



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 10:52 PM UTC

PDB ID : 6VYY / pdb_00006vyy
EMDB ID : EMD-21407
Title : Mycobacterium tuberculosis WT RNAP transcription open promoter complex with Sorangicin
Authors : Lilic, M.; Boyaci, H.; Chen, J.; Darst, S.A.; Campbell, E.A.
Deposited on : 2020-02-18
Resolution : 3.42 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:

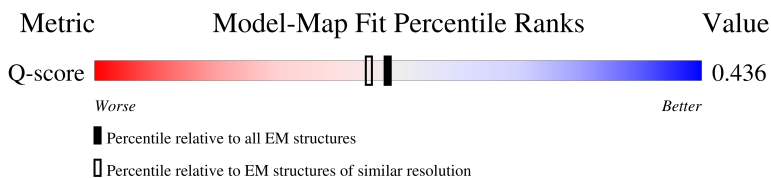
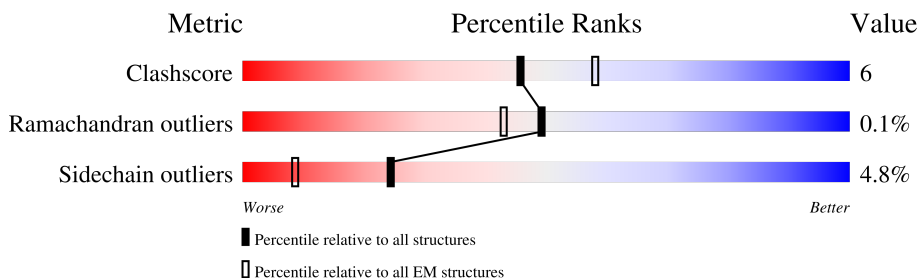
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.42 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	13959 (2.92 - 3.92)

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	347	
1	B	347	
2	C	1179	
3	D	1326	

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Mol	Chain	Length	Quality of chain
4	E	110	55%18%25%
5	F	531	51%9%39%
6	J	111	77%20%..
7	O	90	62%10%28%
8	P	90	64%8%28%
9	M	162	79%18%..

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 30033 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	0	0
			1716	1080	296	338	2		
1	B	237	Total	C	N	O	S	0	0
			1765	1115	301	346	3		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8602	5390	1511	1662	39		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1179	LEU	-	expression tag	UNP V9Z879
C	1180	ALA	-	expression tag	UNP V9Z879
C	1181	ARG	-	expression tag	UNP V9Z879
C	1182	HIS	-	expression tag	UNP V9Z879
C	1183	GLY	-	expression tag	UNP V9Z879
C	1184	GLY	-	expression tag	UNP V9Z879
C	1185	SER	-	expression tag	UNP V9Z879

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1270	Total	C	N	O	S	0	0
			9914	6208	1802	1862	42		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A5U053
D	0	ALA	-	expression tag	UNP A5U053

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP A5U053
D	1318	HIS	-	expression tag	UNP A5U053
D	1319	HIS	-	expression tag	UNP A5U053
D	1320	HIS	-	expression tag	UNP A5U053
D	1321	HIS	-	expression tag	UNP A5U053
D	1322	HIS	-	expression tag	UNP A5U053
D	1323	HIS	-	expression tag	UNP A5U053
D	1324	HIS	-	expression tag	UNP A5U053

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP A0A0T9N9K3

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	322	Total	C	N	O	S	0	0
			2540	1583	459	489	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P9WGI0
F	-1	PRO	-	expression tag	UNP P9WGI0
F	0	HIS	-	expression tag	UNP P9WGI0

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	109	Total	C	N	O	S	0	0
			880	543	166	168	3		

- Molecule 7 is a DNA chain called DNA (65-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	65	Total	C	N	O	P	0	0
			1336	633	243	395	65		

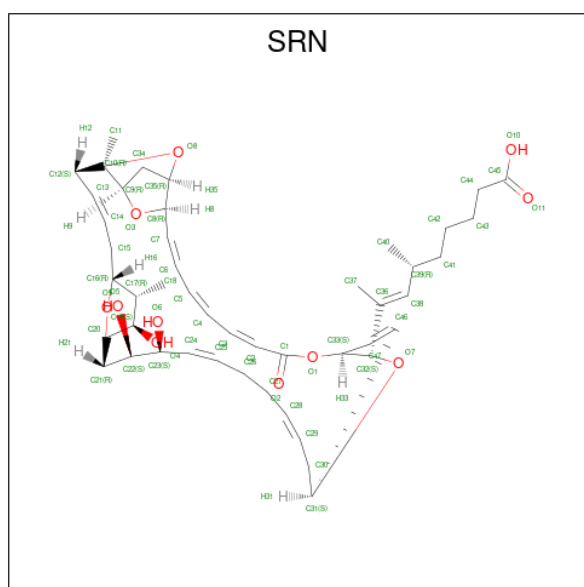
- Molecule 8 is a DNA chain called DNA (65-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	65	Total	C	N	O	P	0	0
			1329	629	250	385	65		

- Molecule 9 is a protein called RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	159	Total	C	N	O	S	0	0
			1241	777	224	239	1		

- Molecule 10 is SORANGICIN A (CCD ID: SRN) (formula: $C_{47}H_{66}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
10	C	1	Total	C	O	0
			58	47	11	

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	D	2	Total	Zn	0
			2	2	

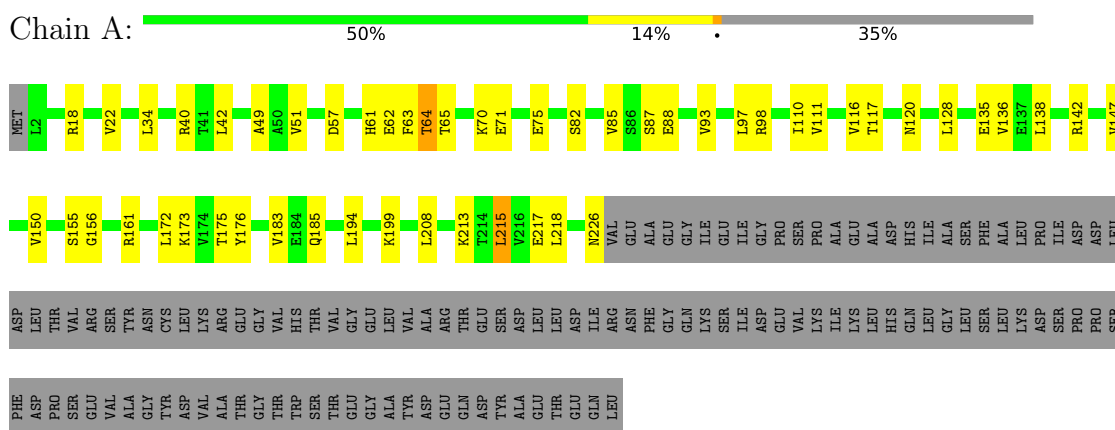
- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
12	D	1	Total	Mg	0
			1	1	

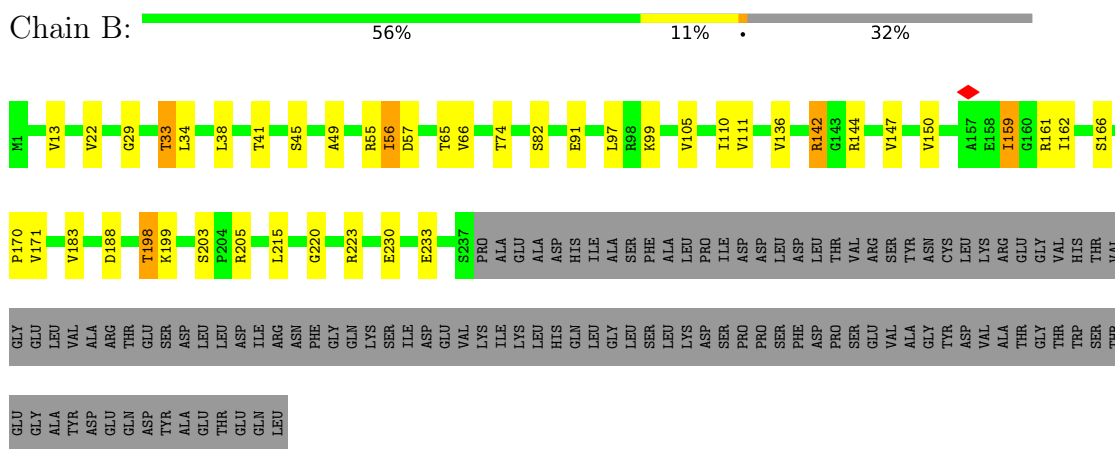
3 Residue-property plots

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.

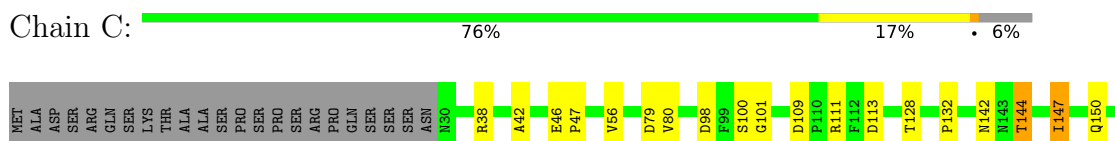
• Molecule 1: DNA-directed RNA polymerase subunit alpha

