



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:36 PM UTC

PDB ID : 6SKZ / pdb_00006skz
EMDB ID : EMD-10232
Title : Structure of the closed conformation of CtTel1
Authors : Jansma, M.; Eustermann, S.E.; Kostrewa, D.; Lammens, K.; Hopfner, K.P.
Deposited on : 2019-08-16
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

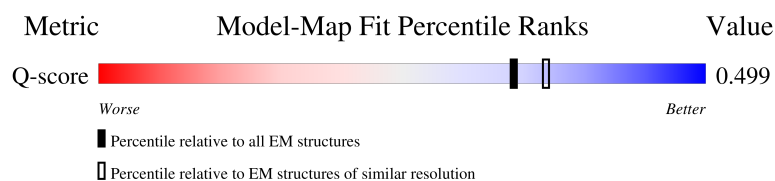
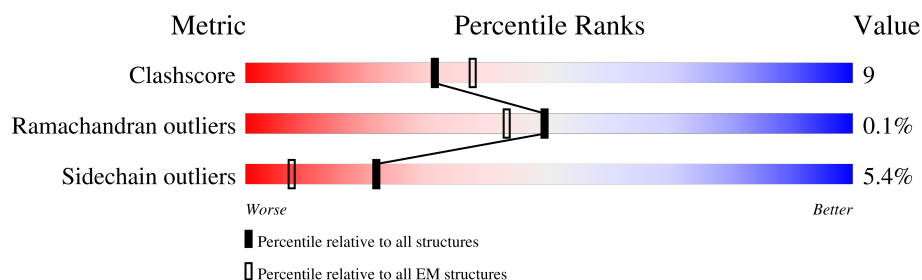
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	2944	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20930 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 Serine/threonine-protein kinase Tel1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2638	Total	C	N	O	S	0	0
			20898	13292	3638	3874	94		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2847	LEU	PHE	conflict	UNP G0S4S9
A	2848	TYR	-	insertion	UNP G0S4S9
A	2849	GLN	-	insertion	UNP G0S4S9
A	2850	TRP	-	insertion	UNP G0S4S9
A	2851	SER	-	insertion	UNP G0S4S9
A	2852	ILE	-	insertion	UNP G0S4S9
A	2853	SER	-	insertion	UNP G0S4S9
A	2854	PRO	-	insertion	UNP G0S4S9
A	2855	VAL	-	insertion	UNP G0S4S9
A	2856	ARG	-	insertion	UNP G0S4S9
A	2857	MET	-	insertion	UNP G0S4S9
A	2858	ALA	-	insertion	UNP G0S4S9
A	2859	LYS	-	insertion	UNP G0S4S9
A	2860	LEU	-	insertion	UNP G0S4S9
A	2861	GLN	-	insertion	UNP G0S4S9
A	2862	ASN	-	insertion	UNP G0S4S9
A	2863	ALA	-	insertion	UNP G0S4S9
A	2864	ARG	-	insertion	UNP G0S4S9
A	2865	GLU	-	insertion	UNP G0S4S9
A	2866	VAL	-	insertion	UNP G0S4S9

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

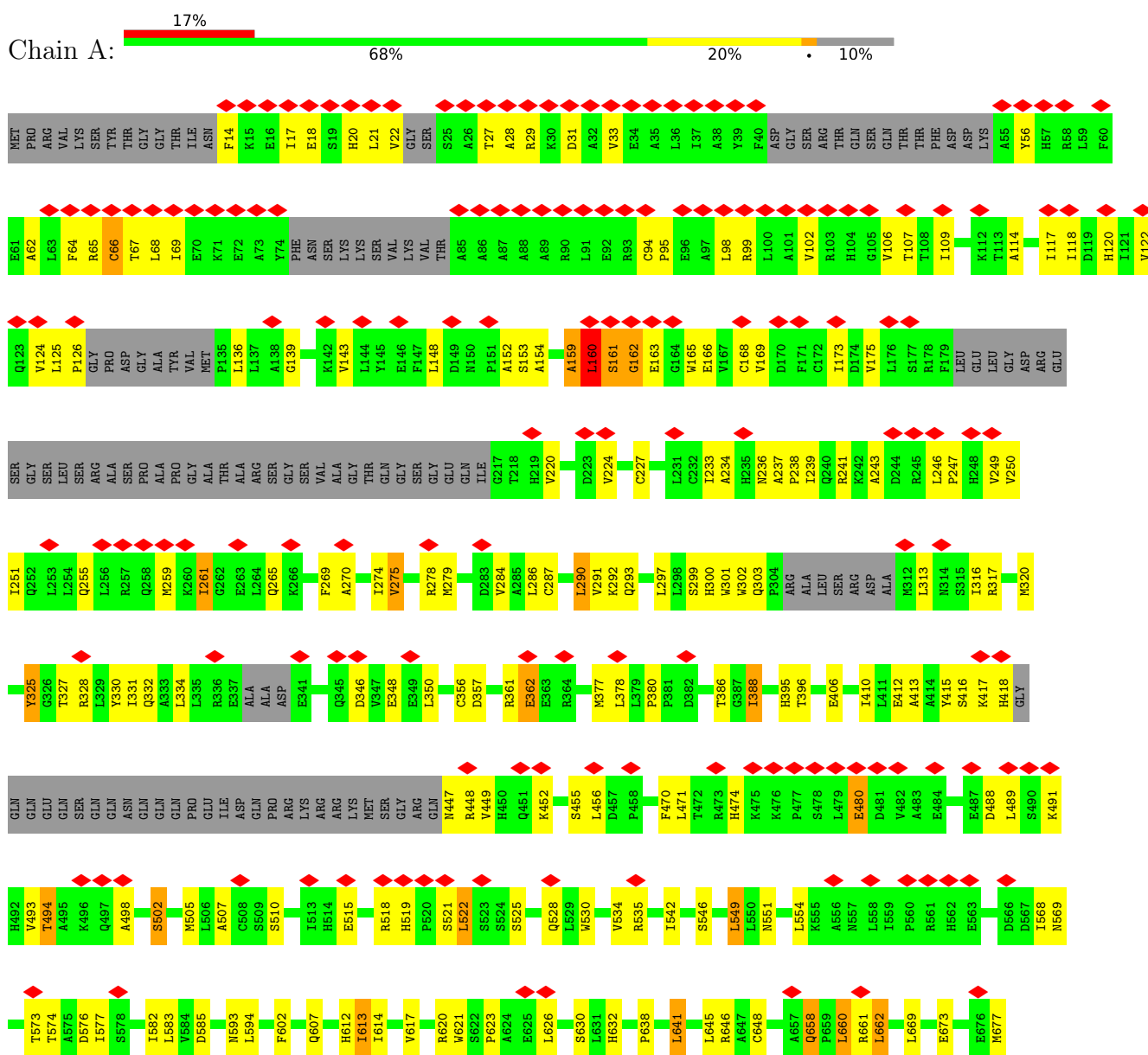
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

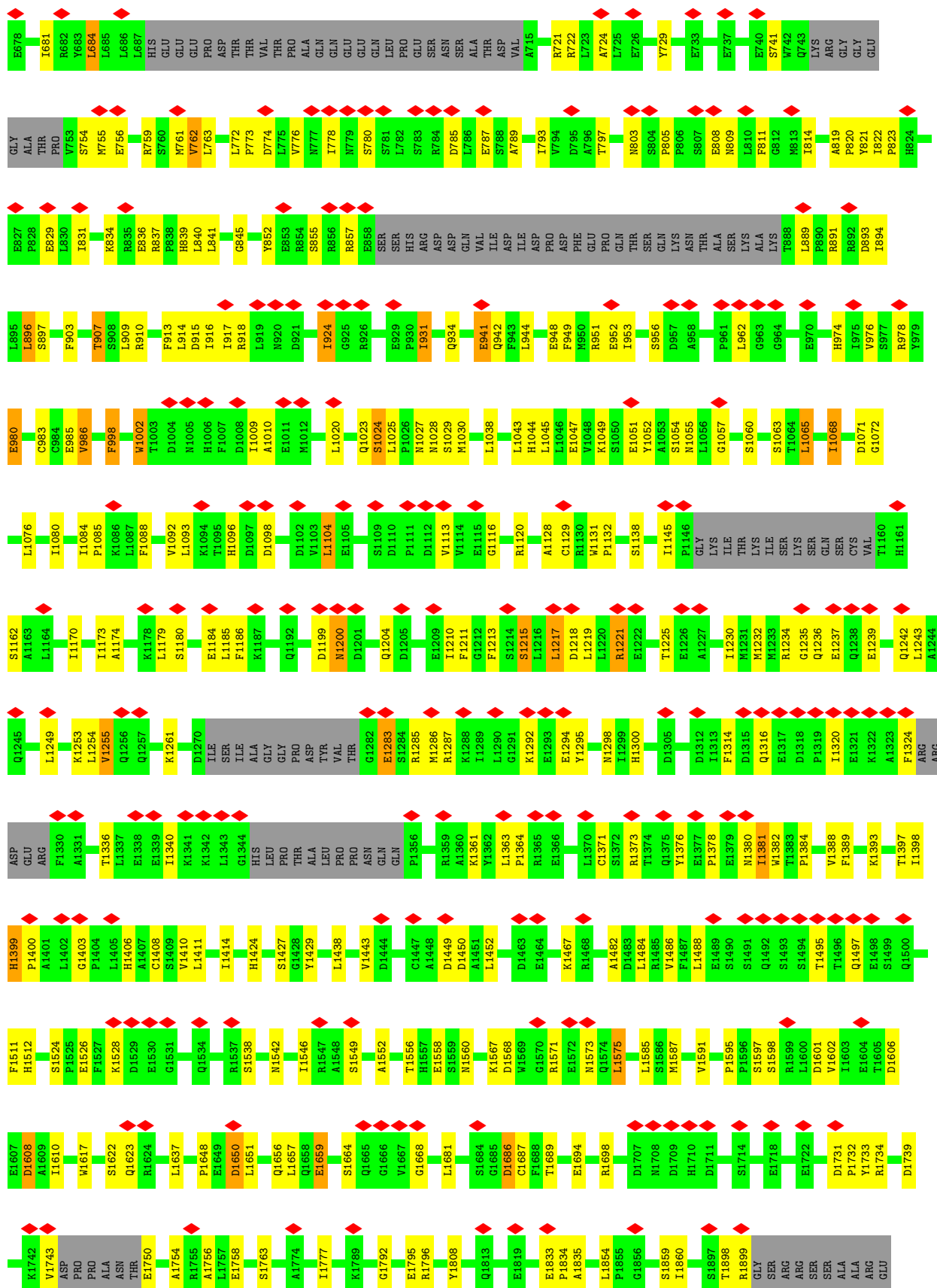
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Mg 1 1	0

