



Full wwPDB EM Validation Report ⓘ

Nov 16, 2024 – 01:24 PM EST

PDB ID : 8TOM
EMDB ID : EMD-41456
Title : Escherichia coli RNA polymerase closed complex intermediate at the lambda PR promoter
Authors : Darst, S.A.; Saecker, R.M.; Mueller, A.U.
Deposited on : 2023-08-03
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

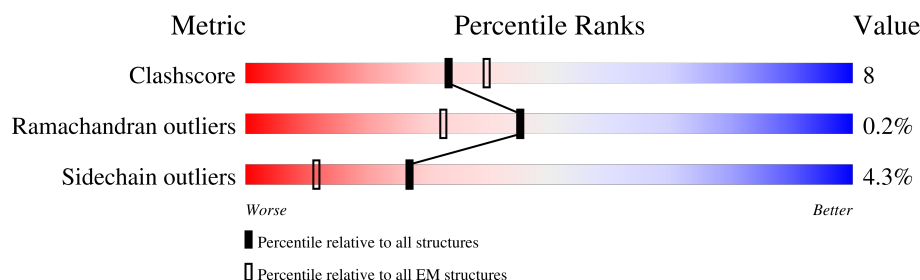
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	<div> <div>6%</div> <div>53%</div> <div>17%</div> <div>30%</div> </div>
1	H	329	<div> <div>11%</div> <div>51%</div> <div>14%</div> <div>33%</div> </div>
1	M	329	<div> <div>22%</div> <div>18%</div> <div>5%</div> <div>78%</div> </div>
2	I	1342	<div> <div>25%</div> <div>79%</div> <div>19%</div> <div>•</div> </div>
3	J	1407	<div> <div>27%</div> <div>78%</div> <div>16%</div> <div>•</div> <div>5%</div> </div>
4	K	91	<div> <div>25%</div> <div>71%</div> <div>10%</div> <div>19%</div> </div>
5	L	613	<div> <div>61%</div> <div>72%</div> <div>17%</div> <div>•</div> <div>10%</div> </div>
6	O	90	<div> <div>29%</div> <div>28%</div> <div>17%</div> <div>56%</div> </div>

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Mol	Chain	Length	Quality of chain
7	P	90	<div><div><div></div><div></div><div></div></div><div>31%36%9%56%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 31753 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	231	Total	C	N	O	S	0	0
			1773	1107	315	345	6		
1	H	219	Total	C	N	O	S	0	0
			1684	1052	295	331	6		
1	M	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
			10563	6629	1841	2050	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1338	Total	C	N	O	S	0	0
			10402	6536	1854	1962	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	74	Total	C	N	O	S	0	0
			595	362	113	119	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	552	Total	C	N	O	S	0	0
			4413	2758	775	853	27		

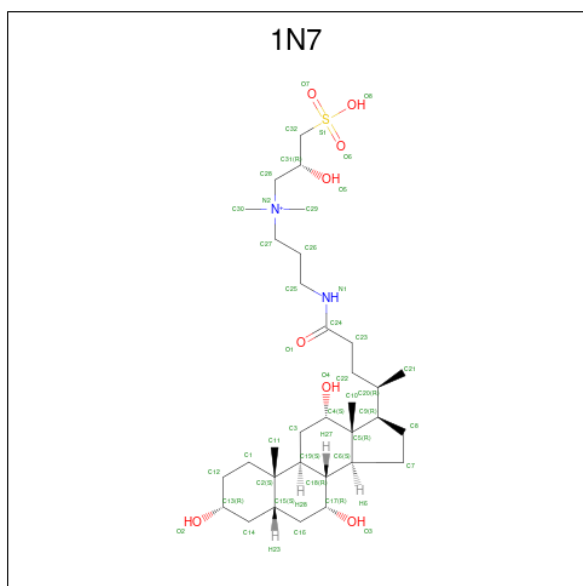
- Molecule 6 is a DNA chain called Nontemplate strand of lambda PR promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	40	Total	C	N	O	P	0	0
			821	392	142	247	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	40	Total	C	N	O	P	0	0
			819	389	157	233	40		

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



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

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

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

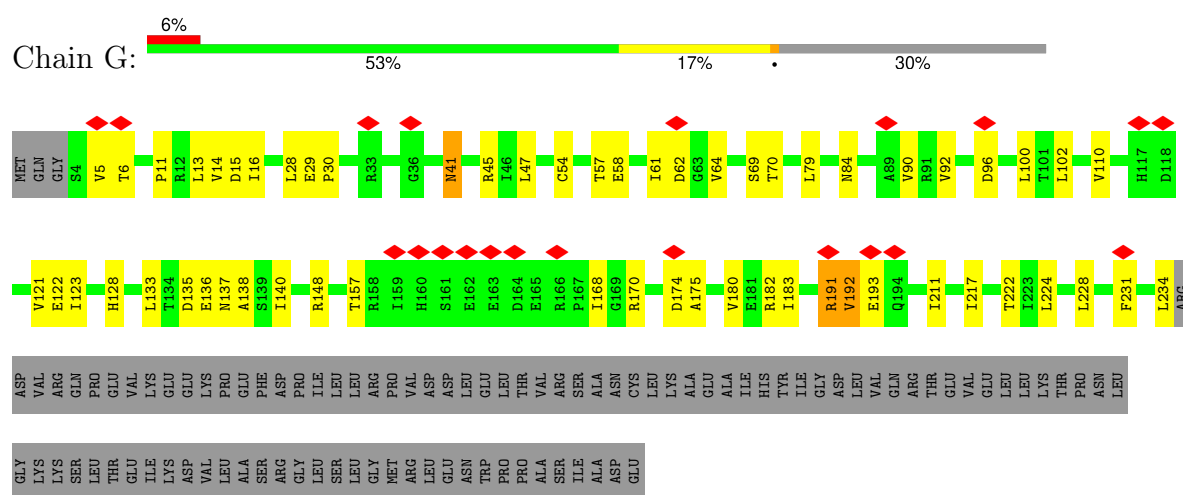
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

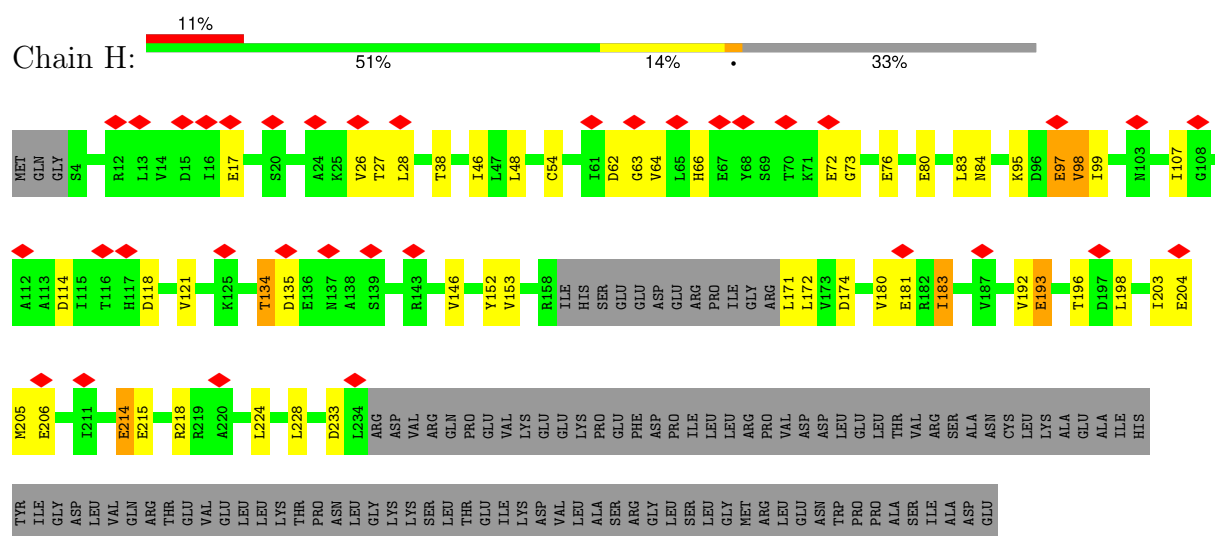
3 Residue-property plots

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



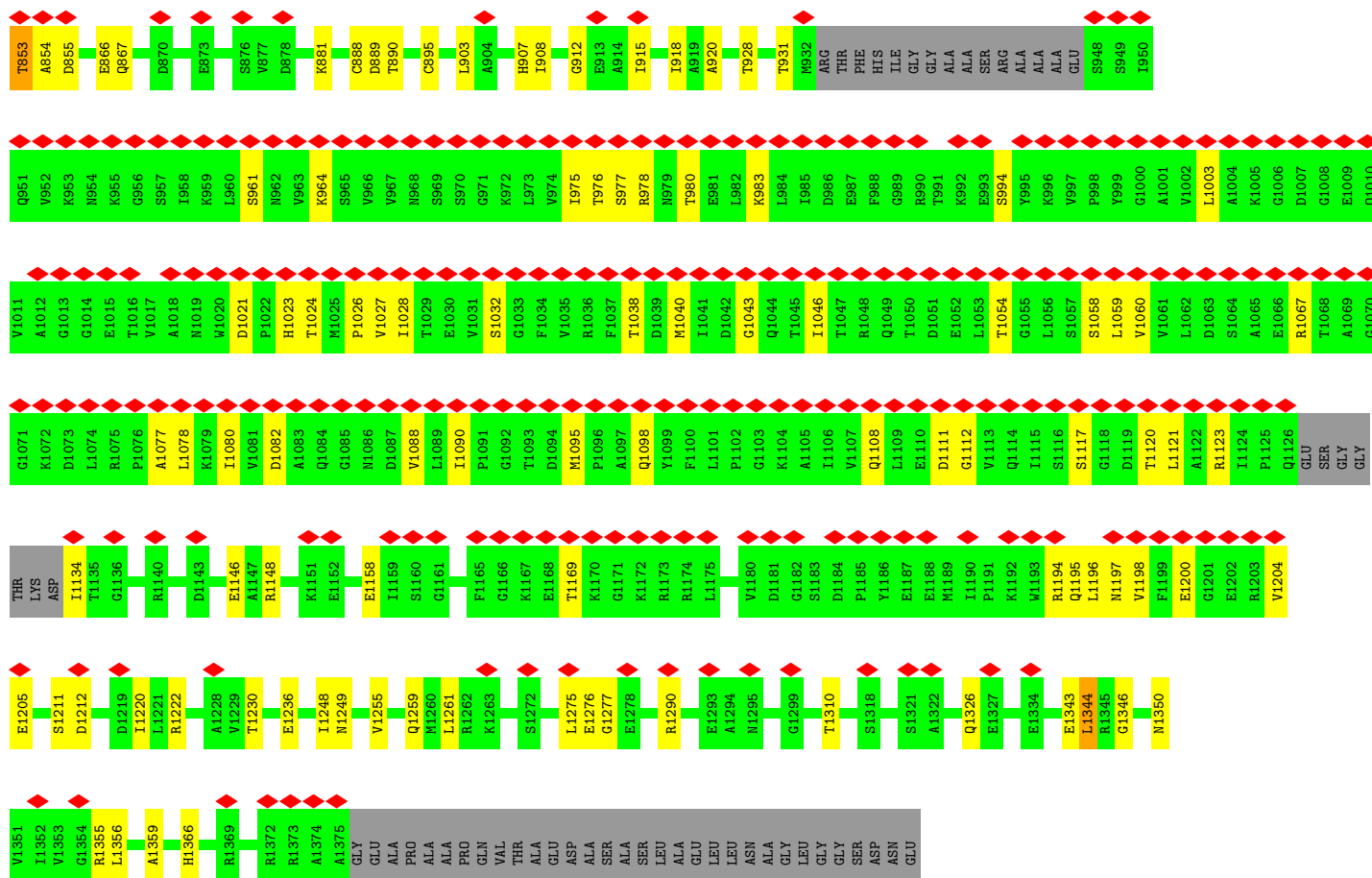
- Molecule 1: DNA-directed RNA polymerase subunit alpha



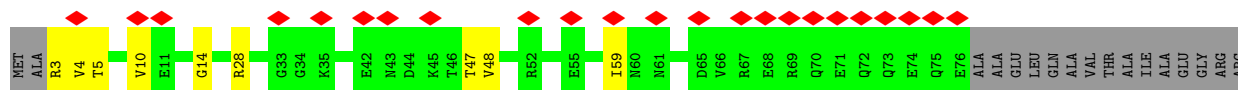
- Molecule 1: DNA-directed RNA polymerase subunit alpha



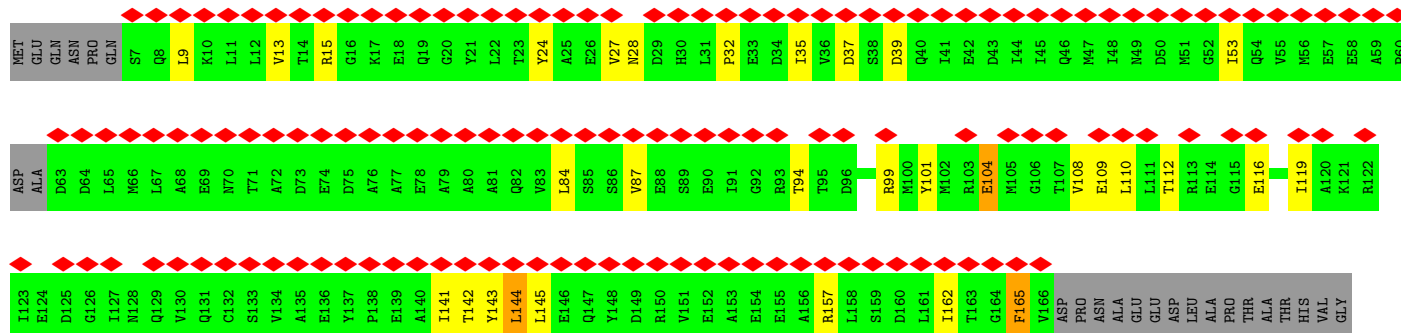


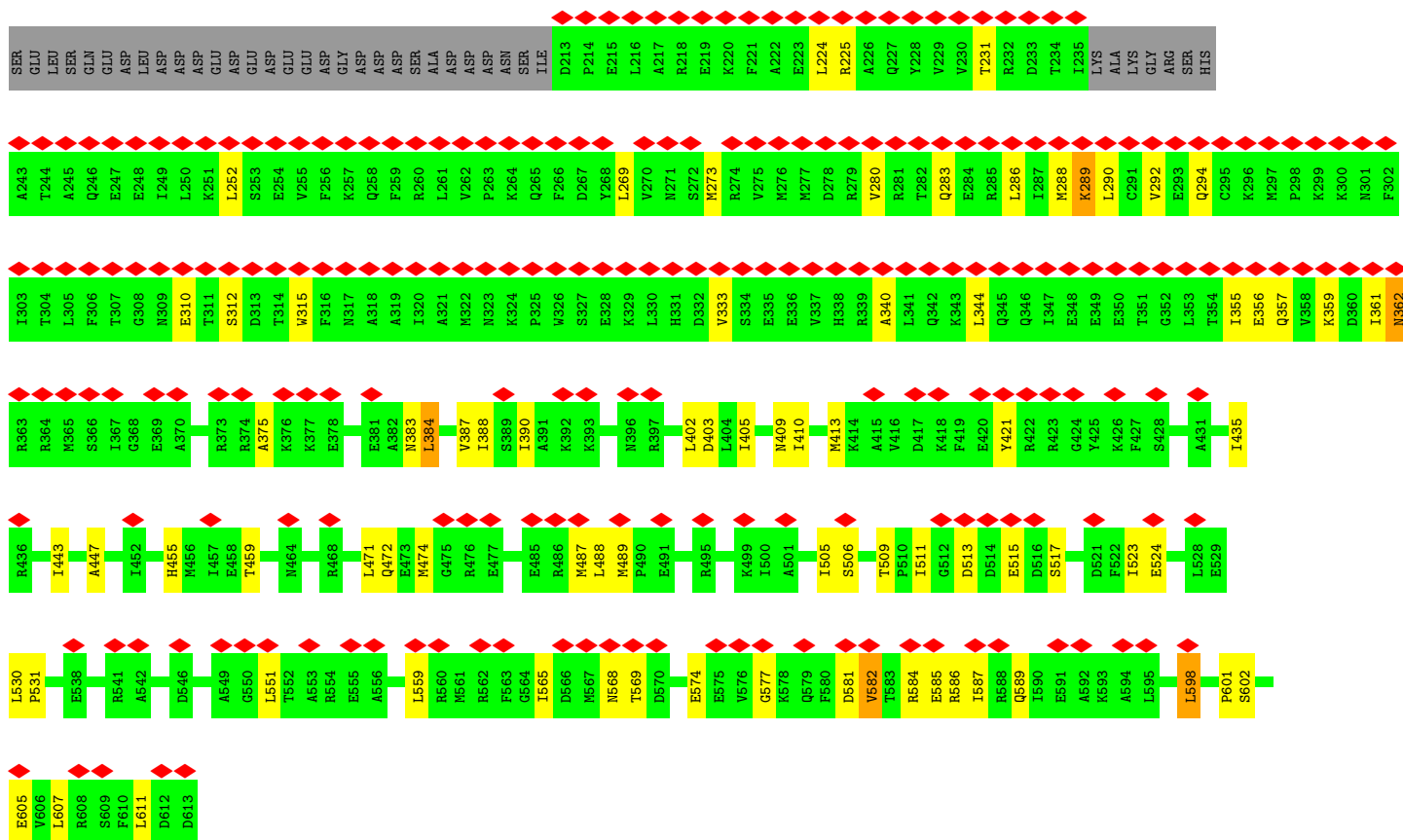


• Molecule 4: DNA-directed RNA polymerase subunit omega

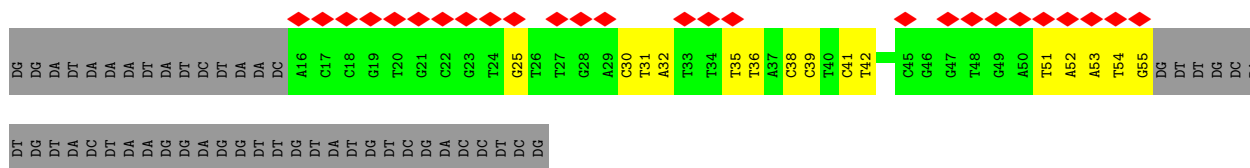
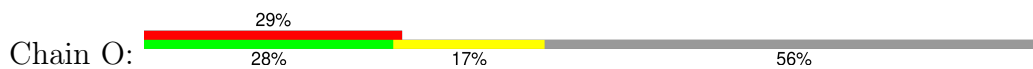


