



Full wwPDB EM Validation Report ⓘ

May 14, 2025 – 05:07 AM EDT

PDB ID : 7MKD / pdb_00007mkd
EMDB ID : EMD-23892
Title : Cryo-EM structure of Escherichia coli RNA polymerase bound to lambda PR promoter DNA (class 1)
Authors : Saecker, R.M.; Darst, S.A.; Chen, J.
Deposited on : 2021-04-23
Resolution : 3.20 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

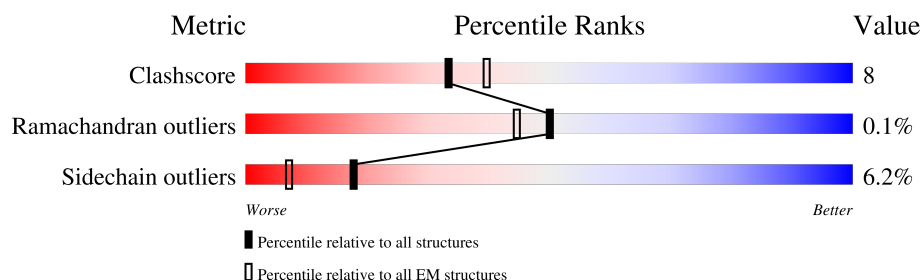
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	
1	R	329	
2	I	1342	
3	J	1407	
4	K	91	
5	L	613	
6	P	90	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	Q	90	<div> <div>61%</div> <div>14%</div> <div>24%</div> </div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 32393 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		
1	R	73	Total	C	N	O	S	0	0
			572	362	100	108	2		

- 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	1336	Total	C	N	O	S	0	0
			10386	6525	1852	1960	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	474	Total	C	N	O	S	0	0
			3847	2409	687	728	23		

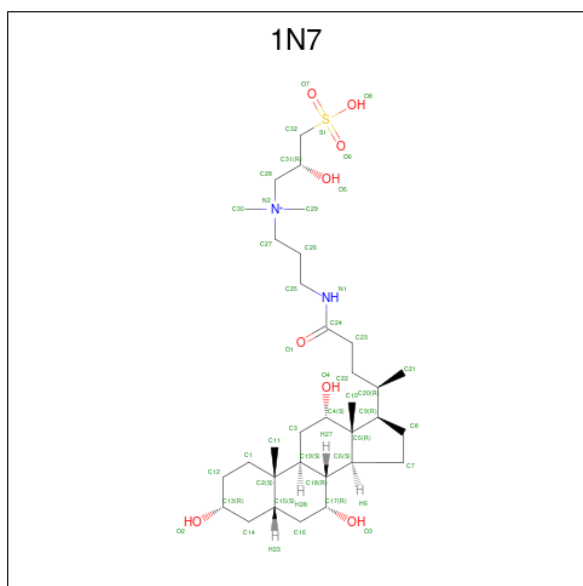
- Molecule 6 is a DNA chain called Nontemplate strand of lambda PR promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	68	Total	C	N	O	P	0	0
			1402	669	246	419	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	68	Total	C	N	O	P	0	0
			1386	660	261	397	68		

- Molecule 8 is CHAPSO (CCD ID: 1N7) (formula: $C_{32}H_{59}N_2O_8S$).



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	Q	1	Total	C	O	0
			27	24	3	

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

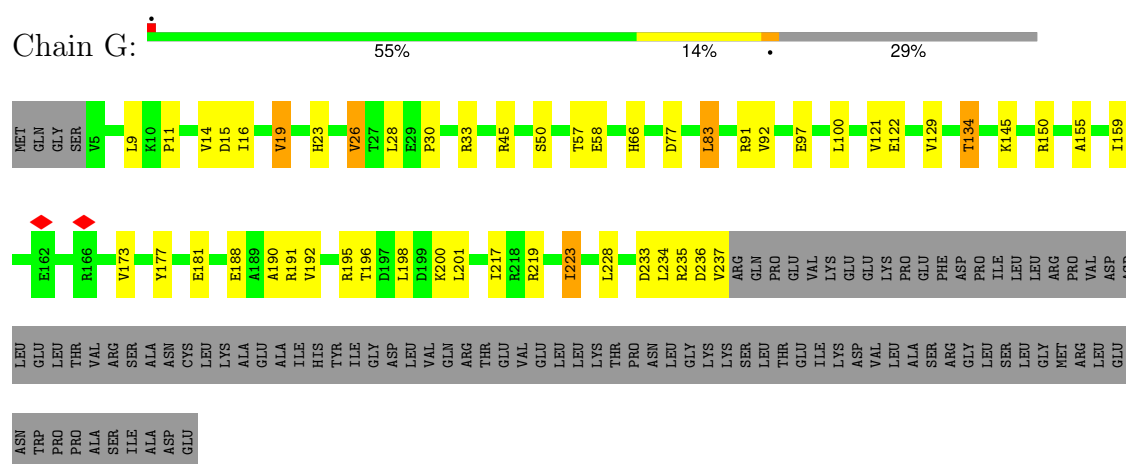
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

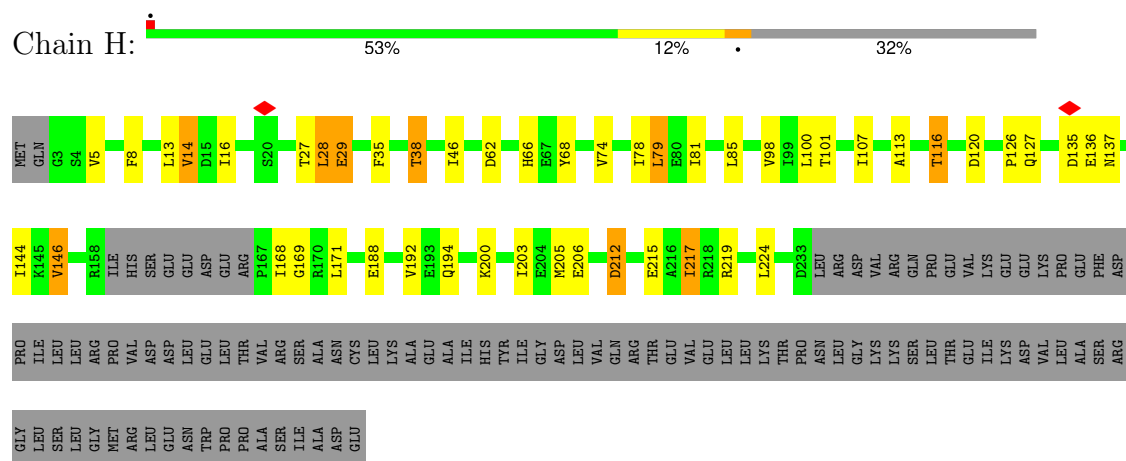
3 Residue-property plots

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.

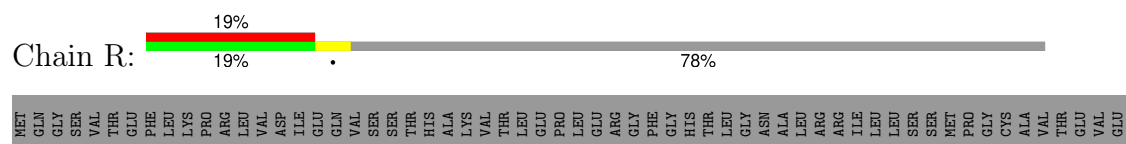
• Molecule 1: DNA-directed RNA polymerase subunit alpha



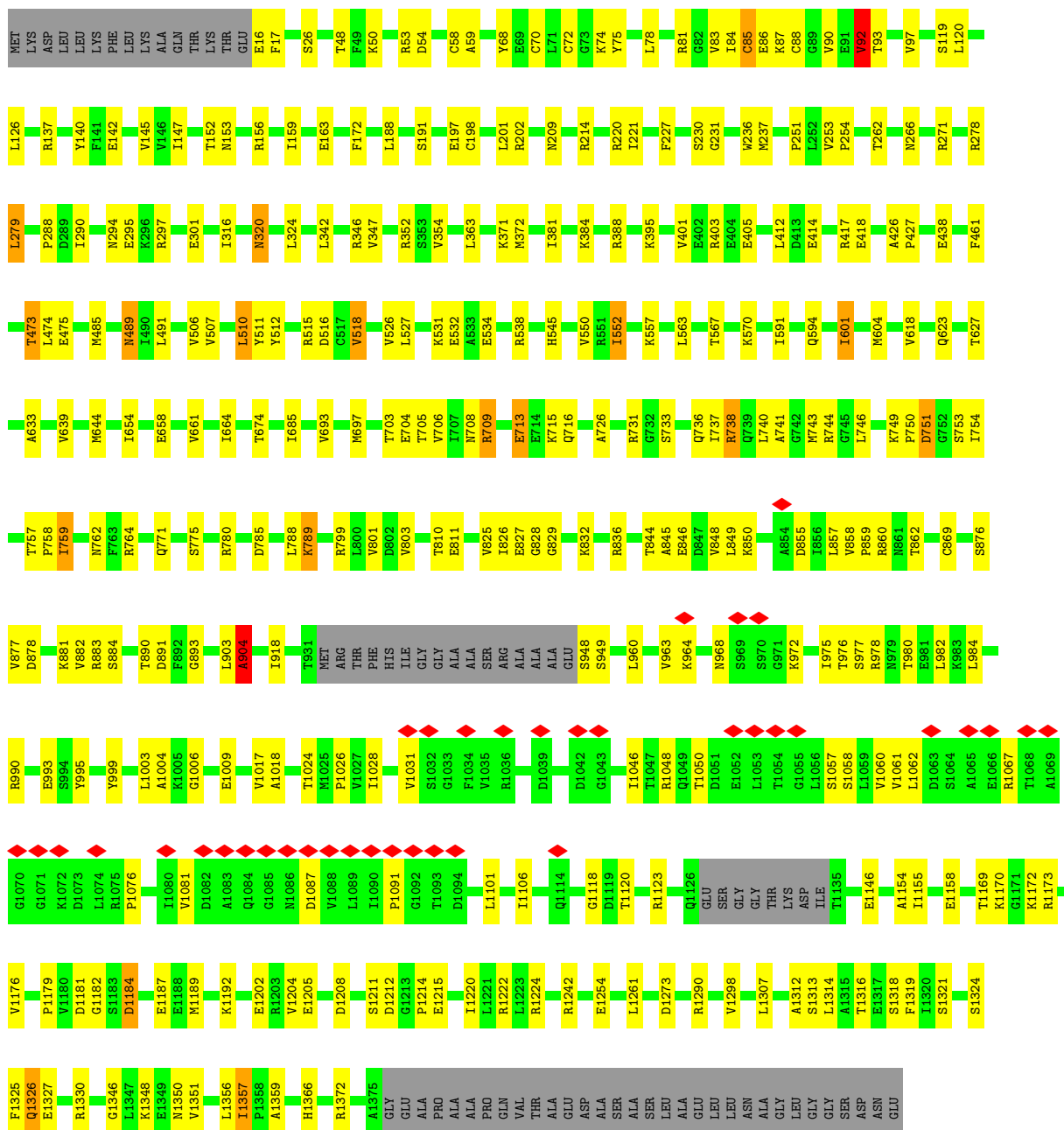
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha

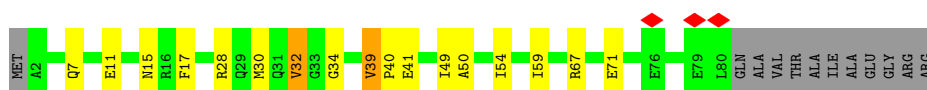


Chain J:  73% 21% 5%



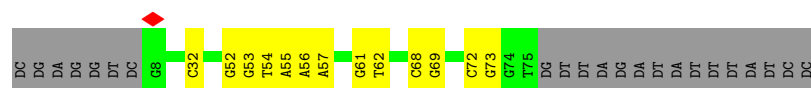
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:  68% 16% 13%



• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:  59% 17% 23%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	267577	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	3.045	Depositor
Minimum map value	-1.788	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	0.27	Depositor
Map size (\AA)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: 1N7, ZN, MG

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	0.38	0/1830	0.49	0/2481
1	H	0.47	0/1734	0.50	0/2349
1	R	0.12	0/579	0.32	0/784
2	I	0.44	5/10736 (0.0%)	0.49	3/14487 (0.0%)
3	J	0.44	0/10543	0.52	5/14236 (0.0%)
4	K	0.28	0/629	0.41	0/847
5	L	0.46	0/3897	0.64	3/5236 (0.1%)
6	P	0.30	0/1570	0.43	0/2425
7	Q	0.28	0/1556	0.41	0/2395
All	All	0.42	5/33074 (0.0%)	0.51	11/45240 (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
3	J	0	4
4	K	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1212	LEU	C-O	-9.00	1.12	1.24
2	I	1212	LEU	CA-C	-8.37	1.42	1.52
2	I	1211	ARG	C-O	-6.78	1.16	1.24
2	I	1210	ILE	C-O	-6.64	1.16	1.24
2	I	1210	ILE	CA-CB	-5.78	1.46	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	86	GLU	N-CA-C	9.98	121.92	111.14
3	J	713	GLU	N-CA-C	9.08	122.51	110.53
5	L	503	GLU	CA-C-N	8.21	130.10	119.84
5	L	503	GLU	C-N-CA	8.21	130.10	119.84
3	J	90	VAL	CB-CA-C	-7.97	101.31	110.96
2	I	1210	ILE	CB-CA-C	-7.80	98.50	111.29
3	J	90	VAL	N-CA-C	5.57	116.75	108.23
2	I	517	GLN	CA-C-N	-5.49	113.97	123.25
2	I	517	GLN	C-N-CA	-5.49	113.97	123.25
5	L	164	GLY	CA-C-O	-5.41	117.59	122.57
3	J	92	VAL	N-CA-C	5.28	115.37	107.51

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	235	ARG	Peptide
3	J	1184	ASP	Peptide
3	J	119	SER	Peptide
3	J	1325	PHE	Peptide
3	J	904	ALA	Peptide
4	K	32	VAL	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	29	0
1	H	1714	0	1748	36	0
1	R	572	0	602	9	0
2	I	10567	0	10585	149	0
3	J	10386	0	10605	206	0
4	K	627	0	634	10	0
5	L	3847	0	3922	70	0
6	P	1402	0	773	16	0
7	Q	1386	0	762	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	54	0	75	19	0
8	Q	27	0	37	10	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
All	All	32393	0	31578	518	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 8.