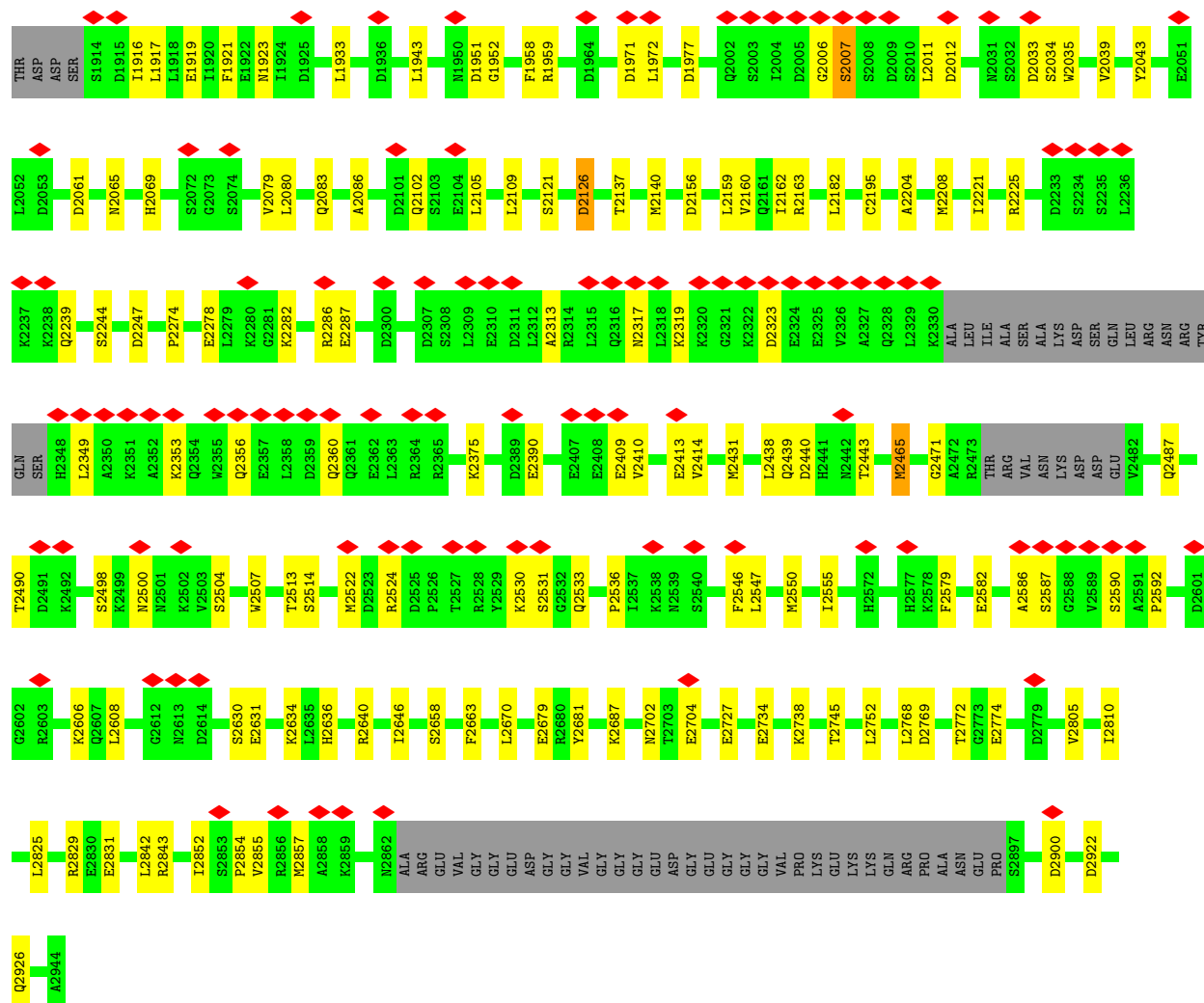
3 Residue-property plots

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: Serine/threonine-protein kinase Tel1







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	132127	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 ($e^-/\text{\AA}^2$)	55.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0126	Depositor
Map size (Å)	372.768, 372.768, 372.768	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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: MG, AGS

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	0.44	0/21306	0.46	2/28856 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2007	SER	N-CA-CB	-6.82	98.97	110.49
1	A	162	GLY	N-CA-C	-5.40	107.75	115.64

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	ALA	Peptide
1	A	2006	GLY	Peptide
1	A	259	MET	Peptide
1	A	361	ARG	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	20898	0	21075	368	0
2	A	31	0	12	1	0
3	A	1	0	0	0	0
All	All	20930	0	21087	369	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 9.