• Molecule 5: RNA polymerase sigma factor RpoD

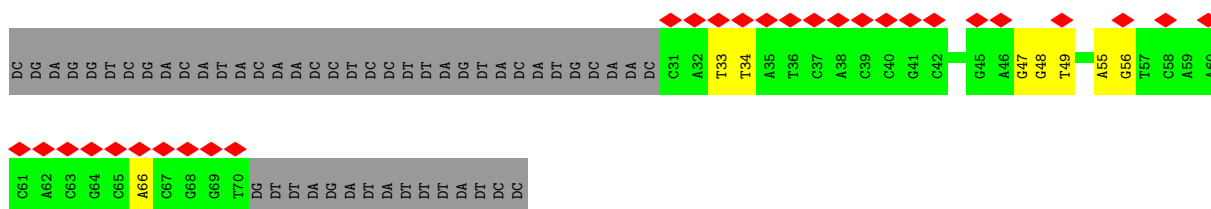
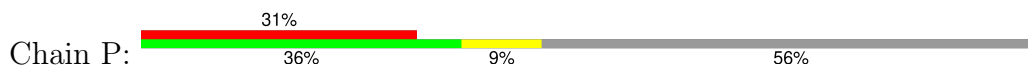




- Molecule 6: Nontemplate strand of lambda PR promoter DNA



- Molecule 7: Template strand of lamdba PR promoter DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	122806	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)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.164	Depositor
Minimum map value	-3.917	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.28	0/1795	0.53	0/2435
1	H	0.26	0/1703	0.52	0/2309
1	M	0.23	0/579	0.50	0/784
2	I	0.29	0/10732	0.50	0/14482
3	J	0.28	0/10559	0.52	0/14257
4	K	0.25	0/597	0.50	0/803
5	L	0.25	0/4468	0.50	0/6016
6	O	0.53	0/918	0.95	0/1416
7	P	0.54	0/920	0.86	0/1416
All	All	0.30	0/32271	0.55	0/43918

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	1
3	J	0	3
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	57	PHE	Peptide
3	J	120	LEU	Peptide

