



Full wwPDB EM Validation Report ⓘ

Aug 7, 2026 – 05:04 AM JST

PDB ID : 9W8S / pdb_00009w8s
EMDB ID : EMD-65750
Title : Structure of mammalian RNA polymerase II stalled by a cisplatin-induced inter-strand crosslink lesion at the +2 position.
Authors : Xu, J.; Zhu, L.
Deposited on : 2025-08-08
Resolution : 3.04 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

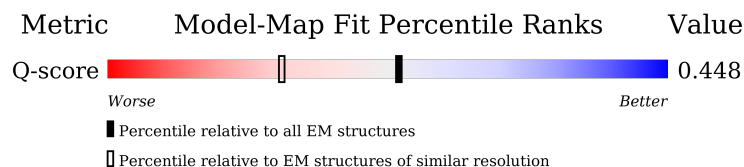
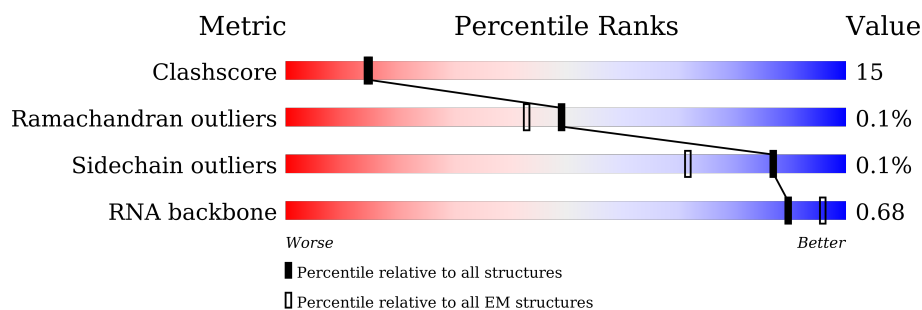
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13952 (2.54 - 3.54)

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	1970	
2	B	1174	
3	C	271	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	171	
8	H	150	
9	I	125	
10	J	67	
11	K	115	
12	L	58	
13	N	18	
14	P	20	
15	T	25	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32013 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1427	Total	C	N	O	S	0	0
			11291	7102	2021	2096	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 13 is a DNA chain called DNA (NTS, non-template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	12	Total	C	N	O	P	0	0
			256	119	58	67	12		

- Molecule 14 is a RNA chain called RNA (5'-R(*UP*AP*CP*AP*AP*UP*GP*UP*UP*GP

*GP*AP*AP*AP*GP*GP*AP*GP*AP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	11	Total	C	N	O	P	0	0
			248	110	55	72	11		

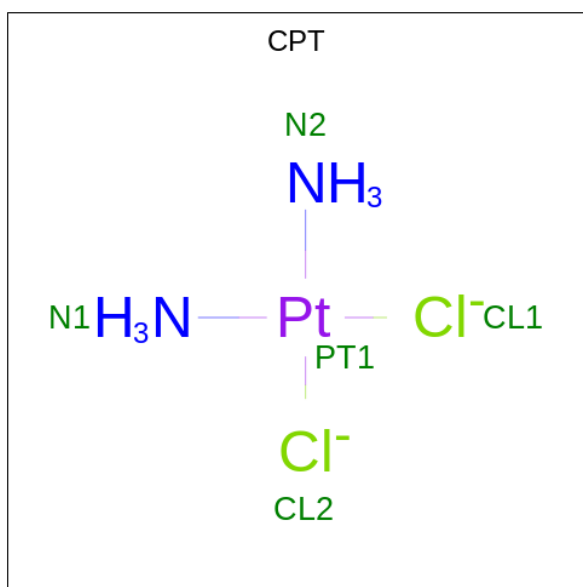
- Molecule 15 is a DNA chain called DNA (TS, template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	22	Total	C	N	O	P	0	0
			431	209	58	142	22		

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	A	2	Total	Zn	0
			2	2	
16	B	1	Total	Zn	0
			1	1	
16	C	1	Total	Zn	0
			1	1	
16	I	2	Total	Zn	0
			2	2	
16	J	1	Total	Zn	0
			1	1	
16	L	1	Total	Zn	0
			1	1	

- Molecule 17 is Cisplatin (CCD ID: CPT) (formula: $\text{Cl}_2\text{H}_6\text{N}_2\text{Pt}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
17	N	1	Total	N	Pt	0
			3	2	1	

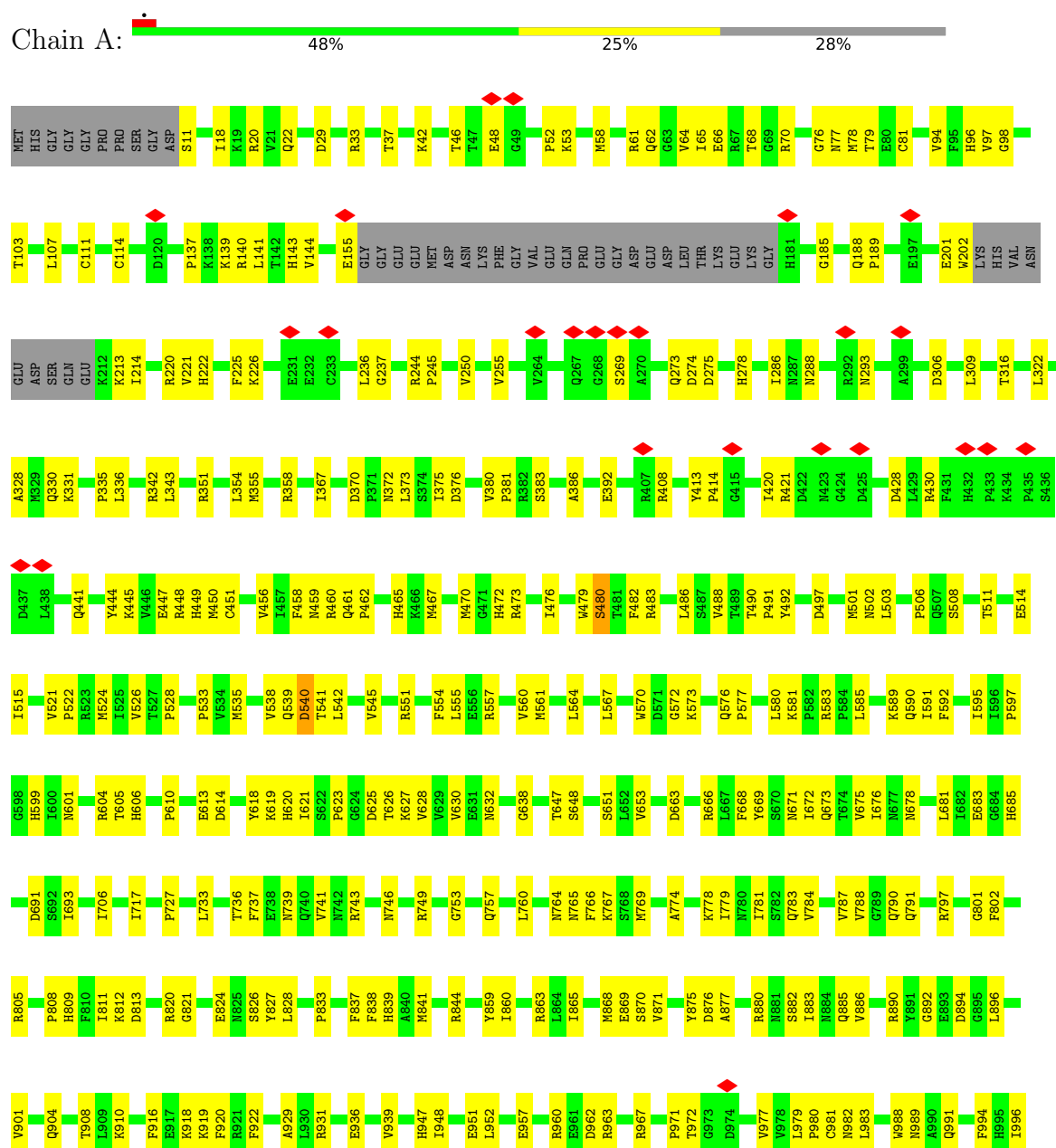
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

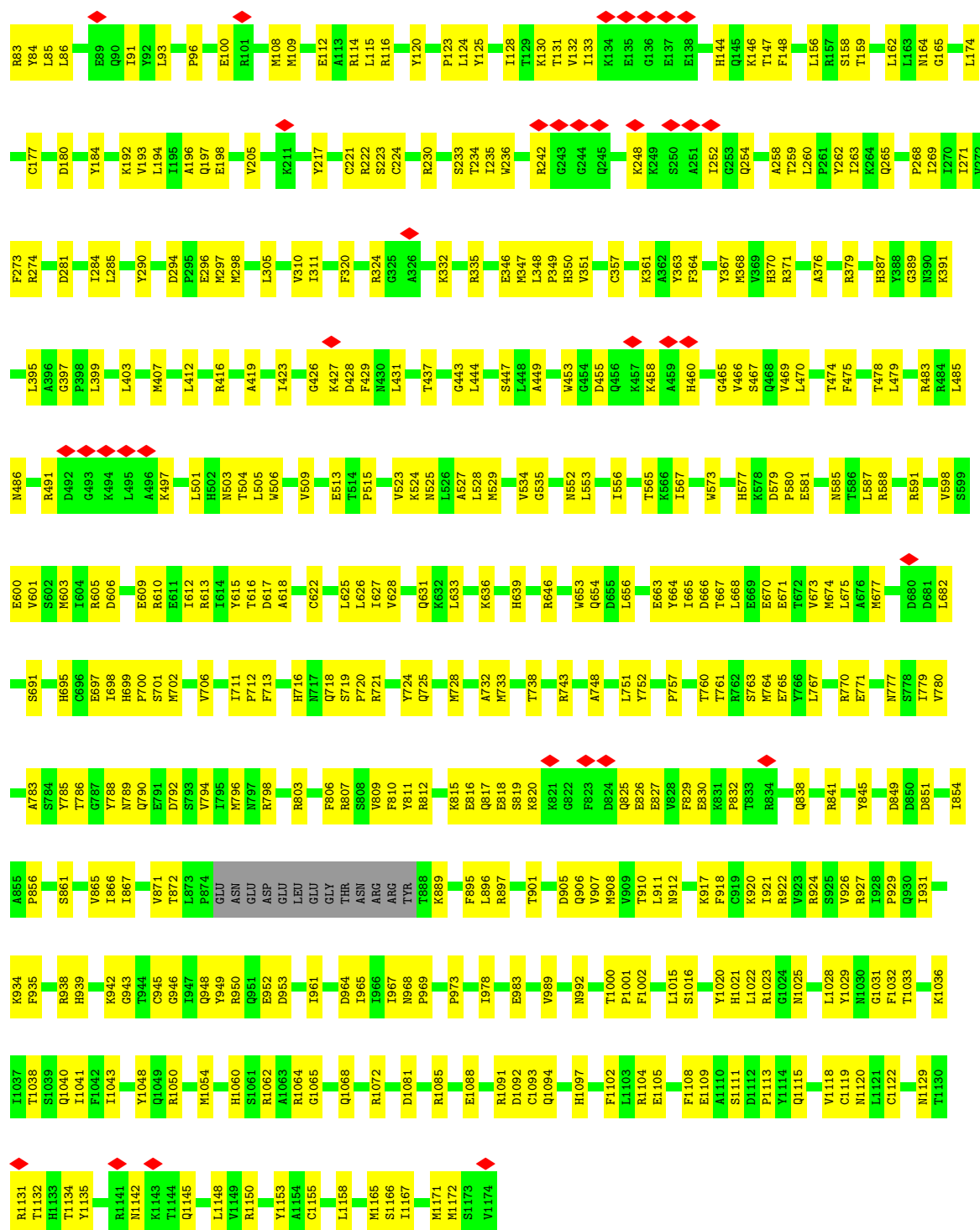
Mol	Chain	Residues	Atoms		AltConf
18	P	1	Total	Mg	0
			1	1	

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.

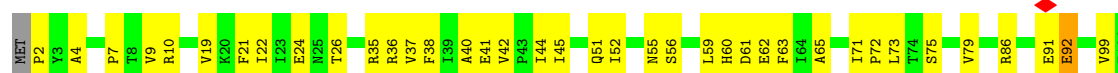
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1

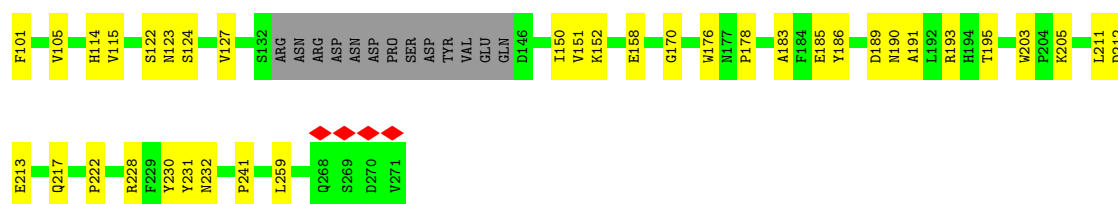




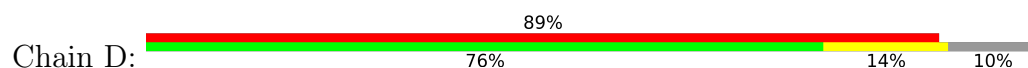
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 68% 27% 5%

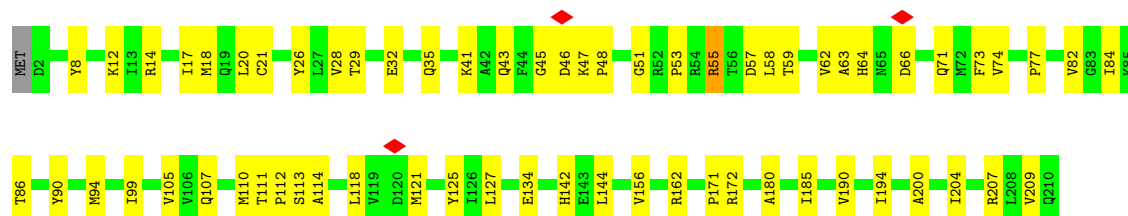




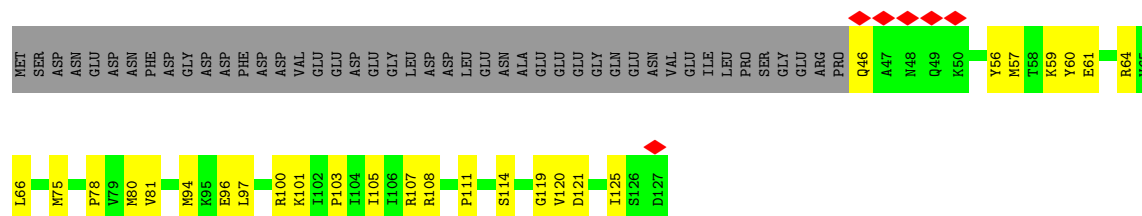
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



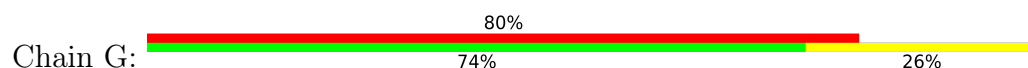
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

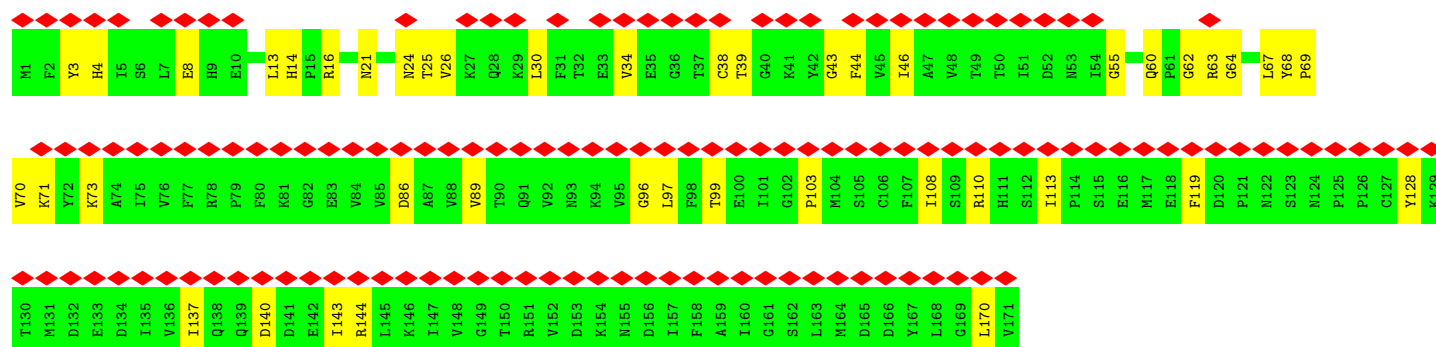


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



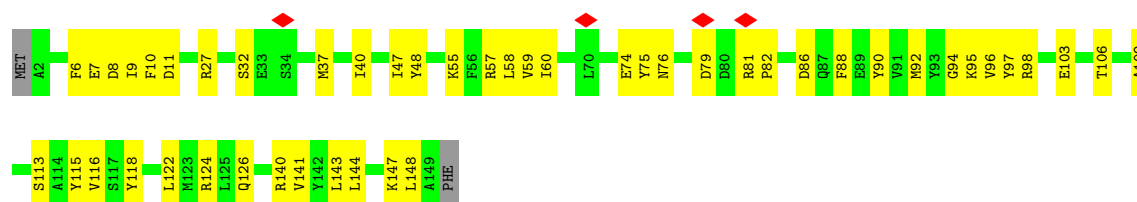
- Molecule 7: DNA-directed RNA polymerase subunit RPB7





