



# Full wwPDB EM Validation Report ⓘ

Jun 26, 2024 – 07:02 PM EDT

PDB ID : 8TO6  
EMDB ID : EMD-41437  
Title : Escherichia coli RNA polymerase unwinding intermediate (I1d) at the lambda PR promoter  
Authors : Darst, S.A.; Saecker, R.M.; Mueller, A.U.  
Deposited on : 2023-08-02  
Resolution : 2.90 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

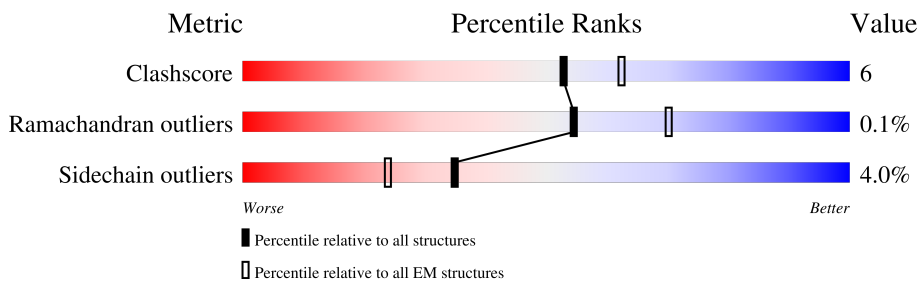
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	M	329	
2	I	1342	
3	J	1407	
4	K	91	
5	L	613	
6	O	105	

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Mol	Chain	Length	Quality of chain
7	P	105	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into two segments: a green segment on the left labeled '37%' and a grey segment on the right labeled '60%'. A small red dot is visible at the beginning of the bar, and a small black dot is visible at the end of the green segment.</p>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 31406 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
			Total	C	N	O	S		
1	G	230	Total 1755	C 1097	N 310	O 342	S 6	0	0
1	H	221	Total 1699	C 1061	N 299	O 333	S 6	0	0
1	M	73	Total 572	C 362	N 100	O 108	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	1336	Total 10530	C 6612	N 1833	O 2042	S 43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	1335	Total 10373	C 6518	N 1848	O 1958	S 49	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	73	Total 582	C 355	N 111	O 115	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	470	Total 3799	C 2383	N 679	O 714	S 23	0	0

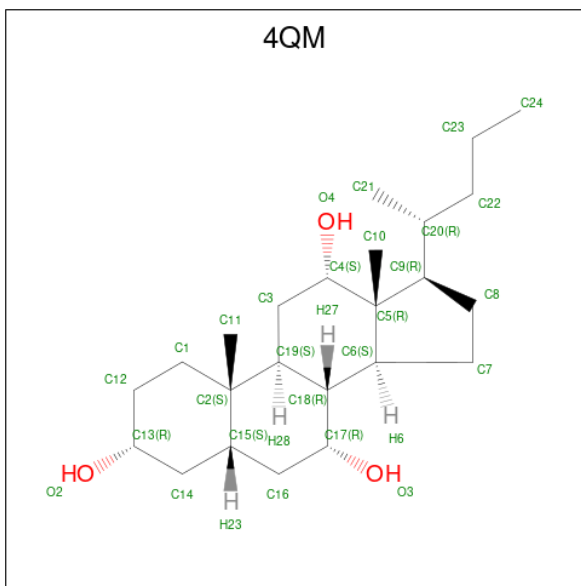
- Molecule 6 is a DNA chain called Nontemplate strand of lambda PR promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	O	56	1150	549	201	344	56	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	P	42	863	409	167	245	42	0	0

- Molecule 8 is (3R,5S,7R,8R,9S,10S,12S,13R,14S,17R)-10,13-dimethyl-17-[(2R)-pentan-2-yl]-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthrene-3,7,12-triol (three-letter code: 4QM) (formula: C<sub>24</sub>H<sub>42</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	I	1	26	23	3	0
8	J	1	27	24	3	0
8	L	1	27	24	3	0

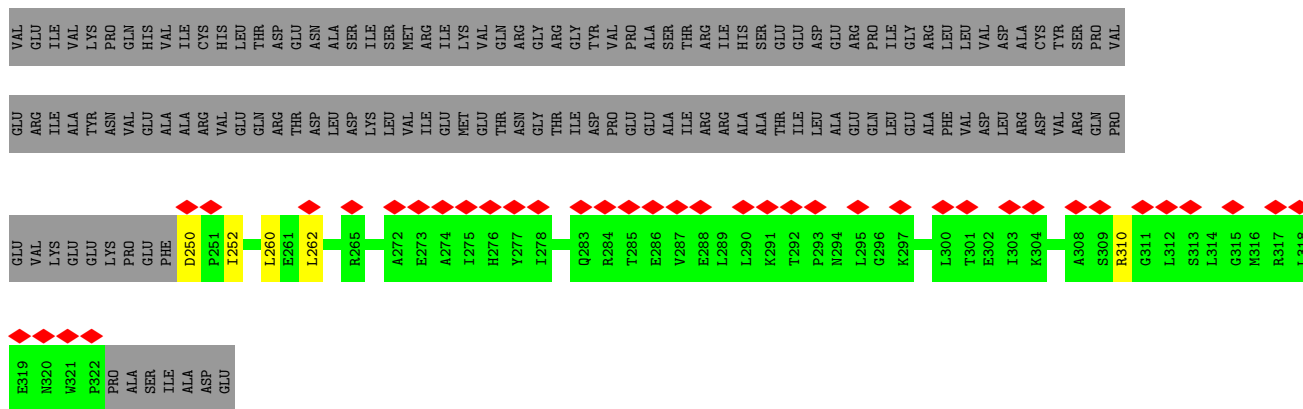
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

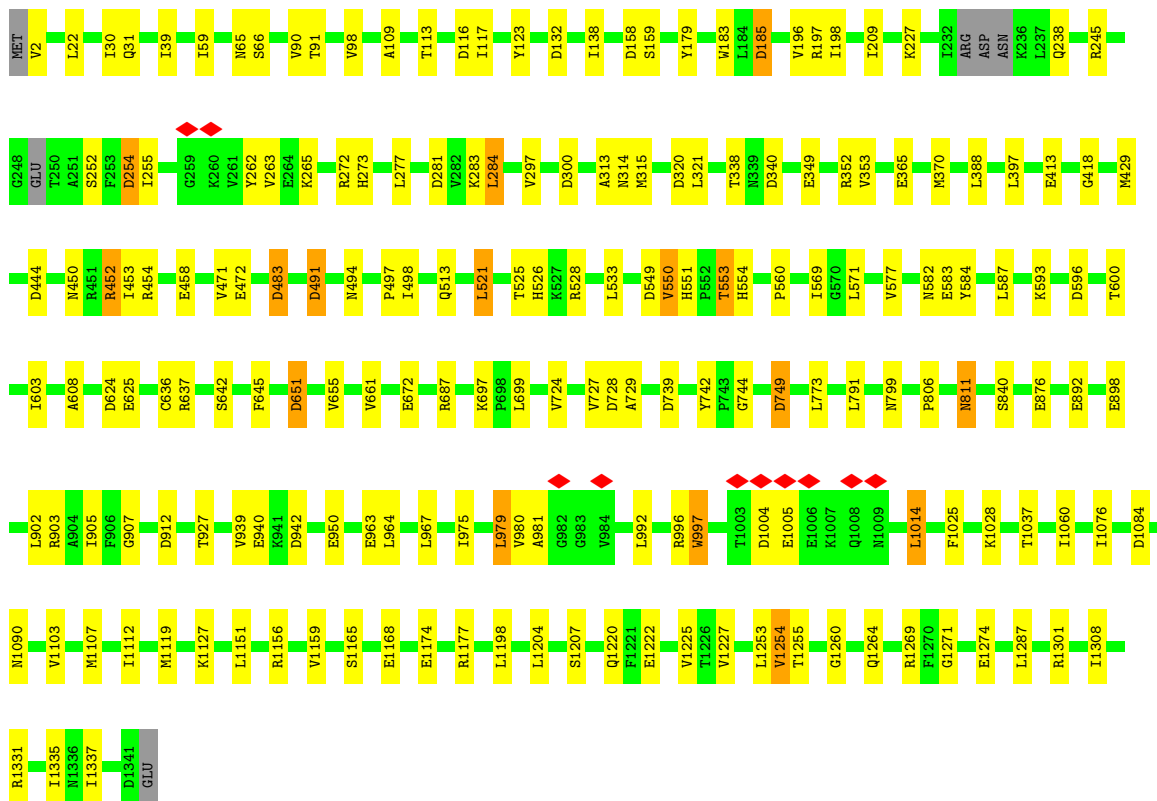
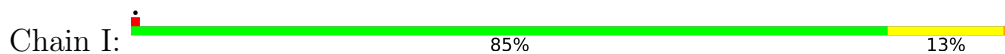
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

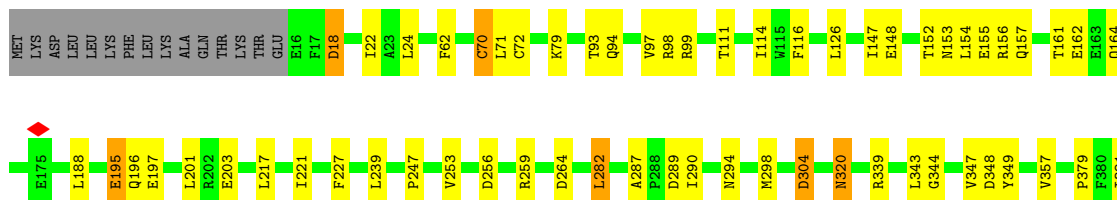
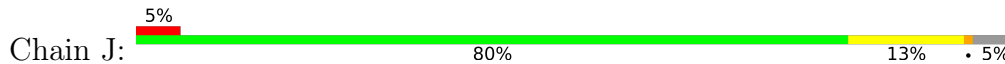




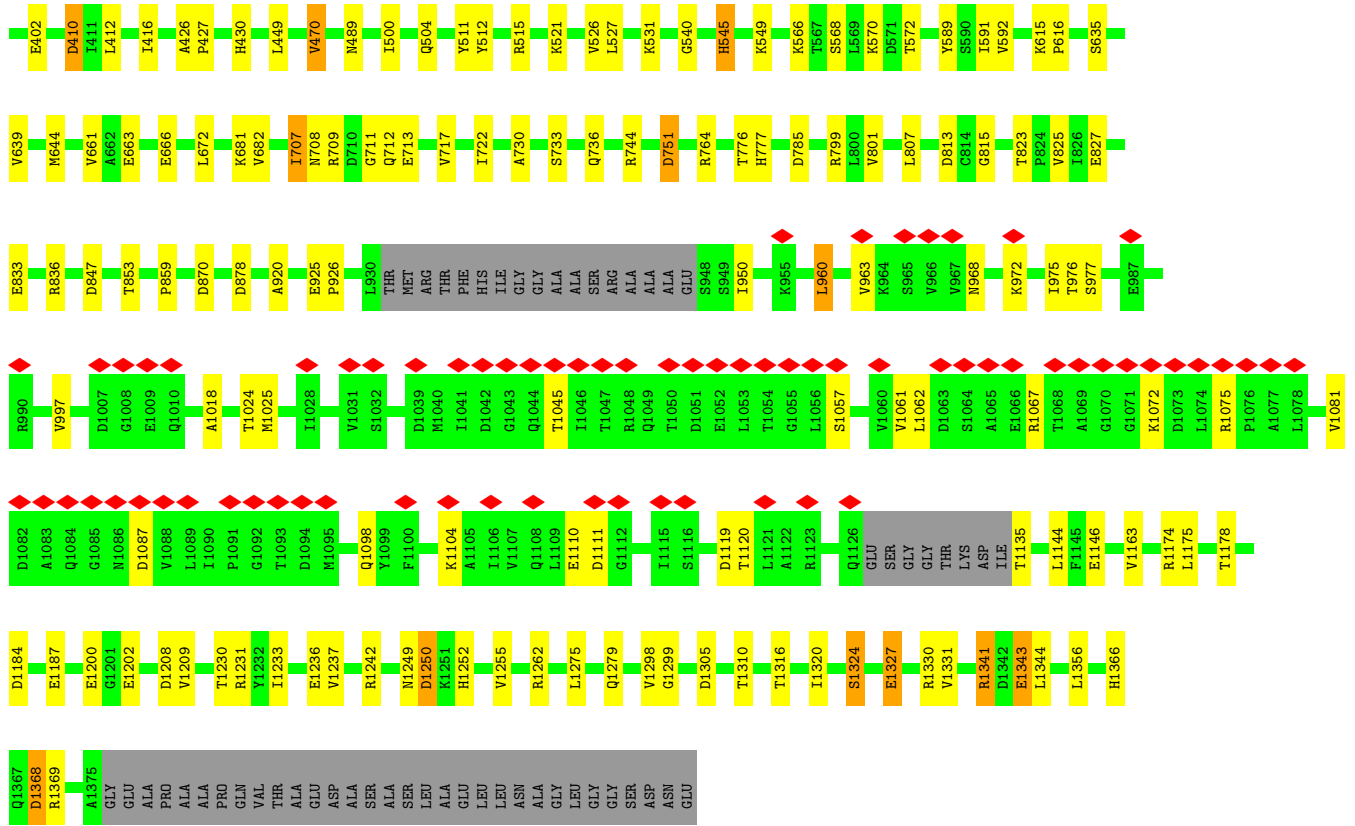
• Molecule 2: DNA-directed RNA polymerase subunit beta