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Mol	Chain	Res	Type	Group
3	J	585	LYS	Peptide
3	J	853	THR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1773	0	1800	42	0
1	H	1684	0	1709	36	0
1	M	572	0	602	11	0
2	I	10563	0	10581	168	0
3	J	10402	0	10625	150	0
4	K	595	0	602	6	0
5	L	4413	0	4416	80	0
6	O	821	0	455	9	0
7	P	819	0	448	6	0
8	I	54	0	75	26	0
8	J	27	0	39	10	0
8	L	27	0	38	14	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
All	All	31753	0	31390	510	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 (510) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:1402:1N7:C3	8:I:1402:1N7:C19	1.82	1.56
8:J:1504:1N7:C3	8:J:1504:1N7:C19	1.83	1.55
8:L:701:1N7:C3	8:L:701:1N7:C19	1.82	1.52
8:I:1401:1N7:C3	8:I:1401:1N7:C19	1.82	1.51
1:G:100:LEU:HD21	1:G:121:VAL:HG21	1.46	0.98
2:I:201:ARG:O	5:L:28:ASN:ND2	2.08	0.86
2:I:528:ARG:NH2	2:I:576:SER:O	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:966:ILE:HG12	8:I:1402:1N7:H7	1.63	0.80
3:J:17:PHE:O	3:J:1355:ARG:NH2	2.15	0.79
1:G:45:ARG:NH2	2:I:1084:ASP:OD1	2.15	0.79
2:I:106:GLU:N	2:I:113:THR:O	2.16	0.78
2:I:318:SER:OG	2:I:320:ASP:OD1	2.02	0.78
2:I:560:PRO:O	3:J:780:ARG:NH2	2.16	0.78
3:J:709:ARG:NH1	3:J:710:ASP:OD2	2.16	0.78
3:J:1058:SER:OG	3:J:1108:GLN:OE1	2.01	0.78
5:L:601:PRO:O	5:L:602:SER:OG	2.01	0.77
1:H:48:LEU:HD13	1:H:183:ILE:HD11	1.66	0.77
3:J:79:LYS:HB2	5:L:569:THR:HG22	1.68	0.76
3:J:853:THR:O	3:J:855:ASP:N	2.18	0.76
5:L:109:GLU:OE1	5:L:109:GLU:N	2.18	0.75
1:M:298:LYS:NZ	7:P:66:DA:OP1	2.20	0.75
2:I:1240:ASP:OD1	2:I:1240:ASP:N	2.20	0.73
8:I:1401:1N7:C3	8:I:1401:1N7:C2	2.66	0.73
3:J:978:ARG:NH2	3:J:1197:ASN:O	2.21	0.73
3:J:591:ILE:HG22	3:J:592:VAL:HG13	1.72	0.72
8:J:1504:1N7:C3	8:J:1504:1N7:C2	2.66	0.72
1:H:192:VAL:HG12	1:H:193:GLU:H	1.53	0.71
3:J:268:LEU:HD21	3:J:324:LEU:HD11	1.72	0.71
1:M:295:LEU:HD21	1:M:300:LEU:HD23	1.71	0.71
3:J:475:GLU:OE2	4:K:28:ARG:NH2	2.23	0.71
3:J:964:LYS:O	3:J:976:THR:OG1	2.06	0.71
3:J:1032:SER:OG	3:J:1117:SER:N	2.23	0.71
1:G:5:VAL:O	1:G:6:THR:OG1	2.07	0.71
2:I:966:ILE:HD11	8:I:1402:1N7:H26	1.73	0.70
1:M:262:LEU:HD21	1:M:306:VAL:HG11	1.73	0.70
2:I:1103:VAL:HG11	2:I:1112:ILE:CD1	2.21	0.70
2:I:728:ASP:OD1	2:I:729:ALA:N	2.24	0.70
3:J:500:ILE:O	3:J:500:ILE:HG22	1.92	0.70
8:I:1402:1N7:C3	8:I:1402:1N7:C2	2.66	0.69
8:L:701:1N7:C3	8:L:701:1N7:C2	2.66	0.69
2:I:1103:VAL:HG11	2:I:1112:ILE:HD12	1.74	0.69
3:J:726:ALA:CB	3:J:737:ILE:HD11	2.23	0.69
8:I:1402:1N7:H5	8:I:1402:1N7:H31	1.74	0.69
2:I:1261:GLY:O	2:I:1263:ALA:N	2.25	0.69
3:J:702:GLN:HG3	3:J:703:THR:HG23	1.73	0.69
2:I:187:GLU:OE1	2:I:187:GLU:N	2.25	0.68
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	1.74	0.68
2:I:758:ARG:NH2	2:I:762:ASN:OD1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:282:VAL:O	1:M:315:GLY:N	2.26	0.68
1:H:95:LYS:NZ	1:H:97:GLU:O	2.26	0.67
5:L:104:GLU:N	5:L:104:GLU:OE1	2.27	0.67
3:J:1158:GLU:OE2	3:J:1222:ARG:NH1	2.28	0.67
8:J:1504:1N7:H5	8:J:1504:1N7:H31	1.76	0.67
5:L:584:ARG:NH1	7:P:56:DG:N7	2.42	0.67
1:H:80:GLU:O	1:H:84:ASN:ND2	2.29	0.65
2:I:651:ASP:OD1	2:I:651:ASP:N	2.27	0.65
2:I:892:GLU:O	2:I:893:THR:OG1	2.08	0.65
1:M:253:LEU:HD21	1:M:312:LEU:HD22	1.78	0.65
2:I:50:GLU:OE1	2:I:54:ARG:NH1	2.29	0.65
2:I:1143:GLU:OE1	2:I:1144:PHE:N	2.30	0.64
5:L:143:TYR:CD2	5:L:269:LEU:HD21	2.33	0.64
3:J:866:GLU:N	3:J:866:GLU:OE1	2.31	0.64
2:I:265:LYS:O	2:I:267:ARG:NH1	2.31	0.63
3:J:661:VAL:HG12	3:J:685:ILE:HD11	1.79	0.63
8:I:1402:1N7:C3	8:I:1402:1N7:C18	2.71	0.63
1:H:98:VAL:HG21	1:H:121:VAL:HG11	1.80	0.62
3:J:262:THR:OG1	3:J:266:ASN:OD1	2.18	0.62
2:I:1002:LEU:HD23	2:I:1003:THR:O	2.00	0.61
1:M:260:LEU:CB	1:M:262:LEU:HD23	2.30	0.61
3:J:975:ILE:HD11	3:J:1003:LEU:HD12	1.81	0.61
3:J:268:LEU:HD21	3:J:324:LEU:CD1	2.31	0.61
3:J:339:ARG:NH2	3:J:1326:GLN:O	2.33	0.61
5:L:101:TYR:OH	5:L:384:LEU:HD13	2.00	0.61
2:I:414:ILE:HG22	2:I:414:ILE:O	2.01	0.61
3:J:678:ARG:NH1	3:J:756:GLU:OE1	2.32	0.61
5:L:505:ILE:CD1	8:L:701:1N7:H25	2.29	0.61
2:I:1043:ALA:HB3	2:I:1046:VAL:HG11	1.83	0.60
3:J:983:LYS:NZ	3:J:994:SER:OG	2.29	0.60
3:J:550:VAL:HG23	3:J:552:ILE:HG23	1.83	0.60
1:G:16:ILE:HG22	1:G:16:ILE:O	2.01	0.60
3:J:762:ASN:OD1	3:J:762:ASN:N	2.31	0.60
5:L:405:ILE:O	5:L:409:ASN:ND2	2.33	0.60
2:I:629:PHE:HE2	2:I:650:VAL:HG21	1.66	0.60
2:I:761:GLN:OE1	2:I:761:GLN:N	2.35	0.59
1:H:152:TYR:OH	3:J:532:GLU:OE2	2.19	0.59
3:J:168:ALA:HB3	3:J:176:PHE:CE2	2.36	0.59
5:L:142:THR:HA	5:L:145:LEU:HD12	1.84	0.59
1:M:260:LEU:HB2	1:M:262:LEU:HD23	1.84	0.59
2:I:1214:ASP:OD1	2:I:1215:GLY:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:620:ASN:ND2	2:I:620:ASN:O	2.35	0.59
2:I:84:GLU:N	2:I:84:GLU:OE1	2.35	0.58
1:G:90:VAL:HG13	1:G:121:VAL:HG13	1.85	0.58
1:H:76:GLU:N	1:H:76:GLU:OE1	2.34	0.58
3:J:424:ASN:OD1	3:J:425:ARG:N	2.36	0.58
8:I:1401:1N7:C3	8:I:1401:1N7:C18	2.70	0.58
1:H:121:VAL:HG23	1:H:121:VAL:O	2.03	0.58
3:J:661:VAL:HG11	3:J:686:TRP:NE1	2.18	0.58
8:L:701:1N7:C3	8:L:701:1N7:C18	2.70	0.58
5:L:280:VAL:HG11	5:L:355:ILE:HG23	1.85	0.58
5:L:551:LEU:HD11	5:L:598:LEU:HD13	1.84	0.58
5:L:585:GLU:OE1	5:L:589:GLN:NE2	2.37	0.58
1:H:66:HIS:O	1:H:171:LEU:HD21	2.03	0.57
2:I:185:ASP:N	2:I:185:ASP:OD1	2.36	0.57
2:I:402:ARG:NH1	2:I:406:ASN:OD1	2.37	0.57
2:I:638:SER:O	2:I:640:GLY:N	2.37	0.57
1:M:284:ARG:NH1	1:M:288:GLU:OE2	2.35	0.57
1:M:270:LEU:O	1:M:274:ALA:N	2.35	0.57
6:O:41:DC:H2'	6:O:42:DT:H72	1.85	0.57
2:I:1043:ALA:HB3	2:I:1046:VAL:CG1	2.35	0.57
1:H:214:GLU:OE2	1:H:218:ARG:NH1	2.37	0.56
8:J:1504:1N7:C3	8:J:1504:1N7:C18	2.71	0.56
3:J:1111:ASP:OD1	3:J:1112:GLY:N	2.38	0.56
3:J:738:ARG:NH1	3:J:744:ARG:O	2.38	0.56
2:I:490:GLN:NE2	5:L:472:GLN:O	2.39	0.56
5:L:141:ILE:HA	5:L:144:LEU:HD23	1.88	0.56
3:J:697:MET:HE1	3:J:741:ALA:HB3	1.88	0.56
1:H:196:THR:HG21	3:J:443:GLU:HG2	1.87	0.56
2:I:976:ARG:O	2:I:980:VAL:HG23	2.06	0.56
2:I:719:LYS:O	2:I:779:ARG:NH1	2.39	0.55
3:J:271:ARG:HH11	3:J:316:ILE:HD12	1.69	0.55
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.87	0.55
2:I:228:VAL:N	2:I:335:THR:O	2.39	0.55
2:I:189:ASP:OD1	2:I:193:ASN:N	2.34	0.55
5:L:505:ILE:HD13	8:L:701:1N7:H25	1.89	0.55
3:J:657:ALA:O	3:J:661:VAL:HG13	2.07	0.55
1:H:181:GLU:O	3:J:535:ARG:NH1	2.40	0.54
2:I:1335:ILE:HG21	3:J:22:ILE:HD11	1.89	0.54
2:I:577:VAL:HG23	2:I:661:VAL:O	2.07	0.54
3:J:975:ILE:HG22	3:J:977:SER:H	1.71	0.54
3:J:726:ALA:HB2	3:J:737:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:871:VAL:O	2:I:944:ARG:NH2	2.40	0.54
3:J:585:LYS:O	3:J:587:LEU:N	2.37	0.54
3:J:122:SER:O	3:J:125:GLY:N	2.41	0.54
5:L:310:GLU:OE2	5:L:355:ILE:HG21	2.07	0.54
2:I:966:ILE:CD1	8:I:1402:1N7:H26	2.37	0.53
1:G:58:GLU:OE1	1:G:170:ARG:NH1	2.41	0.53
2:I:302:ILE:O	2:I:330:HIS:NE2	2.36	0.53
2:I:342:ASP:O	2:I:344:GLY:N	2.41	0.53
2:I:205:PRO:O	2:I:208:ILE:HG22	2.08	0.53
5:L:53:ILE:HD12	5:L:53:ILE:N	2.23	0.53
3:J:816:THR:HG21	3:J:889:ASP:HB2	1.91	0.53
2:I:1013:GLN:O	2:I:1017:GLN:NE2	2.41	0.53
3:J:1200:GLU:OE1	3:J:1200:GLU:N	2.42	0.53
2:I:560:PRO:HB2	3:J:776:THR:HG21	1.91	0.52
3:J:708:ASN:OD1	3:J:708:ASN:N	2.42	0.52
3:J:1021:ASP:OD1	3:J:1023:HIS:ND1	2.42	0.52
2:I:633:LEU:HD12	2:I:633:LEU:O	2.09	0.52
3:J:347:VAL:HG12	3:J:348:ASP:O	2.09	0.52
5:L:581:ASP:O	5:L:582:VAL:HG13	2.09	0.52
1:H:206:GLU:OE1	3:J:531:LYS:NZ	2.27	0.52
5:L:390:ILE:HG21	5:L:435:ILE:HG21	1.91	0.52
3:J:278:ARG:NH1	5:L:403:ASP:OD1	2.42	0.52
4:K:3:ARG:HG3	4:K:48:VAL:HG13	1.92	0.52
2:I:902:LEU:HD21	5:L:611:LEU:HG	1.91	0.52
1:H:62:ASP:OD1	1:H:63:GLY:N	2.42	0.51
2:I:1043:ALA:HB1	2:I:1044:PRO:HD2	1.92	0.51
3:J:817:HIS:O	3:J:881:LYS:NZ	2.42	0.51
2:I:692:THR:HG22	2:I:693:LEU:N	2.26	0.51
1:G:41:ASN:O	1:G:41:ASN:ND2	2.42	0.51
3:J:443:GLU:N	3:J:443:GLU:OE1	2.43	0.51
5:L:224:LEU:CD1	5:L:252:LEU:HD11	2.41	0.51
3:J:1090:ILE:HG22	3:J:1095:MET:O	2.10	0.51
2:I:905:ILE:HD11	5:L:598:LEU:HD23	1.92	0.51
2:I:159:SER:OG	2:I:160:ASP:N	2.43	0.51
5:L:511:ILE:CD1	8:L:701:1N7:H30	2.41	0.51
2:I:715:THR:CG2	2:I:782:VAL:HG13	2.41	0.51
5:L:384:LEU:HD12	5:L:384:LEU:C	2.32	0.51
3:J:1261:LEU:HD12	3:J:1261:LEU:O	2.11	0.50
2:I:692:THR:HG22	2:I:693:LEU:H	1.75	0.50
5:L:312:SER:O	5:L:315:TRP:NE1	2.44	0.50
1:H:214:GLU:OE1	1:H:215:GLU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:47:TYR:CE2	8:I:1401:1N7:H14	2.46	0.50
2:I:836:LEU:HD21	2:I:921:PRO:HD3	1.93	0.50
2:I:557:ARG:NH2	2:I:611:GLU:OE1	2.41	0.50
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.44	0.50
3:J:155:GLU:OE1	3:J:155:GLU:N	2.45	0.50
1:G:224:LEU:HD23	1:H:228:LEU:HD11	1.93	0.50
3:J:491:LEU:HD11	3:J:609:TYR:CE2	2.46	0.50
3:J:975:ILE:N	3:J:975:ILE:HD12	2.26	0.50
1:G:28:LEU:HD12	1:G:28:LEU:N	2.26	0.50
3:J:204:GLU:N	3:J:204:GLU:OE1	2.45	0.50
3:J:1078:LEU:HD21	3:J:1121:LEU:HB3	1.93	0.49
3:J:799:ARG:NH2	3:J:1146:GLU:OE2	2.43	0.49
1:H:73:GLY:O	1:H:134:THR:OG1	2.28	0.49
6:O:53:DA:H2'	6:O:54:DT:H71	1.93	0.49
1:G:182:ARG:O	1:G:183:ILE:HD13	2.13	0.49
2:I:773:LEU:HD23	2:I:774:GLY:N	2.28	0.49
7:P:48:DG:H2'	7:P:49:DT:H72	1.95	0.49
3:J:70:CYS:SG	3:J:72:CYS:N	2.83	0.49
3:J:278:ARG:NH2	5:L:403:ASP:OD1	2.45	0.49
3:J:388:ARG:NH2	3:J:414:GLU:OE1	2.43	0.49
6:O:51:DT:H2''	6:O:52:DA:N7	2.27	0.49
2:I:715:THR:HG22	2:I:716:ALA:H	1.77	0.49
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.94	0.49
4:K:10:VAL:O	4:K:14:GLY:N	2.43	0.49
1:G:137:ASN:ND2	1:G:137:ASN:O	2.46	0.49
3:J:201:LEU:HD22	3:J:217:LEU:CD1	2.43	0.48
5:L:112:THR:OG1	5:L:116:GLU:OE2	2.12	0.48
3:J:502:PRO:HG2	3:J:601:ILE:HD11	1.95	0.48
1:G:192:VAL:HG13	1:G:193:GLU:N	2.28	0.48
3:J:1046:ILE:HG23	3:J:1060:VAL:O	2.13	0.48
2:I:66:SER:HB3	2:I:479:LEU:HD22	1.95	0.48
2:I:329:GLY:O	2:I:331:LYS:NZ	2.43	0.48
2:I:477:GLU:OE1	2:I:478:ARG:N	2.47	0.48
3:J:975:ILE:HG21	3:J:980:THR:OG1	2.13	0.48
8:J:1504:1N7:H31	8:J:1504:1N7:C4	2.43	0.48
5:L:515:GLU:OE1	5:L:515:GLU:N	2.42	0.48
1:G:61:ILE:HG22	1:G:62:ASP:H	1.79	0.48
1:H:153:VAL:HG13	1:H:153:VAL:O	2.13	0.48
2:I:1082:ILE:HD12	2:I:1082:ILE:H	1.78	0.48
5:L:356:GLU:OE1	5:L:356:GLU:N	2.40	0.48
5:L:9:LEU:O	5:L:13:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:505:ILE:HD11	8:L:701:1N7:H25	1.96	0.48
2:I:1212:LEU:HD22	2:I:1225:VAL:CG2	2.44	0.48
3:J:426:ALA:HB3	3:J:427:PRO:CD	2.43	0.48
2:I:65:ASN:ND2	2:I:111:GLU:O	2.41	0.48
3:J:289:ASP:N	3:J:289:ASP:OD1	2.47	0.48
1:H:72:GLU:N	1:H:72:GLU:OE1	2.46	0.47
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.45	0.47
8:J:1504:1N7:C3	8:J:1504:1N7:C1	2.92	0.47
3:J:1046:ILE:HG21	3:J:1059:LEU:HB3	1.97	0.47
1:M:260:LEU:HB3	1:M:262:LEU:HD23	1.96	0.47
6:O:30:DC:C6	6:O:31:DT:H72	2.50	0.47
3:J:1169:THR:HG22	3:J:1169:THR:O	2.15	0.47
1:G:96:ASP:OD1	1:G:148:ARG:NH1	2.46	0.47
1:H:196:THR:OG1	3:J:443:GLU:OE2	2.32	0.47
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.95	0.47
3:J:478:LEU:HG	4:K:47:THR:HG23	1.96	0.47
1:G:14:VAL:HG21	1:G:29:GLU:HB2	1.95	0.47
2:I:1255:THR:O	2:I:1257:GLN:N	2.45	0.47
5:L:283:GLN:HB2	5:L:344:LEU:HD21	1.96	0.47
1:G:54:CYS:SG	1:G:92:VAL:HG22	2.54	0.47
2:I:74:ARG:NH1	2:I:121:GLU:OE2	2.47	0.47
2:I:269:ILE:HG22	2:I:274:ILE:CG1	2.44	0.47
2:I:676:ALA:HB3	3:J:779:ALA:HB2	1.97	0.47
2:I:992:LEU:HD11	2:I:1000:LEU:HD11	1.97	0.47
5:L:288:MET:O	5:L:292:VAL:N	2.36	0.47
5:L:505:ILE:HG22	5:L:506:SER:N	2.30	0.47
6:O:35:DT:H2'	6:O:36:DT:H72	1.96	0.47
3:J:1040:MET:HB3	3:J:1046:ILE:HD11	1.96	0.47
5:L:224:LEU:HD12	5:L:252:LEU:HD11	1.97	0.47
5:L:383:ASN:O	5:L:387:VAL:HG23	2.15	0.47
2:I:475:VAL:HG13	2:I:492:MET:CE	2.45	0.47
2:I:843:THR:OG1	2:I:846:GLY:O	2.20	0.47
8:J:1504:1N7:C3	8:J:1504:1N7:H1	2.45	0.47
2:I:941:LYS:NZ	2:I:949:GLU:OE2	2.46	0.47
1:G:61:ILE:HG22	1:G:62:ASP:N	2.30	0.46
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.97	0.46
3:J:1078:LEU:HD21	3:J:1121:LEU:CB	2.45	0.46
3:J:1344:LEU:H	3:J:1344:LEU:HD22	1.80	0.46
2:I:131:THR:HG22	2:I:132:ASP:N	2.31	0.46
5:L:509:THR:HG23	5:L:509:THR:O	2.15	0.46
2:I:521:LEU:O	2:I:525:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:818:VAL:HG12	2:I:819:SER:O	2.15	0.46
