



Full wwPDB EM Validation Report ⓘ

Sep 16, 2025 – 07:11 pm BST

PDB ID : 9QRL / pdb_00009qrl
EMDB ID : EMD-53319
Title : DNA polymerase with inhibitor #2
Authors : Lamers, M.H.; Urem, M.; Smits, W.K.
Deposited on : 2025-04-03
Resolution : 3.20 Å(reported)
Based on initial model : .

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.dev126
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

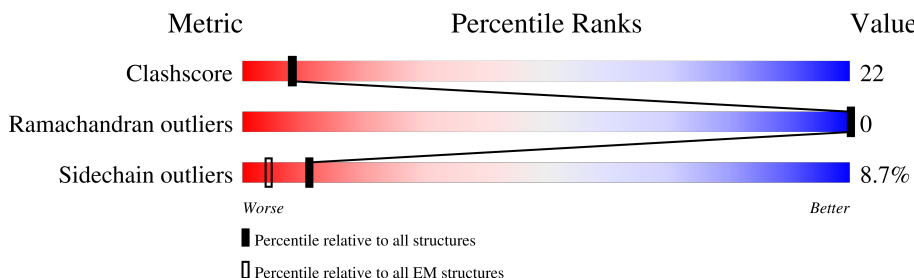
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1474	<div> <div>12%</div> <div>42%</div> <div>28%</div> <div>•</div> <div>26%</div> </div>
2	E	3	<div>100%</div>
3	P	33	<div> <div>9%</div> <div>18%</div> <div>73%</div> </div>
4	T	42	<div> <div>5%</div> <div>14%</div> <div>12%</div> <div>74%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9160 atoms, of which 20 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 polymerase III PolC-type.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1094	Total	C	N	O	S	0	0
			8636	5502	1438	1655	41		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A0A9X4B319
A	-20	GLY	-	expression tag	UNP A0A9X4B319
A	-19	SER	-	expression tag	UNP A0A9X4B319
A	-18	SER	-	expression tag	UNP A0A9X4B319
A	-17	HIS	-	expression tag	UNP A0A9X4B319
A	-16	HIS	-	expression tag	UNP A0A9X4B319
A	-15	HIS	-	expression tag	UNP A0A9X4B319
A	-14	HIS	-	expression tag	UNP A0A9X4B319
A	-13	HIS	-	expression tag	UNP A0A9X4B319
A	-12	HIS	-	expression tag	UNP A0A9X4B319
A	-11	SER	-	expression tag	UNP A0A9X4B319
A	-10	SER	-	expression tag	UNP A0A9X4B319
A	-9	GLY	-	expression tag	UNP A0A9X4B319
A	-8	LEU	-	expression tag	UNP A0A9X4B319
A	-7	VAL	-	expression tag	UNP A0A9X4B319
A	-6	PRO	-	expression tag	UNP A0A9X4B319
A	-5	ARG	-	expression tag	UNP A0A9X4B319
A	-4	GLY	-	expression tag	UNP A0A9X4B319
A	-3	SER	-	expression tag	UNP A0A9X4B319
A	-2	HIS	-	expression tag	UNP A0A9X4B319
A	-1	MET	-	expression tag	UNP A0A9X4B319
A	0	HIS	-	expression tag	UNP A0A9X4B319
A	22	LYS	ARG	conflict	UNP A0A9X4B319
A	218	HIS	-	insertion	UNP A0A9X4B319
A	219	ILE	-	insertion	UNP A0A9X4B319
A	355	THR	ILE	conflict	UNP A0A9X4B319
A	431	ALA	ASP	engineered mutation	UNP A0A9X4B319
A	433	ALA	GLU	engineered mutation	UNP A0A9X4B319

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Chain	Residue	Modelled	Actual	Comment	Reference
A	484	GLY	GLU	conflict	UNP A0A9X4B319
A	857	LYS	GLU	conflict	UNP A0A9X4B319
A	1141	SER	THR	conflict	UNP A0A9X4B319

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	3	Total	C	N	O	P	0	0
			62	30	12	17	3		

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*GP*TP*GP*CP*GP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	9	Total	C	N	O	P	0	0
			187	88	35	55	9		

- Molecule 4 is a DNA chain called DNA (5'-D(P*CP*CP*AP*TP*GP*CP*GP*CP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	11	Total	C	N	O	P	0	0
			220	104	40	65	11		

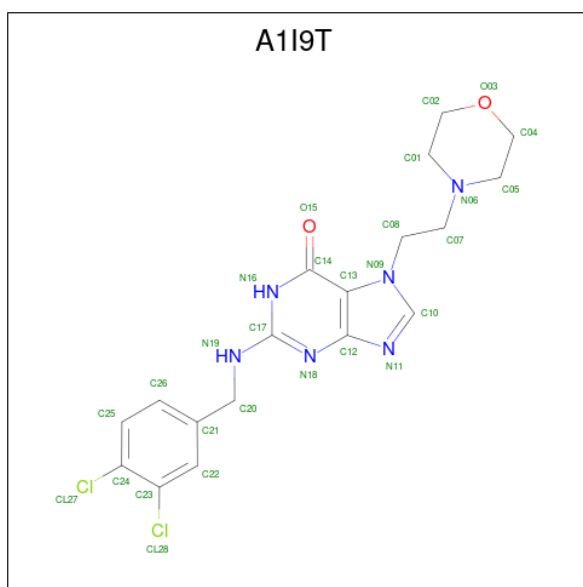
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	4	Total	Zn	0
			4	4	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Mg	0
			2	2	

- Molecule 7 is 2-[(3,4-dichlorophenyl)methylamino]-7-(2-morpholin-4-ylethyl)-1 {H}-purin-6-one (CCD ID: A1I9T) (formula: C₁₈H₂₀Cl₂N₆O₂) (labeled as "Ligand of Interest" by depositor).



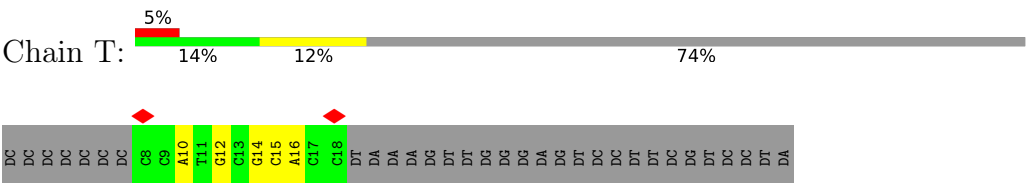
Mol	Chain	Residues	Atoms						AltConf
7	T	1	Total	C	Cl	H	N	O	0
			48	18	2	20	6	2	

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total O 1 1	0

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● Molecule 4: DNA (5'-D(P*CP*CP*AP*TP*GP*CP*GP*CP*AP*CP*C)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	330001	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0116	Depositor
Map size (\AA)	214.016, 214.016, 214.016	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.836, 0.836, 0.836	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, A1I9T

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	7/8818 (0.1%)	0.72	9/11924 (0.1%)
2	E	0.53	0/69	0.79	0/104
3	P	0.32	0/209	0.41	0/321
4	T	0.28	0/245	0.36	0/374
All	All	0.51	7/9341 (0.1%)	0.71	9/12723 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1178	LEU	C-N	8.30	1.44	1.33
1	A	1139	GLY	C-N	-8.23	1.22	1.33
1	A	1286	LEU	C-N	6.52	1.42	1.33
1	A	441	TYR	C-N	-6.48	1.25	1.33
1	A	1129	MET	C-O	6.14	1.31	1.24
1	A	1185	HIS	C-N	-5.53	1.25	1.33
1	A	1149	THR	C-N	5.53	1.41	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1249	ARG	N-CA-C	-6.79	103.88	111.28
1	A	1415	GLU	N-CA-C	-6.32	105.70	113.41
1	A	445	ILE	N-CA-C	-5.70	107.95	113.53
1	A	694	ASP	N-CA-C	-5.62	106.97	113.88
1	A	1133	ALA	CA-C-N	5.59	130.64	121.87
1	A	1133	ALA	C-N-CA	5.59	130.64	121.87
1	A	1195	GLU	N-CA-C	-5.38	105.31	111.07
1	A	1128	VAL	O-C-N	-5.34	116.47	121.87
1	A	1137	VAL	N-CA-C	-5.03	105.64	110.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8636	0	8467	380	0
2	E	62	0	35	5	0
3	P	187	0	102	6	0
4	T	220	0	123	5	0
5	A	4	0	0	0	0
6	A	2	0	0	0	0
7	T	28	20	0	2	0
8	A	1	0	0	0	0
All	All	9140	20	8727	386	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 22.