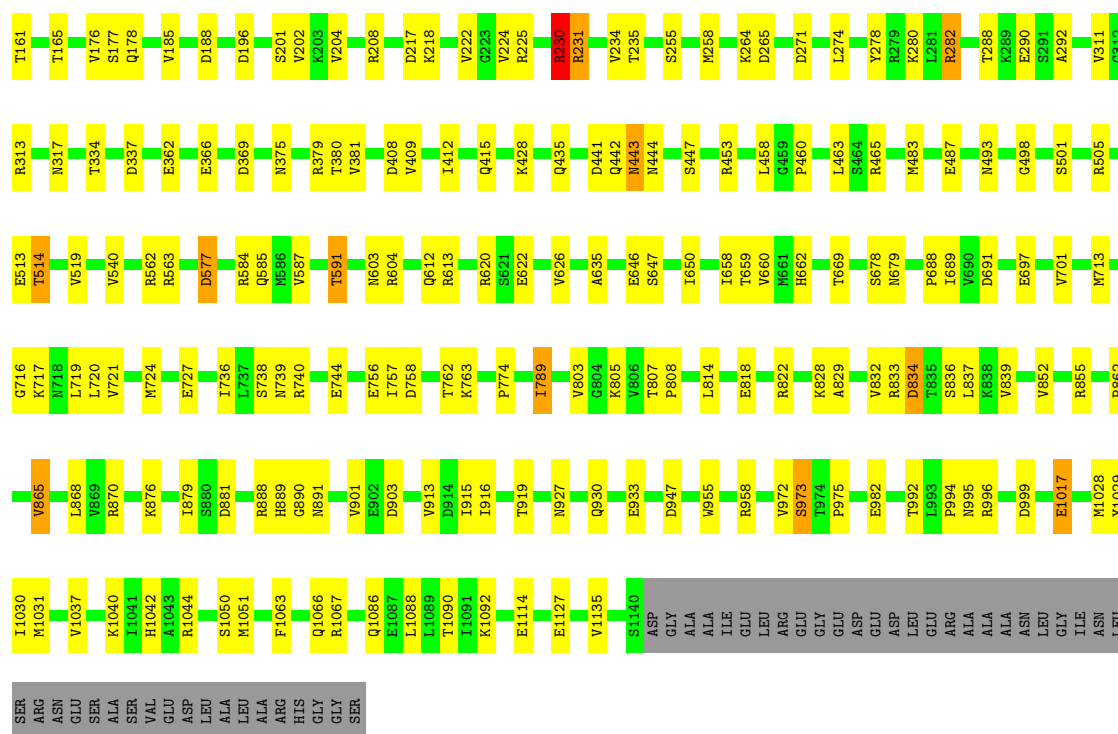


• Molecule 1: DNA-directed RNA polymerase subunit alpha



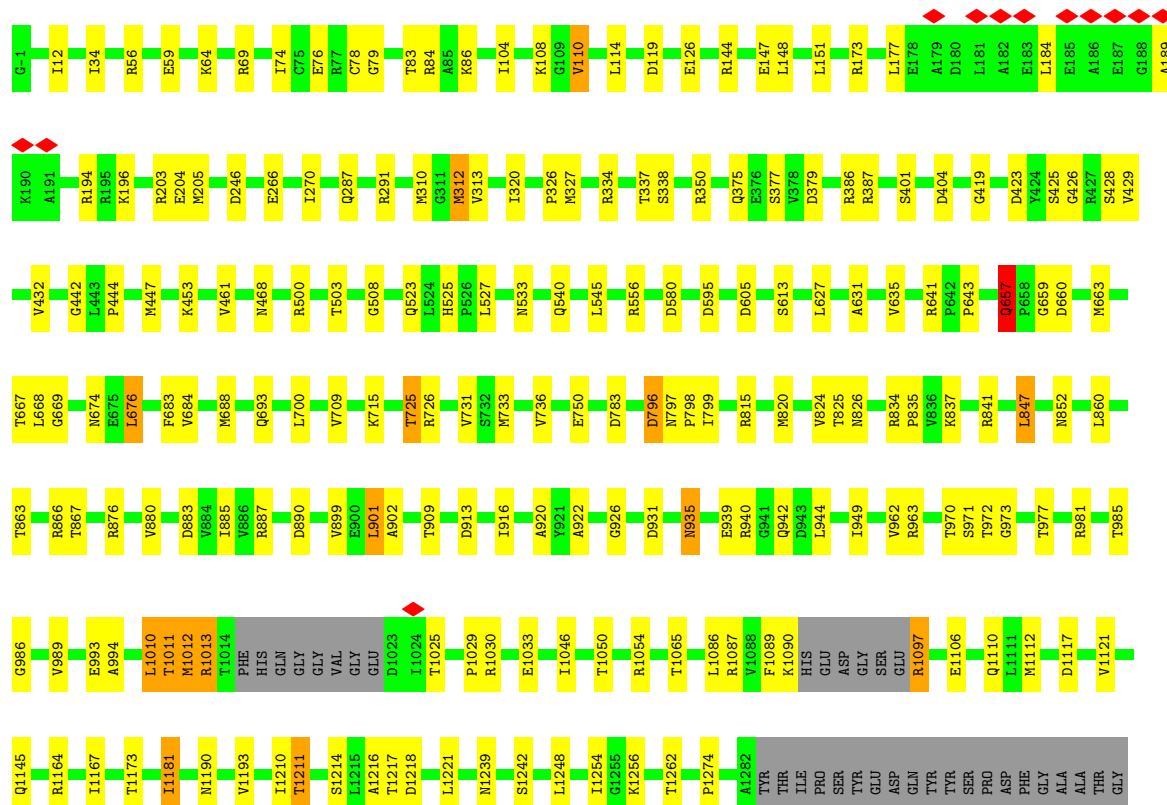
• Molecule 2: DNA-directed RNA polymerase subunit beta





• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 80% 14%





Chain M: 79% 18% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98323	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 ($e^-/\text{\AA}^2$)	66	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	2.695	Depositor
Minimum map value	-0.795	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.433	Depositor
Map size ($\text{\AA}$)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SRN, MG, ZN

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	0.33	0/1742	0.46	0/2370
1	B	0.31	0/1792	0.50	0/2442
2	C	0.34	0/8761	0.53	0/11880
3	D	0.34	0/10078	0.53	3/13624 (0.0%)
4	E	0.31	0/662	0.48	0/901
5	F	0.25	0/2571	0.45	0/3468
6	J	0.22	0/896	0.46	0/1210
7	O	0.30	0/1497	0.51	0/2310
8	P	0.31	0/1491	0.52	0/2297
9	M	0.22	0/1257	0.54	0/1700
All	All	0.32	0/30747	0.52	3/42202 (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
2	C	0	2
3	D	0	3
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1013	ARG	N-CA-C	8.64	122.55	108.99
3	D	916	ILE	N-CA-C	-6.41	106.55	112.96
3	D	657	GLN	N-CA-C	5.13	121.16	109.81