All (518) 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:Q:101:1N7:C19	8:Q:101:1N7:C3	1.82	1.58
8:I:1401:1N7:C3	8:I:1401:1N7:C19	1.82	1.56
8:I:1402:1N7:C3	8:I:1402:1N7:C19	1.83	1.56
3:J:74:LYS:HZ2	3:J:87:LYS:NZ	0.97	1.45
3:J:74:LYS:NZ	3:J:87:LYS:HZ1	1.03	1.42
3:J:74:LYS:NZ	3:J:87:LYS:NZ	1.65	1.16
3:J:137:ARG:HH12	5:L:91:ILE:HG13	1.19	1.06
5:L:470:MET:HE1	5:L:482:GLU:HG3	1.40	1.03
3:J:72:CYS:N	3:J:88:CYS:SG	2.33	0.97
3:J:137:ARG:NH1	5:L:91:ILE:HG13	1.81	0.96
1:H:101:THR:HG22	1:H:116:THR:HG21	1.46	0.96
1:H:101:THR:O	1:H:116:THR:HG22	1.67	0.94
3:J:74:LYS:CE	3:J:87:LYS:NZ	2.34	0.91
3:J:74:LYS:CE	3:J:87:LYS:HZ3	1.89	0.86
3:J:74:LYS:CD	3:J:87:LYS:NZ	2.43	0.81
5:L:470:MET:HE1	5:L:482:GLU:CG	2.11	0.79
3:J:74:LYS:CD	3:J:87:LYS:HZ3	1.96	0.79
5:L:584:ARG:NH1	7:Q:61:DG:N7	2.30	0.79
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.64	0.79
8:Q:101:1N7:C3	8:Q:101:1N7:C2	2.61	0.78
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.67	0.77
3:J:74:LYS:HD2	3:J:87:LYS:HZ3	1.48	0.77
3:J:1290:ARG:HG3	3:J:1290:ARG:HH11	1.49	0.76
3:J:751:ASP:OD1	3:J:751:ASP:N	2.17	0.76
2:I:528:ARG:NH2	2:I:576:SER:O	2.19	0.75
2:I:516:ASP:HA	2:I:761:GLN:NE2	2.02	0.74
8:I:1402:1N7:C3	8:I:1402:1N7:C2	2.64	0.74
3:J:74:LYS:HD2	3:J:87:LYS:NZ	2.03	0.73
1:G:11:PRO:HA	1:G:30:PRO:HD2	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:1401:1N7:C3	8:I:1401:1N7:C2	2.64	0.73
2:I:516:ASP:OD1	2:I:516:ASP:O	2.07	0.72
8:I:1402:1N7:H4	8:I:1402:1N7:H17	1.70	0.72
3:J:74:LYS:HZ2	3:J:87:LYS:HZ3	1.28	0.71
3:J:74:LYS:HZ3	3:J:87:LYS:HZ1	1.34	0.71
3:J:87:LYS:HD3	3:J:87:LYS:N	2.06	0.71
3:J:1351:VAL:HG23	3:J:1357:ILE:HD11	1.72	0.70
2:I:1072:ASN:HD21	2:I:1230:MET:HE1	1.56	0.70
1:G:33:ARG:NH2	1:G:196:THR:OG1	2.24	0.70
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.25	0.69
2:I:699:LEU:HB2	2:I:799:ASN:HD22	1.57	0.68
5:L:148:TYR:HD2	5:L:225:ARG:HH22	1.41	0.68
2:I:1210:ILE:HD11	2:I:1227:VAL:HG11	1.76	0.68
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.76	0.68
2:I:452:ARG:NH1	2:I:584:TYR:O	2.27	0.67
5:L:402:LEU:HD23	5:L:405:ILE:HD11	1.77	0.67
2:I:1088:ASP:OD1	2:I:1088:ASP:N	2.28	0.67
8:I:1401:1N7:C3	8:I:1401:1N7:C18	2.68	0.67
3:J:294:ASN:OD1	5:L:406:GLN:NE2	2.27	0.66
3:J:1003:LEU:HD23	3:J:1018:ALA:HB2	1.78	0.65
5:L:277:MET:HB2	5:L:362:ASN:HD22	1.62	0.65
2:I:103:VAL:HG12	2:I:117:ILE:HG22	1.76	0.65
3:J:799:ARG:NH1	3:J:1146:GLU:OE2	2.29	0.65
2:I:109:ALA:HB1	2:I:112:GLY:HA3	1.77	0.65
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.78	0.65
1:G:223:ILE:HD12	1:H:8:PHE:CZ	2.31	0.64
2:I:24:VAL:HG21	2:I:704:MET:HE1	1.79	0.64
3:J:140:TYR:O	3:J:297:ARG:NH1	2.31	0.63
2:I:1341:ASP:OD1	2:I:1341:ASP:N	2.29	0.63
3:J:644:MET:O	3:J:764:ARG:NH1	2.32	0.63
8:Q:101:1N7:C3	8:Q:101:1N7:C18	2.67	0.63
1:H:206:GLU:OE1	3:J:531:LYS:NZ	2.32	0.63
2:I:452:ARG:NH2	2:I:458:GLU:OE2	2.32	0.63
3:J:552:ILE:HD11	3:J:570:LYS:HG3	1.80	0.63
2:I:728:ASP:OD1	2:I:729:ALA:N	2.32	0.62
3:J:209:ASN:HA	3:J:214:ARG:HH21	1.64	0.62
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.81	0.62
1:G:57:THR:HG22	1:G:58:GLU:HG3	1.83	0.61
3:J:984:LEU:HB2	3:J:993:GLU:HB2	1.81	0.61
3:J:1307:LEU:HB2	3:J:1312:ALA:HB2	1.81	0.61
2:I:159:SER:OG	2:I:160:ASP:N	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1243:MET:HE1	3:J:371:LYS:HB2	1.83	0.61
7:Q:73:DG:H5"	1:R:294:ASN:HA	1.82	0.61
2:I:1070:HIS:NE2	2:I:1114:GLU:OE1	2.32	0.61
3:J:785:ASP:O	3:J:789:LYS:HB3	2.01	0.61
3:J:1290:ARG:HG3	3:J:1290:ARG:NH1	2.16	0.61
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.83	0.60
2:I:1210:ILE:HD11	2:I:1227:VAL:CG1	2.30	0.60
3:J:963:VAL:HG12	3:J:980:THR:HG23	1.83	0.60
1:G:50:SER:HB2	1:G:150:ARG:HD2	1.83	0.60
2:I:81:ASP:OD1	2:I:81:ASP:N	2.32	0.60
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.84	0.60
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.66	0.60
3:J:1062:LEU:O	3:J:1067:ARG:NH2	2.35	0.60
3:J:403:ARG:NH2	3:J:405:GLU:OE2	2.34	0.60
3:J:84:ILE:O	3:J:84:ILE:HG22	2.01	0.60
1:H:66:HIS:ND1	1:H:68:TYR:O	2.35	0.59
2:I:185:ASP:N	2:I:185:ASP:OD1	2.35	0.59
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.84	0.59
3:J:844:THR:OG1	3:J:860:ARG:O	2.16	0.59
1:H:101:THR:CG2	1:H:116:THR:HG21	2.27	0.59
2:I:241:LEU:HD11	2:I:246:LEU:HD21	1.84	0.59
3:J:775:SER:O	3:J:775:SER:OG	2.17	0.59
2:I:400:VAL:HG21	2:I:452:ARG:HD2	1.85	0.59
2:I:272:ARG:NH1	2:I:276:GLN:OE1	2.36	0.59
3:J:1172:LYS:HG2	3:J:1189:MET:HB3	1.84	0.59
5:L:600:HIS:ND1	5:L:601:PRO:O	2.34	0.59
2:I:131:THR:OG1	2:I:135:THR:O	2.20	0.59
2:I:962:GLU:O	2:I:966:ILE:HG12	2.03	0.59
1:G:97:GLU:OE1	1:G:145:LYS:NZ	2.34	0.58
2:I:1072:ASN:ND2	2:I:1111:GLN:OE1	2.34	0.58
3:J:197:GLU:OE2	3:J:220:ARG:NH2	2.35	0.58
5:L:593:LYS:HG3	5:L:596:ARG:HH21	1.67	0.58
2:I:1149:TYR:HB3	2:I:1159:VAL:HG11	1.85	0.58
3:J:845:ALA:HB2	3:J:883:ARG:HG3	1.84	0.58
5:L:346:GLN:NE2	5:L:350:GLU:OE2	2.37	0.58
8:Q:101:1N7:H4	8:Q:101:1N7:H17	1.85	0.58
3:J:74:LYS:NZ	3:J:87:LYS:HZ3	1.79	0.57
3:J:1076:PRO:HG2	3:J:1101:LEU:HB2	1.86	0.57
3:J:1158:GLU:OE1	3:J:1222:ARG:NH1	2.36	0.57
3:J:1357:ILE:HG22	3:J:1359:ALA:H	1.69	0.57
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1050:THR:HA	3:J:1057:SER:HA	1.86	0.57
3:J:749:LYS:HB3	3:J:750:PRO:CD	2.34	0.57
2:I:979:LEU:HD21	2:I:1000:LEU:HD12	1.85	0.57
8:I:1402:1N7:C3	8:I:1402:1N7:C18	2.67	0.57
2:I:192:ASP:OD2	2:I:436:ARG:NH2	2.36	0.57
2:I:1119:MET:HG2	2:I:1204:LEU:HD13	1.87	0.57
2:I:14:ASP:HB3	2:I:1157:GLN:HG2	1.87	0.56
2:I:1142:ARG:NH2	2:I:1164:PHE:O	2.38	0.56
5:L:555:GLU:OE2	5:L:593:LYS:NZ	2.38	0.56
5:L:586:ARG:NH1	6:P:25:DG:OP2	2.36	0.56
3:J:395:LYS:HE2	5:L:536:THR:HG21	1.87	0.56
3:J:948:SER:OG	3:J:949:SER:N	2.39	0.56
5:L:469:GLN:OE1	5:L:486:ARG:NH2	2.36	0.56
3:J:968:ASN:OD1	3:J:972:LYS:N	2.39	0.56
5:L:385:ARG:NH1	6:P:55:DG:N7	2.53	0.56
5:L:584:ARG:NH2	7:Q:61:DG:O6	2.39	0.56
2:I:836:LEU:HD21	2:I:921:PRO:HD3	1.87	0.56
3:J:381:ILE:HD11	3:J:412:LEU:HD13	1.88	0.56
3:J:475:GLU:OE2	4:K:28:ARG:NH2	2.39	0.56
2:I:726:TYR:OH	2:I:728:ASP:OD2	2.24	0.55
2:I:1245:ALA:HB2	3:J:372:MET:HG3	1.87	0.55
3:J:1120:THR:OG1	3:J:1123:ARG:NH1	2.38	0.55
3:J:1220:ILE:HG23	3:J:1224:ARG:HD2	1.88	0.55
2:I:942:ASP:OD1	2:I:942:ASP:N	2.32	0.55
2:I:1240:ASP:OD1	2:I:1240:ASP:N	2.35	0.55
1:H:168:ILE:N	1:H:169:GLY:HA2	2.22	0.55
1:G:219:ARG:O	1:G:223:ILE:HG22	2.07	0.55
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.89	0.55
5:L:596:ARG:HA	5:L:599:ARG:HD2	1.88	0.55
1:H:212:ASP:OD1	1:H:212:ASP:N	2.28	0.55
2:I:324:LYS:O	2:I:327:GLN:NE2	2.40	0.55
5:L:606:VAL:O	5:L:609:SER:OG	2.23	0.55
1:H:98:VAL:HG13	1:H:146:VAL:HG13	1.88	0.55
3:J:54:ASP:OD1	3:J:54:ASP:N	2.40	0.55
3:J:1176:VAL:HG22	3:J:1187:GLU:HB3	1.88	0.55
5:L:320:ILE:HG12	5:L:330:LEU:HD12	1.89	0.54
2:I:235:ASN:HB3	2:I:236:LYS:HG2	1.88	0.54
1:H:107:ILE:HG23	1:H:135:ASP:HB3	1.89	0.54
3:J:1046:ILE:HG22	3:J:1061:VAL:HG22	1.90	0.54
1:G:181:GLU:O	2:I:821:ARG:NH2	2.40	0.54
3:J:516:ASP:OD1	3:J:516:ASP:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:759:ILE:HG22	3:J:771:GLN:HG2	1.88	0.54
3:J:1060:VAL:HG22	3:J:1106:ILE:HG23	1.90	0.54
3:J:1048:ARG:NH2	3:J:1058:SER:O	2.40	0.53
5:L:94:THR:O	5:L:94:THR:HG23	2.07	0.53
1:G:134:THR:O	1:G:134:THR:OG1	2.24	0.53
5:L:215:GLU:HA	5:L:218:ARG:HE	1.73	0.53
3:J:48:THR:O	3:J:50:LYS:N	2.40	0.53
2:I:617:ALA:HB2	2:I:650:VAL:HG21	1.90	0.53
3:J:74:LYS:HZ3	3:J:87:LYS:NZ	1.90	0.53
2:I:551:HIS:ND1	2:I:553:THR:OG1	2.40	0.53
3:J:388:ARG:NH2	3:J:414:GLU:OE1	2.42	0.53
2:I:75:LEU:HD11	2:I:127:ILE:HD11	1.91	0.53
3:J:251:PRO:HG2	5:L:507:MET:HE1	1.90	0.53
1:H:100:LEU:HD12	1:H:144:ILE:HD11	1.90	0.53
3:J:271:ARG:HH11	3:J:316:ILE:HD12	1.74	0.53
3:J:762:ASN:OD1	3:J:762:ASN:N	2.40	0.53
3:J:1314:LEU:HD11	3:J:1326:GLN:HG2	1.90	0.53
1:G:19:VAL:HG13	1:G:23:HIS:HB3	1.91	0.53
5:L:517:SER:O	5:L:517:SER:OG	2.26	0.53
3:J:527:LEU:HD22	3:J:532:GLU:HG2	1.91	0.53
3:J:1031:VAL:HG12	3:J:1091:PRO:HD3	1.91	0.52
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.91	0.52
2:I:941:LYS:NZ	2:I:949:GLU:OE2	2.26	0.52
3:J:417:ARG:HG2	3:J:418:GLU:HG2	1.91	0.52
3:J:137:ARG:HH21	3:J:159:ILE:HD12	1.73	0.52
3:J:884:SER:OG	3:J:1254:GLU:OE1	2.22	0.52
7:Q:61:DG:H2'	7:Q:62:DT:H71	1.90	0.52
2:I:699:LEU:HB2	2:I:799:ASN:ND2	2.25	0.52
3:J:74:LYS:CD	3:J:87:LYS:HZ2	2.23	0.52
5:L:277:MET:HB2	5:L:362:ASN:ND2	2.23	0.52
2:I:1341:ASP:HB3	3:J:17:PHE:HA	1.92	0.52
8:I:1401:1N7:C19	8:I:1401:1N7:C4	2.84	0.52
2:I:196:VAL:HG12	2:I:206:ALA:HA	1.92	0.52
2:I:560:PRO:O	3:J:780:ARG:NH2	2.39	0.52
2:I:1268:GLN:OE1	3:J:352:ARG:NH1	2.37	0.52
3:J:848:VAL:HB	3:J:858:VAL:HG22	1.91	0.52
3:J:1326:GLN:HG3	3:J:1327:GLU:H	1.74	0.52
1:H:120:ASP:OD1	1:H:120:ASP:N	2.38	0.52
3:J:733:SER:OG	3:J:736:GLN:OE1	2.28	0.52
3:J:1321:SER:HA	3:J:1348:LYS:HD2	1.92	0.52
2:I:596:ASP:N	2:I:596:ASP:OD1	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:749:LYS:CB	3:J:750:PRO:CD	2.87	0.51
2:I:735:LYS:HA	2:I:748:ILE:HG22	1.92	0.51
2:I:808:ASN:H	3:J:633:ALA:HB2	1.75	0.51
3:J:876:SER:HA	3:J:990:ARG:HH21	1.75	0.51
6:P:43:DG:H8	6:P:43:DG:H5"	1.75	0.51
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.93	0.51
3:J:1181:ASP:OD1	3:J:1181:ASP:N	2.40	0.51
5:L:547:VAL:HG21	5:L:607:LEU:HD21	1.93	0.51
2:I:730:SER:O	2:I:730:SER:OG	2.29	0.51
8:Q:101:1N7:C3	8:Q:101:1N7:H1	2.40	0.51
3:J:749:LYS:HG2	3:J:750:PRO:HD3	1.93	0.51
1:H:74:VAL:HG11	1:H:81:ILE:HD11	1.93	0.51
2:I:646:SER:OG	2:I:647:ARG:N	2.44	0.51
8:I:1402:1N7:C3	8:I:1402:1N7:C11	2.89	0.51
5:L:105:MET:HE3	5:L:388:ILE:HG13	1.92	0.51
1:G:192:VAL:HG11	1:G:198:LEU:HD12	1.93	0.50
2:I:114:VAL:HG21	2:I:117:ILE:HG23	1.93	0.50
3:J:810:THR:HG22	3:J:893:GLY:HA3	1.93	0.50
2:I:720:ARG:NH2	2:I:745:GLU:OE2	2.44	0.50
5:L:322:MET:O	5:L:324:LYS:NZ	2.38	0.50
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.94	0.50
5:L:161:LEU:HG	5:L:162:ILE:HG23	1.93	0.50
5:L:313:ASP:O	5:L:317:ASN:N	2.39	0.50
1:G:83:LEU:HD23	2:I:694:ARG:HE	1.76	0.50
2:I:18:ARG:O	2:I:1156:ARG:NH1	2.45	0.50
2:I:714:VAL:O	2:I:767:GLN:NE2	2.45	0.50
2:I:1109:ILE:HD12	3:J:644:MET:HE1	1.92	0.50
6:P:63:DG:H2'	6:P:64:DT:H71	1.94	0.50
1:G:16:ILE:HG12	1:G:26:VAL:HG12	1.93	0.50
2:I:68:LEU:HD22	2:I:492:MET:HE3	1.93	0.50
3:J:803:VAL:HA	3:J:1313:SER:HB3	1.94	0.50
3:J:75:TYR:CD2	3:J:85:CYS:HB2	2.47	0.49
3:J:1024:THR:HG22	3:J:1026:PRO:HD3	1.94	0.49
2:I:576:SER:OG	2:I:577:VAL:N	2.42	0.49
1:H:107:ILE:HG12	1:H:135:ASP:HA	1.94	0.49
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.94	0.49
5:L:297:MET:HE3	5:L:302:PHE:HB2	1.94	0.49
3:J:92:VAL:O	3:J:92:VAL:HG22	2.12	0.49
3:J:708:ASN:OD1	3:J:708:ASN:N	2.39	0.49
3:J:709:ARG:O	3:J:709:ARG:CD	2.60	0.49
3:J:977:SER:OG	3:J:980:THR:OG1	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1076:PRO:HB2	3:J:1101:LEU:HD12	1.94	0.49
3:J:1173:ARG:NH2	3:J:1192:LYS:O	2.46	0.49
5:L:511:ILE:HG21	5:L:522:PHE:HE2	1.77	0.49
1:G:28:LEU:HD22	1:G:201:LEU:HD23	1.95	0.49
3:J:346:ARG:NH1	7:Q:32:DC:OP1	2.46	0.49
3:J:511:TYR:CZ	3:J:515:ARG:HD2	2.48	0.49
5:L:432:THR:HG21	6:P:53:DA:C5	2.48	0.49
3:J:744:ARG:HG3	3:J:759:ILE:HG13	1.95	0.48
4:K:50:ALA:O	4:K:54:ILE:HG12	2.13	0.48
1:H:205:MET:HE1	1:H:217:ILE:HG13	1.95	0.48
8:I:1401:1N7:C3	8:I:1401:1N7:H1	2.43	0.48
3:J:749:LYS:HB3	3:J:750:PRO:HD2	1.94	0.48
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.96	0.48
5:L:110:LEU:HD21	5:L:385:ARG:HD2	1.93	0.48
2:I:228:VAL:HG23	2:I:337:PHE:HB2	1.95	0.48
3:J:198:CYS:SG	3:J:202:ARG:NH2	2.86	0.48
3:J:1211:SER:OG	3:J:1212:ASP:N	2.47	0.48
3:J:473:THR:OG1	3:J:474:LEU:N	2.47	0.48
3:J:438:GLU:HG3	3:J:485:MET:HE1	1.94	0.48
1:H:135:ASP:OD1	1:H:135:ASP:N	2.47	0.48
3:J:832:LYS:HE3	3:J:1242:ARG:HD2	1.95	0.48
3:J:850:LYS:HE2	3:J:857:LEU:HD13	1.96	0.48
2:I:487:LEU:HD23	2:I:487:LEU:H	1.79	0.47
3:J:1154:ALA:N	3:J:1214:PRO:O	2.41	0.47
1:R:285:THR:OG1	1:R:286:GLU:N	2.47	0.47
3:J:510:LEU:HD13	3:J:601:ILE:HD11	1.95	0.47
3:J:1081:VAL:HG12	3:J:1087:ASP:HA	1.96	0.47
4:K:32:VAL:O	4:K:34:GLY:N	2.43	0.47
2:I:444:ASP:OD1	2:I:444:ASP:N	2.48	0.47