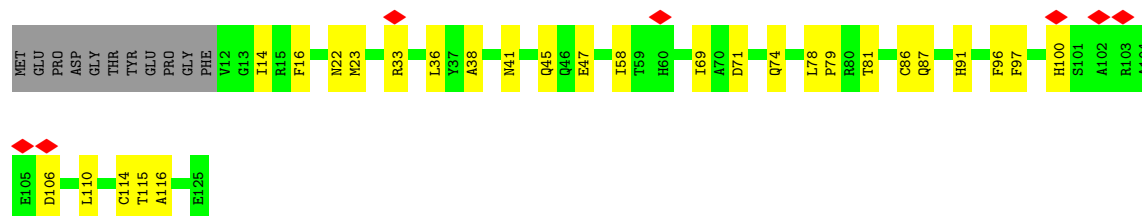
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 67% 32%



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 6% 69% 22% 9%



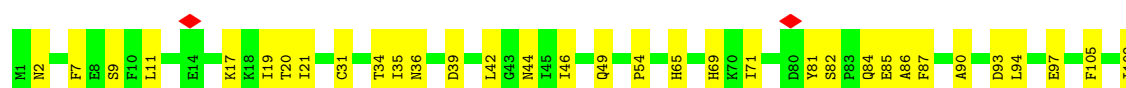
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 69% 31%



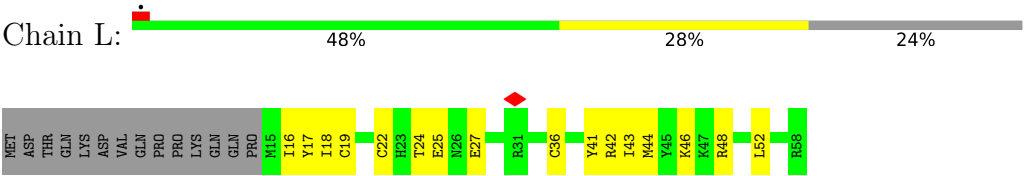
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 71% 29%

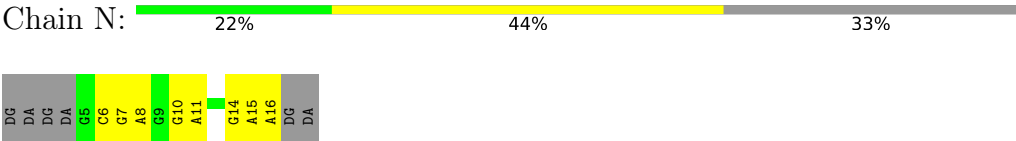




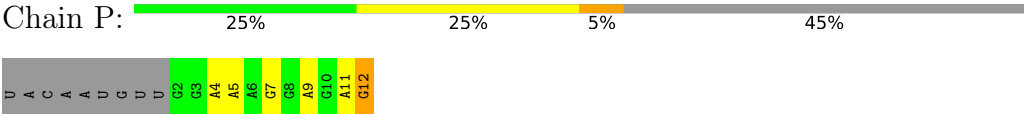
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



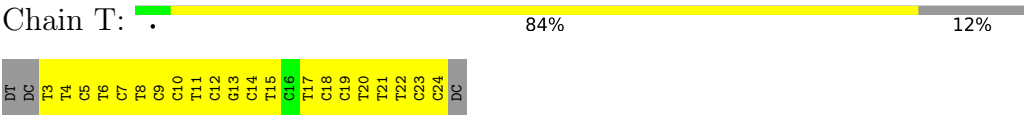
- Molecule 13: DNA (NTS, non-template strand)



- Molecule 14: RNA (5'-R(*UP*AP*CP*AP*AP*UP*GP*UP*UP*GP*GP*AP*AP*AP*GP*GP*AP*GP*AP*G)-3')



- Molecule 15: DNA (TS, template strand)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145135	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)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.569	Depositor
Minimum map value	-0.270	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	297.6, 297.6, 297.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CPT, 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	A	0.24	0/11497	0.44	3/15521 (0.0%)
2	B	0.26	0/9243	0.44	0/12475
3	C	0.27	0/2102	0.47	0/2857
4	D	0.10	0/1019	0.31	0/1374
5	E	0.39	0/1751	0.57	0/2366
6	F	0.21	0/667	0.48	0/901
7	G	0.13	0/1365	0.38	0/1853
8	H	0.28	0/1207	0.58	0/1628
9	I	0.19	0/948	0.38	0/1284
10	J	0.29	0/542	0.51	0/730
11	K	0.22	0/939	0.40	0/1271
12	L	0.20	0/377	0.44	0/500
13	N	0.52	0/290	0.86	0/447
14	P	0.63	0/280	0.91	1/437 (0.2%)
15	T	0.41	0/475	0.72	0/727
All	All	0.26	0/32702	0.47	4/44371 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
5	E	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	SER	N-CA-C	7.52	122.19	112.26
1	A	538	VAL	N-CA-C	5.75	115.83	108.82
1	A	539	GLN	CB-CA-C	-5.49	110.23	116.54
14	P	9	A	O3'-P-O5'	-5.16	96.26	104.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	910	LYS	Peptide
2	B	497	LYS	Peptide
5	E	55	ARG	Sidechain

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	11291	0	11402	397	0
2	B	9062	0	9107	349	0
3	C	2059	0	2007	61	0
4	D	1005	0	964	15	0
5	E	1720	0	1737	52	0
6	F	657	0	684	30	0
7	G	1334	0	1333	33	0
8	H	1186	0	1147	42	0
9	I	927	0	859	25	0
10	J	533	0	553	17	0
11	K	920	0	942	25	0
12	L	372	0	378	17	0
13	N	256	0	133	12	0
14	P	248	0	122	4	0
15	T	431	0	253	35	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	N	3	0	0	0	0
18	P	1	0	0	0	0
All	All	32013	0	31621	959	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 15.