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	1.94	0.46
2:I:98:VAL:HG21	2:I:124:MET:SD	2.54	0.46
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.97	0.46
1:G:11:PRO:HA	1:G:30:PRO:HD2	1.97	0.46
5:L:421:TYR:O	5:L:421:TYR:CG	2.69	0.46
3:J:789:LYS:NZ	3:J:931:THR:HG22	2.30	0.46
5:L:84:LEU:O	5:L:87:VAL:HG12	2.15	0.46
1:H:64:VAL:HG22	1:H:66:HIS:H	1.81	0.46
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.41	0.46
3:J:867:GLN:OE1	3:J:867:GLN:N	2.49	0.46
3:J:1275:LEU:HD23	3:J:1277:GLY:H	1.81	0.46
1:G:191:ARG:NH2	1:G:193:GLU:O	2.45	0.46
1:H:114:ASP:OD1	1:H:114:ASP:N	2.49	0.46
8:I:1401:1N7:C3	8:I:1401:1N7:H1	2.46	0.46
8:I:1402:1N7:H31	8:I:1402:1N7:C4	2.45	0.46
3:J:606:ASN:OD1	3:J:610:ARG:NH1	2.48	0.46
5:L:145:LEU:HD22	5:L:225:ARG:HE	1.80	0.46
8:L:701:1N7:H15	8:L:701:1N7:H27	1.69	0.46
5:L:359:LYS:HA	5:L:362:ASN:OD1	2.16	0.46
3:J:801:VAL:HG12	3:J:920:ALA:HB3	1.97	0.46
3:J:1054:THR:O	3:J:1054:THR:HG22	2.16	0.46
5:L:24:TYR:HA	5:L:27:VAL:HG12	1.98	0.46
5:L:551:LEU:HD11	5:L:598:LEU:CD1	2.46	0.46
6:O:54:DT:H4'	6:O:55:DG:OP1	2.16	0.46
5:L:286:LEU:HD23	5:L:340:ALA:HB2	1.98	0.45
2:I:1024:GLU:O	2:I:1027:LYS:HG2	2.15	0.45
5:L:119:ILE:HG23	5:L:375:ALA:HB1	1.97	0.45
8:L:701:1N7:C3	8:L:701:1N7:C1	2.95	0.45
2:I:802:VAL:HG23	2:I:1098:LEU:HD13	1.98	0.45
2:I:975:ILE:HD11	2:I:1014:LEU:HB3	1.97	0.45
8:I:1401:1N7:C3	8:I:1401:1N7:C1	2.94	0.45
3:J:964:LYS:O	3:J:976:THR:N	2.48	0.45
1:H:118:ASP:HB2	1:H:121:VAL:HG22	1.99	0.45
2:I:966:ILE:HD11	8:I:1402:1N7:C17	2.43	0.45
8:I:1402:1N7:C3	8:I:1402:1N7:H1	2.47	0.45
3:J:888:CYS:SG	3:J:889:ASP:N	2.89	0.45
1:G:110:VAL:HG21	1:G:140:ILE:HD11	1.98	0.45
3:J:253:VAL:HG11	5:L:523:ILE:HD13	1.99	0.45
3:J:796:LEU:CD2	3:J:800:LEU:HD13	2.47	0.45
3:J:1146:GLU:OE1	3:J:1310:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:443:ILE:O	5:L:447:ALA:HB2	2.16	0.45
2:I:886:LYS:NZ	2:I:916:SER:OG	2.49	0.45
8:L:701:1N7:H32	8:L:701:1N7:C24	2.47	0.45
2:I:59:ILE:HG22	2:I:68:LEU:O	2.16	0.45
2:I:163:LYS:O	2:I:164:THR:OG1	2.35	0.45
2:I:272:ARG:HE	2:I:276:GLN:HG3	1.82	0.45
2:I:1210:ILE:HG22	2:I:1211:ARG:N	2.31	0.45
8:I:1401:1N7:H21	8:I:1401:1N7:O3	2.17	0.45
3:J:310:GLY:CA	3:J:315:ALA:HB2	2.46	0.45
1:G:69:SER:OG	1:G:70:THR:N	2.50	0.45
2:I:23:ASP:OD1	2:I:24:VAL:N	2.50	0.45
2:I:180:ARG:NH1	2:I:396:ASP:OD2	2.47	0.45
8:I:1402:1N7:C3	8:I:1402:1N7:C1	2.94	0.45
3:J:154:LEU:HD22	3:J:176:PHE:HE1	1.82	0.45
3:J:289:ASP:HA	3:J:292:VAL:HG22	1.98	0.45
3:J:807:LEU:HD22	3:J:1255:VAL:CG2	2.47	0.45
2:I:892:GLU:O	2:I:893:THR:CB	2.65	0.45
1:H:192:VAL:HG12	1:H:193:GLU:N	2.25	0.45
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.99	0.45
1:G:168:ILE:O	1:G:168:ILE:HG22	2.18	0.44
3:J:653:ILE:HG21	3:J:693:VAL:HG23	1.99	0.44
3:J:1080:ILE:HD11	3:J:1121:LEU:HD11	2.00	0.44
3:J:1195:GLN:OE1	3:J:1196:LEU:N	2.50	0.44
1:G:29:GLU:HB3	1:G:30:PRO:HD3	2.00	0.44
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	2.00	0.44
1:G:13:LEU:HD11	1:G:217:ILE:HD11	1.99	0.44
2:I:158:ASP:OD1	2:I:159:SER:N	2.46	0.44
1:H:107:ILE:HD13	1:H:135:ASP:HA	1.99	0.44
1:H:183:ILE:HG23	1:H:205:MET:HG3	1.99	0.44
1:H:192:VAL:HG23	1:H:198:LEU:HD12	2.00	0.44
2:I:237:LEU:O	2:I:287:VAL:HG22	2.17	0.44
2:I:715:THR:HG22	2:I:716:ALA:N	2.33	0.44
3:J:85:CYS:O	3:J:89:GLY:N	2.43	0.44
5:L:108:VAL:O	5:L:108:VAL:HG13	2.17	0.44
2:I:106:GLU:HB3	2:I:113:THR:HG23	2.00	0.44
2:I:376:PRO:O	2:I:377:THR:OG1	2.32	0.44
2:I:408:SER:O	2:I:431:LYS:NZ	2.42	0.44
5:L:37:ASP:OD2	5:L:99:ARG:NH1	2.50	0.44
5:L:402:LEU:HA	5:L:405:ILE:HG12	2.00	0.44
5:L:513:ASP:OD2	5:L:517:SER:OG	2.24	0.44
1:G:122:GLU:O	1:G:123:ILE:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:61:SER:OG	2:I:62:TYR:N	2.51	0.44
2:I:244:GLU:OE1	2:I:247:ARG:NE	2.47	0.44
2:I:484:LEU:HB3	2:I:486:THR:HG22	1.99	0.44
3:J:839:VAL:HG12	3:J:839:VAL:O	2.17	0.44
3:J:1024:THR:HG23	3:J:1123:ARG:HB3	2.00	0.44
1:G:110:VAL:CG2	1:G:133:LEU:HD23	2.48	0.44
2:I:60:GLN:O	2:I:476:LYS:NZ	2.46	0.44
2:I:218:GLU:OE2	2:I:300:ASP:N	2.51	0.44
3:J:1082:ASP:N	3:J:1088:VAL:HG23	2.33	0.44
2:I:595:THR:O	2:I:596:ASP:C	2.56	0.44
2:I:1103:VAL:N	2:I:1104:PRO:HD2	2.33	0.44
3:J:928:THR:O	3:J:928:THR:HG22	2.18	0.44
5:L:289:LYS:O	5:L:294:GLN:N	2.49	0.44
5:L:455:HIS:O	5:L:459:THR:HG23	2.17	0.44
1:G:102:LEU:C	1:G:102:LEU:HD23	2.39	0.44
2:I:1109:ILE:N	2:I:1109:ILE:HD12	2.33	0.44
8:I:1401:1N7:H15	8:I:1401:1N7:H27	1.69	0.44
3:J:127:LEU:HD21	3:J:234:PRO:HB3	1.99	0.44
2:I:106:GLU:O	2:I:112:GLY:HA2	2.18	0.43
2:I:159:SER:HB2	2:I:442:VAL:HG11	2.00	0.43
3:J:287:ALA:HB2	5:L:413:MET:HE1	2.00	0.43
1:G:224:LEU:HD23	1:H:228:LEU:CD1	2.48	0.43
1:H:192:VAL:O	1:H:193:GLU:C	2.56	0.43
2:I:247:ARG:NH2	2:I:278:GLU:OE2	2.42	0.43
2:I:836:LEU:HD12	2:I:836:LEU:N	2.34	0.43
3:J:500:ILE:O	3:J:500:ILE:CG2	2.63	0.43
8:J:1504:1N7:H13	8:J:1504:1N7:H27	1.67	0.43
4:K:4:VAL:HG13	4:K:5:THR:N	2.33	0.43
5:L:586:ARG:NE	6:O:25:DG:OP2	2.51	0.43
1:G:222:THR:OG1	1:H:233:ASP:OD1	2.32	0.43
1:H:203:ILE:HG22	1:H:204:GLU:N	2.34	0.43
2:I:274:ILE:HA	2:I:277:LEU:HD12	2.01	0.43
2:I:660:VAL:HG11	3:J:769:VAL:HG13	2.01	0.43
2:I:819:SER:OG	2:I:820:GLU:N	2.51	0.43
8:I:1401:1N7:H30	8:I:1401:1N7:H36	1.73	0.43
3:J:97:VAL:HG12	3:J:101:ARG:HE	1.83	0.43
3:J:235:GLU:OE1	3:J:235:GLU:N	2.39	0.43
3:J:320:ASN:OD1	3:J:320:ASN:N	2.49	0.43
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.99	0.43
3:J:697:MET:HG3	3:J:698:MET:N	2.33	0.43
2:I:211:ARG:NE	2:I:354:ASP:OD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:493:ILE:HG23	2:I:493:ILE:O	2.18	0.43
2:I:715:THR:HG21	2:I:782:VAL:HG22	2.01	0.43
1:G:47:LEU:O	1:G:180:VAL:HG21	2.18	0.43
2:I:1069:ARG:NH2	2:I:1114:GLU:OE2	2.41	0.43
2:I:1335:ILE:HG22	2:I:1336:ASN:N	2.33	0.43
2:I:208:ILE:HG23	2:I:209:ILE:N	2.33	0.43
8:I:1401:1N7:H34	8:I:1401:1N7:H10	1.77	0.43
5:L:487:MET:O	5:L:489:MET:N	2.49	0.43
5:L:37:ASP:OD1	5:L:39:ASP:N	2.51	0.43
5:L:94:THR:HG22	5:L:94:THR:O	2.19	0.43
2:I:367:TYR:CZ	2:I:380:ALA:HB1	2.53	0.43
2:I:1011:LEU:O	2:I:1011:LEU:HD23	2.19	0.42
2:I:1115:THR:HG22	2:I:1228:GLY:HA3	2.01	0.42
3:J:321:LYS:O	3:J:321:LYS:HG2	2.19	0.42
3:J:1248:ILE:HG22	3:J:1249:ASN:O	2.19	0.42
5:L:357:GLN:O	5:L:361:ILE:HG23	2.18	0.42
8:L:701:1N7:H21	8:L:701:1N7:H28	1.77	0.42
2:I:230:PHE:HE2	2:I:292:ILE:HD11	1.84	0.42
3:J:97:VAL:CG1	3:J:101:ARG:HE	2.32	0.42
3:J:1038:THR:O	3:J:1077:ALA:HB3	2.18	0.42
5:L:530:LEU:HD12	5:L:530:LEU:H	1.84	0.42
5:L:601:PRO:O	5:L:602:SER:CB	2.66	0.42
8:L:701:1N7:H14	8:L:701:1N7:H29	1.80	0.42
1:G:13:LEU:HD21	1:G:217:ILE:HD11	2.00	0.42
2:I:799:ASN:O	2:I:799:ASN:ND2	2.52	0.42
3:J:201:LEU:HD13	3:J:220:ARG:HG2	2.01	0.42
3:J:412:LEU:O	3:J:412:LEU:HD23	2.20	0.42
8:J:1504:1N7:O3	8:J:1504:1N7:H21	2.18	0.42
6:O:38:DC:H2'	6:O:39:DC:C5	2.54	0.42
2:I:320:ASP:OD1	2:I:320:ASP:N	2.51	0.42
2:I:241:LEU:HD21	2:I:246:LEU:HD21	2.00	0.42
3:J:528:THR:O	3:J:528:THR:OG1	2.26	0.42
2:I:109:ALA:O	2:I:113:THR:HB	2.20	0.42
1:G:28:LEU:N	1:G:28:LEU:CD1	2.83	0.42
1:G:174:ASP:OD1	1:G:174:ASP:N	2.52	0.42
3:J:646:ILE:HD12	3:J:762:ASN:ND2	2.34	0.42
5:L:141:ILE:N	5:L:141:ILE:HD12	2.34	0.42
5:L:290:LEU:HB3	5:L:333:VAL:HG21	2.02	0.42
7:P:33:DT:H4'	7:P:34:DT:OP1	2.19	0.42
1:G:192:VAL:O	1:G:193:GLU:C	2.57	0.42
2:I:67:GLU:OE1	2:I:69:GLN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:122:VAL:HG22	2:I:123:TYR:N	2.35	0.42
2:I:963:GLU:OE1	2:I:964:LEU:N	2.53	0.42
2:I:1288:GLN:OE1	3:J:1356:LEU:HD21	2.20	0.42
3:J:1027:VAL:O	3:J:1027:VAL:HG13	2.20	0.42
8:J:1504:1N7:H27	8:J:1504:1N7:H15	1.57	0.42
5:L:387:VAL:HG22	5:L:435:ILE:CD1	2.50	0.42
1:G:57:THR:HG22	1:G:175:ALA:HB2	2.01	0.42
1:G:135:ASP:OD1	1:G:136:GLU:N	2.52	0.42
2:I:1040:ASP:OD1	2:I:1041:ASP:N	2.53	0.42
2:I:1142:ARG:NH2	2:I:1166:ASP:OD1	2.52	0.42
3:J:814:CYS:HB3	3:J:890:THR:HG23	2.01	0.42
4:K:59:ILE:O	4:K:59:ILE:HG22	2.19	0.42
1:M:300:LEU:O	1:M:303:ILE:HG22	2.20	0.42
1:G:84:ASN:O	1:G:128:HIS:NE2	2.52	0.42
2:I:319:LEU:O	2:I:319:LEU:HD23	2.20	0.42
2:I:1109:ILE:O	2:I:1109:ILE:CG2	2.67	0.42
3:J:741:ALA:O	3:J:762:ASN:ND2	2.50	0.42
3:J:1197:ASN:ND2	3:J:1212:ASP:OD2	2.49	0.42
5:L:568:ASN:O	5:L:569:THR:C	2.59	0.42
8:L:701:1N7:H10	8:L:701:1N7:H33	1.55	0.42
1:G:231:PHE:CZ	1:H:28:LEU:HD22	2.55	0.41
1:H:192:VAL:HG23	1:H:198:LEU:CD1	2.50	0.41
2:I:283:LYS:O	2:I:285:ILE:HG23	2.20	0.41
2:I:638:SER:HB3	2:I:645:PHE:CZ	2.54	0.41
2:I:902:LEU:HD21	5:L:611:LEU:CD2	2.50	0.41
1:G:61:ILE:HB	1:G:64:VAL:HG22	2.02	0.41
1:G:182:ARG:NH1	2:I:1090:ASN:O	2.53	0.41
2:I:836:LEU:HD13	2:I:1054:LEU:HD13	2.01	0.41
2:I:903:ARG:O	2:I:907:GLY:N	2.53	0.41
8:I:1402:1N7:H14	8:I:1402:1N7:H29	1.90	0.41
3:J:811:GLU:OE1	3:J:890:THR:HG22	2.21	0.41
8:L:701:1N7:H21	8:L:701:1N7:O3	2.20	0.41
1:H:26:VAL:HG12	1:H:27:THR:N	2.35	0.41
2:I:471:VAL:HG21	2:I:498:ILE:HD11	2.02	0.41
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.51	0.41
3:J:804:ALA:HB2	3:J:1259:GLN:HG3	2.02	0.41
2:I:651:ASP:O	2:I:652:TYR:CG	2.73	0.41
2:I:901:LEU:HD22	5:L:565:ILE:CD1	2.50	0.41
8:I:1402:1N7:H21	8:I:1402:1N7:O3	2.20	0.41
3:J:907:HIS:CG	3:J:908:ILE:H	2.38	0.41
2:I:81:ASP:OD1	2:I:82:VAL:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:865:LEU:HD21	2:I:882:ILE:O	2.20	0.41
8:I:1402:1N7:C19	8:I:1402:1N7:C4	2.89	0.41
3:J:915:ILE:HA	3:J:918:ILE:CG2	2.50	0.41
3:J:961:SER:O	3:J:980:THR:HA	2.20	0.41
2:I:233:ARG:O	2:I:235:ASN:N	2.52	0.41
2:I:292:ILE:HB	2:I:322:LEU:HD11	2.01	0.41
2:I:1095:ASP:O	2:I:1096:ILE:HD13	2.21	0.41
2:I:1205:PRO:HG3	2:I:1210:ILE:HD13	2.03	0.41
3:J:79:LYS:CB	5:L:569:THR:HG22	2.45	0.41
5:L:577:GLY:HA2	5:L:587:ILE:HD13	2.02	0.41
5:L:602:SER:N	5:L:605:GLU:OE2	2.46	0.41
2:I:197:ARG:HG3	2:I:198:ILE:N	2.36	0.41
2:I:237:LEU:N	2:I:237:LEU:HD22	2.36	0.41
2:I:364:VAL:HG13	2:I:376:PRO:HB3	2.03	0.41
2:I:1060:ILE:HD11	2:I:1076:ILE:HD13	2.02	0.41
3:J:751:ASP:OD1	3:J:751:ASP:N	2.53	0.41
5:L:471:LEU:O	5:L:471:LEU:HD23	2.21	0.41
1:G:157:THR:HG22	1:G:157:THR:O	2.21	0.41
2:I:400:VAL:HG21	2:I:452:ARG:HD3	2.03	0.41
2:I:736:VAL:HG12	2:I:737:ASN:N	2.35	0.41
3:J:282:LEU:HD21	5:L:410:ILE:HG12	2.03	0.41
3:J:510:LEU:HD11	3:J:624:ILE:HG23	2.02	0.41
3:J:1043:GLY:O	3:J:1067:ARG:NH2	2.46	0.41
3:J:1198:VAL:O	3:J:1198:VAL:HG13	2.21	0.41
3:J:1204:VAL:HG22	3:J:1205:GLU:N	2.36	0.41
5:L:162:ILE:HG22	5:L:165:PHE:CE1	2.56	0.41
6:O:32:DA:C2	7:P:55:DA:C2	3.09	0.41
1:H:46:ILE:HD11	1:H:224:LEU:HD13	2.03	0.41
2:I:871:VAL:HG22	2:I:872:TYR:N	2.35	0.41
2:I:1248:THR:HG21	5:L:531:PRO:HG2	2.02	0.41
3:J:412:LEU:HD23	3:J:412:LEU:C	2.41	0.41
3:J:801:VAL:HG12	3:J:920:ALA:CB	2.51	0.41
3:J:1275:LEU:HD23	3:J:1276:GLU:N	2.35	0.41
2:I:839:VAL:HG12	2:I:1049:ILE:HG23	2.02	0.40
8:I:1402:1N7:H15	8:I:1402:1N7:H27	1.66	0.40
3:J:912:GLY:O	3:J:1359:ALA:O	2.40	0.40
2:I:118:LYS:NZ	2:I:487:LEU:O	2.52	0.40
8:I:1401:1N7:H27	8:I:1401:1N7:H13	1.75	0.40
3:J:452:LEU:HD13	3:J:500:ILE:CG2	2.52	0.40
2:I:14:ASP:N	2:I:1157:GLN:OE1	2.51	0.40
2:I:179:TYR:OH	2:I:458:GLU:OE2	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:353:VAL:O	2:I:353:VAL:HG12	2.22	0.40
5:L:32:PRO:HD2	5:L:35:ILE:HD12	2.04	0.40
5:L:488:LEU:HD12	5:L:488:LEU:N	2.37	0.40
7:P:47:DG:H1'	7:P:48:DG:C8	2.56	0.40
1:G:133:LEU:HD12	1:G:138:ALA:HB3	2.03	0.40
1:H:48:LEU:HD13	1:H:183:ILE:CD1	2.43	0.40
2:I:1151:LEU:HD23	2:I:1151:LEU:C	2.42	0.40
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.57	0.40
3:J:120:LEU:N	3:J:120:LEU:HD22	2.37	0.40
3:J:803:VAL:HG13	3:J:804:ALA:N	2.36	0.40
3:J:1211:SER:OG	3:J:1212:ASP:N	2.54	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	229/329 (70%)	204 (89%)	25 (11%)	0	100	100
1	H	215/329 (65%)	188 (87%)	27 (13%)	0	100	100
1	M	71/329 (22%)	70 (99%)	1 (1%)	0	100	100
2	I	1338/1342 (100%)	1215 (91%)	118 (9%)	5 (0%)	30	63
3	J	1332/1407 (95%)	1242 (93%)	87 (6%)	3 (0%)	44	74
4	K	72/91 (79%)	68 (94%)	4 (6%)	0	100	100
5	L	544/613 (89%)	510 (94%)	34 (6%)	0	100	100
All	All	3801/4440 (86%)	3497 (92%)	296 (8%)	8 (0%)	45	74