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	230	ARG	Peptide
2	C	282	ARG	Peptide
3	D	110	VAL	Peptide
3	D	657	GLN	Peptide
3	D	834	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	1716	0	1756	29	0
1	B	1765	0	1794	24	0
2	C	8602	0	8540	126	0
3	D	9914	0	9986	127	0
4	E	649	0	645	11	0
5	F	2540	0	2552	31	0
6	J	880	0	852	16	0
7	O	1336	0	732	7	0
8	P	1329	0	727	5	0
9	M	1241	0	1259	18	0
10	C	58	0	63	10	0
11	D	2	0	0	0	0
12	D	1	0	0	0	0
All	All	30033	0	28906	364	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (364) 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)
10:C:1201:SRN:C10	10:C:1201:SRN:C12	1.76	1.63
3:D:866:ARG:HD3	3:D:1012:MET:CE	1.41	1.49
10:C:1201:SRN:O3	10:C:1201:SRN:C8	1.79	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1201:SRN:O3	10:C:1201:SRN:C9	1.81	1.28
3:D:866:ARG:CD	3:D:1012:MET:HE1	1.72	1.19
3:D:1011:THR:HG23	3:D:1145:GLN:NE2	1.58	1.14
3:D:866:ARG:CD	3:D:1012:MET:CE	2.30	1.10
3:D:866:ARG:HD3	3:D:1012:MET:HE1	0.94	0.94
3:D:1011:THR:CG2	3:D:1145:GLN:NE2	2.34	0.90
3:D:866:ARG:HH11	3:D:1012:MET:CE	1.87	0.88
3:D:1011:THR:CG2	3:D:1145:GLN:HE22	1.86	0.87
10:C:1201:SRN:C10	10:C:1201:SRN:C13	2.51	0.86
3:D:866:ARG:HD3	3:D:1012:MET:HE3	1.60	0.83
3:D:866:ARG:HH11	3:D:1012:MET:HE2	1.44	0.81
10:C:1201:SRN:C12	10:C:1201:SRN:C11	2.61	0.78
1:A:40:ARG:HE	1:B:33:THR:HG22	1.53	0.74
2:C:225:ARG:HE	2:C:230:ARG:HB3	1.53	0.73
10:C:1201:SRN:C12	10:C:1201:SRN:C9	2.55	0.72
2:C:278:TYR:O	2:C:282:ARG:HB2	1.91	0.71
5:F:384:ARG:HG2	5:F:388:GLN:HE22	1.56	0.70
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.79	0.64
3:D:1011:THR:HG21	3:D:1145:GLN:HE22	1.60	0.64
3:D:880:VAL:HG21	3:D:1210:ILE:HB	1.81	0.62
2:C:147:ILE:HG12	9:M:47:ARG:HB2	1.80	0.62
1:A:183:VAL:HG13	1:A:185:GLN:H	1.65	0.62
2:C:453:ARG:NH2	2:C:501:SER:O	2.33	0.61
3:D:688:MET:HB3	3:D:693:GLN:HE21	1.66	0.60
5:F:306:LEU:HD11	5:F:348:THR:HG23	1.82	0.60
3:D:78:CYS:SG	3:D:79:GLY:N	2.76	0.59
3:D:866:ARG:HH11	3:D:1012:MET:HE3	1.65	0.59
2:C:408:ASP:OD1	2:C:408:ASP:N	2.36	0.59
2:C:659:THR:HG22	2:C:669:THR:HG22	1.85	0.59
2:C:1042:HIS:NE2	2:C:1063:PHE:O	2.28	0.59
1:A:64:THR:OG1	1:A:65:THR:N	2.37	0.58
2:C:903:ASP:OD1	2:C:903:ASP:N	2.35	0.58
2:C:369:ASP:O	2:C:375:ASN:ND2	2.36	0.58
2:C:188:ASP:OD1	2:C:188:ASP:N	2.36	0.58
3:D:676:LEU:HD12	3:D:715:LYS:HB3	1.84	0.58
1:A:142:ARG:NH2	1:B:230:GLU:OE1	2.37	0.58
2:C:635:ALA:HB2	2:C:713:MET:HG2	1.84	0.58
2:C:891:ASN:ND2	2:C:930:GLN:OE1	2.35	0.57
2:C:79:ASP:OD1	2:C:79:ASP:N	2.38	0.57
2:C:612:GLN:HA	2:C:1031:MET:HE1	1.87	0.57
3:D:885:ILE:HG22	3:D:994:ALA:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1010:LEU:O	3:D:1011:THR:O	2.22	0.57
3:D:83:THR:OG1	3:D:84:ARG:N	2.38	0.57
4:E:70:GLN:NE2	4:E:73:GLU:OE2	2.38	0.57
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.38	0.57
3:D:899:VAL:HG12	3:D:901:LEU:HB2	1.87	0.57
7:O:22:DG:H2''	7:O:23:DT:H5'	1.86	0.57
5:F:336:ASP:OD1	6:J:88:ARG:NH1	2.38	0.56
2:C:577:ASP:OD1	2:C:577:ASP:N	2.35	0.56
3:D:173:ARG:HG2	3:D:205:MET:HB2	1.86	0.56
3:D:876:ARG:HD3	3:D:1211:THR:HG23	1.86	0.56
3:D:885:ILE:HD11	3:D:887:ARG:HH21	1.68	0.56
5:F:286:ARG:HH11	5:F:290:ARG:HH12	1.53	0.56
3:D:866:ARG:CD	3:D:1012:MET:HE2	2.34	0.56
9:M:112:TRP:O	9:M:116:GLN:HB2	2.05	0.56
3:D:796:ASP:OD1	3:D:796:ASP:N	2.33	0.56
5:F:464:LEU:HD23	5:F:476:ARG:HE	1.71	0.56
2:C:271:ASP:OD1	2:C:271:ASP:N	2.39	0.56
1:B:57:ASP:OD1	1:B:57:ASP:N	2.39	0.56
4:E:47:VAL:HG21	4:E:53:LEU:HB2	1.86	0.56
2:C:144:THR:O	9:M:52:ASN:ND2	2.39	0.56
3:D:468:ASN:OD1	3:D:468:ASN:N	2.38	0.56
1:A:87:SER:OG	1:A:88:GLU:N	2.39	0.55
2:C:38:ARG:NH1	2:C:972:VAL:O	2.38	0.55
2:C:380:THR:OG1	2:C:381:VAL:N	2.40	0.55
9:M:75:ARG:NH2	9:M:158:LEU:O	2.39	0.55
2:C:758:ASP:N	2:C:758:ASP:OD1	2.37	0.55
2:C:201:SER:OG	2:C:202:VAL:N	2.39	0.55
2:C:678:SER:OG	2:C:679:ASN:N	2.40	0.55
2:C:740:ARG:NH1	2:C:744:GLU:OE1	2.39	0.55
3:D:880:VAL:HG22	3:D:1214:SER:HB3	1.88	0.55
2:C:757:ILE:HB	2:C:837:LEU:HD22	1.88	0.55
3:D:147:GLU:O	3:D:151:LEU:HB2	2.06	0.55
1:B:33:THR:OG1	1:B:34:LEU:N	2.39	0.54
2:C:113:ASP:HB2	2:C:132:PRO:HD2	1.89	0.54
2:C:982:GLU:OE1	3:D:841:ARG:NH2	2.40	0.54
3:D:425:SER:OG	3:D:426:GLY:N	2.39	0.54
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.89	0.54
1:B:170:PRO:HA	1:B:199:LYS:HD2	1.89	0.54
3:D:500:ARG:NH1	3:D:533:ASN:O	2.40	0.54
6:J:20:ARG:NH1	6:J:23:ASP:O	2.41	0.54
9:M:121:SER:HB3	9:M:124:GLU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:147:ILE:HD11	9:M:47:ARG:HH11	1.71	0.54
2:C:719:LEU:HD22	2:C:1030:ILE:HD11	1.90	0.54
1:A:217:GLU:HG2	1:B:233:GLU:HA	1.88	0.54
3:D:926:GLY:O	3:D:940:ARG:NH2	2.41	0.54
3:D:350:ARG:HH11	3:D:377:SER:HB3	1.73	0.53
5:F:488:THR:OG1	5:F:491:GLU:OE1	2.25	0.53
2:C:150:GLN:HG3	9:M:44:LEU:HB3	1.91	0.53
2:C:334:THR:HG23	2:C:337:ASP:H	1.74	0.53
5:F:210:GLU:HA	5:F:213:ARG:HB3	1.90	0.53
8:P:107:DA:OP1	9:M:121:SER:OG	2.24	0.53
2:C:736:ILE:HD11	2:C:916:ILE:HD12	1.91	0.53
2:C:101:GLY:O	2:C:142:ASN:ND2	2.41	0.53
3:D:1087:ARG:NH1	3:D:1110:GLN:OE1	2.42	0.53
2:C:756:GLU:OE2	2:C:870:ARG:NH1	2.40	0.52
2:C:995:ASN:N	2:C:995:ASN:OD1	2.39	0.52
1:A:62:GLU:OE2	2:C:876:LYS:NZ	2.41	0.52
2:C:230:ARG:O	2:C:230:ARG:NH1	2.42	0.52
2:C:828:LYS:HE2	2:C:829:ALA:H	1.75	0.52
2:C:444:ASN:N	2:C:444:ASN:OD1	2.42	0.52
1:B:198:THR:OG1	1:B:199:LYS:O	2.28	0.52
2:C:808:PRO:HA	2:C:832:VAL:HG12	1.92	0.52
2:C:955:TRP:O	2:C:958:ARG:NH1	2.43	0.52
3:D:931:ASP:N	3:D:931:ASP:OD1	2.41	0.52
2:C:218:LYS:NZ	8:P:85:DT:OP1	2.39	0.52
2:C:855:ARG:NH1	2:C:865:VAL:O	2.43	0.52
10:C:1201:SRN:O3	10:C:1201:SRN:H6	2.10	0.52
3:D:144:ARG:O	3:D:148:LEU:HB2	2.11	0.52
2:C:789:ILE:HG22	2:C:803:VAL:HG22	1.92	0.51
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.92	0.51
3:D:866:ARG:NH1	3:D:1012:MET:CE	2.67	0.51
5:F:232:LEU:HD22	7:O:55:DG:H2''	1.90	0.51
2:C:178:GLN:OE1	2:C:379:ARG:NH2	2.43	0.51
2:C:881:ASP:N	2:C:881:ASP:OD1	2.42	0.51
5:F:336:ASP:OD1	6:J:89:ARG:NH2	2.43	0.51
1:A:71:GLU:HB3	1:A:75:GLU:HB3	1.93	0.51
3:D:1025:THR:HG21	3:D:1029:PRO:HB2	1.92	0.51
4:E:89:GLU:OE2	4:E:97:ARG:NH1	2.40	0.51
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.93	0.50
7:O:56:DG:H2'	7:O:57:DC:C2	2.45	0.50
1:B:171:VAL:HA	1:B:198:THR:HA	1.92	0.50
5:F:381:ARG:HH21	8:P:104:DC:H1'	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:822:ARG:NH1	2:C:828:LYS:O	2.43	0.50
5:F:311:THR:OG1	5:F:312:GLY:N	2.45	0.50
5:F:463:VAL:O	5:F:466:THR:OG1	2.29	0.50
9:M:147:ASP:OD1	9:M:147:ASP:N	2.44	0.50
2:C:435:GLN:HE21	2:C:460:PRO:HG3	1.77	0.50
2:C:443:ASN:OD1	2:C:443:ASN:N	2.44	0.50
3:D:126:GLU:OE2	3:D:387:ARG:NE	2.43	0.50
1:B:56:ILE:HB	1:B:136:VAL:HG22	1.93	0.50
2:C:442:GLN:NE2	2:C:679:ASN:OD1	2.41	0.50
3:D:184:LEU:O	3:D:194:ARG:NH1	2.44	0.50
2:C:1092:LYS:NZ	3:D:545:LEU:O	2.44	0.50
3:D:750:GLU:OE1	3:D:837:LYS:NZ	2.43	0.50
3:D:922:ALA:HB1	3:D:981:ARG:HB3	1.94	0.50
1:A:82:SER:O	1:A:82:SER:OG	2.27	0.50
2:C:947:ASP:OD1	2:C:947:ASP:N	2.39	0.50
3:D:700:LEU:HD23	3:D:709:VAL:HG22	1.94	0.50
9:M:79:THR:OG1	9:M:109:ARG:NH2	2.45	0.50
5:F:485:GLN:NE2	5:F:486:PRO:O	2.44	0.50
6:J:20:ARG:NH1	6:J:23:ASP:OD1	2.45	0.49
10:C:1201:SRN:O3	10:C:1201:SRN:C6	2.60	0.49
3:D:74:ILE:HD12	6:J:42:VAL:HG13	1.94	0.49
3:D:334:ARG:HD3	5:F:418:ARG:HE	1.77	0.49
9:M:115:ASP:HA	9:M:119:GLY:H	1.75	0.49
1:A:70:LYS:NZ	2:C:691:ASP:OD1	2.45	0.49
5:F:256:GLY:HA2	5:F:284:ILE:HG22	1.94	0.49
3:D:525:HIS:HE1	3:D:527:LEU:HD12	1.77	0.49
3:D:866:ARG:NH1	3:D:1012:MET:HE3	2.27	0.49
1:B:45:SER:O	1:B:45:SER:OG	2.31	0.49
3:D:1089:PHE:O	3:D:1097:ARG:N	2.46	0.49
3:D:108:LYS:O	3:D:386:ARG:NH1	2.46	0.49
3:D:375:GLN:NE2	3:D:379:ASP:OD2	2.45	0.49
5:F:502:ARG:NH2	7:O:23:DT:OP2	2.44	0.49
2:C:231:ARG:HB2	2:C:280:LYS:HE2	1.94	0.49
10:C:1201:SRN:O3	10:C:1201:SRN:C35	2.53	0.49
3:D:444:PRO:HG2	3:D:447:MET:HB3	1.95	0.49
4:E:42:GLU:O	4:E:46:ARG:NH1	2.46	0.49
1:A:49:ALA:HB2	1:A:142:ARG:HD2	1.94	0.49
3:D:935:ASN:OD1	3:D:935:ASN:N	2.42	0.49
3:D:428:SER:OG	3:D:429:VAL:N	2.46	0.48
6:J:63:THR:OG1	6:J:64:LEU:N	2.46	0.48
6:J:64:LEU:HD23	6:J:66:GLU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:VAL:HA	1:B:188:ASP:H	1.77	0.48
2:C:255:SER:HB2	2:C:258:MET:HB2	1.94	0.48
1:A:120:ASN:OD1	1:A:120:ASN:N	2.45	0.48
1:A:40:ARG:HH12	2:C:903:ASP:HB3	1.78	0.48
2:C:38:ARG:HG2	2:C:973:SER:HB3	1.95	0.48
2:C:1067:ARG:NH2	3:D:419:GLY:O	2.45	0.48
3:D:971:SER:OG	3:D:972:THR:N	2.45	0.48
3:D:985:THR:OG1	3:D:986:GLY:N	2.45	0.48
6:J:34:THR:OG1	6:J:36:ASN:OD1	2.31	0.48
3:D:641:ARG:HA	3:D:657:GLN:HG3	1.96	0.47
3:D:1046:ILE:HG22	3:D:1110:GLN:HA	1.95	0.47
9:M:41:GLN:OE1	9:M:133:GLN:NE2	2.44	0.47
2:C:185:VAL:HG12	2:C:204:VAL:HG22	1.97	0.47
3:D:989:VAL:HG22	3:D:993:GLU:HG3	1.96	0.47