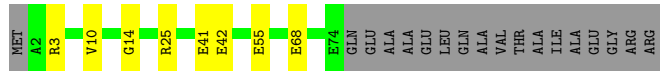
• Molecule 3: DNA-directed RNA polymerase subunit beta'



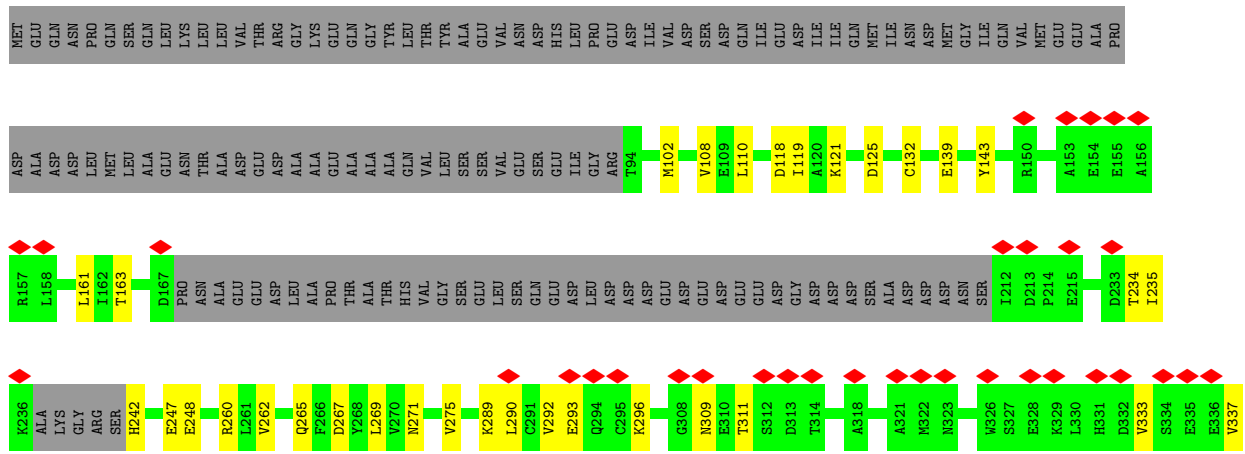




● Molecule 4: DNA-directed RNA polymerase subunit omega



● Molecule 5: RNA polymerase sigma factor RpoD





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111510	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.366	Depositor
Minimum map value	-2.575	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.12	Depositor
Map size ( $\text{\AA}$ )	324.096, 324.096, 324.096	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.84400004, 0.84400004, 0.84400004	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 4QM

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	0.33	0/1777	0.54	0/2412
1	H	0.29	0/1718	0.52	0/2328
1	M	0.23	0/579	0.49	0/784
2	I	0.35	0/10695	0.52	0/14426
3	J	0.33	0/10530	0.54	1/14219 (0.0%)
4	K	0.28	0/584	0.55	0/786
5	L	0.28	0/3849	0.51	0/5175
6	O	0.55	0/1287	0.96	0/1986
7	P	0.51	0/969	0.83	0/1490
All	All	0.35	0/31988	0.57	1/43606 (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
5	L	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	707	ILE	C-N-CA	5.10	134.45	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	L	423	ARG	Sidechain

## 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	1755	0	1771	24	0
1	H	1699	0	1731	33	0
1	M	572	0	602	3	0
2	I	10530	0	10549	106	0
3	J	10373	0	10587	128	0
4	K	582	0	593	5	0
5	L	3799	0	3861	56	0
6	O	1150	0	636	7	0
7	P	863	0	471	3	0
8	I	26	0	0	3	0
8	J	27	0	0	4	0
8	L	27	0	0	4	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
All	All	31406	0	30801	349	0

