



Full wwPDB EM Validation Report ⓘ

Oct 20, 2024 – 05:12 PM EDT

PDB ID : 7MKE
EMDB ID : EMD-23893
Title : Cryo-EM structure of Escherichia coli RNA polymerase bound to lambda PR promoter DNA (class 2)
Authors : Saecker, R.M.; Darst, S.A.; Chen, J.
Deposited on : 2021-04-23
Resolution : 3.70 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
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) : 2.39

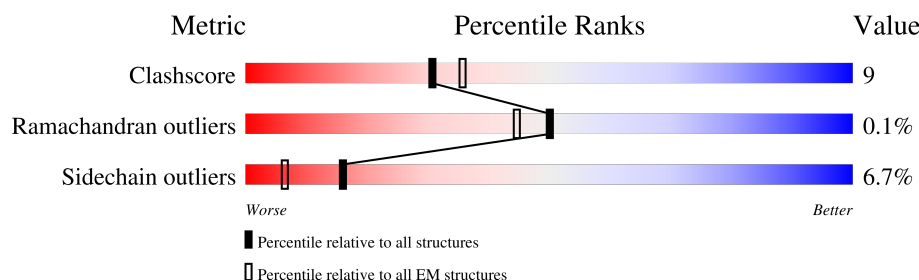
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	G	329	
1	H	329	
2	I	1342	
3	J	1407	
4	K	91	
5	L	613	
6	P	90	
7	Q	90	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 30641 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	G	233	Total	C	N	O	S	0	0
			1808	1126	320	356	6		
1	H	223	Total	C	N	O	S	0	0
			1714	1070	302	336	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1340	Total	C	N	O	S	0	0
			10567	6631	1841	2052	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1335	Total	C	N	O	S	0	0
			10377	6519	1850	1959	49		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1384	VAL	MET	conflict	UNP A0A4S1NBU2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	465	Total	C	N	O	S	0	0
			3781	2373	677	708	23		

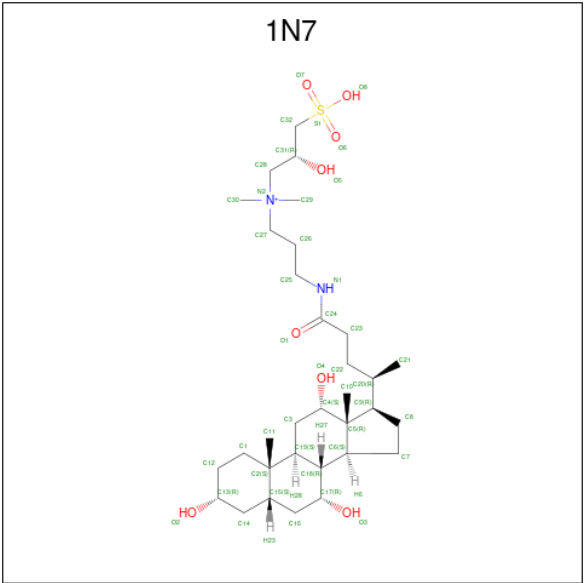
- Molecule 6 is a DNA chain called Nontemplate strand of lambda PR DNA promoter.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	44	Total	C	N	O	P	0	0
			907	434	163	267	43		

- Molecule 7 is a DNA chain called Template strand of lambda PR DNA promoter.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	37	Total	C	N	O	P	0	0
			749	358	142	213	36		

- Molecule 8 is CHAPSO (three-letter code: 1N7) (formula: C₃₂H₅₉N₂O₈S).



Mol	Chain	Residues	Atoms			AltConf
8	I	1	Total	C	O	0
			27	24	3	
8	I	1	Total	C	O	0
			27	24	3	
8	L	1	Total	C	O	0
			27	24	3	
8	L	1	Total	C	O	0
			27	24	3	

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	J	1	Total 1	Mg 1	0

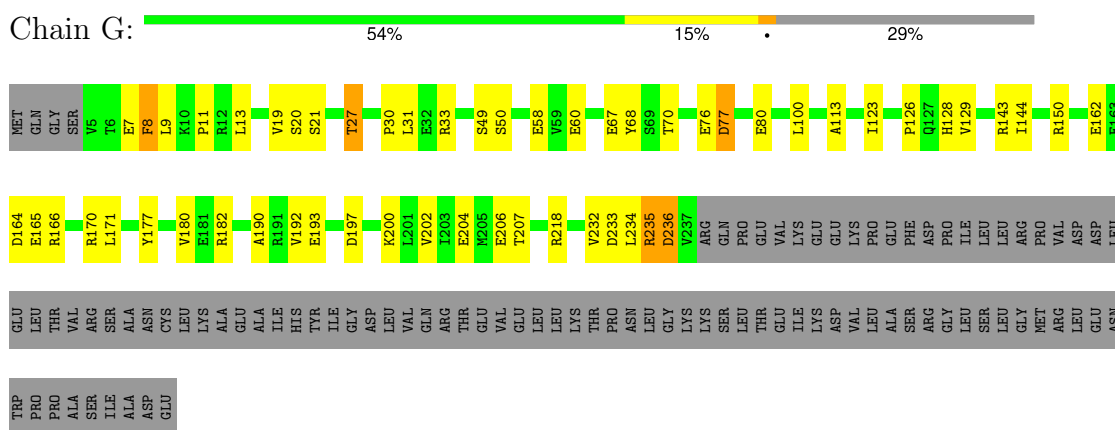
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	J	2	Total 2	Zn 2	0

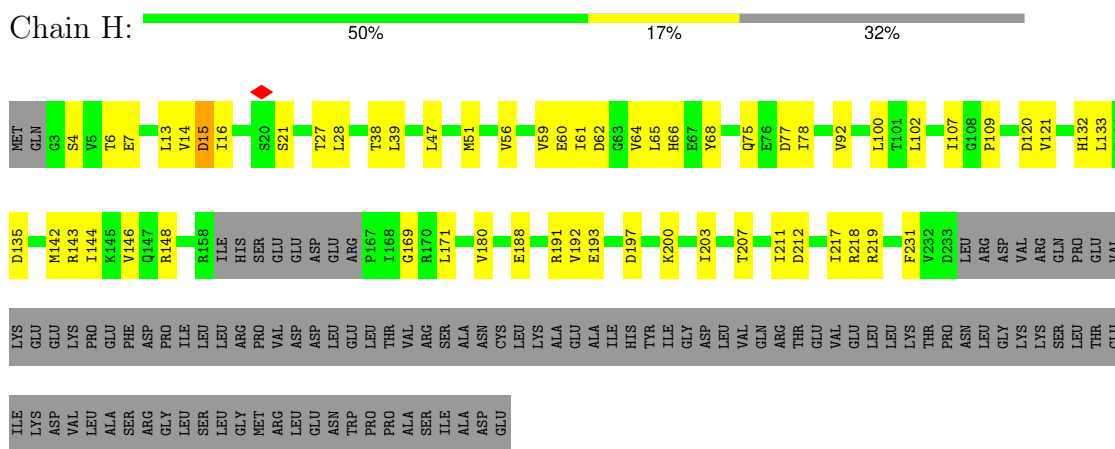
3 Residue-property plots

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.

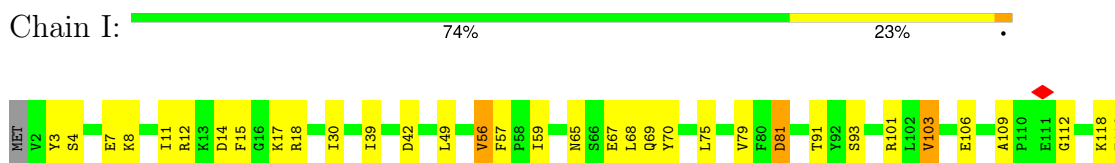
- Molecule 1: DNA-directed RNA polymerase subunit alpha

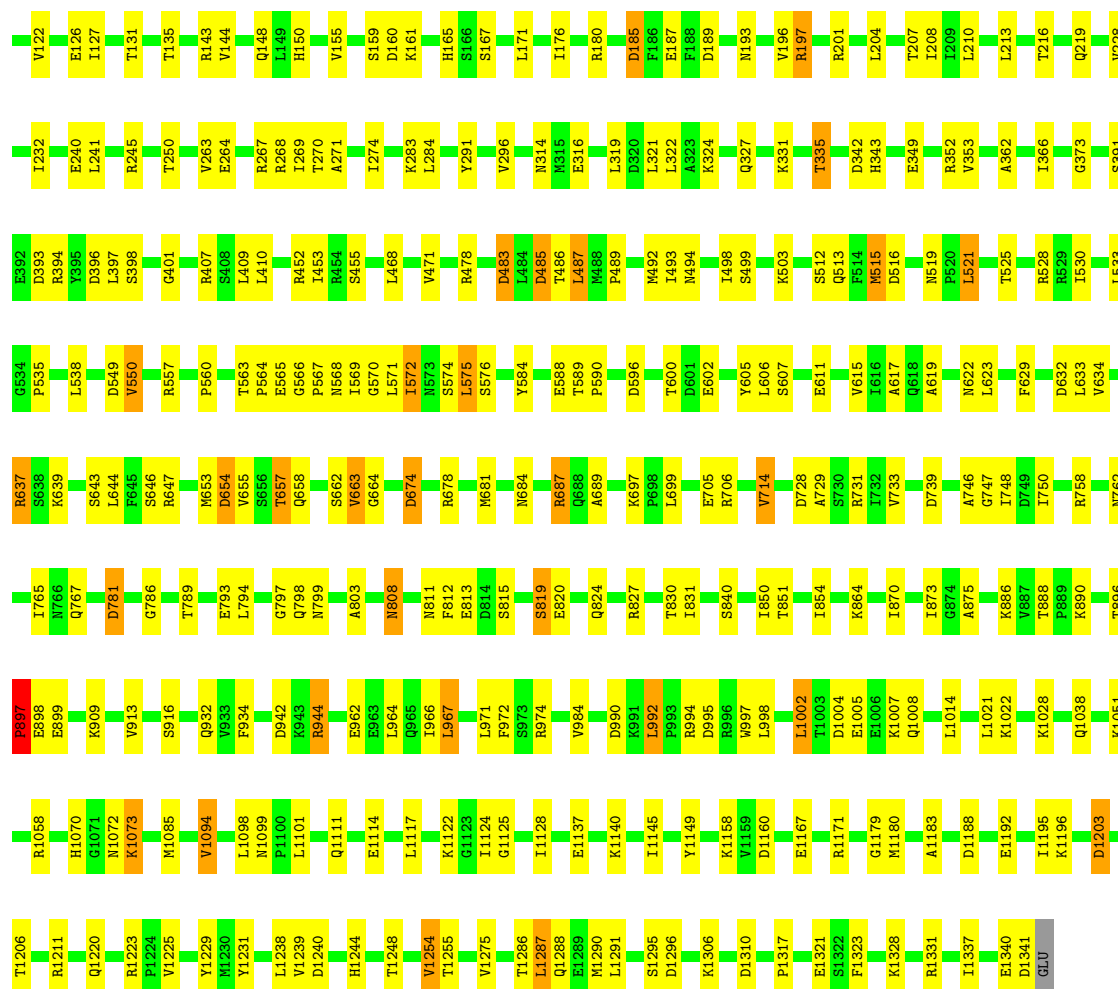


- Molecule 1: DNA-directed RNA polymerase subunit alpha



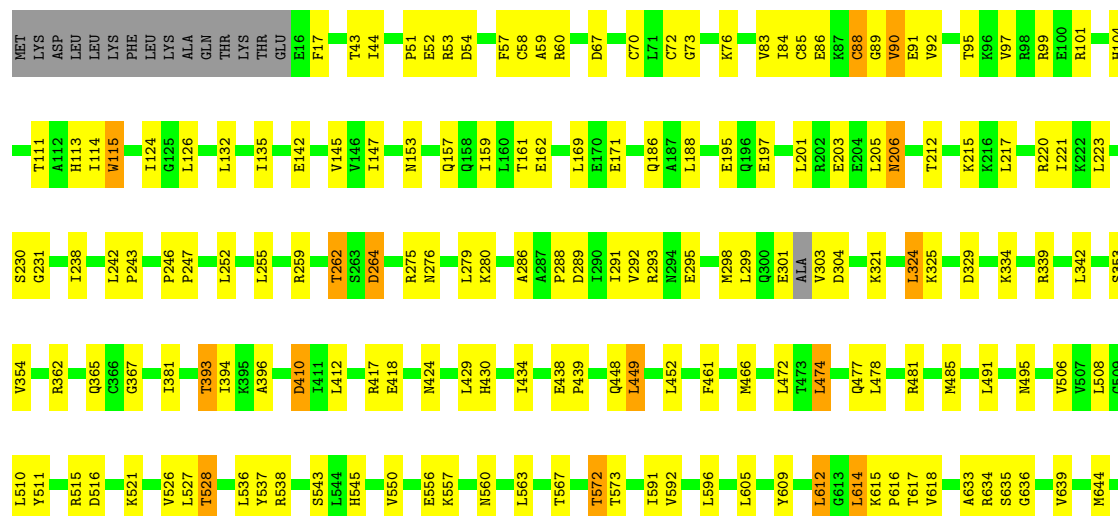
- Molecule 2: DNA-directed RNA polymerase subunit beta

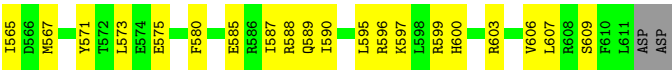




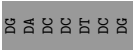
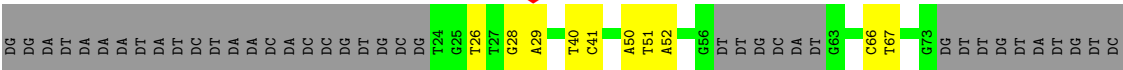
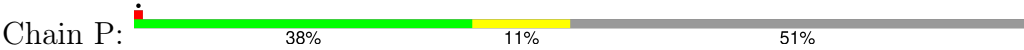
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J: 70% 24% 5%

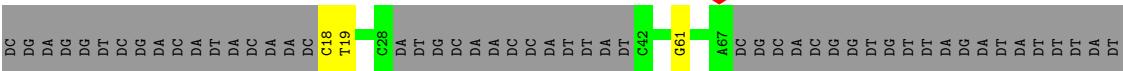




● Molecule 6: Nontemplate strand of lambda PR DNA promoter



● Molecule 7: Template strand of lambda PR DNA promoter



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89914	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 ($e^-/\text{\AA}^2$)	46	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	1.527	Depositor
Minimum map value	-0.556	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1N7, 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	G	0.43	0/1830	0.55	0/2481
1	H	0.38	0/1734	0.55	0/2349
2	I	0.43	0/10736	0.52	1/14487 (0.0%)
3	J	0.41	0/10533	0.52	0/14222
4	K	0.32	0/629	0.48	0/847
5	L	0.29	0/3831	0.45	0/5148
6	P	0.58	0/1016	0.98	0/1567
7	Q	0.57	0/840	0.90	0/1290
All	All	0.42	0/31149	0.55	1/42391 (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	G	0	1
1	H	0	1
2	I	0	3
3	J	0	2
All	All	0	7

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	487	LEU	C-N-CA	6.91	138.98	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	235	ARG	Peptide
1	H	192	VAL	Peptide
2	I	397	LEU	Peptide
2	I	485	ASP	Peptide
2	I	897	PRO	Peptide
3	J	1184	ASP	Peptide
3	J	736	GLN	Peptide