2:C:264:LYS:HD2	2:C:264:LYS:HA	1.74	0.47
2:C:836:SER:OG	2:C:837:LEU:N	2.47	0.47
2:C:891:ASN:HD21	2:C:1028:MET:HE1	1.79	0.47
4:E:48:SER:OG	4:E:49:SER:N	2.47	0.47
1:A:18:ARG:HH12	2:C:996:ARG:HH12	1.63	0.47
2:C:1135:VAL:HG22	3:D:12:ILE:HG13	1.97	0.47
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.95	0.47
3:D:605:ASP:OD1	3:D:605:ASP:N	2.45	0.47
3:D:1217:THR:OG1	3:D:1218:ASP:N	2.48	0.47
5:F:367:ARG:NH2	7:O:45:DG:OP1	2.42	0.47
5:F:464:LEU:HB3	5:F:476:ARG:HH21	1.80	0.47
9:M:111:LEU:HB3	9:M:128:LEU:HD12	1.96	0.47
2:C:915:ILE:HD13	2:C:1030:ILE:HD13	1.96	0.47
3:D:64:LYS:NZ	3:D:76:GLU:OE2	2.46	0.47
3:D:327:MET:HE2	3:D:337:THR:HG22	1.96	0.47
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.97	0.47
2:C:505:ARG:NH2	2:C:513:GLU:OE1	2.48	0.47
2:C:727:GLU:H	3:D:725:THR:HG22	1.80	0.47
2:C:758:ASP:HB3	2:C:868:LEU:HD23	1.97	0.47
3:D:643:PRO:HD3	3:D:683:PHE:HB3	1.96	0.47
6:J:79:ARG:NH1	7:O:48:DT:OP1	2.45	0.47
2:C:994:PRO:HB3	2:C:999:ASP:H	1.80	0.47
3:D:1254:ILE:HD11	3:D:1256:LYS:HD2	1.96	0.46
1:A:40:ARG:NH2	1:B:29:GLY:O	2.38	0.46
1:B:97:LEU:HB3	1:B:110:ILE:HG13	1.96	0.46
2:C:647:SER:HB2	2:C:697:GLU:HA	1.97	0.46
3:D:1054:ARG:HB3	3:D:1065:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:OD1	1:A:57:ASP:N	2.42	0.46
2:C:1088:LEU:HD23	2:C:1092:LYS:HD2	1.97	0.46
3:D:825:THR:OG1	3:D:826:ASN:N	2.48	0.46
2:C:487:GLU:OE2	2:C:613:ARG:NH2	2.48	0.46
3:D:1030:ARG:NH1	3:D:1033:GLU:OE2	2.42	0.46
2:C:891:ASN:OD1	2:C:891:ASN:N	2.40	0.46
3:D:56:ARG:HB2	3:D:59:GLU:HB2	1.97	0.46
3:D:674:ASN:HD21	3:D:684:VAL:H	1.63	0.46
5:F:252:ARG:NE	5:F:287:ASP:OD2	2.47	0.46
9:M:136:VAL:HG21	9:M:151:GLU:HG2	1.97	0.46
3:D:963:ARG:NH1	3:D:977:THR:OG1	2.49	0.46
2:C:587:VAL:HG22	2:C:591:THR:HB	1.98	0.46
3:D:114:LEU:HG	3:D:312:MET:HE2	1.98	0.46
2:C:265:ASP:OD1	2:C:265:ASP:N	2.41	0.46
2:C:620:ARG:HB3	2:C:717:LYS:HZ1	1.81	0.46
2:C:919:THR:HG23	3:D:731:VAL:HG23	1.98	0.46
3:D:69:ARG:HG3	6:J:20:ARG:HH22	1.81	0.46
3:D:660:ASP:OD1	3:D:660:ASP:N	2.49	0.46
2:C:441:ASP:OD2	2:C:447:SER:OG	2.32	0.46
2:C:1066:GLN:NE2	3:D:425:SER:OG	2.40	0.46
5:F:501:GLU:OE2	5:F:504:ARG:NH2	2.45	0.46
5:F:359:MET:O	5:F:363:ALA:HB2	2.16	0.45
2:C:888:ARG:NH2	2:C:933:GLU:OE2	2.45	0.45
3:D:525:HIS:CE1	3:D:527:LEU:HD12	2.51	0.45
3:D:663:MET:HE2	3:D:663:MET:HB3	1.85	0.45
5:F:334:LYS:HG3	6:J:84:MET:HG2	1.98	0.45
2:C:879:ILE:HD12	2:C:879:ILE:HA	1.83	0.45
2:C:889:HIS:NE2	2:C:933:GLU:OE1	2.40	0.45
6:J:89:ARG:HD3	6:J:89:ARG:HA	1.77	0.45
3:D:196:LYS:HD2	3:D:196:LYS:HA	1.77	0.45
3:D:657:GLN:O	3:D:659:GLY:N	2.50	0.45
2:C:927:ASN:OD1	2:C:927:ASN:N	2.49	0.45
3:D:1167:ILE:HD11	3:D:1181:ILE:HD11	1.99	0.45
1:B:159:ILE:H	1:B:159:ILE:HG13	1.51	0.45
2:C:465:ARG:NH1	2:C:493:ASN:OD1	2.37	0.45
2:C:762:THR:OG1	2:C:763:LYS:N	2.50	0.45
3:D:939:GLU:OE2	3:D:942:GLN:NE2	2.48	0.45
1:B:55:ARG:HB3	1:B:161:ARG:HA	1.98	0.45
2:C:109:ASP:OD2	2:C:111:ARG:NH1	2.50	0.45
2:C:514:THR:HG22	2:C:585:GLN:HE21	1.80	0.45
3:D:334:ARG:HD2	3:D:334:ARG:HA	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:114:ARG:HD3	9:M:120:LEU:HD21	1.98	0.45
9:M:146:ASP:O	9:M:149:LYS:N	2.49	0.45
1:B:41:THR:HG21	1:B:215:LEU:HG	1.99	0.45
2:C:724:MET:HE3	2:C:724:MET:HB2	1.81	0.45
3:D:173:ARG:O	3:D:177:LEU:HB2	2.16	0.45
5:F:492:ILE:O	5:F:496:TYR:HB2	2.17	0.45
2:C:274:LEU:HD22	2:C:292:ALA:HB1	1.99	0.44
2:C:774:PRO:HD2	2:C:834:ASP:HB2	1.99	0.44
3:D:173:ARG:NH1	3:D:204:GLU:OE1	2.50	0.44
5:F:372:MET:HE2	5:F:372:MET:HB2	1.89	0.44
8:P:140:DC:H2"	8:P:141:DG:C8	2.52	0.44
5:F:449:ASP:OD1	5:F:449:ASP:N	2.47	0.44
6:J:77:PRO:HA	6:J:78:PRO:HD3	1.90	0.44
1:A:175:THR:OG1	1:A:176:TYR:N	2.51	0.44
2:C:288:THR:OG1	2:C:290:GLU:OE1	2.31	0.44
5:F:382:ILE:HD13	5:F:382:ILE:HA	1.88	0.44
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.99	0.44
3:D:1274:PRO:HG2	4:E:79:VAL:HG21	1.99	0.44
5:F:502:ARG:HA	5:F:502:ARG:HD2	1.81	0.44
2:C:814:LEU:HD12	2:C:818:GLU:HG2	1.99	0.44
3:D:84:ARG:HD2	3:D:86:LYS:HG2	2.00	0.44
3:D:736:VAL:HG22	3:D:799:ILE:HD11	2.00	0.44
3:D:899:VAL:HG11	3:D:920:ALA:HB2	2.00	0.44
3:D:863:THR:O	3:D:867:THR:OG1	2.34	0.44
5:F:328:LEU:HD23	5:F:351:ILE:HD11	2.00	0.44
1:A:213:LYS:NZ	1:B:233:GLU:OE2	2.51	0.43
1:B:34:LEU:O	1:B:38:LEU:HB2	2.18	0.43
2:C:1086:GLN:O	2:C:1090:THR:OG1	2.25	0.43
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.99	0.43
10:C:1201:SRN:H152	10:C:1201:SRN:H181	1.78	0.43
1:A:161:ARG:HE	1:A:161:ARG:HB2	1.65	0.43
2:C:1040:LYS:HD2	3:D:540:GLN:HE22	1.82	0.43
3:D:1054:ARG:N	3:D:1065:THR:O	2.44	0.43
2:C:435:GLN:H	2:C:435:GLN:HG2	1.52	0.43
3:D:627:LEU:HD13	3:D:668:LEU:HD12	2.00	0.43
5:F:432:ASP:OD1	5:F:432:ASP:N	2.51	0.43
2:C:604:ARG:NH2	2:C:890:GLY:O	2.44	0.43
3:D:326:PRO:O	3:D:338:SER:OG	2.36	0.43
1:A:97:LEU:HB2	1:A:110:ILE:HG12	2.00	0.43
3:D:890:ASP:OD1	3:D:977:THR:OG1	2.33	0.43
2:C:716:GLY:N	2:C:1029:TYR:OH	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1050:SER:OG	2:C:1051:MET:N	2.52	0.43
7:O:36:DG:H2"	7:O:37:DC:H5"	2.01	0.43
3:D:847:LEU:HD12	3:D:847:LEU:HA	1.88	0.43
1:A:98:ARG:HG2	1:A:135:GLU:HG2	2.01	0.43
1:A:199:LYS:H	1:A:199:LYS:HG2	1.70	0.43
2:C:646:GLU:HB3	2:C:662:HIS:CE1	2.53	0.43
3:D:119:ASP:OD1	3:D:291:ARG:NH2	2.53	0.42
1:A:51:VAL:HG21	1:A:138:LEU:HD23	2.02	0.42
1:A:61:HIS:HD2	1:A:63:PHE:H	1.66	0.42
4:E:52:ALA:O	4:E:56:TYR:HB2	2.19	0.42
1:A:173:LYS:HE3	1:A:173:LYS:HB2	1.86	0.42
3:D:580:ASP:OD1	3:D:580:ASP:N	2.52	0.42
2:C:98:ASP:OD1	2:C:98:ASP:N	2.53	0.42
3:D:902:ALA:H	3:D:913:ASP:HB2	1.83	0.42
2:C:161:THR:OG1	2:C:165:THR:O	2.31	0.42
3:D:556:ARG:NH2	4:E:35:ILE:O	2.53	0.42
3:D:815:ARG:NH1	3:D:820:MET:O	2.53	0.42
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.91	0.42
6:J:101:ARG:HA	6:J:101:ARG:HD3	1.82	0.42
3:D:203:ARG:HA	3:D:203:ARG:HD2	1.85	0.42
2:C:562:ARG:HD3	3:D:847:LEU:HD11	2.01	0.42
2:C:1017:GLU:H	2:C:1017:GLU:HG2	1.65	0.42
2:C:217:ASP:OD1	2:C:217:ASP:N	2.40	0.41
2:C:689:ILE:HD11	2:C:701:VAL:HG12	2.02	0.41
3:D:641:ARG:O	3:D:683:PHE:N	2.53	0.41
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.46	0.41
2:C:428:LYS:HE2	2:C:428:LYS:HB3	1.95	0.41
2:C:563:ARG:HD3	2:C:563:ARG:HA	1.68	0.41
3:D:189:ALA:O	3:D:194:ARG:NH2	2.53	0.41
3:D:993:GLU:OE2	4:E:51:TYR:OH	2.37	0.41
1:A:208:LEU:HD12	1:A:208:LEU:HA	1.93	0.41
3:D:725:THR:OG1	3:D:726:ARG:NH1	2.53	0.41
5:F:378:LYS:HE2	5:F:378:LYS:HB3	1.84	0.41
1:B:220:GLY:HA2	1:B:223:ARG:HB3	2.02	0.41
2:C:224:VAL:HG21	2:C:234:VAL:HA	2.03	0.41
2:C:862:PRO:HG2	2:C:865:VAL:HG21	2.01	0.41
2:C:1031:MET:HE3	2:C:1031:MET:HB2	1.81	0.41
3:D:1086:LEU:HD12	3:D:1112:MET:HE1	2.02	0.41
3:D:1190:ASN:HA	3:D:1193:VAL:HG12	2.02	0.41
6:J:15:SER:OG	6:J:16:TYR:N	2.53	0.41
1:B:49:ALA:HA	1:B:142:ARG:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:401:SER:OG	3:D:404:ASP:OD2	2.39	0.41
3:D:503:THR:HG23	3:D:508:GLY:HA3	2.03	0.41
3:D:970:THR:OG1	3:D:973:GLY:O	2.31	0.41
1:A:215:LEU:HD13	1:A:215:LEU:HA	1.89	0.41
2:C:313:ARG:NH1	2:C:317:ASN:OD1	2.54	0.41
2:C:435:GLN:HG3	2:C:460:PRO:HD3	2.03	0.41
2:C:483:MET:HE3	2:C:498:GLY:HA3	2.02	0.41
3:D:1050:THR:HG22	3:D:1106:GLU:HA	2.02	0.41
3:D:1221:LEU:HD12	3:D:1221:LEU:HA	1.92	0.41
4:E:60:ARG:HA	4:E:60:ARG:HD2	1.92	0.41
6:J:93:GLU:H	6:J:93:GLU:HG3	1.74	0.41
2:C:46:GLU:HA	2:C:47:PRO:HD3	1.94	0.41
2:C:807:THR:O	2:C:833:ARG:N	2.53	0.41
8:P:122:DT:H2'	8:P:123:DG:C8	2.55	0.41
9:M:38:LYS:HE2	9:M:38:LYS:HB2	1.92	0.41
1:B:82:SER:O	1:B:82:SER:OG	2.36	0.40
2:C:150:GLN:HE22	2:C:415:GLN:HB2	1.86	0.40
3:D:797:ASN:HD22	3:D:798:PRO:HD2	1.86	0.40
5:F:492:ILE:HA	5:F:495:VAL:HG12	2.03	0.40
1:A:155:SER:OG	1:A:156:GLY:N	2.52	0.40
1:B:147:VAL:HG12	1:B:166:SER:HB2	2.03	0.40
2:C:738:SER:OG	2:C:739:ASN:N	2.53	0.40
2:C:1127:GLU:HG2	3:D:320:ILE:HD11	2.03	0.40
2:C:442:GLN:O	2:C:678:SER:OG	2.29	0.40
2:C:650:ILE:HD13	2:C:660:VAL:HG12	2.04	0.40
2:C:721:VAL:HG11	2:C:1028:MET:HB2	2.03	0.40
2:C:757:ILE:HD12	2:C:757:ILE:HA	1.87	0.40
3:D:667:THR:OG1	3:D:669:GLY:N	2.54	0.40
9:M:38:LYS:HA	9:M:45:THR:HA	2.03	0.40
2:C:1044:ARG:NE	3:D:423:ASP:OD1	2.55	0.40
3:D:266:GLU:HA	3:D:310:MET:HE1	2.04	0.40
1:B:203:SER:OG	1:B:205:ARG:NH2	2.54	0.40
2:C:196:ASP:OD1	2:C:196:ASP:N	2.54	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	223/347 (64%)	204 (92%)	19 (8%)	0	100	100
1	B	235/347 (68%)	211 (90%)	24 (10%)	0	100	100
2	C	1109/1179 (94%)	1018 (92%)	90 (8%)	1 (0%)	48	78
3	D	1264/1326 (95%)	1167 (92%)	95 (8%)	2 (0%)	43	71
4	E	81/110 (74%)	74 (91%)	7 (9%)	0	100	100
5	F	320/531 (60%)	307 (96%)	13 (4%)	0	100	100
6	J	107/111 (96%)	98 (92%)	9 (8%)	0	100	100
9	M	157/162 (97%)	147 (94%)	10 (6%)	0	100	100
All	All	3496/4113 (85%)	3226 (92%)	267 (8%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	1011	THR
2	C	231	ARG
3	D	835	PRO