All (386) 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)
1:A:961:THR:HG22	1:A:1233:MET:HE1	1.71	0.72
1:A:1131:ILE:HG13	1:A:1132:PHE:N	2.04	0.71
1:A:1187:THR:HG22	1:A:1273:LYS:HB2	1.73	0.69
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.58	0.69
1:A:345:VAL:HB	1:A:374:ALA:O	1.92	0.68
1:A:1414:LYS:HA	1:A:1440:LEU:HD13	1.75	0.68
1:A:513:ALA:HB3	1:A:538:ASP:HB2	1.74	0.68
1:A:1008:ALA:HB3	3:P:30:DG:OP1	1.93	0.68
1:A:510:ALA:O	1:A:539:THR:HG23	1.94	0.68
1:A:358:ILE:O	1:A:362:VAL:HG23	1.95	0.68
1:A:1233:MET:HG3	1:A:1234:GLU:N	2.08	0.68
1:A:434:THR:HG22	1:A:444:ILE:HA	1.77	0.67
1:A:498:MET:O	1:A:501:GLU:HG3	1.95	0.67
1:A:413:ILE:HG13	1:A:606:ILE:HD11	1.76	0.67
1:A:935:GLY:O	1:A:952:LYS:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:MET:HG2	1:A:1180:ILE:HD12	1.76	0.67
1:A:414:ALA:HB1	1:A:599:HIS:CE1	2.30	0.67
1:A:1414:LYS:HB2	1:A:1442:ASP:OD1	1.94	0.67
1:A:521:ASN:HB3	1:A:531:GLU:OE2	1.94	0.67
1:A:669:CYS:HB3	1:A:699:MET:HE1	1.76	0.67
1:A:1357:MET:HE1	1:A:1384:LEU:HG	1.78	0.66
1:A:1162:VAL:HG22	1:A:1184:SER:HB2	1.78	0.66
1:A:275:SER:HB3	1:A:1031:GLU:HA	1.76	0.66
1:A:761:MET:SD	1:A:765:ASN:ND2	2.68	0.66
1:A:416:ASN:HB2	1:A:535:PRO:HA	1.76	0.66
1:A:858:LYS:HG2	1:A:959:PHE:CZ	2.32	0.65
1:A:704:TYR:HB2	1:A:719:LEU:HD21	1.79	0.65
1:A:1237:ARG:NH2	1:A:1238:LYS:HE2	2.12	0.64
3:P:25:DG:H2''	3:P:26:DG:H5'	1.78	0.64
1:A:612:TYR:CE1	1:A:613:LYS:HG3	2.32	0.64
1:A:688:ASN:HA	1:A:691:LYS:HD2	1.79	0.64
1:A:714:LYS:HD3	1:A:714:LYS:N	2.12	0.64
1:A:1423:VAL:HG11	1:A:1431:MET:HE1	1.79	0.64
1:A:1000:ARG:O	1:A:1081:THR:HA	1.97	0.63
1:A:416:ASN:ND2	1:A:534:ASN:O	2.30	0.63
1:A:1413:SER:HA	1:A:1442:ASP:HB3	1.80	0.63
1:A:342:GLU:HG3	1:A:345:VAL:HG23	1.79	0.63
1:A:1120:THR:O	1:A:1120:THR:HG22	1.98	0.63
1:A:547:TYR:HB3	1:A:550:PHE:CE1	2.34	0.63
1:A:1159:THR:HG21	4:T:10:DA:OP1	1.98	0.62
1:A:1215:ILE:CD1	1:A:1275:MET:HE1	2.30	0.62
1:A:479:THR:HB	1:A:481:ILE:HD12	1.81	0.62
1:A:862:SER:O	1:A:866:ASN:ND2	2.31	0.62
1:A:364:GLN:HG2	1:A:746:LEU:HD11	1.82	0.62
1:A:707:LEU:HD22	1:A:712:LEU:HD12	1.81	0.61
1:A:1023:ASN:HB2	1:A:1025:LEU:HD11	1.83	0.61
1:A:465:ILE:CG2	1:A:492:GLU:HG2	2.31	0.61
1:A:1071:PRO:HD3	1:A:1081:THR:HG23	1.83	0.61
1:A:1312:ASP:HA	1:A:1389:ARG:HH12	1.65	0.60
1:A:1095:LYS:HE3	1:A:1097:ASP:OD1	2.01	0.60
1:A:1023:ASN:CB	1:A:1025:LEU:HD11	2.31	0.60
1:A:1414:LYS:HG3	1:A:1440:LEU:HD12	1.82	0.60
1:A:1418:ALA:HA	1:A:1423:VAL:HG23	1.84	0.60
1:A:647:ARG:O	1:A:648:VAL:HG13	2.02	0.60
1:A:1423:VAL:CG1	1:A:1431:MET:HE1	2.31	0.60
1:A:358:ILE:HD13	1:A:375:ILE:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:ILE:HD12	1:A:1080:LYS:HD3	1.84	0.60
1:A:1228:MET:HE3	1:A:1228:MET:HA	1.84	0.59
1:A:550:PHE:HB2	1:A:553:PHE:CE1	2.38	0.59
1:A:669:CYS:CB	1:A:699:MET:HE1	2.32	0.59
1:A:727:VAL:O	1:A:731:LYS:HG2	2.03	0.59
1:A:1303:TYR:OH	1:A:1356:GLU:OE2	2.21	0.59
1:A:275:SER:HB3	1:A:1031:GLU:CA	2.33	0.58
1:A:497:ARG:HH11	1:A:497:ARG:HG2	1.66	0.58
1:A:779:THR:OG1	1:A:782:GLU:HG3	2.03	0.58
1:A:513:ALA:HB2	1:A:538:ASP:HA	1.84	0.58
1:A:1380:GLU:O	1:A:1380:GLU:HG3	2.02	0.58
1:A:545:TYR:CD1	1:A:546:LEU:HD23	2.38	0.58
1:A:1416:ASP:CG	1:A:1420:ARG:HD2	2.29	0.57
1:A:604:GLU:HG3	1:A:605:HIS:CD2	2.39	0.57
1:A:961:THR:HG21	1:A:1213:ASP:OD2	2.04	0.57
1:A:1248:LEU:HD22	1:A:1252:TYR:CE1	2.40	0.57
1:A:871:ILE:HD12	1:A:971:PRO:HG2	1.86	0.56
1:A:908:GLU:CD	1:A:1290:ARG:HH22	2.13	0.56
3:P:27:DT:H2"	3:P:28:DG:H5"	1.86	0.56
1:A:1272:ILE:HG21	1:A:1275:MET:HG3	1.86	0.56
1:A:546:LEU:HD13	1:A:589:GLU:HG2	1.88	0.56
1:A:553:PHE:N	2:E:1:DT:OP2	2.33	0.56
1:A:731:LYS:HE2	1:A:797:GLU:OE2	2.05	0.56
1:A:1131:ILE:HG21	1:A:1296:VAL:CG2	2.36	0.56
1:A:698:VAL:O	1:A:739:ALA:HA	2.05	0.56
1:A:1237:ARG:HH21	1:A:1238:LYS:HE2	1.71	0.56
1:A:1299:PRO:HB2	1:A:1362:PHE:CZ	2.40	0.56
1:A:1431:MET:HB3	1:A:1437:LEU:HG	1.88	0.56
1:A:681:LYS:CE	1:A:689:ARG:HH22	2.19	0.56
1:A:432:VAL:O	1:A:434:THR:HG23	2.06	0.55
1:A:1085:ASP:OD2	1:A:1087:HIS:ND1	2.29	0.55
1:A:508:LEU:HG	1:A:534:ASN:HD21	1.70	0.55
1:A:482:THR:HG22	1:A:483:ASP:N	2.22	0.55
1:A:669:CYS:CA	1:A:699:MET:HE1	2.36	0.55
1:A:382:GLN:HG2	1:A:1004:ILE:HD11	1.89	0.55
1:A:1367:ILE:HD12	1:A:1388:PHE:HD1	1.71	0.55
1:A:492:GLU:O	1:A:493:GLU:C	2.47	0.55
1:A:659:MET:O	1:A:663:LEU:HD12	2.07	0.55
1:A:413:ILE:HG21	1:A:542:LEU:HD13	1.88	0.55
1:A:878:LEU:HD23	1:A:988:TYR:HD2	1.72	0.55
1:A:1248:LEU:HD22	1:A:1252:TYR:CZ	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1234:GLU:HA	1:A:1237:ARG:HG2	1.88	0.54
1:A:1436:VAL:HG12	1:A:1437:LEU:HD23	1.89	0.54
4:T:15:DC:H2"	4:T:16:DA:OP2	2.07	0.54
1:A:250:VAL:HG22	1:A:269:ILE:HG22	1.90	0.54
1:A:1421:GLY:O	1:A:1422:LYS:HB2	2.08	0.54
1:A:700:PRO:HB3	1:A:786:ALA:HB1	1.91	0.53
1:A:547:TYR:HB3	1:A:550:PHE:CD1	2.43	0.53
1:A:892:ARG:HG2	1:A:1280:HIS:NE2	2.24	0.53
1:A:725:ASN:O	1:A:729:ILE:HG12	2.09	0.53
1:A:1188:ASP:HB3	1:A:1271:LYS:O	2.09	0.53
1:A:378:HIS:CE1	1:A:403:GLU:HG2	2.44	0.53
1:A:1114:SER:HB3	1:A:1301:LEU:CD1	2.38	0.53
1:A:465:ILE:HG21	1:A:492:GLU:HG2	1.90	0.53
1:A:347:SER:O	1:A:354:ALA:HB3	2.08	0.53
1:A:610:ASP:HB3	1:A:613:LYS:HD3	1.91	0.53
1:A:482:THR:HG22	1:A:483:ASP:H	1.73	0.53
1:A:811:GLU:HG2	1:A:812:GLU:N	2.23	0.53
1:A:990:LYS:HG2	1:A:995:GLU:HG3	1.91	0.53
1:A:1095:LYS:NZ	3:P:33:DT:OP1	2.42	0.52
1:A:1423:VAL:HB	1:A:1428:ILE:HD11	1.91	0.52
1:A:1333:ILE:HG21	1:A:1348:LEU:HB2	1.91	0.52
1:A:534:ASN:HB2	1:A:535:PRO:HD2	1.92	0.52
1:A:1023:ASN:HB2	1:A:1025:LEU:CD1	2.38	0.52
1:A:1181:SER:HB3	7:T:1501:A1I9T:CL27	2.46	0.52
1:A:251:PHE:CZ	1:A:268:LYS:HB3	2.44	0.52
1:A:984:GLU:N	1:A:984:GLU:OE1	2.42	0.52
1:A:1008:ALA:HB3	3:P:30:DG:P	2.50	0.52
1:A:430:PHE:CE1	1:A:516:ASP:HB3	2.45	0.52
1:A:986:HIS:O	1:A:989:THR:OG1	2.20	0.52
1:A:706:PRO:O	1:A:710:GLN:HG3	2.10	0.52
1:A:511:HIS:HD2	1:A:555:LEU:HG	1.74	0.52
1:A:526:ARG:HG3	1:A:526:ARG:NH1	2.25	0.52
1:A:875:ALA:O	1:A:879:VAL:HG23	2.10	0.52
1:A:252:ASP:HB3	1:A:268:LYS:HB2	1.92	0.51
1:A:1121:ILE:HD11	1:A:1294:PHE:HE2	1.73	0.51
1:A:1427:LEU:O	1:A:1431:MET:HE3	2.11	0.51
1:A:707:LEU:CD2	1:A:712:LEU:HD12	2.40	0.51
1:A:846:ASP:HB3	1:A:847:PRO:HD3	1.91	0.51
1:A:644:TYR:O	1:A:650:ARG:HB2	2.11	0.51
1:A:363:ALA:O	1:A:367:LYS:HG3	2.10	0.51
1:A:631:LYS:HE3	1:A:1061:ASP:OD1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:MET:HE1	1:A:1231:LYS:HE2	1.92	0.51
1:A:573:ILE:HG23	1:A:574:TYR:N	2.26	0.51
1:A:678:MET:HE2	1:A:686:ALA:CB	2.40	0.51
1:A:508:LEU:HG	1:A:534:ASN:ND2	2.26	0.51
1:A:851:ILE:HD13	1:A:926:PHE:CD2	2.46	0.51
1:A:1149:THR:OG1	1:A:1163:ARG:HG2	2.11	0.51
1:A:850:GLU:OE2	1:A:854:LYS:HG3	2.11	0.51
1:A:1424:SER:O	1:A:1425:LYS:C	2.54	0.51
1:A:529:ILE:HG22	1:A:530:PRO:HD2	1.93	0.51
3:P:25:DG:C2'	3:P:26:DG:H5'	2.41	0.50
1:A:1413:SER:C	1:A:1415:GLU:H	2.18	0.50
1:A:1414:LYS:HA	1:A:1440:LEU:CD1	2.41	0.50
1:A:636:LEU:O	1:A:639:MET:HG2	2.12	0.50
1:A:1102:ASP:HB2	4:T:12:DG:OP1	2.10	0.50
1:A:472:SER:O	1:A:476:VAL:HG23	2.11	0.50
1:A:976:ASN:HB3	1:A:1101:HIS:HB2	1.92	0.50
1:A:669:CYS:HA	1:A:699:MET:HE1	1.94	0.50
1:A:851:ILE:HA	1:A:854:LYS:HZ1	1.75	0.50
1:A:497:ARG:HH11	1:A:497:ARG:CG	2.25	0.50
1:A:1428:ILE:HG23	1:A:1437:LEU:CD1	2.42	0.50
1:A:1231:LYS:O	1:A:1235:THR:HG23	2.11	0.50
1:A:1252:TYR:O	1:A:1256:MET:HG3	2.12	0.50
1:A:1413:SER:HA	1:A:1442:ASP:CB	2.42	0.50
1:A:477:ASP:OD1	1:A:478:LEU:N	2.46	0.49
1:A:575:ASP:OD1	1:A:575:ASP:C	2.54	0.49
1:A:1235:THR:HG21	1:A:1252:TYR:HE2	1.77	0.49
1:A:378:HIS:ND1	1:A:403:GLU:HG2	2.26	0.49
1:A:1152:LEU:HB2	1:A:1356:GLU:OE1	2.12	0.49
1:A:1272:ILE:CG2	1:A:1275:MET:HG3	2.41	0.49
1:A:843:MET:HE2	1:A:844:TYR:OH	2.13	0.49
1:A:1166:LEU:HD23	1:A:1180:ILE:HG13	1.94	0.49
1:A:511:HIS:CD2	1:A:555:LEU:HG	2.47	0.49
1:A:850:GLU:HA	1:A:850:GLU:OE1	2.12	0.49
1:A:1031:GLU:O	1:A:1032:VAL:C	2.52	0.49
1:A:708:ILE:HA	1:A:713:VAL:O	2.12	0.49
1:A:1438:LYS:O	1:A:1439:ASP:C	2.54	0.49
1:A:1178:LEU:HD23	1:A:1285:VAL:HG21	1.95	0.49
1:A:346:HIS:CE1	1:A:378:HIS:CD2	3.00	0.49
1:A:610:ASP:HB2	1:A:614:ARG:NH2	2.28	0.49
1:A:1367:ILE:HG12	1:A:1436:VAL:HG21	1.95	0.49
1:A:843:MET:HE2	1:A:844:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:VAL:HG21	1:A:973:ILE:HG23	1.95	0.48
1:A:1109:MET:SD	1:A:1305:ALA:HA	2.52	0.48
1:A:1318:SER:HB3	1:A:1325:ALA:C	2.38	0.48
1:A:646:GLU:O	1:A:647:ARG:HG2	2.12	0.48
1:A:1000:ARG:HG2	1:A:1048:GLN:HE21	1.77	0.48
1:A:1414:LYS:CA	1:A:1440:LEU:HD13	2.43	0.48
1:A:1304:CYS:HB2	1:A:1384:LEU:HD21	1.95	0.48
1:A:1396:THR:O	1:A:1399:ALA:HB3	2.13	0.48
1:A:433:ALA:HB1	1:A:479:THR:HG21	1.94	0.48
1:A:1146:TYR:HD2	1:A:1330:MET:HE1	1.79	0.48
1:A:1232:ILE:HG12	1:A:1252:TYR:CG	2.49	0.48
1:A:1368:ASP:HB3	1:A:1371:LYS:HB2	1.96	0.48
1:A:1169:THR:HB	1:A:1205:LEU:HD22	1.96	0.48
1:A:610:ASP:HB2	1:A:614:ARG:HH21	1.78	0.48