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

All (349) 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:1401:4QM:C3	8:I:1401:4QM:C19	1.82	1.55
8:J:1504:4QM:C19	8:J:1504:4QM:C3	1.83	1.54
8:L:701:4QM:C3	8:L:701:4QM:C19	1.82	1.50
2:I:1269:ARG:NH1	3:J:344:GLY:O	2.02	0.93
2:I:452:ARG:NH1	2:I:584:TYR:O	2.07	0.87
5:L:234:THR:OG1	5:L:248:GLU:OE1	1.93	0.85
2:I:91:THR:OG1	2:I:138:ILE:O	1.96	0.82
2:I:281:ASP:OD1	2:I:283:LYS:NZ	2.14	0.80
2:I:413:GLU:OE1	2:I:413:GLU:N	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1165:SER:OG	2:I:1168:GLU:OE1	2.00	0.79
2:I:1260:GLY:O	2:I:1264:GLN:NE2	2.16	0.79
3:J:799:ARG:NH1	3:J:1146:GLU:OE2	2.15	0.79
3:J:1072:LYS:O	3:J:1075:ARG:NH1	2.15	0.78
3:J:294:ASN:OD1	5:L:406:GLN:NE2	2.17	0.77
1:G:45:ARG:NH2	2:I:1084:ASP:OD1	2.17	0.77
3:J:833:GLU:OE1	3:J:1242:ARG:NH1	2.18	0.76
2:I:314:ASN:OD1	2:I:352:ARG:NH1	2.19	0.75
5:L:267:ASP:OD1	5:L:271:ASN:ND2	2.20	0.75
2:I:185:ASP:N	2:I:185:ASP:OD1	2.19	0.75
3:J:1174:ARG:NH2	3:J:1187:GLU:OE1	2.20	0.75
2:I:593:LYS:O	2:I:600:THR:OG1	2.05	0.74
2:I:349:GLU:N	2:I:349:GLU:OE1	2.21	0.73
1:G:212:ASP:N	1:G:212:ASP:OD1	2.21	0.73
3:J:1341:ARG:NH1	3:J:1343:GLU:OE1	2.21	0.73
5:L:503:GLU:OE1	5:L:503:GLU:N	2.22	0.73
3:J:712:GLN:OE1	3:J:712:GLN:N	2.22	0.72
3:J:708:ASN:ND2	3:J:712:GLN:O	2.23	0.72
5:L:381:GLU:OE1	5:L:381:GLU:N	2.21	0.72
1:H:41:ASN:OD1	1:H:44:ARG:NH2	2.23	0.71
2:I:560:PRO:HB2	3:J:776:THR:HG21	1.73	0.71
3:J:155:GLU:OE1	3:J:155:GLU:N	2.24	0.71
3:J:1098:GLN:OE1	3:J:1098:GLN:N	2.24	0.71
8:L:701:4QM:C3	8:L:701:4QM:C2	2.67	0.71
8:I:1401:4QM:C3	8:I:1401:4QM:C18	2.69	0.70
2:I:749:ASP:N	2:I:749:ASP:OD1	2.24	0.70
2:I:300:ASP:OD1	2:I:313:ALA:N	2.24	0.69
3:J:572:THR:HG21	3:J:589:TYR:OH	1.91	0.69
3:J:195:GLU:OE1	3:J:196:GLN:N	2.25	0.69
2:I:227:LYS:O	2:I:245:ARG:NH1	2.25	0.69
5:L:108:VAL:HG21	5:L:381:GLU:HB3	1.73	0.69
1:H:191:ARG:NH1	1:H:193:GLU:O	2.26	0.69
8:I:1401:4QM:C3	8:I:1401:4QM:C2	2.69	0.69
8:J:1504:4QM:C3	8:J:1504:4QM:C2	2.67	0.69
2:I:252:SER:O	2:I:265:LYS:NZ	2.19	0.69
3:J:500:ILE:O	3:J:500:ILE:HG22	1.92	0.69
3:J:1057:SER:OG	3:J:1110:GLU:OE2	2.10	0.69
3:J:18:ASP:OD1	3:J:18:ASP:N	2.25	0.68
1:H:77:ASP:OD1	1:H:78:ILE:N	2.27	0.68
5:L:139:GLU:OE1	5:L:139:GLU:N	2.26	0.68
3:J:1200:GLU:OE1	3:J:1200:GLU:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:902:LEU:HD21	5:L:611:LEU:HB2	1.75	0.68
5:L:163:THR:O	5:L:260:ARG:NE	2.26	0.68
2:I:728:ASP:OD1	2:I:729:ALA:N	2.28	0.66
2:I:582:ASN:OD1	2:I:583:GLU:N	2.29	0.66
2:I:1254:VAL:O	3:J:99:ARG:NH2	2.28	0.66
3:J:70:CYS:SG	3:J:71:LEU:N	2.69	0.66
5:L:293:GLU:OE1	5:L:293:GLU:N	2.30	0.65
5:L:429:THR:HG22	6:O:75:DA:H4'	1.78	0.65
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.13	0.64
3:J:1279:GLN:NE2	3:J:1305:ASP:OD2	2.30	0.64
3:J:1062:LEU:O	3:J:1067:ARG:NH2	2.29	0.64
2:I:560:PRO:CB	3:J:776:THR:HG21	2.28	0.64
2:I:491:ASP:N	2:I:491:ASP:OD1	2.29	0.63
1:G:228:LEU:O	1:G:232:VAL:HG23	1.99	0.63
5:L:247:GLU:OE1	5:L:247:GLU:N	2.32	0.63
8:J:1504:4QM:C3	8:J:1504:4QM:C18	2.72	0.63
1:G:137:ASN:N	1:G:137:ASN:OD1	2.31	0.63
2:I:577:VAL:HG23	2:I:661:VAL:O	1.98	0.63
2:I:975:ILE:HG12	2:I:1014:LEU:HD23	1.81	0.63
2:I:198:ILE:HG21	2:I:388:LEU:HD21	1.82	0.62
5:L:508:GLU:N	5:L:508:GLU:OE1	2.33	0.62
2:I:521:LEU:O	2:I:525:THR:HG22	1.99	0.62
5:L:161:LEU:O	5:L:265:GLN:NE2	2.33	0.62
1:G:118:ASP:N	1:G:118:ASP:OD1	2.32	0.62
2:I:444:ASP:O	2:I:450:ASN:ND2	2.32	0.61
3:J:156:ARG:NH1	3:J:157:GLN:OE1	2.34	0.61
3:J:950:ILE:HD12	3:J:1018:ALA:HB3	1.82	0.61
1:H:155:ALA:N	1:H:174:ASP:OD1	2.34	0.61
3:J:827:GLU:OE1	3:J:827:GLU:N	2.33	0.61
5:L:380:VAL:HG13	5:L:412:LEU:HD21	1.82	0.61
2:I:892:GLU:OE1	2:I:892:GLU:N	2.31	0.60
3:J:707:ILE:HD11	3:J:713:GLU:CD	2.22	0.60
1:H:206:GLU:OE2	3:J:531:LYS:NZ	2.22	0.60
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.84	0.60
3:J:256:ASP:OD2	8:J:1504:4QM:O2	2.20	0.60
3:J:568:SER:OG	3:J:570:LYS:NZ	2.35	0.60
1:G:45:ARG:NH1	1:H:34:GLY:O	2.36	0.59
3:J:1327:GLU:OE1	3:J:1330:ARG:NH1	2.35	0.59
3:J:708:ASN:OD1	3:J:709:ARG:N	2.34	0.59
1:H:172:LEU:HD23	1:H:172:LEU:H	1.67	0.59
2:I:1271:GLY:N	2:I:1274:GLU:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1174:GLU:OE2	2:I:1177:ARG:NH1	2.34	0.59
5:L:292:VAL:O	5:L:296:LYS:N	2.34	0.59
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.86	0.58
5:L:426:LYS:NZ	6:O:78:DA:OP1	2.34	0.58
5:L:358:VAL:O	5:L:362:ASN:ND2	2.36	0.58
1:H:202:VAL:HG12	1:H:202:VAL:O	2.04	0.58
8:L:701:4QM:C3	8:L:701:4QM:C18	2.72	0.58
2:I:996:ARG:O	2:I:997:TRP:N	2.37	0.58
1:G:207:THR:HG21	1:G:211:ILE:HG22	1.86	0.57
2:I:453:ILE:HD11	2:I:587:LEU:HD21	1.85	0.57
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.86	0.57
3:J:1368:ASP:OD1	3:J:1369:ARG:N	2.37	0.57
1:G:182:ARG:NH1	2:I:1090:ASN:O	2.37	0.57
3:J:572:THR:HG21	3:J:589:TYR:CE2	2.40	0.57
4:K:10:VAL:O	4:K:14:GLY:N	2.33	0.57
5:L:376:LYS:O	5:L:380:VAL:HG23	2.05	0.56
5:L:383:ASN:CB	5:L:412:LEU:HD13	2.34	0.56
7:P:43:DG:H2'	7:P:44:DT:H72	1.87	0.56
2:I:65:ASN:OD1	2:I:66:SER:N	2.38	0.56
2:I:551:HIS:ND1	2:I:553:THR:OG1	2.32	0.56
2:I:1335:ILE:HG21	3:J:22:ILE:HD11	1.87	0.56
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.89	0.55
3:J:1163:VAL:HG12	3:J:1202:GLU:O	2.06	0.55
3:J:282:LEU:HD23	3:J:287:ALA:HB3	1.89	0.55
5:L:125:ASP:OD2	5:L:371:LYS:NZ	2.40	0.55
3:J:1356:LEU:O	3:J:1366:HIS:NE2	2.37	0.55
1:G:58:GLU:HG2	1:G:172:LEU:HD23	1.89	0.55
2:I:196:VAL:HG21	2:I:209:ILE:CD1	2.37	0.55
2:I:806:PRO:O	2:I:811:ASN:ND2	2.39	0.55
3:J:661:VAL:HG23	3:J:682:VAL:HG22	1.88	0.55
3:J:1249:ASN:OD1	3:J:1250:ASP:N	2.39	0.55
3:J:347:VAL:HG12	3:J:348:ASP:O	2.07	0.55
3:J:960:LEU:HB2	3:J:963:VAL:HG11	1.89	0.54
2:I:525:THR:HG21	2:I:687:ARG:CD	2.37	0.54
1:H:207:THR:HG22	1:H:208:ASN:H	1.72	0.54
3:J:511:TYR:OH	3:J:515:ARG:NH1	2.40	0.54
3:J:960:LEU:O	3:J:960:LEU:HD12	2.07	0.54
2:I:158:ASP:OD1	2:I:159:SER:N	2.41	0.54
2:I:742:TYR:O	2:I:744:GLY:N	2.41	0.54
3:J:111:THR:O	3:J:239:LEU:N	2.41	0.54
3:J:1061:VAL:O	3:J:1104:LYS:N	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:131:CYS:SG	1:H:132:HIS:N	2.81	0.54
3:J:320:ASN:OD1	3:J:320:ASN:N	2.39	0.54
3:J:521:LYS:NZ	3:J:540:GLY:O	2.35	0.53
1:H:89:ALA:HB3	1:H:124:VAL:HG22	1.90	0.53
3:J:707:ILE:HA	3:J:708:ASN:HB2	1.90	0.53
1:G:14:VAL:HG11	1:G:29:GLU:HB2	1.90	0.53
2:I:1004:ASP:OD1	2:I:1004:ASP:N	2.42	0.53
5:L:583:THR:HG21	6:O:52:DT:OP2	2.08	0.53
2:I:980:VAL:HG12	2:I:980:VAL:O	2.09	0.53
3:J:152:THR:OG1	3:J:154:LEU:HD23	2.08	0.53
3:J:259:ARG:CZ	5:L:505:ILE:HD11	2.39	0.53
5:L:383:ASN:HB2	5:L:412:LEU:HD13	1.91	0.53
1:H:35:PHE:HA	1:H:38:THR:HG22	1.90	0.52
5:L:586:ARG:NH1	5:L:589:GLN:OE1	2.38	0.52
2:I:596:ASP:N	2:I:596:ASP:OD1	2.42	0.52
3:J:1144:LEU:HD21	3:J:1236:GLU:HB3	1.91	0.52
6:O:76:DT:H2''	6:O:77:DA:C8	2.44	0.52
1:H:67:GLU:OE2	1:H:82:LEU:HD12	2.09	0.52
5:L:383:ASN:O	5:L:387:VAL:HG23	2.10	0.51
5:L:143:TYR:CD2	5:L:269:LEU:HD21	2.44	0.51
3:J:410:ASP:OD1	3:J:410:ASP:N	2.43	0.51
5:L:415:ALA:O	5:L:416:VAL:C	2.48	0.51
5:L:570:ASP:OD1	5:L:571:TYR:N	2.44	0.51
2:I:2:VAL:O	2:I:2:VAL:HG22	2.10	0.51
3:J:975:ILE:HG22	3:J:977:SER:H	1.76	0.51
2:I:1037:THR:HG22	2:I:1037:THR:O	2.11	0.51
5:L:562:ARG:NH2	7:P:51:DG:OP1	2.43	0.51
1:M:260:LEU:HD23	1:M:262:LEU:HD11	1.92	0.51
2:I:1255:THR:HG23	2:I:1255:THR:O	2.10	0.51
2:I:284:LEU:HD23	2:I:284:LEU:N	2.26	0.50
2:I:483:ASP:OD1	2:I:483:ASP:N	2.41	0.50
1:G:197:ASP:OD1	1:G:197:ASP:N	2.39	0.50
5:L:118:ASP:OD1	5:L:119:ILE:N	2.45	0.50
2:I:903:ARG:O	2:I:907:GLY:N	2.42	0.50
3:J:70:CYS:SG	3:J:72:CYS:N	2.85	0.50
5:L:309:ASN:OD1	5:L:311:THR:OG1	2.26	0.50
3:J:416:ILE:HG22	3:J:416:ILE:O	2.12	0.50
3:J:925:GLU:HG3	3:J:926:PRO:HD3	1.93	0.50
3:J:148:GLU:OE2	3:J:156:ARG:NE	2.42	0.49
3:J:853:THR:HG22	3:J:853:THR:O	2.13	0.49
2:I:964:LEU:HD13	2:I:1025:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:644:MET:O	3:J:764:ARG:NE	2.45	0.49
2:I:340:ASP:OD1	2:I:340:ASP:N	2.44	0.49
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.95	0.49
2:I:196:VAL:HG21	2:I:209:ILE:HD12	1.95	0.49
5:L:337:VAL:O	5:L:341:LEU:HD13	2.13	0.49
1:H:100:LEU:HD23	1:H:115:ILE:HG12	1.94	0.49
4:K:42:GLU:N	4:K:42:GLU:OE1	2.46	0.48
3:J:381:ILE:HD11	3:J:412:LEU:HD13	1.96	0.48
1:G:16:ILE:N	1:G:16:ILE:HD12	2.28	0.48
2:I:553:THR:CG2	2:I:608:ALA:HB1	2.43	0.48
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.95	0.48
1:G:110:VAL:CG2	1:G:133:LEU:HD23	2.43	0.48
2:I:22:LEU:HD13	2:I:603:ILE:HD13	1.95	0.48
2:I:553:THR:HG21	2:I:608:ALA:HB1	1.96	0.48
3:J:572:THR:HG21	3:J:589:TYR:CZ	2.47	0.48
2:I:651:ASP:OD1	2:I:651:ASP:N	2.46	0.48
2:I:254:ASP:OD1	2:I:255:ILE:N	2.45	0.47
3:J:1146:GLU:OE1	3:J:1310:THR:HG22	2.13	0.47
3:J:197:GLU:O	3:J:201:LEU:HD23	2.14	0.47
5:L:395:THR:HG23	5:L:396:ASN:N	2.29	0.47
2:I:109:ALA:HB3	2:I:113:THR:CG2	2.45	0.47
1:G:27:THR:C	1:G:28:LEU:HD12	2.35	0.47
3:J:751:ASP:OD1	3:J:751:ASP:N	2.45	0.47
3:J:801:VAL:HG12	3:J:920:ALA:CB	2.45	0.47
5:L:568:ASN:OD1	5:L:569:THR:N	2.48	0.47
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.97	0.47
2:I:397:LEU:N	2:I:418:GLY:O	2.47	0.47
3:J:836:ARG:NH1	3:J:870:ASP:OD1	2.46	0.47
1:G:15:ASP:C	1:G:16:ILE:HD12	2.35	0.47
1:H:58:GLU:OE1	1:H:170:ARG:NH2	2.48	0.47
2:I:320:ASP:OD1	2:I:321:LEU:N	2.49	0.47
4:K:41:GLU:OE1	4:K:41:GLU:N	2.40	0.46
5:L:118:ASP:O	5:L:121:LYS:HG2	2.15	0.46
1:H:9:LEU:HD21	1:H:12:ARG:NH2	2.30	0.46
2:I:624:ASP:OD1	2:I:625:GLU:N	2.44	0.46
3:J:976:THR:O	3:J:976:THR:HG22	2.16	0.46
3:J:1184:ASP:N	3:J:1184:ASP:OD1	2.49	0.46
3:J:1320:ILE:O	3:J:1324:SER:OG	2.33	0.46
2:I:739:ASP:OD1	2:I:739:ASP:N	2.49	0.46
3:J:153:ASN:C	3:J:154:LEU:HD22	2.36	0.46
3:J:24:LEU:HD21	3:J:116:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:93:GLN:NE2	1:H:122:GLU:OE1	2.49	0.46
2:I:1060:ILE:HD11	2:I:1076:ILE:HD11	1.97	0.46
2:I:939:VAL:HG12	2:I:940:GLU:N	2.31	0.46
3:J:290:ILE:N	3:J:290:ILE:HD12	2.31	0.46
5:L:376:LYS:HG3	5:L:416:VAL:HG11	1.98	0.46
8:L:701:4QM:C3	8:L:701:4QM:C11	2.94	0.46
7:P:43:DG:C2'	7:P:44:DT:H72	2.45	0.45
3:J:1178:THR:HA	3:J:1184:ASP:HB3	1.98	0.45
5:L:163:THR:OG1	5:L:262:VAL:HG22	2.16	0.45
3:J:801:VAL:HG12	3:J:920:ALA:HB3	1.99	0.45
5:L:387:VAL:HG22	5:L:435:ILE:CD1	2.46	0.45
2:I:116:ASP:OD1	2:I:117:ILE:N	2.48	0.45
1:H:29:GLU:HB3	1:H:30:PRO:HD3	1.99	0.45
2:I:353:VAL:HG12	2:I:353:VAL:O	2.16	0.45
3:J:813:ASP:OD1	3:J:815:GLY:N	2.49	0.45
2:I:183:TRP:O	2:I:198:ILE:O	2.34	0.45
1:H:83:LEU:HD11	3:J:526:VAL:CG2	2.47	0.45
2:I:59:ILE:HD13	2:I:472:GLU:HA	1.98	0.45
2:I:255:ILE:HG21	2:I:262:TYR:HB2	1.99	0.45
2:I:876:GLU:HG2	2:I:927:THR:HG22	1.98	0.45
3:J:1111:ASP:N	3:J:1111:ASP:OD1	2.50	0.45
1:H:92:VAL:HG22	1:H:121:VAL:HG12	1.99	0.44
3:J:975:ILE:CD1	3:J:997:VAL:HG11	2.47	0.44
1:G:224:LEU:HD23	1:H:228:LEU:HD11	1.99	0.44
1:H:207:THR:HG22	1:H:208:ASN:N	2.32	0.44
1:M:252:ILE:HD11	1:M:310:ARG:HD3	1.98	0.44
2:I:981:ALA:HB1	2:I:1005:GLU:H	1.83	0.44
3:J:349:TYR:HB3	3:J:470:VAL:HG13	1.99	0.44
5:L:235:ILE:O	5:L:242:HIS:N	2.50	0.44
1:H:71:LYS:O	1:H:74:VAL:HG22	2.17	0.44
5:L:412:LEU:O	5:L:416:VAL:HG23	2.17	0.44
1:H:114:ASP:OD1	1:H:114:ASP:N	2.49	0.44
2:I:132:ASP:OD1	2:I:132:ASP:N	2.48	0.44
2:I:254:ASP:HB2	2:I:263:VAL:HG13	1.99	0.44
2:I:550:VAL:HG13	3:J:777:HIS:CD2	2.53	0.44
3:J:1081:VAL:HG12	3:J:1087:ASP:OD1	2.17	0.44
4:K:25:ARG:NH2	4:K:68:GLU:OE1	2.51	0.44
5:L:403:ASP:N	5:L:403:ASP:OD1	2.50	0.44
1:G:233:ASP:N	1:G:233:ASP:OD1	2.50	0.44
2:I:283:LYS:HB2	2:I:284:LEU:HD23	1.99	0.44
2:I:453:ILE:CD1	2:I:587:LEU:HD21	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1331:ARG:NH2	2:I:1337:ILE:O	2.51	0.44
1:H:14:VAL:HG13	1:H:14:VAL:O	2.18	0.43
1:M:250:ASP:OD1	1:M:252:ILE:HG22	2.17	0.43
3:J:807:LEU:CD2	3:J:1255:VAL:HG23	2.48	0.43
3:J:823:THR:HG22	3:J:878:ASP:O	2.18	0.43
3:J:1024:THR:O	3:J:1025:MET:C	2.57	0.43
6:O:85:DC:O2	6:O:85:DC:O4'	2.36	0.43
2:I:273:HIS:O	2:I:277:LEU:HD13	2.18	0.43
3:J:290:ILE:HD12	3:J:290:ILE:H	1.84	0.43
3:J:1298:VAL:HG22	3:J:1299:GLY:H	1.83	0.43
3:J:847:ASP:OD1	3:J:847:ASP:N	2.51	0.43
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.19	0.43
3:J:572:THR:HG21	3:J:589:TYR:HE2	1.84	0.43
1:G:174:ASP:OD1	1:G:174:ASP:N	2.49	0.43
1:H:198:LEU:N	1:H:198:LEU:HD22	2.33	0.43
3:J:298:MET:SD	5:L:402:LEU:HB3	2.59	0.43
3:J:1208:ASP:OD1	3:J:1209:VAL:N	2.50	0.43
3:J:1327:GLU:OE2	3:J:1331:VAL:HG23	2.18	0.43
1:G:215:GLU:OE2	1:G:219:ARG:NH2	2.52	0.43
2:I:905:ILE:HD11	5:L:598:LEU:HD13	2.00	0.43
3:J:162:GLU:OE1	3:J:162:GLU:N	2.42	0.43
2:I:39:ILE:HG13	2:I:39:ILE:O	2.18	0.42
3:J:825:VAL:O	3:J:825:VAL:HG13	2.20	0.42
1:G:135:ASP:OD1	1:G:136:GLU:N	2.52	0.42
3:J:201:LEU:HB3	3:J:221:ILE:HD11	2.01	0.42
3:J:711:GLY:N	3:J:712:GLN:OE1	2.52	0.42
2:I:30:ILE:HG23	2:I:31:GLN:N	2.34	0.42
2:I:297:VAL:HG12	2:I:315:MET:O	2.19	0.42
5:L:271:ASN:O	5:L:275:VAL:HG23	2.18	0.42
5:L:290:LEU:HB3	5:L:333:VAL:HG21	2.00	0.42
5:L:415:ALA:O	5:L:418:LYS:N	2.37	0.42
5:L:547:VAL:CG1	5:L:598:LEU:HD22	2.49	0.42
2:I:637:ARG:HA	2:I:642:SER:HA	2.01	0.42
3:J:147:ILE:HG13	3:J:147:ILE:O	2.19	0.42
3:J:515:ARG:O	3:J:545:HIS:HB3	2.20	0.42
5:L:582:VAL:HG12	5:L:583:THR:N	2.34	0.42
2:I:979:LEU:O	2:I:979:LEU:HD22	2.20	0.42
2:I:981:ALA:HB1	2:I:1004:ASP:HA	2.01	0.42
3:J:504:GLN:O	3:J:730:ALA:HB1	2.19	0.42
3:J:707:ILE:HD11	3:J:713:GLU:OE2	2.19	0.42
2:I:942:ASP:OD1	2:I:942:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:62:PHE:O	3:J:98:ARG:HA	2.20	0.42
6:O:59:DT:H4'	6:O:60:DT:OP1	2.19	0.42
3:J:591:ILE:HG13	3:J:592:VAL:HG13	2.01	0.42
3:J:1275:LEU:N	3:J:1275:LEU:HD12	2.34	0.42
2:I:905:ILE:O	5:L:599:ARG:NE	2.53	0.41
2:I:1151:LEU:HD12	2:I:1198:LEU:HD13	2.02	0.41
5:L:385:ARG:O	5:L:388:ILE:HG22	2.20	0.41
6:O:83:DT:H2''	6:O:84:DG:N3	2.35	0.41
1:H:102:LEU:HB2	1:H:115:ILE:HD12	2.02	0.41
2:I:569:ILE:HG23	2:I:569:ILE:O	2.21	0.41
4:K:3:ARG:NH2	4:K:55:GLU:OE1	2.53	0.41
5:L:511:ILE:HG23	5:L:512:GLY:N	2.35	0.41
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	2.02	0.41
1:H:47:LEU:HD12	1:H:183:ILE:HD13	2.02	0.41
2:I:494:ASN:OD1	2:I:494:ASN:N	2.53	0.41
1:G:98:VAL:HG22	1:G:99:ILE:N	2.36	0.41
1:G:234:LEU:HB2	1:H:14:VAL:HG21	2.01	0.41
2:I:90:VAL:HG22	2:I:91:THR:N	2.35	0.41
2:I:494:ASN:O	2:I:497:PRO:HD2	2.21	0.41
3:J:975:ILE:HD12	3:J:997:VAL:HG11	2.03	0.41
2:I:724:VAL:HG11	2:I:727:VAL:CG2	2.51	0.41
3:J:114:ILE:HD12	3:J:304:ASP:OD1	2.21	0.41
3:J:253:VAL:HG12	5:L:507:MET:CE	2.51	0.41
3:J:1230:THR:HG23	3:J:1231:ARG:N	2.35	0.41
1:H:20:SER:OG	1:H:21:SER:N	2.54	0.41
2:I:636:CYS:SG	2:I:645:PHE:CD1	3.14	0.41
3:J:357:VAL:O	3:J:449:LEU:O	2.39	0.41
3:J:639:VAL:HG23	3:J:722:ILE:HD11	2.03	0.41
3:J:663:GLU:O	3:J:666:GLU:HG3	2.21	0.41
3:J:672:LEU:N	3:J:672:LEU:HD12	2.36	0.41
3:J:733:SER:OG	3:J:736:GLN:OE1	2.37	0.41
5:L:417:ASP:OD1	5:L:417:ASP:N	2.52	0.41
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	2.02	0.41
3:J:94:GLN:O	3:J:97:VAL:HG12	2.21	0.41
3:J:161:THR:HG23	3:J:164:GLN:H	1.86	0.41
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.03	0.41
3:J:1045:THR:O	3:J:1062:LEU:N	2.46	0.40
5:L:586:ARG:HD3	5:L:589:GLN:HB2	2.01	0.40
1:G:23:HIS:NE2	1:G:204:GLU:OE2	2.52	0.40
2:I:979:LEU:HD23	2:I:981:ALA:O	2.21	0.40
3:J:500:ILE:O	3:J:500:ILE:CG2	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1119:ASP:OD1	3:J:1120:THR:N	2.54	0.40
1:H:212:ASP:OD1	1:H:212:ASP:N	2.54	0.40
2:I:179:TYR:OH	2:I:458:GLU:OE2	2.35	0.40
2:I:471:VAL:HG21	2:I:498:ILE:HD11	2.02	0.40
2:I:727:VAL:HG12	2:I:728:ASP:N	2.36	0.40
3:J:515:ARG:NH2	3:J:717:VAL:HG23	2.36	0.40
3:J:1252:HIS:HA	3:J:1255:VAL:HG12	2.02	0.40
1:H:59:VAL:HG23	1:H:144:ILE:HG22	2.03	0.40
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.57	0.40
3:J:526:VAL:HG12	3:J:549:LYS:HB2	2.04	0.40
1:H:112:ALA:O	1:H:115:ILE:HG22	2.21	0.40
3:J:968:ASN:OD1	3:J:972:LYS:N	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	228/329 (69%)	210 (92%)	18 (8%)	0	100	100
1	H	217/329 (66%)	196 (90%)	21 (10%)	0	100	100
1	M	71/329 (22%)	69 (97%)	2 (3%)	0	100	100
2	I	1326/1342 (99%)	1237 (93%)	88 (7%)	1 (0%)	51	82
3	J	1329/1407 (94%)	1249 (94%)	79 (6%)	1 (0%)	51	82
4	K	71/91 (78%)	68 (96%)	3 (4%)	0	100	100
5	L	462/613 (75%)	440 (95%)	21 (4%)	1 (0%)	47	78
All	All	3704/4440 (83%)	3469 (94%)	232 (6%)	3 (0%)	54	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	898	GLU
5	L	416	VAL
3	J	859	PRO