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	194/297 (65%)	177 (91%)	17 (9%)	9	30
1	B	195/297 (66%)	180 (92%)	15 (8%)	12	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	936/997 (94%)	895 (96%)	41 (4%)	25	50
3	D	1048/1103 (95%)	1008 (96%)	40 (4%)	29	54
4	E	69/89 (78%)	62 (90%)	7 (10%)	7	25
5	F	266/429 (62%)	257 (97%)	9 (3%)	32	56
6	J	92/97 (95%)	86 (94%)	6 (6%)	15	41
9	M	129/131 (98%)	122 (95%)	7 (5%)	20	46
All	All	2929/3440 (85%)	2787 (95%)	142 (5%)	24	48

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	34	LEU
1	A	64	THR
1	A	85	VAL
1	A	93	VAL
1	A	111	VAL
1	A	116	VAL
1	A	117	THR
1	A	128	LEU
1	A	136	VAL
1	A	147	VAL
1	A	150	VAL
1	A	172	LEU
1	A	194	LEU
1	A	215	LEU
1	A	218	LEU
1	A	226	ASN
1	B	13	VAL
1	B	22	VAL
1	B	33	THR
1	B	56	ILE
1	B	65	THR
1	B	66	VAL
1	B	74	THR
1	B	91	GLU
1	B	111	VAL
1	B	142	ARG
1	B	144	ARG
1	B	150	VAL

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Mol	Chain	Res	Type
1	B	159	ILE
1	B	162	ILE
1	B	198	THR
2	C	56	VAL
2	C	80	VAL
2	C	100	SER
2	C	128	THR
2	C	144	THR
2	C	147	ILE
2	C	176	VAL
2	C	177	SER
2	C	208	ARG
2	C	222	VAL
2	C	230	ARG
2	C	235	THR
2	C	311	VAL
2	C	362	GLU
2	C	366	GLU
2	C	409	VAL
2	C	412	ILE
2	C	443	ASN
2	C	458	LEU
2	C	463	LEU
2	C	514	THR
2	C	519	VAL
2	C	540	VAL
2	C	577	ASP
2	C	584	ARG
2	C	591	THR
2	C	603	ASN
2	C	622	GLU
2	C	626	VAL
2	C	789	ILE
2	C	805	LYS
2	C	834	ASP
2	C	839	VAL
2	C	852	VAL
2	C	865	VAL
2	C	901	VAL
2	C	973	SER
2	C	992	THR
2	C	1017	GLU

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Mol	Chain	Res	Type
2	C	1037	VAL
2	C	1114	GLU
3	D	34	ILE
3	D	110	VAL
3	D	246	ASP
3	D	270	ILE
3	D	287	GLN
3	D	312	MET
3	D	313	VAL
3	D	432	VAL
3	D	453	LYS
3	D	461	VAL
3	D	613	SER
3	D	635	VAL
3	D	676	LEU
3	D	725	THR
3	D	733	MET
3	D	783	ASP
3	D	796	ASP
3	D	847	LEU
3	D	860	LEU
3	D	883	ASP
3	D	901	LEU
3	D	909	THR
3	D	935	ASN
3	D	944	LEU
3	D	949	ILE
3	D	962	VAL
3	D	1010	LEU
3	D	1012	MET
3	D	1013	ARG
3	D	1090	LYS
3	D	1097	ARG
3	D	1117	ASP
3	D	1121	VAL
3	D	1173	THR
3	D	1181	ILE
3	D	1211	THR
3	D	1239	ASN
3	D	1242	SER
3	D	1248	LEU
3	D	1262	THR

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Mol	Chain	Res	Type
4	E	31	THR
4	E	33	LEU
4	E	35	ILE
4	E	36	THR
4	E	79	VAL
4	E	102	ASP
4	E	103	LEU
5	F	208	GLU
5	F	237	LYS
5	F	244	GLU
5	F	280	ASP
5	F	421	ILE
5	F	455	LEU
5	F	460	LEU
5	F	464	LEU
5	F	481	LEU
6	J	5	VAL
6	J	10	ARG
6	J	49	GLU
6	J	55	LEU
6	J	63	THR
6	J	65	ILE
9	M	9	VAL
9	M	19	VAL
9	M	35	LEU
9	M	52	ASN
9	M	61	VAL
9	M	111	LEU
9	M	134	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	226	ASN
1	B	36	ASN
1	B	226	ASN
2	C	141	ASN
2	C	169	ASN
2	C	293	GLN
2	C	323	HIS
2	C	419	ASN

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Mol	Chain	Res	Type
2	C	585	GLN
2	C	662	HIS
2	C	755	HIS
2	C	1062	GLN
3	D	213	GLN
3	D	287	GLN
3	D	341	ASN
3	D	368	ASN
3	D	369	ASN
3	D	494	HIS
3	D	653	HIS
3	D	693	GLN
3	D	748	HIS
3	D	797	ASN
3	D	942	GLN
3	D	1084	GLN
3	D	1145	GLN
3	D	1160	GLN
3	D	1227	GLN
5	F	353	GLN
5	F	377	ASN
5	F	388	GLN
5	F	425	GLN
6	J	22	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 3 are 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
10	SRN	C	1201	-	60,62,62	5.11	33 (55%)	61,84,84	1.72	14 (22%)

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
10	SRN	C	1201	-	-	13/52/105/105	0/4/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1201	SRN	O3-C8	20.31	1.79	1.44
10	C	1201	SRN	O3-C9	16.25	1.81	1.45
10	C	1201	SRN	C34-C9	-11.39	1.28	1.52
10	C	1201	SRN	C34-C35	-9.18	1.33	1.52
10	C	1201	SRN	C3-C2	8.98	1.58	1.34
10	C	1201	SRN	C4-C5	7.41	1.56	1.36
10	C	1201	SRN	C13-C14	7.12	1.60	1.31
10	C	1201	SRN	C24-C25	6.34	1.57	1.31
10	C	1201	SRN	C6-C7	6.31	1.56	1.33
10	C	1201	SRN	C8-C7	-6.20	1.29	1.50
10	C	1201	SRN	C12-C13	-5.85	1.30	1.50
10	C	1201	SRN	C28-C29	5.19	1.61	1.31
10	C	1201	SRN	C10-C9	-5.15	1.43	1.53
10	C	1201	SRN	C35-C8	-5.13	1.45	1.53
10	C	1201	SRN	O8-C12	5.02	1.51	1.43
10	C	1201	SRN	O7-C32	4.42	1.51	1.43
10	C	1201	SRN	C11-C10	-4.40	1.44	1.53
10	C	1201	SRN	C3-C4	4.05	1.57	1.44
10	C	1201	SRN	C5-C6	3.99	1.56	1.44
10	C	1201	SRN	C33-C47	-3.92	1.43	1.49
10	C	1201	SRN	C30-C29	3.74	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1201	SRN	C46-C47	3.66	1.44	1.33
10	C	1201	SRN	O1-C1	3.56	1.42	1.34
10	C	1201	SRN	O7-C31	3.46	1.53	1.44
10	C	1201	SRN	C2-C1	3.31	1.55	1.48
10	C	1201	SRN	C23-C24	2.95	1.54	1.50
10	C	1201	SRN	C15-C14	2.79	1.58	1.50
10	C	1201	SRN	O1-C33	2.77	1.50	1.46
10	C	1201	SRN	O8-C35	2.36	1.50	1.44
10	C	1201	SRN	C17-C16	2.32	1.57	1.53
10	C	1201	SRN	C31-C46	2.26	1.53	1.50
10	C	1201	SRN	O6-C23	-2.16	1.39	1.43
10	C	1201	SRN	C22-C21	2.15	1.56	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1201	SRN	C8-C7-C6	-5.34	115.06	125.88
10	C	1201	SRN	C6-C5-C4	-4.39	114.58	124.72
10	C	1201	SRN	C18-C17-C19	-3.40	107.37	111.35
10	C	1201	SRN	C35-O8-C12	3.31	118.31	112.93
10	C	1201	SRN	C23-C24-C25	-3.13	118.20	124.69
10	C	1201	SRN	C3-C4-C5	-2.86	118.11	124.72
10	C	1201	SRN	C9-C34-C35	2.55	110.88	103.67
10	C	1201	SRN	C20-C19-C17	2.52	114.81	111.16
10	C	1201	SRN	C43-C44-C45	-2.27	108.58	114.51
10	C	1201	SRN	O9-C21-C20	2.24	112.32	109.78
10	C	1201	SRN	C12-C13-C14	-2.14	118.82	124.59
10	C	1201	SRN	C4-C3-C2	-2.07	119.76	124.65
10	C	1201	SRN	C30-C31-C46	-2.07	109.36	113.00
10	C	1201	SRN	C16-C15-C14	-2.02	107.97	113.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	1201	SRN	C29-C30-C31-O7
10	C	1201	SRN	C25-C26-C27-C28
10	C	1201	SRN	O1-C1-C2-C3
10	C	1201	SRN	O2-C1-C2-C3
10	C	1201	SRN	C42-C43-C44-C45
10	C	1201	SRN	O2-C1-O1-C33
10	C	1201	SRN	C2-C1-O1-C33