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	893	THR
2	I	1262	LYS
3	J	854	ALA
3	J	586	GLY
2	I	164	THR
2	I	234	ASP
3	J	585	LYS
2	I	1223	ARG

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	195/286 (68%)	187 (96%)	8 (4%)	26	57
1	H	186/286 (65%)	171 (92%)	15 (8%)	9	33
1	M	65/286 (23%)	65 (100%)	0	100	100
2	I	1154/1157 (100%)	1101 (95%)	53 (5%)	23	52
3	J	1121/1168 (96%)	1075 (96%)	46 (4%)	26	57
4	K	65/75 (87%)	65 (100%)	0	100	100
5	L	474/540 (88%)	455 (96%)	19 (4%)	27	58
All	All	3260/3798 (86%)	3119 (96%)	141 (4%)	27	55

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	15	ASP
1	G	41	ASN
1	G	79	LEU
1	G	191	ARG
1	G	192	VAL
1	G	211	ILE
1	G	228	LEU
1	G	234	LEU
1	H	17	GLU
1	H	38	THR

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Mol	Chain	Res	Type
1	H	54	CYS
1	H	83	LEU
1	H	97	GLU
1	H	98	VAL
1	H	99	ILE
1	H	134	THR
1	H	146	VAL
1	H	172	LEU
1	H	174	ASP
1	H	180	VAL
1	H	183	ILE
1	H	193	GLU
1	H	214	GLU
2	I	39	ILE
2	I	47	TYR
2	I	50	GLU
2	I	57	PHE
2	I	67	GLU
2	I	90	VAL
2	I	116	ASP
2	I	150	HIS
2	I	185	ASP
2	I	188	PHE
2	I	197	ARG
2	I	270	THR
2	I	272	ARG
2	I	311	CYS
2	I	331	LYS
2	I	335	THR
2	I	343	HIS
2	I	358	ASP
2	I	388	LEU
2	I	398	SER
2	I	402	ARG
2	I	434	ASP
2	I	472	GLU
2	I	484	LEU
2	I	487	LEU
2	I	488	MET
2	I	513	GLN
2	I	521	LEU
2	I	554	HIS

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Mol	Chain	Res	Type
2	I	576	SER
2	I	609	ILE
2	I	633	LEU
2	I	651	ASP
2	I	699	LEU
2	I	748	ILE
2	I	750	ILE
2	I	764	CYS
2	I	765	ILE
2	I	799	ASN
2	I	800	MET
2	I	830	THR
2	I	909	LYS
2	I	914	LYS
2	I	992	LEU
2	I	1083	GLU
2	I	1143	GLU
2	I	1172	LEU
2	I	1211	ARG
2	I	1240	ASP
2	I	1253	LEU
2	I	1262	LYS
2	I	1296	ASP
2	I	1313	HIS
3	J	46	TYR
3	J	70	CYS
3	J	78	LEU
3	J	93	THR
3	J	130	MET
3	J	172	PHE
3	J	179	LYS
3	J	198	CYS
3	J	222	LYS
3	J	252	LEU
3	J	270	ARG
3	J	284	ASP
3	J	320	ASN
3	J	321	LYS
3	J	430	HIS
3	J	442	ILE
3	J	489	ASN
3	J	506	VAL

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Mol	Chain	Res	Type
3	J	518	VAL
3	J	527	LEU
3	J	545	HIS
3	J	553	THR
3	J	591	ILE
3	J	722	ILE
3	J	744	ARG
3	J	754	ILE
3	J	762	ASN
3	J	770	LEU
3	J	773	PHE
3	J	796	LEU
3	J	807	LEU
3	J	814	CYS
3	J	895	CYS
3	J	903	LEU
3	J	1098	GLN
3	J	1120	THR
3	J	1134	ILE
3	J	1148	ARG
3	J	1194	ARG
3	J	1220	ILE
3	J	1230	THR
3	J	1236	GLU
3	J	1290	ARG
3	J	1343	GLU
3	J	1344	LEU
3	J	1366	HIS
5	L	15	ARG
5	L	104	GLU
5	L	110	LEU
5	L	144	LEU
5	L	157	ARG
5	L	165	PHE
5	L	231	THR
5	L	273	MET
5	L	289	LYS
5	L	362	ASN
5	L	384	LEU
5	L	388	ILE
5	L	474	MET
5	L	524	GLU

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Mol	Chain	Res	Type
5	L	559	LEU
5	L	574	GLU
5	L	582	VAL
5	L	598	LEU
5	L	607	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	1N7	J	1504	-	30,30,46	5.31	15 (50%)	47,48,72	2.64	15 (31%)
8	1N7	I	1401	-	30,30,46	5.31	15 (50%)	47,48,72	2.56	18 (38%)
8	1N7	L	701	-	30,30,46	5.27	15 (50%)	47,48,72	2.59	18 (38%)
8	1N7	I	1402	-	30,30,46	5.26	15 (50%)	47,48,72	2.54	16 (34%)

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	J	1504	-	-	3/7/72/92	0/4/4/4
8	1N7	I	1401	-	-	5/7/72/92	0/4/4/4
8	1N7	L	701	-	-	7/7/72/92	0/4/4/4
8	1N7	I	1402	-	-	4/7/72/92	0/4/4/4

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1504	1N7	C3-C19	18.08	1.83	1.53
8	I	1401	1N7	C3-C19	18.06	1.82	1.53
8	I	1402	1N7	C3-C19	18.03	1.82	1.53
8	L	701	1N7	C3-C19	17.95	1.82	1.53
8	J	1504	1N7	C3-C4	12.63	1.73	1.53
8	I	1401	1N7	C3-C4	12.55	1.73	1.53
8	I	1402	1N7	C3-C4	12.46	1.73	1.53
8	L	701	1N7	C3-C4	12.19	1.73	1.53
8	L	701	1N7	C5-C4	-9.74	1.39	1.54
8	I	1401	1N7	C5-C4	-9.60	1.39	1.54
8	J	1504	1N7	C2-C19	-9.49	1.39	1.56
8	I	1402	1N7	C5-C4	-9.42	1.40	1.54
8	L	701	1N7	C2-C19	-9.42	1.39	1.56
8	J	1504	1N7	C5-C4	-9.36	1.40	1.54
8	I	1401	1N7	C2-C19	-9.26	1.39	1.56
8	I	1402	1N7	C2-C19	-9.18	1.40	1.56
8	L	701	1N7	C8-C7	6.29	1.71	1.54
8	J	1504	1N7	C8-C7	6.27	1.71	1.54
8	I	1401	1N7	C8-C7	6.23	1.71	1.54
8	I	1402	1N7	C8-C7	6.22	1.71	1.54
8	I	1401	1N7	C5-C6	-5.21	1.46	1.55
8	J	1504	1N7	C5-C6	-5.08	1.47	1.55
8	L	701	1N7	C5-C6	-5.07	1.47	1.55
8	J	1504	1N7	C18-C6	-5.02	1.44	1.53
8	I	1402	1N7	C5-C6	-4.98	1.47	1.55
8	I	1401	1N7	C18-C6	-4.84	1.44	1.53
8	L	701	1N7	C18-C6	-4.71	1.44	1.53
8	I	1402	1N7	C18-C6	-4.63	1.45	1.53
8	L	701	1N7	O4-C4	-4.21	1.36	1.43
8	I	1401	1N7	O4-C4	-4.20	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1504	1N7	O4-C4	-4.07	1.36	1.43
8	I	1402	1N7	O4-C4	-4.04	1.37	1.43
8	L	701	1N7	C7-C6	3.31	1.61	1.54
8	I	1402	1N7	C14-C15	-3.30	1.48	1.53
8	I	1401	1N7	C14-C15	-3.30	1.48	1.53
8	L	701	1N7	C14-C15	-3.27	1.48	1.53
8	I	1402	1N7	C7-C6	3.24	1.61	1.54
8	J	1504	1N7	C14-C15	-3.24	1.48	1.53
8	J	1504	1N7	C7-C6	3.21	1.61	1.54
8	I	1401	1N7	C7-C6	3.21	1.60	1.54
8	I	1401	1N7	C2-C15	2.96	1.60	1.55
8	L	701	1N7	C20-C9	-2.94	1.49	1.54
8	I	1401	1N7	C20-C9	-2.88	1.49	1.54
8	I	1402	1N7	C20-C9	-2.83	1.49	1.54
8	J	1504	1N7	C20-C9	-2.76	1.49	1.54
8	J	1504	1N7	C2-C15	2.76	1.59	1.55
8	I	1402	1N7	C2-C15	2.71	1.59	1.55
8	L	701	1N7	C14-C13	2.57	1.56	1.52
8	I	1402	1N7	C5-C9	2.56	1.59	1.55
8	L	701	1N7	C2-C15	2.54	1.59	1.55
8	J	1504	1N7	C5-C9	2.47	1.59	1.55
8	J	1504	1N7	C14-C13	2.44	1.56	1.52
8	I	1402	1N7	C14-C13	2.42	1.56	1.52
8	I	1401	1N7	C14-C13	2.37	1.56	1.52
8	I	1401	1N7	O2-C13	-2.28	1.36	1.43
8	I	1401	1N7	C5-C9	2.27	1.59	1.55
8	I	1402	1N7	O2-C13	-2.25	1.36	1.43
8	J	1504	1N7	O2-C13	-2.23	1.36	1.43
8	L	701	1N7	O2-C13	-2.23	1.36	1.43
8	L	701	1N7	C5-C9	2.22	1.59	1.55

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	1504	1N7	C9-C5-C4	-8.50	110.02	117.67
8	I	1402	1N7	C9-C5-C4	-8.45	110.06	117.67
8	I	1401	1N7	C9-C5-C4	-8.28	110.22	117.67
8	L	701	1N7	C9-C5-C4	-8.27	110.22	117.67
8	L	701	1N7	C5-C9-C20	-6.41	111.72	119.48
8	I	1401	1N7	C5-C9-C20	-6.23	111.94	119.48
8	I	1401	1N7	C7-C6-C18	-5.95	110.19	118.36
8	I	1402	1N7	C7-C6-C18	-5.90	110.26	118.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	701	1N7	C7-C6-C18	-5.81	110.38	118.36
8	J	1504	1N7	C5-C9-C20	-5.75	112.52	119.48
8	J	1504	1N7	C7-C6-C18	-5.70	110.54	118.36
8	I	1402	1N7	C5-C9-C20	-5.58	112.72	119.48
8	I	1402	1N7	C6-C5-C4	5.20	112.17	107.42
8	L	701	1N7	C19-C3-C4	-4.96	107.80	114.29
8	J	1504	1N7	C9-C5-C6	4.81	104.94	100.11
8	J	1504	1N7	C6-C5-C4	4.65	111.67	107.42
8	I	1401	1N7	C9-C5-C6	4.53	104.66	100.11
8	I	1401	1N7	C6-C5-C4	4.52	111.55	107.42
8	L	701	1N7	C6-C5-C4	4.50	111.53	107.42
8	I	1402	1N7	C19-C3-C4	-4.43	108.50	114.29
8	J	1504	1N7	C2-C19-C18	-4.00	107.38	111.84
8	L	701	1N7	C9-C5-C6	3.86	103.99	100.11
8	J	1504	1N7	C5-C6-C18	-3.70	110.03	114.72
8	J	1504	1N7	C7-C6-C5	3.69	107.12	103.54
8	L	701	1N7	C16-C15-C2	-3.50	108.94	112.66
8	I	1402	1N7	C16-C15-C2	-3.39	109.05	112.66
8	I	1402	1N7	C9-C5-C6	3.34	103.46	100.11
8	L	701	1N7	C14-C15-C2	-3.32	109.13	112.66
8	I	1402	1N7	C19-C18-C17	-3.23	107.79	111.86
8	J	1504	1N7	C8-C9-C5	3.22	106.66	103.54
8	J	1504	1N7	C19-C18-C17	-3.17	107.87	111.86
8	J	1504	1N7	C16-C15-C2	-3.13	109.33	112.66
8	I	1401	1N7	C19-C3-C4	-3.06	110.28	114.29
8	I	1401	1N7	C3-C19-C2	-2.98	110.68	113.70
8	L	701	1N7	C21-C20-C9	-2.93	108.49	112.88
8	I	1402	1N7	C3-C19-C2	-2.91	110.75	113.70
8	I	1401	1N7	C21-C20-C9	-2.90	108.53	112.88
8	I	1401	1N7	C16-C15-C2	-2.80	109.68	112.66
8	I	1401	1N7	C7-C6-C5	2.79	106.25	103.54
8	J	1504	1N7	C3-C19-C2	-2.77	110.89	113.70
8	I	1402	1N7	C14-C15-C2	-2.74	109.74	112.66
8	I	1402	1N7	C21-C20-C9	-2.74	108.77	112.88
8	I	1402	1N7	C6-C18-C17	-2.74	108.22	111.85
8	I	1401	1N7	C5-C6-C18	-2.73	111.26	114.72
8	L	701	1N7	C7-C6-C5	2.68	106.14	103.54
8	I	1402	1N7	C8-C9-C5	2.67	106.13	103.54
8	L	701	1N7	C3-C19-C2	-2.65	111.01	113.70
8	I	1401	1N7	C19-C18-C17	-2.62	108.56	111.86
8	L	701	1N7	C6-C18-C17	-2.61	108.39	111.85
8	I	1402	1N7	C2-C19-C18	-2.59	108.95	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1401	1N7	C15-C16-C17	-2.59	111.32	114.40
8	I	1401	1N7	C2-C19-C18	-2.55	109.00	111.84
8	L	701	1N7	C3-C4-C5	-2.50	108.72	111.26
8	J	1504	1N7	C14-C15-C2	-2.45	110.05	112.66
8	J	1504	1N7	C21-C20-C9	-2.45	109.21	112.88
8	L	701	1N7	C12-C1-C2	-2.43	108.64	112.74
8	I	1402	1N7	C15-C16-C17	-2.41	111.53	114.40
8	J	1504	1N7	C15-C16-C17	-2.39	111.56	114.40
8	I	1401	1N7	C8-C9-C5	2.37	105.84	103.54
8	L	701	1N7	C2-C19-C18	-2.27	109.31	111.84
8	L	701	1N7	C8-C9-C5	2.27	105.74	103.54
8	L	701	1N7	C5-C6-C18	-2.22	111.90	114.72
8	I	1401	1N7	C15-C14-C13	-2.20	109.38	112.71
8	I	1401	1N7	C14-C15-C2	-2.13	110.39	112.66
8	I	1401	1N7	C6-C18-C17	-2.10	109.07	111.85
8	I	1402	1N7	C15-C14-C13	-2.09	109.55	112.71
8	L	701	1N7	C15-C16-C17	-2.06	111.94	114.40

There are no chirality outliers.

All (19) torsion outliers are listed below:

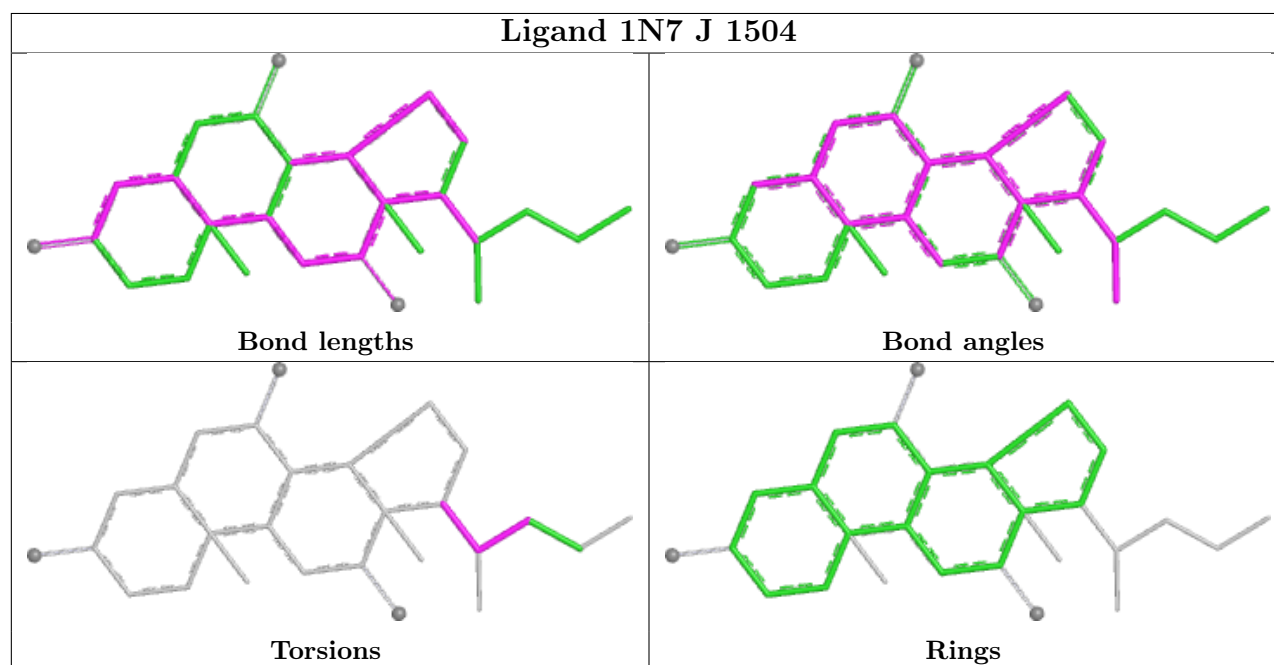
Mol	Chain	Res	Type	Atoms
8	L	701	1N7	C21-C20-C22-C23
8	I	1401	1N7	C21-C20-C9-C5
8	L	701	1N7	C21-C20-C9-C5
8	I	1401	1N7	C21-C20-C9-C8
8	L	701	1N7	C21-C20-C9-C8
8	I	1401	1N7	C22-C20-C9-C5
8	L	701	1N7	C22-C20-C9-C5
8	J	1504	1N7	C21-C20-C22-C23
8	L	701	1N7	C9-C20-C22-C23
8	I	1402	1N7	C21-C20-C22-C23
8	I	1401	1N7	C20-C22-C23-C24
8	L	701	1N7	C22-C20-C9-C8
8	I	1401	1N7	C22-C20-C9-C8
8	J	1504	1N7	C9-C20-C22-C23
8	I	1402	1N7	C21-C20-C9-C5
8	I	1402	1N7	C20-C22-C23-C24
8	I	1402	1N7	C21-C20-C9-C8
8	J	1504	1N7	C21-C20-C9-C5
8	L	701	1N7	C20-C22-C23-C24

There are no ring outliers.