### 5.3.2 Protein sidechains [i](#)

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	191/286 (67%)	180 (94%)	11 (6%)	20	50
1	H	188/286 (66%)	184 (98%)	4 (2%)	53	81
1	M	65/286 (23%)	65 (100%)	0	100	100
2	I	1150/1157 (99%)	1094 (95%)	56 (5%)	25	57
3	J	1117/1168 (96%)	1076 (96%)	41 (4%)	34	68
4	K	63/75 (84%)	63 (100%)	0	100	100
5	L	412/540 (76%)	395 (96%)	17 (4%)	30	64
All	All	3186/3798 (84%)	3057 (96%)	129 (4%)	35	65

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	44	ARG
1	G	50	SER
1	G	56	VAL
1	G	118	ASP
1	G	137	ASN
1	G	160	HIS
1	G	173	VAL
1	G	177	TYR
1	G	211	ILE
1	G	212	ASP
1	G	229	GLU
1	H	9	LEU
1	H	27	THR
1	H	107	ILE
1	H	127	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	I	98	VAL
2	I	123	TYR
2	I	185	ASP
2	I	197	ARG
2	I	238	GLN
2	I	254	ASP
2	I	272	ARG
2	I	284	LEU
2	I	338	THR
2	I	365	GLU
2	I	370	MET
2	I	429	MET
2	I	452	ARG
2	I	454	ARG
2	I	483	ASP
2	I	491	ASP
2	I	513	GLN
2	I	521	LEU
2	I	526	HIS
2	I	528	ARG
2	I	549	ASP
2	I	550	VAL
2	I	553	THR
2	I	554	HIS
2	I	651	ASP
2	I	655	VAL
2	I	672	GLU
2	I	697	LYS
2	I	699	LEU
2	I	749	ASP
2	I	773	LEU
2	I	791	LEU
2	I	799	ASN
2	I	811	ASN
2	I	840	SER
2	I	912	ASP
2	I	950	GLU
2	I	963	GLU
2	I	967	LEU
2	I	979	LEU
2	I	992	LEU
2	I	997	TRP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	I	1014	LEU
2	I	1028	LYS
2	I	1107	MET
2	I	1127	LYS
2	I	1156	ARG
2	I	1159	VAL
2	I	1207	SER
2	I	1220	GLN
2	I	1225	VAL
2	I	1227	VAL
2	I	1253	LEU
2	I	1254	VAL
2	I	1287	LEU
2	I	1301	ARG
3	J	18	ASP
3	J	70	CYS
3	J	79	LYS
3	J	93	THR
3	J	126	LEU
3	J	195	GLU
3	J	203	GLU
3	J	217	LEU
3	J	227	PHE
3	J	264	ASP
3	J	282	LEU
3	J	289	ASP
3	J	304	ASP
3	J	320	ASN
3	J	339	ARG
3	J	343	LEU
3	J	402	GLU
3	J	410	ASP
3	J	430	HIS
3	J	470	VAL
3	J	489	ASN
3	J	527	LEU
3	J	545	HIS
3	J	566	LYS
3	J	635	SER
3	J	681	LYS
3	J	744	ARG
3	J	751	ASP

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Mol	Chain	Res	Type
3	J	785	ASP
3	J	960	LEU
3	J	1135	THR
3	J	1175	LEU
3	J	1250	ASP
3	J	1262	ARG
3	J	1316	THR
3	J	1324	SER
3	J	1327	GLU
3	J	1341	ARG
3	J	1343	GLU
3	J	1344	LEU
3	J	1368	ASP
5	L	102	MET
5	L	110	LEU
5	L	132	CYS
5	L	289	LYS
5	L	376	LYS
5	L	381	GLU
5	L	402	LEU
5	L	403	ASP
5	L	412	LEU
5	L	417	ASP
5	L	463	LEU
5	L	477	GLU
5	L	483	LEU
5	L	517	SER
5	L	566	ASP
5	L	584	ARG
5	L	591	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	J	1195	GLN
3	J	1279	GLN
5	L	362	ASN

### 5.3.3 RNA

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 monosaccharides 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	4QM	I	1401	-	29,29,30	5.10	15 (51%)	47,47,48	1.97	10 (21%)
8	4QM	J	1504	-	30,30,30	5.06	15 (50%)	47,48,48	2.35	13 (27%)
8	4QM	L	701	-	30,30,30	5.01	15 (50%)	47,48,48	2.29	10 (21%)

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	4QM	I	1401	-	-	0/6/71/72	0/4/4/4
8	4QM	J	1504	-	-	4/7/72/72	1/4/4/4
8	4QM	L	701	-	-	5/7/72/72	1/4/4/4