All (369) 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:1528:LYS:NZ	1:A:1573:ASN:OD1	1.96	0.97
1:A:1917:LEU:HD21	1:A:2810:ILE:HD13	1.48	0.93
1:A:2702:ASN:ND2	1:A:2704:GLU:OE1	2.00	0.93
1:A:2012:ASP:OD1	1:A:2034:SER:OG	1.87	0.92
1:A:1528:LYS:HZ3	1:A:1573:ASN:CG	1.88	0.81
1:A:721:ARG:HB3	1:A:778:ILE:HD11	1.63	0.80
1:A:1023:GLN:O	1:A:1027:ASN:ND2	2.15	0.79
1:A:173:ILE:HG23	1:A:249:VAL:HG21	1.67	0.77
1:A:772:LEU:HD13	1:A:787:GLU:HG3	1.66	0.77
1:A:125:LEU:HD12	1:A:126:PRO:HD2	1.65	0.76
1:A:522:LEU:O	1:A:525:SER:HB3	1.87	0.75
1:A:2498:SER:HB3	1:A:2507:TRP:CD1	2.25	0.72
1:A:551:ASN:OD1	1:A:593:ASN:ND2	2.24	0.71
1:A:2586:ALA:HB3	1:A:2592:PRO:HG2	1.71	0.71
1:A:1650:ASP:N	1:A:1650:ASP:OD1	2.22	0.70
1:A:1002:TRP:HB3	1:A:1010:ALA:HA	1.74	0.70
1:A:1917:LEU:HD21	1:A:2810:ILE:CD1	2.20	0.70
1:A:614:ILE:HD13	1:A:724:ALA:HB2	1.74	0.70
1:A:1068:ILE:HG23	1:A:1076:LEU:HD21	1.74	0.69
1:A:474:HIS:O	1:A:474:HIS:ND1	2.26	0.69
1:A:1777:ILE:HD11	1:A:1808:TYR:HB2	1.74	0.68
1:A:646:ARG:NH1	1:A:774:ASP:OD1	2.27	0.68
1:A:1092:VAL:HG11	1:A:1497:GLN:HG2	1.75	0.67
1:A:1528:LYS:NZ	1:A:1573:ASN:CG	2.50	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ALA:HB3	1:A:237:ALA:HB2	1.76	0.67
1:A:20:HIS:HB3	1:A:28:ALA:HB1	1.75	0.67
1:A:303:GLN:O	1:A:317:ARG:NH1	2.27	0.67
1:A:300:HIS:HD1	1:A:301:TRP:CD1	2.13	0.66
1:A:811:PHE:HA	1:A:814:ILE:HG22	1.78	0.66
1:A:1295:TYR:OH	1:A:1373:ARG:NH2	2.29	0.66
1:A:1199:ASP:OD1	1:A:1200:ASN:ND2	2.29	0.66
1:A:67:THR:HG1	1:A:94:CYS:HG	1.41	0.65
1:A:2349:LEU:HG	1:A:2353:LYS:HE3	1.79	0.64
1:A:805:PRO:HG2	1:A:808:GLU:HG3	1.79	0.64
1:A:1024:SER:O	1:A:1029:SER:OG	2.14	0.64
1:A:822:ILE:HG23	1:A:914:LEU:HD11	1.80	0.64
1:A:729:TYR:OH	1:A:785:ASP:HB3	1.97	0.64
1:A:1002:TRP:H	1:A:1002:TRP:CD1	2.14	0.64
1:A:1731:ASP:HB3	1:A:1732:PRO:HD3	1.78	0.63
1:A:2465:MET:HG2	1:A:2507:TRP:CE3	2.33	0.63
1:A:1215:SER:OG	1:A:1218:ASP:N	2.29	0.63
1:A:1538:SER:O	1:A:1542:ASN:ND2	2.31	0.63
1:A:1060:SER:O	1:A:1063:SER:OG	2.16	0.63
1:A:1294:GLU:OE2	1:A:1298:ASN:ND2	2.30	0.63
1:A:1236:GLN:O	1:A:1239:GLU:N	2.32	0.62
1:A:910:ARG:NH1	1:A:952:GLU:OE1	2.33	0.62
1:A:931:ILE:HD12	1:A:934:GLN:HE22	1.63	0.62
1:A:1180:SER:HB2	1:A:1184:GLU:HG3	1.81	0.61
1:A:1484:LEU:HD11	1:A:1511:PHE:CD1	2.35	0.61
1:A:1486:VAL:HG23	1:A:1587:MET:HE3	1.81	0.61
1:A:2204:ALA:HB3	1:A:2239:GLN:HE22	1.65	0.61
2:A:3001:AGS:O1B	2:A:3001:AGS:O2G	2.18	0.61
1:A:160:LEU:HD22	1:A:160:LEU:H	1.65	0.61
1:A:2282:LYS:NZ	1:A:2287:GLU:OE1	2.31	0.61
1:A:1921:PHE:HD2	1:A:1933:LEU:HD22	1.65	0.61
1:A:2126:ASP:N	1:A:2126:ASP:OD1	2.33	0.61
1:A:638:PRO:HD3	1:A:763:LEU:HD22	1.82	0.60
1:A:1051:GLU:OE1	1:A:1055:ASN:ND2	2.34	0.60
1:A:1656:GLN:NE2	1:A:1659:GLU:HG3	2.16	0.60
1:A:2636:HIS:NE2	1:A:2831:GLU:OE2	2.31	0.60
1:A:2500:ASN:O	1:A:2504:SER:OG	2.20	0.60
1:A:494:THR:O	1:A:494:THR:OG1	2.20	0.60
1:A:1482:ALA:HB1	1:A:1587:MET:SD	2.42	0.60
1:A:18:GLU:HG3	1:A:62:ALA:HB2	1.84	0.59
1:A:2244:SER:OG	1:A:2247:ASP:OD2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2465:MET:HG2	1:A:2507:TRP:HE3	1.66	0.58
1:A:891:ARG:NH1	1:A:893:ASP:OD2	2.37	0.58
1:A:95:PRO:HG2	1:A:136:LEU:HD21	1.85	0.58
1:A:1919:GLU:O	1:A:1923:ASN:ND2	2.32	0.58
1:A:2769:ASP:OD2	1:A:2772:THR:OG1	2.21	0.58
1:A:756:GLU:OE1	1:A:759:ARG:NH1	2.36	0.58
1:A:1217:LEU:O	1:A:1221:ARG:NH1	2.36	0.58
1:A:1382:TRP:O	1:A:1424:HIS:ND1	2.36	0.58
1:A:261:ILE:HG13	1:A:301:TRP:HZ3	1.68	0.58
1:A:238:PRO:HG3	1:A:1028:ASN:HD21	1.67	0.58
1:A:498:ALA:O	1:A:502:SER:HB2	2.04	0.57
1:A:239:ILE:HD12	1:A:278:ARG:HG3	1.85	0.57
1:A:2524:ARG:HH11	1:A:2590:SER:HB2	1.69	0.57
1:A:1072:GLY:HA3	1:A:1076:LEU:HD23	1.86	0.57
1:A:803:ASN:OD1	1:A:857:ARG:NH1	2.33	0.57
1:A:1255:VAL:HG13	1:A:1286:MET:HE1	1.86	0.57
1:A:2313:ALA:O	1:A:2317:ASN:ND2	2.38	0.57
1:A:386:THR:HG21	1:A:470:PHE:CD1	2.41	0.56
1:A:1758:GLU:HG2	1:A:1835:ALA:HB2	1.88	0.56
1:A:2102:GLN:NE2	1:A:2156:ASP:OD2	2.31	0.56
1:A:448:ARG:O	1:A:452:LYS:HG2	2.05	0.56
1:A:94:CYS:HB3	1:A:95:PRO:HD3	1.86	0.56
1:A:852:TYR:OH	1:A:934:GLN:OE1	2.11	0.56
1:A:722:ARG:NH2	1:A:780:SER:OG	2.38	0.55
1:A:953:ILE:O	1:A:956:SER:OG	2.21	0.55
1:A:1622:SER:OG	1:A:1623:GLN:N	2.37	0.55
1:A:325:TYR:OH	1:A:406:GLU:OE1	2.21	0.55
1:A:1959:ARG:NH2	1:A:1977:ASP:OD1	2.39	0.55
1:A:302:TRP:NE1	1:A:357:ASP:OD2	2.39	0.55
1:A:974:HIS:ND1	1:A:974:HIS:O	2.40	0.55
1:A:1484:LEU:HD11	1:A:1511:PHE:HD1	1.72	0.55
1:A:1429:TYR:OH	1:A:1694:GLU:OE1	2.20	0.55
1:A:2550:MET:HG2	1:A:2579:PHE:CE2	2.41	0.55
1:A:161:SER:HB2	1:A:163:GLU:H	1.73	0.54
1:A:2631:GLU:OE2	1:A:2634:LYS:NZ	2.38	0.54
1:A:139:GLY:O	1:A:143:VAL:HG23	2.08	0.54
1:A:660:LEU:HD21	1:A:820:PRO:HG3	1.87	0.54
1:A:2061:ASP:O	1:A:2065:ASN:ND2	2.40	0.54
1:A:455:SER:OG	1:A:456:LEU:N	2.40	0.54
1:A:1608:ASP:OD1	1:A:1608:ASP:N	2.37	0.54
1:A:2375:LYS:HE3	1:A:2410:VAL:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:LEU:HD11	1:A:944:LEU:HD12	1.89	0.54
1:A:1597:SER:OG	1:A:1598:SER:N	2.41	0.54
1:A:1951:ASP:OD1	1:A:1952:GLY:N	2.39	0.54
1:A:1316:GLN:OE1	1:A:1316:GLN:N	2.38	0.53
1:A:2498:SER:HB3	1:A:2507:TRP:HD1	1.69	0.53
1:A:2679:GLU:OE1	1:A:2687:LYS:NZ	2.36	0.53
1:A:1043:LEU:HG	1:A:1065:LEU:HD11	1.90	0.53
1:A:1860:ILE:HD13	1:A:2727:GLU:HB3	1.90	0.53
1:A:220:VAL:O	1:A:224:VAL:HG23	2.08	0.53
1:A:568:ILE:HG23	1:A:594:LEU:HD22	1.91	0.53
1:A:1025:LEU:HD11	1:A:1068:ILE:HD11	1.91	0.52
1:A:21:LEU:HB3	1:A:66:CYS:HB2	1.92	0.52
1:A:301:TRP:HB3	1:A:320:MET:HE1	1.91	0.52
1:A:931:ILE:HA	1:A:934:GLN:HE21	1.75	0.52
1:A:261:ILE:HG13	1:A:301:TRP:CZ3	2.44	0.52
1:A:417:LYS:HG3	1:A:418:HIS:HD2	1.75	0.52
1:A:2109:LEU:HD21	1:A:2163:ARG:HD2	1.91	0.52
1:A:948:GLU:OE2	1:A:951:ARG:NH1	2.43	0.52
1:A:29:ARG:O	1:A:33:VAL:HG23	2.10	0.51
1:A:313:LEU:O	1:A:317:ARG:HG2	2.11	0.51
1:A:823:PRO:HB2	1:A:829:GLU:HG2	1.91	0.51
1:A:377:MET:HE1	1:A:820:PRO:HB3	1.92	0.51
1:A:1316:GLN:H	1:A:1316:GLN:CD	2.18	0.51
1:A:2670:LEU:HD12	1:A:2768:LEU:HD11	1.92	0.51
1:A:896:LEU:HD22	1:A:986:VAL:HG11	1.92	0.51
1:A:1606:ASP:O	1:A:1610:ILE:HG13	2.10	0.51
1:A:2843:ARG:NH2	1:A:2900:ASP:OD1	2.43	0.51
1:A:519:HIS:CD2	1:A:521:SER:H	2.29	0.51
1:A:542:ILE:O	1:A:546:SER:OG	2.22	0.51
1:A:931:ILE:HD12	1:A:934:GLN:NE2	2.25	0.51
1:A:1235:GLY:HA2	1:A:1285:ARG:HH12	1.75	0.51
1:A:316:ILE:HG23	1:A:320:MET:HE3	1.93	0.51
1:A:505:MET:HG2	1:A:549:LEU:HD12	1.92	0.51
1:A:2286:ARG:HD3	1:A:2390:GLU:OE2	2.11	0.51
1:A:1754:ALA:C	1:A:1756:ALA:H	2.19	0.51
1:A:348:GLU:HB2	1:A:415:TYR:CZ	2.46	0.50
1:A:525:SER:O	1:A:528:GLN:HB2	2.11	0.50
1:A:2550:MET:HG2	1:A:2579:PHE:HE2	1.76	0.50
1:A:841:LEU:HD13	1:A:918:ARG:HB2	1.94	0.50
1:A:1113:VAL:HG12	1:A:1116:GLY:H	1.76	0.50
1:A:1567:LYS:HE2	1:A:1571:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1648:PRO:HG2	1:A:1651:LEU:HD12	1.92	0.50
1:A:118:ILE:O	1:A:122:VAL:HG23	2.11	0.50
1:A:573:THR:HA	1:A:612:HIS:CD2	2.46	0.50
1:A:836:GLU:OE1	1:A:837:ARG:NH1	2.44	0.50
1:A:99:ARG:HA	1:A:102:VAL:HG12	1.93	0.50
1:A:2530:LYS:HB2	1:A:2533:GLN:HG2	1.93	0.50
1:A:1371:CYS:HB2	1:A:1378:PRO:HG3	1.94	0.50
1:A:1249:LEU:HD11	1:A:1253:LYS:HD3	1.94	0.50
1:A:677:MET:O	1:A:681:ILE:HG12	2.12	0.50
1:A:2531:SER:HB3	1:A:2587:SER:HA	1.94	0.49
1:A:269:PHE:CE2	1:A:320:MET:HE2	2.47	0.49
1:A:2035:TRP:HB2	1:A:2086:ALA:HB2	1.94	0.49
1:A:1170:ILE:HG23	1:A:1185:LEU:HD23	1.93	0.49
1:A:2204:ALA:HB3	1:A:2239:GLN:NE2	2.27	0.49
1:A:1204:GLN:HG3	1:A:1242:GLN:HE21	1.78	0.49
1:A:2745:THR:HG21	1:A:2774:GLU:HB2	1.95	0.49
1:A:2536:PRO:HA	1:A:2582:GLU:HA	1.94	0.49
1:A:20:HIS:O	1:A:29:ARG:NE	2.45	0.49
1:A:22:VAL:HG21	1:A:65:ARG:HB2	1.96	0.48
1:A:519:HIS:CD2	1:A:521:SER:HB3	2.48	0.48
1:A:2606:LYS:HB2	1:A:2663:PHE:HB3	1.94	0.48
1:A:574:THR:HG22	1:A:576:ASP:H	1.78	0.48
1:A:1030:MET:HE1	1:A:1038:LEU:HD22	1.94	0.48
1:A:626:LEU:O	1:A:630:SER:HB3	2.14	0.48
1:A:1287:ARG:HD2	1:A:1292:LYS:HZ2	1.78	0.48
1:A:1921:PHE:HE2	1:A:1933:LEU:HD13	1.79	0.48
1:A:246:LEU:HB3	1:A:247:PRO:HD3	1.96	0.48
1:A:673:GLU:OE2	1:A:891:ARG:NH1	2.47	0.48
1:A:845:GLY:HA3	1:A:918:ARG:NH2	2.29	0.48
1:A:1336:THR:O	1:A:1340:ILE:HG13	2.14	0.48
1:A:2011:LEU:HD12	1:A:2011:LEU:O	2.14	0.48
1:A:95:PRO:HA	1:A:98:LEU:HB3	1.95	0.47
1:A:1232:MET:HE1	1:A:1286:MET:HG2	1.96	0.47
1:A:1399:HIS:CG	1:A:1400:PRO:HD2	2.49	0.47
1:A:661:ARG:NH2	1:A:952:GLU:OE2	2.48	0.47
1:A:1132:PRO:HB2	1:A:1403:GLY:HA2	1.96	0.47
1:A:1381:ILE:HB	1:A:1733:TYR:OH	2.15	0.47
1:A:2221:ILE:O	1:A:2225:ARG:HG2	2.14	0.47
1:A:120:HIS:CE1	1:A:124:VAL:HG21	2.49	0.47