All (959) 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)
2:B:230:ARG:HH21	2:B:349:PRO:HG3	1.22	1.04
13:N:15:DA:H2''	13:N:16:DA:H5'	1.40	1.02
1:A:948:ILE:HG12	1:A:1007:ILE:HD11	1.47	0.94
15:T:4:DT:H2''	15:T:5:DC:H5''	1.52	0.92
2:B:115:LEU:HB3	2:B:908:MET:HE1	1.54	0.90
13:N:16:DA:N6	15:T:3:DT:O4	2.06	0.88
2:B:159:THR:HA	2:B:164:ASN:HD22	1.41	0.86
8:H:32:SER:HB3	8:H:37:MET:H	1.41	0.85
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.60	0.84
1:A:1087:VAL:HG12	1:A:1400:LEU:HD22	1.57	0.84
1:A:784:VAL:HG13	2:B:978:ILE:HD11	1.60	0.83
15:T:10:DC:H2'	15:T:11:DT:H71	1.59	0.83
1:A:1468:THR:HG23	6:F:64:ARG:HB2	1.60	0.83
1:A:1457:ASN:HD22	1:A:1465:PRO:HD3	1.43	0.83
1:A:589:LYS:HZ3	1:A:638:GLY:H	1.24	0.83
2:B:109:MET:HE2	2:B:174:LEU:HD13	1.58	0.83
1:A:863:ARG:NH2	1:A:1129:ASN:OD1	2.11	0.83
2:B:230:ARG:NH2	2:B:349:PRO:HG3	1.94	0.82
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.61	0.81
2:B:631:GLN:NE2	2:B:691:SER:O	2.12	0.81
1:A:1474:LEU:HB2	6:F:105:ILE:HG13	1.64	0.80
2:B:1031:GLY:O	3:C:36:ARG:NH2	2.14	0.80
2:B:230:ARG:HH22	2:B:233:SER:CB	1.93	0.80
2:B:910:THR:HG22	12:L:43:ILE:HA	1.64	0.79
1:A:98:GLY:HA3	1:A:1440:MET:HE2	1.64	0.79
13:N:10:DG:H2'	13:N:11:DA:C8	2.18	0.79
15:T:10:DC:H2''	15:T:11:DT:C6	2.18	0.78
2:B:827:GLU:HG2	2:B:871:VAL:HG22	1.65	0.78
1:A:585:LEU:HD22	8:H:47:ILE:HD11	1.65	0.78
5:E:18:MET:HE2	5:E:32:GLU:HG2	1.66	0.77
3:C:205:LYS:NZ	3:C:212:ASP:O	2.17	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:63:ALA:HA	5:E:71:GLN:HA	1.66	0.77
1:A:877:ALA:HB3	1:A:890:ARG:HH11	1.49	0.77
15:T:4:DT:C2'	15:T:5:DC:H5''	2.14	0.76
1:A:274:ASP:OD2	1:A:342:ARG:NH2	2.18	0.76
1:A:894:ASP:OD1	1:A:1396:ARG:NH1	2.17	0.75
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.02	0.75
1:A:1262:MET:HE2	1:A:1264:SER:HB3	1.69	0.75
5:E:112:PRO:HG3	15:T:3:DT:H5''	1.69	0.74
1:A:876:ASP:O	1:A:890:ARG:NH1	2.21	0.74
1:A:554:PHE:HB3	1:A:585:LEU:HD23	1.69	0.74
2:B:626:LEU:HG	2:B:698:ILE:HD13	1.70	0.74
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.69	0.73
13:N:15:DA:C2'	13:N:16:DA:H5'	2.16	0.73
2:B:274:ARG:NH1	2:B:311:ILE:O	2.20	0.73
2:B:474:THR:OG1	2:B:732:ALA:O	2.07	0.73
9:I:115:THR:HG22	9:I:116:ALA:H	1.53	0.73
2:B:37:LYS:NZ	2:B:664:TYR:OH	2.17	0.73
2:B:274:ARG:NH2	2:B:281:ASP:OD1	2.21	0.73
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.62	0.72
2:B:260:LEU:HD22	2:B:347:MET:HE1	1.71	0.72
1:A:201:GLU:OE2	1:A:213:LYS:NZ	2.22	0.72
2:B:65:ILE:HB	2:B:86:LEU:HB2	1.72	0.72
2:B:777:ASN:O	10:J:47:ARG:NH1	2.22	0.72
2:B:796:MET:HE3	2:B:948:GLN:HE21	1.55	0.71
2:B:193:VAL:HG21	2:B:470:LEU:HD13	1.73	0.71
2:B:1036:LYS:NZ	3:C:186:TYR:O	2.21	0.71
1:A:545:VAL:HG22	1:A:676:ILE:HD13	1.73	0.71
1:A:1093:GLN:HE22	2:B:1093:CYS:HA	1.55	0.71
1:A:614:ASP:O	1:A:619:LYS:NZ	2.24	0.71
1:A:576:GLN:O	1:A:590:GLN:NE2	2.24	0.71
15:T:4:DT:H2''	15:T:5:DC:C5'	2.20	0.71
3:C:4:ALA:HB2	11:K:93:ASP:HB3	1.73	0.71
1:A:1138:SER:OG	1:A:1360:ASN:ND2	2.25	0.70
15:T:11:DT:H2'	15:T:12:DC:C6	2.26	0.70
1:A:1055:ALA:O	1:A:1059:ARG:NH1	2.25	0.70
15:T:12:DC:H2''	15:T:13:DG:C8	2.27	0.70
1:A:621:ILE:HD11	8:H:124:ARG:HB2	1.74	0.70
5:E:171:PRO:HB2	5:E:207:ARG:HD3	1.74	0.69
13:N:11:DA:H61	15:T:8:DT:H3	1.39	0.69
2:B:1115:GLN:HB3	2:B:1148:LEU:HD11	1.75	0.69
2:B:636:LYS:H	2:B:639:HIS:HD2	1.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:PHE:HD2	2:B:284:ILE:HG23	1.58	0.69
13:N:15:DA:H8	13:N:15:DA:H5''	1.57	0.69
2:B:357:CYS:SG	2:B:361:LYS:NZ	2.66	0.68
8:H:40:ILE:HD12	8:H:124:ARG:HD3	1.74	0.68
1:A:1184:THR:OG1	1:A:1190:GLN:NE2	2.26	0.68
1:A:1412:MET:SD	1:A:1422:GLN:NE2	2.66	0.68
1:A:524:MET:HE1	2:B:1097:HIS:HE1	1.59	0.68
5:E:55:ARG:HA	5:E:58:LEU:HD12	1.76	0.68
2:B:230:ARG:HH22	2:B:233:SER:HB3	1.57	0.68
1:A:458:PHE:HB3	1:A:472:HIS:HD2	1.59	0.68
8:H:7:GLU:HG2	8:H:59:VAL:HG22	1.76	0.68
1:A:601:ASN:HB3	1:A:988:TRP:CZ3	2.29	0.67
5:E:121:MET:HE2	5:E:125:TYR:HB2	1.75	0.67
2:B:486:ASN:OD1	2:B:491:ARG:NH2	2.24	0.67
3:C:72:PRO:HG3	10:J:13:ILE:HD11	1.77	0.67
2:B:677:MET:H	2:B:682:LEU:HD22	1.60	0.67
12:L:17:TYR:HB3	12:L:44:MET:HB3	1.75	0.67
2:B:627:ILE:HD11	2:B:663:GLU:HB2	1.77	0.67
3:C:259:LEU:HD11	11:K:42:LEU:HD21	1.75	0.67
1:A:78:MET:O	2:B:1072:ARG:NH2	2.27	0.67
1:A:904:GLN:NE2	1:A:981:CYS:O	2.28	0.66
8:H:96:VAL:HA	8:H:116:VAL:HA	1.75	0.66
1:A:1211:LEU:HD11	1:A:1258:ARG:HB3	1.75	0.66
15:T:11:DT:H2''	15:T:12:DC:O5'	1.94	0.66
2:B:587:LEU:HB3	2:B:603:MET:SD	2.36	0.66
2:B:935:PHE:HE1	2:B:1050:ARG:HG3	1.61	0.66
1:A:766:PHE:HE2	1:A:784:VAL:HG11	1.61	0.66
1:A:904:GLN:HE21	1:A:982:ASN:HA	1.61	0.66
2:B:580:PRO:HB2	2:B:605:ARG:HE	1.61	0.66
1:A:802:PHE:HE2	1:A:808:PRO:HD3	1.61	0.65
15:T:23:DC:H2'	15:T:24:DC:C6	2.31	0.65
1:A:885:GLN:HE22	1:A:1408:ARG:HH12	1.44	0.65
12:L:36:CYS:HB2	12:L:44:MET:HE1	1.79	0.65
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.61	0.65
3:C:24:GLU:HG2	3:C:228:ARG:HG2	1.78	0.65
15:T:11:DT:H4'	15:T:12:DC:OP1	1.96	0.65
1:A:605:THR:HA	1:A:627:LYS:HA	1.78	0.65
2:B:310:VAL:HG23	2:B:311:ILE:HD12	1.78	0.65
5:E:29:THR:HG23	5:E:32:GLU:HB2	1.78	0.65
1:A:42:LYS:O	1:A:288:ASN:ND2	2.24	0.65
4:D:70:ARG:NH2	7:G:140:ASP:O	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD21	1:A:221:VAL:HG13	1.79	0.65
2:B:534:VAL:N	2:B:600:GLU:OE2	2.29	0.65
1:A:551:ARG:HH12	8:H:27:ARG:HH21	1.45	0.64
4:D:90:LYS:NZ	4:D:126:GLU:OE2	2.27	0.64
6:F:105:ILE:HG22	6:F:119:GLY:HA2	1.79	0.64
1:A:381:PRO:HB3	1:A:480:SER:HA	1.79	0.64
2:B:1022:LEU:HD12	2:B:1023:ARG:HG2	1.79	0.64
1:A:727:PRO:HA	1:A:736:THR:HG21	1.80	0.64
1:A:560:VAL:HG22	1:A:591:ILE:HD11	1.79	0.64
2:B:114:ARG:NH2	2:B:184:TYR:OH	2.31	0.64
2:B:585:ASN:OD1	2:B:588:ARG:NH2	2.30	0.64
7:G:97:LEU:HB2	7:G:108:ILE:HB	1.80	0.64
10:J:40:LEU:HD22	10:J:45:CYS:HB3	1.79	0.63
15:T:7:DC:H2"	15:T:8:DT:C6	2.33	0.63
1:A:141:LEU:HD13	1:A:1445:HIS:HE1	1.63	0.63
2:B:849:ASP:OD2	12:L:46:LYS:NZ	2.31	0.63
1:A:358:ARG:HA	2:B:1085:ARG:HA	1.81	0.63
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.30	0.63
3:C:51:GLN:HE21	12:L:52:LEU:HB3	1.63	0.63
2:B:222:ARG:HG2	2:B:234:THR:HG22	1.80	0.63
2:B:505:LEU:HD22	2:B:509:VAL:HB	1.81	0.63
1:A:581:LYS:NZ	8:H:86:ASP:O	2.32	0.62
1:A:833:PRO:HB2	2:B:677:MET:HE2	1.80	0.62
3:C:59:LEU:HD12	3:C:151:VAL:HG23	1.81	0.62
1:A:375:ILE:HD11	1:A:669:TYR:HB2	1.81	0.62
1:A:717:ILE:HG12	1:A:737:PHE:HZ	1.63	0.62
9:I:97:PHE:HB2	9:I:100:HIS:HE2	1.64	0.62
1:A:877:ALA:HB3	1:A:890:ARG:NH1	2.13	0.62
2:B:989:VAL:HG22	2:B:1015:LEU:HB2	1.82	0.62
1:A:140:ARG:HD2	1:A:237:GLY:HA2	1.81	0.62
2:B:794:VAL:O	2:B:946:GLY:N	2.32	0.62
2:B:407:MET:HE1	2:B:444:LEU:HG	1.80	0.61
2:B:625:LEU:HD12	2:B:665:ILE:HD12	1.82	0.61
5:E:18:MET:HE3	5:E:28:VAL:HG13	1.82	0.61
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.27	0.61
2:B:809:VAL:HG22	2:B:926:VAL:HG12	1.82	0.61
1:A:330:GLN:HB3	1:A:336:LEU:HD21	1.82	0.61
1:A:459:ASN:OD1	1:A:460:ARG:N	2.33	0.61
1:A:1077:ASN:HB3	6:F:56:TYR:HE2	1.66	0.61
6:F:81:VAL:HG21	6:F:96:GLU:HA	1.81	0.61
1:A:467:MET:SD	1:A:524:MET:HE2	2.41	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:LYS:HB3	2:B:41:ARG:HG3	1.82	0.61
2:B:581:GLU:OE2	9:I:74:GLN:NE2	2.31	0.61
1:A:706:ILE:HG21	1:A:824:GLU:HG3	1.83	0.61
1:A:757:GLN:HE22	1:A:778:LYS:HB3	1.66	0.61
1:A:890:ARG:HE	1:A:1023:VAL:HG22	1.64	0.61
13:N:10:DG:H2'	13:N:11:DA:H8	1.61	0.61
8:H:88:PHE:CD2	8:H:144:LEU:HB3	2.36	0.61
1:A:733:LEU:HB3	9:I:106:ASP:HB2	1.83	0.61
2:B:506:TRP:NE1	2:B:697:GLU:OE2	2.29	0.61
1:A:805:ARG:NH2	2:B:673:VAL:O	2.32	0.60
1:A:1454:VAL:HA	1:A:1465:PRO:HD2	1.81	0.60
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.63	0.60
1:A:18:ILE:H	1:A:1462:GLN:HE22	1.49	0.60
1:A:567:LEU:HD21	1:A:595:ILE:HG12	1.83	0.60
1:A:1348:SER:O	5:E:12:LYS:NZ	2.34	0.60
1:A:1458:ILE:HD12	2:B:1091:ARG:HH21	1.65	0.60
1:A:589:LYS:NZ	1:A:625:ASP:OD1	2.35	0.60
1:A:757:GLN:NE2	1:A:778:LYS:HB3	2.17	0.60
2:B:907:VAL:HG22	2:B:921:ILE:HG12	1.82	0.60
1:A:1386:ILE:HD12	1:A:1398:LEU:HD21	1.82	0.60
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.35	0.60
2:B:764:MET:HE1	2:B:938:ARG:HH11	1.66	0.60
1:A:376:ASP:O	1:A:473:ARG:N	2.32	0.60
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.84	0.60
1:A:533:PRO:O	1:A:647:THR:OG1	2.16	0.60
2:B:816:GLU:HG2	2:B:867:ILE:HG21	1.84	0.60
2:B:1062:ARG:NH1	2:B:1081:ASP:O	2.35	0.60
2:B:230:ARG:HH21	2:B:349:PRO:CG	2.08	0.59
2:B:565:THR:HA	2:B:610:ARG:HG2	1.84	0.59
2:B:924:ARG:HH12	3:C:62:GLU:CD	2.11	0.59
3:C:123:ASN:OD1	3:C:124:SER:N	2.35	0.59
15:T:11:DT:H2'	15:T:12:DC:C5	2.36	0.59
12:L:18:ILE:HG12	12:L:25:GLU:HG2	1.83	0.59
2:B:713:PHE:HB3	2:B:716:HIS:HD2	1.67	0.59
5:E:26:TYR:HD1	5:E:64:HIS:HA	1.66	0.59
1:A:76:GLY:HA2	1:A:81:CYS:HB2	1.85	0.59
1:A:461:GLN:HE22	1:A:502:ASN:HD22	1.50	0.59
1:A:555:LEU:HD12	1:A:591:ILE:HD12	1.85	0.59
1:A:871:VAL:HG11	1:A:1400:LEU:HD11	1.83	0.59
2:B:91:ILE:HD11	2:B:124:LEU:HD21	1.84	0.59
2:B:1028:LEU:HB2	2:B:1041:ILE:HD13	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:LEU:HB2	2:B:263:ILE:HD12	1.84	0.59
2:B:819:SER:H	2:B:827:GLU:HB2	1.67	0.59
2:B:794:VAL:HG22	2:B:967:ILE:HG22	1.85	0.58
11:K:49:GLN:HB2	11:K:94:LEU:HD21	1.85	0.58
1:A:576:GLN:HA	8:H:75:TYR:HB2	1.85	0.58
1:A:678:ASN:HA	1:A:681:LEU:HD13	1.84	0.58
2:B:159:THR:HA	2:B:164:ASN:ND2	2.17	0.58
8:H:58:LEU:HD11	8:H:143:LEU:HD11	1.84	0.58
1:A:957:GLU:HG2	1:A:960:ARG:HH21	1.68	0.58
3:C:193:ARG:NH1	3:C:217:GLN:OE1	2.28	0.58
13:N:15:DA:H5"	13:N:15:DA:C8	2.38	0.58
1:A:70:ARG:HH12	2:B:1131:ARG:CZ	2.17	0.58
1:A:1024:ASN:O	5:E:162:ARG:NH2	2.36	0.58
2:B:625:LEU:HD13	2:B:675:LEU:HD21	1.83	0.58
2:B:764:MET:HE1	2:B:938:ARG:NH1	2.17	0.58
1:A:528:PRO:HG2	1:A:1090:LEU:HD11	1.85	0.58
2:B:598:VAL:HG12	2:B:600:GLU:H	1.68	0.58
2:B:743:ARG:O	2:B:922:ARG:NH1	2.36	0.58
3:C:22:ILE:HG12	3:C:230:TYR:HD1	1.67	0.58
7:G:96:GLY:HA3	7:G:108:ILE:O	2.04	0.58
1:A:1417:HIS:O	1:A:1421:ARG:HG2	2.04	0.58
2:B:217:TYR:CE2	2:B:376:ALA:HA	2.38	0.58
2:B:296:GLU:OE1	2:B:379:ARG:NH2	2.29	0.58
1:A:971:PRO:O	1:A:972:THR:OG1	2.21	0.58
1:A:1476:ASP:HB2	6:F:105:ILE:HG23	1.86	0.58
2:B:236:TRP:HB2	2:B:259:THR:HB	1.86	0.58
2:B:761:THR:HG23	2:B:1000:THR:HA	1.86	0.58
1:A:1307:VAL:HG22	1:A:1338:THR:HG22	1.86	0.58
2:B:780:VAL:HG21	2:B:1048:TYR:CE1	2.39	0.58
2:B:748:ALA:HB3	2:B:811:TYR:HB2	1.84	0.57
1:A:1148:ALA:HB1	1:A:1333:GLU:HB2	1.86	0.57
2:B:298:MET:HB3	9:I:14:ILE:HD12	1.84	0.57
2:B:780:VAL:HG22	2:B:965:ILE:HB	1.86	0.57
2:B:423:ILE:HD11	2:B:429:PHE:HB2	1.84	0.57
2:B:780:VAL:HA	2:B:965:ILE:O	2.04	0.57
11:K:7:PHE:HB2	11:K:11:LEU:HD12	1.85	0.57
1:A:1344:MET:HE2	5:E:134:GLU:HA	1.86	0.57
1:A:1357:THR:O	5:E:142:HIS:NE2	2.29	0.57
2:B:924:ARG:NH1	3:C:62:GLU:OE2	2.37	0.57
1:A:451:CYS:HA	1:A:476:ILE:HD11	1.85	0.57
1:A:618:TYR:HE1	8:H:40:ILE:HD13	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:752:TYR:HE1	3:C:60:HIS:CE1	2.22	0.57
7:G:4:HIS:CE1	7:G:73:LYS:HB3	2.40	0.57
1:A:330:GLN:HG3	1:A:331:LYS:H	1.68	0.57
2:B:628:VAL:HG22	2:B:633:LEU:HD23	1.85	0.57
1:A:46:THR:OG1	1:A:273:GLN:NE2	2.38	0.57
1:A:460:ARG:HB2	1:A:501:MET:HE2	1.87	0.57
3:C:7:PRO:HA	3:C:24:GLU:O	2.05	0.57
2:B:1028:LEU:HD11	2:B:1043:ILE:HD11	1.86	0.57
3:C:190:ASN:ND2	3:C:195:THR:O	2.29	0.57
2:B:265:GLN:HE21	2:B:324:ARG:HE	1.52	0.57
7:G:30:LEU:HD22	7:G:70:VAL:HG11	1.87	0.57
1:A:931:ARG:HD3	1:A:939:VAL:HG11	1.87	0.57
11:K:46:ILE:HG21	11:K:87:PHE:HE1	1.70	0.57
2:B:794:VAL:HG13	2:B:965:ILE:HG23	1.87	0.56
1:A:62:GLN:HE22	1:A:255:VAL:HG12	1.70	0.56
2:B:50:PHE:HB2	2:B:397:GLY:HA2	1.87	0.56
2:B:721:ARG:HD3	2:B:724:TYR:HD2	1.71	0.56
2:B:242:ARG:HB3	2:B:254:GLN:HG3	1.87	0.56
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.87	0.56
1:A:675:VAL:HG23	1:A:676:ILE:HG13	1.88	0.56
1:A:885:GLN:HE22	1:A:1408:ARG:NH1	2.03	0.56
1:A:413:TYR:OH	1:A:450:MET:O	2.22	0.56
1:A:595:ILE:HD11	1:A:675:VAL:HG21	1.85	0.56
2:B:866:ILE:HG22	2:B:867:ILE:HG13	1.88	0.56
1:A:461:GLN:HE22	1:A:502:ASN:ND2	2.04	0.56
2:B:112:GLU:HG3	12:L:43:ILE:HD11	1.88	0.56
2:B:771:GLU:O	10:J:55:LEU:HD21	2.06	0.56
1:A:370:ASP:OD2	1:A:373:LEU:HG	2.05	0.56
1:A:1258:ARG:HH22	1:A:1260:ARG:HH21	1.54	0.56
14:P:11:A:H2'	14:P:12:G:O4'	2.05	0.56
2:B:865:VAL:HG22	2:B:895:PHE:CE1	2.41	0.56
2:B:1142:ASN:HD21	2:B:1145:GLN:HG3	1.70	0.56
1:A:557:ARG:O	1:A:561:MET:HG2	2.06	0.55
1:A:827:TYR:HB2	2:B:978:ILE:HD12	1.86	0.55
2:B:622:CYS:HB3	2:B:666:ASP:HB3	1.87	0.55
12:L:22:CYS:SG	12:L:24:THR:OG1	2.59	0.55
14:P:4:A:H2'	14:P:5:A:C8	2.41	0.55
5:E:17:ILE:HA	5:E:20:LEU:HD12	1.88	0.55
7:G:14:HIS:HD2	7:G:16:ARG:HG2	1.72	0.55
1:A:749:ARG:NH2	1:A:779:ILE:HD11	2.20	0.55
1:A:1262:MET:HB3	1:A:1265:ASP:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1454:VAL:HG13	1:A:1464:ALA:HB1	1.88	0.55
4:D:111:SER:HB2	4:D:131:LEU:HD21	1.87	0.55
1:A:859:TYR:CE2	1:A:863:ARG:HD2	2.42	0.55
1:A:1429:LYS:HB2	1:A:1438:VAL:HG11	1.88	0.55
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.87	0.55
3:C:59:LEU:HD13	3:C:63:PHE:CE2	2.41	0.55
9:I:86:CYS:HB2	9:I:114:CYS:SG	2.46	0.55
1:A:672:ILE:HG23	1:A:676:ILE:HD12	1.87	0.55
1:A:766:PHE:CE2	1:A:784:VAL:HG11	2.41	0.55
2:B:130:LYS:NZ	2:B:429:PHE:O	2.40	0.55
1:A:1479:LYS:HD2	6:F:103:PRO:HA	1.88	0.55
2:B:419:ALA:O	2:B:423:ILE:HG12	2.07	0.55
6:F:100:ARG:HG2	6:F:125:ILE:HD12	1.86	0.55
1:A:535:MET:O	1:A:669:TYR:OH	2.24	0.55
2:B:779:ILE:O	2:B:964:ASP:N	2.40	0.55
1:A:904:GLN:NE2	1:A:982:ASN:HA	2.22	0.55
2:B:230:ARG:NH2	2:B:233:SER:OG	2.38	0.55
5:E:8:TYR:CZ	5:E:12:LYS:HE3	2.42	0.55
8:H:94:GLY:HA3	8:H:118:TYR:HA	1.89	0.55
9:I:69:ILE:HG22	9:I:71:ASP:H	1.71	0.55
15:T:7:DC:C2'	15:T:8:DT:C6	2.89	0.55
15:T:10:DC:C2'	15:T:11:DT:H71	2.34	0.55
1:A:472:HIS:CE1	1:A:521:VAL:HG21	2.42	0.55
8:H:10:PHE:CE1	8:H:32:SER:HB2	2.42	0.55
1:A:330:GLN:HG3	1:A:331:LYS:N	2.22	0.54
1:A:428:ASP:OD2	1:A:430:ARG:NH1	2.40	0.54
2:B:281:ASP:HB2	9:I:22:ASN:HA	1.89	0.54
2:B:1032:PHE:HA	3:C:36:ARG:HH22	1.72	0.54
1:A:1139:LEU:HB3	1:A:1338:THR:OG1	2.07	0.54
1:A:1139:LEU:HD13	1:A:1359:SER:HB3	1.88	0.54
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.42	0.54
1:A:890:ARG:HH21	1:A:1023:VAL:HG13	1.73	0.54
2:B:1016:SER:HB2	2:B:1022:LEU:HB3	1.88	0.54
1:A:462:PRO:HG3	14:P:12:G:H21	1.73	0.54
1:A:1416:ARG:HE	15:T:12:DC:H5'	1.73	0.54
1:A:791:GLN:HE21	1:A:839:HIS:HA	1.73	0.54
2:B:248:LYS:O	2:B:252:ILE:HG12	2.08	0.54
6:F:66:LEU:HD11	6:F:97:LEU:HD22	1.90	0.54
1:A:863:ARG:NH2	1:A:1414:ILE:O	2.36	0.54
5:E:55:ARG:NH1	5:E:107:GLN:HE21	2.05	0.54
15:T:8:DT:H2'	15:T:9:DC:C6	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:20:DT:H2''	15:T:21:DT:H5'	1.89	0.54
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	1.90	0.54