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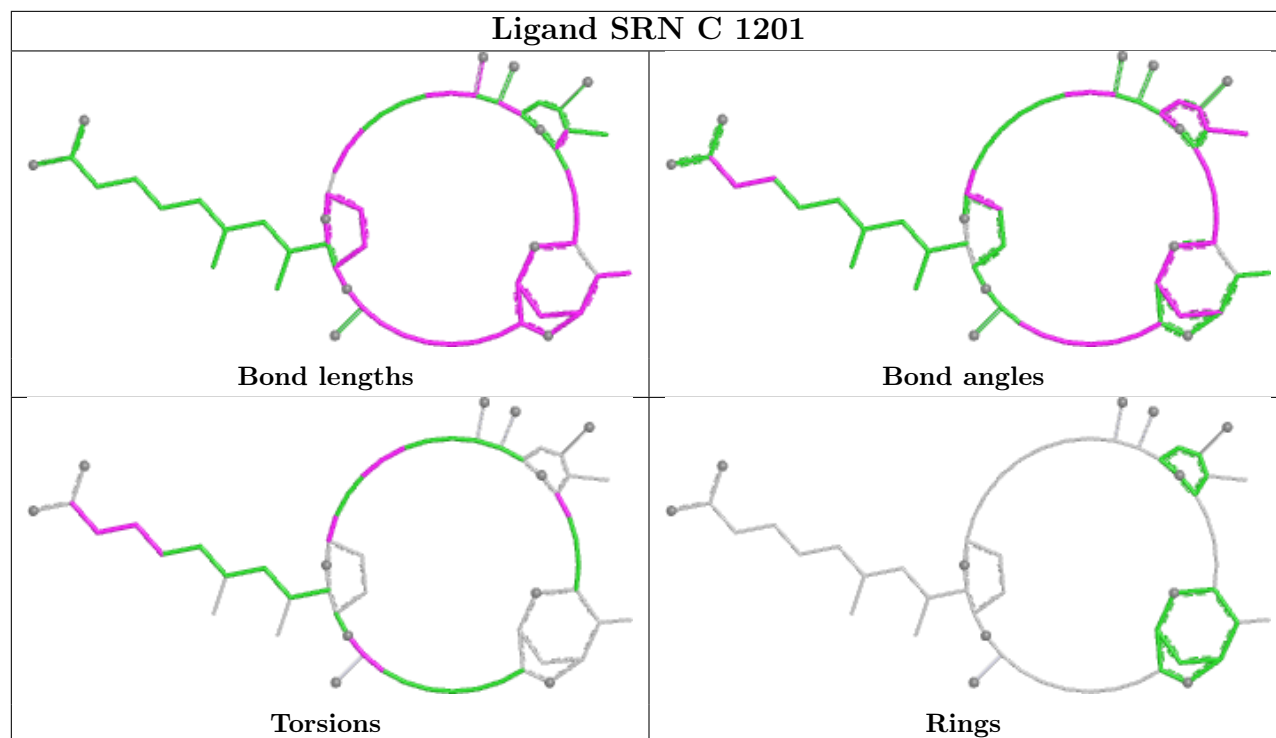
Mol	Chain	Res	Type	Atoms
10	C	1201	SRN	C43-C44-C45-O10
10	C	1201	SRN	C26-C27-C28-C29
10	C	1201	SRN	C43-C44-C45-O11
10	C	1201	SRN	C41-C42-C43-C44
10	C	1201	SRN	C14-C15-C16-O9
10	C	1201	SRN	C14-C15-C16-C17

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1201	SRN	10	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.

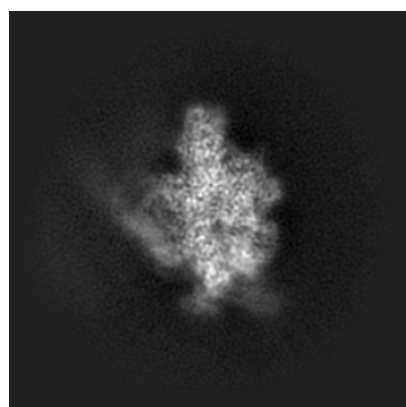
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21407. These allow visual inspection of the internal detail of the map and identification of artifacts.

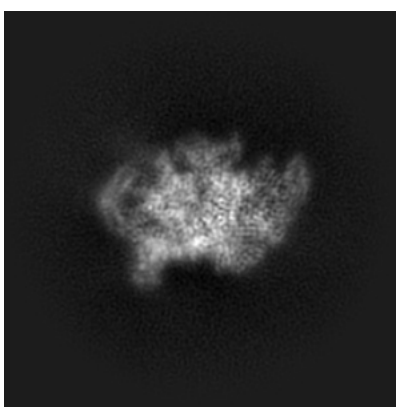
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

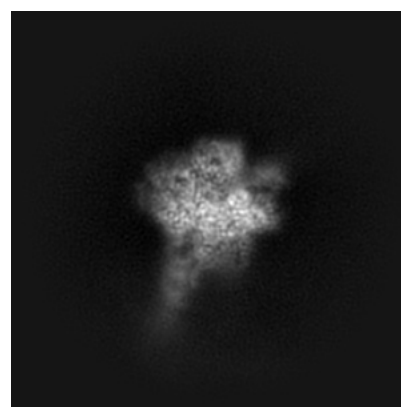
6.1.1 Primary map



X



Y

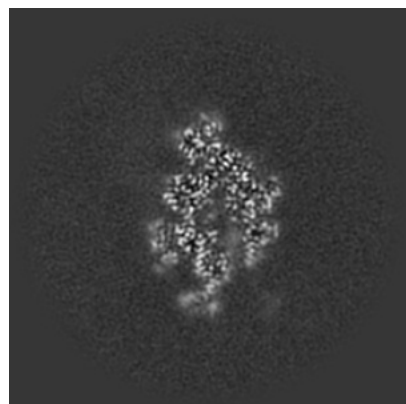


Z

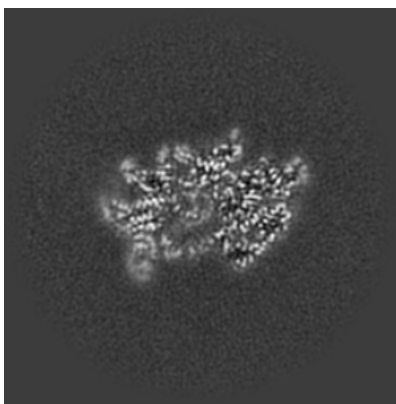
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

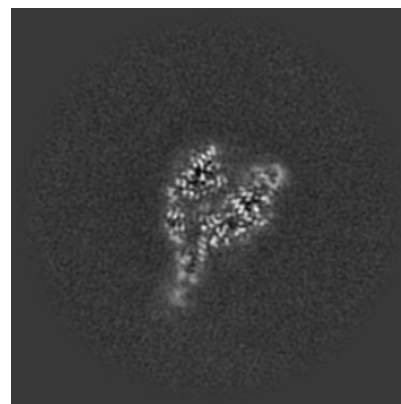
6.2.1 Primary map



X Index: 150



Y Index: 150

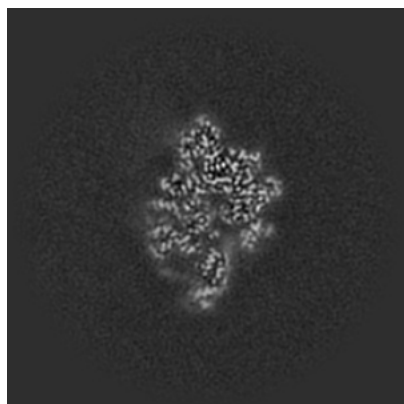


Z Index: 150

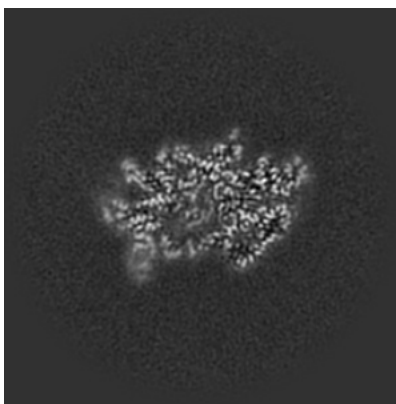
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

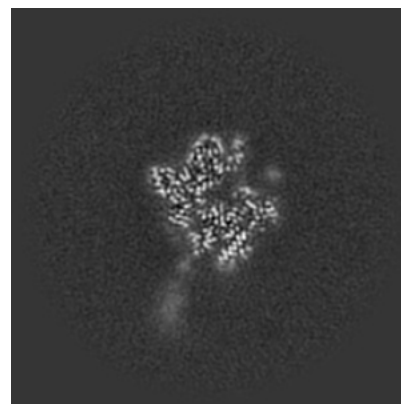
6.3.1 Primary map



X Index: 144



Y Index: 149

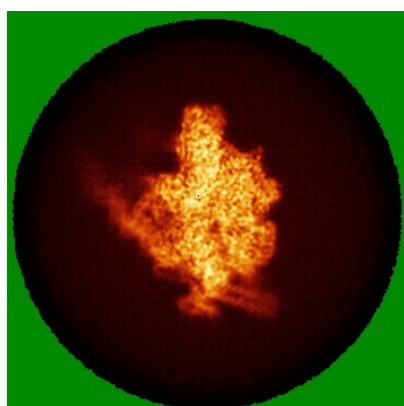


Z Index: 163

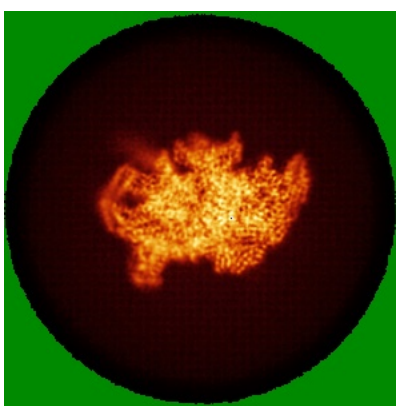
The images above show the largest variance slices of the map in three orthogonal directions.