1:A:165:TRP:CH2	1:A:169:VAL:HG21	2.49	0.47
1:A:175:VAL:HG11	1:A:224:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLN:HG2	1:A:301:TRP:CZ3	2.50	0.47
1:A:292:LYS:HE3	1:A:334:LEU:HD22	1.97	0.47
1:A:1917:LEU:CD2	1:A:2810:ILE:HD13	2.34	0.47
1:A:1080:ILE:O	1:A:1084:ILE:N	2.48	0.47
1:A:2471:GLY:HA3	1:A:2490:THR:HG21	1.96	0.47
1:A:789:ALA:O	1:A:793:ILE:HG13	2.15	0.46
1:A:291:VAL:HG21	1:A:330:TYR:HB3	1.97	0.46
1:A:348:GLU:HB2	1:A:415:TYR:OH	2.16	0.46
1:A:1054:SER:O	1:A:1057:GLY:N	2.46	0.46
1:A:2854:PRO:HA	1:A:2857:MET:HB3	1.97	0.46
1:A:1020:LEU:HA	1:A:1024:SER:HB2	1.97	0.46
1:A:1204:GLN:HG3	1:A:1242:GLN:NE2	2.30	0.46
1:A:102:VAL:O	1:A:106:VAL:HB	2.15	0.46
1:A:362:GLU:N	1:A:362:GLU:OE1	2.49	0.46
1:A:1186:PHE:HB2	1:A:1211:PHE:CD1	2.51	0.46
1:A:1389:PHE:HE1	1:A:1393:LYS:HE2	1.81	0.46
1:A:1549:SER:HB2	1:A:1591:VAL:O	2.16	0.46
1:A:299:SER:HB2	1:A:350:LEU:HD12	1.97	0.46
1:A:762:VAL:HG23	1:A:797:THR:HG21	1.98	0.46
1:A:903:PHE:O	1:A:907:THR:OG1	2.31	0.46
1:A:569:ASN:O	1:A:573:THR:OG1	2.24	0.46
1:A:2922:ASP:O	1:A:2926:GLN:HG2	2.16	0.46
1:A:14:PHE:O	1:A:18:GLU:N	2.47	0.45
1:A:406:GLU:O	1:A:410:ILE:HG13	2.17	0.45
1:A:480:GLU:H	1:A:480:GLU:HG3	1.38	0.45
1:A:2825:LEU:O	1:A:2829:ARG:HG2	2.16	0.45
1:A:99:ARG:HB3	1:A:143:VAL:HG22	1.98	0.45
1:A:1044:HIS:ND1	1:A:1047:GLU:OE1	2.30	0.45
1:A:148:LEU:HD12	1:A:227:CYS:HB2	1.99	0.45
1:A:894:ILE:N	1:A:985:GLU:OE1	2.50	0.45
1:A:2530:LYS:HB2	1:A:2533:GLN:CG	2.46	0.45
1:A:328:ARG:O	1:A:332:GLN:NE2	2.49	0.45
1:A:519:HIS:HD2	1:A:521:SER:HB3	1.80	0.45
1:A:1104:LEU:HD21	1:A:1120:ARG:HH12	1.81	0.45
1:A:1363:LEU:HB3	1:A:1364:PRO:HD3	1.98	0.45
1:A:1556:THR:O	1:A:1560:ASN:ND2	2.49	0.45
1:A:2274:PRO:O	1:A:2278:GLU:HG2	2.17	0.45
1:A:1225:THR:HG22	1:A:1261:LYS:HD2	1.98	0.45
1:A:2513:THR:HG21	1:A:2555:ILE:CD1	2.47	0.45
1:A:2734:GLU:O	1:A:2738:LYS:HG2	2.16	0.45
1:A:247:PRO:HB3	1:A:290:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ALA:O	1:A:274:ILE:HD12	2.16	0.45
1:A:1558:GLU:OE1	1:A:1558:GLU:N	2.29	0.45
1:A:1763:SER:OG	1:A:1795:GLU:OE2	2.30	0.45
1:A:2319:LYS:HE3	1:A:2360:GLN:HE22	1.80	0.45
1:A:2546:PHE:HD2	1:A:2547:LEU:HD12	1.82	0.45
1:A:645:LEU:HA	1:A:648:CYS:SG	2.57	0.45
1:A:2323:ASP:HA	1:A:2356:GLN:HE21	1.82	0.45
1:A:2431:MET:HE3	1:A:2431:MET:HB3	1.90	0.45
1:A:1657:LEU:HD23	1:A:1657:LEU:HA	1.79	0.45
1:A:519:HIS:HD2	1:A:521:SER:H	1.64	0.45
1:A:1217:LEU:HD22	1:A:1221:ARG:HH11	1.80	0.45
1:A:761:MET:HB2	1:A:761:MET:HE3	1.58	0.44
1:A:941:GLU:HG2	1:A:942:GLN:HG3	2.00	0.44
1:A:1384:PRO:O	1:A:1388:VAL:HG23	2.17	0.44
1:A:18:GLU:HA	1:A:21:LEU:HD12	1.98	0.44
1:A:488:ASP:O	1:A:491:LYS:HB3	2.16	0.44
1:A:621:TRP:CE2	1:A:623:PRO:HG3	2.52	0.44
1:A:1659:GLU:H	1:A:1659:GLU:HG2	1.47	0.44
1:A:2702:ASN:OD1	1:A:2702:ASN:N	2.50	0.44
1:A:114:ALA:O	1:A:118:ILE:HG13	2.17	0.44
1:A:284:VAL:HG21	1:A:684:LEU:HD22	1.99	0.44
1:A:1088:PHE:HB3	1:A:1096:HIS:CE1	2.53	0.44
1:A:1601:ASP:OD1	1:A:1602:VAL:N	2.51	0.44
1:A:2121:SER:HB3	1:A:2640:ARG:NE	2.32	0.44
1:A:1129:CYS:SG	1:A:1173:ILE:HA	2.56	0.44
1:A:1287:ARG:HD2	1:A:1292:LYS:NZ	2.32	0.44
1:A:153:SER:OG	1:A:154:ALA:N	2.49	0.44
1:A:236:ASN:HD22	1:A:1029:SER:HA	1.83	0.44
1:A:1449:ASP:OD1	1:A:1450:ASP:N	2.50	0.44
1:A:2409:GLU:O	1:A:2413:GLU:HG2	2.17	0.44
1:A:2513:THR:HG21	1:A:2555:ILE:HD11	1.99	0.44
1:A:287:CYS:O	1:A:291:VAL:HG13	2.17	0.43
1:A:1512:HIS:C	1:A:1512:HIS:CD2	2.96	0.43
1:A:1552:ALA:HB3	1:A:1595:PRO:HD3	2.00	0.43
1:A:2105:LEU:HG	1:A:2160:VAL:HG21	1.99	0.43
1:A:1215:SER:OG	1:A:1217:LEU:N	2.51	0.43
1:A:949:PHE:O	1:A:953:ILE:HG12	2.19	0.43
1:A:1393:LYS:HA	1:A:1393:LYS:HD3	1.76	0.43
1:A:64:PHE:HZ	1:A:117:ILE:HG12	1.82	0.43
1:A:166:GLU:HB2	1:A:241:ARG:NH2	2.33	0.43
1:A:386:THR:O	1:A:388:ILE:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:ILE:N	1:A:1085:PRO:HD2	2.33	0.43
1:A:1088:PHE:HB2	1:A:1131:TRP:NE1	2.33	0.43
1:A:1128:ALA:HB2	1:A:1138:SER:CB	2.48	0.43
1:A:1971:ASP:OD1	1:A:1972:LEU:N	2.52	0.43
1:A:2522:MET:HE3	1:A:2658:SER:HB3	2.00	0.43
1:A:102:VAL:HG11	1:A:143:VAL:HG13	2.01	0.43
1:A:778:ILE:HG22	1:A:780:SER:H	1.83	0.43
1:A:819:ALA:O	1:A:821:TYR:N	2.52	0.43
1:A:2375:LYS:HG2	1:A:2414:VAL:HG21	2.00	0.43
1:A:620:ARG:HD3	1:A:620:ARG:HA	1.83	0.43
1:A:2162:ILE:HD11	1:A:2195:CYS:SG	2.58	0.43
1:A:574:THR:HG22	1:A:577:ILE:H	1.83	0.43
1:A:1104:LEU:HD21	1:A:1120:ARG:NH1	2.33	0.43
1:A:1943:LEU:HD13	1:A:1958:PHE:HB2	2.01	0.43
1:A:162:GLY:O	1:A:241:ARG:NH2	2.47	0.43
1:A:507:ALA:O	1:A:510:SER:OG	2.23	0.43
1:A:1686:ASP:OD1	1:A:1686:ASP:N	2.29	0.43
1:A:585:ASP:OD1	1:A:585:ASP:N	2.52	0.42
1:A:1484:LEU:O	1:A:1488:LEU:HG	2.18	0.42
1:A:1916:ILE:HD12	1:A:1916:ILE:HA	1.90	0.42
1:A:2842:LEU:HD12	1:A:2842:LEU:HA	1.89	0.42
1:A:68:LEU:HD23	1:A:68:LEU:HA	1.81	0.42
1:A:1174:ALA:O	1:A:1179:LEU:HB2	2.19	0.42
1:A:1283:GLU:H	1:A:1283:GLU:HG3	1.61	0.42
1:A:118:ILE:HD13	1:A:168:CYS:SG	2.60	0.42
1:A:2852:ILE:HG23	1:A:2857:MET:HE3	2.01	0.42
1:A:152:ALA:CB	1:A:980:GLU:HG2	2.49	0.42
1:A:243:ALA:HB1	1:A:279:MET:SD	2.60	0.42
1:A:772:LEU:HD23	1:A:772:LEU:HA	1.77	0.42
1:A:913:PHE:O	1:A:917:ILE:HG12	2.19	0.42
1:A:1213:PHE:HD2	1:A:1219:LEU:HD12	1.84	0.42
1:A:1898:THR:OG1	1:A:1899:ARG:N	2.53	0.42
1:A:327:THR:HG22	1:A:331:ILE:HG13	2.01	0.42
1:A:998:PHE:O	1:A:1002:TRP:NE1	2.53	0.42
1:A:1575:LEU:HD12	1:A:1575:LEU:HA	1.74	0.42
1:A:159:ALA:O	1:A:161:SER:N	2.53	0.42
1:A:255:GLN:HA	1:A:297:LEU:HD22	2.02	0.42
1:A:1210:ILE:H	1:A:1210:ILE:HG13	1.65	0.42
1:A:1833:GLU:N	1:A:1834:PRO:HD2	2.35	0.42
1:A:1921:PHE:CE2	1:A:1933:LEU:HD13	2.55	0.42
1:A:2630:SER:OG	1:A:2646:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:TRP:O	1:A:534:VAL:HG23	2.20	0.42
1:A:978:ARG:C	1:A:980:GLU:H	2.27	0.42
1:A:2140:MET:HE3	1:A:2140:MET:HB3	1.86	0.42
1:A:641:LEU:HD13	1:A:641:LEU:HA	1.86	0.41
1:A:669:LEU:HD23	1:A:669:LEU:HA	1.87	0.41
1:A:772:LEU:O	1:A:776:VAL:HG23	2.20	0.41
1:A:924:ILE:H	1:A:924:ILE:HG13	1.68	0.41
1:A:1049:LYS:HG2	1:A:1052:TYR:HB2	2.02	0.41
1:A:489:LEU:O	1:A:493:VAL:HG23	2.20	0.41
1:A:1438:LEU:HD23	1:A:1438:LEU:HA	1.86	0.41
1:A:1733:TYR:HB3	1:A:1734:ARG:H	1.71	0.41
1:A:841:LEU:HD23	1:A:841:LEU:HA	1.90	0.41
1:A:1664:SER:O	1:A:1668:GLY:HA2	2.21	0.41
1:A:2182:LEU:HD12	1:A:2182:LEU:HA	1.87	0.41
1:A:931:ILE:HA	1:A:934:GLN:NE2	2.35	0.41
1:A:380:PRO:HG3	1:A:662:LEU:HD11	2.01	0.41
1:A:515:GLU:HG2	1:A:518:ARG:NH2	2.35	0.41
1:A:1236:GLN:O	1:A:1237:GLU:C	2.64	0.41
1:A:1467:LYS:O	1:A:1524:SER:OG	2.27	0.41
1:A:1542:ASN:O	1:A:1546:ILE:HG23	2.20	0.41
1:A:1750:GLU:OE1	1:A:1750:GLU:HA	2.21	0.41
1:A:2440:ASP:OD1	1:A:2440:ASP:N	2.45	0.41
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.87	0.41
1:A:894:ILE:HA	1:A:894:ILE:HD12	1.79	0.41
1:A:1452:LEU:HD22	1:A:1511:PHE:CG	2.55	0.41
1:A:2208:MET:HB2	1:A:2208:MET:HE3	1.72	0.41
1:A:1859:SER:HB2	1:A:2681:TYR:CE1	2.56	0.41
1:A:2039:VAL:HG13	1:A:2043:TYR:CE2	2.55	0.41
1:A:2159:LEU:HD12	1:A:2159:LEU:HA	1.83	0.41
1:A:582:ILE:HD11	1:A:632:HIS:CD2	2.56	0.41
1:A:773:PRO:HD3	1:A:839:HIS:CD2	2.55	0.41
1:A:1199:ASP:HA	1:A:1234:ARG:CZ	2.51	0.41
1:A:1249:LEU:HD21	1:A:1253:LYS:HG2	2.03	0.41
1:A:840:LEU:HD12	1:A:840:LEU:HA	1.86	0.41
1:A:1651:LEU:HD22	1:A:2080:LEU:HD11	2.03	0.41
1:A:1686:ASP:O	1:A:1689:THR:N	2.53	0.41
1:A:2105:LEU:HD12	1:A:2105:LEU:HA	1.89	0.41
1:A:233:ILE:HG23	1:A:274:ILE:HD13	2.03	0.41
1:A:755:MET:HG3	1:A:756:GLU:HG2	2.02	0.41
1:A:2033:ASP:HB3	1:A:2069:HIS:CE1	2.56	0.41
1:A:2286:ARG:HD3	1:A:2390:GLU:CD	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:HG3	1:A:275:VAL:HG11	2.03	0.40
1:A:1686:ASP:O	1:A:1687:CYS:C	2.63	0.40
1:A:378:LEU:HD23	1:A:658:GLN:C	2.46	0.40
1:A:1698:ARG:NH1	1:A:1739:ASP:OD2	2.55	0.40
1:A:413:ALA:HB2	1:A:471:LEU:HD11	2.01	0.40
1:A:934:GLN:HE21	1:A:934:GLN:HB2	1.68	0.40
1:A:1092:VAL:HA	1:A:1495:THR:O	2.20	0.40
1:A:1617:TRP:HB2	1:A:1637:LEU:HD21	2.02	0.40
1:A:1792:GLY:O	1:A:1796:ARG:HG3	2.22	0.40
1:A:2438:LEU:O	1:A:2439:GLN:HG3	2.20	0.40
1:A:2079:VAL:O	1:A:2083:GLN:HG2	2.21	0.40
1:A:2513:THR:HG23	1:A:2550:MET:HE1	2.02	0.40
1:A:412:GLU:OE2	1:A:416:SER:OG	2.36	0.40
1:A:613:ILE:O	1:A:617:VAL:HG23	2.22	0.40
1:A:1484:LEU:HD23	1:A:1484:LEU:HA	1.93	0.40
1:A:2043:TYR:HH	1:A:2137:THR:HG1	1.66	0.40
1:A:2349:LEU:CG	1:A:2353:LYS:HE3	2.49	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	2596/2944 (88%)	2401 (92%)	193 (7%)	2 (0%)	48 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2007	SER
1	A	160	LEU