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	G	1808	0	1835	28	0
1	H	1714	0	1748	36	0
2	I	10567	0	10585	189	0
3	J	10377	0	10588	191	0
4	K	627	0	634	7	0
5	L	3781	0	3862	62	0
6	P	907	0	502	6	0
7	Q	749	0	413	2	0
8	I	54	0	74	21	0
8	L	54	0	74	17	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
All	All	30641	0	30315	529	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 (529) 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)
8:I:1402:1N7:C3	8:I:1402:1N7:C19	1.82	1.56
8:L:702:1N7:C19	8:L:702:1N7:C3	1.82	1.54
8:L:701:1N7:C3	8:L:701:1N7:C19	1.82	1.54
8:I:1401:1N7:C3	8:I:1401:1N7:C19	1.82	1.54
3:J:85:CYS:HB3	3:J:88:CYS:SG	1.97	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:701:1N7:C3	8:L:701:1N7:C2	2.63	0.76
8:L:702:1N7:C3	8:L:702:1N7:C2	2.62	0.75
5:L:310:GLU:H	5:L:315:TRP:HE1	1.34	0.75
8:I:1401:1N7:C3	8:I:1401:1N7:C2	2.63	0.73
3:J:85:CYS:SG	3:J:86:GLU:N	2.64	0.71
8:I:1402:1N7:C3	8:I:1402:1N7:C2	2.64	0.71
1:H:75:GLN:HE22	1:H:132:HIS:HB2	1.55	0.70
1:H:109:PRO:HA	1:H:132:HIS:HA	1.72	0.70
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.75	0.69
8:L:702:1N7:C3	8:L:702:1N7:C18	2.69	0.68
3:J:973:LEU:HB3	3:J:1003:LEU:HB2	1.73	0.68
1:H:15:ASP:N	1:H:15:ASP:OD1	2.26	0.68
3:J:145:VAL:HG23	3:J:159:ILE:HG22	1.75	0.68
3:J:58:CYS:SG	3:J:59:ALA:N	2.67	0.68
3:J:762:ASN:OD1	3:J:762:ASN:N	2.27	0.68
8:I:1401:1N7:C3	8:I:1401:1N7:C18	2.67	0.67
8:I:1402:1N7:C3	8:I:1402:1N7:C18	2.67	0.66
4:K:25:ARG:HE	4:K:64:LEU:HD13	1.60	0.65
2:I:528:ARG:NH2	2:I:576:SER:O	2.29	0.65
3:J:1357:ILE:HG22	3:J:1359:ALA:H	1.61	0.65
5:L:163:THR:HG23	5:L:262:VAL:HG12	1.79	0.65
5:L:141:ILE:HG13	5:L:252:LEU:HD21	1.80	0.64
5:L:423:ARG:NH1	6:P:50:DA:N7	2.46	0.64
2:I:1211:ARG:NH1	2:I:1220:GLN:OE1	2.30	0.64
2:I:1223:ARG:HH22	3:J:721:SER:HB3	1.62	0.63
3:J:516:ASP:OD1	3:J:516:ASP:N	2.31	0.63
2:I:398:SER:HB3	2:I:401:GLY:H	1.64	0.62
3:J:393:THR:HG23	3:J:396:ALA:H	1.64	0.62
1:G:164:ASP:HA	1:G:166:ARG:HH11	1.64	0.62
1:G:235:ARG:H	1:H:218:ARG:HH21	1.47	0.62
2:I:811:ASN:O	2:I:1099:ASN:ND2	2.32	0.62
2:I:1072:ASN:ND2	2:I:1111:GLN:OE1	2.33	0.62
1:G:234:LEU:H	1:H:218:ARG:HE	1.46	0.62
2:I:678:ARG:NH1	2:I:681:MET:SD	2.73	0.62
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.81	0.62
2:I:662:SER:OG	2:I:663:VAL:N	2.32	0.62
8:L:701:1N7:C3	8:L:701:1N7:C18	2.70	0.61
3:J:653:ILE:HG12	3:J:692:ARG:HH21	1.65	0.61
2:I:758:ARG:NH2	2:I:762:ASN:OD1	2.33	0.61
3:J:393:THR:OG1	3:J:394:ILE:N	2.31	0.60
3:J:708:ASN:OD1	3:J:708:ASN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1025:MET:HB3	3:J:1124:ILE:HB	1.83	0.60
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.83	0.60
1:G:11:PRO:HA	1:G:30:PRO:HD2	1.83	0.60
2:I:1124:ILE:HG21	2:I:1180:MET:HE1	1.84	0.60
3:J:1219:ASP:OD1	3:J:1222:ARG:NH2	2.35	0.60
8:L:702:1N7:H4	8:L:702:1N7:H17	1.82	0.60
3:J:1279:GLN:NE2	3:J:1305:ASP:OD2	2.34	0.60
3:J:301:GLU:O	3:J:303:VAL:N	2.34	0.60
3:J:381:ILE:HD11	3:J:412:LEU:HD13	1.83	0.60
1:H:64:VAL:HG12	1:H:66:HIS:H	1.66	0.60
2:I:1341:ASP:OD1	2:I:1341:ASP:N	2.34	0.60
3:J:1152:GLU:OE1	3:J:1194:ARG:NH1	2.35	0.59
2:I:557:ARG:NH2	2:I:607:SER:O	2.35	0.59
3:J:741:ALA:O	3:J:762:ASN:ND2	2.33	0.59
1:H:102:LEU:HB3	1:H:142:MET:HG3	1.83	0.59
3:J:1161:GLY:HA3	3:J:1179:PRO:HA	1.84	0.59
2:I:568:ASN:OD1	2:I:568:ASN:N	2.36	0.59
2:I:165:HIS:ND1	2:I:167:SER:OG	2.32	0.59
3:J:795:TYR:OH	3:J:799:ARG:NH1	2.36	0.59
5:L:145:LEU:HB3	5:L:225:ARG:HH21	1.66	0.59
2:I:263:VAL:HG11	2:I:269:ILE:HG13	1.85	0.59
8:L:701:1N7:C3	8:L:701:1N7:H1	2.33	0.59
3:J:982:LEU:HD23	3:J:995:TYR:HB2	1.84	0.59
2:I:870:ILE:HB	2:I:944:ARG:HD3	1.84	0.59
3:J:1189:MET:SD	3:J:1189:MET:N	2.75	0.59
1:H:61:ILE:HG22	1:H:64:VAL:H	1.67	0.58
2:I:197:ARG:NH1	2:I:201:ARG:O	2.35	0.58
2:I:629:PHE:O	2:I:647:ARG:NH1	2.35	0.58
2:I:67:GLU:OE2	2:I:69:GLN:NE2	2.35	0.58
3:J:84:ILE:HG22	3:J:91:GLU:HB2	1.85	0.58
3:J:1194:ARG:NH2	3:J:1211:SER:OG	2.35	0.58
5:L:562:ARG:NH2	7:Q:61:DG:OP2	2.36	0.58
3:J:665:GLN:OE1	3:J:678:ARG:NH2	2.36	0.58
3:J:417:ARG:NH1	4:K:43:ASN:O	2.36	0.58
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.85	0.58
1:H:191:ARG:NH2	1:H:193:GLU:O	2.34	0.58
8:I:1402:1N7:H4	8:I:1402:1N7:H17	1.85	0.58
5:L:292:VAL:HA	5:L:297:MET:HB3	1.84	0.58
6:P:40:DT:H2''	6:P:41:DC:H5'	1.86	0.58
2:I:122:VAL:HG11	2:I:493:ILE:HD13	1.86	0.58
2:I:964:LEU:HD11	2:I:1021:LEU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:293:ARG:NH1	5:L:104:GLU:OE2	2.37	0.57
1:G:27:THR:HG22	1:G:202:VAL:HG22	1.86	0.57
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.85	0.57
3:J:1174:ARG:NH1	3:J:1189:MET:SD	2.77	0.57
2:I:632:ASP:OD1	2:I:647:ARG:NH2	2.37	0.57
3:J:288:PRO:HB3	5:L:377:LYS:HG3	1.85	0.57
3:J:1285:VAL:O	3:J:1289:ASN:ND2	2.38	0.57
2:I:1070:HIS:NE2	2:I:1114:GLU:OE1	2.36	0.57
2:I:196:VAL:N	2:I:204:LEU:O	2.36	0.57
3:J:609:TYR:HE1	3:J:614:LEU:HD12	1.69	0.57
3:J:826:ILE:HG22	3:J:828:GLY:H	1.70	0.57
5:L:358:VAL:O	5:L:362:ASN:ND2	2.38	0.57
1:G:113:ALA:HB2	1:G:126:PRO:HB3	1.87	0.56
3:J:661:VAL:HG23	3:J:682:VAL:HG22	1.87	0.56
1:G:60:GLU:OE2	1:G:143:ARG:NH2	2.37	0.56
3:J:511:TYR:OH	3:J:515:ARG:NH1	2.37	0.56
3:J:1149:ARG:HD3	3:J:1150:PRO:HD2	1.86	0.56
5:L:141:ILE:HG21	5:L:252:LEU:HD11	1.87	0.56
3:J:72:CYS:SG	3:J:88:CYS:HB3	2.46	0.56
2:I:494:ASN:OD1	5:L:468:ARG:NH1	2.39	0.56
5:L:587:ILE:HA	5:L:590:ILE:HD12	1.88	0.56
1:H:4:SER:N	1:H:7:GLU:OE1	2.36	0.56
3:J:54:ASP:OD1	3:J:54:ASP:N	2.39	0.56
5:L:340:ALA:HA	5:L:343:LYS:HD2	1.87	0.56
2:I:499:SER:OG	2:I:503:LYS:NZ	2.38	0.55
2:I:574:SER:OG	2:I:575:LEU:N	2.38	0.55
3:J:325:LYS:HG3	3:J:329:ASP:HB2	1.87	0.55
5:L:394:TYR:OH	5:L:436:ARG:NH1	2.40	0.55
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.87	0.55
3:J:644:MET:O	3:J:764:ARG:NH1	2.39	0.55
1:G:58:GLU:OE2	1:G:170:ARG:NH1	2.36	0.55
5:L:311:THR:O	5:L:345:GLN:NE2	2.40	0.55
2:I:59:ILE:HD12	2:I:68:LEU:HD23	1.88	0.55
2:I:728:ASP:OD1	2:I:729:ALA:N	2.39	0.55
2:I:798:GLN:NE2	2:I:827:ARG:O	2.40	0.55
2:I:748:ILE:HG23	2:I:974:ARG:HH22	1.69	0.55
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.89	0.54
1:G:218:ARG:NH1	1:H:231:PHE:O	2.41	0.54
1:H:107:ILE:HG23	1:H:135:ASP:HA	1.88	0.54
2:I:808:ASN:H	3:J:633:ALA:HB2	1.70	0.54
2:I:1128:ILE:HD12	2:I:1145:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:276:ASN:OD1	3:J:280:LYS:NZ	2.32	0.54
5:L:562:ARG:NH1	5:L:571:TYR:O	2.40	0.54
2:I:321:LEU:HD23	2:I:324:LYS:HD2	1.88	0.54
5:L:597:LYS:O	5:L:603:ARG:NH2	2.40	0.54
2:I:452:ARG:NH1	2:I:584:TYR:O	2.41	0.54
3:J:891:ASP:OD1	3:J:891:ASP:N	2.40	0.54
3:J:1341:ARG:NH1	3:J:1343:GLU:OE2	2.40	0.54
3:J:1155:ILE:HG13	3:J:1210:ILE:HB	1.88	0.54
1:G:233:ASP:N	1:G:233:ASP:OD1	2.39	0.54
2:I:14:ASP:HA	2:I:1183:ALA:HB3	1.90	0.54
3:J:88:CYS:SG	3:J:89:GLY:N	2.81	0.54
3:J:201:LEU:HB3	3:J:221:ILE:HD11	1.90	0.54
3:J:1250:ASP:OD1	3:J:1250:ASP:N	2.41	0.54
2:I:319:LEU:HD23	2:I:322:LEU:HD12	1.88	0.53
3:J:845:ALA:HB3	3:J:881:LYS:HG2	1.90	0.53
2:I:18:ARG:NH2	2:I:622:ASN:OD1	2.41	0.53
3:J:1005:LYS:HG3	3:J:1011:VAL:HG12	1.91	0.53
2:I:812:PHE:O	2:I:1099:ASN:ND2	2.41	0.53
3:J:572:THR:OG1	3:J:573:THR:N	2.37	0.53
3:J:876:SER:HA	3:J:990:ARG:HH21	1.72	0.53
1:G:33:ARG:NH2	1:G:197:ASP:O	2.41	0.53
2:I:67:GLU:HB3	2:I:103:VAL:HG23	1.90	0.53
2:I:521:LEU:HD11	2:I:664:GLY:HA2	1.90	0.53
8:I:1402:1N7:C3	8:I:1402:1N7:H1	2.39	0.53
3:J:478:LEU:HG	4:K:47:THR:HG23	1.91	0.53
3:J:142:GLU:OE2	5:L:103:ARG:NH2	2.41	0.53
2:I:81:ASP:OD1	2:I:81:ASP:N	2.28	0.53
5:L:293:GLU:OE2	5:L:299:LYS:NZ	2.41	0.53
2:I:131:THR:OG1	2:I:135:THR:O	2.26	0.53
2:I:180:ARG:NH2	2:I:393:ASP:O	2.41	0.53
3:J:1057:SER:O	3:J:1108:GLN:NE2	2.42	0.53
2:I:118:LYS:HD3	2:I:489:PRO:HD3	1.90	0.52
2:I:324:LYS:O	2:I:327:GLN:NE2	2.42	0.52
2:I:706:ARG:NH1	2:I:793:GLU:OE2	2.42	0.52
3:J:259:ARG:NH1	5:L:503:GLU:O	2.36	0.52
2:I:483:ASP:OD1	2:I:483:ASP:N	2.40	0.52
1:G:180:VAL:HG12	1:G:207:THR:HG22	1.92	0.52
2:I:811:ASN:ND2	2:I:1098:LEU:O	2.41	0.52
3:J:113:HIS:CE1	3:J:115:TRP:HB2	2.45	0.52
3:J:1173:ARG:NH2	3:J:1192:LYS:O	2.43	0.52
2:I:674:ASP:OD1	2:I:674:ASP:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:803:ALA:HB2	2:I:1094:VAL:HG21	1.92	0.52
1:H:65:LEU:HD11	1:H:169:GLY:H	1.75	0.52
2:I:600:THR:HG22	2:I:602:GLU:H	1.73	0.52
3:J:73:GLY:O	3:J:76:LYS:NZ	2.34	0.52
1:H:188:GLU:OE2	1:H:200:LYS:NZ	2.42	0.52
2:I:564:PRO:HA	2:I:684:ASN:HD21	1.74	0.52
3:J:1063:ASP:OD1	3:J:1063:ASP:N	2.39	0.52
2:I:250:THR:HA	2:I:268:ARG:HA	1.92	0.52
6:P:51:DT:H2'	6:P:52:DA:C8	2.45	0.52
2:I:155:VAL:HG23	2:I:176:ILE:HG12	1.91	0.52
3:J:528:THR:O	3:J:528:THR:OG1	2.25	0.52
3:J:1176:VAL:HG13	3:J:1187:GLU:HB3	1.91	0.52
3:J:1234:VAL:O	3:J:1238:GLN:HB2	2.10	0.52
1:G:76:GLU:HB3	1:G:80:GLU:HB3	1.92	0.52
1:H:56:VAL:HG22	1:H:146:VAL:HG12	1.91	0.52
3:J:977:SER:OG	3:J:980:THR:OG1	2.28	0.52
5:L:571:TYR:HB3	5:L:575:GLU:HB3	1.90	0.52
2:I:714:VAL:O	2:I:767:GLN:NE2	2.35	0.51
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.92	0.51
5:L:165:PHE:O	5:L:260:ARG:NH2	2.44	0.51
2:I:747:GLY:O	2:I:974:ARG:NH1	2.42	0.51
3:J:560:ASN:OD1	3:J:560:ASN:N	2.39	0.51
5:L:145:LEU:HD13	5:L:225:ARG:HE	1.75	0.51
5:L:555:GLU:OE1	5:L:597:LYS:NZ	2.39	0.51
1:H:197:ASP:N	1:H:197:ASP:OD1	2.41	0.51
2:I:17:LYS:N	2:I:1188:ASP:OD2	2.43	0.51
2:I:39:ILE:HD11	2:I:75:LEU:HG	1.93	0.51
3:J:410:ASP:OD1	3:J:410:ASP:N	2.41	0.51
3:J:557:LYS:HB3	3:J:563:LEU:HD23	1.91	0.51
3:J:759:ILE:HG22	3:J:771:GLN:HG2	1.92	0.51
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.93	0.51
1:H:211:ILE:HG21	1:H:219:ARG:HH12	1.75	0.51
2:I:208:ILE:HD11	2:I:366:ILE:HB	1.93	0.51
2:I:932:GLN:HB2	2:I:1051:LYS:HB2	1.91	0.51
2:I:207:THR:HA	2:I:210:LEU:HD12	1.91	0.51
2:I:897:PRO:O	2:I:899:GLU:N	2.43	0.51
8:I:1401:1N7:H4	8:I:1401:1N7:H17	1.93	0.51
5:L:334:SER:O	5:L:338:HIS:HB2	2.10	0.51
5:L:262:VAL:HG23	5:L:265:GLN:H	1.76	0.51
2:I:1286:THR:O	2:I:1290:MET:HB2	2.10	0.51
2:I:159:SER:OG	2:I:160:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1004:ASP:OD1	2:I:1004:ASP:N	2.40	0.50
8:L:702:1N7:C3	8:L:702:1N7:H1	2.40	0.50
3:J:753:SER:OG	3:J:754:ILE:N	2.44	0.50
3:J:857:LEU:HD21	3:J:871:LEU:HG	1.92	0.50
5:L:161:LEU:HG	5:L:162:ILE:HG23	1.91	0.50
3:J:424:ASN:HB2	3:J:434:ILE:HG12	1.94	0.50
3:J:789:LYS:NZ	3:J:930:LEU:O	2.42	0.50
2:I:185:ASP:N	2:I:185:ASP:OD1	2.45	0.50
3:J:286:ALA:O	5:L:377:LYS:NZ	2.45	0.50
2:I:942:ASP:OD1	2:I:942:ASP:N	2.38	0.50
2:I:1203:ASP:OD1	2:I:1203:ASP:N	2.45	0.50
3:J:201:LEU:HD11	3:J:217:LEU:HD22	1.94	0.50
8:L:701:1N7:C3	8:L:701:1N7:C1	2.89	0.50
2:I:12:ARG:NH2	2:I:793:GLU:OE1	2.44	0.50
2:I:733:VAL:HG22	2:I:750:ILE:HG12	1.94	0.50
2:I:962:GLU:O	2:I:966:ILE:HG13	2.12	0.50
3:J:252:LEU:HD12	3:J:262:THR:HB	1.93	0.50
2:I:296:VAL:HA	2:I:316:GLU:HA	1.94	0.49
2:I:646:SER:OG	2:I:647:ARG:N	2.45	0.49
3:J:968:ASN:OD1	3:J:972:LYS:N	2.45	0.49
3:J:1095:MET:SD	3:J:1098:GLN:NE2	2.74	0.49
5:L:589:GLN:NE2	6:P:26:DT:O4	2.45	0.49
2:I:109:ALA:HB1	2:I:112:GLY:HA3	1.95	0.49
3:J:264:ASP:HB3	3:J:324:LEU:HD12	1.94	0.49
2:I:1167:GLU:OE2	2:I:1171:ARG:NH2	2.44	0.49
2:I:820:GLU:OE1	2:I:824:GLN:NE2	2.40	0.49
5:L:402:LEU:HD13	5:L:405:ILE:HD11	1.95	0.49
2:I:148:GLN:NE2	2:I:535:PRO:O	2.40	0.49
5:L:560:ARG:HA	5:L:565:ILE:HD12	1.95	0.49
2:I:14:ASP:OD1	2:I:15:PHE:N	2.45	0.49
2:I:75:LEU:HD11	2:I:127:ILE:HD11	1.94	0.49
2:I:966:ILE:HG23	8:I:1402:1N7:H7	1.93	0.49
8:I:1401:1N7:C3	8:I:1401:1N7:H1	2.42	0.49
3:J:537:TYR:OH	3:J:634:ARG:NH2	2.44	0.49
3:J:1000:GLY:HA3	3:J:1026:PRO:HG3	1.94	0.49
2:I:232:ILE:HB	2:I:331:LYS:HG3	1.94	0.49
3:J:959:LYS:NZ	3:J:961:SER:OG	2.45	0.49
5:L:585:GLU:OE2	5:L:588:ARG:NH2	2.41	0.49
2:I:781:ASP:OD1	2:I:781:ASP:N	2.43	0.49
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.95	0.48
2:I:228:VAL:HG22	2:I:245:ARG:HH12	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:519:ASN:ND2	2:I:689:ALA:O	2.46	0.48
3:J:952:VAL:HG22	3:J:954:ASN:H	1.78	0.48
2:I:1323:PHE:HA	3:J:342:LEU:HD11	1.95	0.48
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.94	0.48
3:J:1082:ASP:OD1	3:J:1082:ASP:N	2.44	0.48
5:L:595:LEU:HB3	5:L:599:ARG:HH21	1.76	0.48
3:J:43:THR:OG1	3:J:44:ILE:N	2.47	0.48
3:J:230:SER:OG	3:J:231:GLY:N	2.46	0.48
3:J:242:LEU:HD12	3:J:243:PRO:HD2	1.96	0.48
3:J:888:CYS:SG	3:J:889:ASP:N	2.86	0.48
5:L:479:THR:HG23	5:L:482:GLU:H	1.78	0.48
6:P:28:DG:H2'	6:P:29:DA:C8	2.48	0.48
3:J:161:THR:OG1	3:J:162:GLU:N	2.46	0.48
5:L:606:VAL:O	5:L:609:SER:OG	2.31	0.48
3:J:1076:PRO:HG2	3:J:1101:LEU:HB2	1.96	0.48
1:G:20:SER:OG	1:G:21:SER:N	2.47	0.48
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.96	0.48
2:I:1328:LYS:HD3	2:I:1328:LYS:HA	1.68	0.48