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

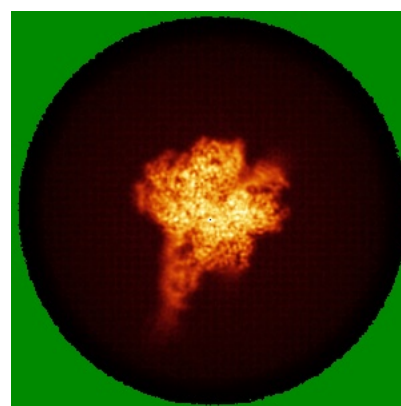
6.4.1 Primary map



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 0.433. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

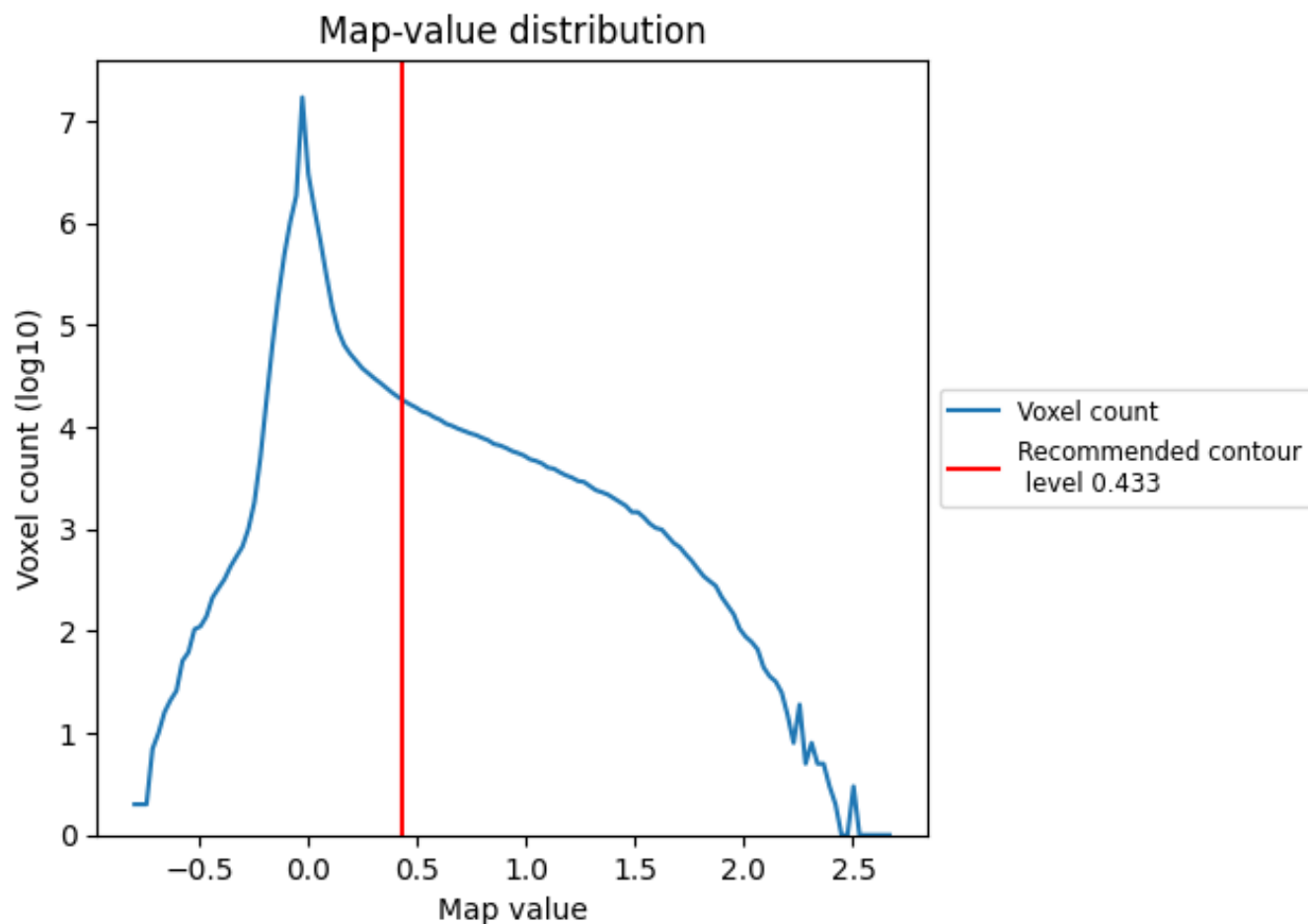
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

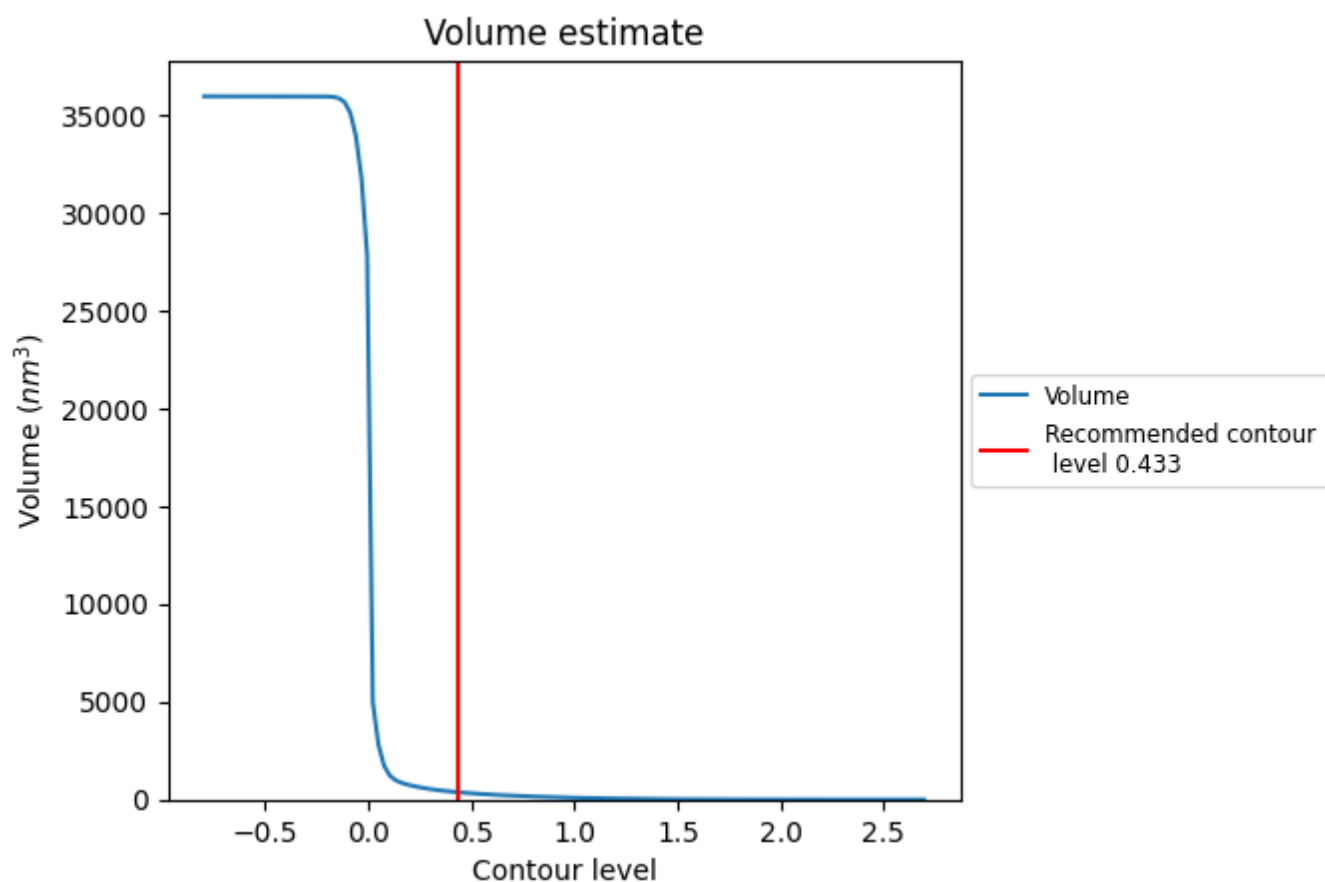
This section contains the results of statistical analysis of the map.

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.

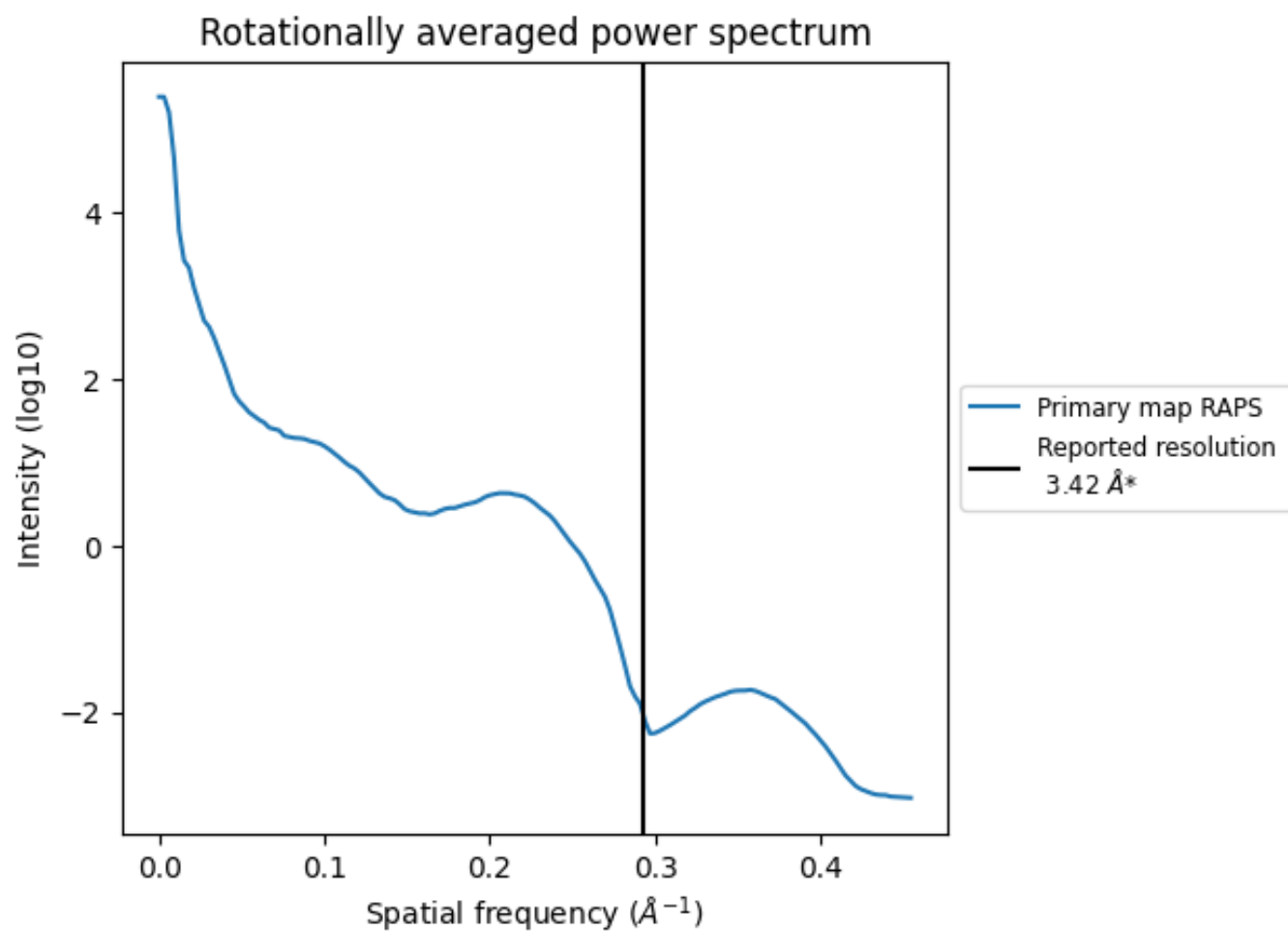
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 376 nm³; this corresponds to an approximate mass of 340 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 0.292 Å⁻¹