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	2281/2529 (90%)	2158 (95%)	123 (5%)	20	47

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	27	THR
1	A	31	ASP
1	A	56	TYR
1	A	66	CYS
1	A	69	ILE
1	A	107	THR
1	A	109	ILE
1	A	160	LEU
1	A	161	SER
1	A	250	VAL
1	A	251	ILE
1	A	261	ILE
1	A	275	VAL
1	A	286	LEU
1	A	290	LEU
1	A	293	GLN
1	A	325	TYR
1	A	346	ASP
1	A	356	CYS
1	A	362	GLU
1	A	388	ILE
1	A	395	HIS
1	A	396	THR
1	A	447	ASN
1	A	449	VAL
1	A	480	GLU
1	A	494	THR
1	A	502	SER
1	A	522	LEU

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Mol	Chain	Res	Type
1	A	535	ARG
1	A	549	LEU
1	A	554	LEU
1	A	583	LEU
1	A	602	PHE
1	A	607	GLN
1	A	613	ILE
1	A	641	LEU
1	A	658	GLN
1	A	660	LEU
1	A	662	LEU
1	A	684	LEU
1	A	741	SER
1	A	754	SER
1	A	762	VAL
1	A	809	ASN
1	A	831	ILE
1	A	834	LYS
1	A	855	SER
1	A	896	LEU
1	A	897	SER
1	A	907	THR
1	A	909	LEU
1	A	915	ASP
1	A	916	ILE
1	A	924	ILE
1	A	931	ILE
1	A	941	GLU
1	A	962	LEU
1	A	976	VAL
1	A	980	GLU
1	A	983	CYS
1	A	986	VAL
1	A	998	PHE
1	A	1002	TRP
1	A	1009	ILE
1	A	1024	SER
1	A	1045	LEU
1	A	1065	LEU
1	A	1068	ILE
1	A	1071	ASP
1	A	1093	LEU

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Mol	Chain	Res	Type
1	A	1098	ASP
1	A	1104	LEU
1	A	1145	ILE
1	A	1162	SER
1	A	1200	ASN
1	A	1215	SER
1	A	1217	LEU
1	A	1221	ARG
1	A	1230	ILE
1	A	1243	LEU
1	A	1254	LEU
1	A	1255	VAL
1	A	1283	GLU
1	A	1300	HIS
1	A	1314	PHE
1	A	1320	ILE
1	A	1324	PHE
1	A	1361	LYS
1	A	1376	TYR
1	A	1380	ASN
1	A	1381	ILE
1	A	1397	THR
1	A	1398	ILE
1	A	1399	HIS
1	A	1406	HIS
1	A	1408	CYS
1	A	1410	VAL
1	A	1411	LEU
1	A	1414	ILE
1	A	1427	SER
1	A	1443	VAL
1	A	1526	GLU
1	A	1568	ASP
1	A	1575	LEU
1	A	1585	LEU
1	A	1608	ASP
1	A	1650	ASP
1	A	1659	GLU
1	A	1681	LEU
1	A	1686	ASP
1	A	1743	VAL
1	A	1854	LEU

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Mol	Chain	Res	Type
1	A	2126	ASP
1	A	2443	THR
1	A	2465	MET
1	A	2487	GLN
1	A	2514	SER
1	A	2608	LEU
1	A	2752	LEU
1	A	2805	VAL
1	A	2855	VAL

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

Mol	Chain	Res	Type
1	A	120	HIS
1	A	376	ASN
1	A	395	HIS
1	A	418	HIS
1	A	450	HIS
1	A	519	HIS
1	A	612	HIS
1	A	632	HIS
1	A	658	GLN
1	A	839	HIS
1	A	934	GLN
1	A	1000	ASN
1	A	1027	ASN
1	A	1028	ASN
1	A	1035	GLN
1	A	1078	HIS
1	A	1096	HIS
1	A	1161	HIS
1	A	1175	GLN
1	A	1512	HIS
1	A	1560	ASN
1	A	1656	GLN
1	A	1765	HIS
1	A	2031	ASN
1	A	2060	HIS
1	A	2065	ASN
1	A	2179	GLN
1	A	2239	GLN
1	A	2255	GLN

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Mol	Chain	Res	Type
1	A	2302	GLN
1	A	2317	ASN
1	A	2354	GLN
1	A	2356	GLN
1	A	2360	GLN
1	A	2446	GLN
1	A	2487	GLN
1	A	2518	HIS
1	A	2553	ASN
1	A	2624	GLN
1	A	2641	GLN
1	A	2678	HIS
1	A	2754	HIS
1	A	2770	HIS
1	A	2849	GLN
1	A	2925	ASN
1	A	2926	GLN

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	AGS	A	3001	3	32,33,33	0.91	4 (12%)	45,52,52	0.76	1 (2%)

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	AGS	A	3001	3	-	10/21/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	AGS	PB-O3A	-2.66	1.56	1.59
2	A	3001	AGS	PB-O3B	-2.41	1.56	1.59
2	A	3001	AGS	PA-O3A	-2.09	1.57	1.59
2	A	3001	AGS	PG-S1G	2.09	1.95	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	AGS	PB-O3B-PG	-3.87	119.00	133.17

There are no chirality outliers.

All (10) torsion outliers are listed below:

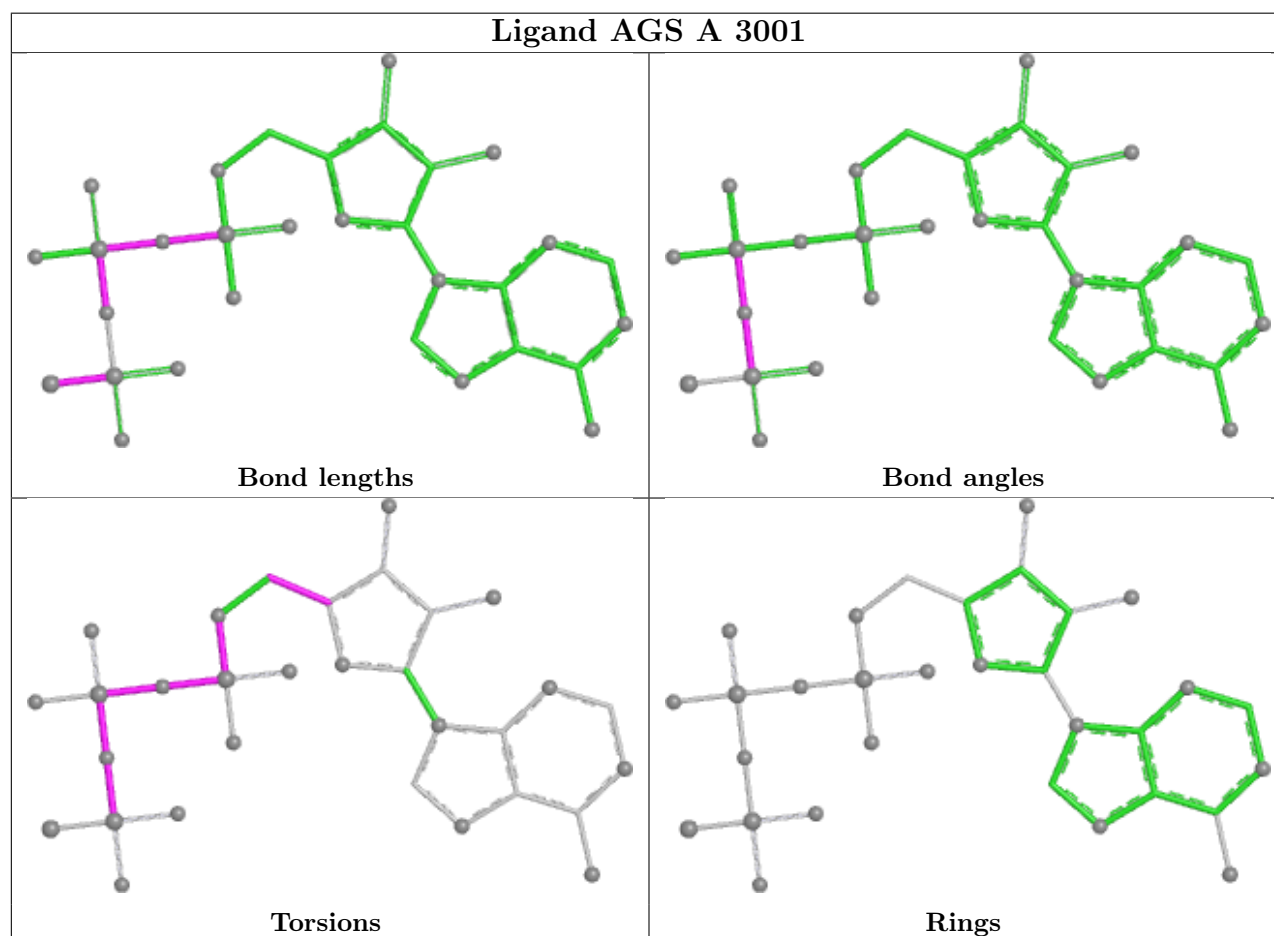
Mol	Chain	Res	Type	Atoms
2	A	3001	AGS	PB-O3B-PG-O2G
2	A	3001	AGS	PB-O3B-PG-O3G
2	A	3001	AGS	C5'-O5'-PA-O1A
2	A	3001	AGS	C5'-O5'-PA-O3A
2	A	3001	AGS	O4'-C4'-C5'-O5'
2	A	3001	AGS	C3'-C4'-C5'-O5'
2	A	3001	AGS	PB-O3A-PA-O5'
2	A	3001	AGS	PA-O3A-PB-O2B
2	A	3001	AGS	PG-O3B-PB-O2B
2	A	3001	AGS	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	AGS	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

There are no chain breaks in this entry.