3:J:886:VAL:HG11	3:J:1230:THR:HG21	1.94	0.48
8:L:701:1N7:H17	8:L:701:1N7:H4	1.96	0.48
2:I:786:GLY:N	2:I:789:THR:OG1	2.47	0.47
1:G:49:SER:OG	1:G:50:SER:N	2.46	0.47
2:I:65:ASN:ND2	2:I:106:GLU:O	2.46	0.47
2:I:611:GLU:OE1	2:I:637:ARG:NH2	2.47	0.47
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.96	0.47
2:I:478:ARG:O	2:I:478:ARG:NH1	2.41	0.47
8:I:1401:1N7:C19	8:I:1401:1N7:C4	2.87	0.47
3:J:53:ARG:HE	3:J:60:ARG:HD3	1.79	0.47
4:K:8:ASP:OD1	4:K:8:ASP:N	2.47	0.47
2:I:746:ALA:HB1	2:I:974:ARG:HH21	1.79	0.47
2:I:1122:LYS:HG2	2:I:1229:TYR:CZ	2.49	0.47
8:L:701:1N7:H14	8:L:701:1N7:H29	1.78	0.47
3:J:806:ASP:OD1	3:J:806:ASP:N	2.44	0.47
5:L:108:VAL:HG21	5:L:381:GLU:HB3	1.96	0.47
2:I:485:ASP:HB3	2:I:487:LEU:HB3	1.96	0.47
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.41	0.47
8:I:1401:1N7:C3	8:I:1401:1N7:C1	2.93	0.47
3:J:203:GLU:O	3:J:206:ASN:ND2	2.42	0.47
3:J:964:LYS:HG2	3:J:977:SER:HB3	1.95	0.47
5:L:525:ASP:OD1	5:L:526:THR:N	2.48	0.47
2:I:1137:GLU:OE1	2:I:1140:LYS:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:279:LEU:HD12	3:J:295:GLU:HG3	1.97	0.47
5:L:152:GLU:OE1	5:L:218:ARG:NH1	2.47	0.47
2:I:118:LYS:NZ	2:I:486:THR:O	2.47	0.47
2:I:143:ARG:NH2	2:I:512:SER:O	2.44	0.47
2:I:588:GLU:HG2	2:I:605:TYR:HB3	1.96	0.47
2:I:596:ASP:N	2:I:596:ASP:OD1	2.48	0.47
2:I:811:ASN:HA	2:I:815:SER:HB2	1.96	0.47
3:J:538:ARG:HD2	3:J:538:ARG:HA	1.70	0.47
2:I:864:LYS:HE3	2:I:875:ALA:HB1	1.96	0.47
3:J:720:ASN:O	3:J:723:TYR:N	2.42	0.47
1:G:197:ASP:OD1	1:G:197:ASP:N	2.46	0.46
2:I:189:ASP:OD1	2:I:193:ASN:N	2.41	0.46
2:I:1192:GLU:OE2	3:J:764:ARG:NE	2.42	0.46
2:I:619:ALA:HB2	2:I:654:ASP:HB3	1.98	0.46
3:J:1041:ILE:N	3:J:1045:THR:OG1	2.48	0.46
2:I:4:SER:N	2:I:7:GLU:OE1	2.38	0.46
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.98	0.46
2:I:797:GLY:N	2:I:1231:TYR:OH	2.38	0.46
3:J:104:HIS:HA	3:J:243:PRO:HA	1.97	0.46
3:J:612:LEU:HD12	3:J:616:PRO:HG2	1.98	0.46
8:L:702:1N7:C3	8:L:702:1N7:C1	2.93	0.46
1:H:60:GLU:N	1:H:143:ARG:O	2.40	0.46
3:J:495:ASN:N	3:J:495:ASN:OD1	2.49	0.46
3:J:527:LEU:HB2	3:J:550:VAL:HG12	1.97	0.46
3:J:703:THR:O	3:J:703:THR:OG1	2.32	0.46
5:L:596:ARG:HA	5:L:599:ARG:HD2	1.97	0.46
1:G:8:PHE:HD1	1:G:8:PHE:HA	1.61	0.46
1:G:13:LEU:HB2	1:H:231:PHE:HE1	1.81	0.46
3:J:556:GLU:OE1	3:J:557:LYS:N	2.46	0.46
3:J:683:ILE:HD11	3:J:754:ILE:HB	1.98	0.46
2:I:264:GLU:HB2	2:I:267:ARG:HB2	1.98	0.46
2:I:992:LEU:HG	2:I:997:TRP:HE1	1.80	0.46
2:I:3:TYR:O	2:I:8:LYS:NZ	2.32	0.45
5:L:127:ILE:HA	5:L:130:VAL:HG22	1.98	0.45
2:I:1196:LYS:HD2	2:I:1206:THR:HG22	1.98	0.45
3:J:132:LEU:HA	3:J:135:ILE:HD12	1.98	0.45
5:L:552:THR:HB	5:L:555:GLU:HB3	1.98	0.45
2:I:568:ASN:HD22	2:I:572:ILE:HD11	1.80	0.45
3:J:1067:ARG:HD3	3:J:1072:LYS:HA	1.98	0.45
3:J:1162:ILE:N	3:J:1178:THR:O	2.49	0.45
3:J:1230:THR:HG22	3:J:1257:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:633:LEU:HB3	2:I:644:LEU:HD12	1.99	0.45
2:I:731:ARG:NH1	2:I:962:GLU:OE1	2.49	0.45
8:I:1402:1N7:H1	8:I:1402:1N7:H3	1.97	0.45
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.97	0.45
3:J:1021:ASP:HB3	3:J:1024:THR:HB	1.98	0.45
5:L:600:HIS:HB3	5:L:603:ARG:HH21	1.81	0.45
3:J:658:GLU:HA	3:J:661:VAL:HG12	1.99	0.45
2:I:101:ARG:NE	2:I:119:GLU:OE2	2.49	0.45
2:I:971:LEU:HD21	2:I:1014:LEU:HB3	1.98	0.45
3:J:418:GLU:O	3:J:481:ARG:NH2	2.49	0.45
8:L:702:1N7:C3	8:L:702:1N7:C11	2.95	0.45
3:J:1002:VAL:N	3:J:1019:ASN:O	2.50	0.45
2:I:11:ILE:O	2:I:1149:TYR:OH	2.33	0.45
2:I:1058:ARG:NE	2:I:1240:ASP:OD2	2.50	0.45
2:I:1117:LEU:HD13	2:I:1195:ILE:HG12	1.98	0.45
2:I:798:GLN:OE1	2:I:827:ARG:NE	2.48	0.44
3:J:767:LEU:HD12	3:J:772:TYR:HD1	1.82	0.44
1:H:66:HIS:ND1	1:H:68:TYR:O	2.40	0.44
2:I:316:GLU:HB3	2:I:352:ARG:HH22	1.82	0.44
2:I:566:GLY:HA3	2:I:567:PRO:HD3	1.89	0.44
3:J:334:LYS:HG2	3:J:339:ARG:HD2	1.99	0.44
3:J:635:SER:OG	3:J:636:GLY:N	2.50	0.44
3:J:1356:LEU:HD23	3:J:1356:LEU:HA	1.85	0.44
4:K:38:LEU:N	4:K:53:GLU:OE2	2.41	0.44
5:L:133:SER:HB3	5:L:364:ARG:HE	1.82	0.44
8:L:702:1N7:C3	8:L:702:1N7:H17	2.47	0.44
1:G:236:ASP:OD1	1:G:236:ASP:N	2.48	0.44
3:J:1175:LEU:HD13	3:J:1175:LEU:HA	1.89	0.44
1:G:190:ALA:HB2	1:G:200:LYS:HB3	1.99	0.44
3:J:362:ARG:H	3:J:365:GLN:HE21	1.65	0.44
3:J:763:PHE:HE1	3:J:767:LEU:HD11	1.82	0.44
1:G:31:LEU:HD23	1:G:31:LEU:HA	1.83	0.44
1:H:62:ASP:OD1	1:H:62:ASP:N	2.49	0.44
2:I:453:ILE:HD12	2:I:530:ILE:HD12	1.99	0.44
2:I:1028:LYS:HE2	2:I:1028:LYS:HB3	1.80	0.44
3:J:605:LEU:HD23	3:J:605:LEU:HA	1.82	0.44
8:L:702:1N7:H1	8:L:702:1N7:H3	1.99	0.44
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.99	0.44
3:J:53:ARG:HA	3:J:54:ASP:HA	1.58	0.44
3:J:1163:VAL:HG23	3:J:1177:ILE:HG13	1.99	0.44
5:L:422:ARG:HA	5:L:422:ARG:HD3	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:135:ASP:OD1	1:H:135:ASP:N	2.46	0.44
2:I:187:GLU:OE2	2:I:197:ARG:NE	2.50	0.44
2:I:271:ALA:HA	2:I:274:ILE:HD12	1.99	0.44
3:J:1282:TYR:CE2	3:J:1286:LYS:HD3	2.53	0.44
5:L:399:LEU:HD23	5:L:443:ILE:HD13	1.99	0.44
2:I:453:ILE:HD13	2:I:453:ILE:HA	1.79	0.44
2:I:886:LYS:NZ	2:I:916:SER:O	2.43	0.44
2:I:1254:VAL:HG22	2:I:1255:THR:HG23	2.00	0.44
3:J:850:LYS:HE3	3:J:855:ASP:HB3	2.00	0.44
1:G:182:ARG:NH1	1:G:206:GLU:OE1	2.47	0.43
2:I:93:SER:HB2	2:I:126:GLU:HB3	2.00	0.43
2:I:160:ASP:N	2:I:171:LEU:O	2.51	0.43
2:I:560:PRO:HB2	3:J:776:THR:HG21	2.00	0.43
2:I:748:ILE:HD11	2:I:967:LEU:HD22	2.00	0.43
5:L:547:VAL:HG21	5:L:607:LEU:HD11	2.00	0.43
2:I:962:GLU:OE2	8:I:1402:1N7:O2	2.37	0.43
8:I:1402:1N7:C3	8:I:1402:1N7:C1	2.96	0.43
5:L:162:ILE:HD12	5:L:164:GLY:H	1.83	0.43
5:L:163:THR:OG1	5:L:261:LEU:O	2.36	0.43
1:H:39:LEU:HD23	1:H:39:LEU:HA	1.73	0.43
8:I:1402:1N7:H34	8:I:1402:1N7:H10	1.65	0.43
2:I:678:ARG:HD3	2:I:678:ARG:HA	1.72	0.43
3:J:1184:ASP:O	3:J:1186:TYR:N	2.51	0.43
3:J:1314:LEU:HD12	3:J:1314:LEU:HA	1.84	0.43
1:H:203:ILE:HG21	1:H:217:ILE:HD11	2.00	0.43
2:I:739:ASP:OD1	2:I:739:ASP:N	2.51	0.43
3:J:135:ILE:H	3:J:135:ILE:HG13	1.69	0.43
5:L:483:LEU:HD13	5:L:483:LEU:HA	1.85	0.43
1:G:77:ASP:OD1	1:G:77:ASP:N	2.50	0.43
1:G:162:GLU:HG2	1:G:165:GLU:HB2	2.01	0.43
1:H:64:VAL:HG21	1:H:78:ILE:HD11	2.00	0.43
3:J:52:GLU:OE1	3:J:53:ARG:N	2.52	0.43
3:J:1143:ASP:OD2	3:J:1148:ARG:NH1	2.52	0.43
5:L:105:MET:HE1	5:L:385:ARG:HG3	2.00	0.43
2:I:1058:ARG:HD3	2:I:1238:LEU:HD13	2.01	0.43
3:J:186:GLN:HG3	3:J:238:ILE:HB	2.00	0.43
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.87	0.43
3:J:1144:LEU:HD11	3:J:1236:GLU:HG3	2.00	0.43
5:L:449:THR:OG1	5:L:450:ILE:N	2.52	0.43
2:I:208:ILE:HG13	2:I:362:ALA:HB1	2.00	0.43
3:J:1295:ASN:OD1	3:J:1296:GLY:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:153:ASN:ND2	3:J:171:GLU:OE2	2.52	0.42
3:J:814:CYS:SG	3:J:815:GLY:N	2.92	0.42
2:I:617:ALA:HB3	2:I:653:MET:HA	2.00	0.42
3:J:972:LYS:HA	3:J:972:LYS:HD3	1.85	0.42
3:J:983:LYS:HG3	3:J:991:THR:HG23	2.00	0.42
8:L:701:1N7:H10	8:L:701:1N7:H34	1.39	0.42
1:H:61:ILE:HD13	1:H:142:MET:HB3	2.01	0.42
1:H:66:HIS:HD1	1:H:68:TYR:H	1.67	0.42
1:H:92:VAL:O	1:H:148:ARG:NH2	2.52	0.42
2:I:512:SER:O	2:I:512:SER:OG	2.35	0.42
8:I:1401:1N7:H33	8:I:1401:1N7:H10	1.49	0.42
3:J:84:ILE:HA	3:J:91:GLU:HA	2.00	0.42
3:J:212:THR:HA	3:J:215:LYS:HE2	2.01	0.42
3:J:321:LYS:HA	3:J:321:LYS:HD3	1.83	0.42
3:J:591:ILE:HG23	3:J:592:VAL:HG13	2.01	0.42
3:J:811:GLU:OE2	3:J:890:THR:OG1	2.23	0.42
5:L:232:ARG:HA	5:L:235:ILE:HG23	1.99	0.42
8:I:1402:1N7:H36	8:I:1402:1N7:H30	1.79	0.42
2:I:565:GLU:HA	2:I:569:ILE:HG12	2.01	0.42
2:I:684:ASN:OD1	2:I:687:ARG:NH1	2.52	0.42
8:I:1402:1N7:C3	8:I:1402:1N7:C11	2.97	0.42
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	2.01	0.42
5:L:359:LYS:HA	5:L:362:ASN:HD21	1.85	0.42
2:I:549:ASP:OD1	2:I:550:VAL:N	2.52	0.42
3:J:511:TYR:HE1	3:J:724:MET:HG2	1.84	0.42
4:K:12:LYS:HD3	4:K:12:LYS:HA	1.89	0.42
5:L:306:PHE:HA	5:L:315:TRP:CG	2.55	0.42
7:Q:18:DC:H1'	7:Q:19:DT:H5'	2.01	0.42
2:I:813:GLU:HB3	3:J:461:PHE:HD1	1.84	0.42
3:J:17:PHE:HZ	3:J:1353:VAL:HG11	1.83	0.42
3:J:968:ASN:HD21	3:J:970:SER:HB2	1.85	0.42
5:L:385:ARG:HA	5:L:388:ILE:HG22	2.00	0.42
2:I:373:GLY:H	5:L:93:ARG:HD2	1.84	0.42
3:J:996:LYS:HA	3:J:996:LYS:HD2	1.85	0.42
3:J:1079:LYS:HE2	3:J:1079:LYS:HB3	1.81	0.42
2:I:268:ARG:NH2	2:I:269:ILE:O	2.53	0.42
2:I:934:PHE:HE2	2:I:1051:LYS:HD2	1.85	0.42
2:I:1005:GLU:HG3	2:I:1007:LYS:H	1.85	0.42
3:J:1157:ALA:N	3:J:1208:ASP:O	2.53	0.42
3:J:1162:ILE:HG22	3:J:1178:THR:HB	2.02	0.42
3:J:1262:ARG:HE	3:J:1262:ARG:HB3	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:ARG:H	1:G:166:ARG:HD2	1.85	0.41
2:I:525:THR:HG21	2:I:687:ARG:HD2	2.02	0.41
8:I:1402:1N7:C3	8:I:1402:1N7:H17	2.49	0.41
3:J:452:LEU:HA	3:J:452:LEU:HD23	1.86	0.41
3:J:521:LYS:HB2	3:J:521:LYS:HE3	1.87	0.41
3:J:861:ASN:OD1	3:J:883:ARG:NH1	2.53	0.41
3:J:1241:TYR:HD1	3:J:1241:TYR:HA	1.71	0.41
1:H:77:ASP:OD1	1:H:78:ILE:N	2.51	0.41
2:I:241:LEU:N	2:I:283:LYS:O	2.53	0.41
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.54	0.41
5:L:277:MET:SD	5:L:277:MET:N	2.92	0.41
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	2.01	0.41
1:H:171:LEU:HD12	1:H:171:LEU:HA	1.90	0.41
2:I:972:PHE:CE2	2:I:994:ARG:HB3	2.56	0.41
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.96	0.41
3:J:615:LYS:HG2	4:K:5:THR:HG21	2.01	0.41
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.55	0.41
2:I:342:ASP:OD2	2:I:343:HIS:NE2	2.53	0.41
2:I:563:THR:HG21	2:I:570:GLY:H	1.86	0.41
2:I:1321:GLU:OE2	3:J:99:ARG:NH2	2.34	0.41
3:J:289:ASP:HA	3:J:292:VAL:HG22	2.03	0.41
3:J:963:VAL:HB	3:J:980:THR:HG23	2.01	0.41
1:H:100:LEU:HB2	1:H:144:ILE:HG12	2.02	0.41
3:J:67:ASP:OD1	3:J:95:THR:N	2.50	0.41
3:J:188:LEU:HA	3:J:188:LEU:HD23	1.83	0.41
3:J:1036:ARG:HE	3:J:1081:VAL:HG11	1.85	0.41
2:I:471:VAL:HB	2:I:498:ILE:HD11	2.03	0.41
2:I:890:LYS:HD2	2:I:890:LYS:HA	1.82	0.41
2:I:995:ASP:OD1	2:I:995:ASP:N	2.54	0.41
1:G:67:GLU:HB3	1:G:171:LEU:HD22	2.01	0.41
2:I:56:VAL:HG11	2:I:468:LEU:HD13	2.01	0.41
2:I:228:VAL:O	2:I:335:THR:OG1	2.32	0.41
2:I:268:ARG:CZ	2:I:270:THR:HA	2.51	0.41
2:I:349:GLU:O	2:I:353:VAL:HG23	2.20	0.41
2:I:1073:LYS:H	2:I:1073:LYS:HG3	1.43	0.41
2:I:1295:SER:OG	2:I:1296:ASP:OD1	2.32	0.41
3:J:362:ARG:HE	3:J:362:ARG:HB2	1.60	0.41
5:L:220:LYS:HB3	5:L:259:PHE:CZ	2.55	0.41
2:I:57:PHE:HD2	2:I:70:TYR:HB2	1.85	0.41
2:I:314:ASN:HD21	2:I:352:ARG:HG3	1.86	0.41
2:I:657:THR:HG21	2:I:1188:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:705:GLU:HB3	2:I:794:LEU:H	1.86	0.41
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	2.03	0.41
3:J:195:GLU:H	3:J:195:GLU:HG2	1.55	0.41
3:J:197:GLU:OE2	3:J:220:ARG:NH1	2.46	0.41
3:J:291:ILE:HG23	5:L:406:GLN:HE22	1.86	0.41
3:J:1058:SER:OG	3:J:1108:GLN:OE1	2.36	0.41
3:J:1146:GLU:HB2	3:J:1148:ARG:HG3	2.03	0.41
5:L:270:VAL:O	5:L:274:ARG:HG2	2.21	0.41
5:L:320:ILE:HG12	5:L:330:LEU:HD12	2.02	0.41
1:H:133:LEU:HD12	1:H:133:LEU:HA	1.91	0.40
2:I:410:LEU:HD12	2:I:410:LEU:HA	1.85	0.40
2:I:492:MET:SD	2:I:492:MET:N	2.84	0.40
2:I:873:ILE:HD13	2:I:873:ILE:HA	1.89	0.40
2:I:1002:LEU:N	2:I:1008:GLN:OE1	2.54	0.40
2:I:1306:LYS:O	2:I:1310:ASP:HB2	2.21	0.40
3:J:472:LEU:O	3:J:477:GLN:NE2	2.54	0.40
1:G:68:TYR:HE2	2:I:831:ILE:HD13	1.86	0.40
1:H:47:LEU:HD23	1:H:51:MET:SD	2.62	0.40
2:I:49:LEU:HD23	2:I:49:LEU:HA	1.91	0.40
2:I:519:ASN:HD21	2:I:689:ALA:HB3	1.86	0.40
2:I:1288:GLN:NE2	2:I:1317:PRO:HB3	2.35	0.40
3:J:51:PRO:HB2	3:J:57:PHE:O	2.22	0.40
3:J:88:CYS:SG	3:J:90:VAL:N	2.94	0.40
3:J:449:LEU:HD13	3:J:466:MET:HE1	2.03	0.40
3:J:1256:ILE:HD13	3:J:1256:ILE:HA	1.90	0.40
1:G:100:LEU:O	1:G:144:ILE:N	2.55	0.40
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.94	0.40
2:I:240:GLU:HA	2:I:284:LEU:HA	2.03	0.40
6:P:66:DC:H2'	6:P:67:DT:H71	2.02	0.40
2:I:216:THR:H	2:I:219:GLN:NE2	2.19	0.40
2:I:639:LYS:HE2	2:I:639:LYS:HB2	1.93	0.40
2:I:699:LEU:HB2	2:I:799:ASN:HD22	1.87	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	G	231/329 (70%)	198 (86%)	33 (14%)	0	100	100
1	H	219/329 (67%)	195 (89%)	24 (11%)	0	100	100
2	I	1338/1342 (100%)	1208 (90%)	128 (10%)	2 (0%)	48	78
3	J	1327/1407 (94%)	1225 (92%)	102 (8%)	0	100	100
4	K	77/91 (85%)	68 (88%)	9 (12%)	0	100	100
5	L	459/613 (75%)	432 (94%)	27 (6%)	0	100	100
All	All	3651/4111 (89%)	3326 (91%)	323 (9%)	2 (0%)	50	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	898	GLU
2	I	897	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	G	201/286 (70%)	184 (92%)	17 (8%)	8	33
1	H	190/286 (66%)	177 (93%)	13 (7%)	13	40
2	I	1155/1157 (100%)	1076 (93%)	79 (7%)	13	40
3	J	1118/1168 (96%)	1034 (92%)	84 (8%)	11	37
4	K	67/75 (89%)	62 (92%)	5 (8%)	11	37
5	L	411/540 (76%)	398 (97%)	13 (3%)	34	57
All	All	3142/3512 (90%)	2931 (93%)	211 (7%)	16	40