1:A:1208:SER:O	1:A:1260:ARG:NH1	2.41	0.53
8:H:79:ASP:O	8:H:82:PRO:HD2	2.07	0.53
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.43	0.53
1:A:1102:MET:HE2	1:A:1120:GLY:HA2	1.90	0.53
1:A:1487:PRO:HG2	6:F:78:PRO:HA	1.91	0.53
1:A:1155:LYS:HD2	1:A:1158:LEU:HD23	1.91	0.53
2:B:125:TYR:HB3	2:B:146:LYS:HA	1.90	0.53
2:B:820:LYS:HG3	2:B:826:GLU:HG2	1.91	0.53
2:B:961:ILE:HD11	10:J:42:ARG:HB2	1.90	0.53
1:A:691:ASP:CG	1:A:765:ASN:HD22	2.16	0.53
1:A:952:LEU:HD21	1:A:1006:PRO:HB2	1.90	0.53
3:C:56:SER:OG	3:C:158:GLU:N	2.33	0.53
8:H:11:ASP:OD1	8:H:55:LYS:HG2	2.08	0.53
1:A:52:PRO:HG3	1:A:58:MET:HE3	1.90	0.53
2:B:332:LYS:HA	2:B:335:ARG:HE	1.72	0.53
2:B:826:GLU:H	2:B:872:THR:HG22	1.74	0.53
2:B:1119:CYS:HB3	2:B:1122:CYS:SG	2.48	0.53
5:E:41:LYS:HG3	5:E:46:ASP:HA	1.90	0.53
2:B:601:VAL:HG22	2:B:616:THR:HG23	1.90	0.53
4:D:90:LYS:HB3	4:D:122:PHE:CZ	2.44	0.53
1:A:1189:ASP:HA	1:A:1192:TRP:CZ2	2.44	0.53
1:A:370:ASP:OD1	11:K:65:HIS:NE2	2.42	0.53
2:B:712:PRO:O	2:B:939:HIS:HE1	1.92	0.53
7:G:86:ASP:OD1	7:G:144:ARG:NH1	2.41	0.53
1:A:957:GLU:HG2	1:A:960:ARG:NH2	2.23	0.52
1:A:1171:ALA:N	1:A:1215:GLU:O	2.41	0.52
9:I:86:CYS:SG	9:I:87:GLN:N	2.82	0.52
1:A:11:SER:N	2:B:1135:TYR:OH	2.42	0.52
2:B:83:ARG:HB2	2:B:133:ILE:HB	1.90	0.52
2:B:838:GLN:N	2:B:889:LYS:O	2.40	0.52
1:A:653:VAL:HG22	1:A:668:PHE:HE2	1.73	0.52
1:A:766:PHE:HB3	1:A:781:ILE:HG12	1.92	0.52
2:B:699:HIS:HD2	2:B:701:SER:OG	1.91	0.52
2:B:789:ASN:O	2:B:968:ASN:HB2	2.09	0.52
5:E:86:THR:HG22	5:E:90:TYR:CE2	2.44	0.52
1:A:1376:LYS:HD2	5:E:144:LEU:HA	1.90	0.52
2:B:1105:GLU:HG3	2:B:1109:GLU:HB2	1.90	0.52
2:B:26:CYS:HG	2:B:27:TRP:CD1	2.28	0.52
2:B:116:ARG:NE	2:B:911:LEU:O	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:PHE:CD2	2:B:284:ILE:HG23	2.41	0.52
2:B:305:LEU:HD12	9:I:23:MET:HE3	1.90	0.52
13:N:7:DG:H4'	13:N:8:DA:OP1	2.10	0.52
1:A:96:HIS:NE2	2:B:1165:MET:O	2.42	0.52
2:B:194:LEU:HD23	2:B:467:SER:HB3	1.92	0.52
2:B:949:TYR:HB3	2:B:953:ASP:HB2	1.92	0.52
5:E:111:THR:HG23	5:E:114:ALA:H	1.75	0.52
1:A:420:ILE:HB	1:A:445:LYS:HB2	1.92	0.52
6:F:57:MET:HE1	6:F:120:VAL:HG13	1.91	0.52
1:A:375:ILE:HD12	1:A:666:ARG:HA	1.92	0.52
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.43	0.52
1:A:841:MET:SD	2:B:503:ASN:ND2	2.83	0.52
1:A:998:PRO:HA	1:A:1059:ARG:HG3	1.92	0.52
11:K:17:LYS:O	11:K:36:ASN:ND2	2.42	0.52
1:A:65:ILE:HG22	1:A:66:GLU:HG3	1.91	0.52
1:A:1161:LEU:HD22	1:A:1346:VAL:HG22	1.92	0.52
2:B:812:ARG:HH12	2:B:897:ARG:HG3	1.75	0.52
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.35	0.51
1:A:1077:ASN:HB3	6:F:56:TYR:CE2	2.45	0.51
1:A:1147:SER:HA	1:A:1153:ARG:HB2	1.91	0.51
2:B:1094:GLN:HE22	2:B:1102:PHE:HE2	1.58	0.51
1:A:570:TRP:CZ3	1:A:572:GLY:HA2	2.45	0.51
2:B:812:ARG:NH1	2:B:897:ARG:HG3	2.25	0.51
2:B:992:ASN:HD21	2:B:1020:TYR:HE2	1.55	0.51
1:A:1358:THR:HG23	5:E:144:LEU:HD11	1.93	0.51
2:B:817:GLN:OE1	2:B:912:ASN:ND2	2.43	0.51
1:A:514:GLU:OE2	1:A:1468:THR:HG21	2.10	0.51
1:A:764:ASN:OD1	1:A:765:ASN:N	2.44	0.51
1:A:802:PHE:HE2	1:A:808:PRO:CD	2.24	0.51
10:J:5:VAL:HG12	10:J:6:ARG:HG2	1.92	0.51
11:K:19:ILE:HG12	11:K:35:ILE:HD12	1.92	0.51
1:A:1457:ASN:ND2	1:A:1465:PRO:HD3	2.21	0.51
2:B:109:MET:HG3	2:B:174:LEU:HD22	1.93	0.51
9:I:97:PHE:HB2	9:I:100:HIS:NE2	2.25	0.51
1:A:372:ASN:ND2	2:B:788:TYR:OH	2.42	0.51
2:B:51:ILE:HG23	2:B:93:LEU:HD12	1.93	0.51
2:B:82:PRO:HA	2:B:133:ILE:O	2.11	0.51
2:B:803:ARG:NH2	10:J:10:CYS:O	2.43	0.51
7:G:30:LEU:O	7:G:34:VAL:HG22	2.10	0.51
1:A:1049:LEU:HA	1:A:1054:MET:HE3	1.92	0.51
3:C:35:ARG:HA	3:C:38:PHE:CD2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:VAL:HG21	2:B:91:ILE:HD12	1.93	0.51
1:A:996:ILE:HD13	1:A:1060:LEU:HA	1.92	0.51
2:B:706:VAL:HG13	2:B:767:LEU:HD22	1.92	0.51
2:B:85:LEU:HB2	2:B:131:THR:OG1	2.11	0.50
2:B:918:PHE:HE2	2:B:920:LYS:HE3	1.76	0.50
2:B:927:ARG:HD2	2:B:1054:MET:SD	2.50	0.50
1:A:97:VAL:HG21	1:A:322:LEU:HD11	1.94	0.50
2:B:403:LEU:HD21	2:B:447:SER:OG	2.11	0.50
3:C:75:SER:HB3	3:C:79:VAL:CG2	2.40	0.50
6:F:66:LEU:HD21	6:F:97:LEU:HB2	1.93	0.50
1:A:458:PHE:HB3	1:A:472:HIS:CD2	2.43	0.50
1:A:573:LYS:NZ	8:H:74:GLU:OE2	2.27	0.50
1:A:601:ASN:HB3	1:A:988:TRP:CE3	2.47	0.50
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.44	0.50
5:E:35:GLN:NE2	5:E:43:GLN:OE1	2.45	0.50
1:A:20:ARG:NH2	2:B:1172:MET:SD	2.85	0.50
1:A:526:VAL:HA	1:A:533:PRO:HA	1.92	0.50
1:A:1485:GLU:HB3	6:F:78:PRO:HB3	1.93	0.50
2:B:552:ASN:O	2:B:556:ILE:HG13	2.12	0.50
3:C:59:LEU:HD13	3:C:63:PHE:HE2	1.76	0.50
10:J:3:ILE:HD13	10:J:18:TRP:HB2	1.94	0.50
11:K:21:ILE:HG21	11:K:84:GLN:HE21	1.77	0.50
1:A:1016:LEU:HD21	1:A:1072:ILE:HG21	1.93	0.50
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.93	0.50
8:H:81:ARG:CG	8:H:82:PRO:HD3	2.42	0.50
1:A:351:ARG:HG3	2:B:1088:GLU:OE2	2.12	0.50
1:A:370:ASP:CG	11:K:65:HIS:HE2	2.18	0.50
1:A:583:ARG:HG3	1:A:585:LEU:HD13	1.94	0.50
1:A:620:HIS:O	8:H:97:TYR:OH	2.22	0.50
1:A:739:ASN:O	1:A:743:ARG:HG2	2.12	0.50
1:A:875:TYR:HA	1:A:1083:PRO:HB3	1.93	0.50
1:A:1440:MET:SD	2:B:1167:ILE:HD11	2.51	0.50
2:B:389:GLY:HA3	2:B:668:LEU:HB3	1.94	0.50
3:C:228:ARG:NH1	3:C:230:TYR:OH	2.45	0.50
5:E:17:ILE:HD13	5:E:74:VAL:HG11	1.93	0.50
7:G:99:THR:HG21	7:G:143:ILE:HD11	1.93	0.50
1:A:653:VAL:HG11	1:A:669:TYR:CZ	2.47	0.50
1:A:1026:ASP:O	1:A:1031:ARG:NH1	2.44	0.50
2:B:144:HIS:ND1	2:B:431:LEU:HD12	2.26	0.50
2:B:785:TYR:OH	2:B:953:ASP:O	2.21	0.50
3:C:62:GLU:HA	3:C:65:ALA:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:17:ILE:HG21	5:E:74:VAL:HG11	1.93	0.50
13:N:14:DG:H2'	13:N:15:DA:OP2	2.10	0.50
1:A:813:ASP:OD2	9:I:100:HIS:NE2	2.45	0.50
2:B:760:THR:OG1	2:B:764:MET:SD	2.65	0.50
7:G:110:ARG:HA	7:G:113:ILE:HD12	1.93	0.50
1:A:386:ALA:O	1:A:449:HIS:ND1	2.41	0.49
1:A:1141:VAL:HG13	1:A:1352:VAL:HG13	1.93	0.49
2:B:841:ARG:HD2	2:B:895:PHE:CZ	2.47	0.49
1:A:542:LEU:HD23	1:A:774:ALA:HA	1.93	0.49
1:A:908:THR:HG23	1:A:916:PHE:HE1	1.76	0.49
2:B:792:ASP:O	2:B:943:GLY:HA3	2.12	0.49
1:A:511:THR:HG21	2:B:1105:GLU:OE1	2.12	0.49
1:A:741:VAL:HG11	1:A:797:ARG:NH1	2.27	0.49
1:A:811:ILE:HG21	9:I:79:PRO:HB3	1.94	0.49
2:B:56:GLN:OE1	2:B:91:ILE:HG22	2.12	0.49
2:B:399:LEU:HB3	2:B:453:TRP:CZ2	2.48	0.49
2:B:712:PRO:HG2	2:B:939:HIS:CE1	2.47	0.49
2:B:911:LEU:HD12	12:L:42:ARG:HH11	1.76	0.49
6:F:66:LEU:HD13	6:F:94:MET:SD	2.53	0.49
1:A:671:ASN:O	1:A:675:VAL:HG22	2.12	0.49
1:A:1258:ARG:NH2	1:A:1260:ARG:HH21	2.09	0.49
2:B:670:GLU:O	2:B:673:VAL:HG12	2.12	0.49
2:B:1129:ASN:HB3	2:B:1132:THR:HB	1.93	0.49
2:B:810:PHE:HZ	2:B:812:ARG:HH21	1.61	0.49
2:B:845:TYR:CE1	2:B:865:VAL:HG21	2.47	0.49
1:A:685:HIS:NE2	1:A:769:MET:HE3	2.27	0.49
2:B:205:VAL:O	2:B:371:ARG:NH1	2.46	0.49
2:B:1115:GLN:HG2	2:B:1150:ARG:HG2	1.94	0.49
3:C:52:ILE:HG21	3:C:55:ASN:HB2	1.95	0.49
1:A:880:ARG:NH1	6:F:111:PRO:HB2	2.28	0.49
1:A:1030:SER:HG	5:E:162:ARG:HE	1.52	0.49
1:A:1180:ASN:HB2	1:A:1183:SER:HB3	1.94	0.49
4:D:79:THR:HG23	4:D:137:LYS:HB3	1.94	0.49
5:E:185:ILE:HG21	5:E:209:VAL:HG21	1.94	0.49
15:T:18:DC:H2'	15:T:19:DC:C6	2.48	0.49
1:A:375:ILE:HD11	1:A:669:TYR:CB	2.43	0.49
1:A:441:GLN:HG2	1:A:444:TYR:CE2	2.48	0.49
1:A:467:MET:SD	1:A:524:MET:HB3	2.52	0.49
1:A:1366:PHE:HB2	1:A:1374:VAL:HG21	1.95	0.49
11:K:39:ASP:O	11:K:71:ILE:HD11	2.13	0.49
1:A:1473:LEU:HD11	6:F:64:ARG:HG2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:617:ASP:OD1	2:B:618:ALA:N	2.46	0.48
1:A:286:ILE:HD13	1:A:309:LEU:HG	1.95	0.48
1:A:693:ILE:HG12	1:A:828:LEU:HD21	1.93	0.48
15:T:10:DC:H2''	15:T:11:DT:H6	1.75	0.48
1:A:222:HIS:O	1:A:226:LYS:HG3	2.14	0.48
1:A:717:ILE:HG12	1:A:737:PHE:CZ	2.46	0.48
3:C:44:ILE:HG23	3:C:176:TRP:HD1	1.78	0.48
15:T:8:DT:H2'	15:T:9:DC:C5	2.47	0.48
1:A:70:ARG:HH22	2:B:1131:ARG:HH22	1.61	0.48
1:A:1179:PRO:HB2	9:I:33:ARG:HD3	1.96	0.48
1:A:1451:MET:HE2	1:A:1460:LEU:HD12	1.94	0.48
2:B:297:MET:HE3	2:B:379:ARG:NH1	2.28	0.48
2:B:19:PRO:C	2:B:21:LEU:H	2.22	0.48
2:B:783:ALA:O	2:B:789:ASN:ND2	2.46	0.48
2:B:1115:GLN:HE21	2:B:1150:ARG:HE	1.61	0.48
1:A:273:GLN:HB2	1:A:278:HIS:CE1	2.48	0.48
1:A:827:TYR:CB	2:B:978:ILE:HD12	2.43	0.48
3:C:40:ALA:O	3:C:170:GLY:N	2.44	0.48
8:H:6:PHE:HB3	8:H:60:ILE:HB	1.95	0.48
1:A:155:GLU:HA	1:A:185:GLY:HA2	1.96	0.48
1:A:1416:ARG:O	1:A:1420:ASN:HB2	2.14	0.48
2:B:509:VAL:HG11	2:B:524:LYS:HB3	1.94	0.48
1:A:18:ILE:N	1:A:1462:GLN:HE22	2.11	0.48
1:A:931:ARG:HH11	1:A:936:GLU:HG3	1.78	0.48
2:B:798:ARG:HB2	2:B:948:GLN:HB3	1.96	0.48
1:A:844:ARG:HG2	2:B:501:LEU:H	1.79	0.48
1:A:947:HIS:NE2	1:A:951:GLU:OE2	2.46	0.48
1:A:1005:HIS:CD2	1:A:1007:ILE:HB	2.49	0.48
2:B:1038:THR:HA	3:C:195:THR:HA	1.96	0.48
2:B:1118:VAL:HG21	2:B:1171:MET:SD	2.53	0.48
3:C:2:PRO:HB3	11:K:54:PRO:HD2	1.95	0.48
3:C:189:ASP:O	3:C:191:ALA:N	2.47	0.48
4:D:31:THR:HG22	7:G:3:TYR:HE1	1.79	0.48
4:D:60:VAL:HG13	7:G:103:PRO:HB3	1.96	0.48
5:E:84:ILE:HD11	5:E:113:SER:HB3	1.94	0.48
15:T:3:DT:H2''	15:T:4:DT:OP2	2.14	0.48
1:A:577:PRO:HG2	1:A:580:LEU:HD23	1.95	0.47
1:A:809:HIS:HE2	2:B:506:TRP:NE1	2.11	0.47
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.96	0.47
2:B:192:LYS:HE2	2:B:469:VAL:HG22	1.95	0.47
2:B:294:ASP:OD2	2:B:379:ARG:NH1	2.41	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:905:ASP:OD2	2:B:922:ARG:NH2	2.41	0.47
2:B:906:GLN:OE1	2:B:922:ARG:NH2	2.46	0.47
5:E:64:HIS:CD2	5:E:66:ASP:HB2	2.49	0.47
1:A:597:PRO:HD3	1:A:668:PHE:CD1	2.50	0.47
1:A:627:LYS:HG2	1:A:628:VAL:H	1.80	0.47
1:A:801:GLY:HA3	2:B:503:ASN:HB2	1.95	0.47
1:A:1098:PRO:O	1:A:1102:MET:HG3	2.14	0.47
1:A:1355:VAL:HA	5:E:142:HIS:HA	1.96	0.47
2:B:1132:THR:HG22	2:B:1134:THR:HG23	1.97	0.47
4:D:16:ASP:OD2	4:D:18:SER:OG	2.23	0.47
9:I:91:HIS:HB3	9:I:114:CYS:SG	2.54	0.47
1:A:269:SER:HB3	2:B:825:GLN:HE22	1.78	0.47
1:A:916:PHE:CE1	1:A:963:ARG:HD2	2.50	0.47
2:B:351:VAL:HG11	2:B:361:LYS:HA	1.95	0.47
2:B:1129:ASN:HD22	2:B:1134:THR:HG1	1.58	0.47
5:E:18:MET:HE2	5:E:32:GLU:CG	2.38	0.47
7:G:89:VAL:HA	7:G:99:THR:HG22	1.96	0.47
7:G:137:ILE:HD11	7:G:170:LEU:HB2	1.96	0.47
2:B:934:LYS:HZ1	2:B:942:LYS:HD2	1.79	0.47
2:B:935:PHE:CE1	2:B:1050:ARG:HG3	2.46	0.47
8:H:48:TYR:OH	8:H:147:LYS:HG3	2.15	0.47
10:J:1:MET:HA	10:J:55:LEU:HB2	1.97	0.47
10:J:16:ASN:OD1	10:J:17:LYS:HG3	2.15	0.47
15:T:7:DC:H2"	15:T:8:DT:H6	1.78	0.47
1:A:869:GLU:OE1	1:A:1455:SER:OG	2.32	0.47
2:B:290:TYR:HE2	2:B:370:HIS:CG	2.32	0.47
2:B:348:LEU:HD23	2:B:351:VAL:HG21	1.97	0.47
2:B:364:PHE:O	2:B:367:TYR:HB3	2.14	0.47
2:B:1033:THR:HA	11:K:44:ASN:ND2	2.30	0.47
1:A:367:ILE:HG22	1:A:482:PHE:HB2	1.97	0.47
1:A:837:PHE:HB2	2:B:506:TRP:HZ3	1.80	0.47
1:A:1035:GLU:O	1:A:1039:LEU:HB2	2.15	0.47
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.96	0.47
2:B:265:GLN:NE2	2:B:324:ARG:HE	2.13	0.47
2:B:751:LEU:HD11	2:B:806:PHE:HA	1.95	0.47
3:C:86:ARG:NE	11:K:11:LEU:HD21	2.30	0.47
2:B:470:LEU:HD11	2:B:478:THR:HG23	1.96	0.47
2:B:950:ARG:HE	2:B:952:GLU:CD	2.22	0.47
7:G:13:LEU:HD21	7:G:26:VAL:HG22	1.97	0.47
1:A:784:VAL:HG13	2:B:978:ILE:CD1	2.40	0.47
1:A:1375:ARG:NE	1:A:1403:ASP:OD1	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:968:ASN:OD1	2:B:969:PRO:HD2	2.14	0.47
13:N:6:DC:H4'	13:N:7:DG:OP1	2.14	0.47
1:A:222:HIS:CD2	1:A:226:LYS:HE3	2.50	0.47
1:A:541:THR:HG21	1:A:673:GLN:HA	1.97	0.47
1:A:1130:ILE:HD13	1:A:1411:LEU:HD22	1.96	0.47
2:B:389:GLY:O	2:B:668:LEU:HD23	2.15	0.47
1:A:865:ILE:HD13	2:B:1092:ASP:HB3	1.97	0.46
1:A:1173:THR:HG23	1:A:1214:VAL:HG12	1.97	0.46
2:B:535:GLY:N	2:B:600:GLU:OE2	2.33	0.46
8:H:113:SER:HB3	8:H:126:GLN:HG2	1.96	0.46
1:A:316:THR:HG21	1:A:328:ALA:HB2	1.97	0.46
1:A:592:PHE:CD1	1:A:595:ILE:HD12	2.50	0.46
1:A:839:HIS:HE2	2:B:718:GLN:HA	1.80	0.46
1:A:1375:ARG:HH12	1:A:1379:GLU:CD	2.23	0.46
2:B:108:MET:O	2:B:162:LEU:HD12	2.16	0.46
2:B:193:VAL:O	2:B:467:SER:HA	2.15	0.46
5:E:48:PRO:HA	5:E:53:PRO:HG2	1.97	0.46
11:K:46:ILE:HG21	11:K:87:PHE:CE1	2.50	0.46
1:A:506:PRO:HG3	1:A:515:ILE:HD12	1.96	0.46
7:G:119:PHE:HB2	7:G:128:TYR:HE1	1.81	0.46
1:A:380:VAL:HG11	1:A:450:MET:HE3	1.96	0.46
1:A:604:ARG:O	1:A:628:VAL:N	2.47	0.46
2:B:665:ILE:HD11	2:B:695:HIS:NE2	2.30	0.46
2:B:780:VAL:HG21	2:B:1048:TYR:HE1	1.79	0.46
3:C:26:THR:HG23	11:K:97:GLU:OE2	2.15	0.46
5:E:21:CYS:SG	5:E:62:VAL:HG21	2.55	0.46
9:I:97:PHE:HD1	9:I:100:HIS:HD2	1.62	0.46
11:K:105:PHE:CE2	11:K:109:ILE:HD11	2.50	0.46
1:A:1436:VAL:O	1:A:1440:MET:HG2	2.16	0.46
2:B:55:VAL:HG12	2:B:91:ILE:HD13	1.97	0.46
2:B:144:HIS:CE1	2:B:431:LEU:HD12	2.51	0.46
7:G:55:GLY:HA3	7:G:69:PRO:HG2	1.97	0.46
1:A:623:PRO:HA	8:H:27:ARG:NH2	2.30	0.46
1:A:1189:ASP:HA	1:A:1192:TRP:CH2	2.51	0.46
1:A:1471:PHE:CE2	6:F:64:ARG:HD3	2.51	0.46
2:B:713:PHE:HB3	2:B:716:HIS:CD2	2.48	0.46
7:G:60:GLN:OE1	7:G:63:ARG:HD2	2.16	0.46
8:H:98:ARG:HD2	8:H:115:TYR:CD2	2.51	0.46
1:A:648:SER:OG	1:A:651:SER:OG	2.27	0.46
5:E:21:CYS:SG	5:E:26:TYR:HB2	2.56	0.46
12:L:41:TYR:CE2	12:L:43:ILE:HB	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:ARG:HH22	1:A:779:ILE:HD11	1.81	0.46
2:B:515:PRO:HG3	2:B:523:VAL:HB	1.98	0.46
2:B:907:VAL:HG13	2:B:921:ILE:HG12	1.98	0.46
3:C:19:VAL:HG12	3:C:21:PHE:HD1	1.81	0.46
1:A:456:VAL:HG21	1:A:503:LEU:HD11	1.98	0.46
2:B:427:LYS:HG3	2:B:428:ASP:H	1.81	0.46
2:B:455:ASP:HB2	2:B:458:LYS:HB2	1.97	0.46
2:B:779:ILE:HD12	10:J:43:TYR:HE2	1.81	0.46
3:C:35:ARG:HB3	3:C:231:TYR:HE2	1.81	0.46
5:E:118:LEU:HD22	5:E:127:LEU:HB2	1.97	0.46
8:H:95:LYS:HB2	8:H:140:ARG:NH1	2.31	0.46
9:I:36:LEU:HD23	9:I:47:GLU:HA	1.97	0.46
1:A:103:THR:HG23	1:A:225:PHE:CE2	2.51	0.45
1:A:1082:HIS:CD2	6:F:59:LYS:HE3	2.51	0.45
2:B:197:GLN:NE2	2:B:466:VAL:HG22	2.31	0.45
2:B:817:GLN:HE22	2:B:912:ASN:HD21	1.65	0.45
4:D:84:ARG:NH1	4:D:97:LEU:HD22	2.31	0.45
9:I:38:ALA:HB2	9:I:45:GLN:HG2	1.98	0.45
9:I:97:PHE:CD1	9:I:100:HIS:HD2	2.34	0.45
1:A:515:ILE:HD11	2:B:1102:PHE:CD1	2.51	0.45
1:A:1082:HIS:HD2	6:F:59:LYS:HE3	1.81	0.45
1:A:1321:ILE:HD12	1:A:1331:LEU:HD12	1.98	0.45
4:D:93:HIS:CD2	4:D:94:LYS:H	2.34	0.45
8:H:40:ILE:HB	8:H:124:ARG:HB3	1.98	0.45
1:A:358:ARG:NH2	2:B:1068:GLN:OE1	2.50	0.45
1:A:488:VAL:O	1:A:491:PRO:HD2	2.16	0.45
1:A:599:HIS:ND1	1:A:632:ASN:OD1	2.49	0.45
1:A:994:PHE:CD2	1:A:1064:ALA:HA	2.52	0.45
2:B:407:MET:HE3	2:B:443:GLY:HA3	1.97	0.45
2:B:992:ASN:OD1	10:J:43:TYR:HB3	2.17	0.45
3:C:71:ILE:HD11	3:C:150:ILE:HG12	1.99	0.45
4:D:64:THR:HG21	7:G:46:ILE:HG23	1.97	0.45
1:A:479:TRP:HB2	1:A:483:ARG:NH2	2.31	0.45
1:A:508:SER:HB3	1:A:511:THR:HG22	1.98	0.45
1:A:733:LEU:HA	1:A:736:THR:HG22	1.98	0.45
1:A:918:LYS:O	1:A:1052:ARG:NE	2.49	0.45
1:A:1086:MET:SD	1:A:1466:ALA:HA	2.57	0.45
2:B:809:VAL:HG21	3:C:60:HIS:CE1	2.52	0.45
1:A:769:MET:SD	2:B:973:PRO:HG3	2.57	0.45
1:A:977:VAL:HG11	1:A:1040:LEU:HD21	1.98	0.45
1:A:983:LEU:HD12	1:A:1044:HIS:CD2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASP:HB3	1:A:33:ARG:HH12	1.81	0.45