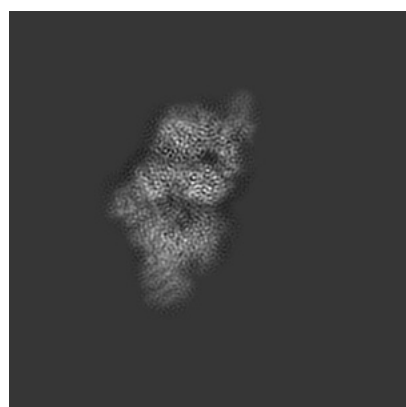
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10232. These allow visual inspection of the internal detail of the map and identification of artifacts.

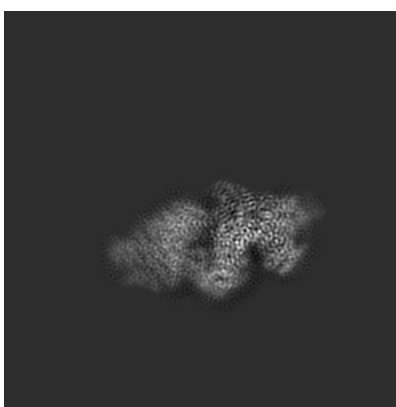
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

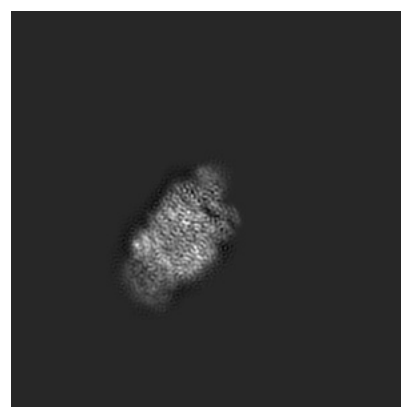
6.1.1 Primary map



X



Y

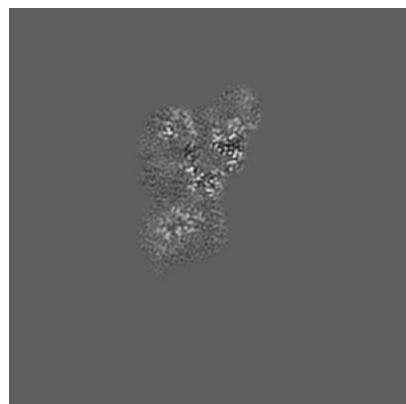


Z

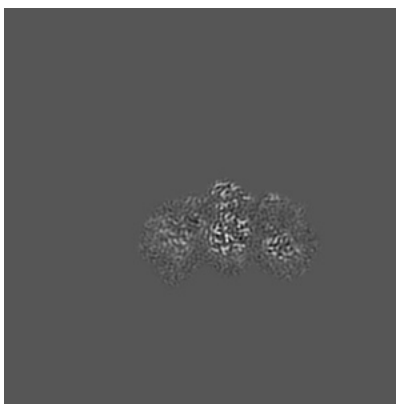
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

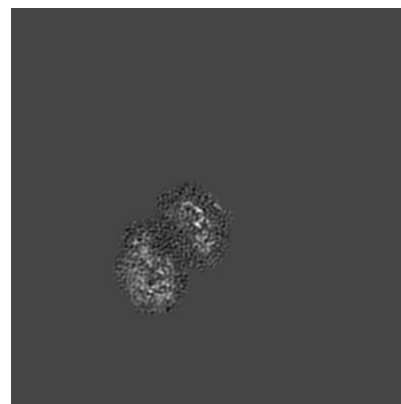
6.2.1 Primary map



X Index: 176



Y Index: 176

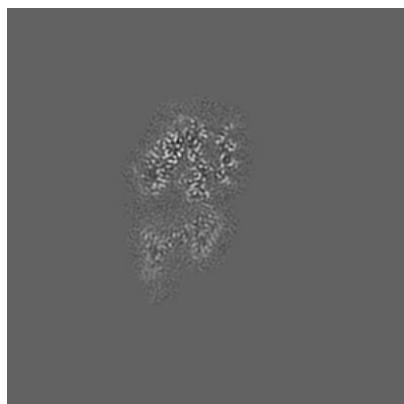


Z Index: 176

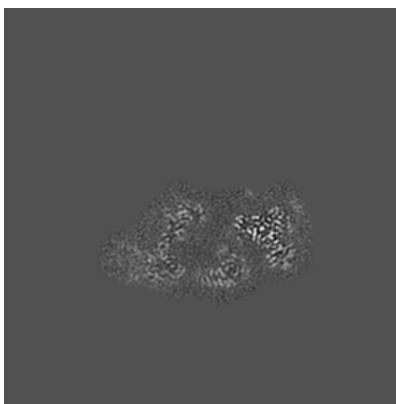
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

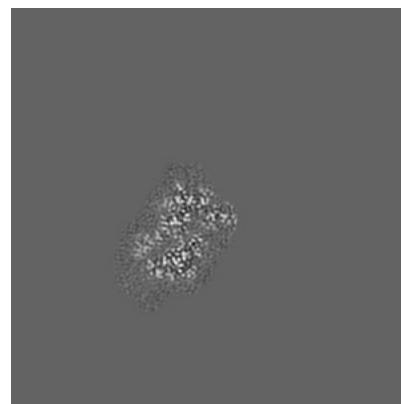
6.3.1 Primary map



X Index: 154



Y Index: 147

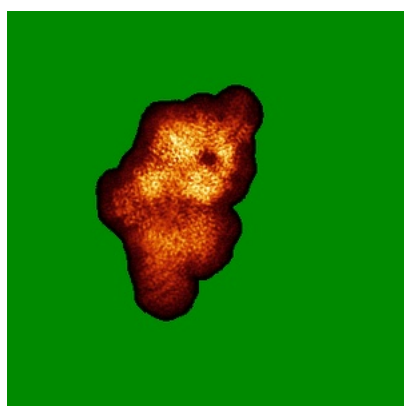


Z Index: 205

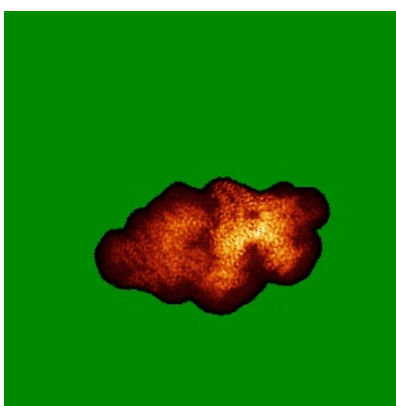
The images above show the largest variance slices of the map in three orthogonal directions.

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

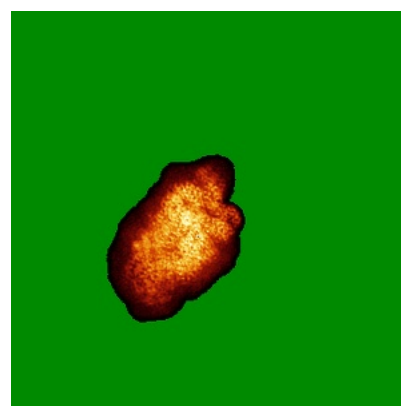
6.4.1 Primary map



X



Y

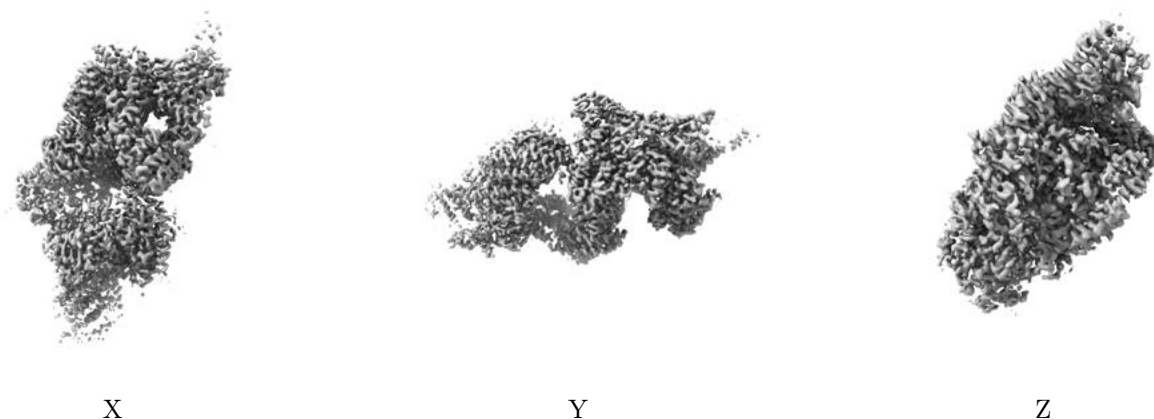


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0126. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

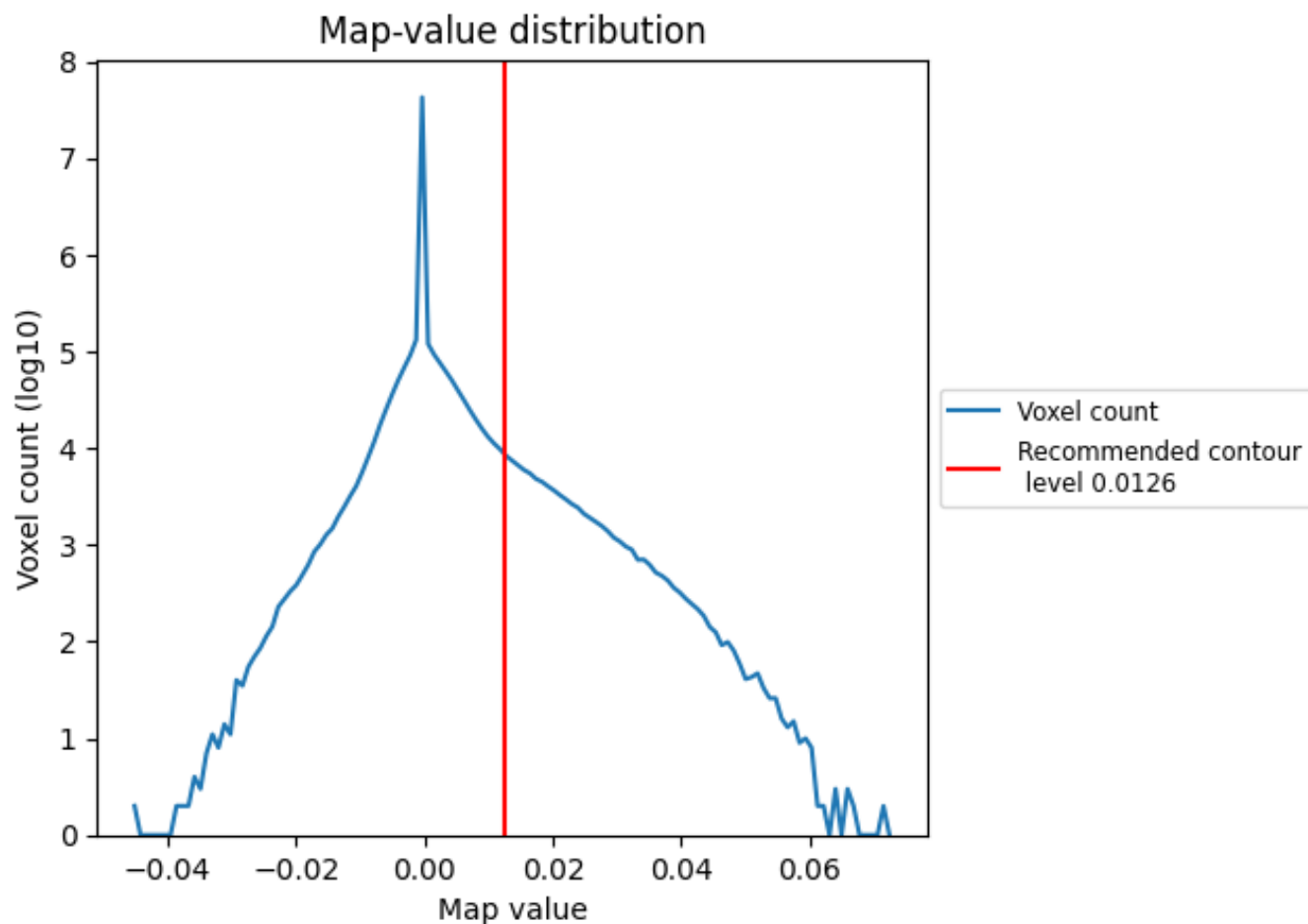
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