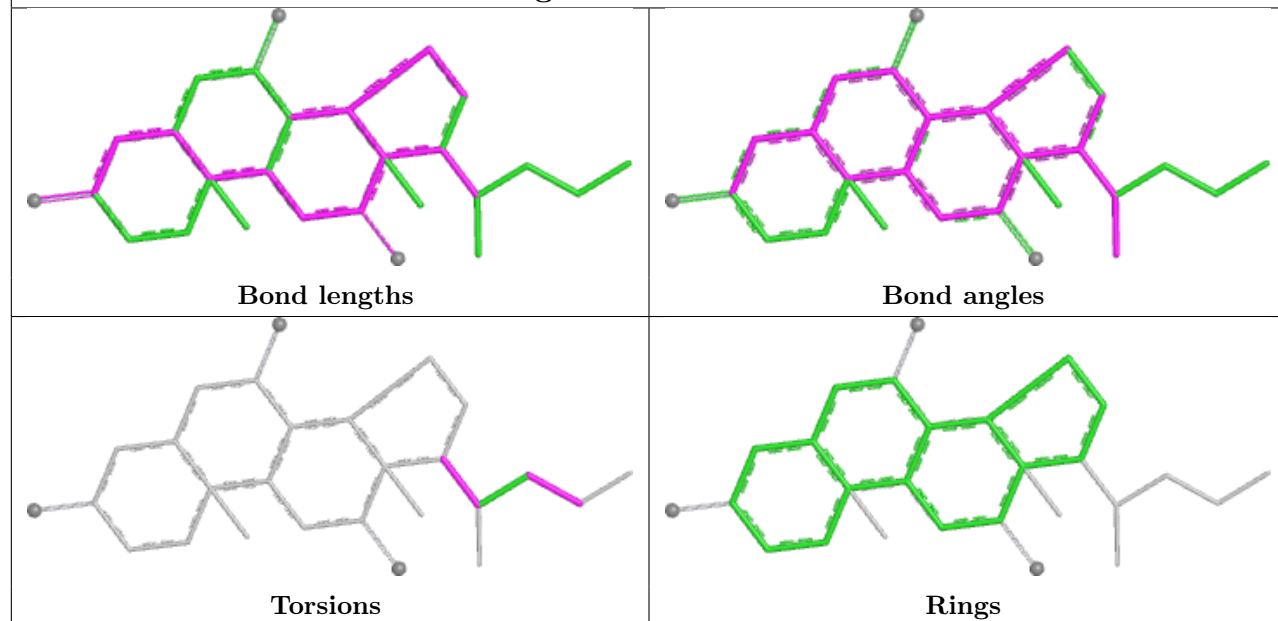
4 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	1504	1N7	10	0
8	I	1401	1N7	11	0
8	L	701	1N7	14	0
8	I	1402	1N7	15	0

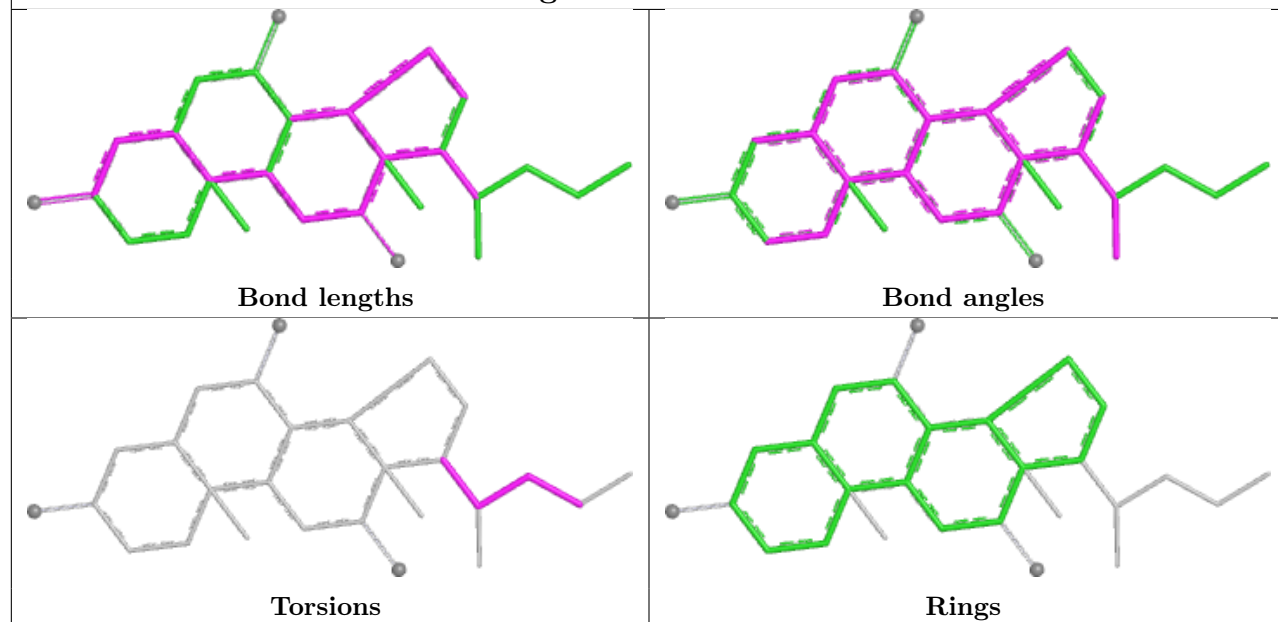
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

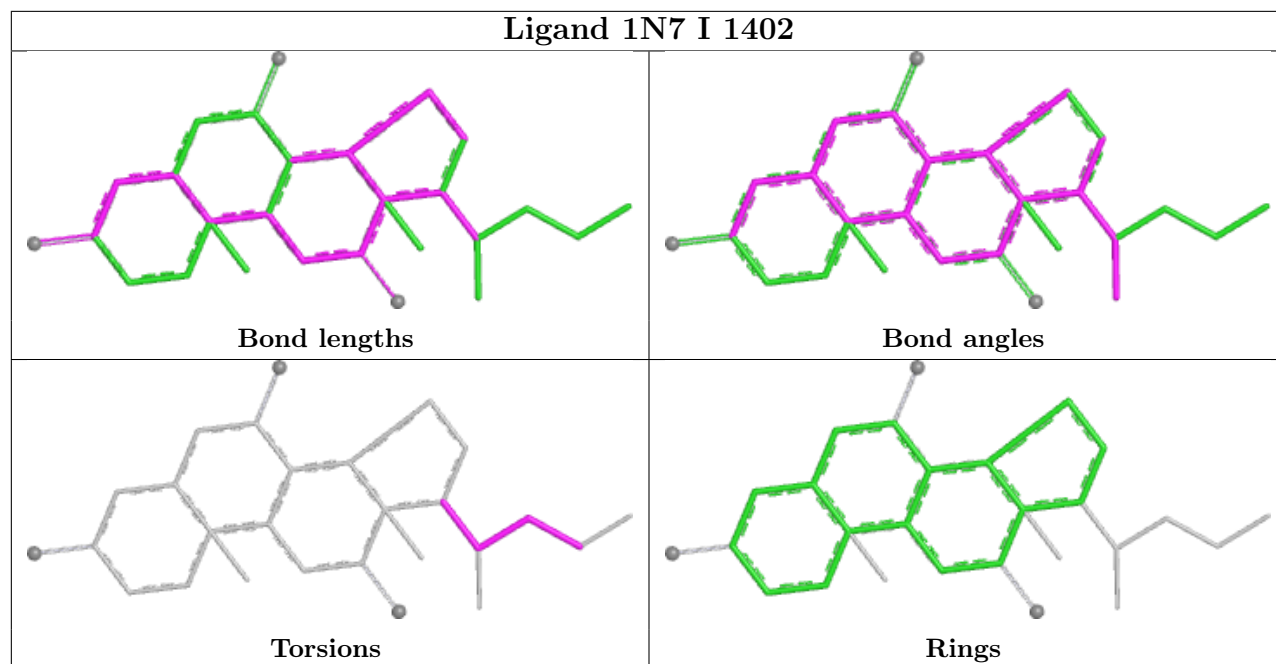


Ligand 1N7 I 1401



Ligand 1N7 L 701





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.

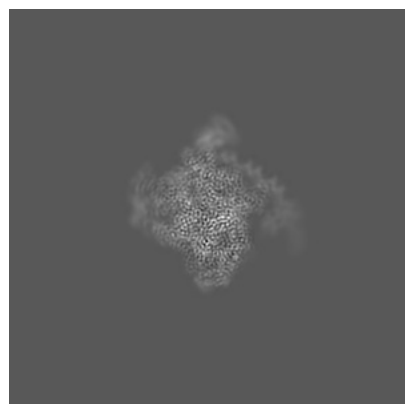
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41456. These allow visual inspection of the internal detail of the map and identification of artifacts.

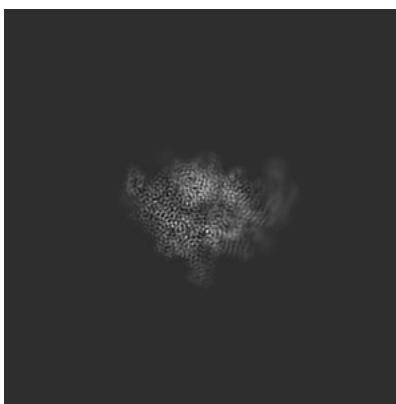
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

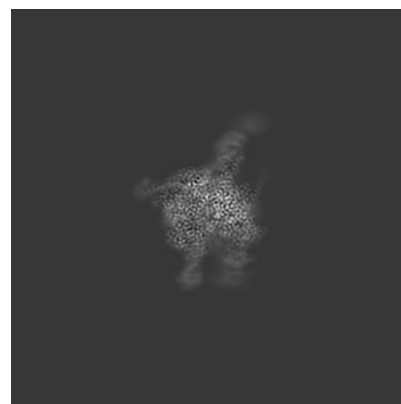
6.1.1 Primary map



X

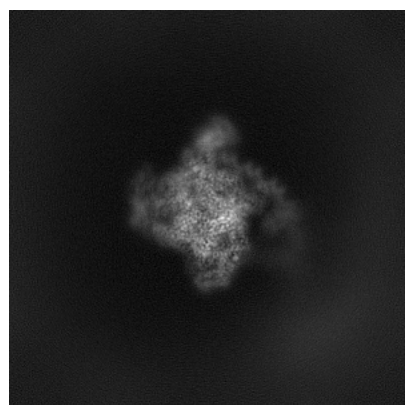


Y

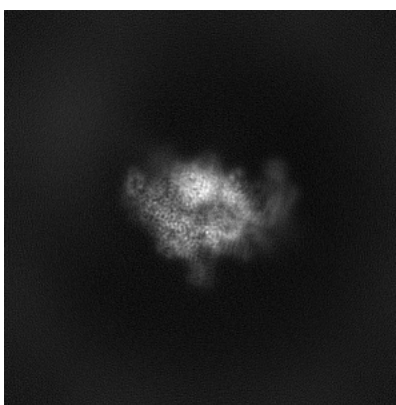


Z

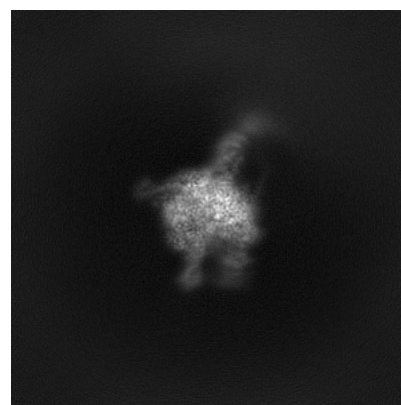
6.1.2 Raw map



X



Y

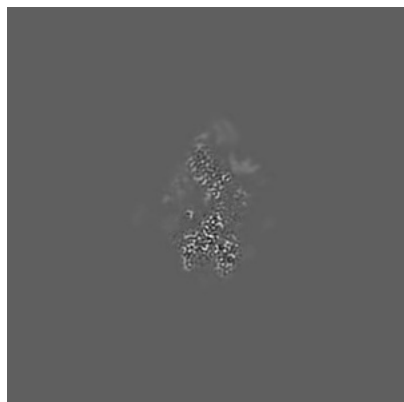


Z

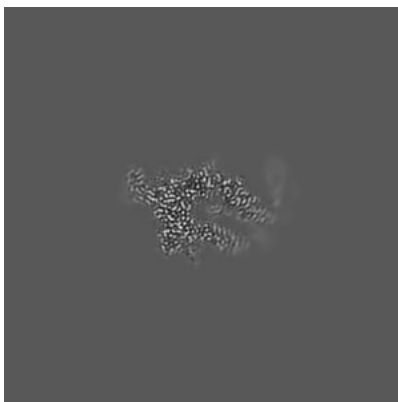
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

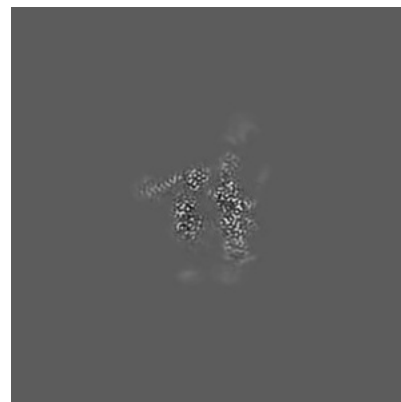
6.2.1 Primary map



X Index: 192

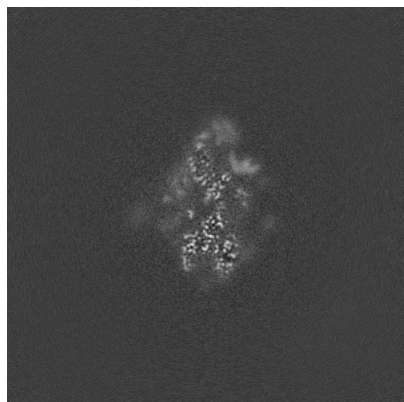


Y Index: 192

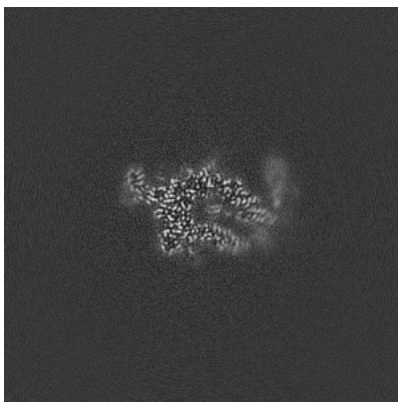


Z Index: 192

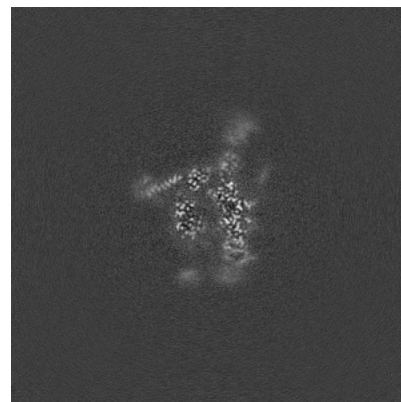
6.2.2 Raw map



X Index: 192



Y Index: 192

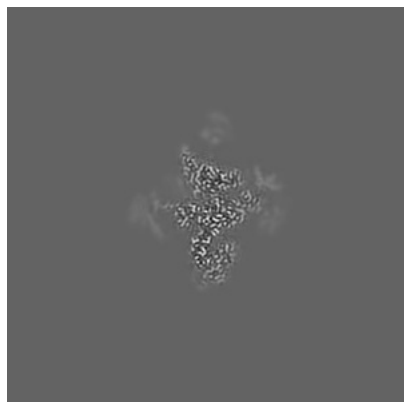


Z Index: 192

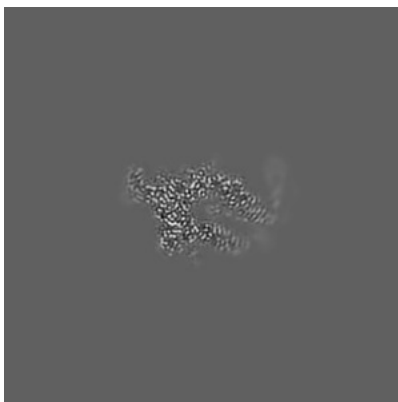
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