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1504	4QM	C3-C19	17.75	1.83	1.53
8	L	701	4QM	C3-C19	17.54	1.82	1.53
8	I	1401	4QM	C3-C19	17.53	1.82	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1504	4QM	C3-C4	11.76	1.73	1.53
8	I	1401	4QM	C3-C4	11.63	1.72	1.53
8	L	701	4QM	C3-C4	11.52	1.72	1.53
8	L	701	4QM	C5-C4	-9.35	1.39	1.54
8	I	1401	4QM	C5-C4	-9.29	1.40	1.54
8	J	1504	4QM	C5-C4	-9.20	1.40	1.54
8	J	1504	4QM	C2-C19	-8.23	1.41	1.56
8	I	1401	4QM	C2-C19	-7.94	1.41	1.56
8	L	701	4QM	C2-C19	-7.92	1.41	1.56
8	J	1504	4QM	C8-C7	6.19	1.71	1.54
8	L	701	4QM	C8-C7	6.12	1.70	1.54
8	I	1401	4QM	C8-C7	6.08	1.70	1.54
8	I	1401	4QM	C5-C6	-4.16	1.48	1.55
8	J	1504	4QM	C5-C6	-4.15	1.48	1.55
8	I	1401	4QM	O4-C4	-4.13	1.36	1.43
8	L	701	4QM	C5-C6	-4.09	1.48	1.55
8	L	701	4QM	O4-C4	-4.09	1.36	1.43
8	J	1504	4QM	O4-C4	-4.06	1.36	1.43
8	J	1504	4QM	C18-C6	-4.04	1.46	1.53
8	I	1401	4QM	C18-C6	-3.96	1.46	1.53
8	L	701	4QM	C18-C6	-3.78	1.46	1.53
8	J	1504	4QM	C7-C6	3.50	1.61	1.54
8	L	701	4QM	C7-C6	3.45	1.61	1.54
8	I	1401	4QM	C7-C6	3.24	1.61	1.54
8	I	1401	4QM	C5-C9	3.19	1.61	1.55
8	I	1401	4QM	C14-C15	-3.13	1.48	1.53
8	L	701	4QM	C5-C9	3.05	1.60	1.55
8	L	701	4QM	C2-C15	3.00	1.60	1.55
8	J	1504	4QM	C14-C15	-3.00	1.49	1.53
8	J	1504	4QM	C5-C9	2.96	1.60	1.55
8	I	1401	4QM	C2-C15	2.91	1.60	1.55
8	L	701	4QM	C14-C15	-2.90	1.49	1.53
8	J	1504	4QM	C2-C15	2.83	1.60	1.55
8	L	701	4QM	C14-C13	2.69	1.56	1.51
8	J	1504	4QM	C14-C13	2.49	1.56	1.51
8	I	1401	4QM	O2-C13	-2.27	1.36	1.43
8	L	701	4QM	O2-C13	-2.21	1.36	1.43
8	J	1504	4QM	O2-C13	-2.19	1.36	1.43
8	I	1401	4QM	C14-C13	2.17	1.55	1.51
8	L	701	4QM	C10-C5	2.10	1.57	1.54
8	I	1401	4QM	C20-C9	-2.06	1.50	1.54
8	J	1504	4QM	C16-C15	2.04	1.57	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	701	4QM	C9-C5-C4	-7.45	110.86	117.67
8	J	1504	4QM	C9-C5-C4	-7.12	111.17	117.67
8	L	701	4QM	C6-C5-C4	6.85	113.78	107.40
8	I	1401	4QM	C9-C5-C4	-6.54	111.70	117.67
8	L	701	4QM	C7-C6-C18	-5.62	110.47	118.33
8	I	1401	4QM	C7-C6-C18	-5.51	110.62	118.33
8	J	1504	4QM	C6-C5-C4	5.25	112.29	107.40
8	J	1504	4QM	C7-C6-C18	-5.19	111.08	118.33
8	J	1504	4QM	C5-C9-C20	-4.98	113.55	119.50
8	J	1504	4QM	C19-C3-C4	-4.36	108.54	114.30
8	I	1401	4QM	C6-C5-C4	4.36	111.47	107.40
8	I	1401	4QM	C19-C3-C4	-4.28	108.64	114.30
8	L	701	4QM	C19-C3-C4	-4.26	108.67	114.30
8	L	701	4QM	C15-C16-C17	-3.92	110.14	114.46
8	J	1504	4QM	C21-C20-C9	-3.82	107.07	112.92
8	J	1504	4QM	C19-C18-C17	-3.65	107.51	111.88
8	L	701	4QM	C3-C19-C2	-3.29	110.34	113.73
8	L	701	4QM	C5-C9-C20	-3.15	115.73	119.50
8	I	1401	4QM	C3-C19-C18	-2.77	106.82	110.88
8	J	1504	4QM	C3-C19-C2	-2.69	110.96	113.73
8	I	1401	4QM	C9-C5-C6	2.56	102.67	100.09
8	J	1504	4QM	C14-C15-C2	-2.56	109.94	112.66
8	I	1401	4QM	C5-C9-C20	-2.43	116.59	119.50
8	J	1504	4QM	C22-C20-C9	2.40	115.23	110.28
8	J	1504	4QM	C15-C14-C13	-2.39	109.25	112.76
8	J	1504	4QM	C1-C2-C19	-2.34	107.67	111.35
8	L	701	4QM	C16-C15-C2	-2.25	110.27	112.66
8	I	1401	4QM	C19-C18-C17	-2.13	109.33	111.88
8	J	1504	4QM	C9-C5-C6	2.12	102.23	100.09
8	I	1401	4QM	C21-C20-C9	-2.09	109.72	112.92
8	I	1401	4QM	C16-C15-C2	-2.07	110.45	112.66
8	L	701	4QM	C5-C6-C18	2.07	117.38	114.74
8	L	701	4QM	C21-C20-C9	-2.04	109.80	112.92

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	J	1504	4QM	C22-C20-C9-C5
8	J	1504	4QM	C21-C20-C9-C8
8	J	1504	4QM	C22-C20-C9-C8

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Mol	Chain	Res	Type	Atoms
8	J	1504	4QM	C21-C20-C9-C5
8	L	701	4QM	C21-C20-C9-C5
8	L	701	4QM	C9-C20-C22-C23
8	L	701	4QM	C22-C20-C9-C5
8	L	701	4QM	C21-C20-C9-C8
8	L	701	4QM	C22-C20-C9-C8

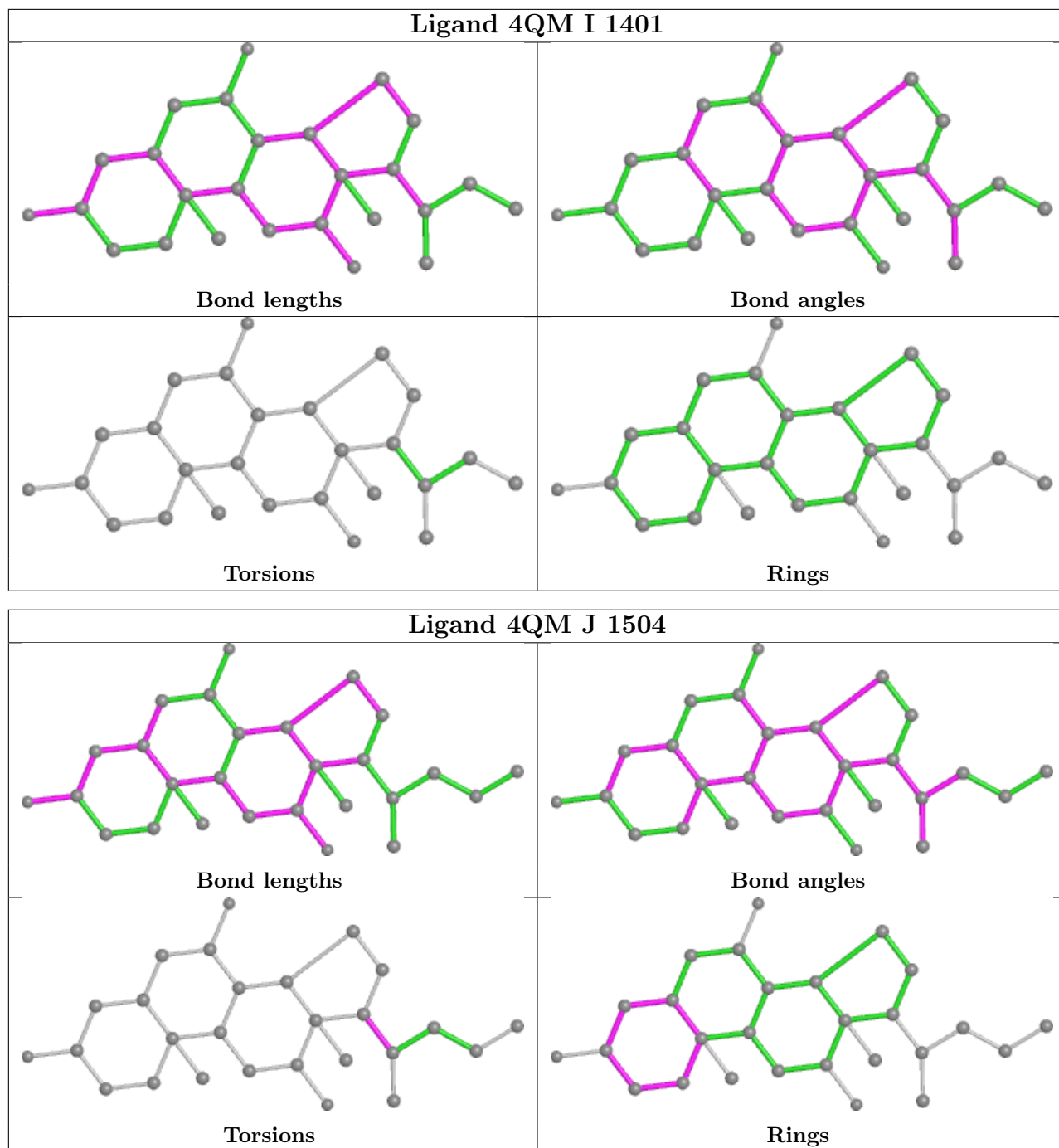
All (2) ring outliers are listed below:

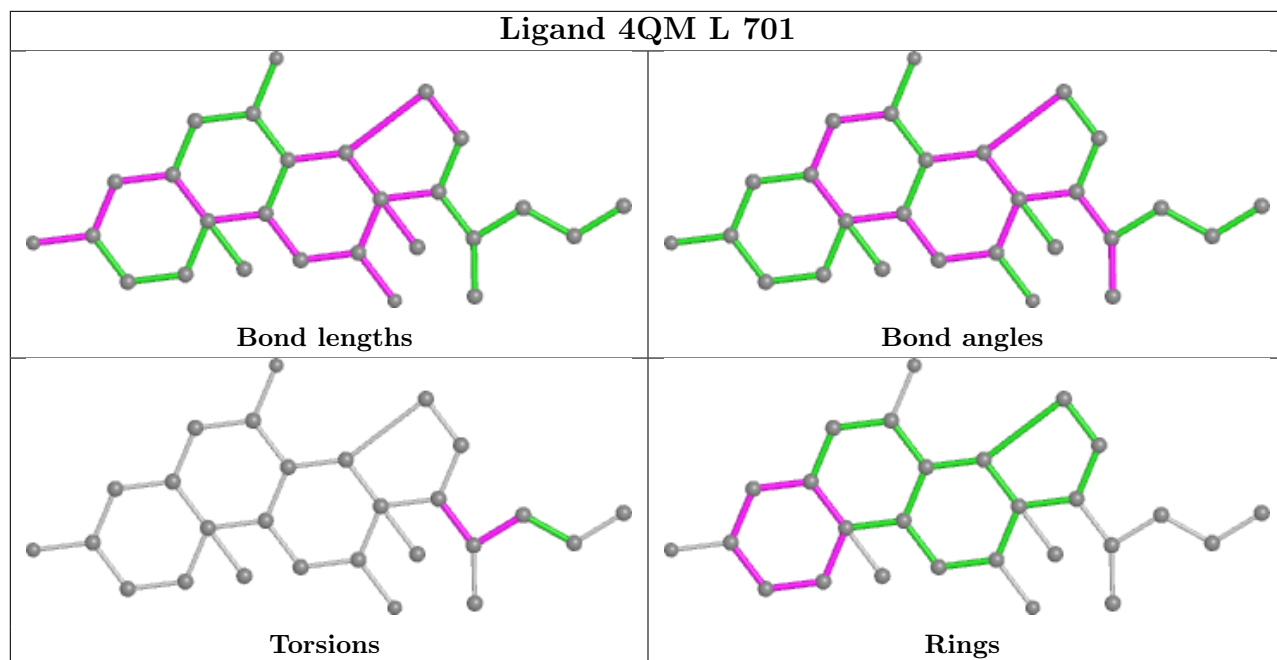
Mol	Chain	Res	Type	Atoms
8	J	1504	4QM	C1-C12-C13-C14-C15-C2
8	L	701	4QM	C1-C12-C13-C14-C15-C2

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1401	4QM	3	0
8	J	1504	4QM	4	0
8	L	701	4QM	4	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	2
5	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	1009:ASN	C	1010:GLN	N	4.89
1	L	586:ARG	C	587:ILE	N	4.05
1	I	996:ARG	C	997:TRP	N	3.59



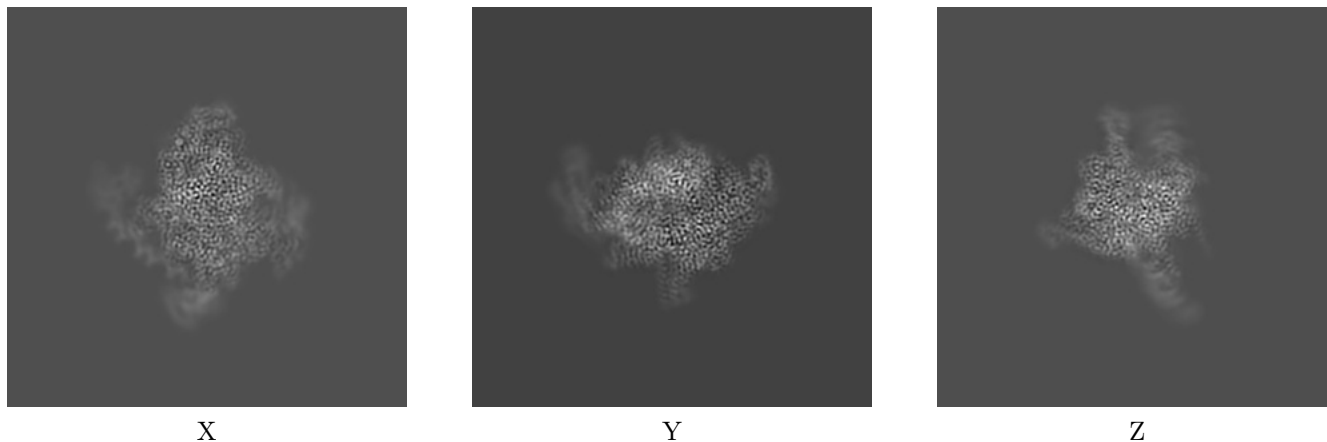
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41437. These allow visual inspection of the internal detail of the map and identification of artifacts.