3:J:557:LYS:HB3	3:J:563:LEU:HD12	1.96	0.47
1:H:127:GLN:N	1:H:127:GLN:OE1	2.47	0.47
2:I:244:GLU:OE1	2:I:244:GLU:N	2.44	0.47
3:J:53:ARG:HA	3:J:54:ASP:HA	1.59	0.47
3:J:227:PHE:HZ	3:J:237:MET:HE3	1.79	0.47
3:J:363:LEU:HD23	3:J:618:VAL:HG13	1.96	0.47
3:J:741:ALA:O	3:J:762:ASN:ND2	2.47	0.47
3:J:1205:GLU:N	3:J:1208:ASP:OD2	2.47	0.47
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.96	0.47
8:Q:101:1N7:C3	8:Q:101:1N7:C1	2.92	0.47
3:J:709:ARG:O	3:J:709:ARG:HD3	2.15	0.47
3:J:836:ARG:HG3	3:J:869:CYS:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:THR:HG22	1:H:116:THR:CG2	2.33	0.47
2:I:453:ILE:HD13	2:I:530:ILE:HD12	1.97	0.47
5:L:584:ARG:HG2	5:L:585:GLU:N	2.30	0.47
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.97	0.46
5:L:600:HIS:CE1	1:R:259:ASP:HA	2.50	0.46
2:I:322:LEU:O	2:I:326:SER:OG	2.27	0.46
2:I:611:GLU:OE2	2:I:637:ARG:NH2	2.48	0.46
2:I:966:ILE:HD12	8:I:1402:1N7:H24	1.96	0.46
3:J:120:LEU:HD23	3:J:120:LEU:HA	1.66	0.46
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.39	0.46
2:I:1122:LYS:HG2	2:I:1229:TYR:CZ	2.50	0.46
3:J:1028:ILE:HB	3:J:1118:GLY:HA2	1.96	0.46
5:L:558:VAL:HG23	5:L:576:VAL:HG11	1.96	0.46
2:I:8:LYS:HE2	2:I:1164:PHE:CE1	2.51	0.46
2:I:478:ARG:O	2:I:478:ARG:NH1	2.41	0.46
2:I:545:PHE:CE1	3:J:788:LEU:HD13	2.50	0.46
2:I:990:ASP:OD1	2:I:990:ASP:N	2.48	0.46
1:H:192:VAL:O	1:H:194:GLN:N	2.49	0.46
2:I:421:SER:OG	2:I:424:ASP:OD2	2.32	0.46
8:I:1401:1N7:C3	8:I:1401:1N7:C1	2.93	0.46
3:J:661:VAL:HG12	3:J:685:ILE:HD11	1.97	0.46
2:I:1213:TYR:HA	2:I:1220:GLN:HA	1.98	0.46
3:J:1356:LEU:HD23	3:J:1356:LEU:HA	1.79	0.46
7:Q:56:DA:H2"	7:Q:57:DA:C8	2.51	0.46
1:R:290:LEU:HG	1:R:300:LEU:HD22	1.97	0.46
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.24	0.46
2:I:201:ARG:HG3	2:I:202:ARG:H	1.81	0.45
4:K:15:ASN:C	4:K:17:PHE:H	2.24	0.45
2:I:484:LEU:HB2	2:I:485:ASP:HA	1.98	0.45
2:I:731:ARG:NH2	2:I:962:GLU:OE1	2.49	0.45
2:I:756:TYR:H	2:I:766:ASN:HB2	1.81	0.45
1:H:35:PHE:HA	1:H:38:THR:HG23	1.97	0.45
3:J:279:LEU:HG	3:J:295:GLU:HG3	1.99	0.45
3:J:1169:THR:OG1	6:P:76:DT:OP1	2.34	0.45
2:I:23:ASP:OD1	2:I:23:ASP:N	2.49	0.45
8:I:1402:1N7:H14	8:I:1402:1N7:H29	1.77	0.45
3:J:1169:THR:OG1	3:J:1170:LYS:N	2.48	0.45
6:P:41:DC:H2"	6:P:42:DT:H72	1.99	0.45
1:H:46:ILE:HD11	1:H:224:LEU:HD13	1.97	0.45
3:J:1004:ALA:N	3:J:1017:VAL:O	2.48	0.45
5:L:320:ILE:HA	5:L:327:SER:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:VAL:HG22	1:G:15:ASP:H	1.82	0.45
2:I:11:ILE:O	2:I:1149:TYR:OH	2.24	0.45
2:I:75:LEU:HD13	2:I:75:LEU:HA	1.80	0.45
3:J:846:GLU:HG2	3:J:881:LYS:HB3	1.98	0.45
3:J:982:LEU:N	3:J:995:TYR:O	2.44	0.45
1:R:250:ASP:HB3	1:R:253:LEU:HD22	1.99	0.45
1:R:254:LEU:HD23	1:R:254:LEU:H	1.81	0.45
2:I:1210:ILE:CD1	2:I:1227:VAL:HG21	2.46	0.45
3:J:715:LYS:HE3	3:J:715:LYS:HB3	1.75	0.45
3:J:1330:ARG:HE	3:J:1330:ARG:HB2	1.56	0.45
1:H:203:ILE:HG21	1:H:217:ILE:HD11	1.98	0.45
3:J:1179:PRO:HB2	3:J:1182:GLY:H	1.82	0.45
3:J:1215:GLU:OE1	3:J:1215:GLU:N	2.50	0.45
6:P:31:DT:H2"	6:P:32:DA:C8	2.52	0.45
1:H:215:GLU:OE2	1:H:219:ARG:NE	2.43	0.45
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.98	0.45
3:J:709:ARG:O	3:J:709:ARG:CG	2.62	0.45
2:I:104:ILE:HD11	2:I:116:ASP:HB3	1.98	0.44
2:I:146:VAL:HG21	2:I:513:GLN:HE21	1.82	0.44
3:J:87:LYS:HD3	3:J:87:LYS:H	1.78	0.44
3:J:534:GLU:O	3:J:538:ARG:HG2	2.17	0.44
2:I:1106:ARG:HH21	3:J:731:ARG:HH22	1.64	0.44
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.51	0.44
3:J:654:ILE:O	3:J:658:GLU:HG2	2.18	0.44
7:Q:54:DT:H2"	7:Q:55:DA:C8	2.52	0.44
2:I:1210:ILE:HD11	2:I:1227:VAL:HG21	2.00	0.44
3:J:230:SER:OG	3:J:231:GLY:N	2.50	0.44
3:J:705:THR:HG21	3:J:716:GLN:HE21	1.81	0.44
5:L:166:VAL:HG22	5:L:260:ARG:HD3	2.00	0.44
8:Q:101:1N7:C3	8:Q:101:1N7:C11	2.96	0.44
2:I:937:ASP:N	2:I:937:ASP:OD1	2.49	0.44
2:I:1107:MET:HG2	3:J:740:LEU:HD21	1.99	0.44
3:J:826:ILE:HG22	3:J:828:GLY:H	1.82	0.44
5:L:451:ARG:NH2	6:P:45:DC:OP1	2.49	0.44
1:R:259:ASP:O	1:R:310:ARG:NH2	2.51	0.44
3:J:964:LYS:O	3:J:976:THR:N	2.46	0.44
8:Q:101:1N7:H1	8:Q:101:1N7:H3	1.99	0.44
3:J:827:GLU:HG3	3:J:829:GLY:H	1.82	0.44
4:K:67:ARG:O	4:K:71:GLU:HG2	2.18	0.44
5:L:262:VAL:HG12	5:L:264:LYS:H	1.82	0.44
1:G:234:LEU:HD23	1:G:234:LEU:HA	1.87	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:960:LEU:HD21	2:I:1028:LYS:HB3	2.00	0.44
5:L:511:ILE:HG21	5:L:522:PHE:CE2	2.52	0.44
2:I:582:ASN:OD1	2:I:583:GLU:N	2.46	0.44
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.99	0.44
7:Q:68:DC:H2"	7:Q:69:DG:C8	2.53	0.44
2:I:529:ARG:HD3	2:I:572:ILE:HG22	1.99	0.43
2:I:714:VAL:HB	2:I:787:PRO:HD2	2.00	0.43
2:I:1072:ASN:ND2	2:I:1230:MET:HE1	2.28	0.43
2:I:1212:LEU:HD21	2:I:1227:VAL:HG11	2.00	0.43
3:J:855:ASP:OD1	3:J:855:ASP:N	2.51	0.43
5:L:597:LYS:HB2	5:L:597:LYS:HE3	1.78	0.43
2:I:118:LYS:HB3	2:I:118:LYS:HE2	1.82	0.43
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.50	0.43
3:J:1356:LEU:O	3:J:1366:HIS:NE2	2.51	0.43
2:I:479:LEU:HD23	2:I:479:LEU:HA	1.88	0.43
3:J:507:VAL:HG12	3:J:601:ILE:HG21	2.01	0.43
3:J:1006:GLY:N	3:J:1009:GLU:OE1	2.42	0.43
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	2.00	0.43
1:H:79:LEU:HA	1:H:79:LEU:HD13	1.78	0.43
2:I:483:ASP:OD1	2:I:483:ASP:N	2.49	0.43
3:J:16:GLU:HB3	3:J:17:PHE:H	1.57	0.43
3:J:708:ASN:HA	3:J:713:GLU:HA	2.00	0.43
3:J:1357:ILE:HD13	3:J:1357:ILE:HA	1.71	0.43
5:L:584:ARG:NH2	7:Q:61:DG:N7	2.66	0.43
7:Q:72:DC:P	1:R:298:LYS:HD3	2.58	0.43
1:G:217:ILE:HD13	1:G:217:ILE:HA	1.83	0.43
3:J:83:VAL:O	3:J:83:VAL:HG13	2.18	0.43
3:J:1061:VAL:HG12	3:J:1067:ARG:HH21	1.82	0.43
6:P:22:DC:H5"	1:R:264:VAL:HG12	2.00	0.43
3:J:384:LYS:HB2	3:J:384:LYS:HE2	1.87	0.43
1:G:91:ARG:NH2	1:G:122:GLU:OE2	2.41	0.43
2:I:402:ARG:HD2	2:I:402:ARG:HA	1.81	0.43
3:J:511:TYR:O	3:J:515:ARG:HG3	2.19	0.43
6:P:17:DC:H2"	6:P:18:DC:C5	2.54	0.43
8:Q:101:1N7:C3	8:Q:101:1N7:H17	2.49	0.43
2:I:693:LEU:HB2	2:I:829:THR:O	2.18	0.43
8:I:1402:1N7:C3	8:I:1402:1N7:H1	2.49	0.43
3:J:693:VAL:HG21	3:J:743:MET:HE3	1.99	0.43
1:G:155:ALA:O	1:G:159:ILE:HG22	2.19	0.43
3:J:527:LEU:HB2	3:J:550:VAL:HG12	2.01	0.43
3:J:664:ILE:HD13	3:J:664:ILE:HA	1.92	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:224:LEU:HA	5:L:224:LEU:HD23	1.78	0.43
5:L:426:LYS:HB3	5:L:426:LYS:HE2	1.76	0.43
6:P:43:DG:H5"	6:P:43:DG:C8	2.51	0.43
1:G:100:LEU:HD21	1:G:121:VAL:HG11	2.01	0.42
2:I:590:PRO:HG3	2:I:605:TYR:CE2	2.54	0.42
2:I:912:ASP:OD1	2:I:912:ASP:N	2.39	0.42
3:J:68:TYR:HA	3:J:92:VAL:CG2	2.47	0.42
3:J:68:TYR:CA	3:J:92:VAL:HG23	2.48	0.42
3:J:518:VAL:HG13	3:J:709:ARG:HB3	2.00	0.42
5:L:258:GLN:HE21	5:L:258:GLN:HB3	1.48	0.42
3:J:859:PRO:HD2	3:J:862:THR:HG21	2.02	0.42
1:G:66:HIS:HD2	2:I:929:ILE:HG22	1.83	0.42
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.18	0.42
3:J:978:ARG:HD3	3:J:999:TYR:HB2	1.99	0.42
5:L:315:TRP:HZ2	5:L:341:LEU:HD11	1.84	0.42
8:Q:101:1N7:H33	8:Q:101:1N7:H10	1.53	0.42
2:I:1210:ILE:HD11	2:I:1227:VAL:CG2	2.50	0.42
1:G:9:LEU:HD23	1:G:9:LEU:HA	1.81	0.42
2:I:250:THR:HA	2:I:268:ARG:HA	2.00	0.42
2:I:545:PHE:HE1	3:J:788:LEU:HD13	1.85	0.42
8:I:1401:1N7:H30	8:I:1401:1N7:H36	1.64	0.42
3:J:320:ASN:OD1	3:J:320:ASN:N	2.38	0.42
5:L:463:LEU:HD21	5:L:498:LEU:HD21	2.00	0.42
5:L:573:LEU:HG	5:L:584:ARG:HB2	2.00	0.42
2:I:998:LEU:HB3	2:I:1015:ALA:HB2	2.00	0.42
3:J:147:ILE:HG22	3:J:188:LEU:HG	2.02	0.42
5:L:101:TYR:HE2	5:L:388:ILE:HD11	1.84	0.42
5:L:235:ILE:HD12	5:L:235:ILE:HA	1.68	0.42
5:L:312:SER:OG	5:L:313:ASP:N	2.52	0.42
1:G:191:ARG:HD3	1:G:191:ARG:HA	1.84	0.42
3:J:1314:LEU:HD21	3:J:1326:GLN:HB3	2.00	0.42
2:I:53:PHE:O	2:I:57:PHE:HB2	2.19	0.42
2:I:101:ARG:NH2	2:I:119:GLU:OE2	2.45	0.42
3:J:1273:ASP:OD1	3:J:1273:ASP:N	2.48	0.42
3:J:1318:SER:OG	3:J:1319:PHE:N	2.52	0.42
2:I:690:VAL:CG2	2:I:1236:ASN:HB3	2.50	0.42
5:L:387:VAL:HG13	5:L:408:GLY:HA3	2.01	0.42
1:G:45:ARG:HE	1:H:38:THR:HG22	1.85	0.42
1:H:8:PHE:N	1:H:8:PHE:CD1	2.87	0.42
1:H:29:GLU:HB3	1:H:200:LYS:HG3	2.02	0.42
3:J:221:ILE:HD13	3:J:221:ILE:HA	1.94	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:355:ILE:HD13	5:L:355:ILE:HA	1.94	0.42
1:H:85:LEU:HA	1:H:85:LEU:HD23	1.84	0.41
2:I:788:SER:O	2:I:788:SER:OG	2.38	0.41
2:I:826:ASP:OD1	2:I:829:THR:OG1	2.30	0.41
3:J:278:ARG:HH11	3:J:278:ARG:HD2	1.75	0.41
3:J:811:GLU:OE1	3:J:890:THR:OG1	2.25	0.41
5:L:163:THR:HG23	5:L:262:VAL:HG22	2.02	0.41
8:I:1401:1N7:H1	8:I:1401:1N7:H3	2.01	0.41
3:J:142:GLU:OE2	5:L:103:ARG:NH2	2.53	0.41
3:J:511:TYR:OH	3:J:515:ARG:NH1	2.53	0.41
5:L:512:GLY:N	5:L:517:SER:OG	2.48	0.41
3:J:156:ARG:NH2	3:J:191:SER:OG	2.38	0.41
3:J:704:GLU:O	3:J:706:VAL:HG13	2.20	0.41
5:L:90:GLU:OE1	5:L:90:GLU:HA	2.19	0.41
5:L:441:ARG:HH12	5:L:454:VAL:HG21	1.86	0.41
2:I:1132:LEU:HD13	2:I:1141:LEU:HD11	2.01	0.41
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.21	0.41
3:J:489:ASN:OD1	3:J:489:ASN:N	2.54	0.41
3:J:591:ILE:HD11	3:J:604:MET:HA	2.02	0.41
5:L:141:ILE:O	5:L:145:LEU:HG	2.21	0.41
7:Q:52:DG:H4'	7:Q:53:DG:OP1	2.21	0.41
2:I:772:SER:OG	2:I:775:GLU:OE1	2.36	0.41
2:I:1222:GLU:H	2:I:1222:GLU:HG3	1.60	0.41
3:J:26:SER:HB3	3:J:236:TRP:CZ2	2.56	0.41
4:K:59:ILE:HD13	4:K:59:ILE:HA	1.94	0.41
5:L:315:TRP:CE2	5:L:316:PHE:HB2	2.55	0.41
5:L:315:TRP:HE1	5:L:341:LEU:HD21	1.85	0.41
6:P:22:DC:H2''	6:P:23:DG:C8	2.55	0.41
1:G:190:ALA:HB2	1:G:200:LYS:HB2	2.03	0.41
1:H:66:HIS:CE1	1:H:68:TYR:HB2	2.55	0.41
2:I:1210:ILE:CD1	2:I:1227:VAL:CG2	2.99	0.41
3:J:152:THR:OG1	3:J:153:ASN:N	2.54	0.41
3:J:978:ARG:NH2	3:J:1202:GLU:OE2	2.53	0.41
5:L:161:LEU:HD12	5:L:265:GLN:HE22	1.86	0.41
1:G:192:VAL:HG13	1:G:195:ARG:HB3	2.01	0.41
1:H:62:ASP:OD1	1:H:62:ASP:N	2.53	0.41
2:I:397:LEU:N	2:I:398:SER:HA	2.36	0.41
3:J:58:CYS:SG	3:J:59:ALA:N	2.92	0.41
4:K:30:MET:HE1	4:K:49:ILE:HB	2.03	0.41
4:K:41:GLU:H	4:K:41:GLU:HG2	1.72	0.41
2:I:638:SER:HB2	2:I:645:PHE:HE2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:288:PRO:HB3	5:L:377:LYS:HG3	2.02	0.41
3:J:878:ASP:OD2	3:J:990:ARG:HA	2.21	0.41
5:L:314:THR:O	5:L:318:ALA:HB3	2.21	0.41
1:H:136:GLU:HG2	1:H:137:ASN:H	1.86	0.41
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.37	0.41
2:I:347:ILE:HD13	2:I:347:ILE:HA	1.81	0.41
2:I:799:ASN:OD1	2:I:799:ASN:N	2.46	0.41
2:I:805:MET:HE3	2:I:805:MET:HB2	1.76	0.41
2:I:843:THR:OG1	2:I:846:GLY:O	2.36	0.41
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.97	0.41
3:J:623:GLN:O	3:J:627:THR:HG22	2.21	0.41
1:G:223:ILE:HD11	1:H:35:PHE:CZ	2.56	0.40
2:I:800:MET:HB3	2:I:800:MET:HE2	1.58	0.40
8:I:1401:1N7:H4	8:I:1401:1N7:H17	2.03	0.40
3:J:697:MET:SD	3:J:741:ALA:HB3	2.61	0.40
3:J:1372:ARG:HD3	3:J:1372:ARG:HA	1.94	0.40
6:P:32:DA:C8	6:P:32:DA:H5'	2.55	0.40
1:G:66:HIS:CD2	2:I:929:ILE:HG22	2.57	0.40
1:H:14:VAL:HB	1:H:28:LEU:HB3	2.02	0.40
1:H:78:ILE:HD13	1:H:78:ILE:HA	1.90	0.40
2:I:210:LEU:HD23	2:I:210:LEU:HA	1.90	0.40
2:I:813:GLU:HB2	3:J:461:PHE:CD2	2.56	0.40
2:I:1103:VAL:HG21	2:I:1112:ILE:HD11	2.02	0.40
3:J:87:LYS:N	3:J:87:LYS:CD	2.73	0.40
5:L:300:LYS:O	5:L:304:THR:N	2.53	0.40
6:P:40:DT:H2''	6:P:41:DC:C6	2.56	0.40
1:H:113:ALA:HB2	1:H:126:PRO:HB3	2.02	0.40
2:I:538:LEU:HD13	2:I:543:ALA:HB2	2.02	0.40
8:I:1402:1N7:C3	8:I:1402:1N7:H17	2.39	0.40
8:I:1402:1N7:H10	8:I:1402:1N7:H34	1.33	0.40
3:J:83:VAL:O	3:J:83:VAL:CG1	2.69	0.40
3:J:737:ILE:HG22	3:J:738:ARG:H	1.87	0.40
6:P:18:DC:H2''	6:P:19:DG:C8	2.56	0.40
2:I:844:LYS:H	2:I:844:LYS:HG2	1.75	0.40
2:I:974:ARG:HD3	2:I:974:ARG:HA	1.92	0.40
2:I:1210:ILE:H	2:I:1210:ILE:HG12	1.51	0.40
3:J:726:ALA:HB2	3:J:737:ILE:HD11	2.04	0.40
4:K:7:GLN:O	4:K:11:GLU:HG2	2.22	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%)	204 (88%)	27 (12%)	0	100	100
1	H	219/329 (67%)	207 (94%)	12 (6%)	0	100	100
1	R	71/329 (22%)	69 (97%)	2 (3%)	0	100	100
2	I	1338/1342 (100%)	1224 (92%)	114 (8%)	0	100	100
3	J	1330/1407 (94%)	1249 (94%)	79 (6%)	2 (0%)	44	75
4	K	77/91 (85%)	68 (88%)	9 (12%)	0	100	100
5	L	466/613 (76%)	441 (95%)	25 (5%)	0	100	100
All	All	3732/4440 (84%)	3462 (93%)	268 (7%)	2 (0%)	50	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	1326	GLN
3	J	904	ALA

