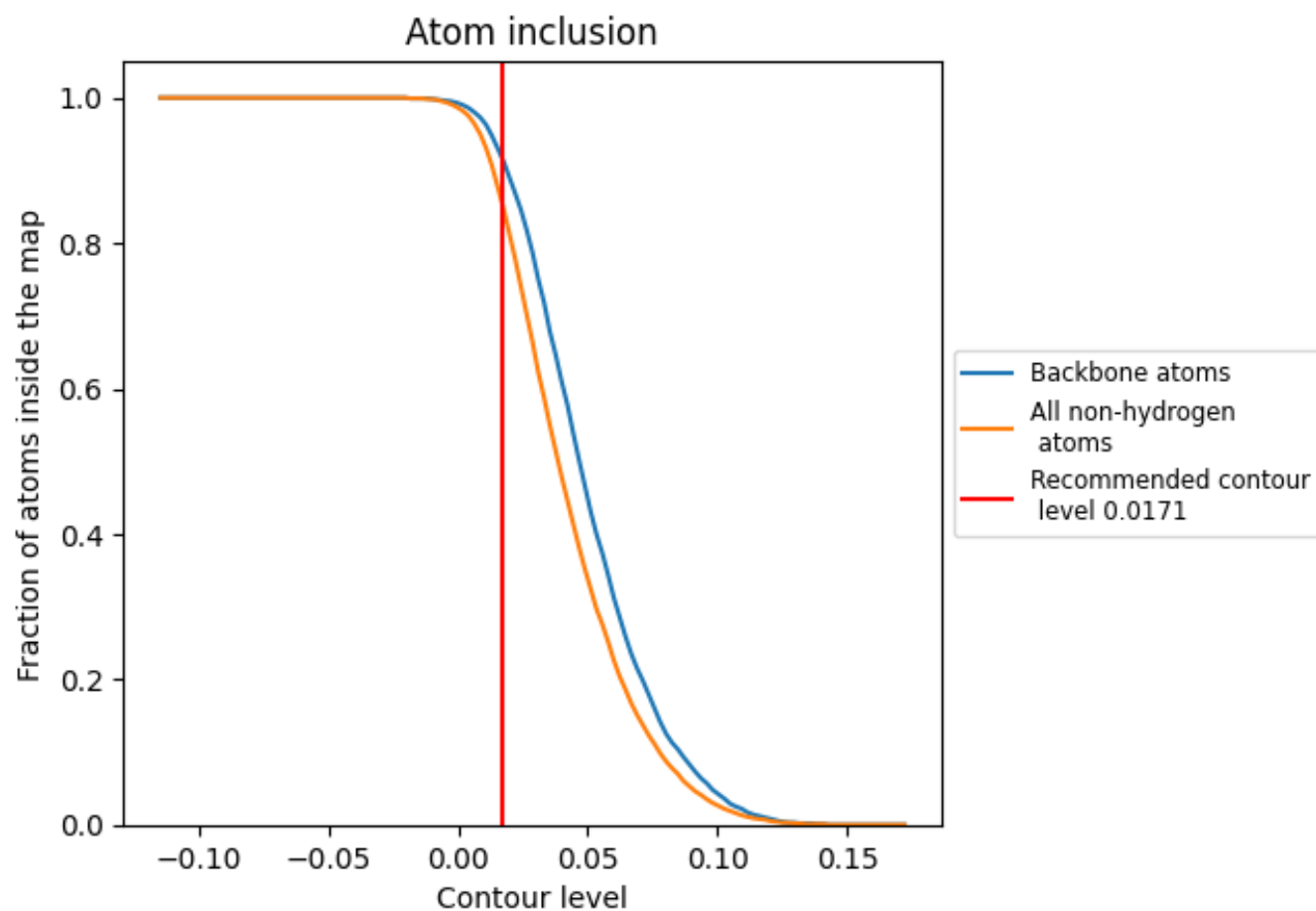
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0171).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 85% 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 (0.0171) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8530	<div><div></div></div> 0.4770
A	<div><div></div></div> 0.8530	<div><div></div></div> 0.4770