1:A:335:PRO:HD3	2:B:460:HIS:CE1	2.52	0.45
1:A:1441:GLU:OE2	1:A:1445:HIS:NE2	2.49	0.45
2:B:513:GLU:HG2	2:B:525:ASN:HD22	1.82	0.45
2:B:1029:TYR:OH	3:C:185:GLU:HG3	2.17	0.45
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.31	0.45
1:A:991:GLN:HA	1:A:996:ILE:HD12	1.99	0.45
1:A:1186:VAL:HB	1:A:1189:ASP:CG	2.42	0.45
2:B:796:MET:HE1	2:B:929:PRO:HB2	1.98	0.45
3:C:99:VAL:HG11	3:C:127:VAL:HG21	1.98	0.45
1:A:1288:ILE:HG22	1:A:1292:MET:HE2	1.98	0.45
1:A:1471:PHE:CZ	6:F:61:GLU:HA	2.52	0.45
1:A:1479:LYS:NZ	6:F:121:ASP:OD2	2.32	0.45
1:A:1486:ILE:HG13	1:A:1487:PRO:HD3	1.98	0.45
2:B:856:PRO:HG2	12:L:48:ARG:HA	1.98	0.45
3:C:10:ARG:NH1	3:C:24:GLU:OE2	2.50	0.45
3:C:91:GLU:HG2	3:C:92:GLU:HG2	1.97	0.45
7:G:67:LEU:HD23	7:G:69:PRO:HD3	1.99	0.45
2:B:148:PHE:CD2	2:B:437:THR:HG21	2.52	0.45
2:B:1032:PHE:HA	3:C:36:ARG:NH2	2.31	0.45
2:B:1165:MET:O	2:B:1166:SER:OG	2.30	0.45
11:K:20:THR:OG1	11:K:34:THR:HB	2.17	0.45
15:T:5:DC:H2''	15:T:6:DT:O5'	2.17	0.45
1:A:64:VAL:HG21	1:A:76:GLY:HA3	1.99	0.44
1:A:375:ILE:HG23	1:A:488:VAL:HG22	1.98	0.44
1:A:805:ARG:NH1	2:B:674:MET:SD	2.89	0.44
1:A:1194:ASN:O	1:A:1198:GLU:HG3	2.17	0.44
2:B:42:GLN:HG3	2:B:43:GLN:N	2.32	0.44
2:B:567:ILE:HA	2:B:612:ILE:O	2.18	0.44
2:B:1104:ARG:O	2:B:1108:PHE:N	2.50	0.44
4:D:64:THR:HG21	7:G:46:ILE:HD12	1.98	0.44
7:G:21:ASN:O	7:G:25:THR:OG1	2.32	0.44
1:A:37:THR:HA	1:A:61:ARG:HD2	2.00	0.44
1:A:486:LEU:HA	1:A:486:LEU:HD23	1.71	0.44
3:C:7:PRO:HB3	3:C:26:THR:OG1	2.18	0.44
6:F:46:GLN:HG3	6:F:114:SER:OG	2.18	0.44
13:N:7:DG:H2''	13:N:8:DA:O5'	2.17	0.44
1:A:606:HIS:HB3	1:A:626:THR:OG1	2.17	0.44
2:B:177:CYS:SG	2:B:738:THR:OG1	2.52	0.44
1:A:383:SER:N	11:K:2:ASN:OD1	2.46	0.44
1:A:821:GLY:HA2	1:A:838:PHE:CD2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:CYS:O	2:B:350:HIS:HB3	2.18	0.44
2:B:465:GLY:HA2	14:P:7:G:H5''	1.99	0.44
2:B:752:TYR:CE2	2:B:807:ARG:HD2	2.53	0.44
7:G:21:ASN:OD1	7:G:24:ASN:HB2	2.17	0.44
1:A:521:VAL:N	1:A:522:PRO:HD2	2.32	0.44
1:A:753:GLY:O	1:A:757:GLN:HG3	2.18	0.44
1:A:788:VAL:HG23	1:A:826:SER:HA	1.98	0.44
1:A:1284:PHE:CE2	1:A:1288:ILE:HD11	2.52	0.44
2:B:711:ILE:HG12	2:B:725:GLN:HG2	1.98	0.44
2:B:1072:ARG:HB2	2:B:1153:TYR:CD2	2.53	0.44
9:I:22:ASN:ND2	9:I:41:ASN:HD22	2.15	0.44
1:A:137:PRO:HA	1:A:140:ARG:HG2	1.99	0.44
1:A:663:ASP:OD1	1:A:666:ARG:NH2	2.50	0.44
1:A:1163:HIS:CE1	1:A:1297:THR:HG23	2.52	0.44
2:B:509:VAL:CG1	2:B:524:LYS:HB3	2.47	0.44
2:B:1111:SER:O	2:B:1113:PRO:HD3	2.16	0.44
5:E:82:VAL:HB	5:E:110:MET:SD	2.58	0.44
12:L:16:ILE:HG12	12:L:27:GLU:HG2	2.00	0.44
1:A:244:ARG:HD3	1:A:245:PRO:HD2	1.99	0.44
1:A:760:LEU:HD13	1:A:767:LYS:HB2	1.98	0.44
1:A:870:SER:HB2	1:A:882:SER:HB3	2.00	0.44
1:A:929:ALA:N	8:H:106:THR:HG22	2.33	0.44
1:A:1130:ILE:HD13	1:A:1411:LEU:HB3	2.00	0.44
2:B:258:ALA:HB2	2:B:269:ILE:HD13	2.00	0.44
5:E:90:TYR:O	5:E:94:MET:HG2	2.18	0.44
8:H:32:SER:HB3	8:H:37:MET:N	2.21	0.44
1:A:488:VAL:HG12	1:A:492:TYR:HE2	1.83	0.44
1:A:1209:PRO:HG2	1:A:1210:TRP:CD1	2.52	0.44
2:B:606:ASP:OD2	2:B:609:GLU:HB2	2.16	0.44
2:B:631:GLN:HE22	2:B:691:SER:C	2.21	0.44
1:A:354:LEU:HD21	2:B:1155:CYS:N	2.33	0.44
2:B:262:TYR:CD2	2:B:346:GLU:HG3	2.53	0.44
2:B:412:LEU:O	2:B:416:ARG:HG2	2.18	0.44
2:B:719:SER:OG	2:B:720:PRO:HD3	2.18	0.44
5:E:180:ALA:HA	5:E:185:ILE:HD12	1.99	0.44
1:A:343:LEU:HD22	2:B:1158:LEU:HD12	2.00	0.43
1:A:583:ARG:NH1	3:C:222:PRO:O	2.51	0.43
2:B:230:ARG:NH2	2:B:233:SER:HB3	2.29	0.43
5:E:82:VAL:HG13	5:E:86:THR:HB	2.00	0.43
8:H:57:ARG:HH22	8:H:88:PHE:HE1	1.66	0.43
15:T:7:DC:H2'	15:T:8:DT:C7	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:19:DC:H2'	15:T:20:DT:C6	2.53	0.43
1:A:141:LEU:HD13	1:A:1445:HIS:CE1	2.50	0.43
1:A:1382:LEU:HD13	1:A:1401:LEU:HD23	2.00	0.43
2:B:198:GLU:OE2	2:B:391:LYS:NZ	2.34	0.43
2:B:761:THR:HG22	2:B:763:SER:H	1.82	0.43
9:I:81:THR:HG23	9:I:96:PHE:HE1	1.83	0.43
11:K:21:ILE:HG23	11:K:31:CYS:SG	2.58	0.43
1:A:70:ARG:HD3	1:A:77:ASN:H	1.83	0.43
1:A:447:GLU:OE1	2:B:1064:ARG:NH2	2.37	0.43
1:A:497:ASP:OD1	1:A:497:ASP:N	2.49	0.43
2:B:164:ASN:OD1	2:B:165:GLY:N	2.51	0.43
2:B:653:TRP:CE3	2:B:656:LEU:HD23	2.53	0.43
2:B:699:HIS:ND1	2:B:700:PRO:HD2	2.34	0.43
15:T:12:DC:H6	15:T:12:DC:H2'	1.70	0.43
15:T:17:DT:H2'	15:T:18:DC:C6	2.54	0.43
1:A:883:ILE:HD11	1:A:1424:THR:HG22	2.01	0.43
2:B:854:ILE:O	2:B:907:VAL:HG21	2.17	0.43
8:H:60:ILE:HG23	8:H:141:VAL:HG13	2.01	0.43
1:A:460:ARG:HD2	1:A:501:MET:HE2	2.01	0.43
1:A:1181:PRO:HB3	1:A:1197:TYR:CE2	2.54	0.43
5:E:156:VAL:HG22	5:E:190:VAL:HB	2.01	0.43
11:K:9:SER:HA	11:K:69:HIS:CG	2.53	0.43
1:A:860:ILE:HD11	1:A:1125:LYS:HG3	2.01	0.43
1:A:1212:LEU:HB2	1:A:1285:LEU:HD11	2.00	0.43
1:A:1248:ASN:HD21	1:A:1256:VAL:HB	1.83	0.43
2:B:114:ARG:O	2:B:920:LYS:NZ	2.51	0.43
7:G:8:GLU:OE2	7:G:71:LYS:HG2	2.19	0.43
1:A:408:ARG:HH11	1:A:414:PRO:HB2	1.83	0.43
1:A:1163:HIS:HB2	1:A:1301:ILE:O	2.19	0.43
2:B:733:MET:HE1	2:B:1054:MET:SD	2.59	0.43
2:B:757:PRO:HA	2:B:777:ASN:HD21	1.83	0.43
2:B:1028:LEU:HD12	2:B:1041:ILE:HB	2.01	0.43
3:C:72:PRO:HG3	10:J:13:ILE:CD1	2.46	0.43
15:T:4:DT:C1'	15:T:5:DC:H5''	2.49	0.43
1:A:70:ARG:HH12	2:B:1131:ARG:NH1	2.16	0.43
1:A:77:ASN:C	1:A:79:THR:H	2.27	0.43
1:A:274:ASP:OD1	1:A:275:ASP:N	2.50	0.43
1:A:470:MET:HB3	1:A:521:VAL:HG22	2.00	0.43
1:A:1054:MET:SD	1:A:1060:LEU:HD12	2.59	0.43
2:B:196:ALA:HB3	2:B:485:LEU:HD23	2.01	0.43
2:B:553:LEU:HD11	2:B:573:TRP:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:910:THR:HG21	12:L:43:ILE:HG12	2.00	0.43
2:B:1001:PRO:HB2	2:B:1002:PHE:CD2	2.53	0.43
2:B:1060:HIS:HE1	2:B:1081:ASP:HA	1.84	0.43
5:E:47:LYS:O	5:E:51:GLY:HA3	2.18	0.43
1:A:66:GLU:C	1:A:68:THR:H	2.27	0.43
1:A:868:MET:HE3	1:A:1401:LEU:HD13	2.00	0.42
2:B:35:ASP:OD2	2:B:646:ARG:NH2	2.52	0.42
2:B:93:LEU:HD23	2:B:123:PRO:O	2.19	0.42
2:B:613:ARG:HD3	2:B:615:TYR:OH	2.19	0.42
2:B:1120:ASN:HD22	2:B:1145:GLN:HB2	1.82	0.42
8:H:8:ASP:OD1	8:H:9:ILE:N	2.52	0.42
1:A:293:ASN:ND2	1:A:306:ASP:OD2	2.52	0.42
1:A:683:GLU:HA	2:B:1038:THR:HB	2.01	0.42
5:E:57:ASP:C	5:E:59:THR:N	2.77	0.42
7:G:38:CYS:HB2	7:G:44:PHE:CD2	2.55	0.42
1:A:103:THR:HG23	1:A:225:PHE:HE2	1.83	0.42
1:A:1282:ASP:OD1	1:A:1283:VAL:N	2.50	0.42
2:B:785:TYR:CD2	2:B:786:THR:HG23	2.54	0.42
2:B:816:GLU:HB2	2:B:867:ILE:HD13	2.00	0.42
8:H:76:ASN:HB2	8:H:79:ASP:OD2	2.18	0.42
1:A:139:LYS:HG2	1:A:143:HIS:CD2	2.54	0.42
1:A:141:LEU:HD12	1:A:236:LEU:O	2.19	0.42
1:A:355:MET:O	2:B:1091:ARG:HD2	2.19	0.42
1:A:621:ILE:HD11	8:H:124:ARG:HD2	2.01	0.42
1:A:653:VAL:HG11	1:A:669:TYR:OH	2.19	0.42
1:A:1474:LEU:HD11	6:F:107:ARG:NE	2.35	0.42
2:B:529:MET:HG2	2:B:702:MET:HB3	2.01	0.42
2:B:818:GLU:HB2	2:B:829:PHE:CE2	2.55	0.42
2:B:866:ILE:HD11	2:B:896:LEU:HG	2.00	0.42
15:T:4:DT:H1'	15:T:5:DC:H5''	2.00	0.42
1:A:458:PHE:CB	1:A:472:HIS:HD2	2.28	0.42
1:A:1228:MET:HE3	1:A:1247:PHE:HB2	2.00	0.42
1:A:94:VAL:O	1:A:250:VAL:N	2.51	0.42
1:A:490:THR:OG1	1:A:491:PRO:HD3	2.19	0.42
1:A:1212:LEU:HB2	1:A:1285:LEU:HD21	2.02	0.42
2:B:42:GLN:HE22	2:B:483:ARG:HA	1.85	0.42
2:B:1021:HIS:CD2	2:B:1025:ASN:HB2	2.55	0.42
5:E:57:ASP:C	5:E:59:THR:H	2.27	0.42
8:H:98:ARG:HB3	8:H:115:TYR:HD2	1.84	0.42
8:H:103:GLU:HB3	8:H:109:ALA:HB2	2.02	0.42
1:A:1181:PRO:HG3	1:A:1207:ILE:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1394:ASN:OD1	1:A:1395:TYR:N	2.53	0.42
1:A:1464:ALA:C	1:A:1466:ALA:H	2.28	0.42
2:B:66:ASP:OD1	2:B:85:LEU:HD22	2.20	0.42
2:B:128:ILE:HD12	2:B:147:THR:HG21	2.02	0.42
2:B:156:LEU:HD22	2:B:184:TYR:CE1	2.54	0.42
2:B:193:VAL:HG23	2:B:470:LEU:HB2	2.01	0.42
2:B:285:LEU:HD22	9:I:16:PHE:HZ	1.83	0.42
2:B:428:ASP:CG	2:B:429:PHE:H	2.28	0.42
2:B:475:PHE:CE2	2:B:479:LEU:HD11	2.54	0.42
2:B:483:ARG:NH1	2:B:706:VAL:HG23	2.34	0.42
2:B:931:ILE:HA	2:B:945:CYS:HB3	2.02	0.42
7:G:39:THR:O	7:G:43:GLY:N	2.50	0.42
8:H:88:PHE:HD2	8:H:144:LEU:HB3	1.81	0.42
1:A:802:PHE:HE1	2:B:504:THR:HG22	1.84	0.42
1:A:880:ARG:HG2	1:A:886:VAL:HA	2.02	0.42
1:A:892:GLY:HA3	1:A:1396:ARG:HH11	1.85	0.42
1:A:1205:ALA:HB1	1:A:1267:ASN:HB2	2.02	0.42
2:B:48:ASP:OD1	2:B:158:SER:HB2	2.20	0.42
2:B:96:PRO:HG2	2:B:120:TYR:CZ	2.55	0.42
2:B:221:CYS:HB3	2:B:368:MET:HE2	2.02	0.42
5:E:55:ARG:HA	5:E:55:ARG:HD2	1.75	0.42
7:G:14:HIS:CD2	7:G:16:ARG:HG2	2.54	0.42
8:H:58:LEU:HD12	8:H:144:LEU:O	2.20	0.42
15:T:14:DC:H2'	15:T:15:DT:C6	2.55	0.42
1:A:96:HIS:HB2	1:A:250:VAL:HG23	2.01	0.42
1:A:506:PRO:HB2	1:A:511:THR:HG23	2.02	0.42
1:A:783:GLN:HA	1:A:787:VAL:O	2.19	0.42
3:C:205:LYS:NZ	3:C:213:GLU:HA	2.34	0.42
1:A:11:SER:N	2:B:1135:TYR:HH	2.17	0.42
1:A:610:PRO:HG2	1:A:613:GLU:HG3	2.01	0.42
1:A:896:LEU:HD23	1:A:1080:ILE:HA	2.01	0.42
2:B:84:TYR:CD1	2:B:132:VAL:HG12	2.55	0.42
2:B:223:SER:OG	2:B:349:PRO:HD2	2.20	0.42
2:B:806:PHE:O	2:B:1050:ARG:NH1	2.53	0.42
2:B:907:VAL:HB	12:L:46:LYS:CB	2.50	0.42
6:F:81:VAL:HG22	6:F:101:LYS:HD3	2.01	0.42
8:H:57:ARG:HB2	8:H:148:LEU:HD11	2.01	0.42
10:J:9:THR:HB	10:J:44:CYS:HB2	2.00	0.42
1:A:1085:GLU:HA	6:F:60:TYR:CE2	2.55	0.41
1:A:1409:GLY:HA2	5:E:172:ARG:O	2.19	0.41
2:B:196:ALA:HB2	2:B:395:LEU:HD23	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:861:SER:O	2:B:896:LEU:HD12	2.19	0.41
11:K:81:TYR:CE2	11:K:86:ALA:HB2	2.55	0.41
11:K:82:SER:HB3	11:K:85:GLU:HG3	2.01	0.41
1:A:189:PRO:HD3	1:A:202:TRP:NE1	2.34	0.41
1:A:812:LYS:HB2	9:I:78:LEU:HD23	2.02	0.41
1:A:979:LEU:HB3	1:A:980:PRO:HD2	2.02	0.41
1:A:1178:ASP:HB2	1:A:1260:ARG:HH22	1.85	0.41
2:B:271:ILE:HD13	2:B:320:PHE:CE2	2.54	0.41
2:B:818:GLU:OE1	2:B:917:LYS:HB3	2.21	0.41
2:B:1040:GLN:HG2	3:C:203:TRP:CZ2	2.55	0.41
3:C:114:HIS:CE1	3:C:152:LYS:HE2	2.55	0.41
4:D:32:LEU:HD11	7:G:4:HIS:HB2	2.01	0.41
8:H:58:LEU:HD11	8:H:143:LEU:CD1	2.48	0.41
1:A:916:PHE:CE1	1:A:920:PHE:HD2	2.37	0.41
1:A:967:ARG:NH2	1:A:1326:GLY:O	2.53	0.41
2:B:36:GLU:OE2	2:B:654:GLN:HB2	2.20	0.41
2:B:177:CYS:HB3	2:B:180:ASP:HB2	2.02	0.41
2:B:952:GLU:HG2	3:C:40:ALA:HB2	2.02	0.41
3:C:44:ILE:HD12	3:C:178:PRO:HA	2.01	0.41
10:J:44:CYS:O	10:J:47:ARG:HG2	2.20	0.41
1:A:746:ASN:HA	1:A:749:ARG:HG2	2.02	0.41
1:A:919:LYS:C	1:A:1052:ARG:HD3	2.45	0.41
1:A:922:PHE:CD2	1:A:952:LEU:HD23	2.55	0.41
1:A:1013:VAL:HG11	1:A:1046:ARG:HG2	2.03	0.41
1:A:1309:MET:HG2	1:A:1334:TRP:CE3	2.56	0.41
2:B:363:TYR:HB3	2:B:573:TRP:CZ3	2.55	0.41
2:B:861:SER:HA	2:B:901:THR:HA	2.01	0.41
4:D:38:HIS:O	4:D:42:GLU:HG2	2.20	0.41
1:A:551:ARG:NH2	8:H:122:LEU:HD12	2.35	0.41
1:A:962:ASP:CG	1:A:1046:ARG:HH21	2.29	0.41
2:B:36:GLU:OE1	2:B:653:TRP:HB3	2.19	0.41
2:B:91:ILE:HG12	2:B:124:LEU:HD11	2.02	0.41
3:C:101:PHE:CE2	3:C:122:SER:HB3	2.55	0.41
3:C:189:ASP:OD2	3:C:211:LEU:HG	2.21	0.41
6:F:61:GLU:OE2	6:F:108:ARG:NE	2.53	0.41
8:H:90:TYR:HE2	8:H:92:MET:HE2	1.84	0.41
8:H:98:ARG:HD2	8:H:115:TYR:HD2	1.86	0.41
1:A:141:LEU:HA	1:A:144:VAL:HG22	2.01	0.41
1:A:564:LEU:HD13	1:A:570:TRP:CZ2	2.55	0.41
1:A:760:LEU:HD11	1:A:781:ILE:HG21	2.02	0.41
1:A:790:GLN:NE2	1:A:797:ARG:HG3	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:ASP:HB3	5:E:200:ALA:HB2	2.02	0.41
1:A:1022:ILE:HD11	1:A:1076:PHE:HZ	1.85	0.41
1:A:1167:ARG:HG3	9:I:58:ILE:HD13	2.02	0.41
1:A:1191:GLU:O	1:A:1195:VAL:HG23	2.20	0.41
2:B:294:ASP:O	2:B:298:MET:HG2	2.21	0.41
2:B:389:GLY:HA2	2:B:667:THR:OG1	2.20	0.41
2:B:509:VAL:HG13	2:B:525:ASN:O	2.21	0.41
3:C:45:ILE:HG22	3:C:73:LEU:HD12	2.02	0.41
9:I:96:PHE:HD2	9:I:110:LEU:HD22	1.86	0.41
10:J:54:ASP:OD2	10:J:57:GLU:HG2	2.21	0.41
1:A:214:ILE:HD12	1:A:220:ARG:NH1	2.36	0.41
2:B:911:LEU:HD23	2:B:917:LYS:HA	2.03	0.41
5:E:29:THR:CG2	5:E:32:GLU:HB2	2.49	0.41
5:E:45:GLY:HA3	5:E:53:PRO:HD3	2.02	0.41
5:E:194:ILE:HG12	5:E:204:ILE:HG12	2.02	0.41
2:B:728:MET:SD	2:B:942:LYS:HB3	2.61	0.41
5:E:73:PHE:HB2	5:E:99:ILE:HD12	2.03	0.41
7:G:62:GLY:O	7:G:63:ARG:HG2	2.20	0.41
1:A:20:ARG:NH1	1:A:22:GLN:OE1	2.54	0.41
1:A:392:GLU:HB2	1:A:448:ARG:NH1	2.36	0.41
1:A:601:ASN:HA	1:A:630:VAL:O	2.21	0.41
1:A:797:ARG:HG2	1:A:820:ARG:HB3	2.01	0.41
2:B:100:GLU:CD	12:L:42:ARG:HE	2.29	0.41
2:B:268:PRO:HD2	2:B:271:ILE:HD12	2.02	0.41
2:B:636:LYS:H	2:B:639:HIS:CD2	2.29	0.41
2:B:677:MET:CE	2:B:700:PRO:HB3	2.51	0.41
2:B:924:ARG:HH22	3:C:61:ASP:HB2	1.84	0.41
2:B:1119:CYS:SG	2:B:1142:ASN:ND2	2.94	0.41
5:E:14:ARG:O	5:E:18:MET:HG2	2.20	0.41
5:E:77:PRO:HD2	5:E:105:VAL:O	2.21	0.41
7:G:13:LEU:HD13	7:G:68:TYR:HD2	1.86	0.41
12:L:19:CYS:HB2	12:L:36:CYS:SG	2.61	0.41
1:A:48:GLU:OE2	1:A:53:LYS:NZ	2.53	0.41
1:A:894:ASP:O	1:A:1022:ILE:HD13	2.21	0.41
1:A:1216:LEU:HB2	1:A:1255:LEU:HD23	2.03	0.41
2:B:577:HIS:HE1	2:B:579:ASP:HB3	1.86	0.41
2:B:830:GLU:O	2:B:832:PRO:HD3	2.20	0.41
6:F:75:MET:HE2	7:G:14:HIS:CE1	2.56	0.41
7:G:62:GLY:C	7:G:64:GLY:H	2.28	0.41
10:J:24:LEU:HD22	10:J:29:TYR:CD2	2.55	0.41
11:K:90:ALA:O	11:K:94:LEU:HG	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ASP:HB2	2:B:790:GLN:NE2	2.37	0.40
2:B:1129:ASN:ND2	2:B:1134:THR:OG1	2.38	0.40
4:D:31:THR:HG22	7:G:3:TYR:CE1	2.57	0.40
15:T:7:DC:H2'	15:T:8:DT:H72	2.02	0.40
1:A:604:ARG:HH11	1:A:651:SER:HA	1.86	0.40
1:A:791:GLN:NE2	1:A:839:HIS:HA	2.36	0.40
1:A:1211:LEU:HD22	1:A:1258:ARG:HH21	1.85	0.40
2:B:483:ARG:NH2	2:B:527:ALA:O	2.51	0.40
1:A:370:ASP:OD1	2:B:788:TYR:HE2	2.05	0.40
1:A:890:ARG:NE	1:A:1023:VAL:HG22	2.35	0.40
1:A:901:VAL:HG12	1:A:980:PRO:HA	2.03	0.40
1:A:1480:CYS:HA	6:F:80:MET:CE	2.51	0.40
2:B:449:ALA:HB1	15:T:22:DT:H5''	2.03	0.40
2:B:752:TYR:HE1	3:C:60:HIS:HE1	1.67	0.40
5:E:55:ARG:HH12	5:E:107:GLN:HG2	1.86	0.40
1:A:465:HIS:NE2	1:A:467:MET:HB2	2.37	0.40
2:B:528:LEU:HB2	2:B:702:MET:HE3	2.03	0.40
2:B:815:LYS:NZ	2:B:920:LYS:HE2	2.37	0.40
1:A:70:ARG:HH22	2:B:1131:ARG:NH2	2.20	0.40
1:A:524:MET:CE	2:B:1097:HIS:HE1	2.32	0.40
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	2.02	0.40
1:A:1214:VAL:CG2	1:A:1257:LEU:HB3	2.51	0.40
2:B:423:ILE:O	2:B:426:GLY:N	2.54	0.40
2:B:765:GLU:HG3	2:B:770:ARG:NH2	2.37	0.40
2:B:1062:ARG:CZ	2:B:1065:GLY:H	2.35	0.40
6:F:66:LEU:HD23	6:F:66:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1417/1970 (72%)	1357 (96%)	59 (4%)	1 (0%)	48	78
2	B	1128/1174 (96%)	1067 (95%)	61 (5%)	0	100	100
3	C	253/271 (93%)	241 (95%)	11 (4%)	1 (0%)	30	61
4	D	126/142 (89%)	123 (98%)	3 (2%)	0	100	100
5	E	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
6	F	80/127 (63%)	78 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
8	H	146/150 (97%)	139 (95%)	7 (5%)	0	100	100
9	I	112/125 (90%)	106 (95%)	6 (5%)	0	100	100
10	J	65/67 (97%)	60 (92%)	5 (8%)	0	100	100
11	K	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
12	L	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
All	All	3858/4580 (84%)	3676 (95%)	180 (5%)	2 (0%)	49	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	CYS
3	C	92	GLU