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	7	GLU
1	G	8	PHE
1	G	9	LEU
1	G	19	VAL
1	G	27	THR
1	G	70	THR
1	G	77	ASP
1	G	123	ILE
1	G	128	HIS
1	G	129	VAL
1	G	150	ARG
1	G	177	TYR
1	G	192	VAL
1	G	193	GLU
1	G	204	GLU
1	G	232	VAL
1	G	236	ASP
1	H	6	THR
1	H	13	LEU
1	H	14	VAL
1	H	15	ASP
1	H	16	ILE
1	H	21	SER
1	H	27	THR
1	H	28	LEU
1	H	38	THR
1	H	59	VAL
1	H	120	ASP
1	H	207	THR
1	H	212	ASP
2	I	30	ILE
2	I	42	ASP
2	I	56	VAL
2	I	79	VAL
2	I	81	ASP
2	I	91	THR
2	I	103	VAL
2	I	150	HIS
2	I	161	LYS
2	I	185	ASP
2	I	197	ARG
2	I	213	LEU
2	I	291	TYR

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Mol	Chain	Res	Type
2	I	335	THR
2	I	391	SER
2	I	394	ARG
2	I	396	ASP
2	I	407	ARG
2	I	409	LEU
2	I	455	SER
2	I	483	ASP
2	I	513	GLN
2	I	515	MET
2	I	516	ASP
2	I	521	LEU
2	I	538	LEU
2	I	550	VAL
2	I	572	ILE
2	I	575	LEU
2	I	589	THR
2	I	606	LEU
2	I	615	VAL
2	I	623	LEU
2	I	634	VAL
2	I	637	ARG
2	I	643	SER
2	I	654	ASP
2	I	657	THR
2	I	658	GLN
2	I	663	VAL
2	I	674	ASP
2	I	687	ARG
2	I	697	LYS
2	I	714	VAL
2	I	765	ILE
2	I	781	ASP
2	I	808	ASN
2	I	819	SER
2	I	830	THR
2	I	851	THR
2	I	854	ILE
2	I	888	THR
2	I	896	THR
2	I	909	LYS
2	I	913	VAL

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Mol	Chain	Res	Type
2	I	944	ARG
2	I	967	LEU
2	I	984	VAL
2	I	990	ASP
2	I	992	LEU
2	I	998	LEU
2	I	1002	LEU
2	I	1022	LYS
2	I	1038	GLN
2	I	1073	LYS
2	I	1094	VAL
2	I	1158	LYS
2	I	1160	ASP
2	I	1203	ASP
2	I	1225	VAL
2	I	1239	VAL
2	I	1244	HIS
2	I	1248	THR
2	I	1254	VAL
2	I	1287	LEU
2	I	1291	LEU
2	I	1331	ARG
2	I	1337	ILE
2	I	1340	GLU
3	J	70	CYS
3	J	83	VAL
3	J	88	CYS
3	J	90	VAL
3	J	92	VAL
3	J	111	THR
3	J	114	ILE
3	J	115	TRP
3	J	124	ILE
3	J	126	LEU
3	J	147	ILE
3	J	157	GLN
3	J	169	LEU
3	J	205	LEU
3	J	206	ASN
3	J	223	LEU
3	J	255	LEU
3	J	262	THR

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Mol	Chain	Res	Type
3	J	264	ASP
3	J	299	LEU
3	J	304	ASP
3	J	324	LEU
3	J	353	SER
3	J	354	VAL
3	J	393	THR
3	J	410	ASP
3	J	429	LEU
3	J	430	HIS
3	J	449	LEU
3	J	474	LEU
3	J	485	MET
3	J	506	VAL
3	J	510	LEU
3	J	526	VAL
3	J	528	THR
3	J	536	LEU
3	J	543	SER
3	J	545	HIS
3	J	567	THR
3	J	572	THR
3	J	596	LEU
3	J	612	LEU
3	J	614	LEU
3	J	617	THR
3	J	618	VAL
3	J	639	VAL
3	J	674	THR
3	J	683	ILE
3	J	684	ASP
3	J	691	ASP
3	J	705	THR
3	J	706	VAL
3	J	707	ILE
3	J	708	ASN
3	J	717	VAL
3	J	727	ASP
3	J	733	SER
3	J	746	LEU
3	J	751	ASP
3	J	762	ASN

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Mol	Chain	Res	Type
3	J	783	LEU
3	J	802	ASP
3	J	806	ASP
3	J	817	HIS
3	J	831	VAL
3	J	835	LEU
3	J	869	CYS
3	J	882	VAL
3	J	885	VAL
3	J	891	ASP
3	J	918	ILE
3	J	962	ASN
3	J	966	VAL
3	J	987	GLU
3	J	1031	VAL
3	J	1034	PHE
3	J	1250	ASP
3	J	1258	ARG
3	J	1261	LEU
3	J	1273	ASP
3	J	1298	VAL
3	J	1327	GLU
3	J	1344	LEU
3	J	1366	HIS
4	K	4	VAL
4	K	5	THR
4	K	8	ASP
4	K	13	ILE
4	K	36	ASP
5	L	98	VAL
5	L	100	MET
5	L	163	THR
5	L	277	MET
5	L	363	ARG
5	L	399	LEU
5	L	476	ARG
5	L	515	GLU
5	L	552	THR
5	L	558	VAL
5	L	567	MET
5	L	573	LEU
5	L	580	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	519	ASN
3	J	335	GLN
3	J	1289	ASN
5	L	362	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](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z > 2$
8	1N7	I	1401	-	30,30,46	5.20	15 (50%)	47,48,72	2.47	13 (27%)
8	1N7	L	701	-	30,30,46	5.25	17 (56%)	47,48,72	2.55	16 (34%)
8	1N7	I	1402	-	30,30,46	5.20	15 (50%)	47,48,72	2.64	18 (38%)
8	1N7	L	702	-	30,30,46	5.18	14 (46%)	47,48,72	2.50	18 (38%)