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%)	187 (93%)	14 (7%)	12	42
1	H	190/286 (66%)	175 (92%)	15 (8%)	10	38
1	R	65/286 (23%)	65 (100%)	0	100	100
2	I	1155/1157 (100%)	1076 (93%)	79 (7%)	13	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	1119/1168 (96%)	1062 (95%)	57 (5%)	20	53
4	K	67/75 (89%)	66 (98%)	1 (2%)	60	81
5	L	421/540 (78%)	389 (92%)	32 (8%)	11	39
All	All	3218/3798 (85%)	3020 (94%)	198 (6%)	18	47

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	19	VAL
1	G	26	VAL
1	G	77	ASP
1	G	83	LEU
1	G	92	VAL
1	G	129	VAL
1	G	134	THR
1	G	173	VAL
1	G	177	TYR
1	G	188	GLU
1	G	223	ILE
1	G	233	ASP
1	G	236	ASP
1	G	237	VAL
1	H	5	VAL
1	H	13	LEU
1	H	14	VAL
1	H	16	ILE
1	H	27	THR
1	H	28	LEU
1	H	29	GLU
1	H	38	THR
1	H	79	LEU
1	H	116	THR
1	H	146	VAL
1	H	171	LEU
1	H	188	GLU
1	H	212	ASP
1	H	217	ILE
2	I	11	ILE
2	I	17	LYS
2	I	18	ARG
2	I	29	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	46	GLN
2	I	56	VAL
2	I	60	GLN
2	I	75	LEU
2	I	79	VAL
2	I	90	VAL
2	I	104	ILE
2	I	122	VAL
2	I	131	THR
2	I	170	VAL
2	I	185	ASP
2	I	216	THR
2	I	239	MET
2	I	292	ILE
2	I	322	LEU
2	I	354	ASP
2	I	365	GLU
2	I	377	THR
2	I	448	LEU
2	I	456	VAL
2	I	471	VAL
2	I	483	ASP
2	I	491	ASP
2	I	493	ILE
2	I	538	LEU
2	I	550	VAL
2	I	553	THR
2	I	563	THR
2	I	575	LEU
2	I	600	THR
2	I	610	GLU
2	I	615	VAL
2	I	623	LEU
2	I	630	VAL
2	I	660	VAL
2	I	663	VAL
2	I	727	VAL
2	I	748	ILE
2	I	753	LEU
2	I	764	CYS
2	I	766	ASN
2	I	785	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	791	LEU
2	I	799	ASN
2	I	800	MET
2	I	802	VAL
2	I	817	LEU
2	I	823	VAL
2	I	856	ASN
2	I	888	THR
2	I	901	LEU
2	I	953	LEU
2	I	963	GLU
2	I	966	ILE
2	I	971	LEU
2	I	979	LEU
2	I	992	LEU
2	I	998	LEU
2	I	1046	VAL
2	I	1056	VAL
2	I	1060	ILE
2	I	1088	ASP
2	I	1157	GLN
2	I	1161	LEU
2	I	1210	ILE
2	I	1217	THR
2	I	1222	GLU
2	I	1225	VAL
2	I	1240	ASP
2	I	1254	VAL
2	I	1291	LEU
2	I	1293	VAL
2	I	1327	LEU
2	I	1332	SER
2	I	1341	ASP
3	J	70	CYS
3	J	78	LEU
3	J	81	ARG
3	J	85	CYS
3	J	92	VAL
3	J	93	THR
3	J	97	VAL
3	J	126	LEU
3	J	145	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	163	GLU
3	J	172	PHE
3	J	201	LEU
3	J	279	LEU
3	J	290	ILE
3	J	301	GLU
3	J	320	ASN
3	J	324	LEU
3	J	342	LEU
3	J	347	VAL
3	J	354	VAL
3	J	401	VAL
3	J	473	THR
3	J	489	ASN
3	J	506	VAL
3	J	510	LEU
3	J	518	VAL
3	J	526	VAL
3	J	545	HIS
3	J	552	ILE
3	J	567	THR
3	J	594	GLN
3	J	601	ILE
3	J	639	VAL
3	J	674	THR
3	J	703	THR
3	J	709	ARG
3	J	738	ARG
3	J	751	ASP
3	J	753	SER
3	J	754	ILE
3	J	757	THR
3	J	759	ILE
3	J	789	LYS
3	J	825	VAL
3	J	849	LEU
3	J	877	VAL
3	J	882	VAL
3	J	891	ASP
3	J	903	LEU
3	J	918	ILE
3	J	1155	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	1204	VAL
3	J	1261	LEU
3	J	1298	VAL
3	J	1316	THR
3	J	1324	SER
3	J	1357	ILE
4	K	39	VAL
5	L	89	SER
5	L	91	ILE
5	L	93	ARG
5	L	98	VAL
5	L	166	VAL
5	L	215	GLU
5	L	216	LEU
5	L	219	GLU
5	L	223	GLU
5	L	224	LEU
5	L	232	ARG
5	L	235	ILE
5	L	236	LYS
5	L	244	THR
5	L	246	GLN
5	L	252	LEU
5	L	254	GLU
5	L	255	VAL
5	L	258	GLN
5	L	260	ARG
5	L	452	ILE
5	L	457	ILE
5	L	504	PRO
5	L	505	ILE
5	L	511	ILE
5	L	569	THR
5	L	581	ASP
5	L	584	ARG
5	L	585	GLU
5	L	587	ILE
5	L	591	GLU
5	L	595	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	66	HIS
1	G	147	GLN
1	H	37	HIS
2	I	273	HIS
2	I	387	ASN
2	I	517	GLN
2	I	684	ASN
2	I	808	ASN
2	I	856	ASN
2	I	1129	ASN
2	I	1264	GLN
3	J	465	GLN
3	J	469	HIS
3	J	720	ASN
3	J	771	GLN
4	K	31	GLN
5	L	258	GLN
5	L	294	GLN
5	L	400	GLN
5	L	464	ASN
1	R	268	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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	1402	-	30,30,46	5.25	17 (56%)	47,48,72	2.60	19 (40%)
8	1N7	I	1401	-	30,30,46	5.17	16 (53%)	47,48,72	2.36	13 (27%)
8	1N7	Q	101	-	30,30,46	5.16	16 (53%)	47,48,72	2.39	14 (29%)