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	A	1252/1749 (72%)	1251 (100%)	1 (0%)	88	91
2	B	993/1027 (97%)	992 (100%)	1 (0%)	88	91
3	C	234/248 (94%)	234 (100%)	0	100	100
4	D	106/126 (84%)	106 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	147/152 (97%)	147 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	103/112 (92%)	103 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/104 (100%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
All	All	3427/4063 (84%)	3425 (100%)	2 (0%)	87	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	540	ASP
2	B	235	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	143	HIS
1	A	222	HIS
1	A	273	GLN
1	A	330	GLN
1	A	353	ASN
1	A	472	HIS
1	A	493	ASN
1	A	502	ASN
1	A	504	HIS
1	A	620	HIS
1	A	673	GLN
1	A	791	GLN
1	A	804	HIS
1	A	1032	GLN
1	A	1034	GLN
1	A	1044	HIS
1	A	1082	HIS
1	A	1093	GLN
1	A	1163	HIS
1	A	1180	ASN
1	A	1190	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1360	ASN
1	A	1457	ASN
1	A	1462	GLN
2	B	245	GLN
2	B	265	GLN
2	B	312	GLN
2	B	518	HIS
2	B	525	ASN
2	B	639	HIS
2	B	649	ASN
2	B	699	HIS
2	B	817	GLN
2	B	825	GLN
2	B	912	ASN
2	B	948	GLN
2	B	986	GLN
2	B	1097	HIS
2	B	1115	GLN
2	B	1117	HIS
3	C	5	ASN
3	C	51	GLN
3	C	265	HIS
4	D	93	HIS
4	D	129	GLN
4	D	135	GLN
5	E	35	GLN
5	E	43	GLN
5	E	148	HIS
6	F	46	GLN
7	G	4	HIS
7	G	14	HIS
9	I	41	ASN
9	I	118	HIS
10	J	52	HIS
11	K	76	GLN
11	K	84	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	10/20 (50%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	12	G