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
8	1N7	I	1401	-	-	7/7/72/92	0/4/4/4
8	1N7	L	701	-	-	6/7/72/92	0/4/4/4
8	1N7	I	1402	-	-	4/7/72/92	0/4/4/4
8	1N7	L	702	-	-	6/7/72/92	0/4/4/4

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	701	1N7	C3-C19	17.98	1.82	1.53
8	I	1402	1N7	C3-C19	17.79	1.82	1.53
8	L	702	1N7	C3-C19	17.76	1.82	1.53
8	I	1401	1N7	C3-C19	17.65	1.82	1.53
8	L	701	1N7	C3-C4	12.31	1.73	1.53
8	I	1402	1N7	C3-C4	12.24	1.73	1.53
8	I	1401	1N7	C3-C4	12.20	1.73	1.53
8	L	702	1N7	C3-C4	12.19	1.73	1.53
8	I	1401	1N7	C5-C4	-10.04	1.39	1.54
8	L	701	1N7	C5-C4	-9.92	1.39	1.54
8	I	1402	1N7	C5-C4	-9.45	1.40	1.54
8	L	702	1N7	C5-C4	-9.35	1.40	1.54
8	L	701	1N7	C2-C19	-9.16	1.40	1.56
8	L	702	1N7	C2-C19	-9.12	1.40	1.56
8	I	1401	1N7	C2-C19	-9.08	1.40	1.56
8	I	1402	1N7	C2-C19	-8.84	1.40	1.56
8	I	1401	1N7	C8-C7	6.17	1.70	1.54
8	L	701	1N7	C8-C7	6.03	1.70	1.54
8	L	702	1N7	C8-C7	5.99	1.70	1.54
8	I	1402	1N7	C8-C7	5.91	1.70	1.54
8	I	1401	1N7	C5-C6	-4.92	1.47	1.55
8	I	1402	1N7	C5-C6	-4.72	1.47	1.55
8	L	702	1N7	C5-C6	-4.61	1.47	1.55
8	I	1402	1N7	C18-C6	-4.47	1.45	1.53
8	L	701	1N7	C5-C6	-4.42	1.48	1.55
8	I	1401	1N7	C18-C6	-4.34	1.45	1.53
8	L	701	1N7	O4-C4	-4.23	1.36	1.43
8	L	702	1N7	C18-C6	-4.20	1.45	1.53
8	I	1401	1N7	O4-C4	-4.19	1.36	1.43
8	L	702	1N7	O4-C4	-4.18	1.36	1.43
8	I	1402	1N7	O4-C4	-4.18	1.36	1.43
8	L	701	1N7	C18-C6	-4.17	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	1402	1N7	C2-C15	3.84	1.61	1.55
8	L	702	1N7	C2-C15	3.60	1.61	1.55
8	I	1402	1N7	C5-C9	3.58	1.61	1.55
8	L	701	1N7	C5-C9	3.30	1.61	1.55
8	L	702	1N7	C5-C9	3.30	1.61	1.55
8	L	702	1N7	C7-C6	3.28	1.61	1.54
8	L	701	1N7	C14-C15	-3.24	1.48	1.53
8	I	1402	1N7	C14-C15	-3.21	1.48	1.53
8	I	1401	1N7	C7-C6	3.20	1.60	1.54
8	L	701	1N7	C7-C6	3.16	1.60	1.54
8	L	701	1N7	C2-C15	3.12	1.60	1.55
8	I	1401	1N7	C2-C15	3.07	1.60	1.55
8	I	1402	1N7	C7-C6	3.00	1.60	1.54
8	I	1401	1N7	C14-C15	-2.93	1.49	1.53
8	L	702	1N7	C14-C15	-2.92	1.49	1.53
8	I	1401	1N7	C5-C9	2.53	1.59	1.55
8	I	1402	1N7	O2-C13	-2.47	1.36	1.43
8	L	701	1N7	O2-C13	-2.40	1.36	1.43
8	L	702	1N7	C16-C15	2.36	1.57	1.53
8	L	702	1N7	O2-C13	-2.30	1.36	1.43
8	L	701	1N7	C16-C15	2.30	1.57	1.53
8	I	1401	1N7	O2-C13	-2.26	1.36	1.43
8	L	701	1N7	C10-C5	2.19	1.57	1.54
8	I	1401	1N7	C14-C13	2.18	1.55	1.52
8	I	1402	1N7	C1-C2	2.12	1.57	1.54
8	I	1402	1N7	C10-C5	2.12	1.57	1.54
8	L	701	1N7	C1-C2	2.09	1.57	1.54
8	L	701	1N7	C14-C13	2.08	1.55	1.52
8	I	1401	1N7	C16-C15	2.03	1.57	1.53

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	701	1N7	C9-C5-C4	-9.62	109.01	117.67
8	I	1401	1N7	C9-C5-C4	-9.27	109.33	117.67
8	L	702	1N7	C9-C5-C4	-8.66	109.88	117.67
8	I	1402	1N7	C9-C5-C4	-8.16	110.32	117.67
8	I	1402	1N7	C19-C18-C17	-5.72	104.66	111.86
8	L	701	1N7	C9-C5-C6	5.68	105.81	100.11
8	L	702	1N7	C6-C5-C4	5.35	112.31	107.42
8	L	702	1N7	C3-C19-C2	-5.12	108.51	113.70
8	L	701	1N7	C5-C9-C20	-5.00	113.43	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1401	1N7	C7-C6-C18	-4.86	111.69	118.36
8	L	702	1N7	C5-C9-C20	-4.78	113.69	119.48
8	I	1401	1N7	C5-C9-C20	-4.76	113.72	119.48
8	I	1401	1N7	C3-C19-C2	-4.72	108.91	113.70
8	L	701	1N7	C3-C19-C2	-4.68	108.95	113.70
8	I	1402	1N7	C19-C3-C4	-4.64	108.22	114.29
8	I	1401	1N7	C19-C3-C4	-4.63	108.24	114.29
8	I	1402	1N7	C9-C5-C6	4.55	104.68	100.11
8	I	1402	1N7	C7-C6-C18	-4.55	112.11	118.36
8	L	702	1N7	C7-C6-C18	-4.34	112.41	118.36
8	L	702	1N7	C19-C3-C4	-4.32	108.64	114.29
8	I	1402	1N7	C14-C13-C12	-4.31	105.36	110.62
8	I	1401	1N7	C6-C5-C4	4.08	111.14	107.42
8	I	1402	1N7	C3-C19-C2	-4.07	109.57	113.70
8	I	1402	1N7	C8-C7-C6	-4.01	97.30	105.14
8	L	701	1N7	C8-C9-C5	3.96	107.38	103.54
8	I	1401	1N7	C21-C20-C9	-3.93	106.99	112.88
8	L	701	1N7	C7-C6-C18	-3.80	113.14	118.36
8	L	702	1N7	C8-C9-C5	3.67	107.10	103.54
8	I	1402	1N7	C1-C2-C15	3.43	112.68	107.75
8	L	701	1N7	C8-C7-C6	-3.39	98.50	105.14
8	I	1402	1N7	C6-C18-C17	-3.39	107.36	111.85
8	I	1401	1N7	C19-C18-C17	-3.35	107.64	111.86
8	I	1402	1N7	C15-C14-C13	-3.29	107.74	112.71
8	L	702	1N7	C9-C5-C6	3.29	103.41	100.11
8	I	1402	1N7	C21-C20-C22	-3.29	105.25	110.34
8	L	702	1N7	C8-C7-C6	-3.28	98.73	105.14
8	I	1402	1N7	C3-C19-C18	-3.22	106.13	110.89
8	L	701	1N7	C1-C2-C15	3.13	112.25	107.75
8	L	701	1N7	C19-C18-C17	-3.12	107.93	111.86
8	L	701	1N7	C14-C13-C12	-3.10	106.84	110.62
8	L	701	1N7	C19-C3-C4	-2.99	110.38	114.29
8	I	1401	1N7	C3-C19-C18	-2.87	106.65	110.89
8	I	1402	1N7	C19-C2-C15	2.73	112.31	108.51
8	I	1401	1N7	C9-C5-C6	2.72	102.84	100.11
8	I	1402	1N7	C1-C12-C13	-2.65	106.97	110.48
8	I	1402	1N7	C8-C9-C5	2.62	106.08	103.54
8	L	702	1N7	C14-C13-C12	-2.57	107.49	110.62
8	L	702	1N7	C3-C19-C18	-2.55	107.12	110.89
8	L	702	1N7	C21-C20-C9	-2.54	109.07	112.88
8	L	701	1N7	C21-C20-C9	-2.53	109.09	112.88
8	L	701	1N7	C15-C14-C13	-2.46	108.99	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	702	1N7	C21-C20-C22	-2.45	106.54	110.34
8	L	702	1N7	C1-C2-C15	2.40	111.20	107.75
8	L	701	1N7	C1-C12-C13	-2.30	107.43	110.48
8	I	1401	1N7	C14-C13-C12	-2.22	107.91	110.62
8	L	701	1N7	C14-C15-C2	-2.18	110.34	112.66
8	L	702	1N7	C16-C15-C14	-2.16	108.76	111.23
8	I	1402	1N7	C1-C2-C19	-2.13	108.03	111.34
8	I	1402	1N7	C10-C5-C4	2.12	111.18	109.06
8	I	1401	1N7	C16-C15-C2	-2.12	110.41	112.66
8	L	702	1N7	C19-C2-C15	2.11	111.45	108.51
8	L	702	1N7	C1-C2-C19	-2.07	108.12	111.34
8	L	702	1N7	C19-C18-C17	-2.06	109.26	111.86
8	L	701	1N7	C3-C19-C18	-2.06	107.85	110.89
8	I	1401	1N7	C1-C2-C15	2.02	110.65	107.75

There are no chirality outliers.

All (23) torsion outliers are listed below:

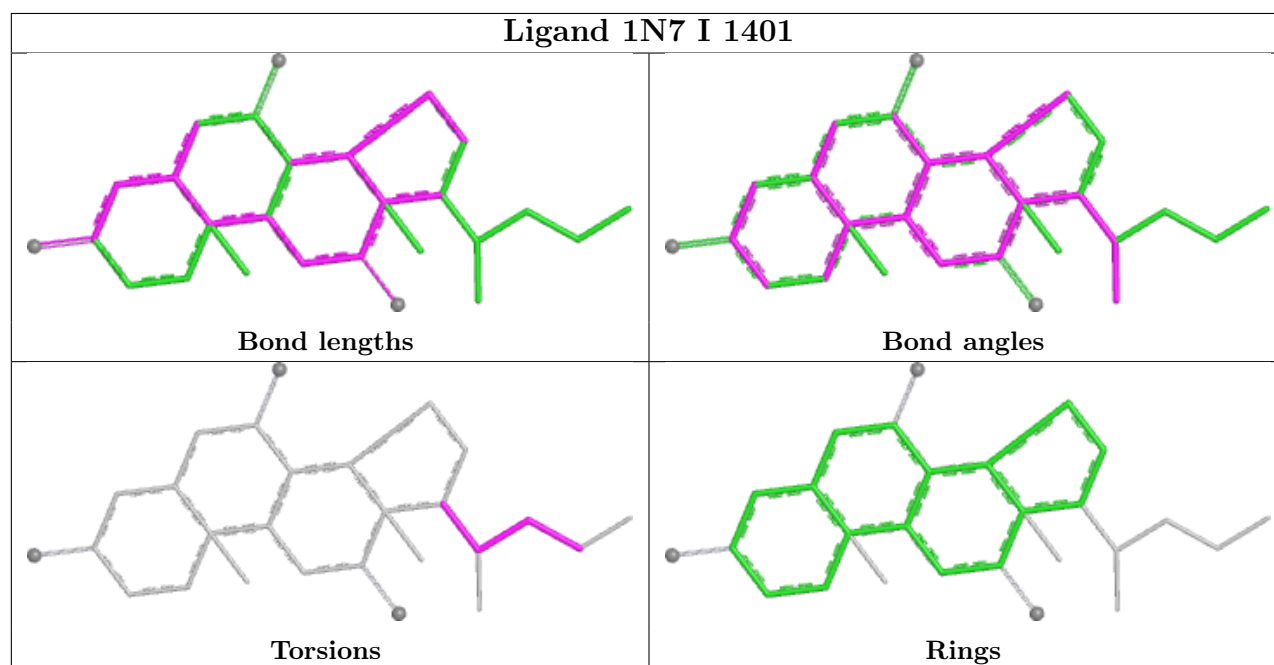
Mol	Chain	Res	Type	Atoms
8	I	1401	1N7	C21-C20-C9-C5
8	I	1401	1N7	C22-C20-C9-C5
8	I	1401	1N7	C21-C20-C9-C8
8	I	1401	1N7	C22-C20-C9-C8
8	L	702	1N7	C21-C20-C9-C5
8	L	702	1N7	C21-C20-C9-C8
8	L	701	1N7	C21-C20-C9-C5
8	I	1401	1N7	C21-C20-C22-C23
8	L	701	1N7	C21-C20-C9-C8
8	L	702	1N7	C22-C20-C9-C8
8	L	701	1N7	C22-C20-C9-C5
8	L	702	1N7	C22-C20-C9-C5
8	L	701	1N7	C22-C20-C9-C8
8	L	701	1N7	C9-C20-C22-C23
8	L	701	1N7	C21-C20-C22-C23
8	I	1401	1N7	C9-C20-C22-C23
8	L	702	1N7	C21-C20-C22-C23
8	L	702	1N7	C9-C20-C22-C23
8	I	1401	1N7	C20-C22-C23-C24
8	I	1402	1N7	C21-C20-C9-C8
8	I	1402	1N7	C21-C20-C9-C5
8	I	1402	1N7	C22-C20-C9-C8
8	I	1402	1N7	C22-C20-C9-C5