1:A:820:LEU:HA	1:A:1092:ASN:HA	1.94	0.48
1:A:1243:LYS:NZ	1:A:1243:LYS:HB3	2.29	0.48
1:A:851:ILE:HA	1:A:854:LYS:NZ	2.28	0.48
1:A:952:LYS:HE3	1:A:1124:ASP:OD2	2.14	0.48
1:A:1224:LEU:HD23	1:A:1228:MET:HG2	1.96	0.48
1:A:1417:LEU:HG	1:A:1423:VAL:HG21	1.96	0.48
1:A:844:TYR:CD2	1:A:852:ILE:HD13	2.49	0.47
1:A:381:ALA:HB1	1:A:384:PHE:CD2	2.49	0.47
1:A:1049:HIS:HD2	1:A:1086:PHE:CE2	2.32	0.47
1:A:1439:ASP:O	1:A:1440:LEU:C	2.56	0.47
1:A:416:ASN:HD22	1:A:536:VAL:HG23	1.78	0.47
1:A:550:PHE:HB2	1:A:553:PHE:CZ	2.49	0.47
1:A:1215:ILE:HD11	1:A:1275:MET:HE1	1.96	0.47
1:A:660:ARG:NH2	1:A:694:ASP:OD1	2.48	0.47
1:A:582:LEU:O	1:A:585:ILE:N	2.47	0.47
1:A:935:GLY:HA3	1:A:953:ASP:O	2.15	0.47
1:A:1394:LEU:O	1:A:1394:LEU:HD12	2.15	0.47
1:A:446:GLU:CD	1:A:572:ALA:HB3	2.39	0.47
1:A:529:ILE:CG2	1:A:530:PRO:HD2	2.44	0.47
1:A:646:GLU:C	1:A:648:VAL:H	2.22	0.47
1:A:701:LYS:HD3	1:A:720:GLU:HG2	1.95	0.47
1:A:1007:VAL:O	1:A:1040:THR:HG23	2.15	0.47
1:A:249:TYR:N	1:A:270:THR:O	2.47	0.47
1:A:558:LEU:HD12	1:A:586:PHE:HZ	1.80	0.47
1:A:581:HIS:O	1:A:585:ILE:HD13	2.15	0.47
1:A:1167:GLU:O	1:A:1170:HIS:NE2	2.48	0.47
1:A:1281:ALA:HA	7:T:1501:A1I9T:CL27	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:SER:HB3	1:A:1325:ALA:HB1	1.96	0.47
1:A:1431:MET:CB	1:A:1437:LEU:HG	2.44	0.47
1:A:510:ALA:C	1:A:539:THR:HG23	2.39	0.47
1:A:599:HIS:O	1:A:602:LEU:HB2	2.15	0.47
1:A:977:PHE:CD1	1:A:1098:ILE:HG23	2.50	0.47
1:A:1178:LEU:HD21	1:A:1282:ALA:HA	1.95	0.47
1:A:1227:GLY:O	1:A:1231:LYS:HG3	2.15	0.47
1:A:1027:PHE:CB	1:A:1032:VAL:HG23	2.45	0.47
1:A:679:MET:HB2	1:A:722:ILE:HD13	1.97	0.46
1:A:1000:ARG:HB3	1:A:1081:THR:HG22	1.97	0.46
1:A:1330:MET:HE3	1:A:1352:GLU:HG2	1.98	0.46
1:A:561:LYS:HE3	1:A:561:LYS:HB2	1.36	0.46
1:A:251:PHE:CZ	1:A:1034:ARG:HB2	2.50	0.46
1:A:1027:PHE:HB3	1:A:1032:VAL:HG23	1.97	0.46
1:A:1121:ILE:CD1	1:A:1290:ARG:HG3	2.45	0.46
1:A:271:ASP:C	1:A:273:THR:H	2.23	0.46
1:A:1241:TRP:HZ2	1:A:1253:LEU:HD21	1.80	0.46
1:A:685:GLU:HA	1:A:685:GLU:OE1	2.15	0.46
1:A:545:TYR:HD1	1:A:546:LEU:HD23	1.80	0.46
1:A:1120:THR:O	1:A:1120:THR:CG2	2.63	0.46
1:A:1367:ILE:HG12	1:A:1436:VAL:CG2	2.44	0.46
1:A:344:HIS:HB2	1:A:740:THR:HB	1.97	0.46
1:A:1135:PRO:HB3	1:A:1145:ILE:HD11	1.98	0.46
1:A:1398:VAL:HA	1:A:1401:GLN:HB2	1.97	0.46
1:A:800:VAL:O	1:A:804:ASN:ND2	2.37	0.46
1:A:917:TYR:HA	1:A:923:TYR:O	2.16	0.46
1:A:573:ILE:HG23	1:A:574:TYR:H	1.81	0.45
1:A:1413:SER:O	1:A:1415:GLU:HG3	2.16	0.45
1:A:716:GLU:O	1:A:720:GLU:HG3	2.16	0.45
1:A:1111:GLN:HG3	1:A:1116:ILE:O	2.16	0.45
1:A:1180:ILE:HD13	1:A:1180:ILE:HA	1.82	0.45
1:A:1367:ILE:HD12	1:A:1388:PHE:CD1	2.50	0.45
1:A:375:ILE:HG23	1:A:375:ILE:O	2.16	0.45
1:A:381:ALA:HB1	1:A:384:PHE:CE2	2.51	0.45
1:A:870:VAL:O	1:A:874:ILE:HG13	2.16	0.45
1:A:990:LYS:HG3	1:A:998:VAL:CG2	2.46	0.45
1:A:1244:ILE:O	1:A:1249:ARG:NH2	2.49	0.45
1:A:269:ILE:O	1:A:269:ILE:HG13	2.15	0.45
1:A:345:VAL:HG21	1:A:373:ILE:HD11	1.98	0.45
1:A:685:GLU:O	1:A:689:ARG:HG3	2.16	0.45
1:A:1203:ALA:HB2	1:A:1264:TRP:CZ2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:LYS:HE2	1:A:657:LYS:HB2	1.42	0.45
1:A:690:ALA:O	1:A:735:LYS:HE3	2.16	0.45
1:A:755:LYS:NZ	1:A:755:LYS:HB3	2.32	0.45
1:A:841:LYS:HG2	1:A:846:ASP:HA	1.99	0.45
1:A:895:VAL:HG23	1:A:973:ILE:HG12	1.98	0.45
1:A:962:PHE:O	1:A:969:LYS:HE2	2.16	0.45
1:A:1051:GLY:O	1:A:1098:ILE:N	2.42	0.45
1:A:1312:ASP:HA	1:A:1389:ARG:NH1	2.31	0.45
1:A:1300:ILE:HG23	1:A:1301:LEU:HD23	1.99	0.44
1:A:1315:ASP:OD1	1:A:1317:VAL:HB	2.16	0.44
1:A:348:ASN:HB2	1:A:1042:VAL:HA	1.98	0.44
1:A:1204:THR:OG1	1:A:1207:GLU:HG3	2.17	0.44
1:A:1423:VAL:O	1:A:1428:ILE:HD11	2.17	0.44
1:A:1129:MET:HA	1:A:1132:PHE:HD1	1.82	0.44
1:A:413:ILE:HG12	1:A:541:GLU:HB3	1.99	0.44
1:A:452:MET:HE2	1:A:452:MET:HB2	1.88	0.44
1:A:496:LEU:HD11	1:A:523:SER:HB3	1.99	0.44
1:A:921:CYS:O	1:A:922:GLN:HB2	2.16	0.44
1:A:1135:PRO:HD3	1:A:1148:LYS:O	2.18	0.44
1:A:1166:LEU:HD22	1:A:1171:PRO:HG3	1.99	0.44
1:A:539:THR:HG21	1:A:579:THR:CG2	2.47	0.44
1:A:781:ASP:OD1	1:A:781:ASP:N	2.49	0.44
1:A:855:ARG:NH2	1:A:911:PRO:HB2	2.33	0.44
1:A:1131:ILE:N	1:A:1137:VAL:HG11	2.32	0.44
1:A:1023:ASN:HB3	1:A:1025:LEU:HD11	1.97	0.44
1:A:1397:ASN:HA	1:A:1400:LYS:HD2	2.00	0.44
1:A:429:VAL:HA	1:A:509:VAL:HB	1.99	0.44
1:A:451:LYS:HE2	1:A:451:LYS:HB2	1.72	0.44
1:A:510:ALA:HB3	1:A:513:ALA:HA	2.00	0.44
1:A:990:LYS:HA	1:A:998:VAL:HG21	2.00	0.44
1:A:1241:TRP:CD1	1:A:1270:SER:HA	2.52	0.44
1:A:513:ALA:H	1:A:538:ASP:CG	2.24	0.44
1:A:714:LYS:N	1:A:714:LYS:CD	2.81	0.43
1:A:903:MET:HE2	1:A:903:MET:HA	2.00	0.43
1:A:558:LEU:HD22	1:A:558:LEU:HA	1.82	0.43
1:A:787:PHE:O	1:A:795:ALA:HB2	2.18	0.43
1:A:1142:GLN:HE21	1:A:1148:LYS:HD3	1.83	0.43
1:A:427:TYR:CD1	1:A:507:ILE:HB	2.54	0.43
1:A:492:GLU:C	1:A:494:GLU:N	2.76	0.43
1:A:591:MET:HB2	1:A:591:MET:HE2	1.76	0.43
1:A:1007:VAL:HG22	1:A:1044:ARG:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1142:GLN:H	1:A:1142:GLN:HG3	1.51	0.43
1:A:1212:ARG:HA	1:A:1275:MET:HE3	2.00	0.43
1:A:774:ASP:O	1:A:778:ARG:NH1	2.49	0.43
1:A:855:ARG:HH22	1:A:911:PRO:HB2	1.84	0.43
1:A:674:ILE:HG22	1:A:726:LEU:CD2	2.49	0.43
1:A:819:GLU:HG2	1:A:821:TYR:CZ	2.54	0.43
1:A:644:TYR:HB2	1:A:650:ARG:O	2.19	0.43
1:A:669:CYS:HA	1:A:699:MET:CE	2.49	0.43
1:A:1267:ASP:O	1:A:1271:LYS:HG2	2.18	0.43
1:A:610:ASP:O	1:A:611:SER:C	2.61	0.43
1:A:1307:PHE:CE2	1:A:1364:PHE:HE1	2.37	0.43
1:A:585:ILE:N	1:A:585:ILE:HD12	2.33	0.42
1:A:1017:LYS:HD3	1:A:1017:LYS:HA	1.89	0.42
1:A:1213:ASP:OD1	1:A:1278:LYS:N	2.42	0.42
1:A:402:VAL:HG12	1:A:633:LEU:HD11	2.00	0.42
1:A:1048:GLN:HE21	1:A:1048:GLN:HB3	1.51	0.42
1:A:1224:LEU:HD11	1:A:1256:MET:HA	2.01	0.42
1:A:437:LEU:HG	2:E:3:DA:C2	2.55	0.42
1:A:811:GLU:HG2	1:A:812:GLU:H	1.83	0.42
1:A:960:GLU:HG2	1:A:965:PHE:CD1	2.54	0.42
1:A:1031:GLU:O	1:A:1034:ARG:N	2.52	0.42
1:A:1209:ILE:HG22	1:A:1275:MET:SD	2.60	0.42
1:A:666:GLY:HA3	1:A:695:TYR:CZ	2.55	0.42
1:A:821:TYR:HB3	1:A:1057:PRO:HG3	2.00	0.42
1:A:1114:SER:HB3	1:A:1301:LEU:HD13	2.02	0.42
1:A:656:LEU:O	1:A:660:ARG:HB3	2.20	0.42
1:A:1427:LEU:C	1:A:1431:MET:HE3	2.45	0.42
1:A:1315:ASP:O	1:A:1316:LEU:HB3	2.19	0.42
1:A:1416:ASP:O	1:A:1420:ARG:HG3	2.19	0.42
1:A:515:PHE:CE2	2:E:3:DA:H5''	2.55	0.42
1:A:1228:MET:HG3	1:A:1232:ILE:HD11	2.02	0.42
1:A:543:ALA:HB1	1:A:558:LEU:HD11	2.02	0.42
1:A:1166:LEU:CD2	1:A:1171:PRO:HG3	2.50	0.42
1:A:851:ILE:HG23	1:A:852:ILE:N	2.34	0.42
1:A:433:ALA:HA	2:E:3:DA:O3'	2.19	0.41
1:A:634:PHE:O	1:A:638:SER:OG	2.33	0.41
1:A:678:MET:HE2	1:A:686:ALA:HB3	2.01	0.41
1:A:832:ILE:HD13	1:A:832:ILE:HA	1.82	0.41
1:A:1043:LYS:HE3	1:A:1046:THR:HG23	2.02	0.41
4:T:16:DA:C8	4:T:16:DA:H5'	2.55	0.41
1:A:1235:THR:HG21	1:A:1252:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:TYR:HD1	1:A:507:ILE:HB	1.84	0.41
1:A:449:ALA:HB2	1:A:499:PHE:HE1	1.86	0.41
1:A:513:ALA:HB3	1:A:538:ASP:CB	2.47	0.41
1:A:630:LEU:HD21	1:A:815:PRO:HA	2.02	0.41
1:A:1433:ASP:OD1	1:A:1434:ASN:OD1	2.38	0.41
1:A:437:LEU:HD22	2:E:2:DA:C4	2.54	0.41
1:A:755:LYS:HB3	1:A:755:LYS:HZ1	1.84	0.41
1:A:929:ASP:OD1	1:A:931:THR:OG1	2.26	0.41
1:A:895:VAL:CG2	1:A:973:ILE:HG12	2.49	0.41
1:A:1354:ALA:HA	1:A:1364:PHE:HZ	1.86	0.41
1:A:1355:ASN:O	1:A:1359:GLU:HG2	2.21	0.41
1:A:655:GLN:O	1:A:659:MET:HG3	2.20	0.41
1:A:1316:LEU:HA	1:A:1319:MET:HB2	2.02	0.41
1:A:497:ARG:CG	1:A:497:ARG:NH1	2.83	0.41
1:A:681:LYS:HD2	1:A:689:ARG:NH2	2.35	0.41
1:A:723:ILE:O	1:A:727:VAL:HG23	2.20	0.41
1:A:1095:LYS:HE2	1:A:1095:LYS:HB3	1.96	0.41
4:T:14:DG:H2"	4:T:15:DC:C6	2.56	0.41
1:A:908:GLU:HG2	1:A:1286:LEU:HD13	2.02	0.41
1:A:1241:TRP:HH2	1:A:1256:MET:HE2	1.86	0.41
1:A:1249:ARG:HB2	1:A:1249:ARG:CZ	2.51	0.41
1:A:492:GLU:O	1:A:494:GLU:N	2.54	0.41
1:A:550:PHE:CD1	1:A:550:PHE:N	2.89	0.41
1:A:885:ASP:N	1:A:885:ASP:OD1	2.54	0.41
1:A:936:PHE:N	1:A:936:PHE:CD1	2.88	0.41
1:A:1196:GLU:O	1:A:1197:LEU:C	2.63	0.41
1:A:1212:ARG:NH2	1:A:1237:ARG:HH11	2.18	0.41
1:A:1247:GLU:OE1	1:A:1247:GLU:N	2.34	0.41
1:A:416:ASN:ND2	1:A:536:VAL:HG23	2.36	0.40
1:A:432:VAL:HG12	1:A:447:LEU:HG	2.02	0.40
1:A:710:GLN:O	1:A:711:GLU:HB2	2.22	0.40
1:A:915:HIS:C	1:A:938:MET:HE1	2.46	0.40
1:A:1241:TRP:CH2	1:A:1256:MET:HE2	2.56	0.40
1:A:449:ALA:CB	1:A:499:PHE:HE1	2.35	0.40
1:A:1224:LEU:HD23	1:A:1228:MET:CG	2.51	0.40
1:A:822:THR:HG22	1:A:1094:LEU:HD21	2.04	0.40
1:A:1241:TRP:HZ2	1:A:1253:LEU:CD2	2.34	0.40
1:A:1357:MET:HE1	1:A:1384:LEU:CG	2.48	0.40
1:A:534:ASN:OD1	1:A:534:ASN:N	2.47	0.40
1:A:701:LYS:HE3	1:A:701:LYS:HB2	1.82	0.40
1:A:1129:MET:HB3	1:A:1129:MET:HE3	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1281:ALA:O	1:A:1285:VAL:HG23	2.22	0.40
1:A:1380:GLU:O	1:A:1380:GLU:CG	2.70	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	A	1074/1474 (73%)	1030 (96%)	44 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	929/1272 (73%)	848 (91%)	81 (9%)	8	32