There are no RNA pucker outliers to report.

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 10 ligands modelled in this entry, 9 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	$\# Z > 2$
17	CPT	N	101	15,13	0,2,4	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

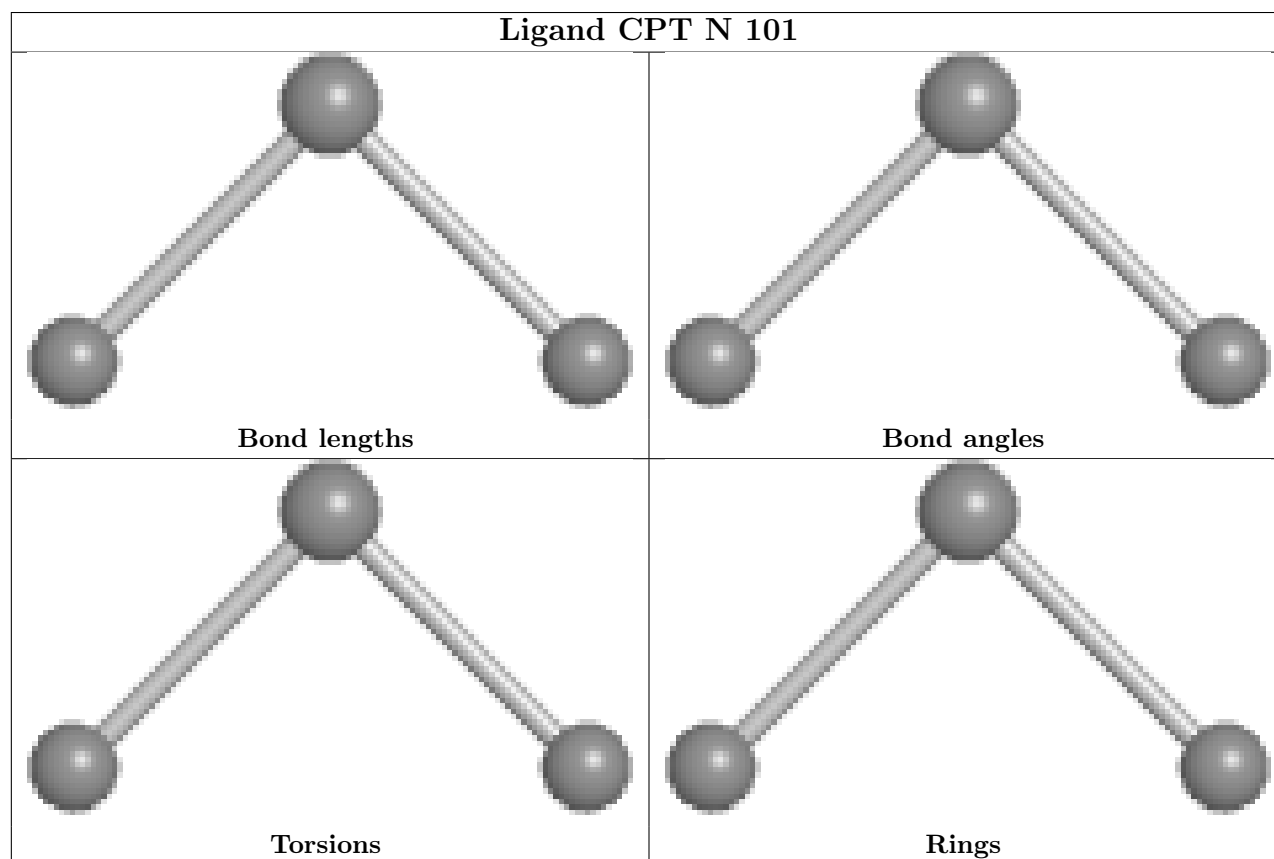
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

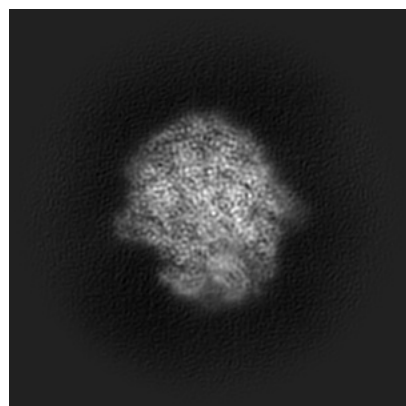
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65750. These allow visual inspection of the internal detail of the map and identification of artifacts.

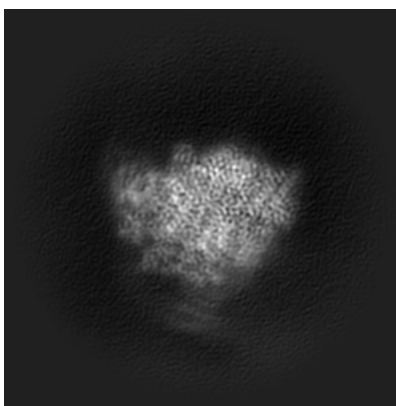
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

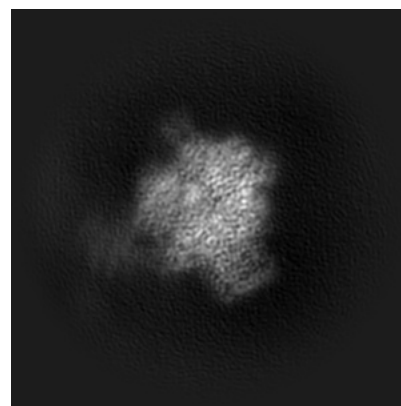
6.1.1 Primary map



X

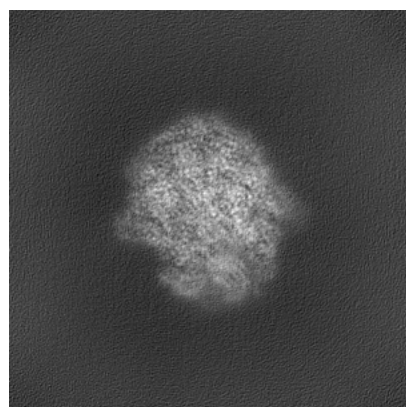


Y

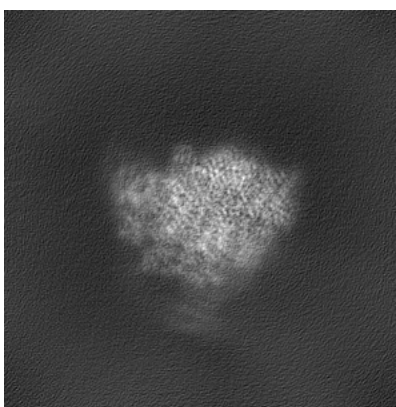


Z

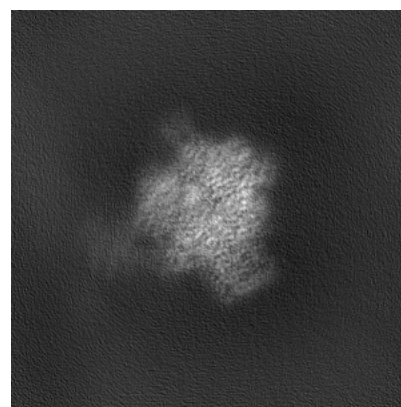
6.1.2 Raw map



X



Y

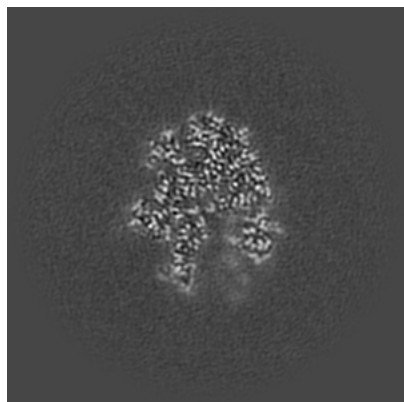


Z

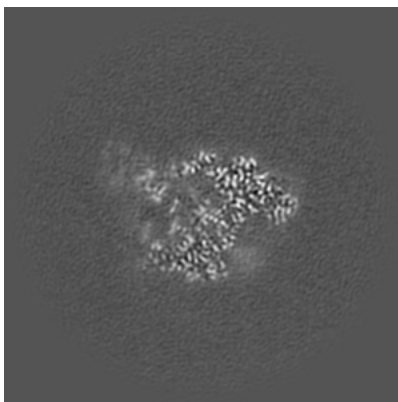
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

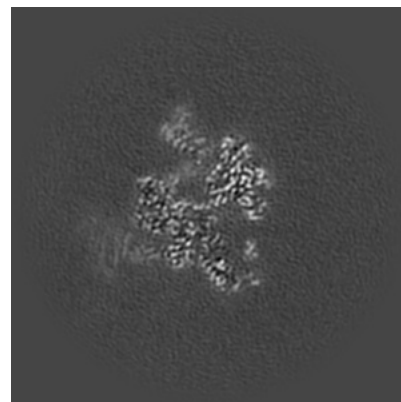
6.2.1 Primary map



X Index: 160

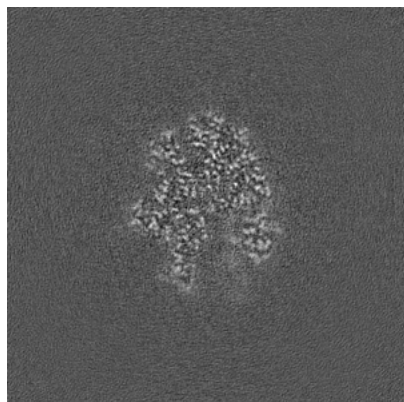


Y Index: 160

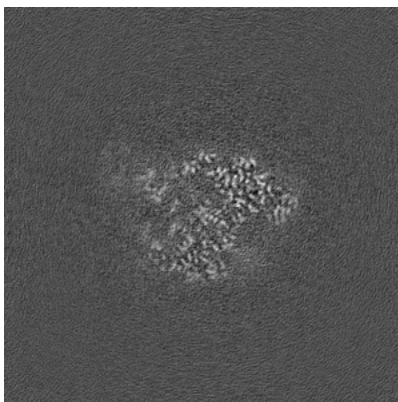


Z Index: 160

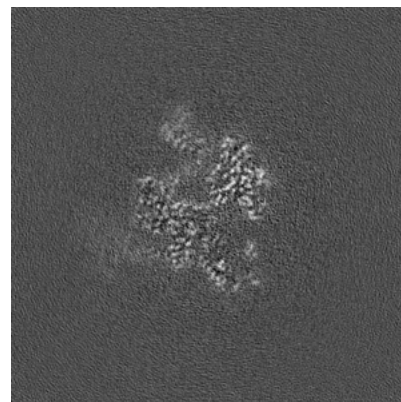
6.2.2 Raw map



X Index: 160



Y Index: 160

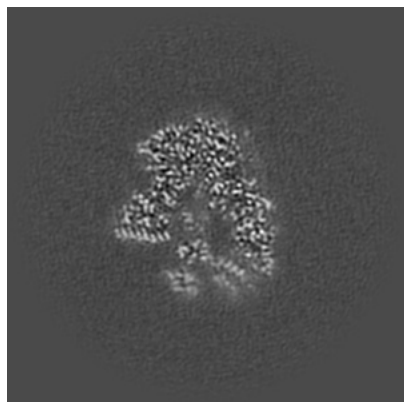


Z Index: 160

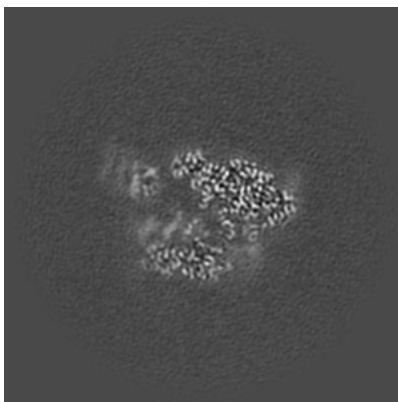
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

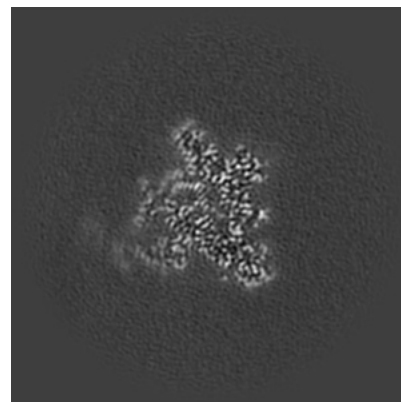
6.3.1 Primary map



X Index: 169

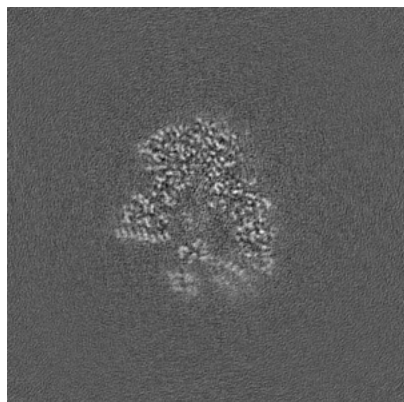


Y Index: 165

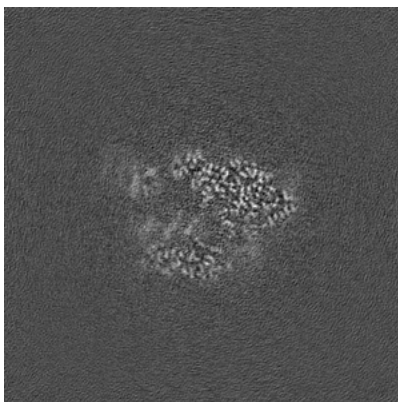


Z Index: 172

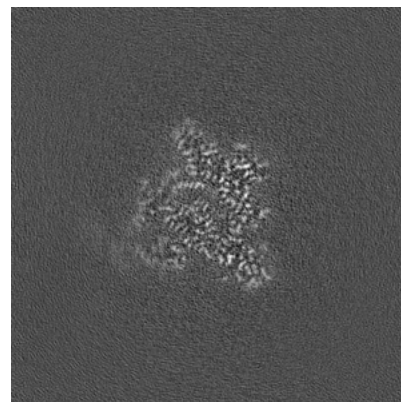
6.3.2 Raw map



X Index: 169



Y Index: 165

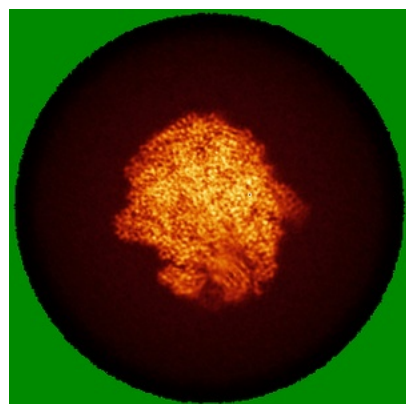


Z Index: 171

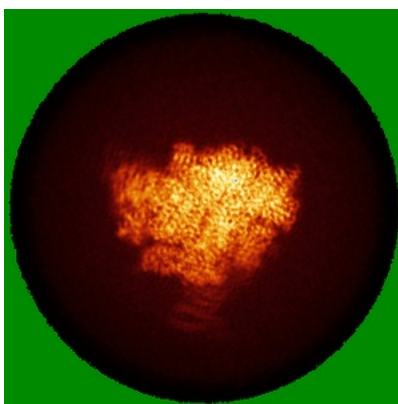
The images above show the largest variance slices of the map in three orthogonal directions.