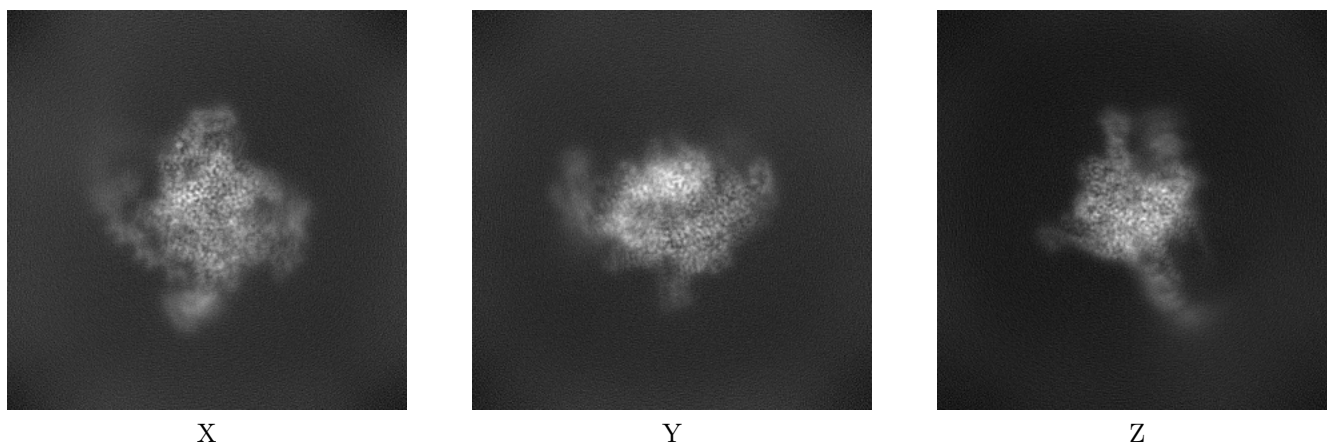
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



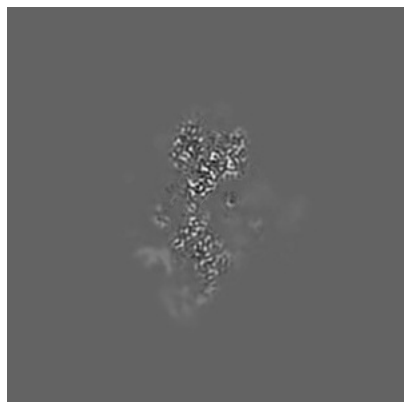
#### 6.1.2 Raw map



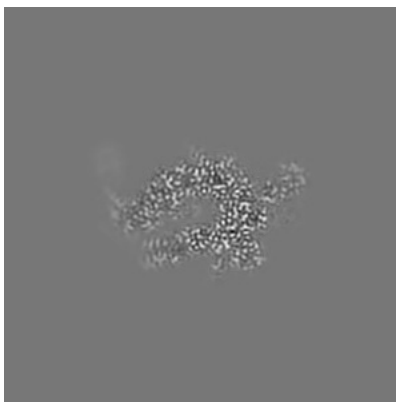
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

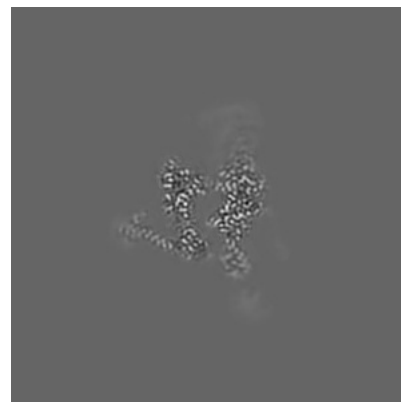
### 6.2.1 Primary map



X Index: 192

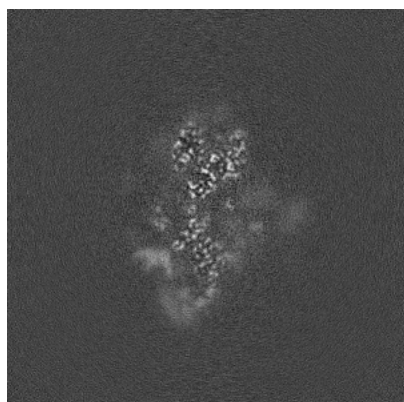


Y Index: 192

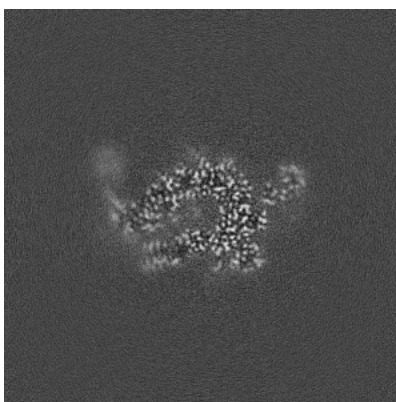


Z Index: 192

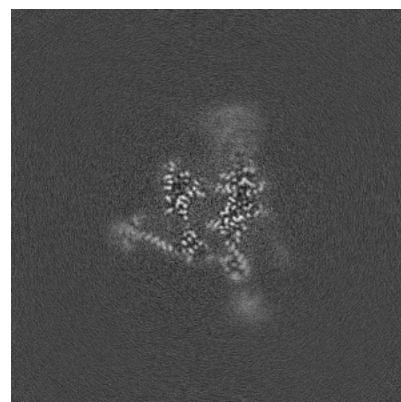
### 6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

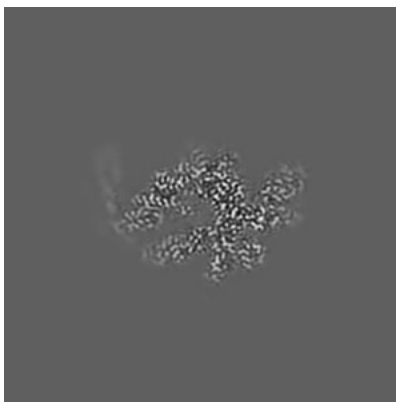
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

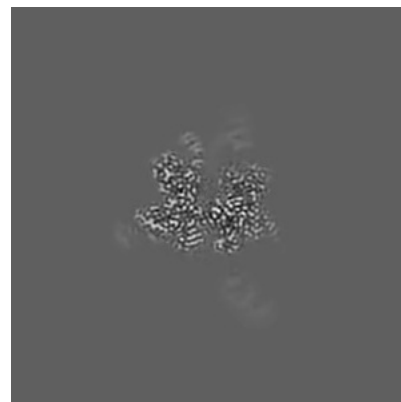
### 6.3.1 Primary map



X Index: 171

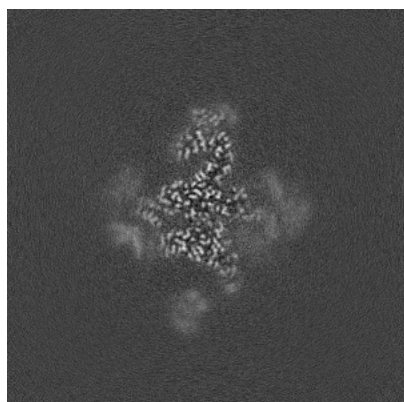


Y Index: 186

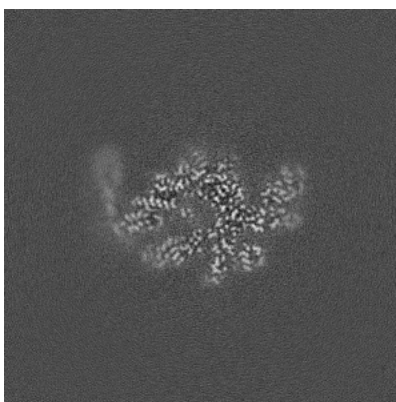


Z Index: 206

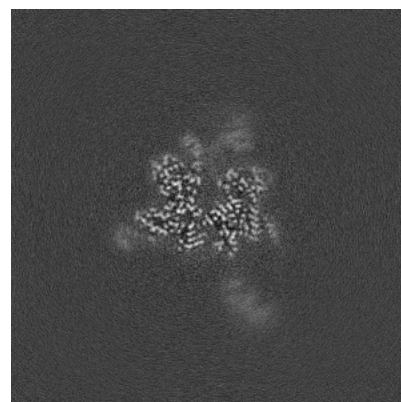
### 6.3.2 Raw map



X Index: 210



Y Index: 186

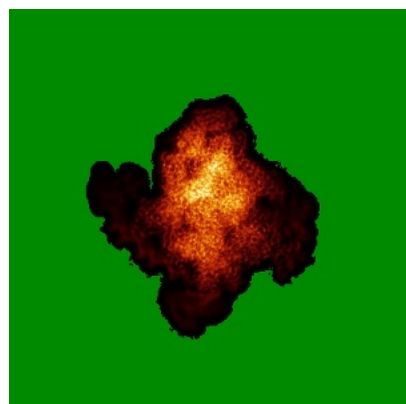


Z Index: 205

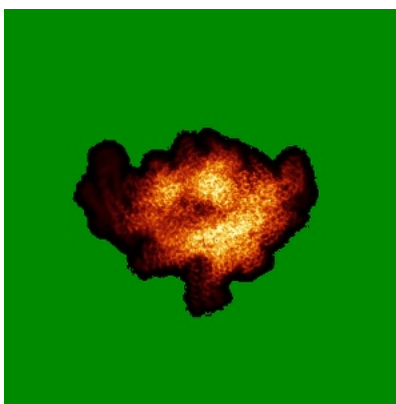
The images above show the largest variance slices of the map in three orthogonal directions.

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

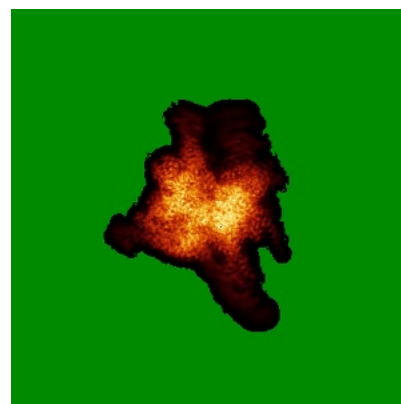
### 6.4.1 Primary map



X

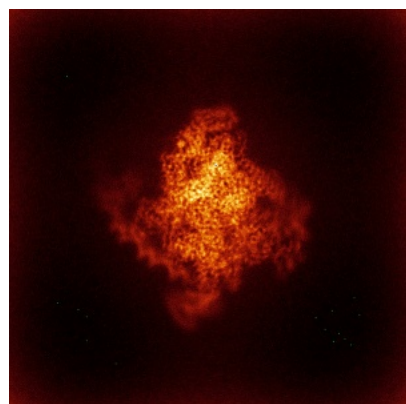


Y

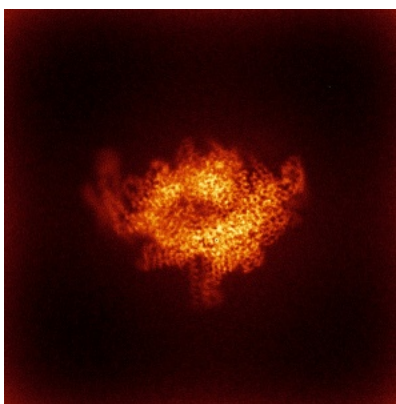


Z

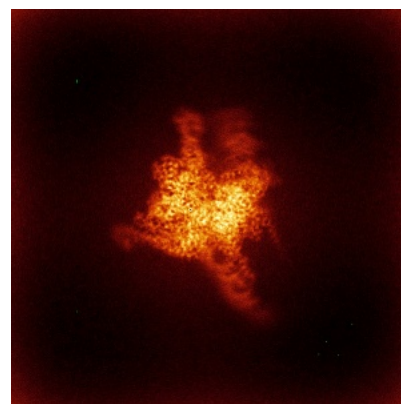
### 6.4.2 Raw map



X



Y

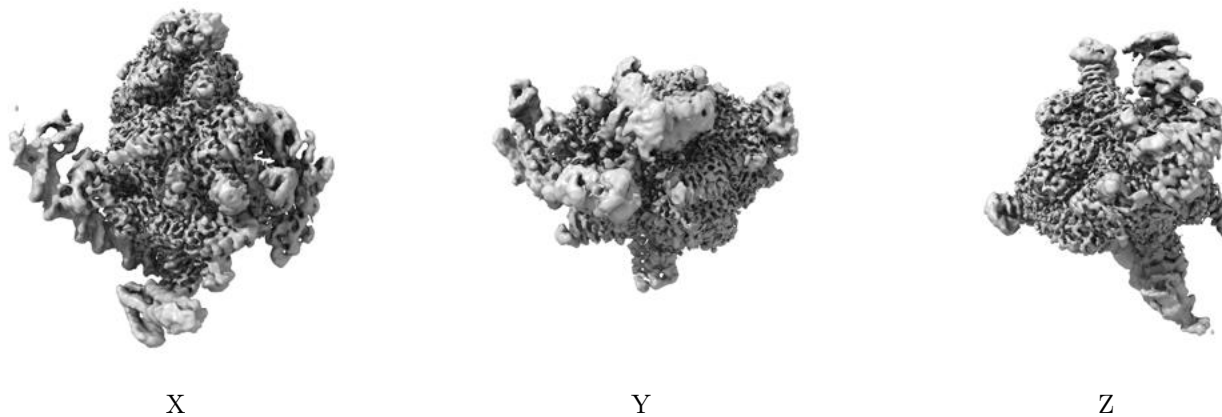


Z

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.