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	1402	-	-	7/7/72/92	0/4/4/4
8	1N7	I	1401	-	-	5/7/72/92	0/4/4/4
8	1N7	Q	101	-	-	7/7/72/92	0/4/4/4

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	1402	1N7	C3-C19	18.12	1.83	1.53
8	I	1401	1N7	C3-C19	17.57	1.82	1.53
8	Q	101	1N7	C3-C19	17.49	1.82	1.53
8	I	1402	1N7	C3-C4	12.69	1.73	1.53
8	Q	101	1N7	C3-C4	11.95	1.72	1.53
8	I	1401	1N7	C3-C4	11.86	1.72	1.53
8	I	1401	1N7	C5-C4	-9.97	1.39	1.54
8	Q	101	1N7	C5-C4	-9.59	1.39	1.54
8	Q	101	1N7	C2-C19	-9.39	1.39	1.56
8	I	1401	1N7	C2-C19	-9.13	1.40	1.56
8	I	1402	1N7	C5-C4	-9.06	1.40	1.54
8	I	1402	1N7	C2-C19	-8.81	1.40	1.56
8	Q	101	1N7	C8-C7	6.23	1.71	1.54
8	I	1401	1N7	C8-C7	6.10	1.70	1.54
8	I	1402	1N7	C8-C7	6.03	1.70	1.54
8	I	1402	1N7	C5-C6	-4.96	1.47	1.55
8	Q	101	1N7	C5-C6	-4.85	1.47	1.55
8	I	1401	1N7	C5-C6	-4.75	1.47	1.55
8	I	1402	1N7	C18-C6	-4.65	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	1401	1N7	C18-C6	-4.44	1.45	1.53
8	I	1401	1N7	O4-C4	-4.42	1.36	1.43
8	Q	101	1N7	C18-C6	-4.39	1.45	1.53
8	Q	101	1N7	O4-C4	-4.22	1.36	1.43
8	I	1402	1N7	O4-C4	-4.00	1.37	1.43
8	I	1402	1N7	C2-C15	3.90	1.61	1.55
8	Q	101	1N7	C7-C6	3.29	1.61	1.54
8	I	1401	1N7	C14-C15	-3.28	1.48	1.53
8	I	1401	1N7	C7-C6	3.19	1.60	1.54
8	I	1402	1N7	C5-C9	3.12	1.60	1.55
8	Q	101	1N7	C2-C15	3.07	1.60	1.55
8	Q	101	1N7	C14-C15	-3.04	1.49	1.53
8	I	1402	1N7	C7-C6	3.04	1.60	1.54
8	I	1401	1N7	C2-C15	2.90	1.59	1.55
8	I	1402	1N7	C14-C15	-2.89	1.49	1.53
8	Q	101	1N7	C5-C9	2.65	1.59	1.55
8	I	1401	1N7	C5-C9	2.49	1.59	1.55
8	I	1401	1N7	C20-C9	-2.47	1.50	1.54
8	I	1402	1N7	O2-C13	-2.46	1.36	1.43
8	I	1401	1N7	O2-C13	-2.41	1.36	1.43
8	Q	101	1N7	O2-C13	-2.31	1.36	1.43
8	I	1402	1N7	C1-C2	2.18	1.57	1.54
8	Q	101	1N7	C14-C13	2.17	1.55	1.52
8	I	1401	1N7	C16-C15	2.12	1.57	1.53
8	I	1402	1N7	C16-C15	2.11	1.57	1.53
8	I	1401	1N7	C14-C13	2.09	1.55	1.52
8	I	1402	1N7	C20-C9	-2.06	1.50	1.54
8	Q	101	1N7	C16-C15	2.06	1.57	1.53
8	Q	101	1N7	C20-C9	-2.04	1.50	1.54
8	I	1402	1N7	C10-C5	2.03	1.57	1.54

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1402	1N7	C9-C5-C4	-8.54	109.99	117.67
8	Q	101	1N7	C9-C5-C4	-7.58	110.85	117.67
8	I	1401	1N7	C9-C5-C4	-6.79	111.56	117.67
8	I	1401	1N7	C6-C5-C4	6.03	112.92	107.42
8	I	1401	1N7	C7-C6-C18	-5.80	110.40	118.36
8	I	1401	1N7	C19-C3-C4	-5.71	106.83	114.29
8	Q	101	1N7	C6-C5-C4	5.50	112.44	107.42
8	Q	101	1N7	C3-C19-C2	-5.26	108.36	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Q	101	1N7	C7-C6-C18	-5.19	111.23	118.36
8	I	1402	1N7	C5-C9-C20	-5.19	113.19	119.48
8	I	1402	1N7	C9-C5-C6	5.18	105.31	100.11
8	Q	101	1N7	C19-C3-C4	-4.97	107.79	114.29
8	Q	101	1N7	C5-C9-C20	-4.67	113.82	119.48
8	I	1402	1N7	C3-C19-C2	-4.47	109.16	113.70
8	I	1402	1N7	C7-C6-C18	-4.44	112.27	118.36
8	I	1401	1N7	C3-C19-C2	-4.02	109.62	113.70
8	I	1402	1N7	C19-C18-C17	-4.01	106.81	111.86
8	I	1402	1N7	C8-C9-C5	3.88	107.30	103.54
8	I	1401	1N7	C21-C20-C9	-3.74	107.26	112.88
8	I	1401	1N7	C5-C9-C20	-3.57	115.16	119.48
8	I	1402	1N7	C14-C13-C12	-3.45	106.41	110.62
8	I	1402	1N7	C6-C5-C4	3.44	110.56	107.42
8	I	1402	1N7	C8-C7-C6	-3.24	98.81	105.14
8	I	1402	1N7	C3-C19-C18	-3.21	106.14	110.89
8	I	1401	1N7	C6-C18-C17	-3.03	107.83	111.85
8	Q	101	1N7	C19-C18-C17	-2.96	108.13	111.86
8	Q	101	1N7	C3-C19-C18	-2.92	106.58	110.89
8	I	1401	1N7	C3-C19-C18	-2.74	106.84	110.89
8	I	1402	1N7	C19-C2-C15	2.71	112.28	108.51
8	Q	101	1N7	C9-C5-C6	2.68	102.80	100.11
8	I	1402	1N7	C11-C2-C19	-2.66	107.60	111.18
8	I	1401	1N7	C19-C18-C17	-2.58	108.61	111.86
8	I	1402	1N7	C16-C17-C18	-2.58	108.68	111.50
8	Q	101	1N7	C14-C13-C12	-2.51	107.56	110.62
8	I	1401	1N7	C14-C13-C12	-2.43	107.65	110.62
8	Q	101	1N7	C6-C18-C17	-2.30	108.80	111.85
8	I	1401	1N7	C21-C20-C22	-2.29	106.79	110.34
8	Q	101	1N7	C21-C20-C9	-2.26	109.49	112.88
8	I	1402	1N7	C1-C2-C15	2.24	110.95	107.75
8	I	1402	1N7	C21-C20-C9	-2.19	109.60	112.88
8	Q	101	1N7	C16-C15-C2	-2.19	110.33	112.66
8	I	1401	1N7	C8-C7-C6	-2.13	100.97	105.14
8	Q	101	1N7	C1-C12-C13	-2.08	107.72	110.48
8	I	1402	1N7	C19-C3-C4	-2.07	111.58	114.29
8	I	1402	1N7	C6-C18-C17	-2.03	109.15	111.85
8	I	1402	1N7	C21-C20-C22	-2.01	107.23	110.34

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1401	1N7	C21-C20-C9-C5
8	Q	101	1N7	C21-C20-C9-C5
8	I	1401	1N7	C21-C20-C9-C8
8	I	1402	1N7	C21-C20-C9-C8
8	I	1402	1N7	C21-C20-C9-C5
8	Q	101	1N7	C21-C20-C9-C8
8	I	1401	1N7	C22-C20-C9-C5
8	I	1402	1N7	C22-C20-C9-C5
8	Q	101	1N7	C22-C20-C9-C5
8	Q	101	1N7	C21-C20-C22-C23
8	I	1401	1N7	C22-C20-C9-C8
8	Q	101	1N7	C22-C20-C9-C8
8	Q	101	1N7	C9-C20-C22-C23
8	I	1402	1N7	C22-C20-C9-C8
8	I	1402	1N7	C21-C20-C22-C23
8	Q	101	1N7	C20-C22-C23-C24
8	I	1402	1N7	C9-C20-C22-C23
8	I	1401	1N7	C21-C20-C22-C23
8	I	1402	1N7	C20-C22-C23-C24

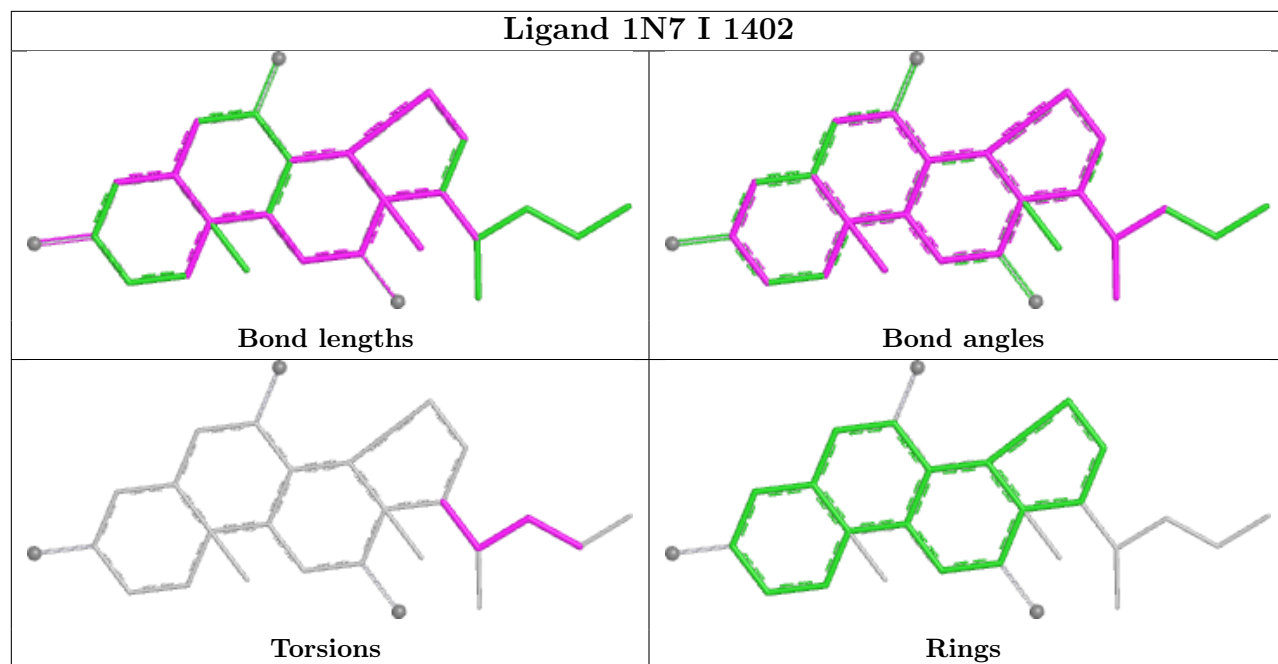
There are no ring outliers.