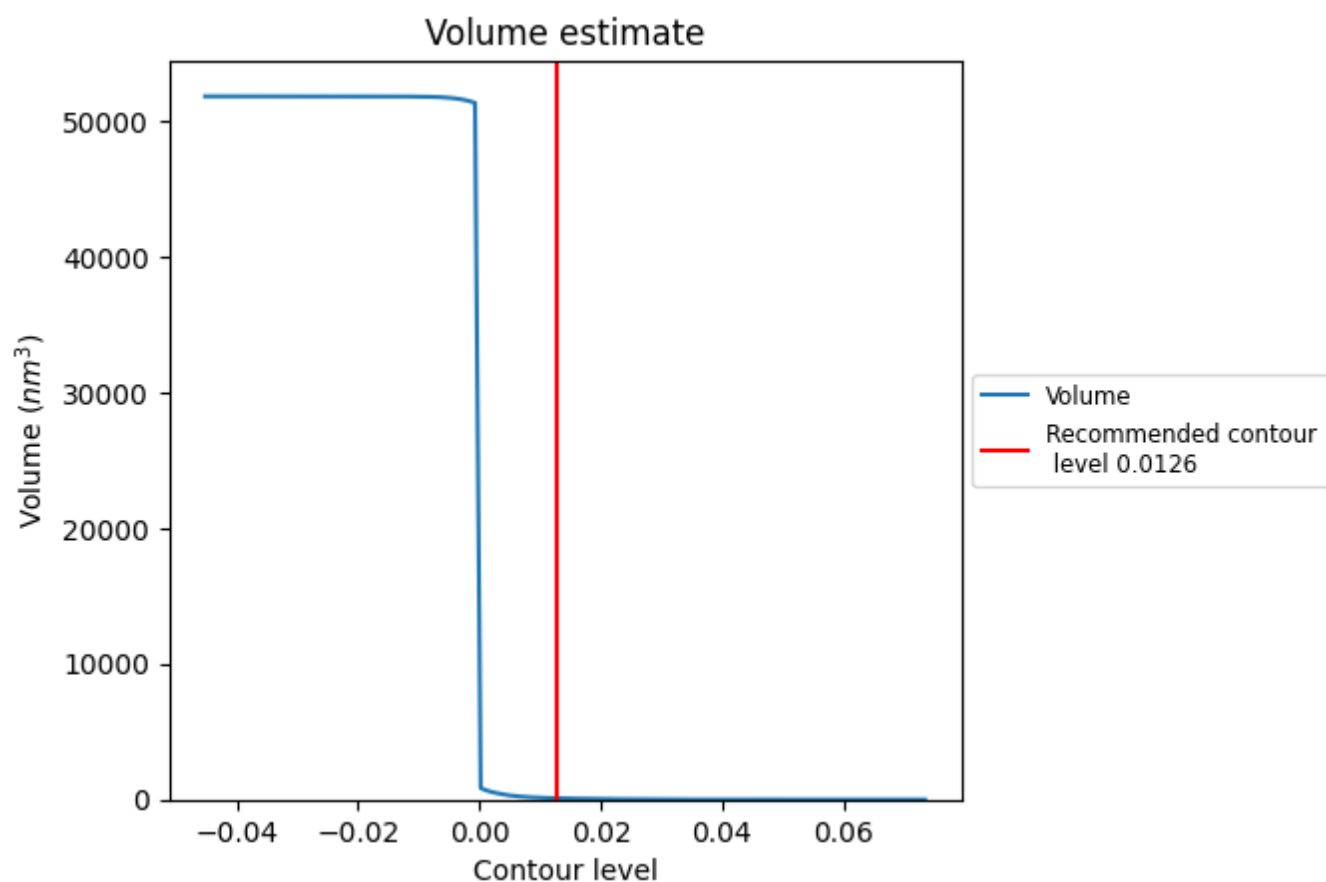
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

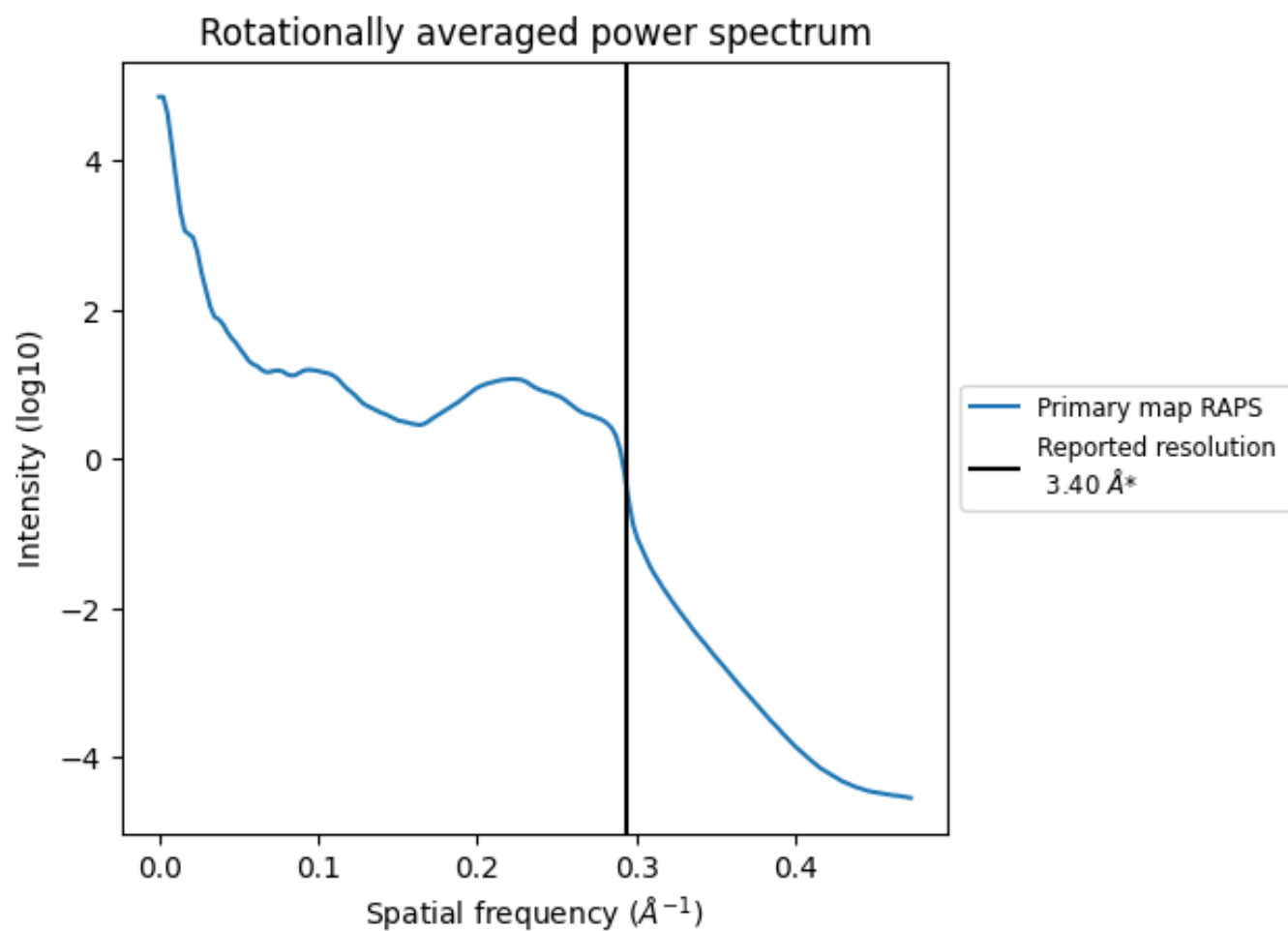
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm³; this corresponds to an approximate mass of 88 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 ⓘ