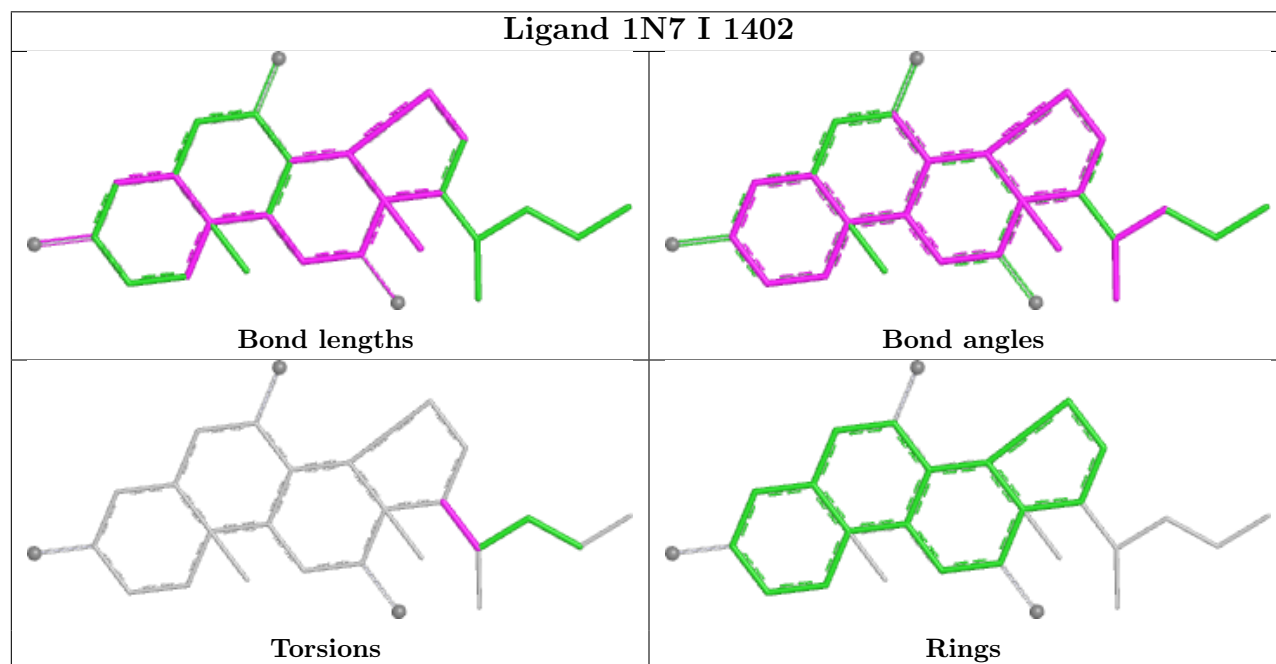
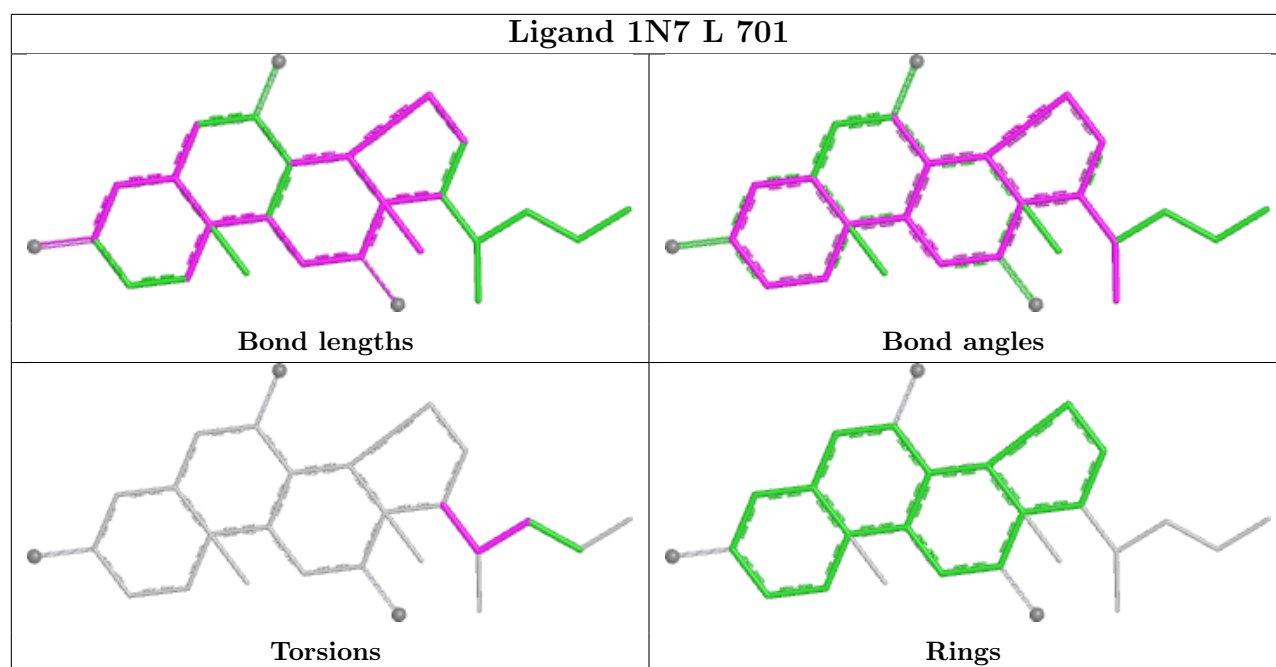
There are no ring outliers.

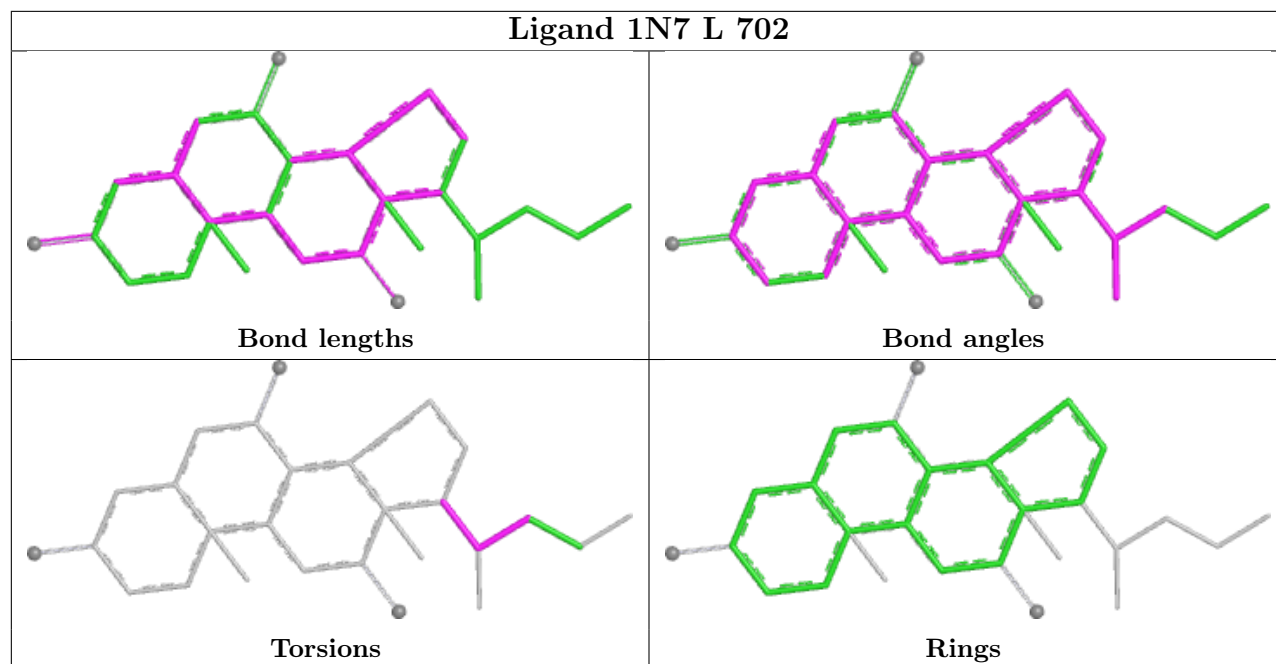
4 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1401	1N7	8	0
8	L	701	1N7	8	0
8	I	1402	1N7	13	0
8	L	702	1N7	9	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.

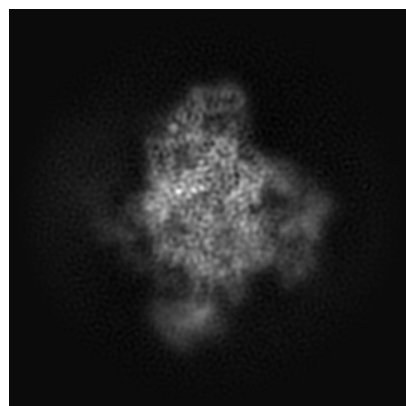
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23893. These allow visual inspection of the internal detail of the map and identification of artifacts.

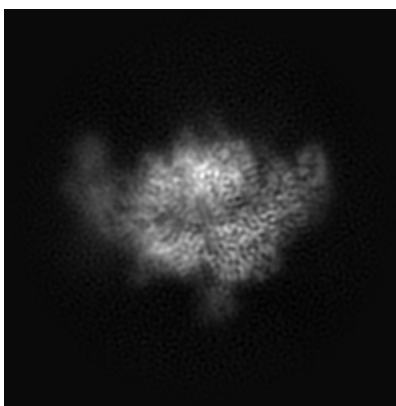
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

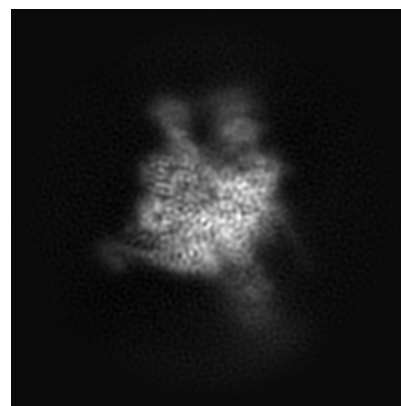
6.1.1 Primary map



X

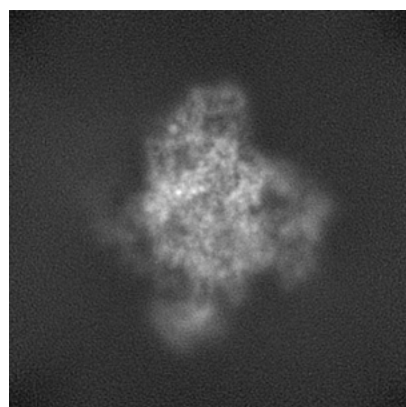


Y

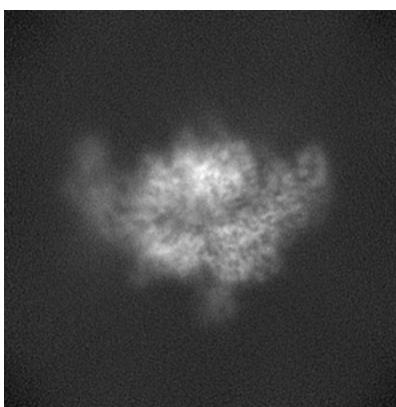


Z

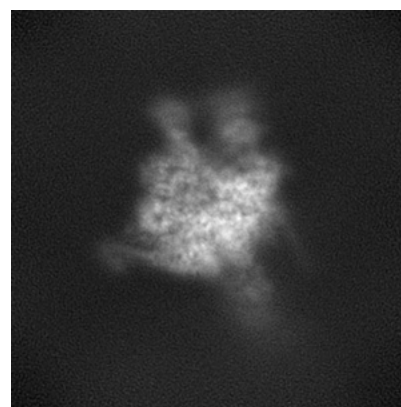
6.1.2 Raw map



X



Y

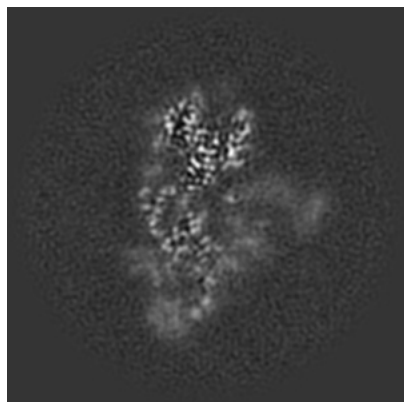


Z

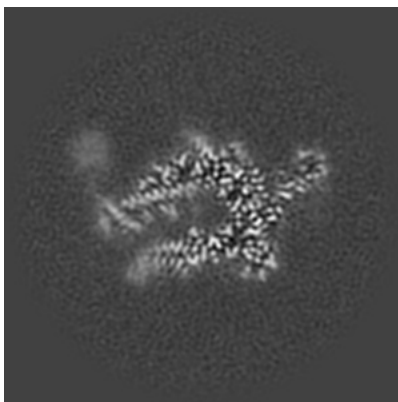
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

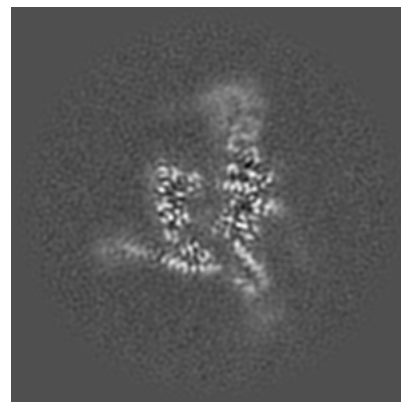
6.2.1 Primary map



X Index: 128

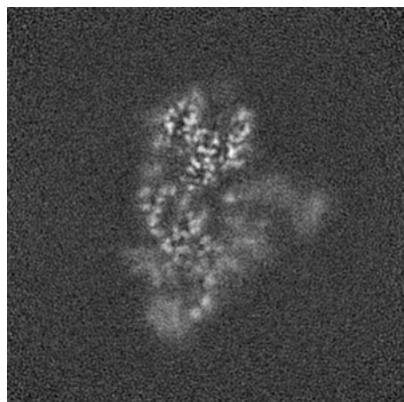


Y Index: 128

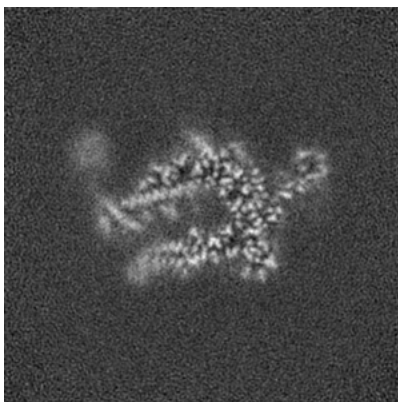


Z Index: 128

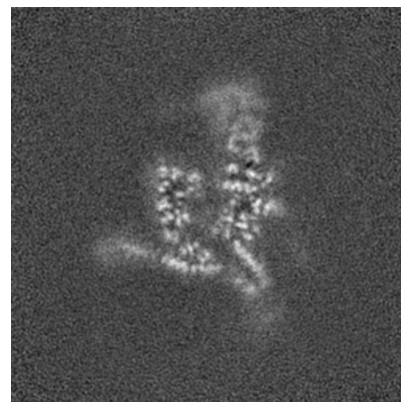
6.2.2 Raw map



X Index: 128



Y Index: 128

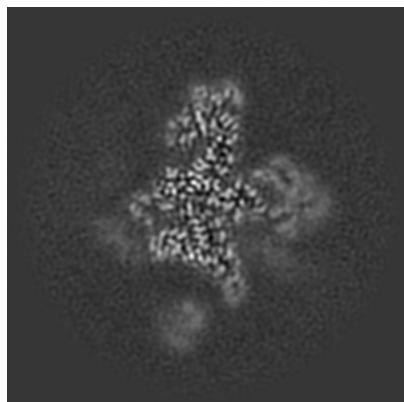


Z Index: 128

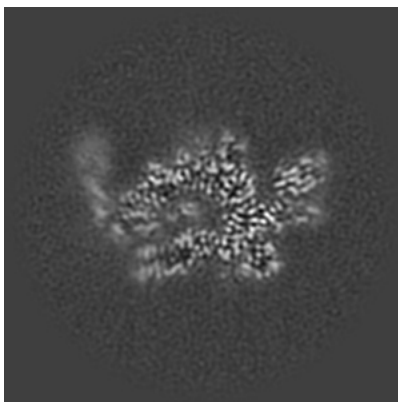
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

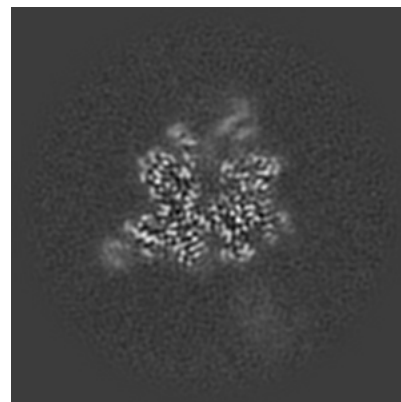
6.3.1 Primary map



X Index: 145

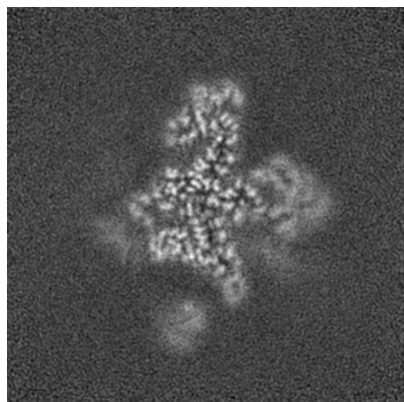


Y Index: 123

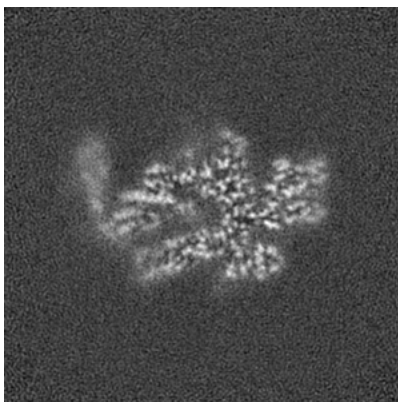


Z Index: 143

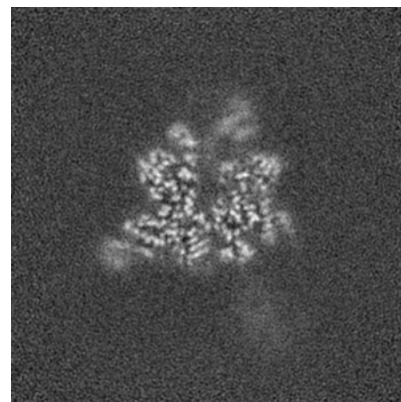
6.3.2 Raw map



X Index: 145



Y Index: 120

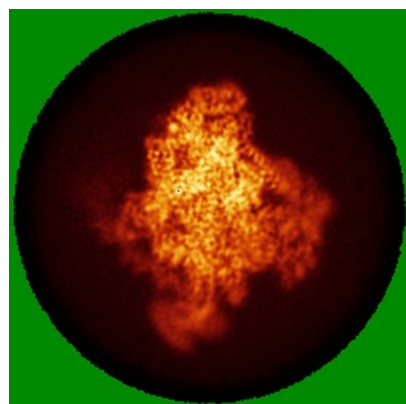


Z Index: 142

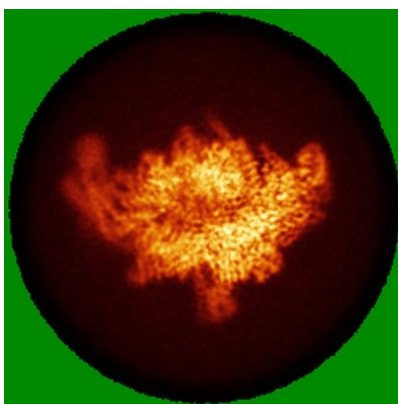
The images above show the largest variance slices of the map in three orthogonal directions.