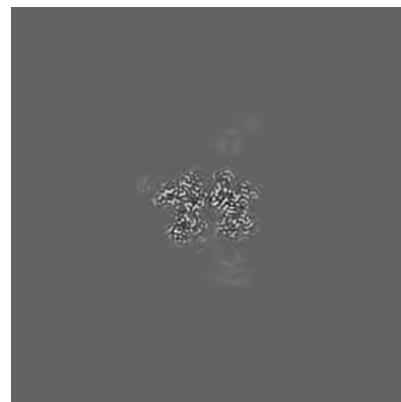
6.3.1 Primary map



X Index: 206

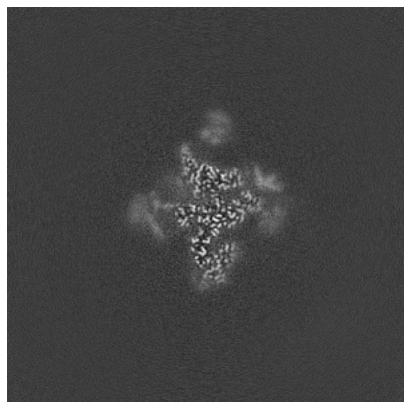


Y Index: 191

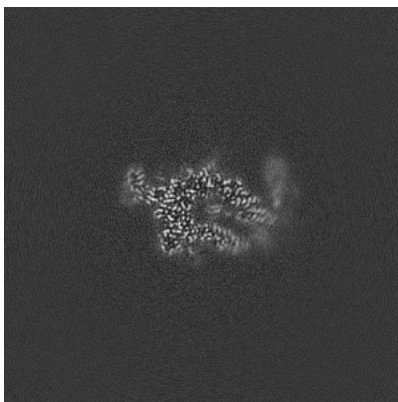


Z Index: 180

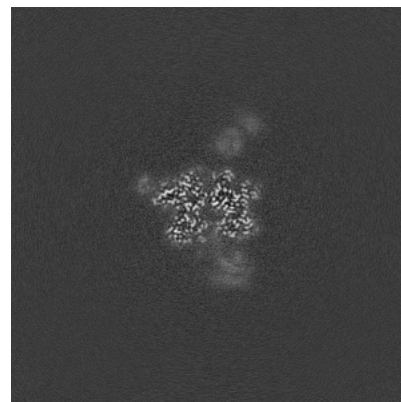
6.3.2 Raw map



X Index: 206



Y Index: 192

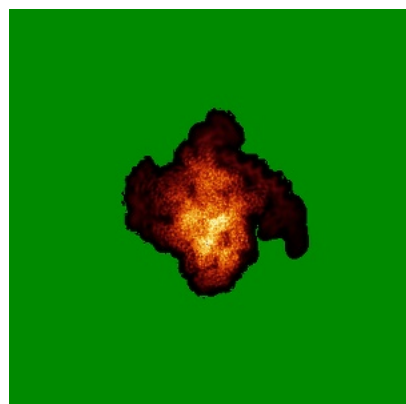


Z Index: 180

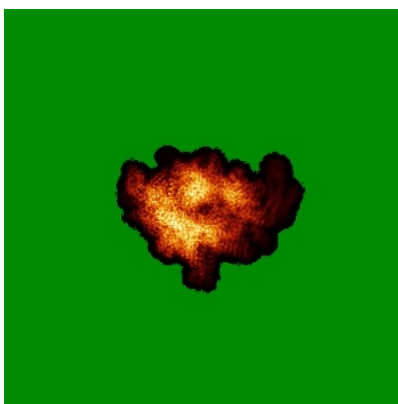
The images above show the largest variance slices of the map in three orthogonal directions.

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

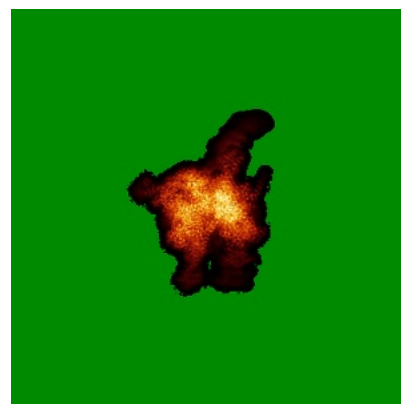
6.4.1 Primary map



X

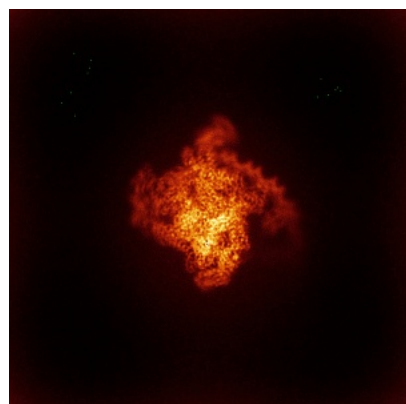


Y



Z

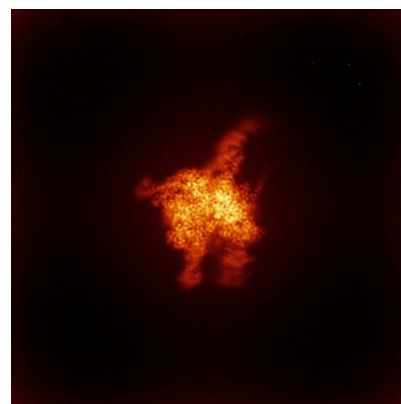
6.4.2 Raw map



X



Y

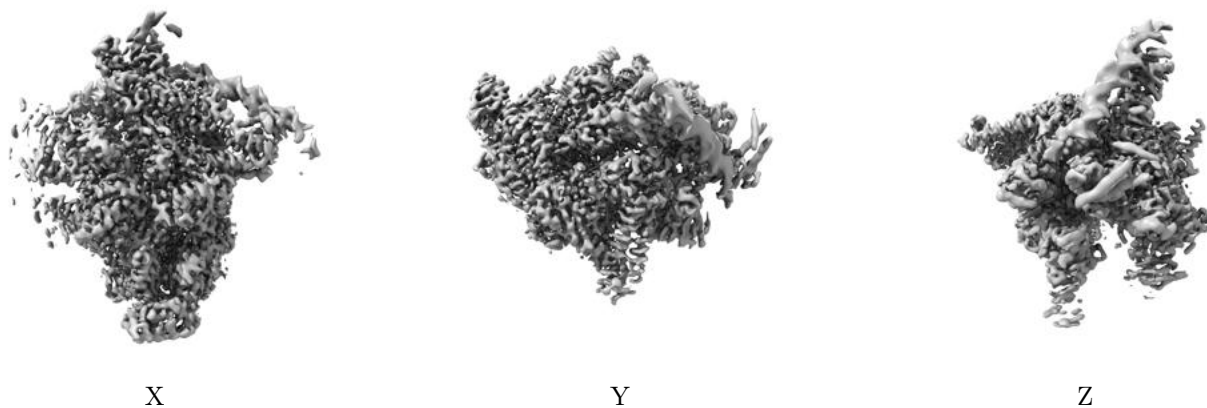


Z

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 0.5. 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.

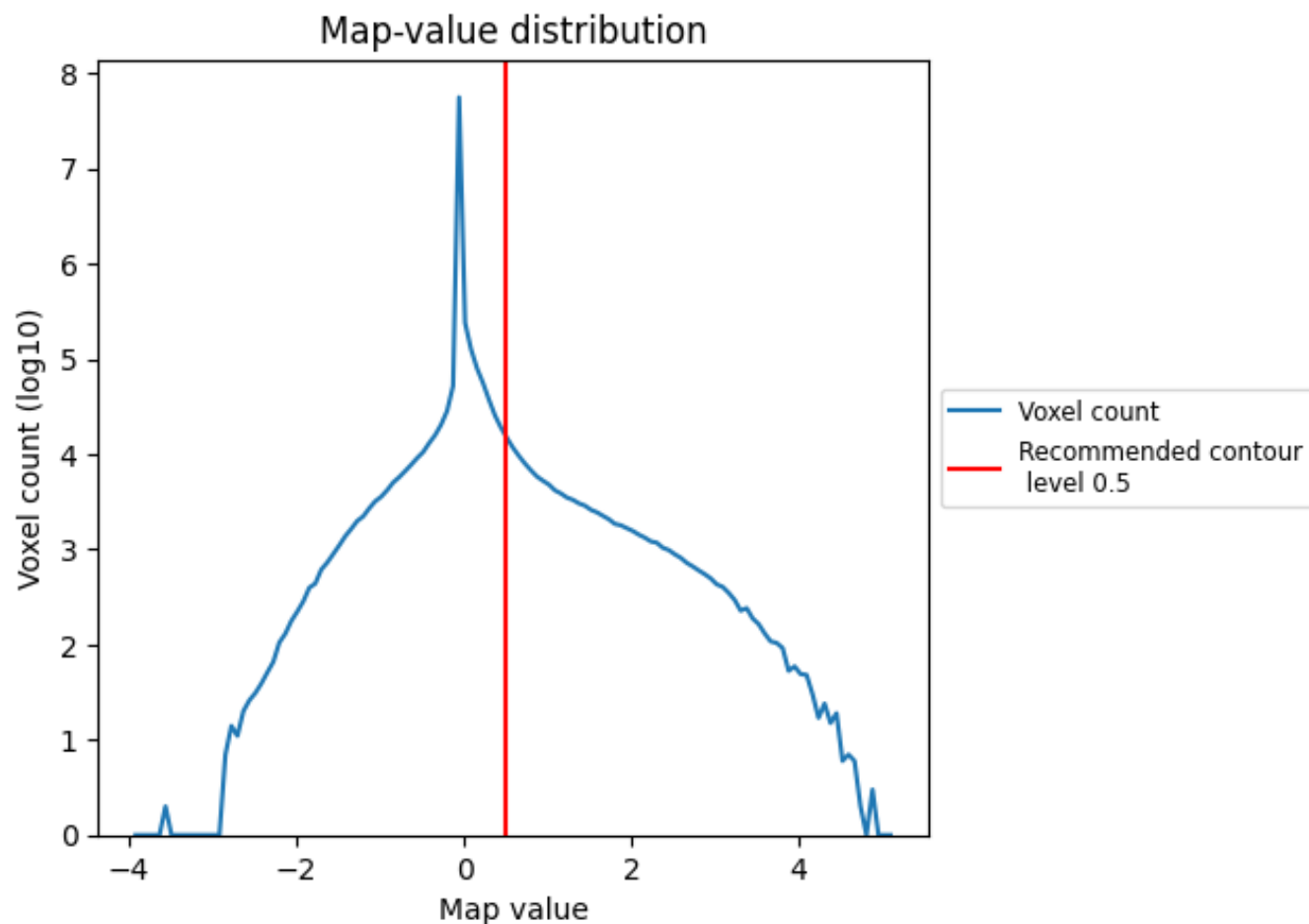
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

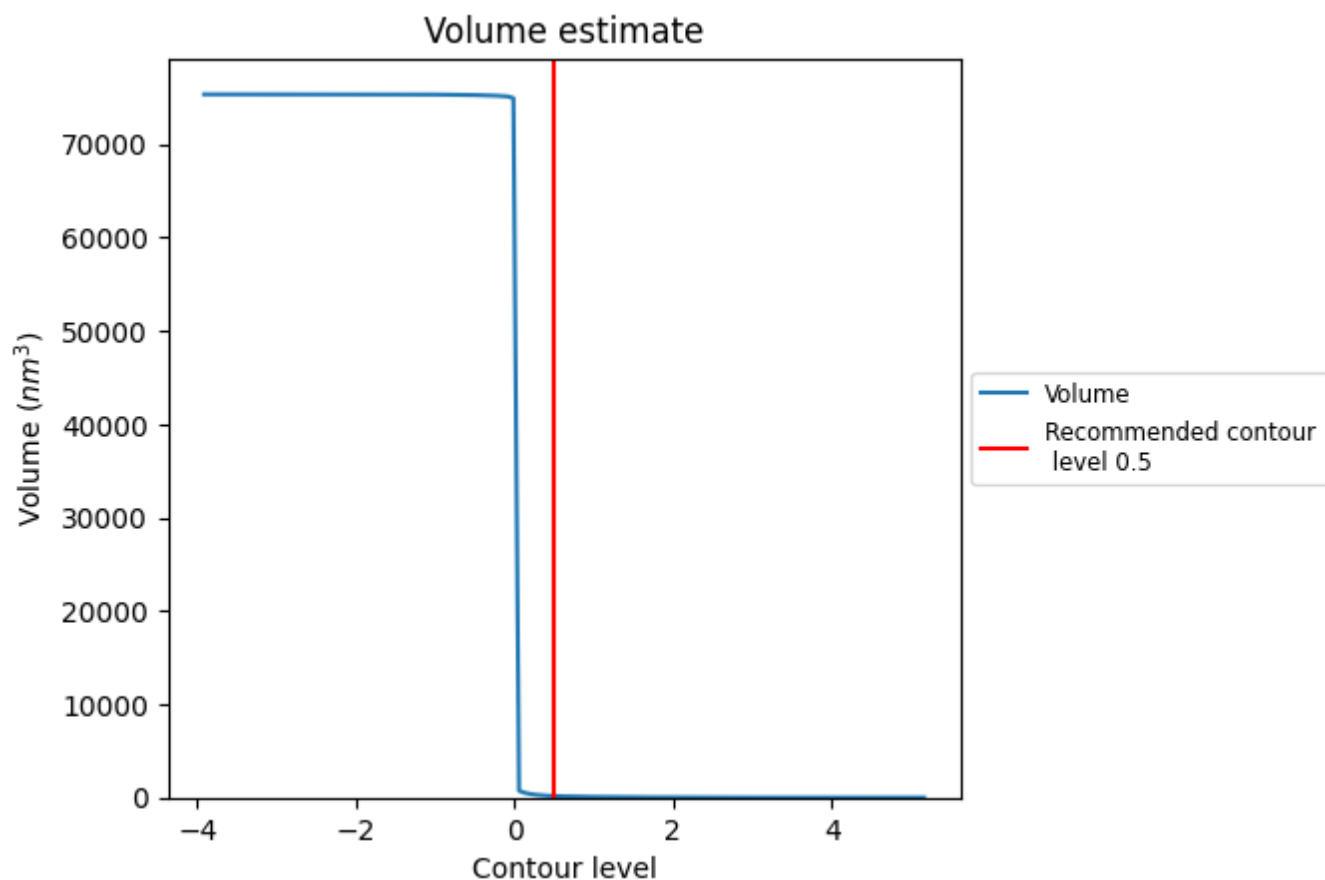
This section contains the results of statistical analysis of the map.

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.