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	LYS
1	A	276	PHE
1	A	277	ILE
1	A	397	LYS

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Mol	Chain	Res	Type
1	A	432	VAL
1	A	435	THR
1	A	444	ILE
1	A	447	LEU
1	A	451	LYS
1	A	475	THR
1	A	478	LEU
1	A	479	THR
1	A	490	LYS
1	A	491	SER
1	A	507	ILE
1	A	539	THR
1	A	555	LEU
1	A	558	LEU
1	A	560	LYS
1	A	561	LYS
1	A	606	ILE
1	A	611	SER
1	A	613	LYS
1	A	616	ARG
1	A	647	ARG
1	A	657	LYS
1	A	659	MET
1	A	661	GLU
1	A	665	ILE
1	A	673	GLU
1	A	683	VAL
1	A	687	ARG
1	A	731	LYS
1	A	732	SER
1	A	749	GLU
1	A	758	ILE
1	A	888	LEU
1	A	892	ARG
1	A	938	MET
1	A	952	LYS
1	A	974	ASP
1	A	1011	THR
1	A	1048	GLN
1	A	1054	ILE
1	A	1090	HIS
1	A	1127	GLU

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Mol	Chain	Res	Type
1	A	1129	MET
1	A	1131	ILE
1	A	1137	VAL
1	A	1142	GLN
1	A	1143	GLU
1	A	1144	GLN
1	A	1180	ILE
1	A	1188	ASP
1	A	1199	ARG
1	A	1212	ARG
1	A	1213	ASP
1	A	1220	ILE
1	A	1224	LEU
1	A	1233	MET
1	A	1250	GLU
1	A	1256	MET
1	A	1270	SER
1	A	1271	LYS
1	A	1290	ARG
1	A	1318	SER
1	A	1323	LYS
1	A	1327	LYS
1	A	1338	LEU
1	A	1366	MET
1	A	1371	LYS
1	A	1378	VAL
1	A	1394	LEU
1	A	1400	LYS
1	A	1406	ARG
1	A	1423	VAL
1	A	1424	SER
1	A	1426	THR
1	A	1427	LEU
1	A	1429	GLU
1	A	1432	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	HIS
1	A	416	ASN
1	A	511	HIS

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Continued from previous page...