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

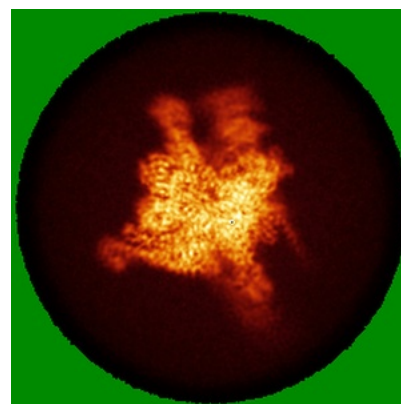
6.4.1 Primary map



X

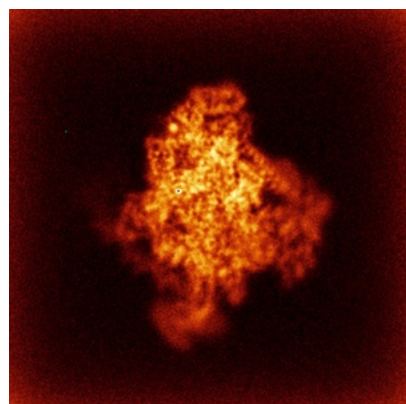


Y

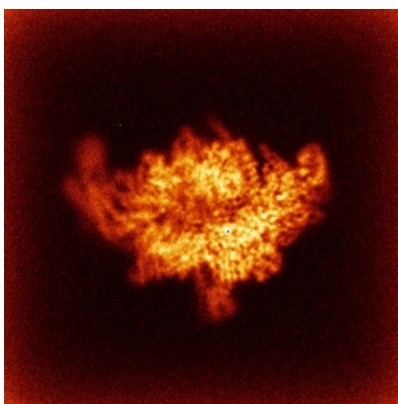


Z

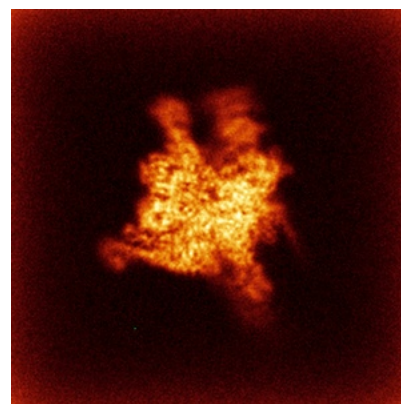
6.4.2 Raw map



X



Y

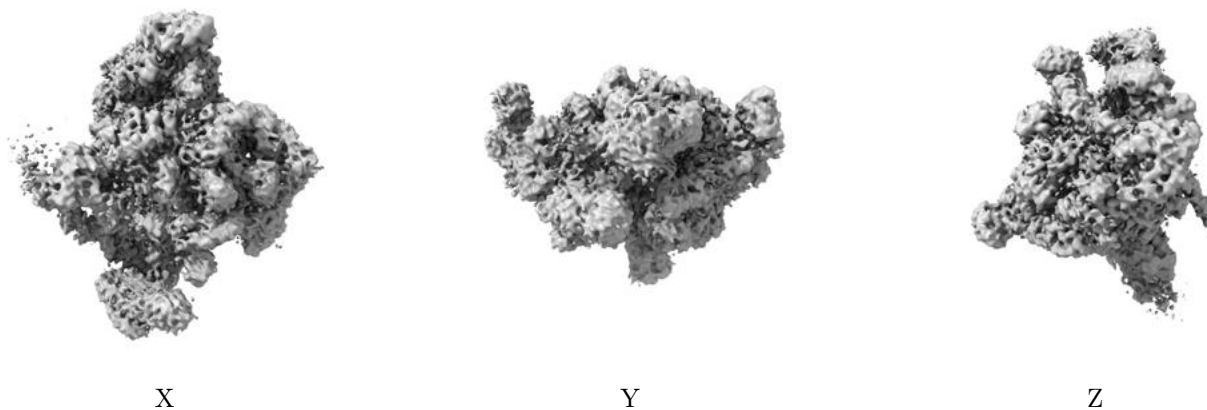


Z

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.

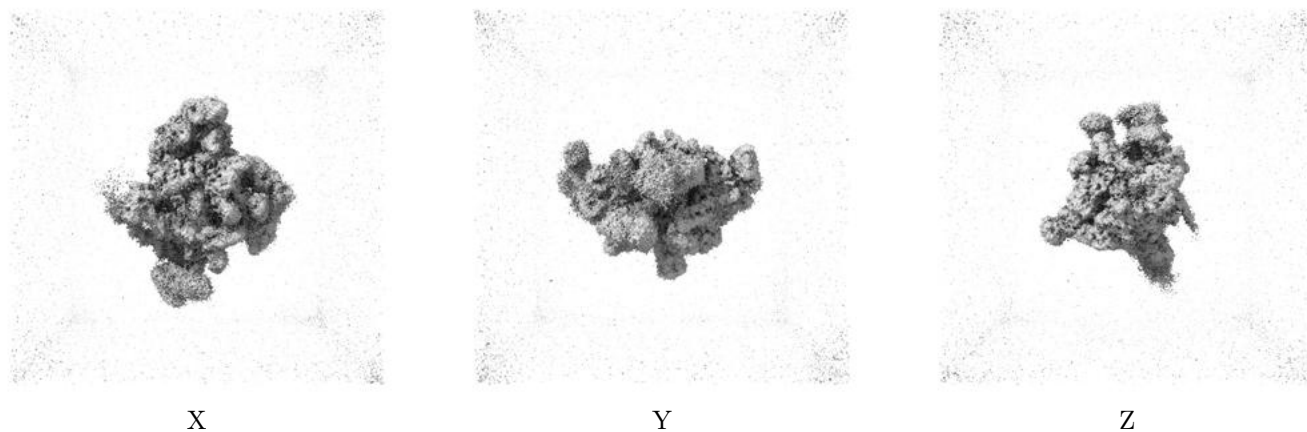
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. 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.

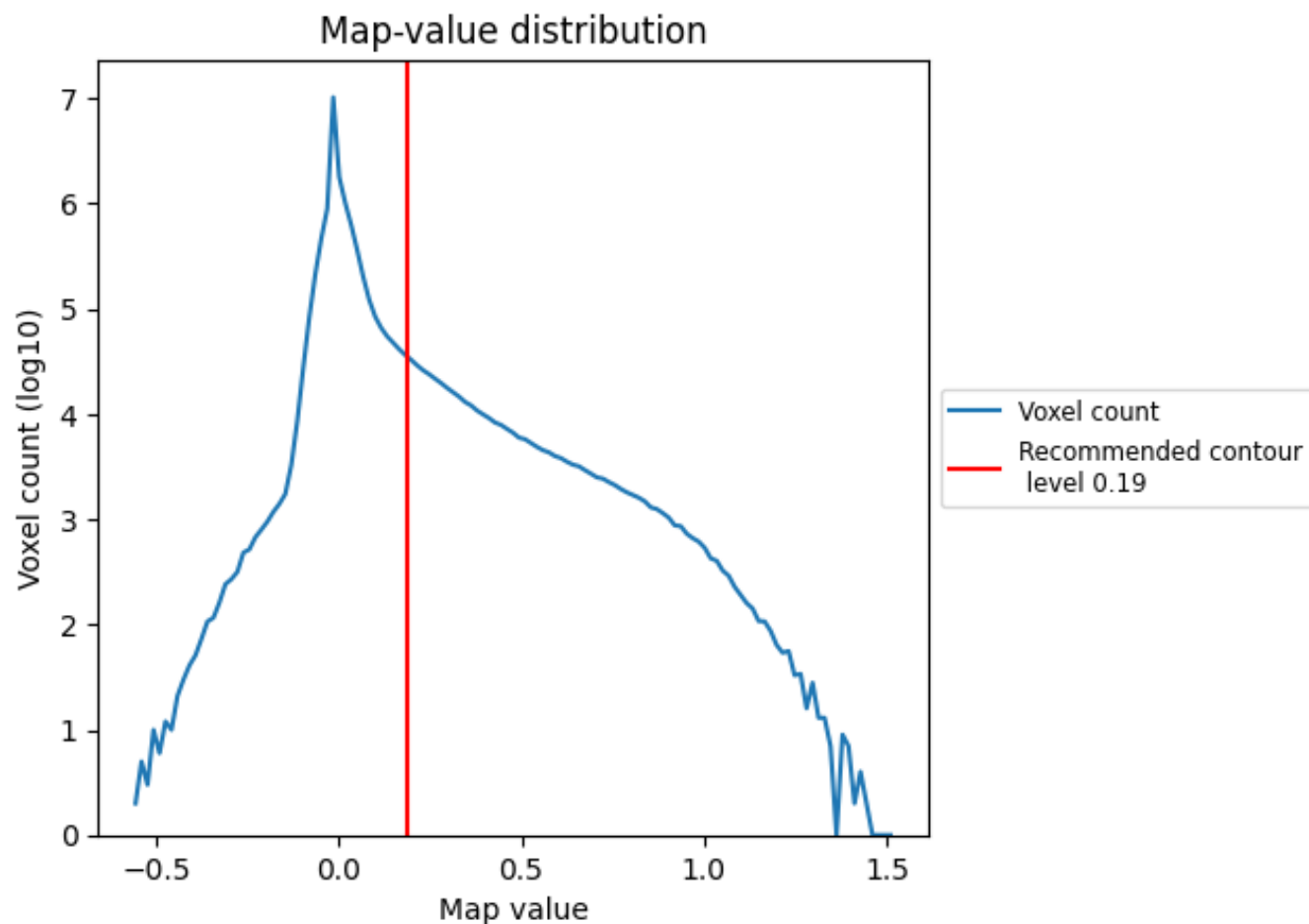
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

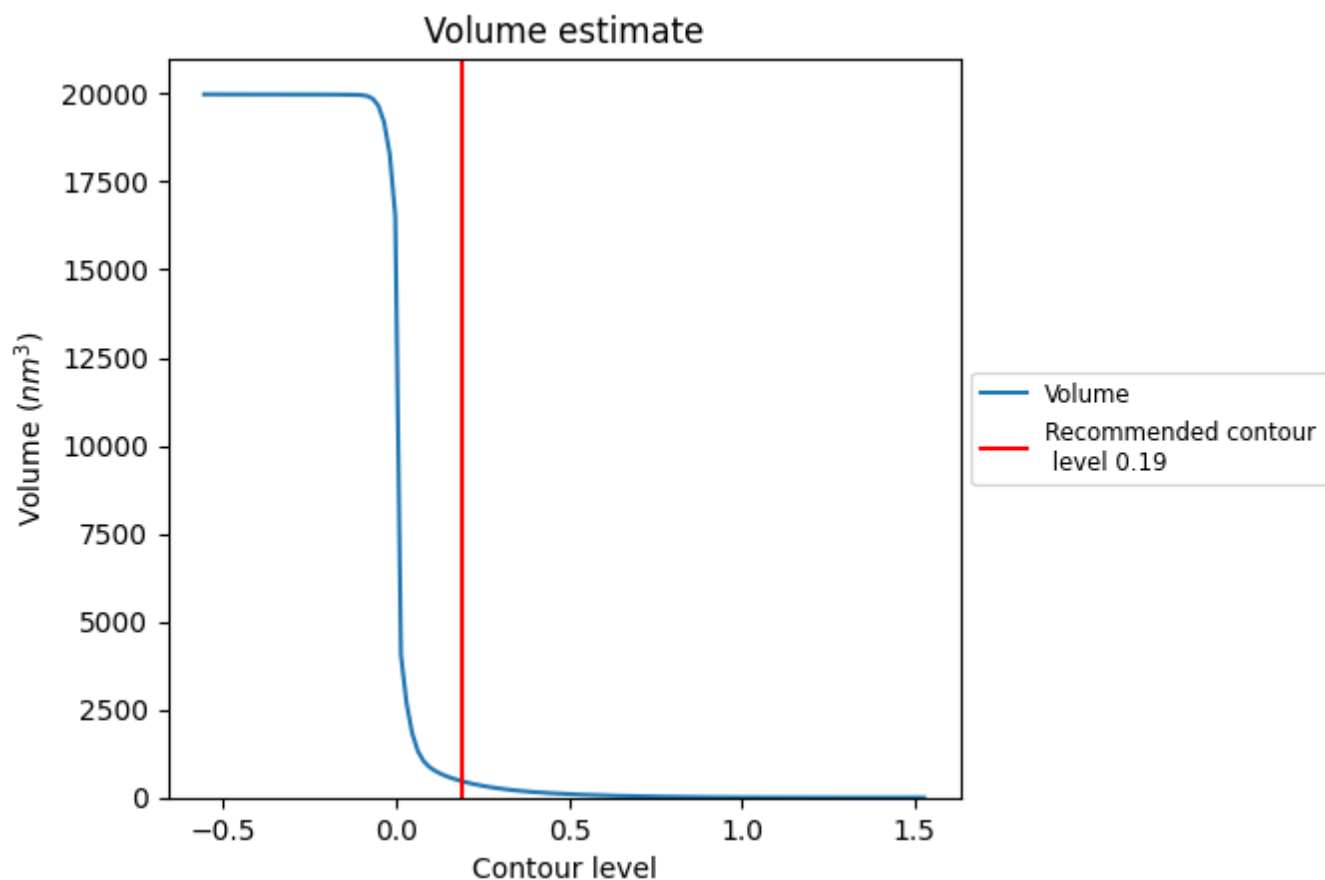
This section contains the results of statistical analysis of the map.

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.