3 monomers are involved in 29 short contacts:

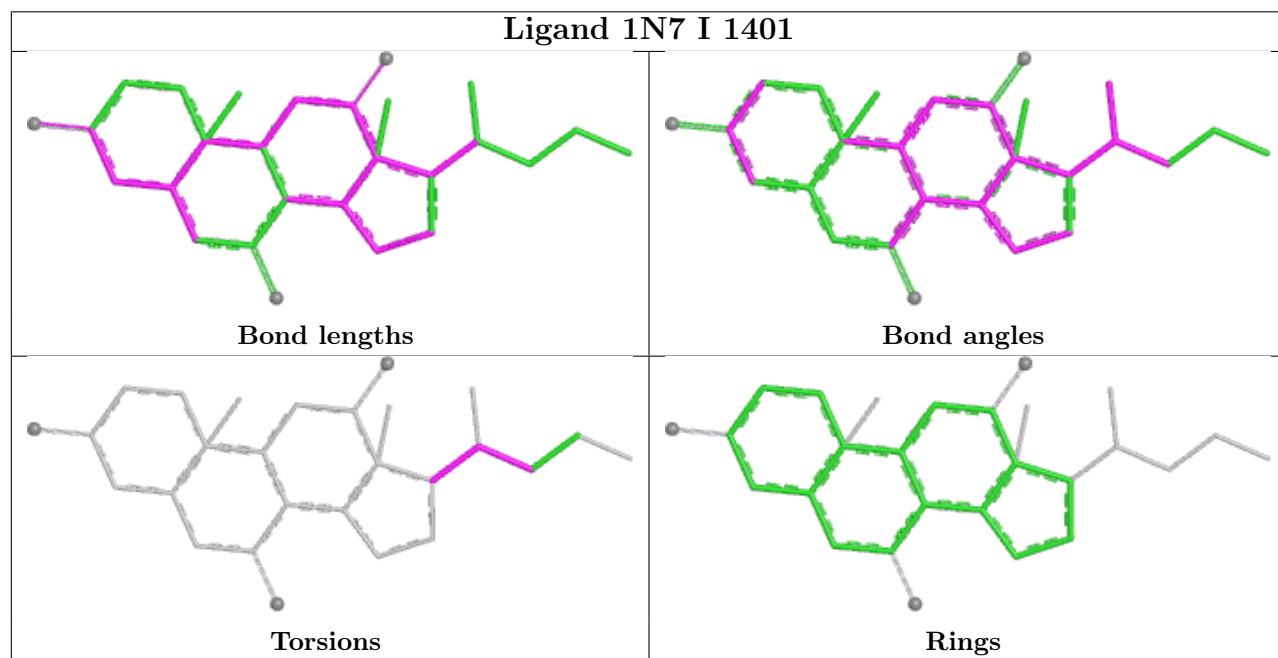
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1402	1N7	10	0
8	I	1401	1N7	9	0
8	Q	101	1N7	10	0

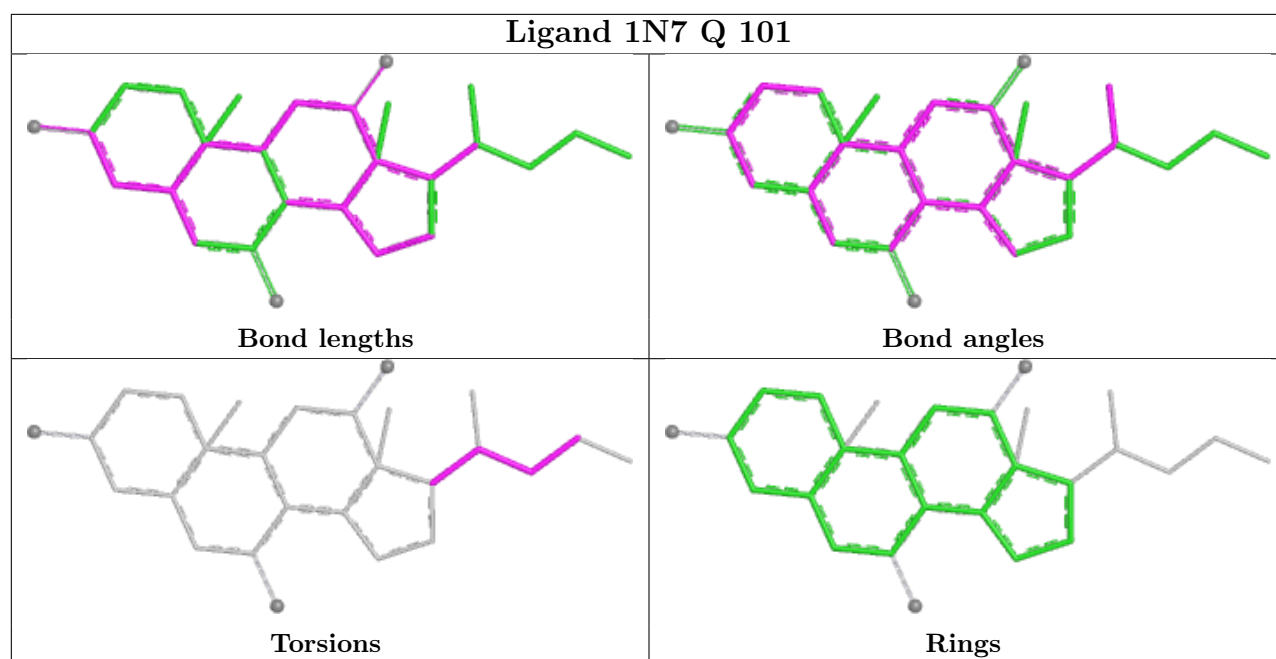
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 1N7 I 1402



Ligand 1N7 I 1401





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.

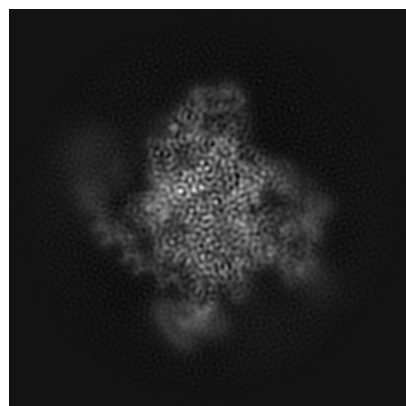
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23892. These allow visual inspection of the internal detail of the map and identification of artifacts.

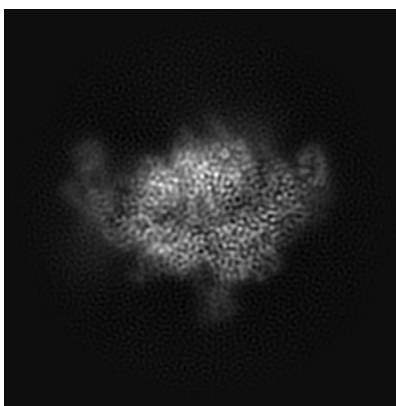
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

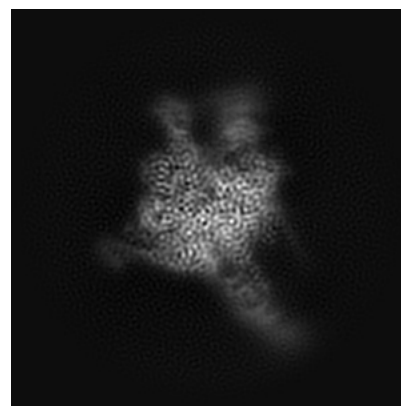
6.1.1 Primary map



X

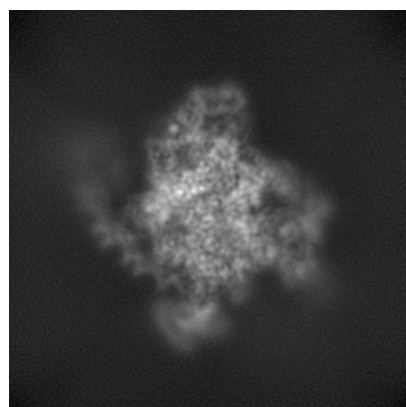


Y

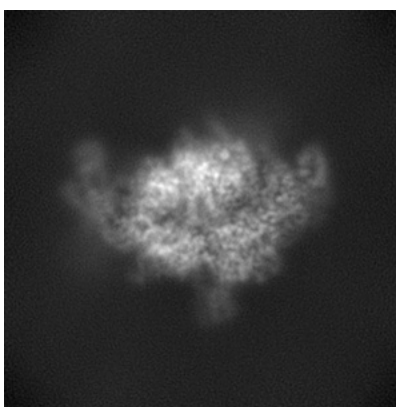


Z

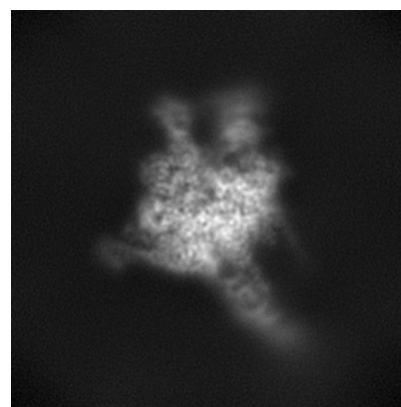
6.1.2 Raw map



X



Y

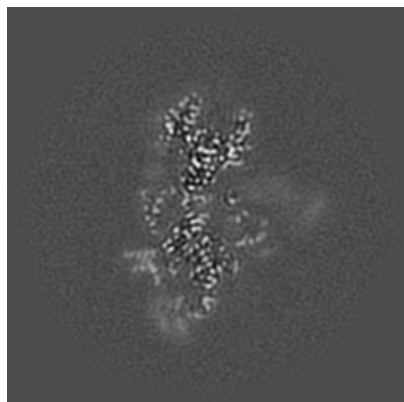


Z

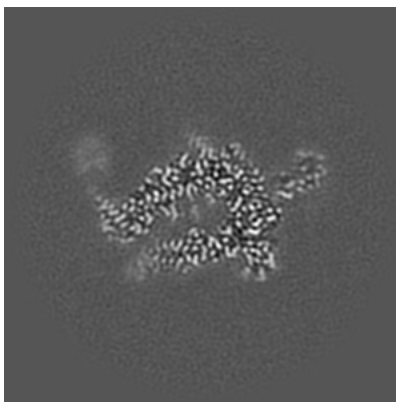
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

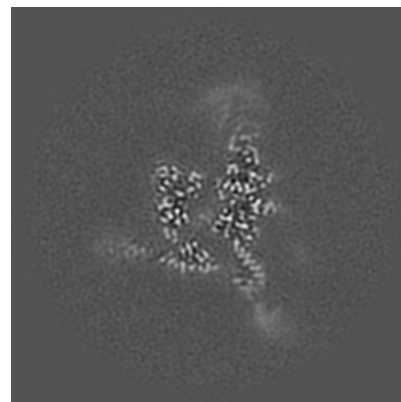
6.2.1 Primary map



X Index: 128

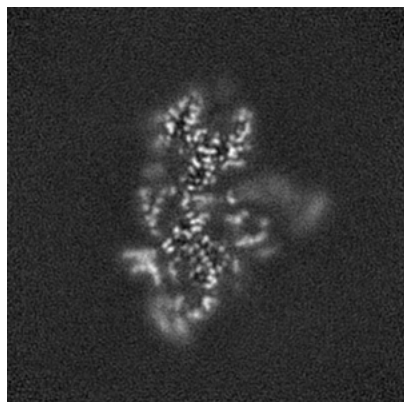


Y Index: 128

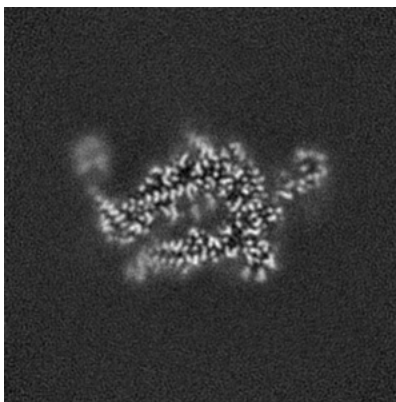


Z Index: 128

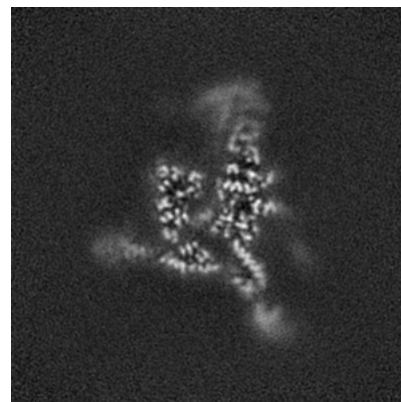
6.2.2 Raw map



X Index: 128



Y Index: 128

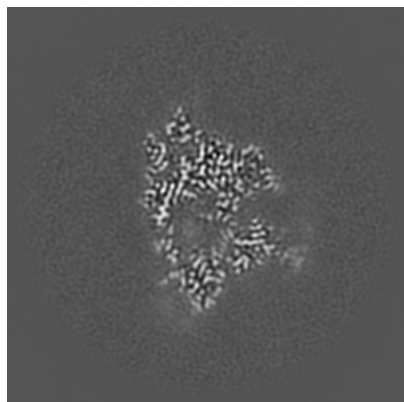


Z Index: 128

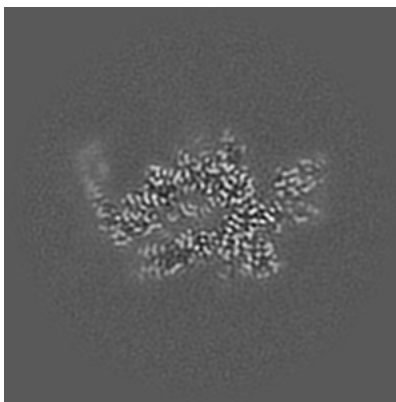
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

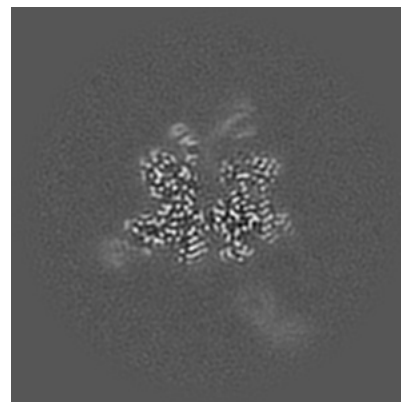
6.3.1 Primary map



X Index: 114

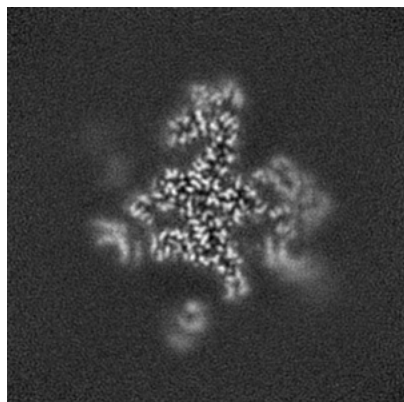


Y Index: 123

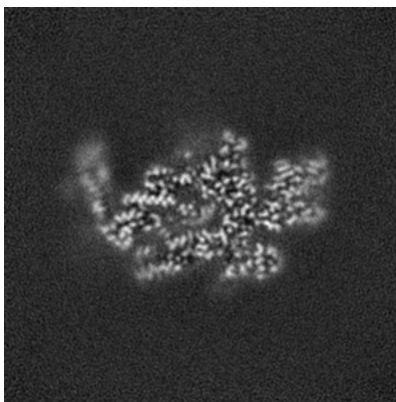


Z Index: 142

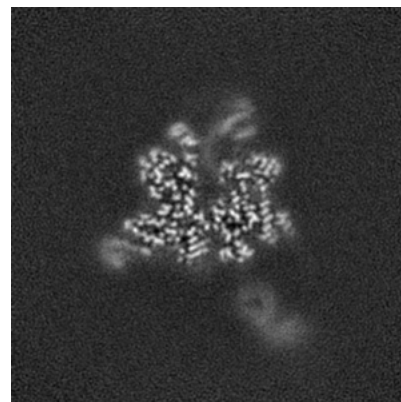
6.3.2 Raw map



X Index: 145



Y Index: 121

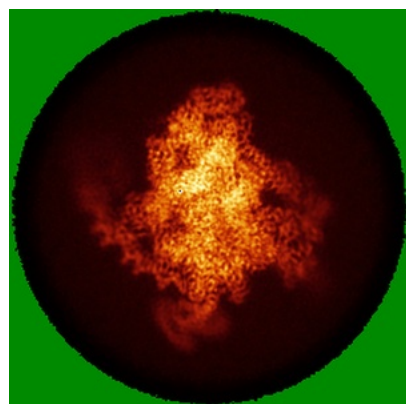


Z Index: 142

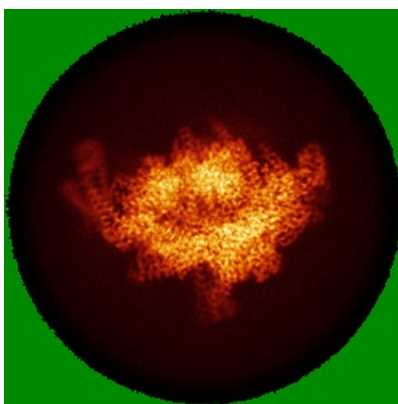
The images above show the largest variance slices of the map in three orthogonal directions.