Mol	Chain	Res	Type
1	A	601	GLN
1	A	641	ASN
1	A	1048	GLN
1	A	1142	GLN
1	A	1347	GLN
1	A	1397	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	A1I9T	T	1501	-	26,31,31	2.57	11 (42%)	25,43,43	1.37	5 (20%)

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
7	A1I9T	T	1501	-	-	3/10/18/18	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	1501	A1I9T	C07-N06	-6.53	1.32	1.47
7	T	1501	A1I9T	C17-N16	5.05	1.44	1.36
7	T	1501	A1I9T	C17-N19	4.63	1.44	1.34
7	T	1501	A1I9T	C20-C21	3.89	1.59	1.51
7	T	1501	A1I9T	C05-N06	-3.62	1.36	1.46
7	T	1501	A1I9T	C14-N16	2.87	1.42	1.37
7	T	1501	A1I9T	C13-C14	2.80	1.52	1.45
7	T	1501	A1I9T	C01-N06	-2.77	1.39	1.46
7	T	1501	A1I9T	O15-C14	-2.49	1.18	1.23
7	T	1501	A1I9T	C20-N19	2.15	1.50	1.46
7	T	1501	A1I9T	C12-N18	2.04	1.48	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	1501	A1I9T	C08-C07-N06	-2.68	105.71	112.51
7	T	1501	A1I9T	C20-C21-C26	-2.27	116.20	120.91
7	T	1501	A1I9T	O03-C04-C05	-2.26	106.81	111.80
7	T	1501	A1I9T	C23-C22-C21	-2.19	118.96	120.46
7	T	1501	A1I9T	C02-C01-N06	2.16	113.37	110.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	T	1501	A1I9T	C08-C07-N06-C05
7	T	1501	A1I9T	N06-C07-C08-N09
7	T	1501	A1I9T	C08-C07-N06-C01

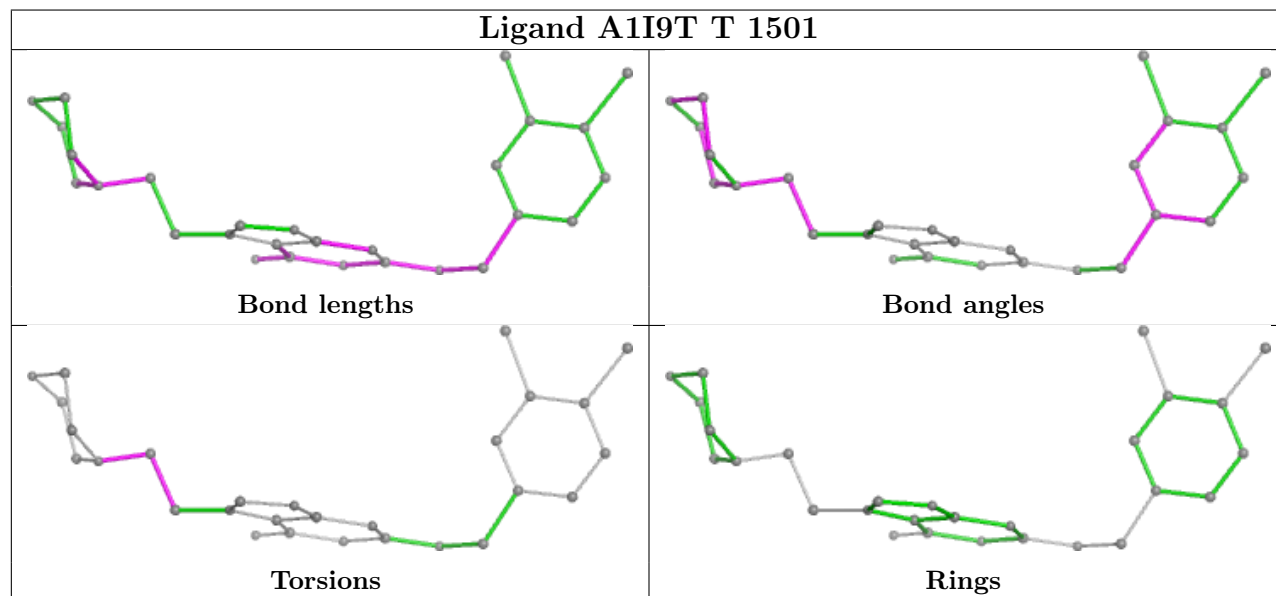
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	1501	A1I9T	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

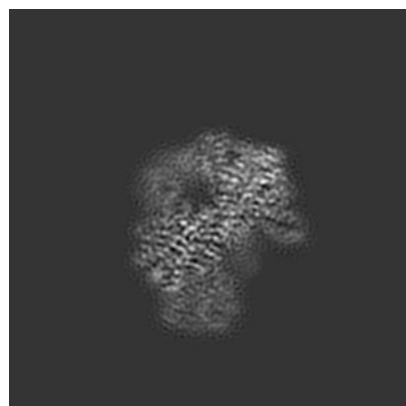
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53319. These allow visual inspection of the internal detail of the map and identification of artifacts.

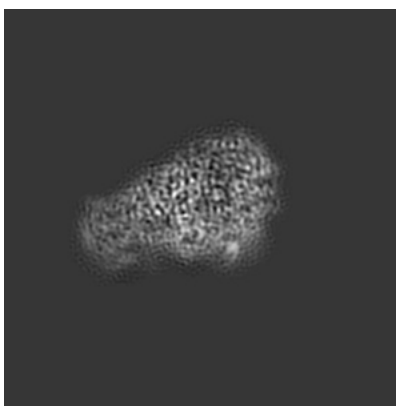
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

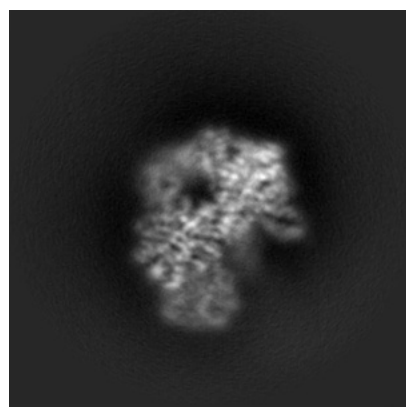


Y

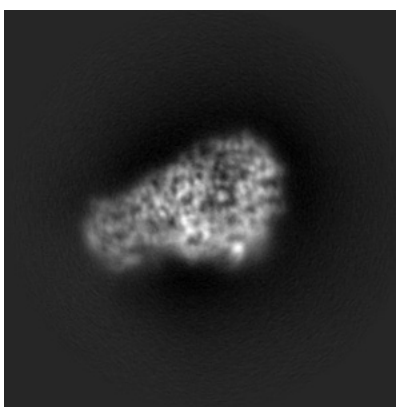


Z

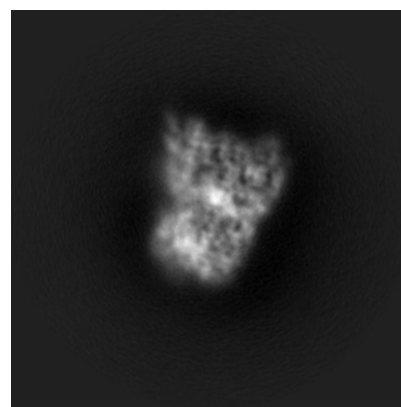
6.1.2 Raw map



X



Y

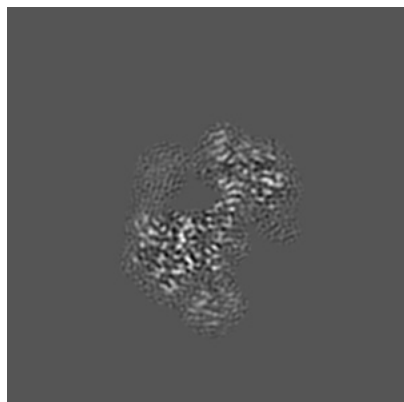


Z

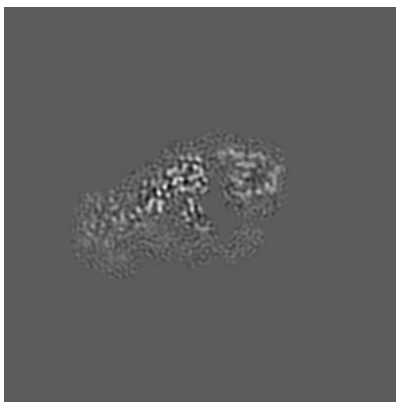
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

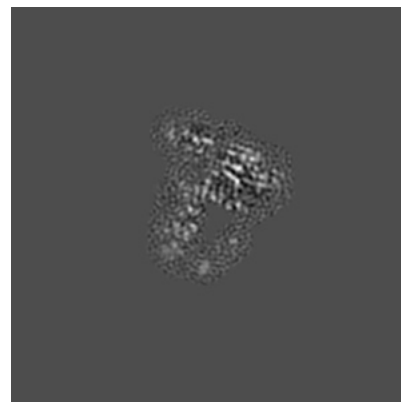
6.2.1 Primary map



X Index: 128

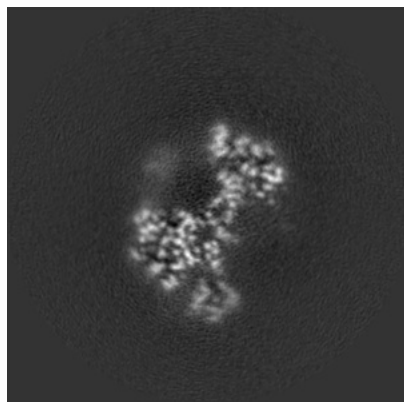


Y Index: 128

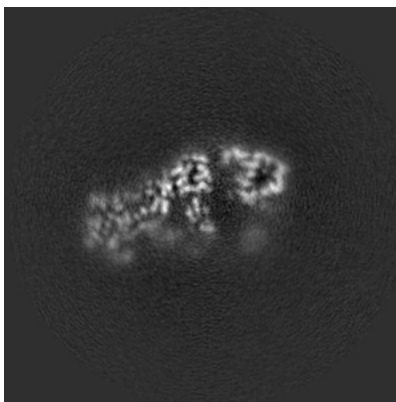


Z Index: 128

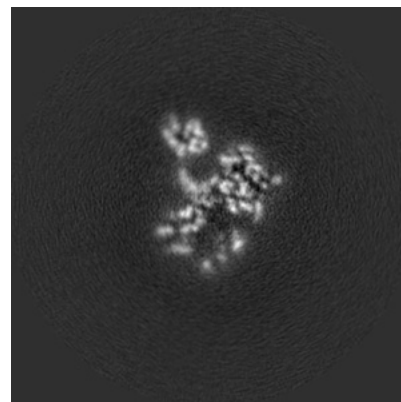
6.2.2 Raw map



X Index: 128



Y Index: 128

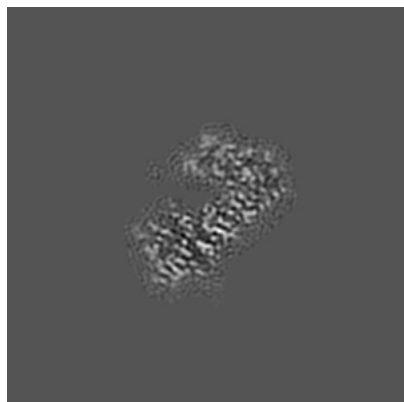


Z Index: 128

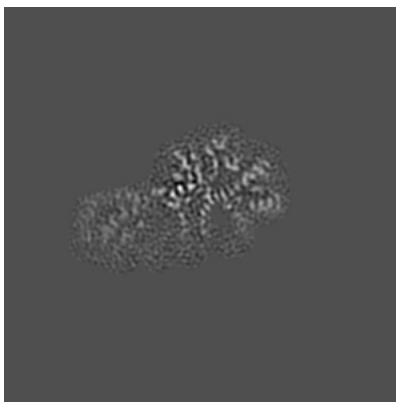
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