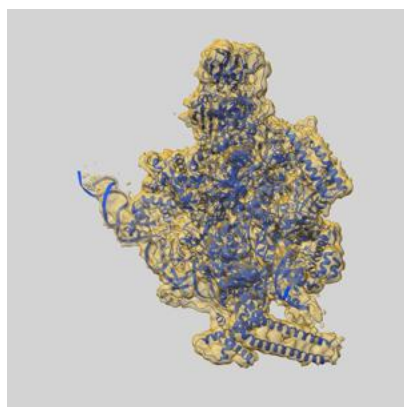
8 Fourier-Shell correlation

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

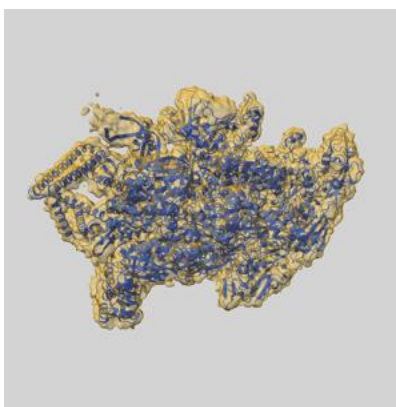
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21407 and PDB model 6VVY. Per-residue inclusion information can be found in section [3](#) on page [8](#).

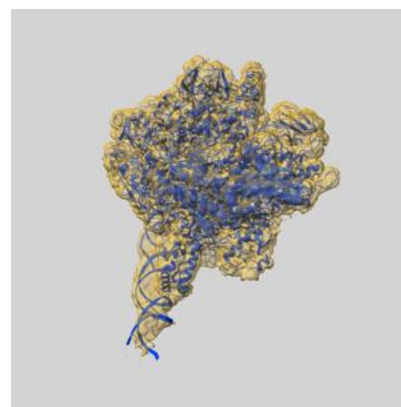
9.1 Map-model overlay [i](#)



X



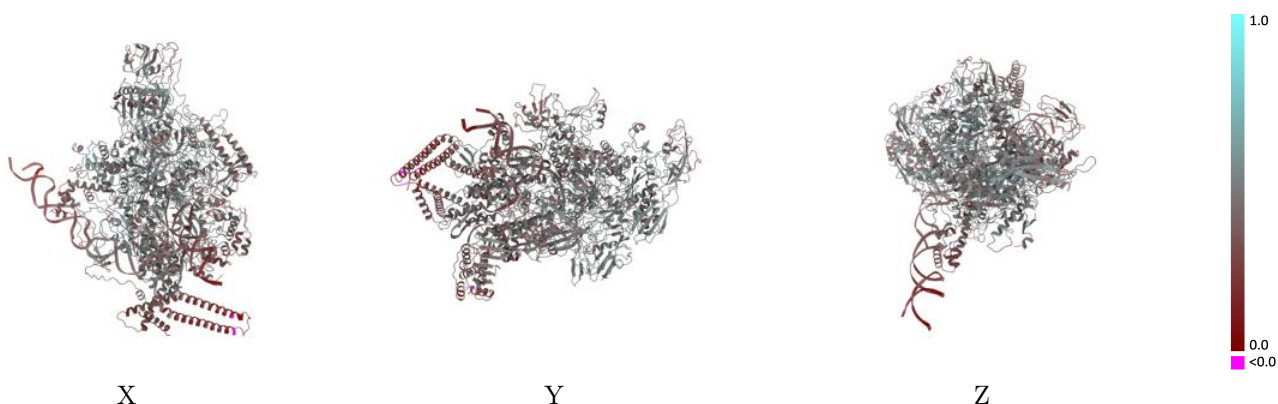
Y



Z

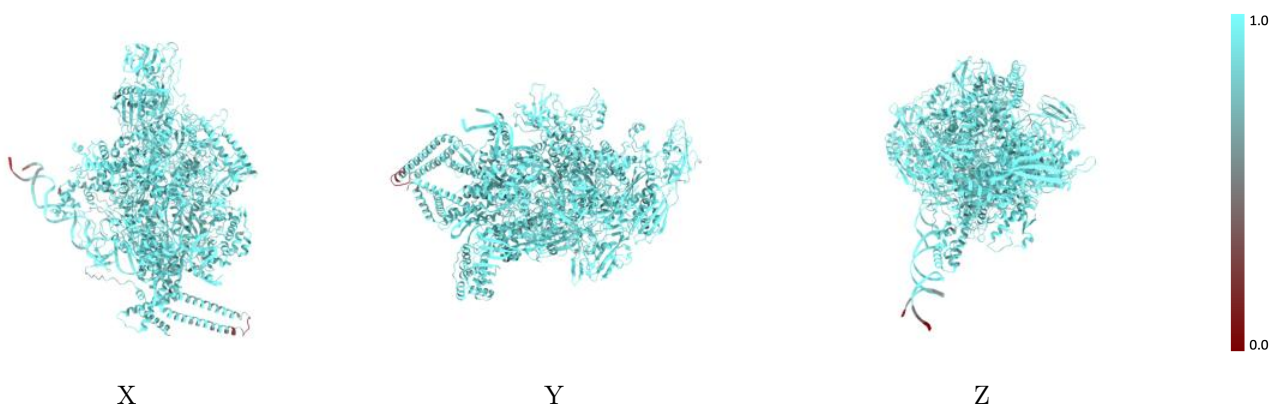
The images above show the 3D surface view of the map at the recommended contour level 0.433 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



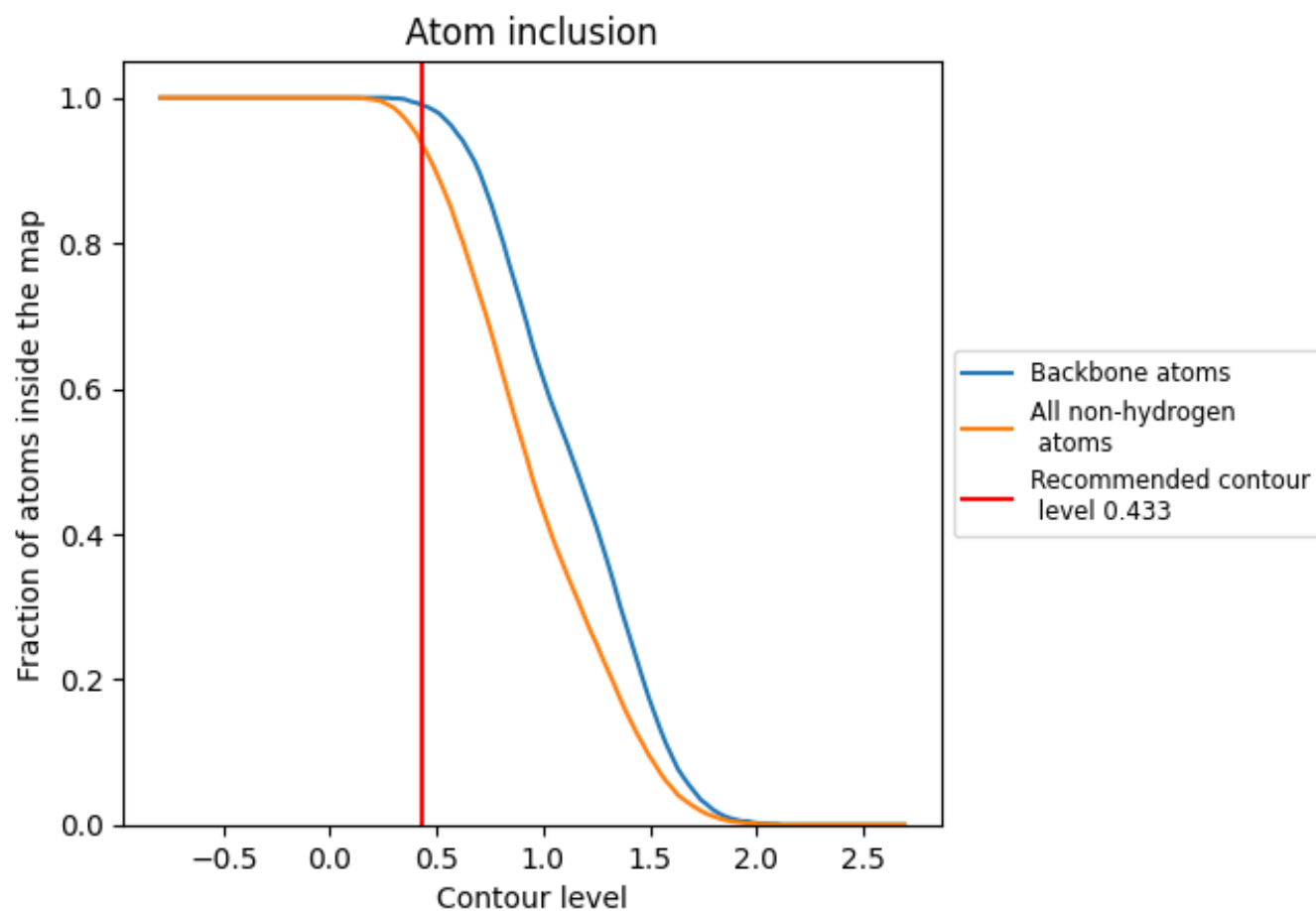
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.433).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.433) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9350	0.4360
A	0.9630	0.4850
B	0.9440	0.4540
C	0.9440	0.4710
D	0.9380	0.4540
E	0.9500	0.4740
F	0.9250	0.3900
J	0.8740	0.3920
M	0.9080	0.3480
O	0.9190	0.3050
P	0.9100	0.3090

1.0

0.0

<0.0