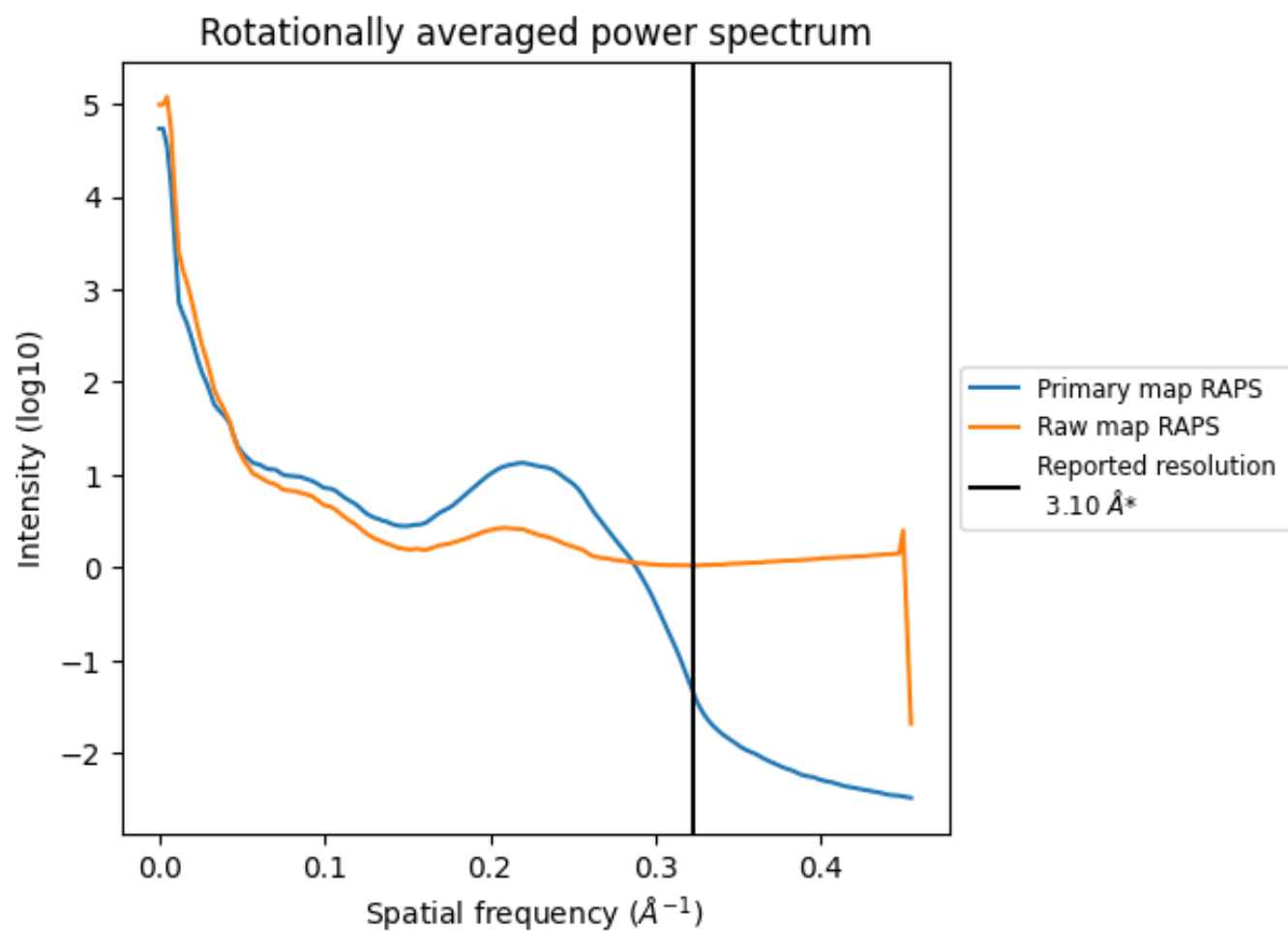
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm³; this corresponds to an approximate mass of 147 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 ⓘ

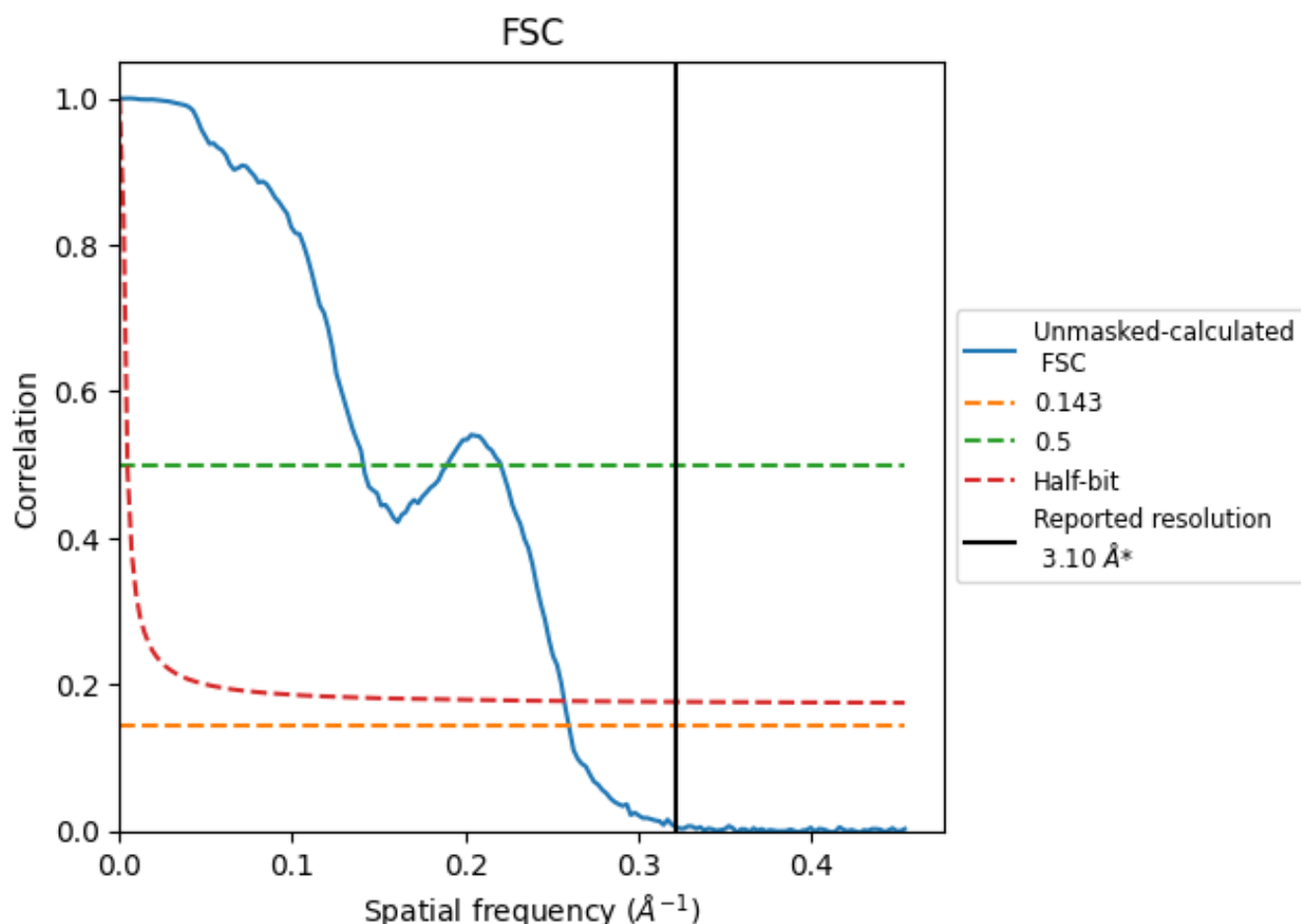


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

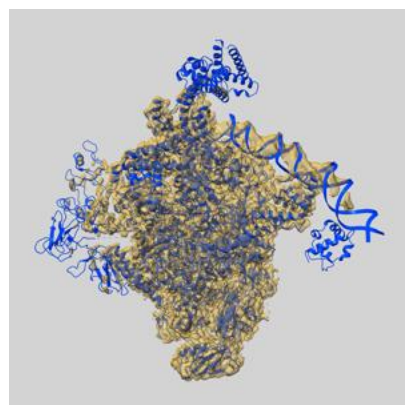
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.84	7.09	3.89

*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 3.84 differs from the reported value 3.1 by more than 10 %

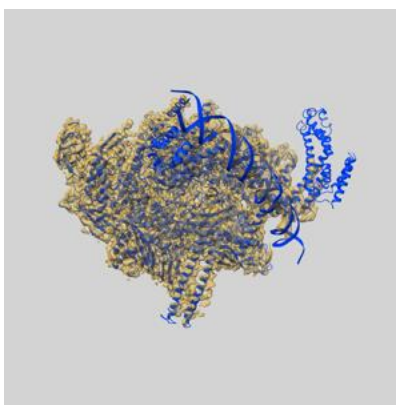
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41456 and PDB model 8TOM. Per-residue inclusion information can be found in section [3](#) on page [7](#).

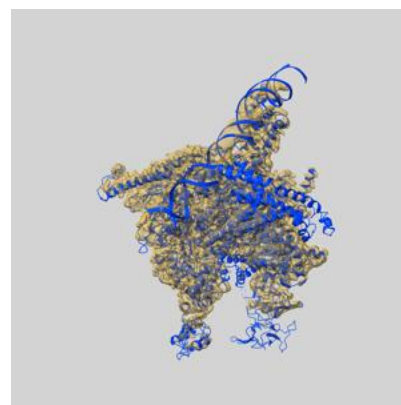
9.1 Map-model overlay [i](#)



X



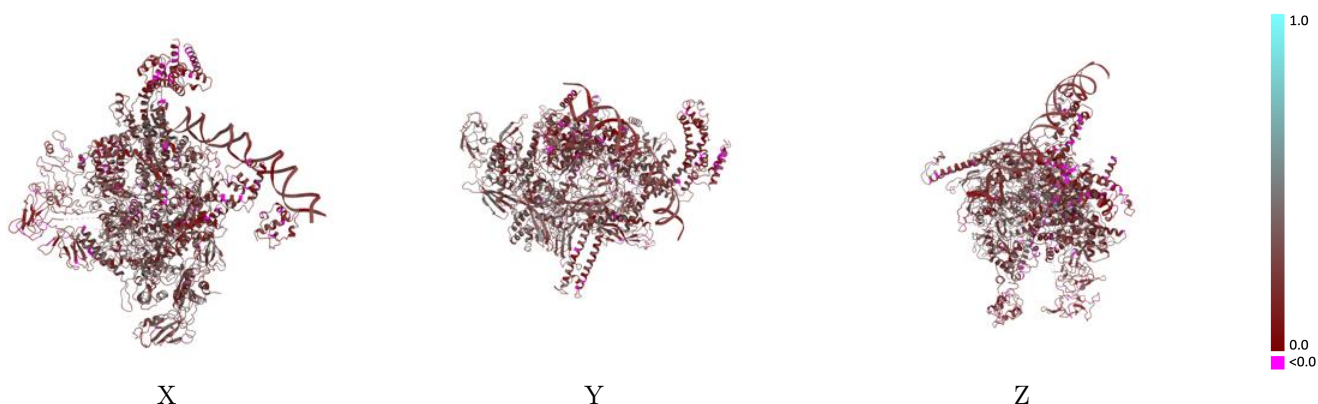
Y



Z

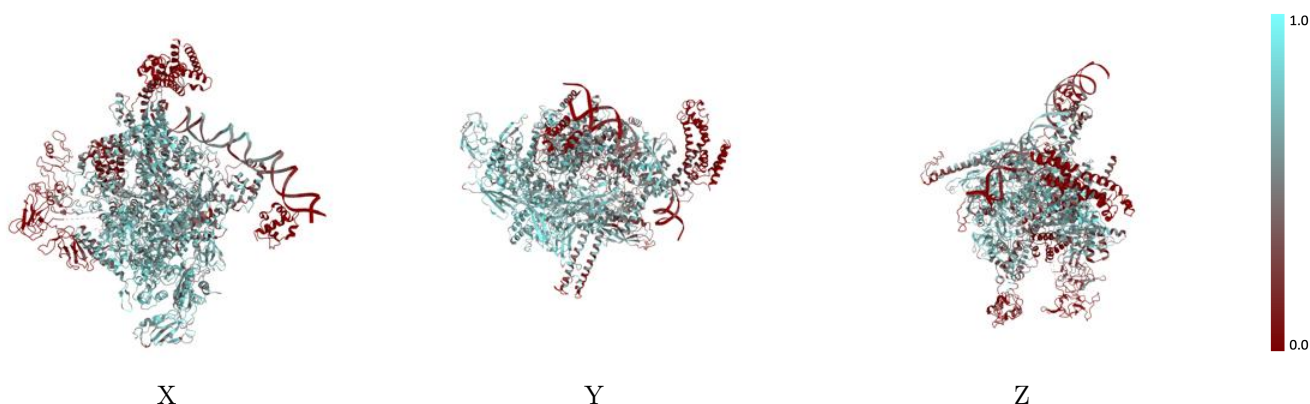
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



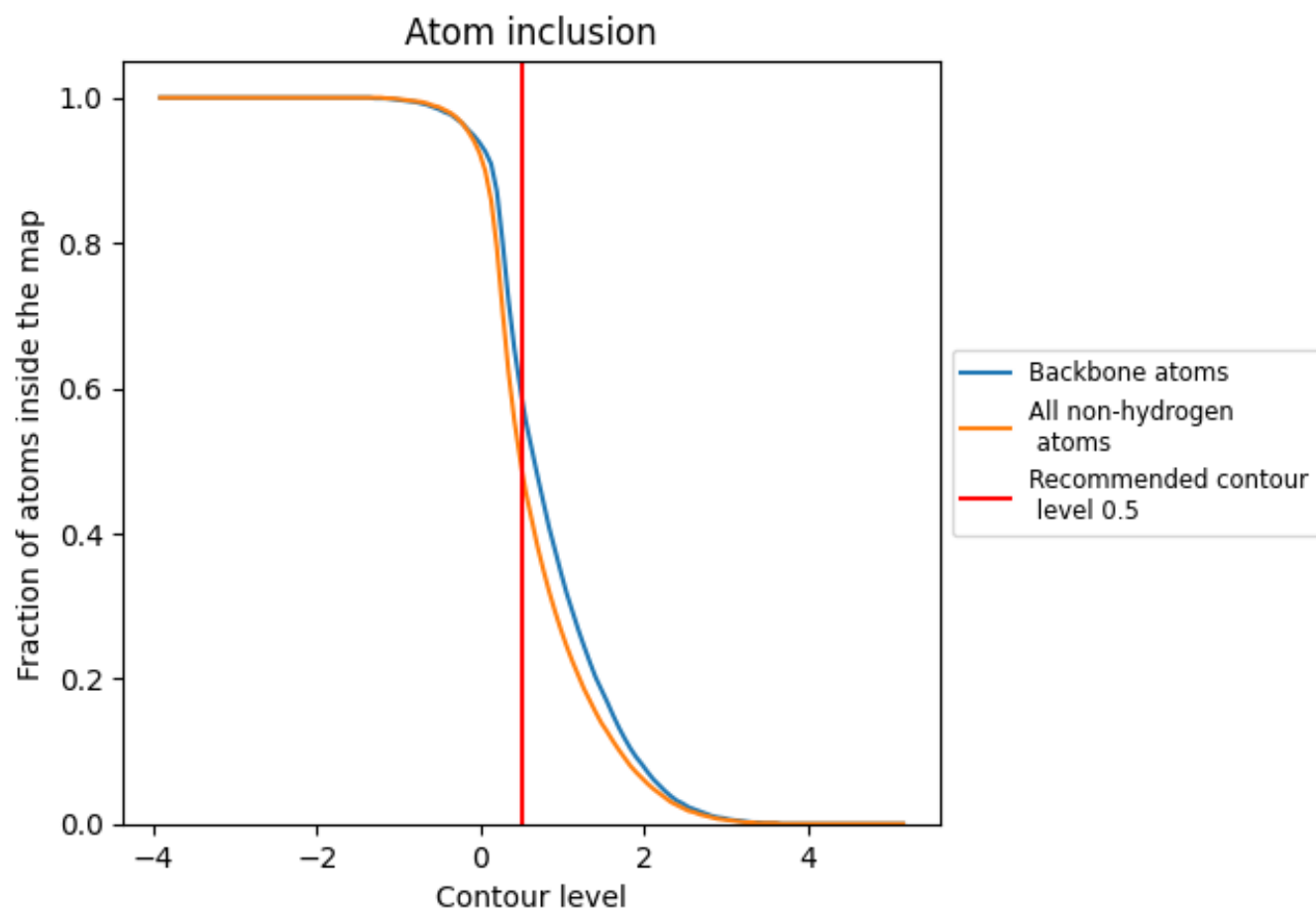
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 49% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4890	<div></div> 0.2530
G	<div></div> 0.6680	<div></div> 0.3080
H	<div></div> 0.6200	<div></div> 0.2930
I	<div></div> 0.5540	<div></div> 0.2690
J	<div></div> 0.5310	<div></div> 0.2580
K	<div></div> 0.5110	<div></div> 0.2090
L	<div></div> 0.2570	<div></div> 0.1950
M	<div></div> 0.0000	<div></div> 0.1560
O	<div></div> 0.2740	<div></div> 0.2160
P	<div></div> 0.2710	<div></div> 0.2180

1.0

0.0

<0.0