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

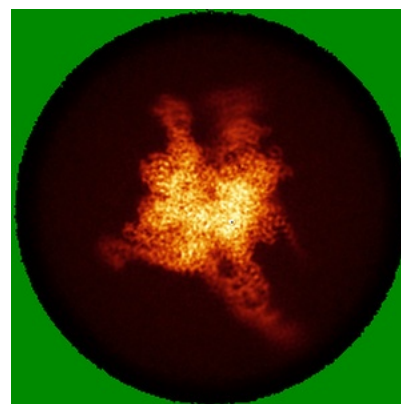
6.4.1 Primary map



X

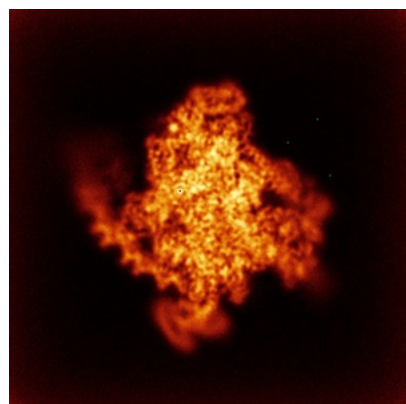


Y

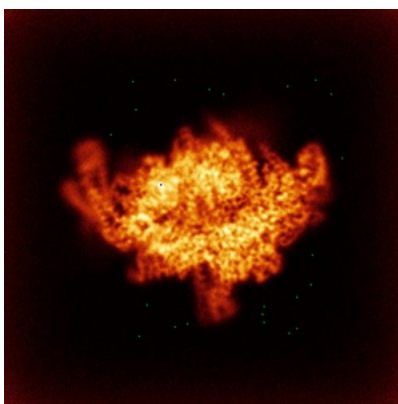


Z

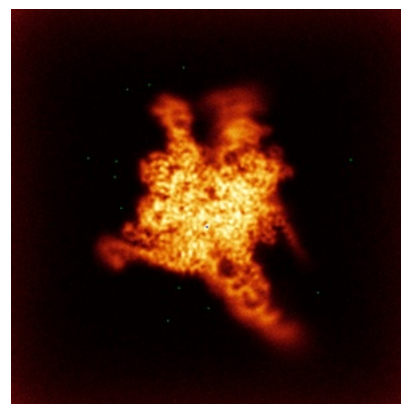
6.4.2 Raw map



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.

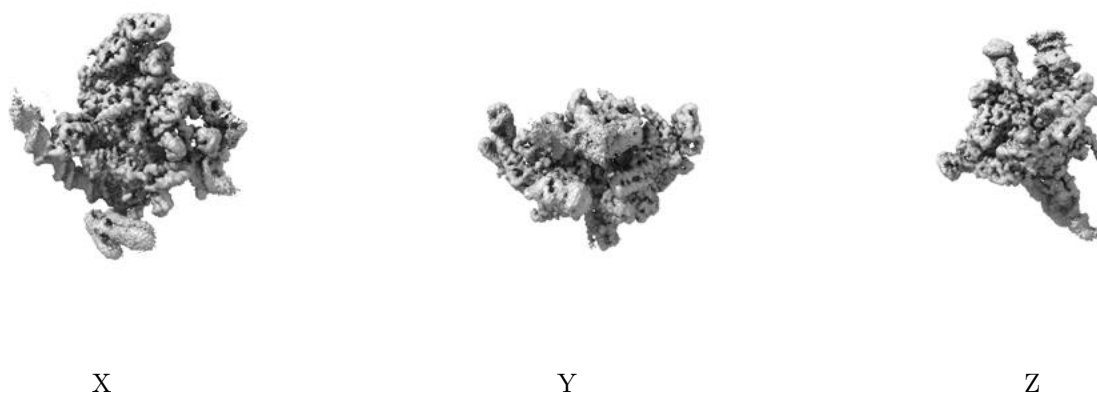
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.27. 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.

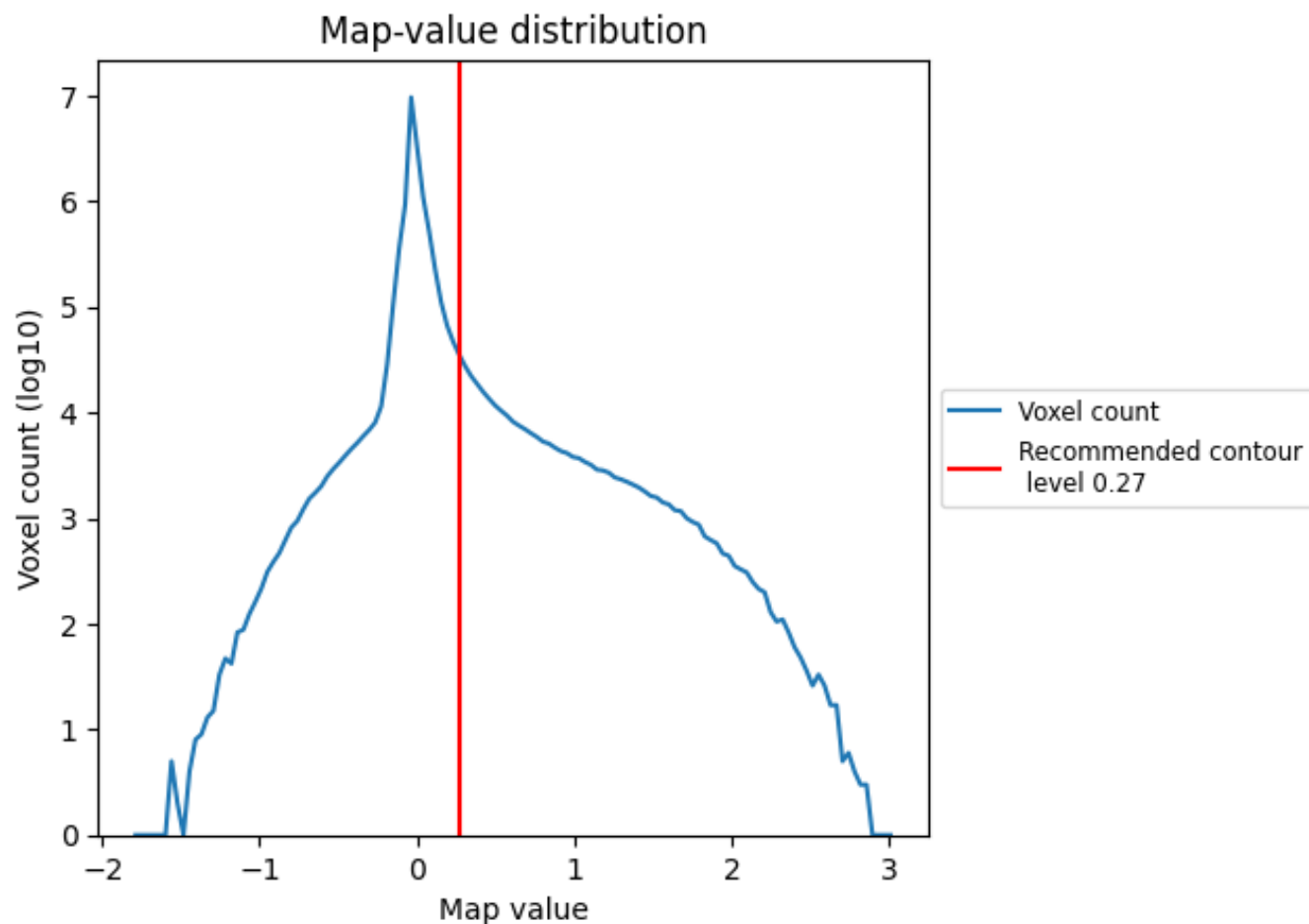
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

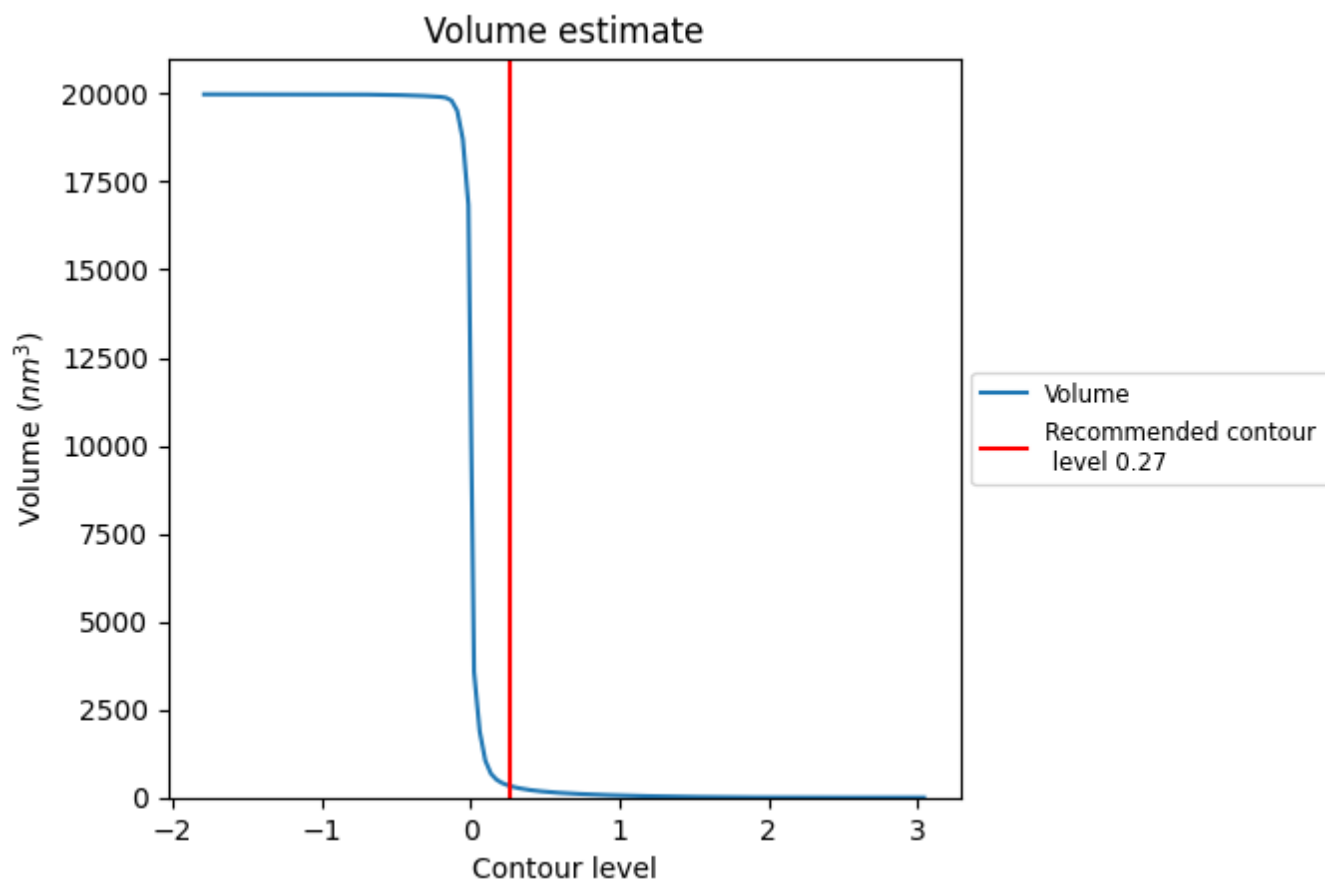
This section contains the results of statistical analysis of the map.

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.

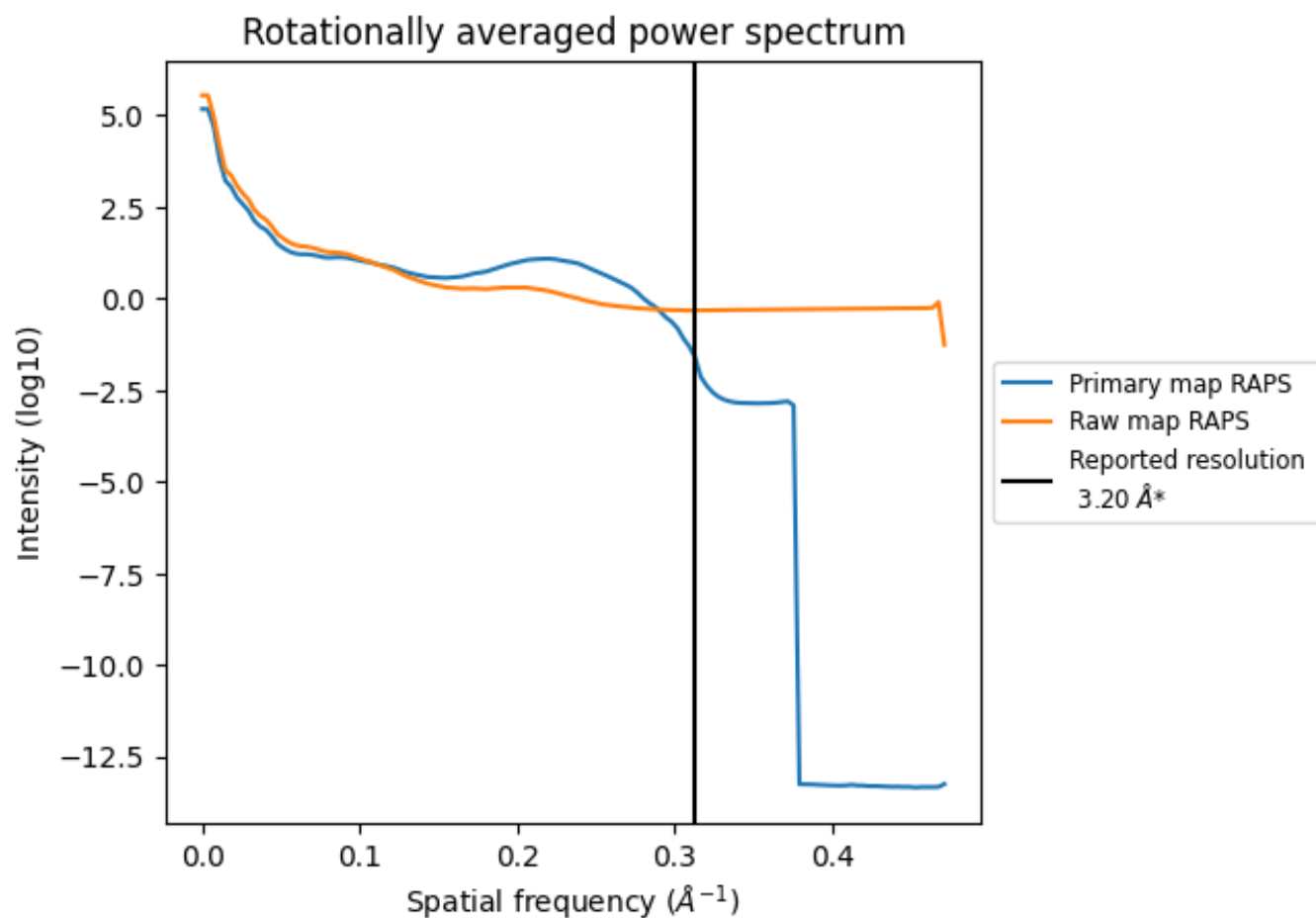
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 325 nm³; this corresponds to an approximate mass of 294 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 ⓘ