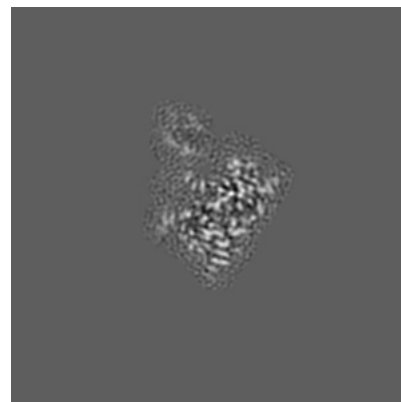
6.3.1 Primary map



X Index: 140

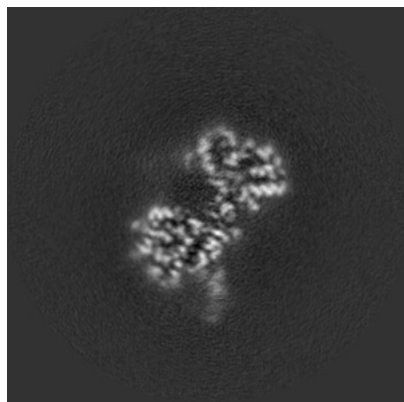


Y Index: 136

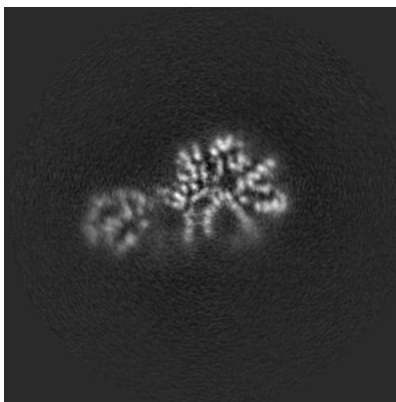


Z Index: 119

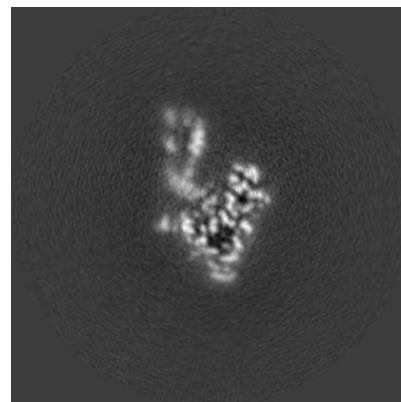
6.3.2 Raw map



X Index: 136



Y Index: 137

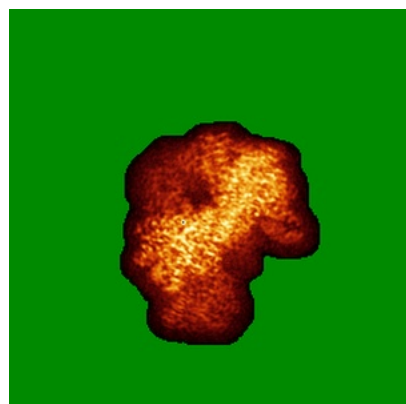


Z Index: 117

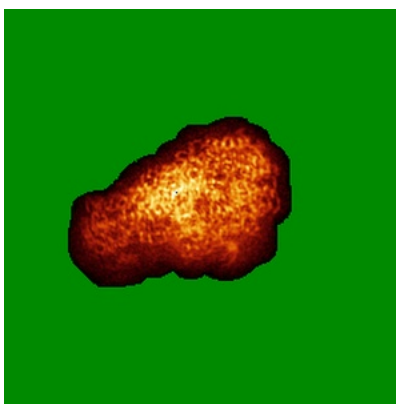
The images above show the largest variance slices of the map in three orthogonal directions.

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

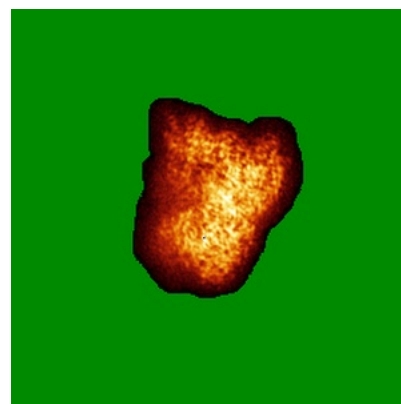
6.4.1 Primary map



X

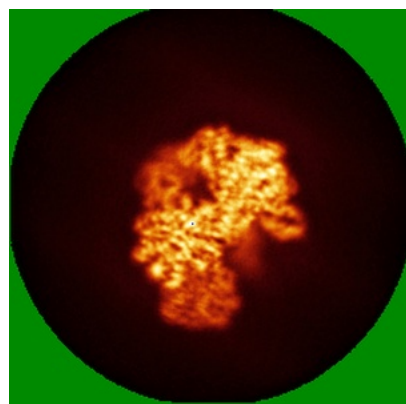


Y

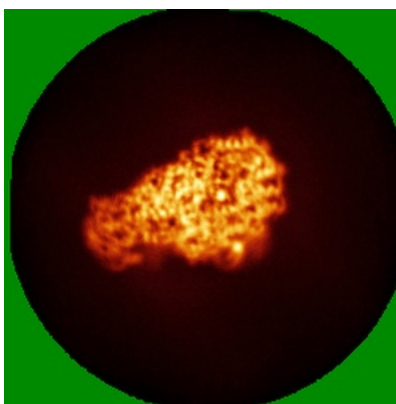


Z

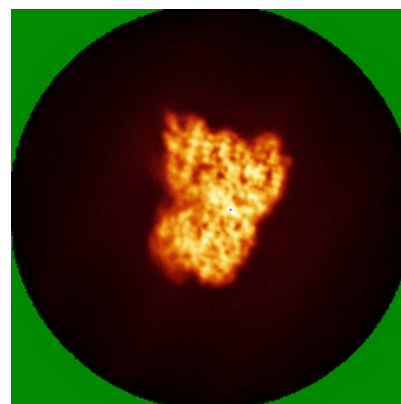
6.4.2 Raw map



X



Y

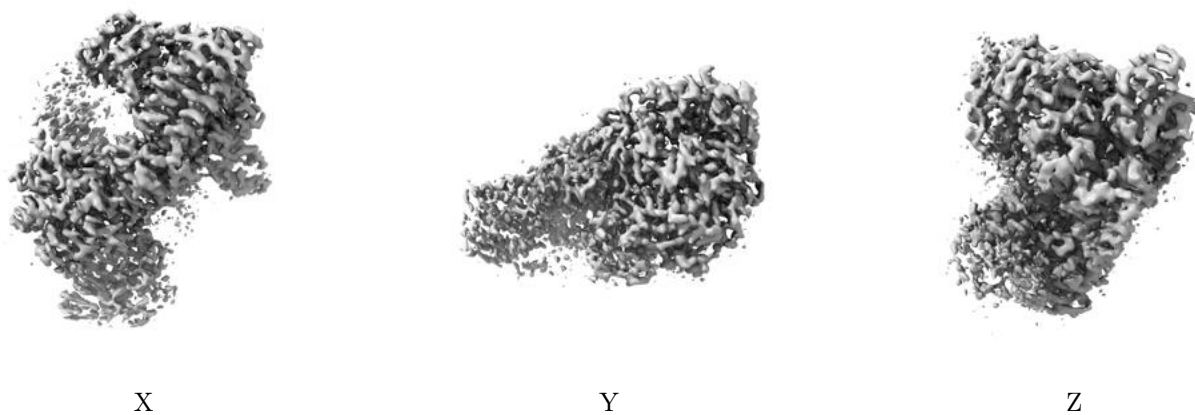


Z

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.

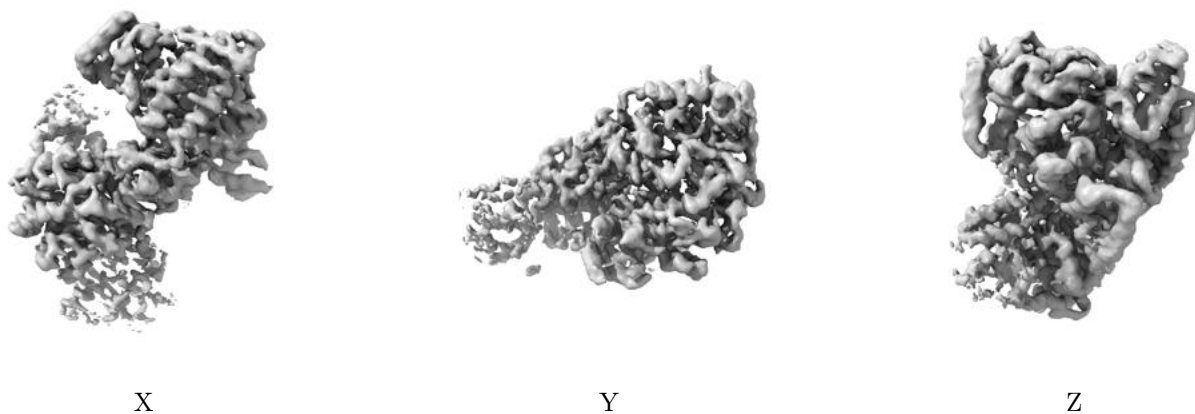
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0116. 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.

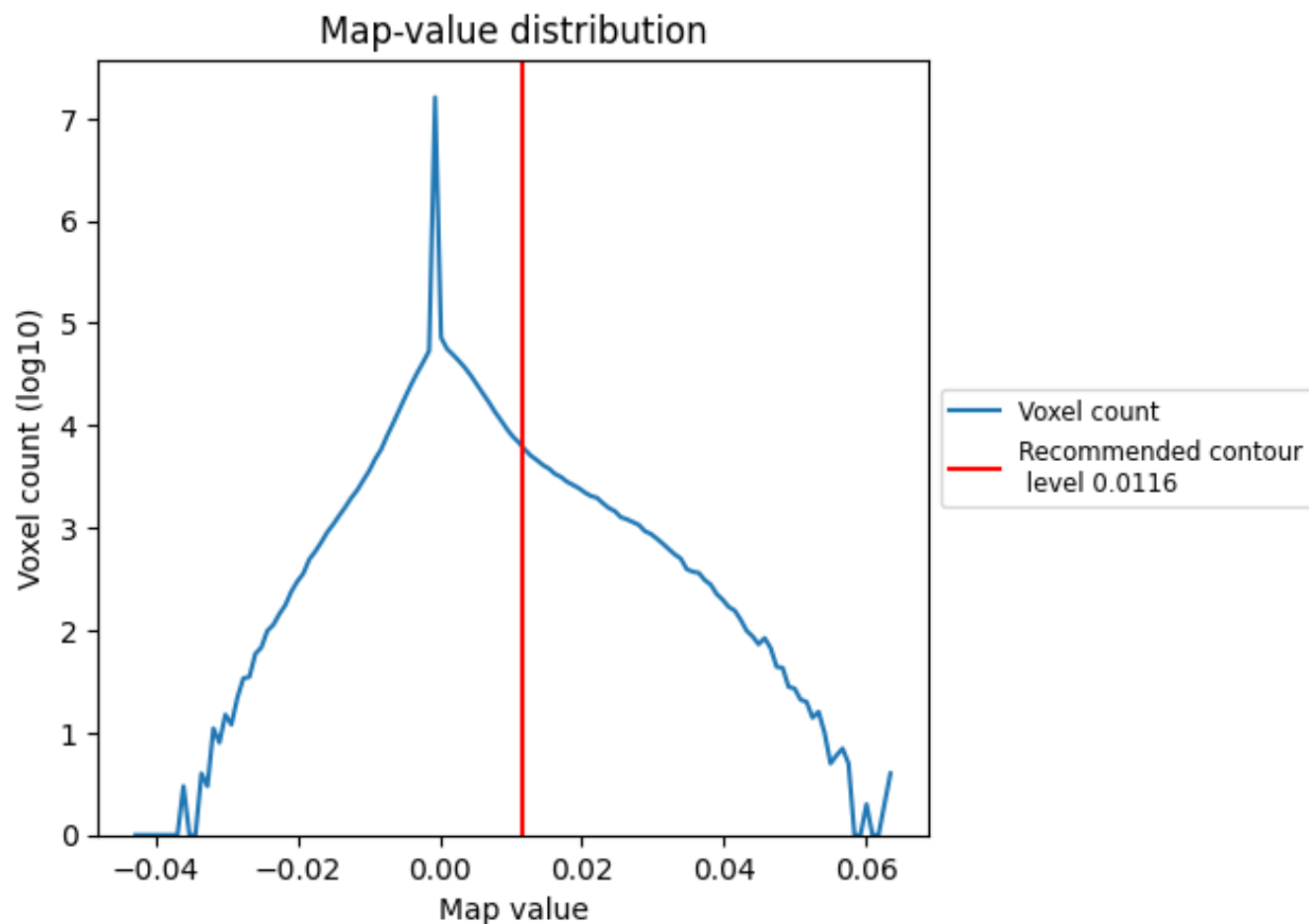
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