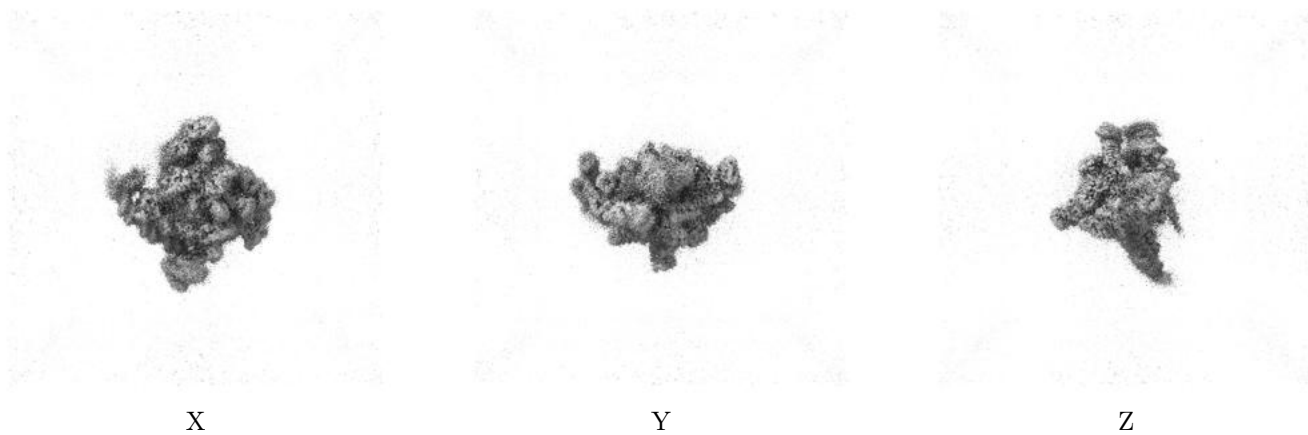
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

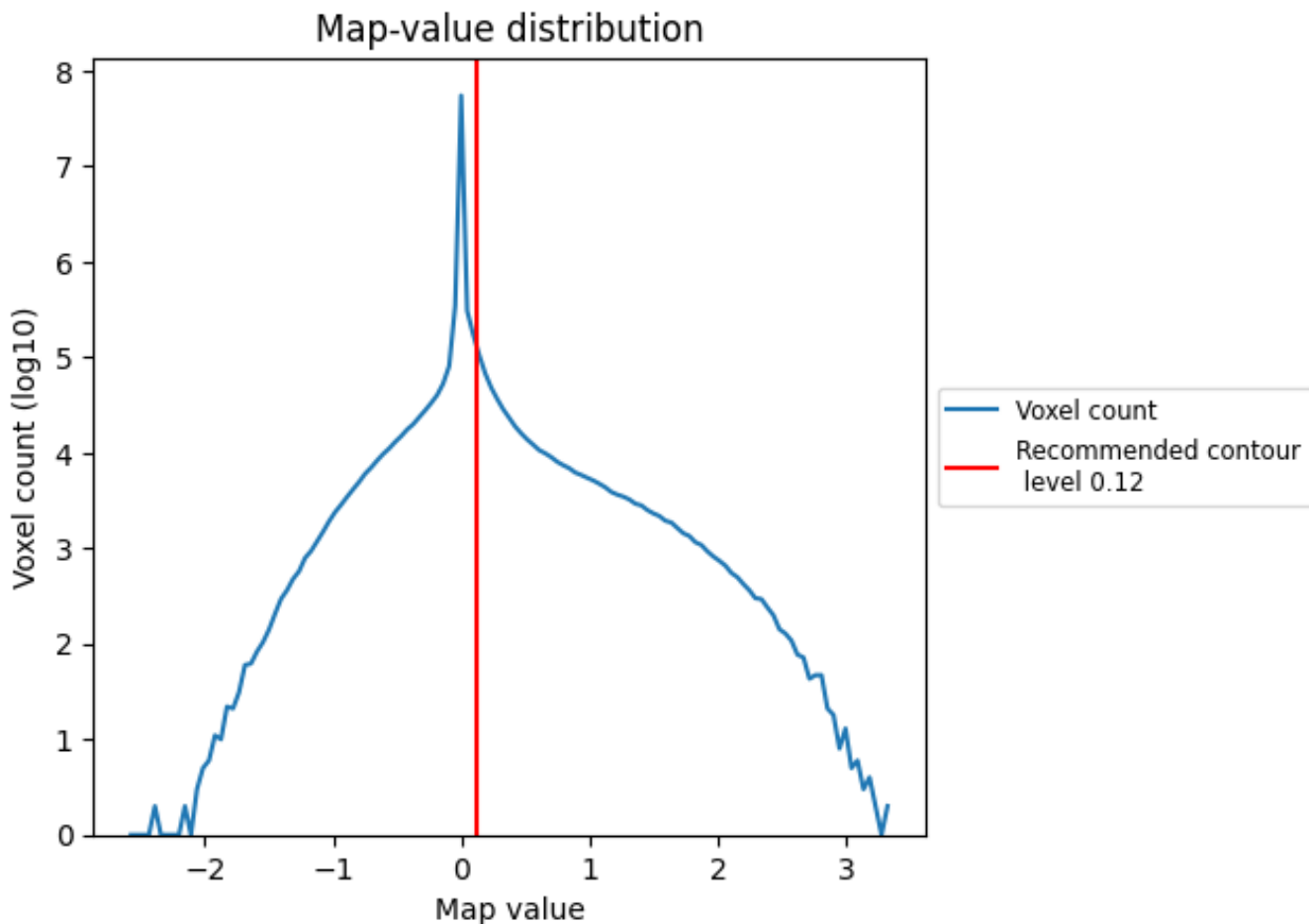
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

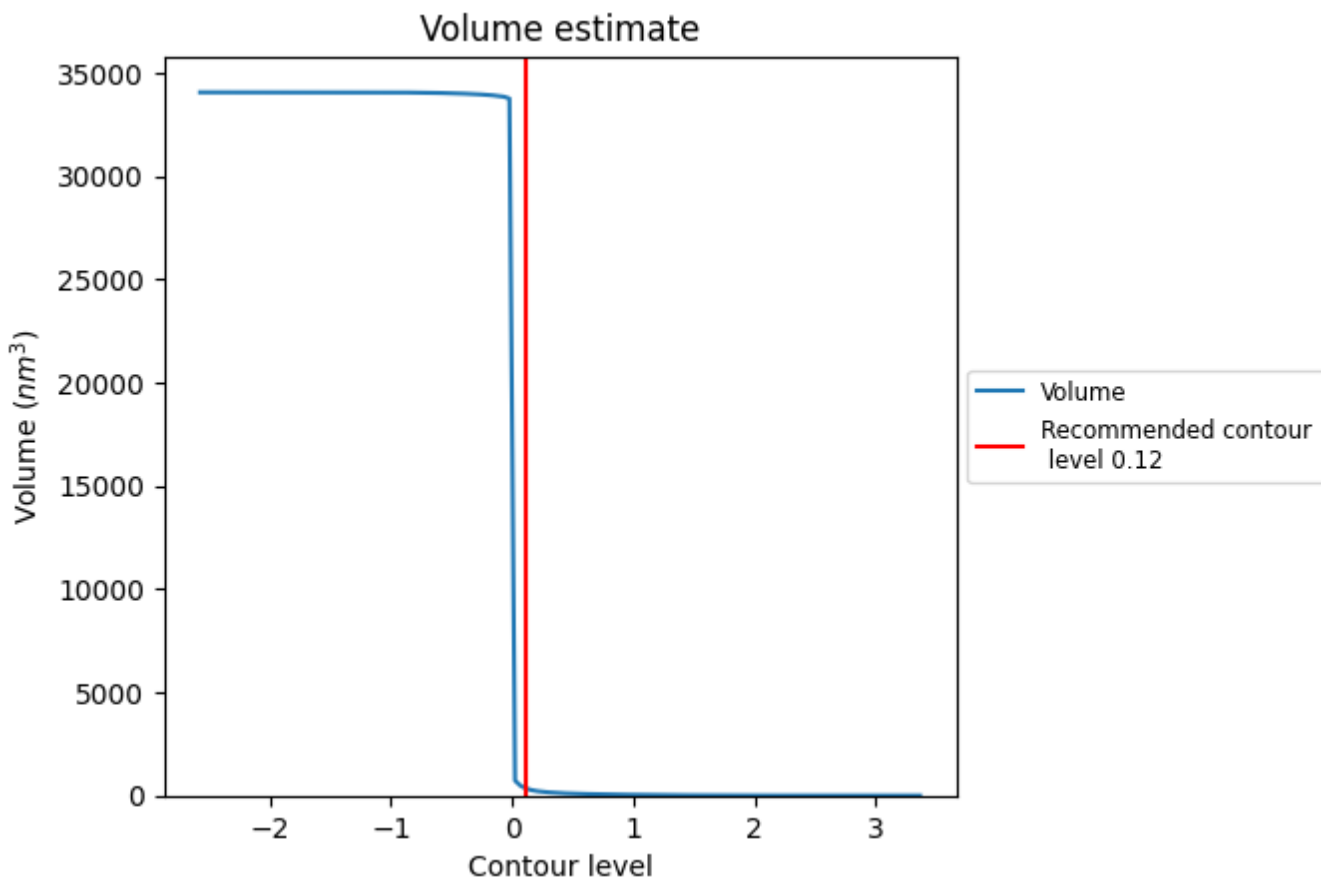
This section contains the results of statistical analysis of the map.

### 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.

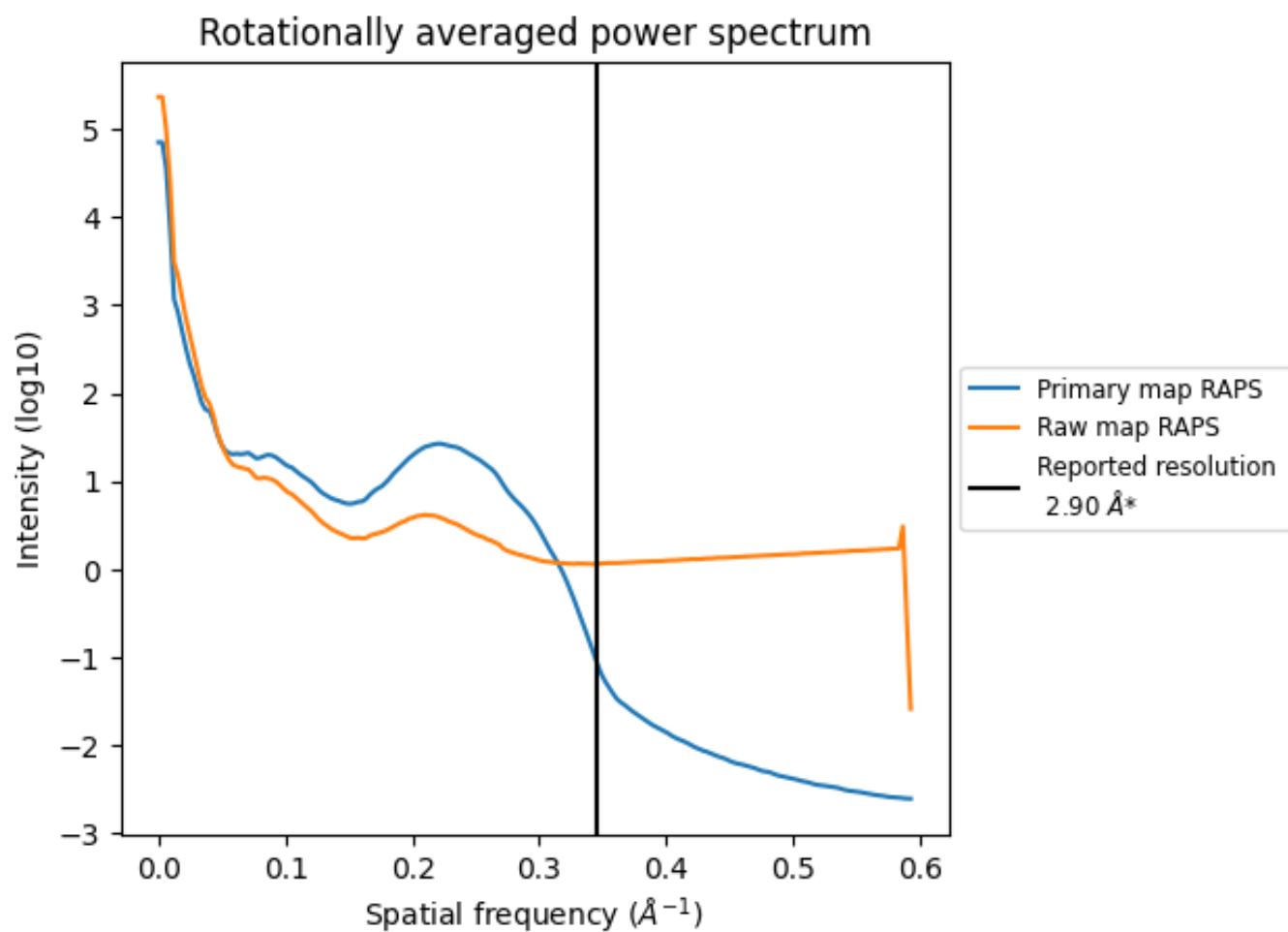
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 336 nm<sup>3</sup>; this corresponds to an approximate mass of 303 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 i