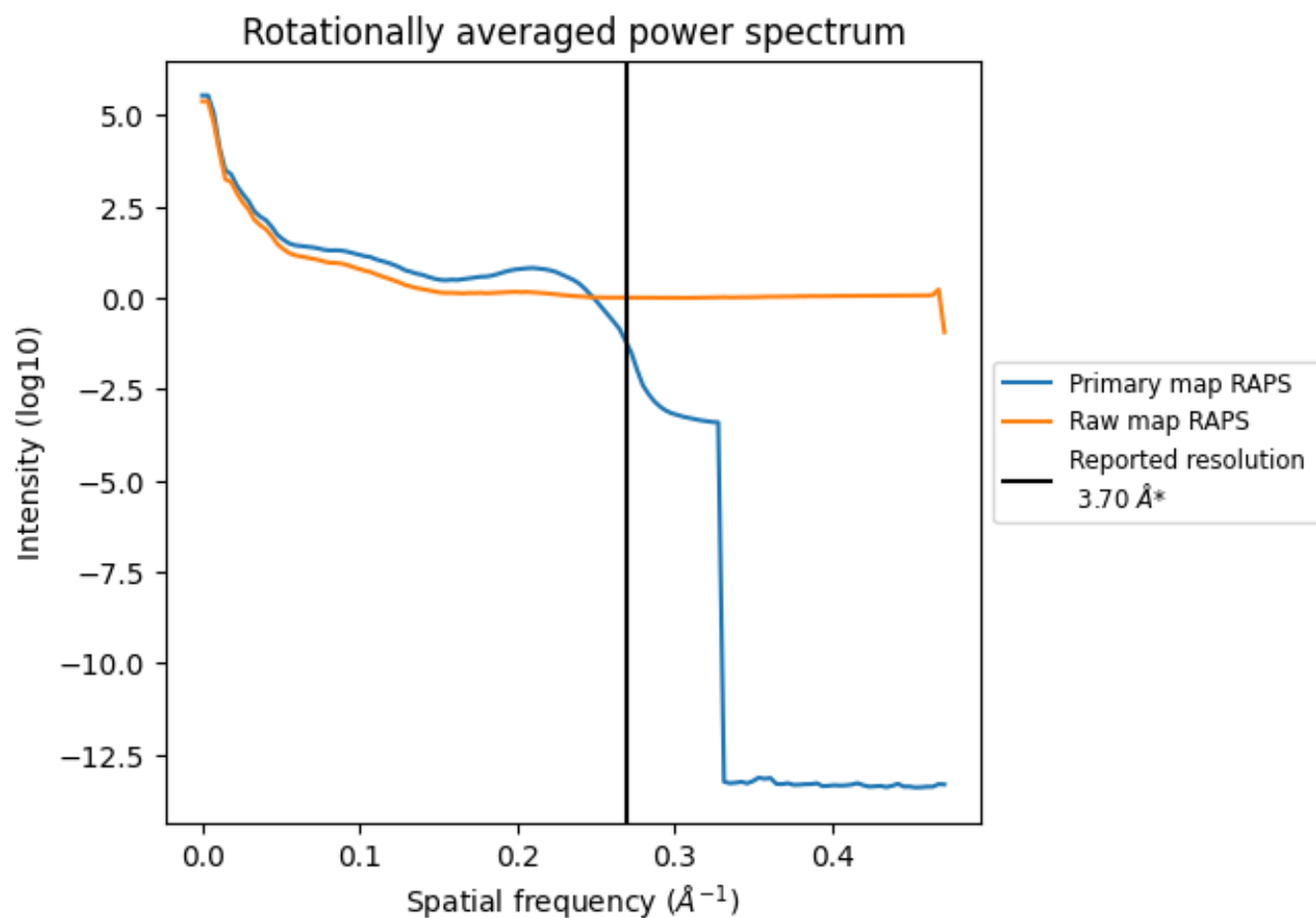
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 464 nm^3 ; this corresponds to an approximate mass of 419 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 ⓘ

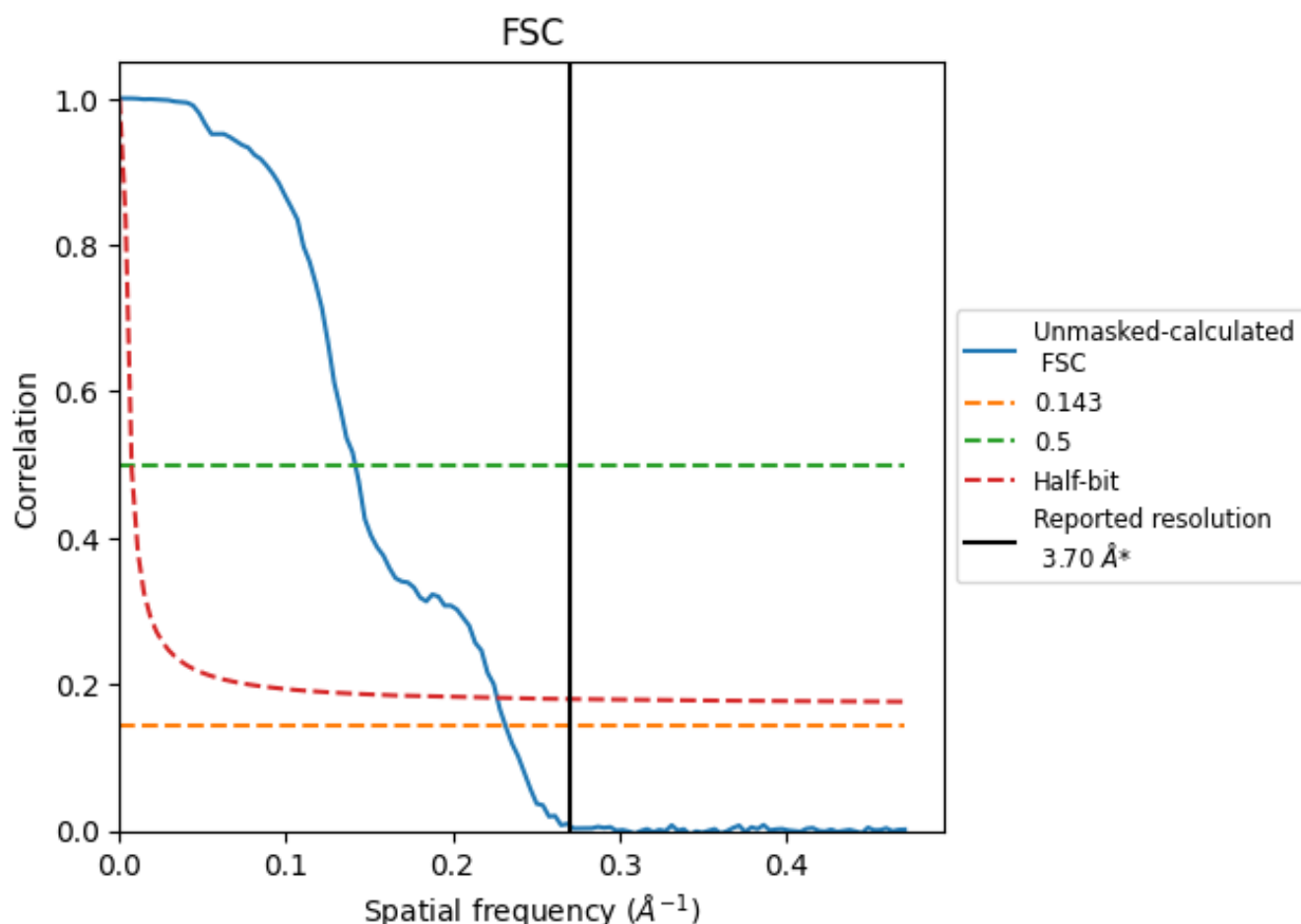


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

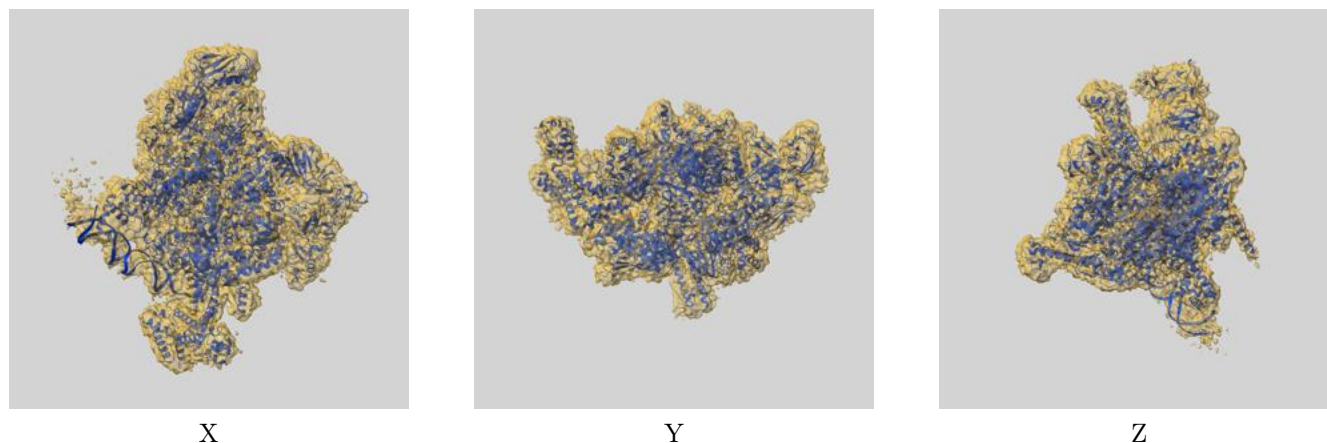
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.31	7.06	4.41

*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 4.31 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

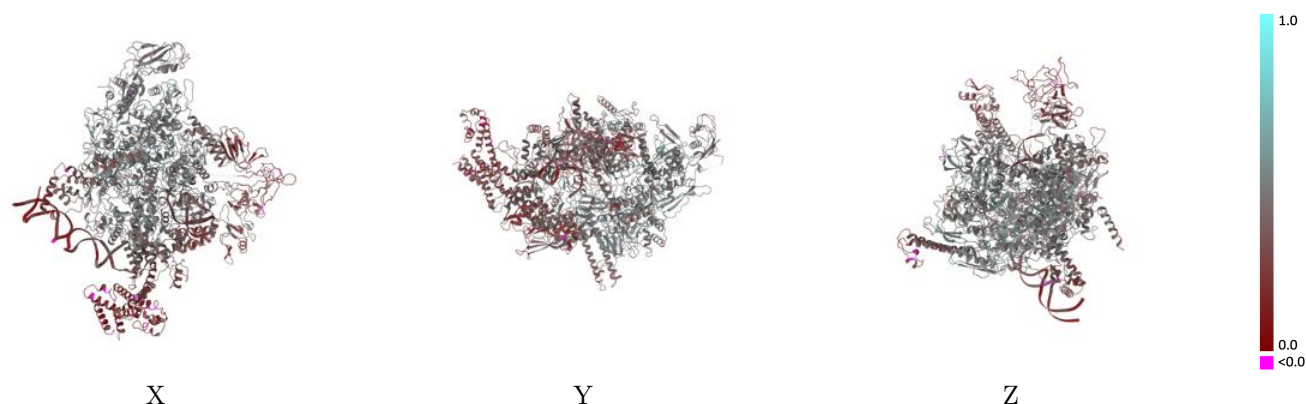
This section contains information regarding the fit between EMDB map EMD-23893 and PDB model 7MKE. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



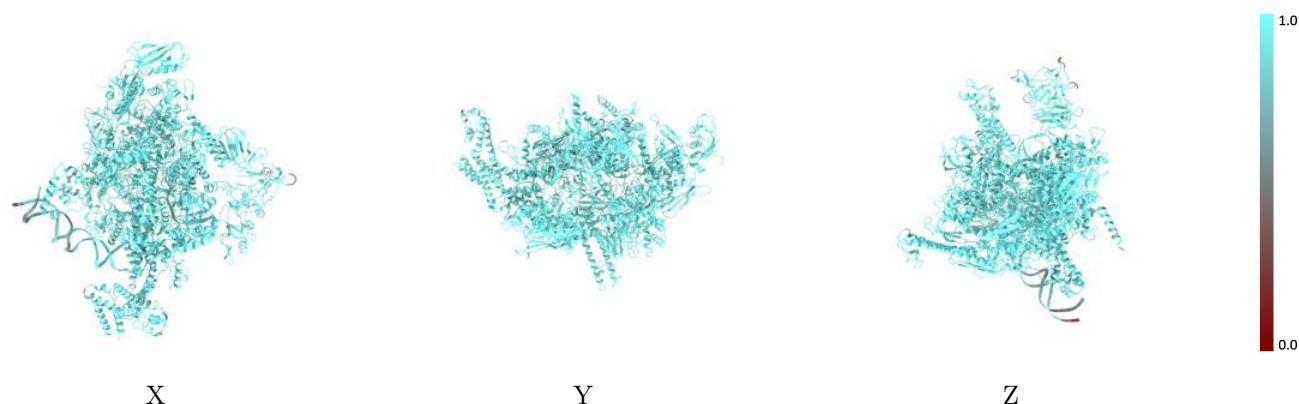
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



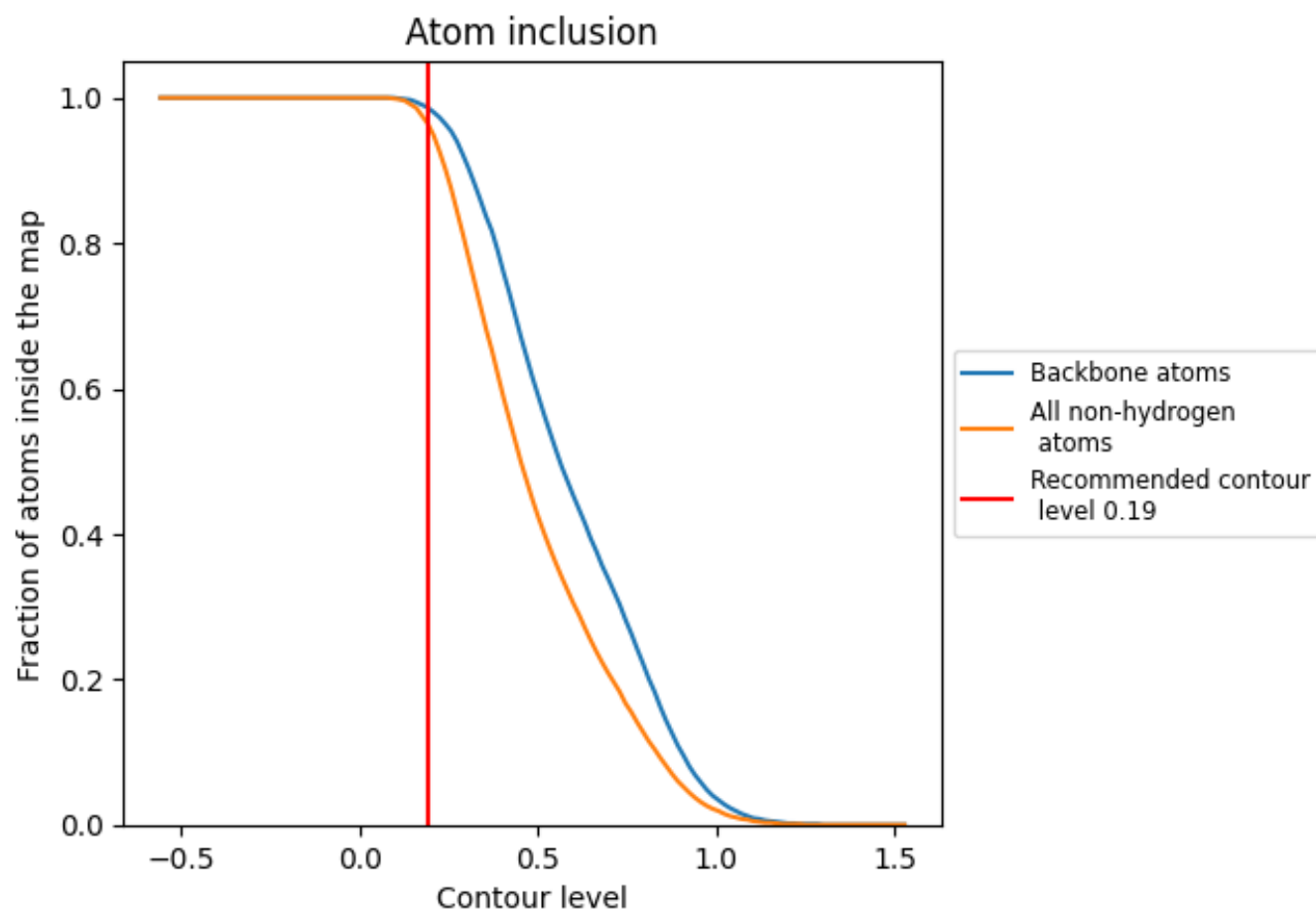
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9660</div>	<div><div></div>0.4120</div>
G	<div><div></div>0.9900</div>	<div><div></div>0.4850</div>
H	<div><div></div>0.9840</div>	<div><div></div>0.4530</div>
I	<div><div></div>0.9800</div>	<div><div></div>0.4440</div>
J	<div><div></div>0.9730</div>	<div><div></div>0.4250</div>
K	<div><div></div>0.9130</div>	<div><div></div>0.4300</div>
L	<div><div></div>0.9560</div>	<div><div></div>0.3010</div>
P	<div><div></div>0.8180</div>	<div><div></div>0.2570</div>
Q	<div><div></div>0.8640</div>	<div><div></div>0.2600</div>

1.0

0.0

<0.0