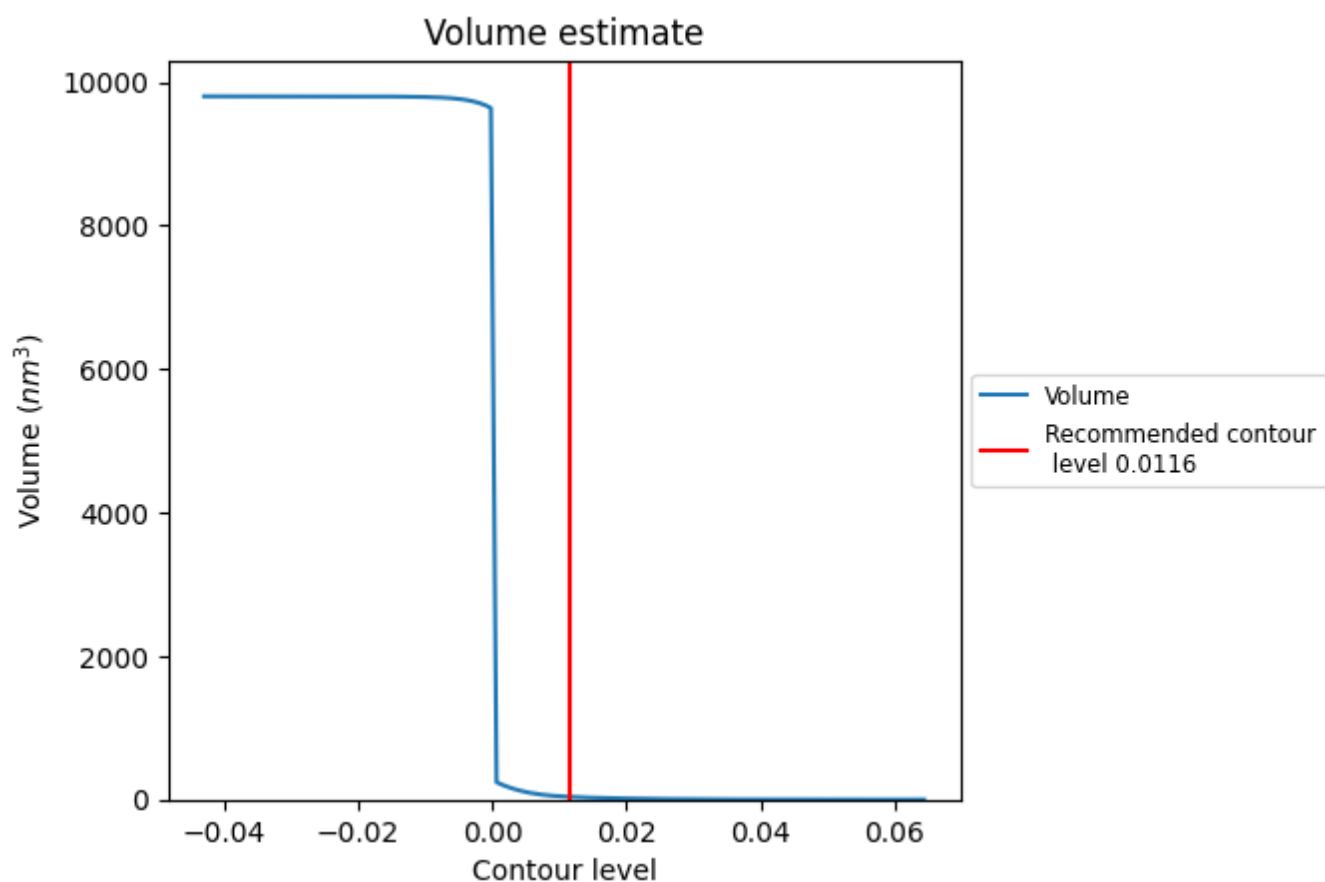
This section contains the results of statistical analysis of the map.

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.

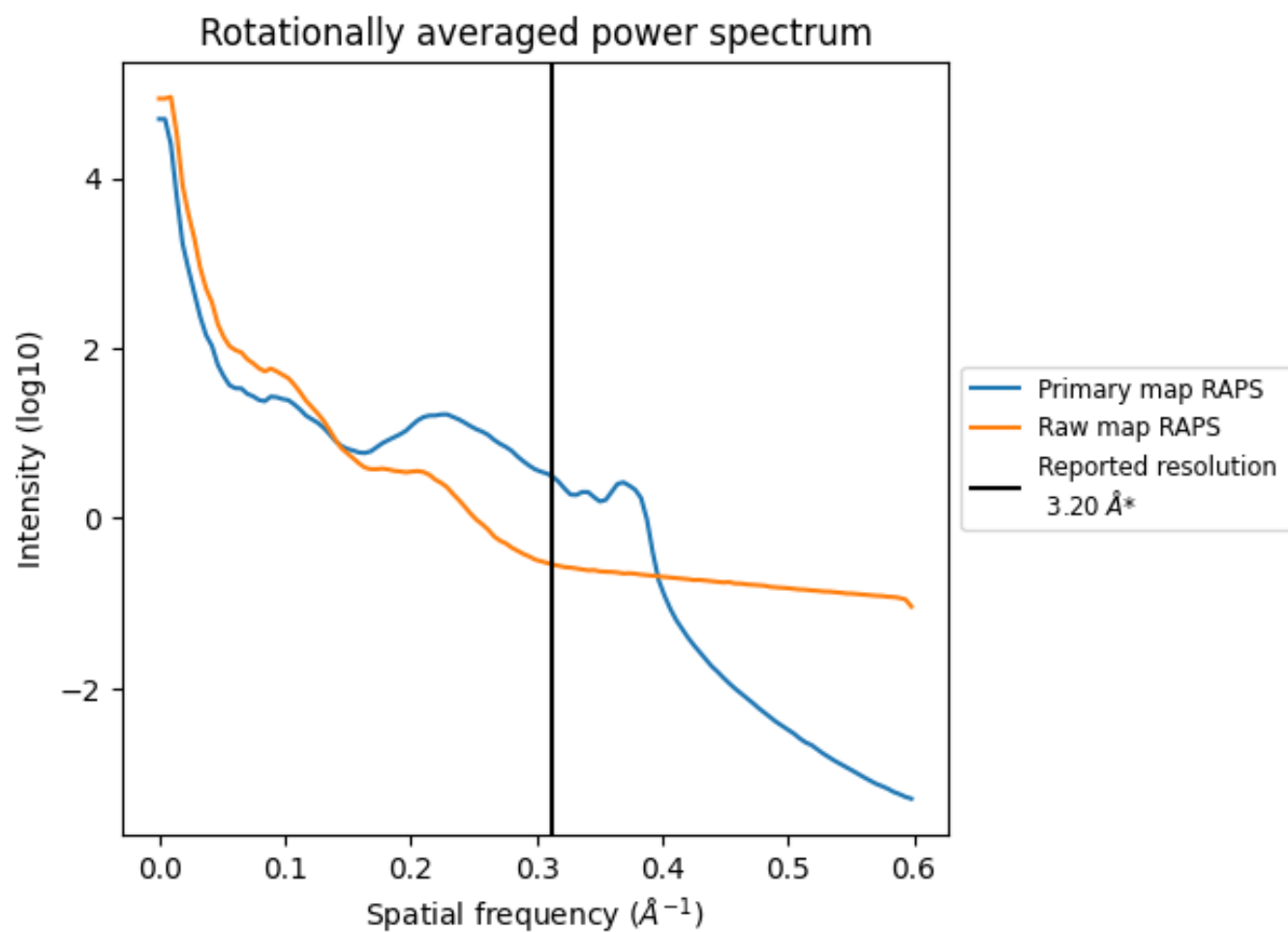
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38 nm³; this corresponds to an approximate mass of 34 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