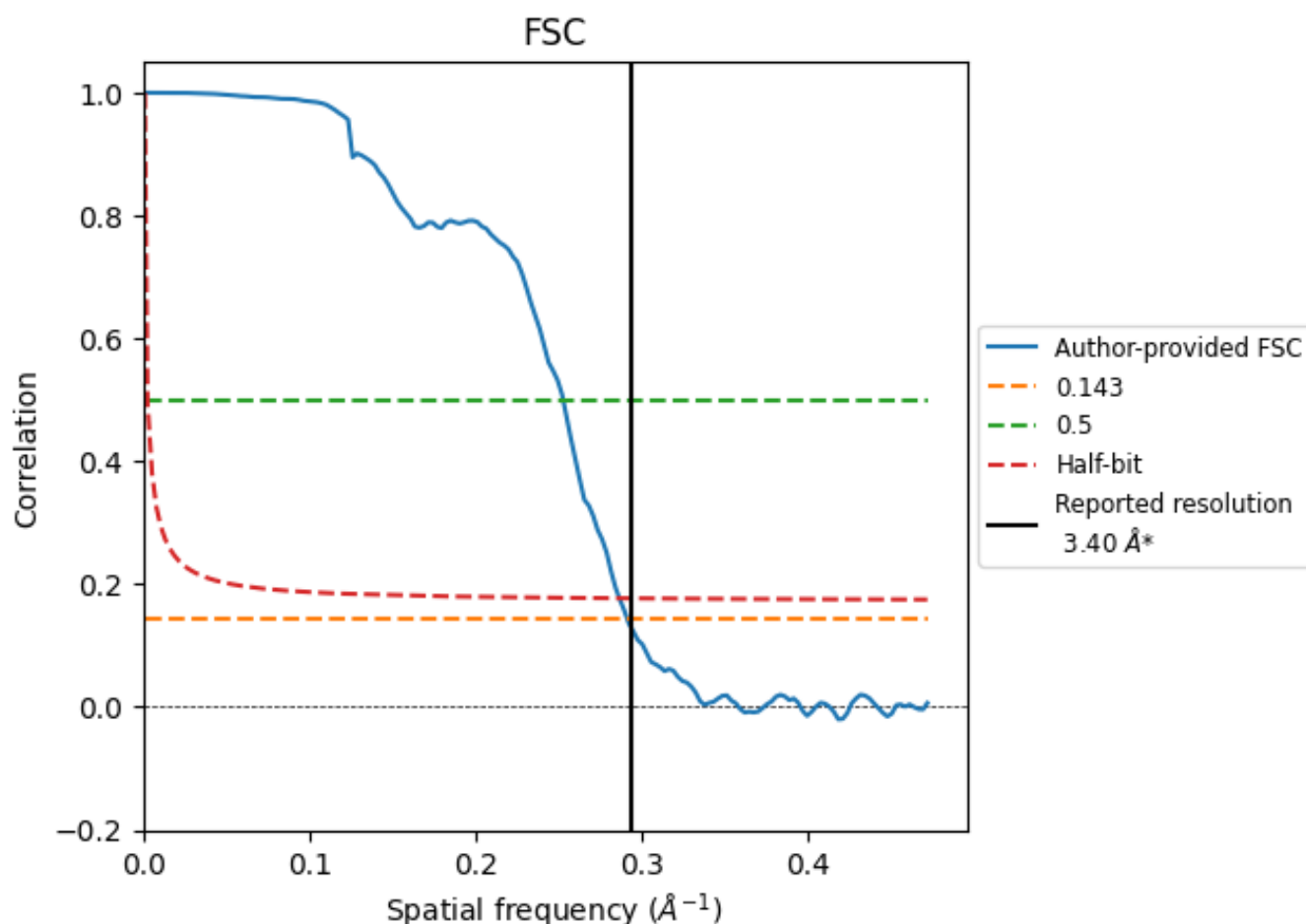


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

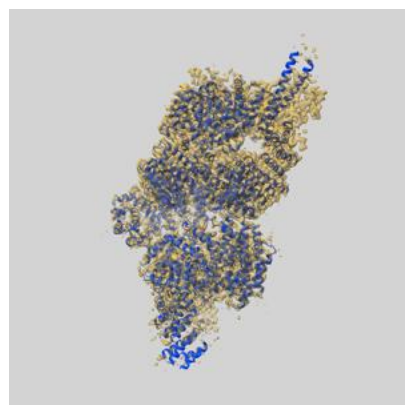
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	3.96	3.49
Unmasked-calculated*	-	-	-

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

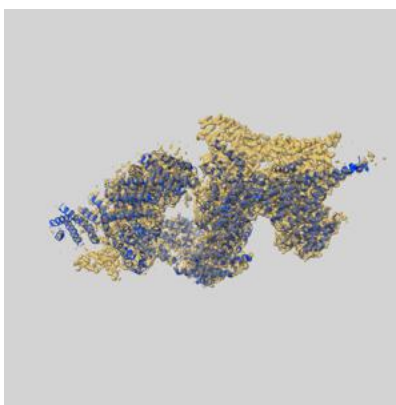
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10232 and PDB model 6SKZ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

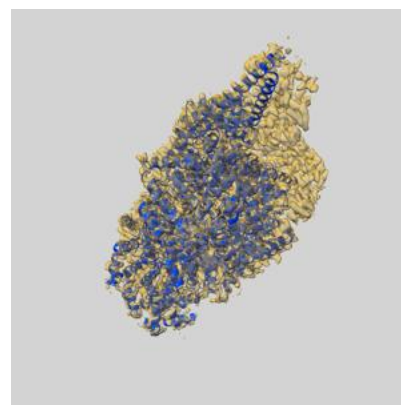
9.1 Map-model overlay [i](#)



X



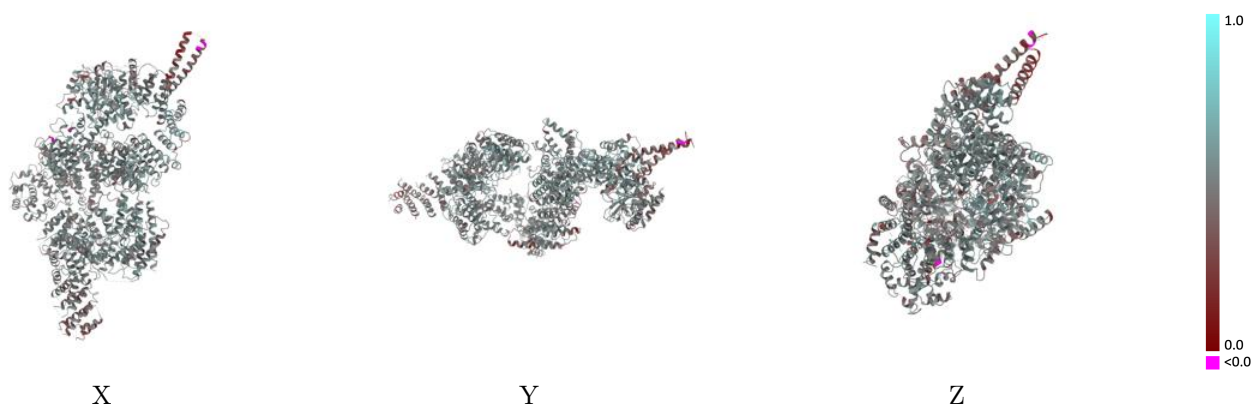
Y



Z

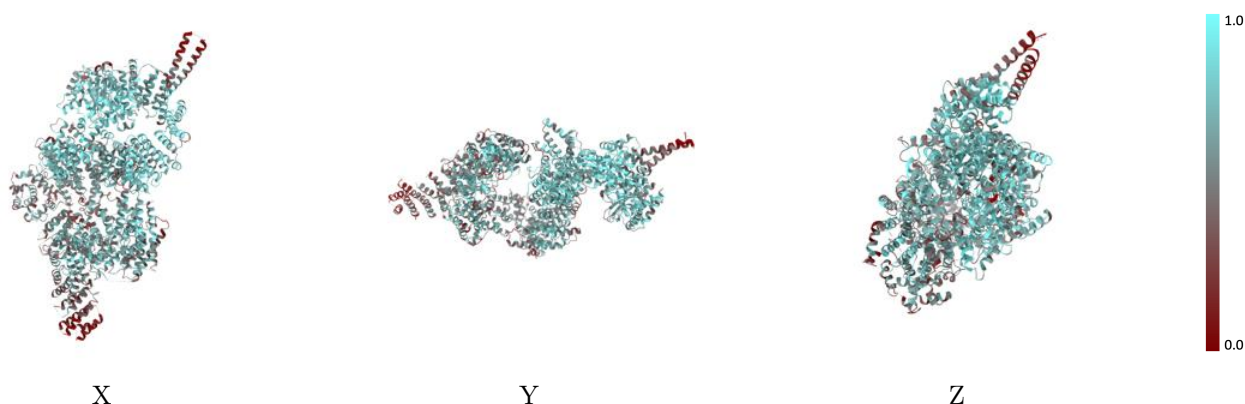
The images above show the 3D surface view of the map at the recommended contour level 0.0126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



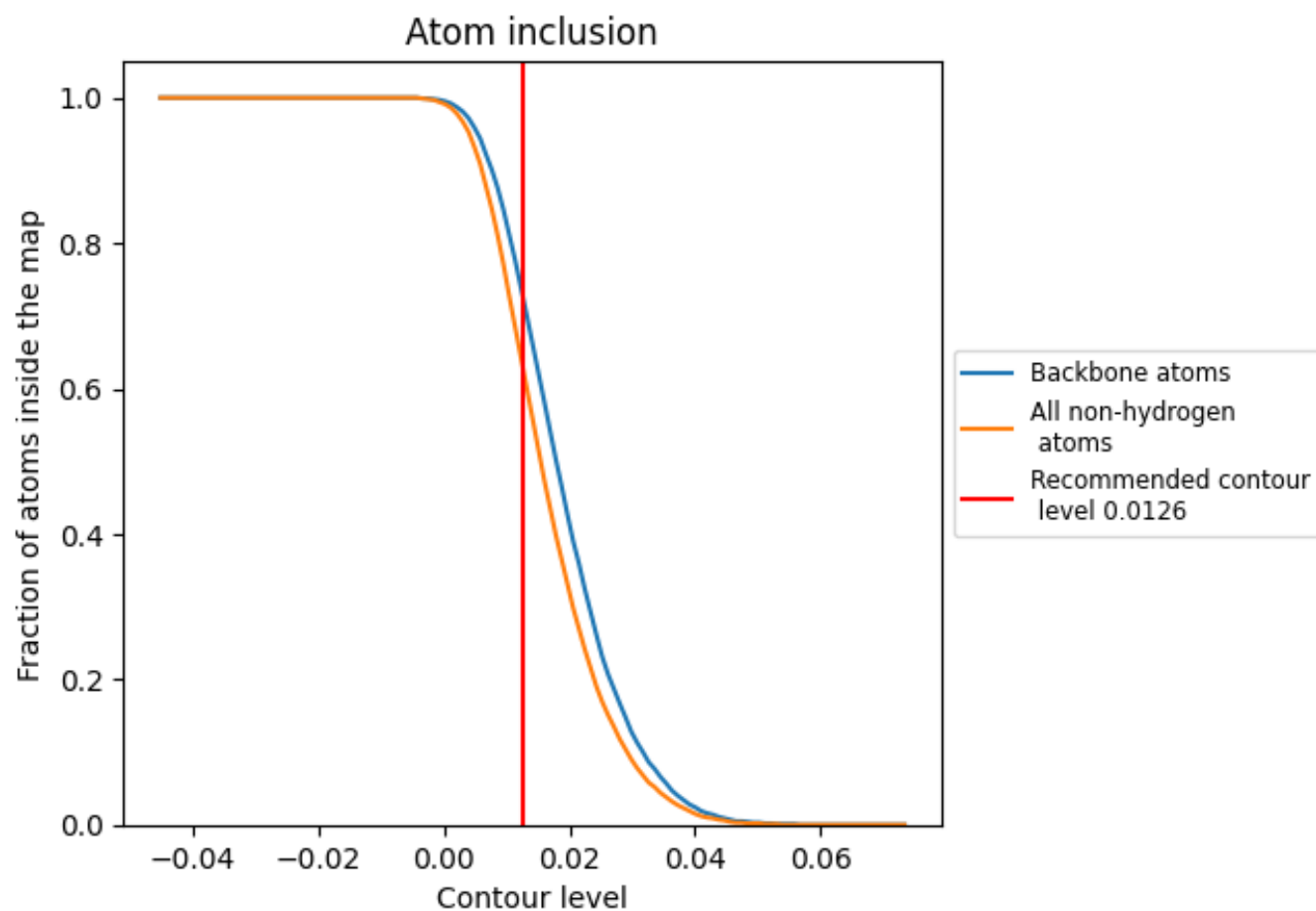
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0126).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 63% 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 (0.0126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6270	0.4990
A	0.6270	0.4990