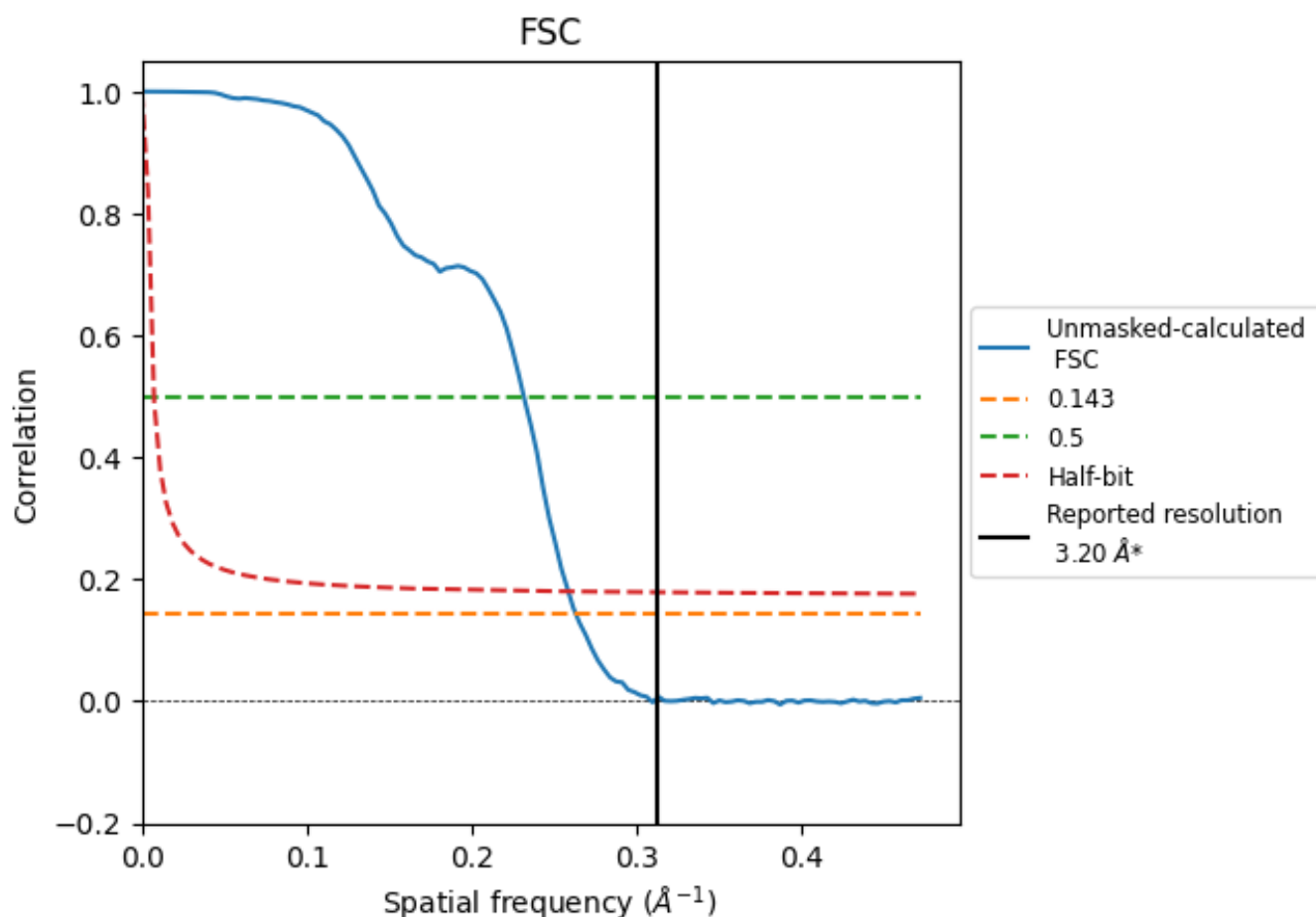


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

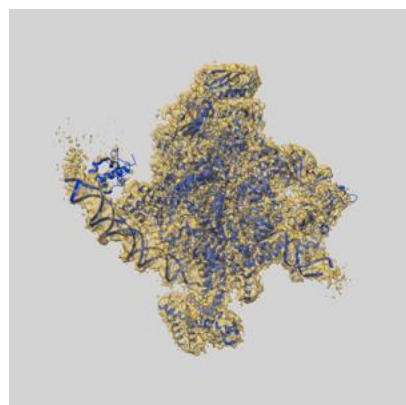
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	4.32	3.87

*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 3.80 differs from the reported value 3.2 by more than 10 %

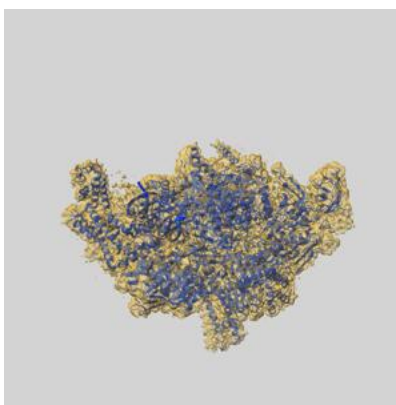
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23892 and PDB model 7MKD. Per-residue inclusion information can be found in section [3](#) on page [7](#).

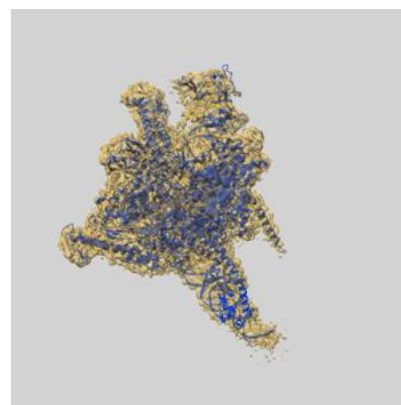
9.1 Map-model overlay [i](#)



X



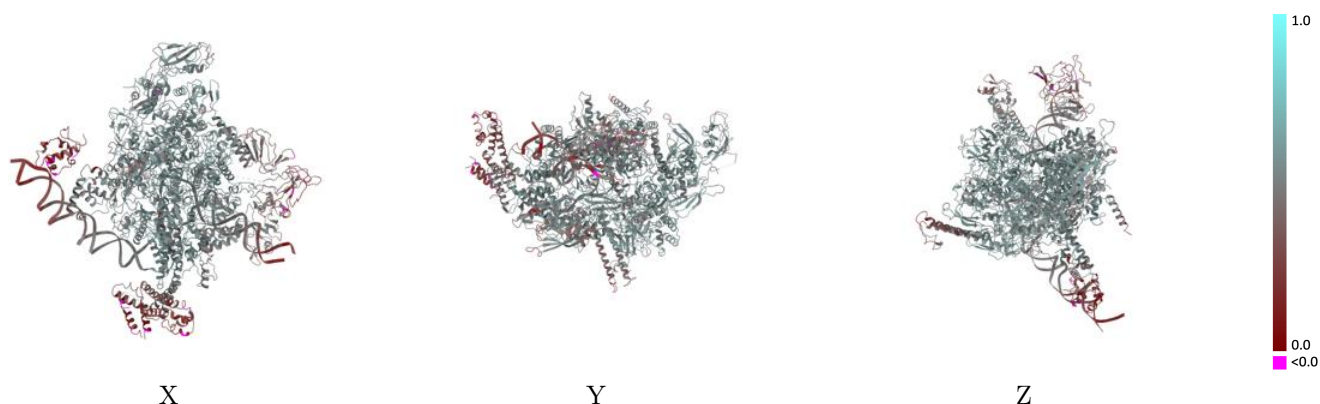
Y



Z

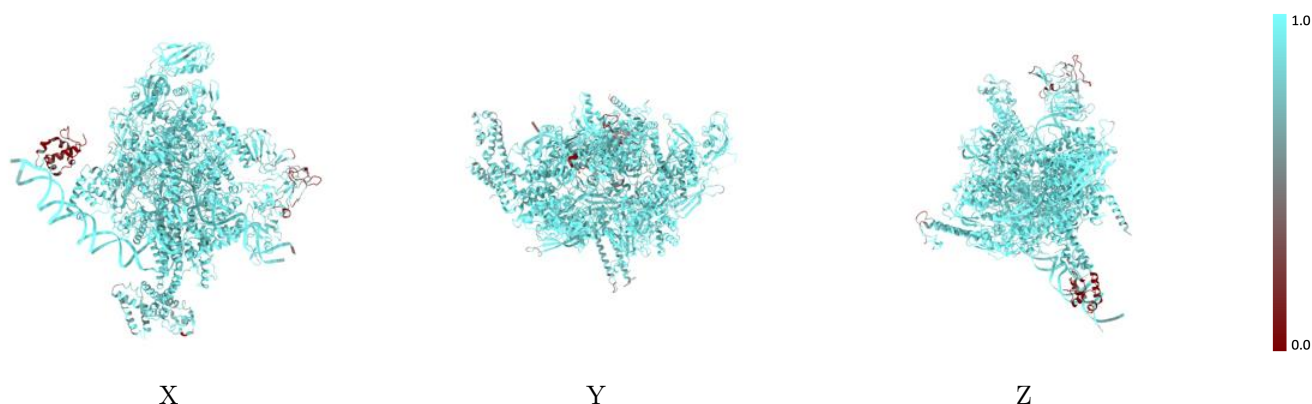
The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



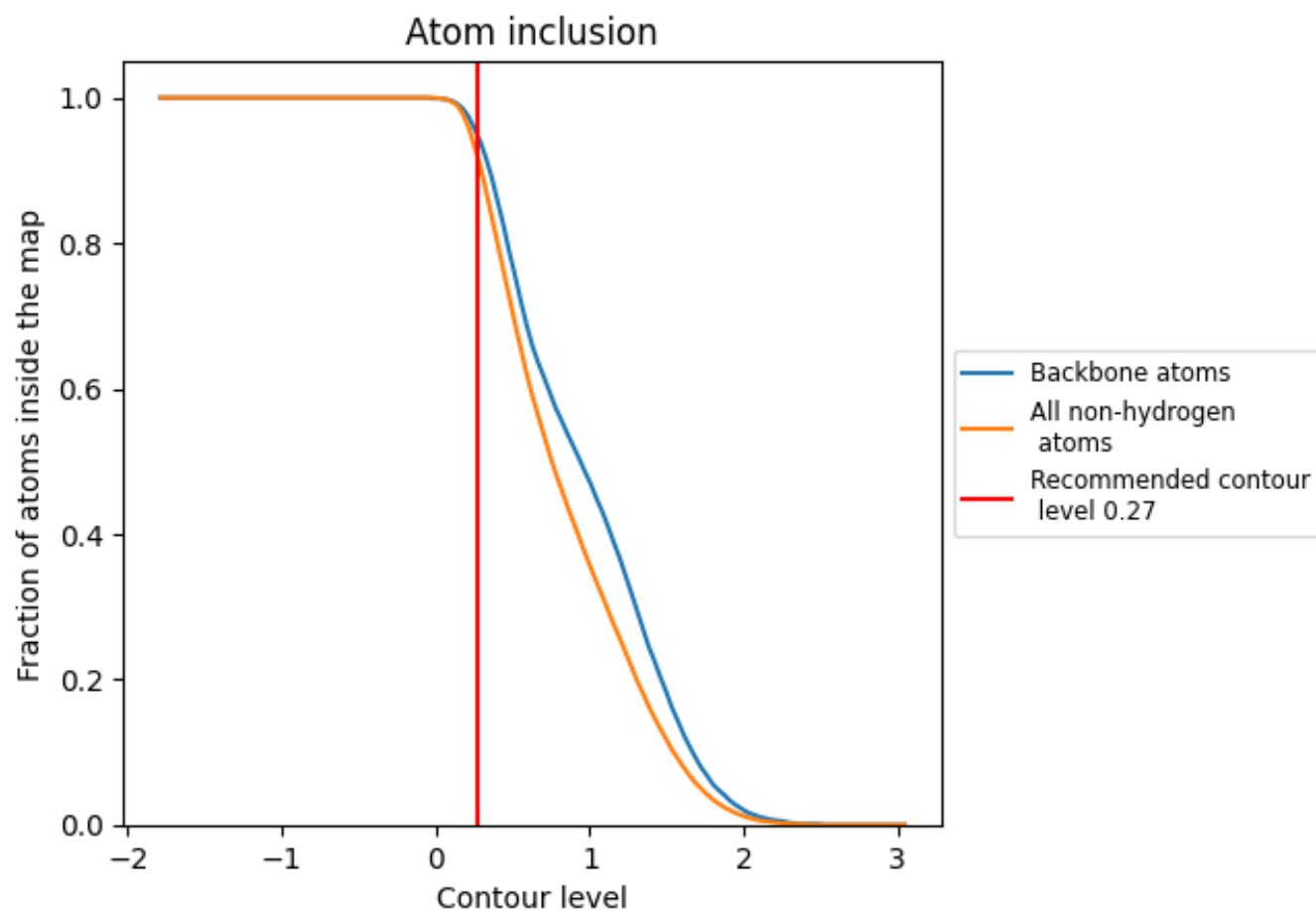
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.27).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9200	<div></div> 0.4950
G	<div></div> 0.9500	<div></div> 0.5360
H	<div></div> 0.9520	<div></div> 0.5220
I	<div></div> 0.9470	<div></div> 0.5280
J	<div></div> 0.9250	<div></div> 0.5160
K	<div></div> 0.8870	<div></div> 0.5060
L	<div></div> 0.8970	<div></div> 0.4120
P	<div></div> 0.9560	<div></div> 0.4270
Q	<div></div> 0.9620	<div></div> 0.4220
R	<div></div> 0.1550	<div></div> 0.1870

1.0

0.0

<0.0