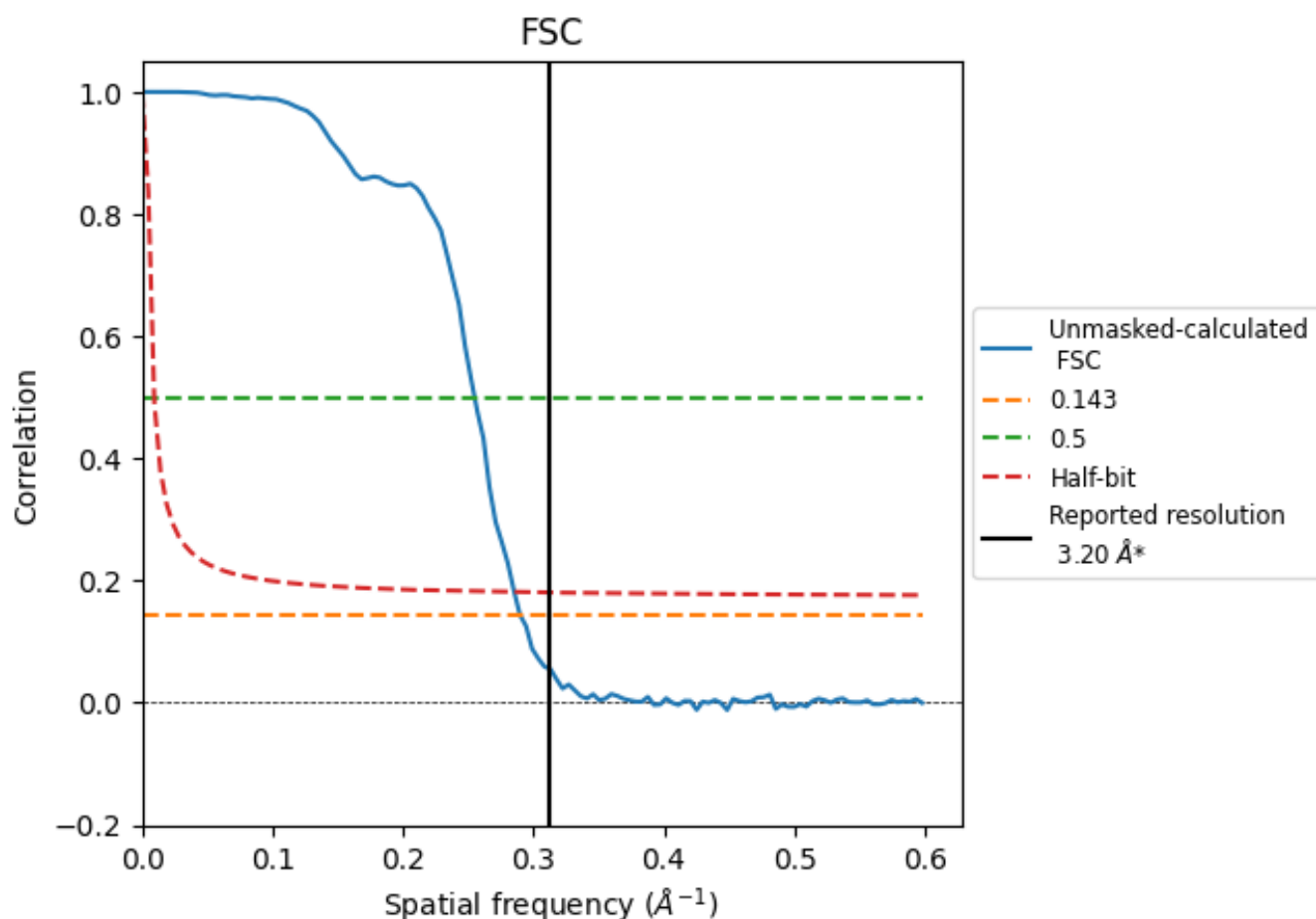


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

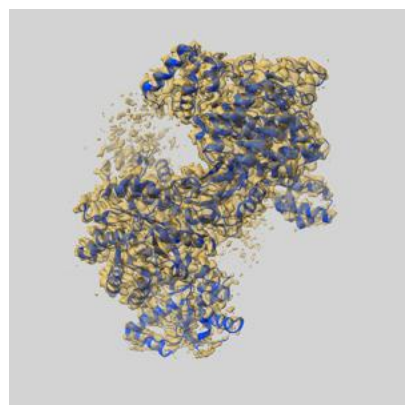
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.45	3.92	3.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

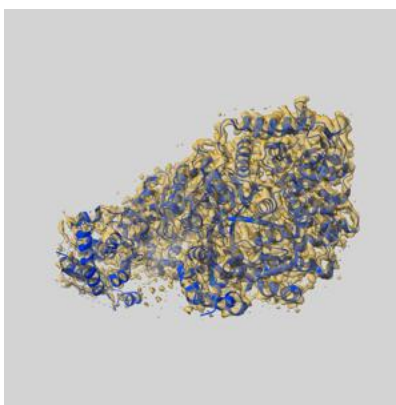
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53319 and PDB model 9QRL. Per-residue inclusion information can be found in section 3 on page 6.

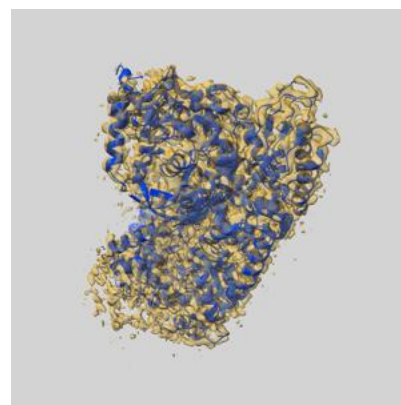
9.1 Map-model overlay [i](#)



X



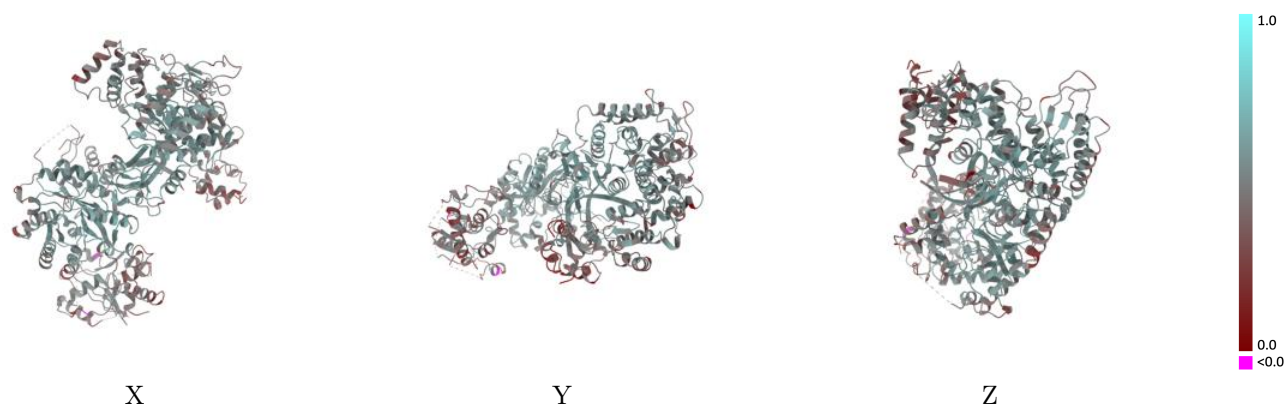
Y



Z

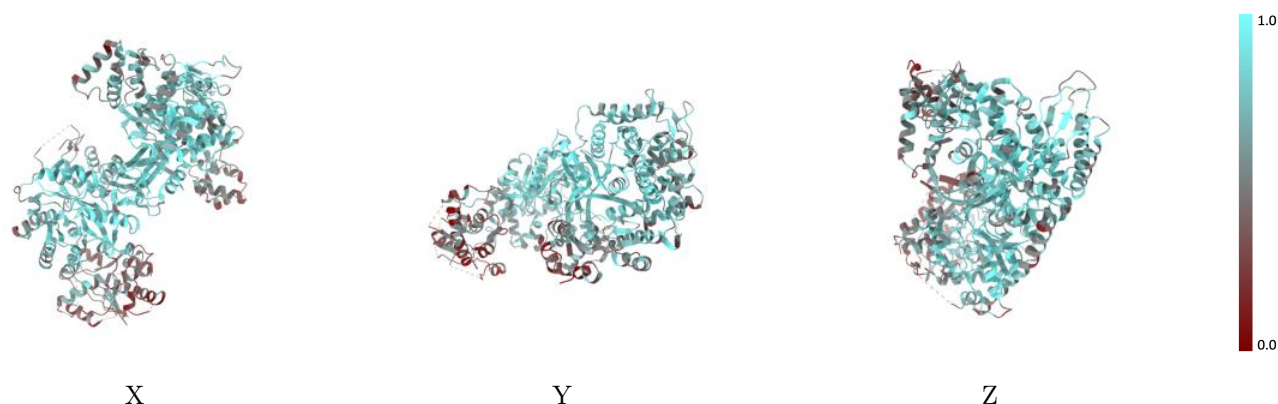
The images above show the 3D surface view of the map at the recommended contour level 0.0116 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



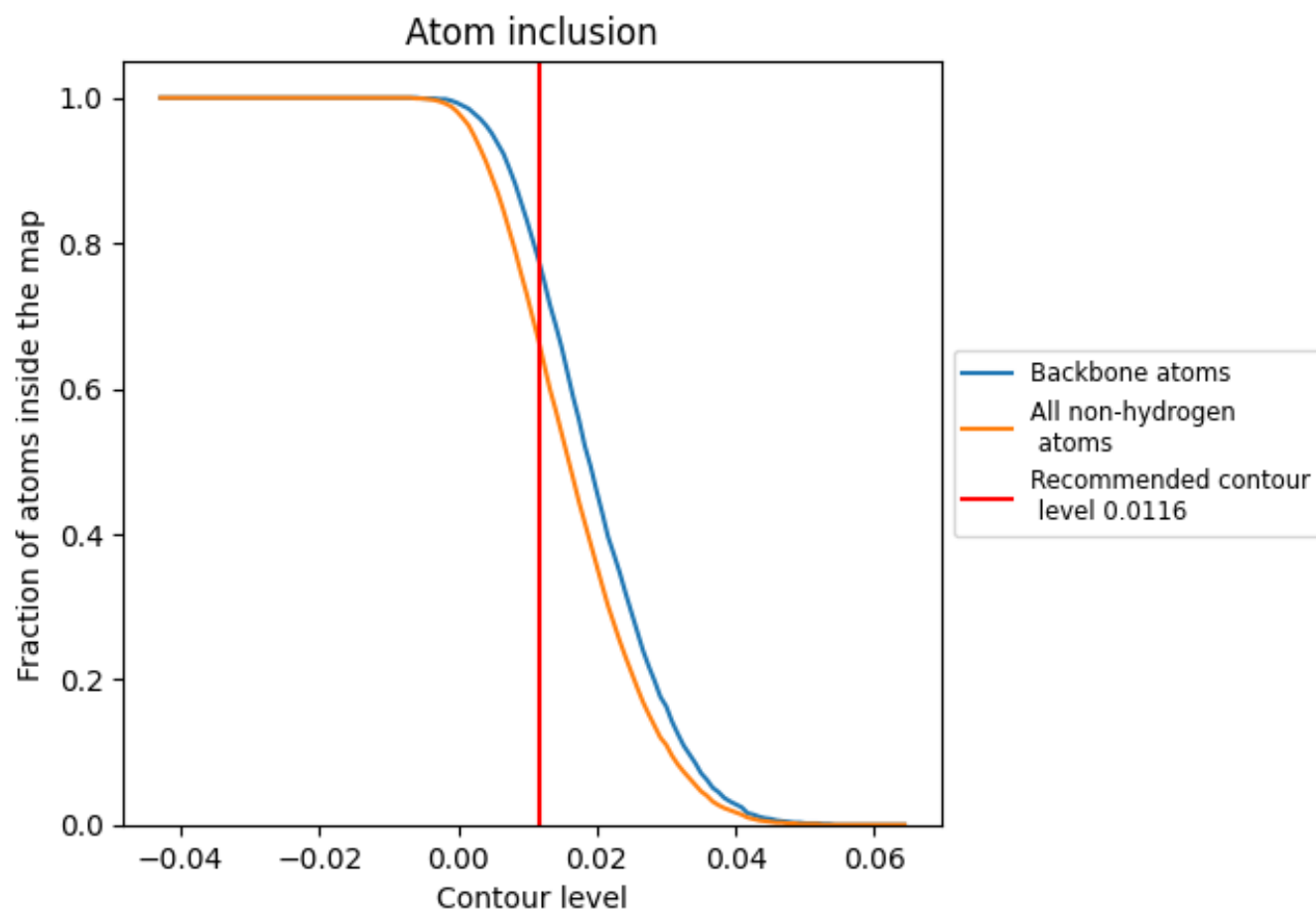
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0116).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 67% 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 (0.0116) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6660	<div></div> 0.4920
A	<div></div> 0.6650	<div></div> 0.4890
E	<div></div> 0.5000	<div></div> 0.5150
P	<div></div> 0.7110	<div></div> 0.5330
T	<div></div> 0.7060	<div></div> 0.5370