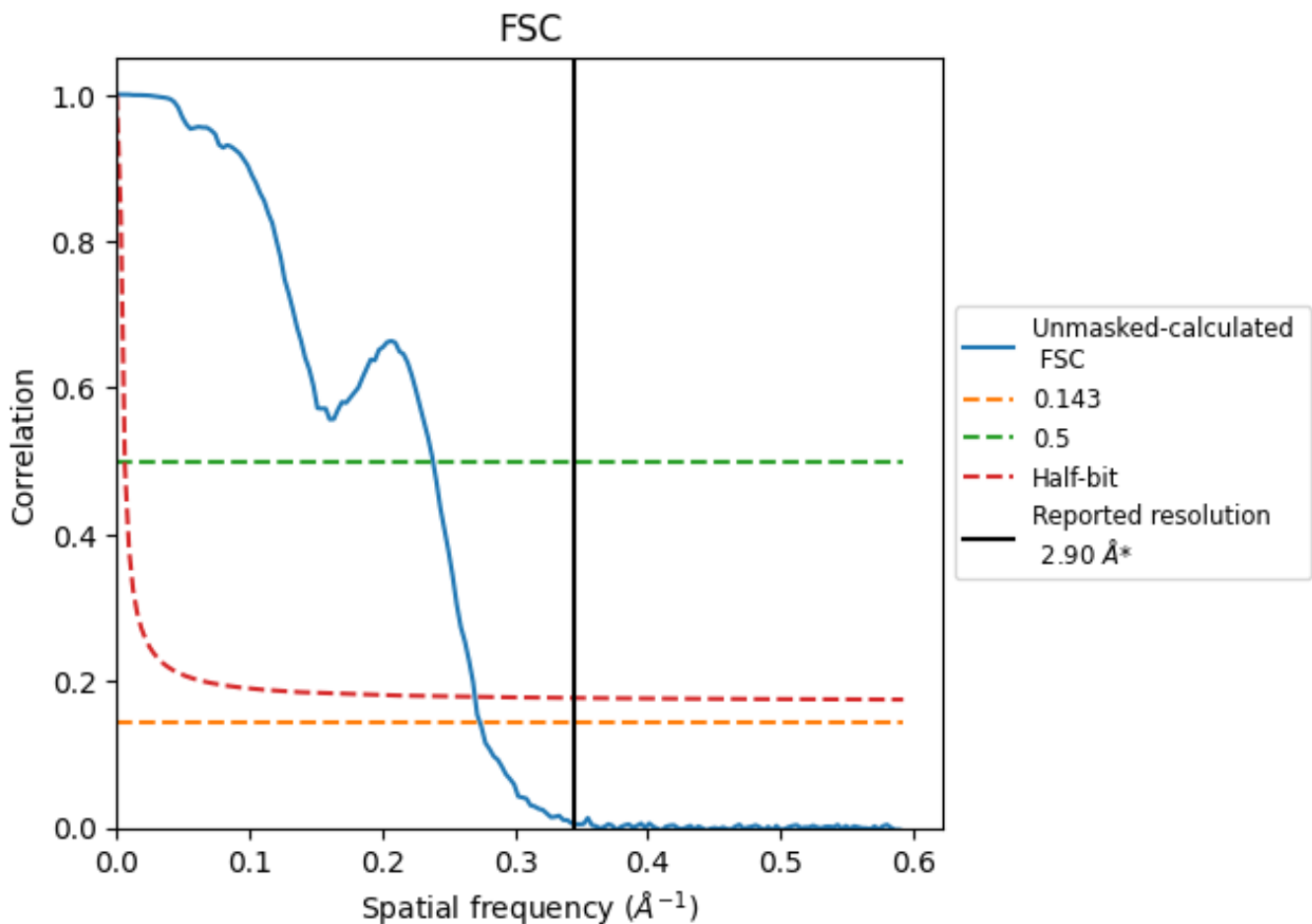
\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>



## 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 0.345 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

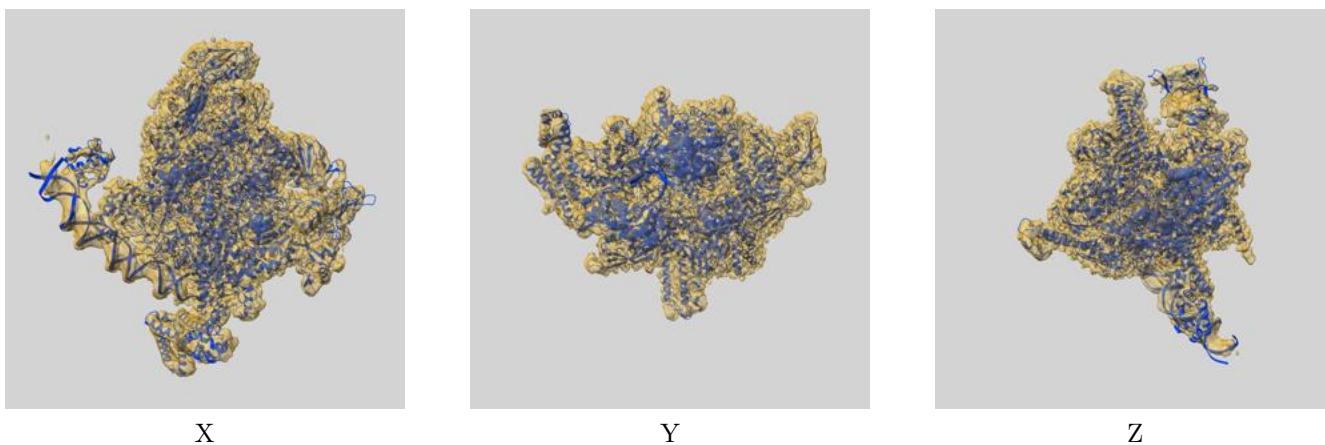
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.65	4.20	3.71

\*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 3.65 differs from the reported value 2.9 by more than 10 %

## 9 Map-model fit [i](#)

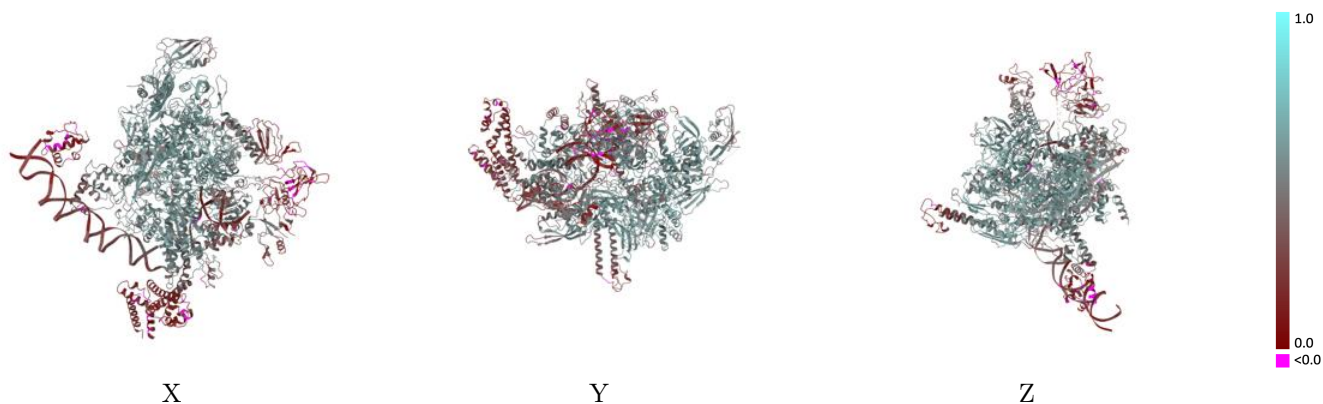
This section contains information regarding the fit between EMDB map EMD-41437 and PDB model 8TO6. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



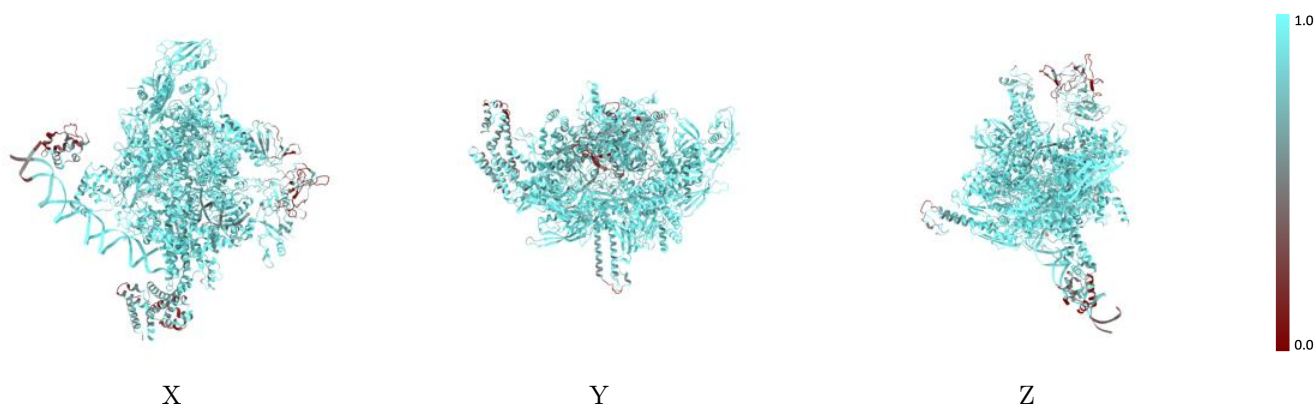
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



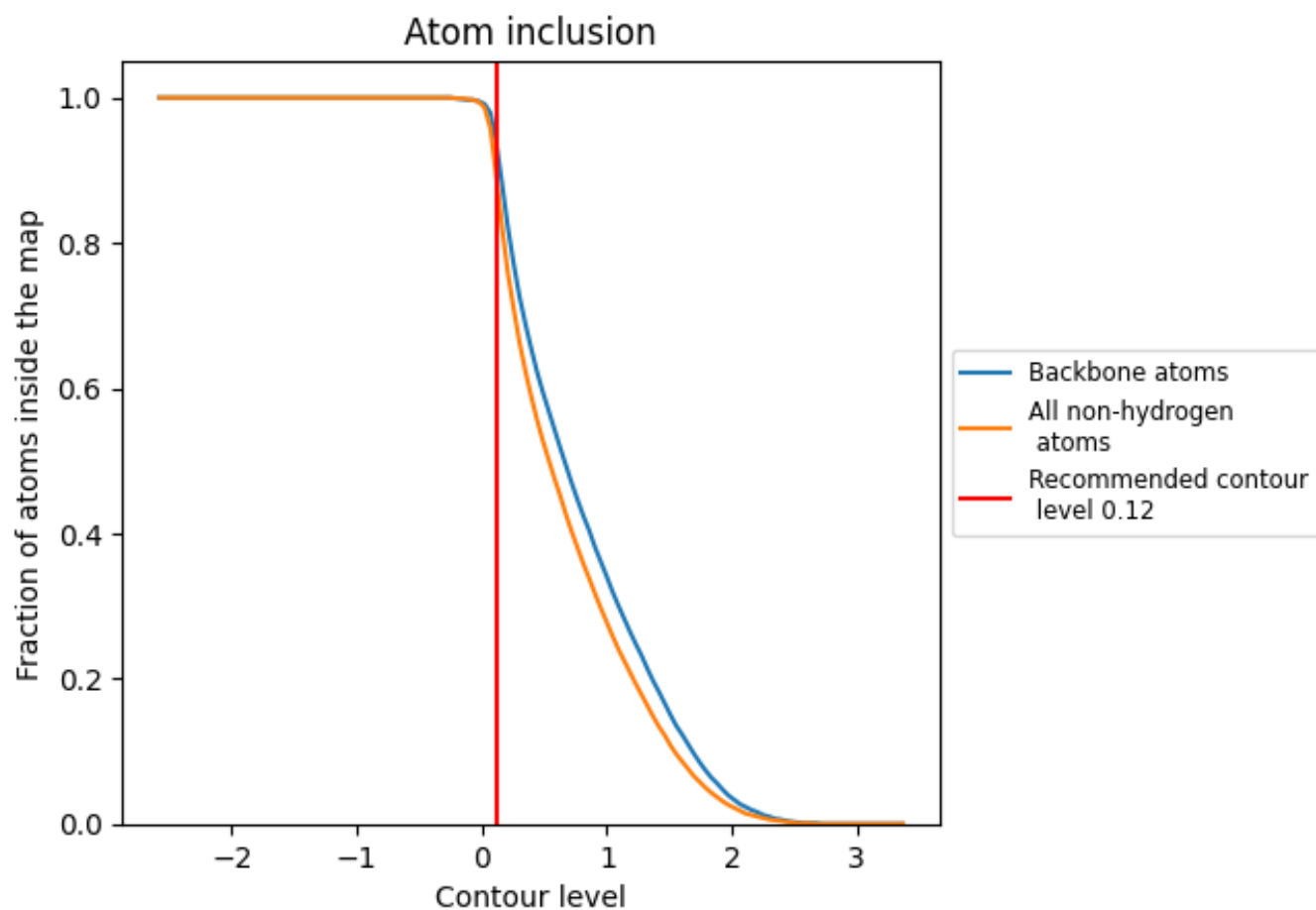
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).





















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.4650
G	 0.9630	 0.5610
H	 0.9380	 0.5150
I	 0.9350	 0.5240
J	 0.8840	 0.4790
K	 0.9360	 0.5380
L	 0.8100	 0.3460
M	 0.3860	 0.1280
O	 0.8000	 0.2610
P	 0.8590	 0.2480