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

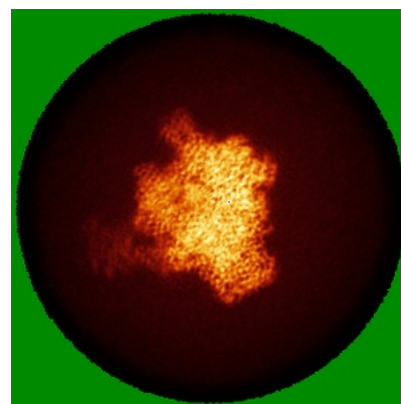
6.4.1 Primary map



X

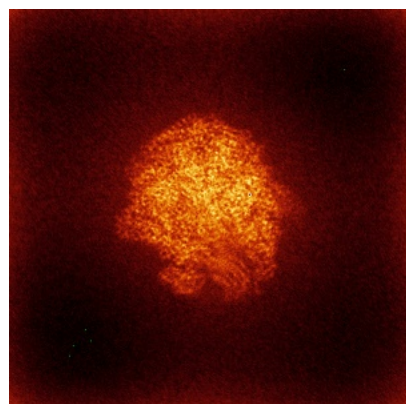


Y

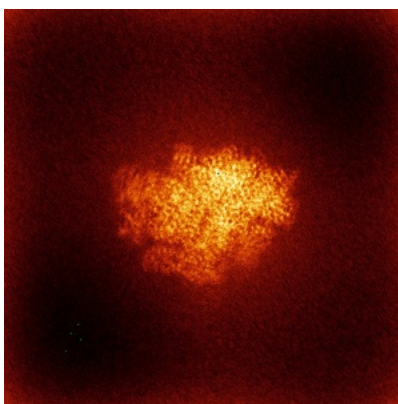


Z

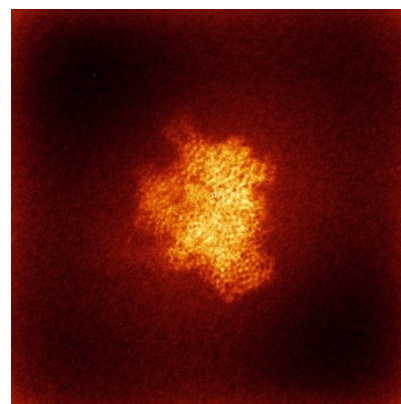
6.4.2 Raw map



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.

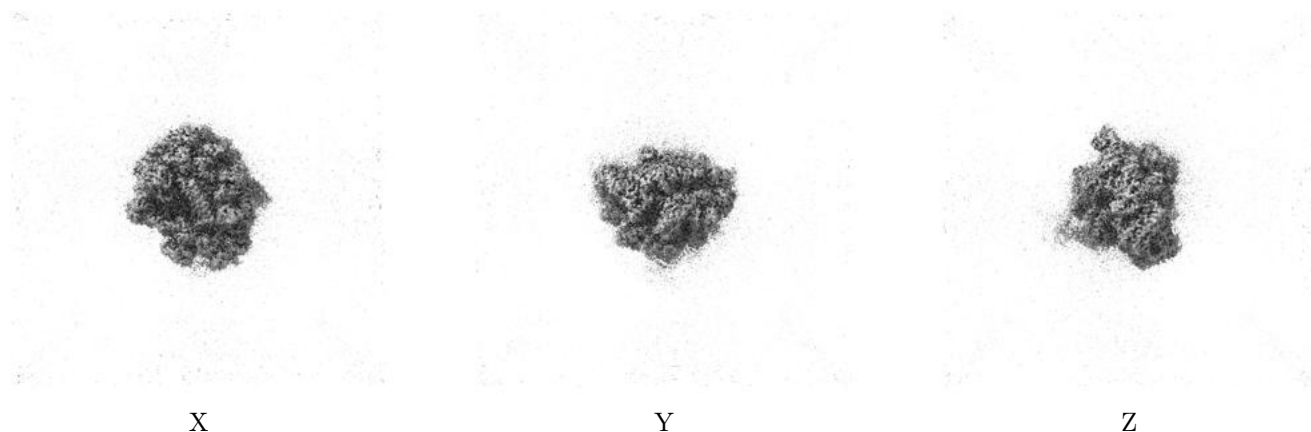
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

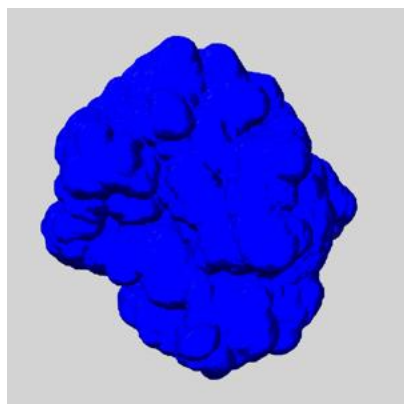
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

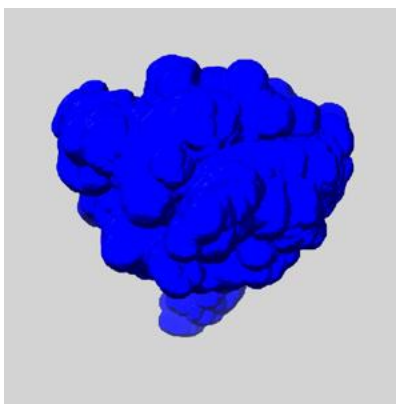
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

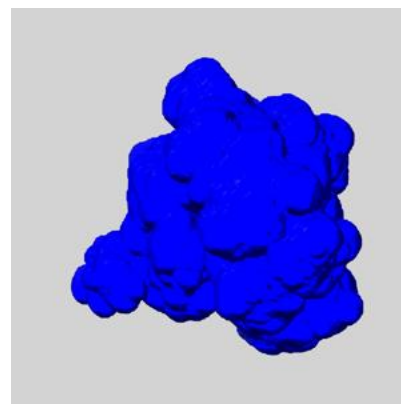
6.6.1 emd_65750_msk_1.map [i](#)



X



Y

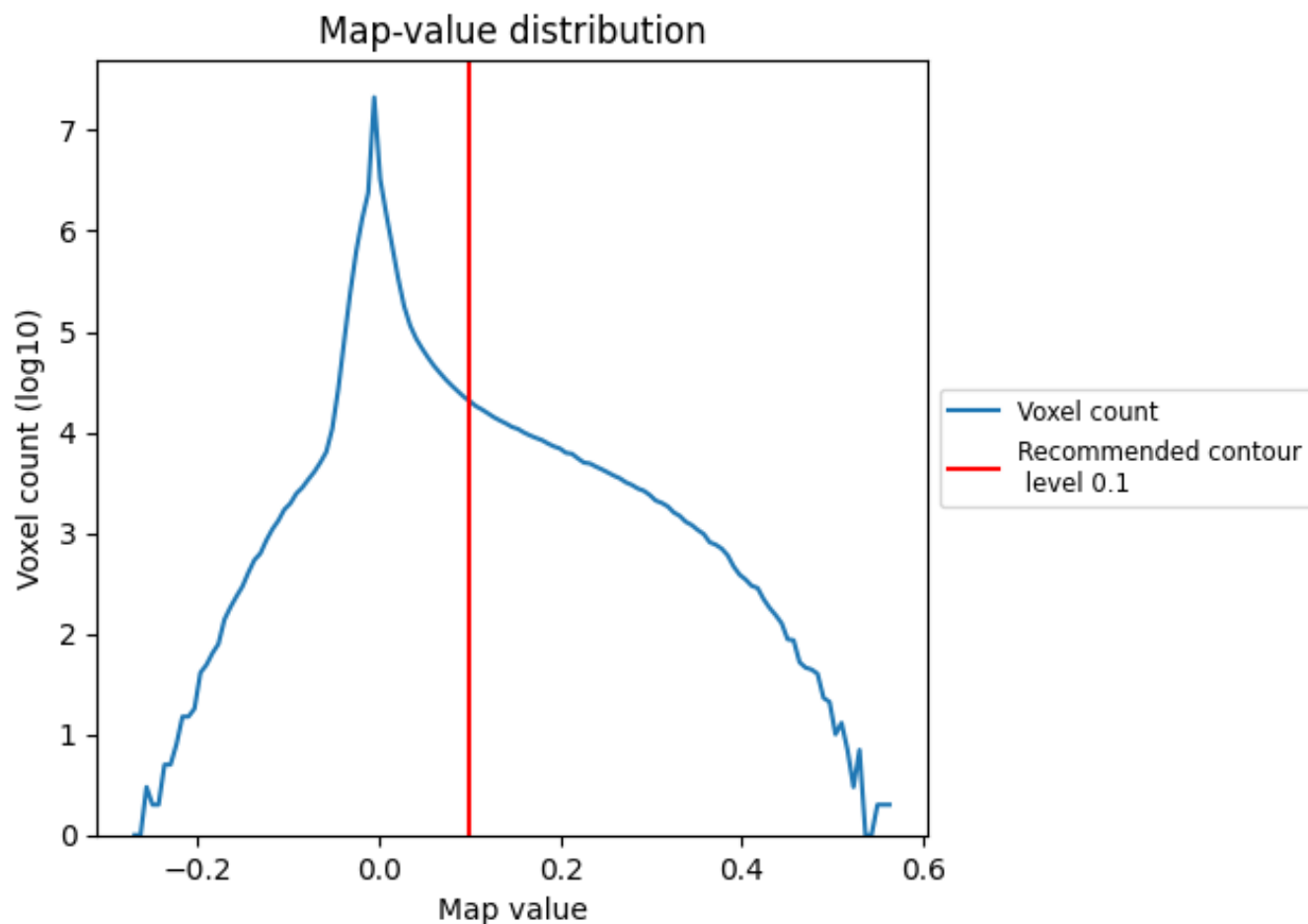


Z

7 Map analysis [i](#)

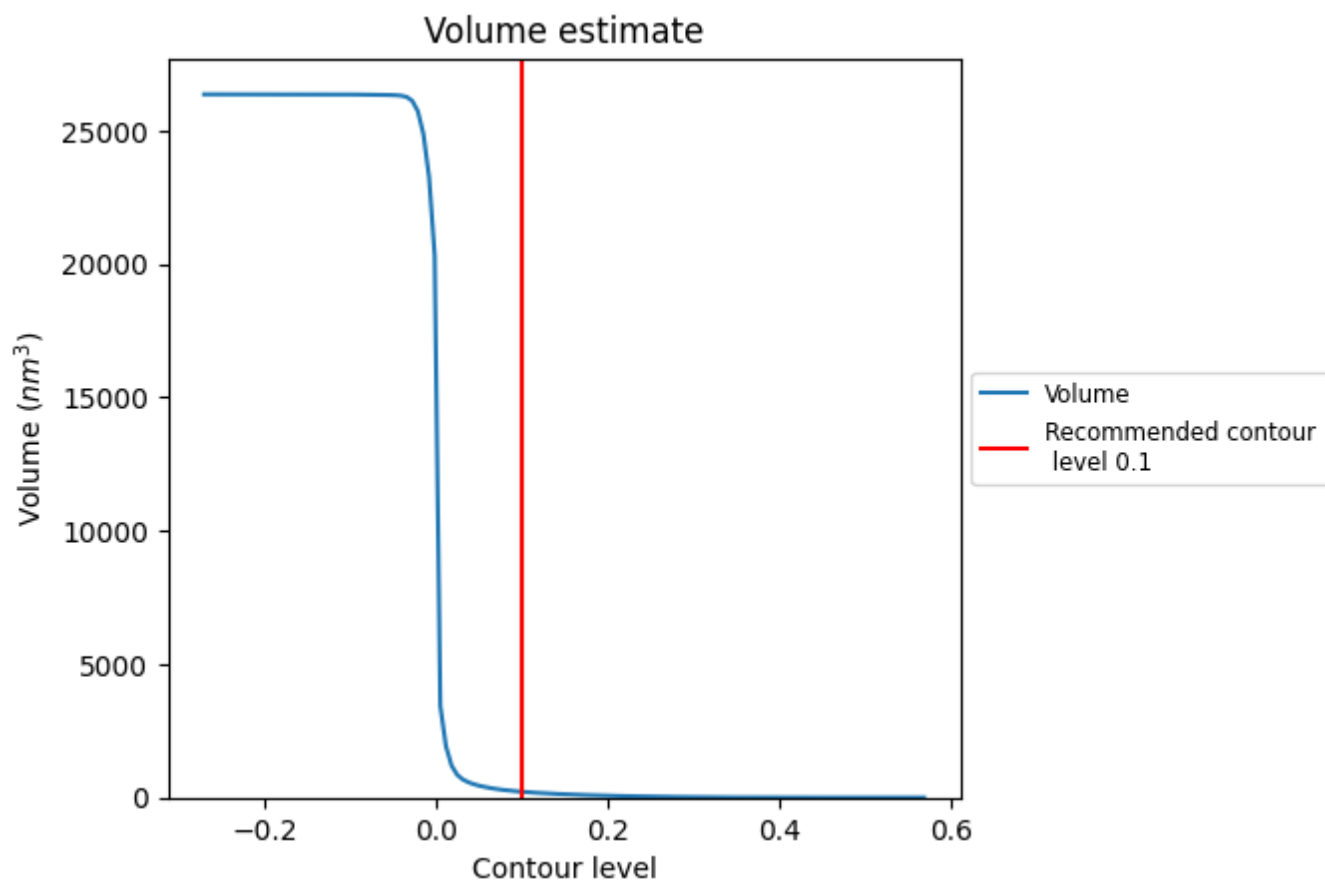
This section contains the results of statistical analysis of the map.

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.

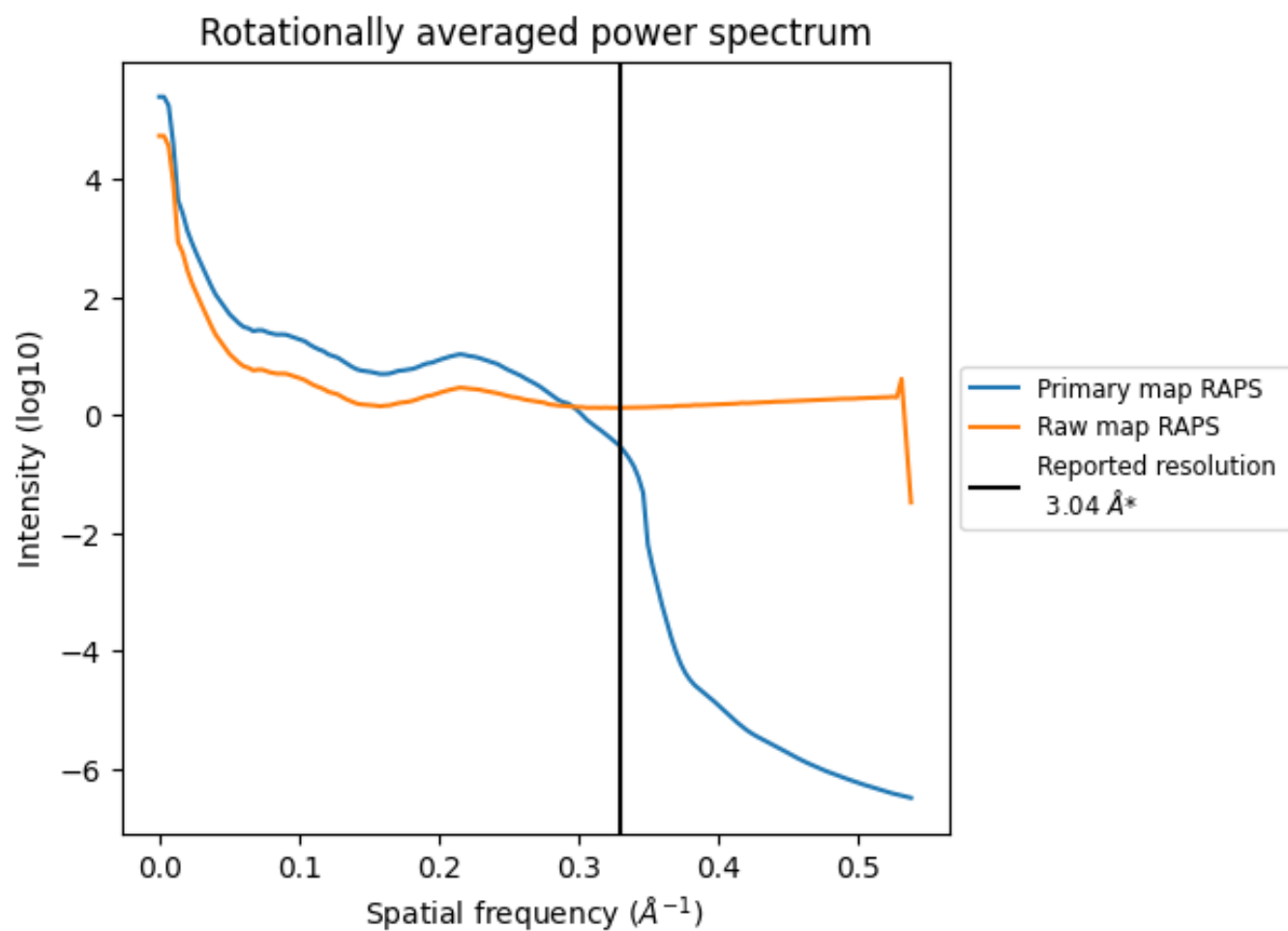
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm^3 ; this corresponds to an approximate mass of 198 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

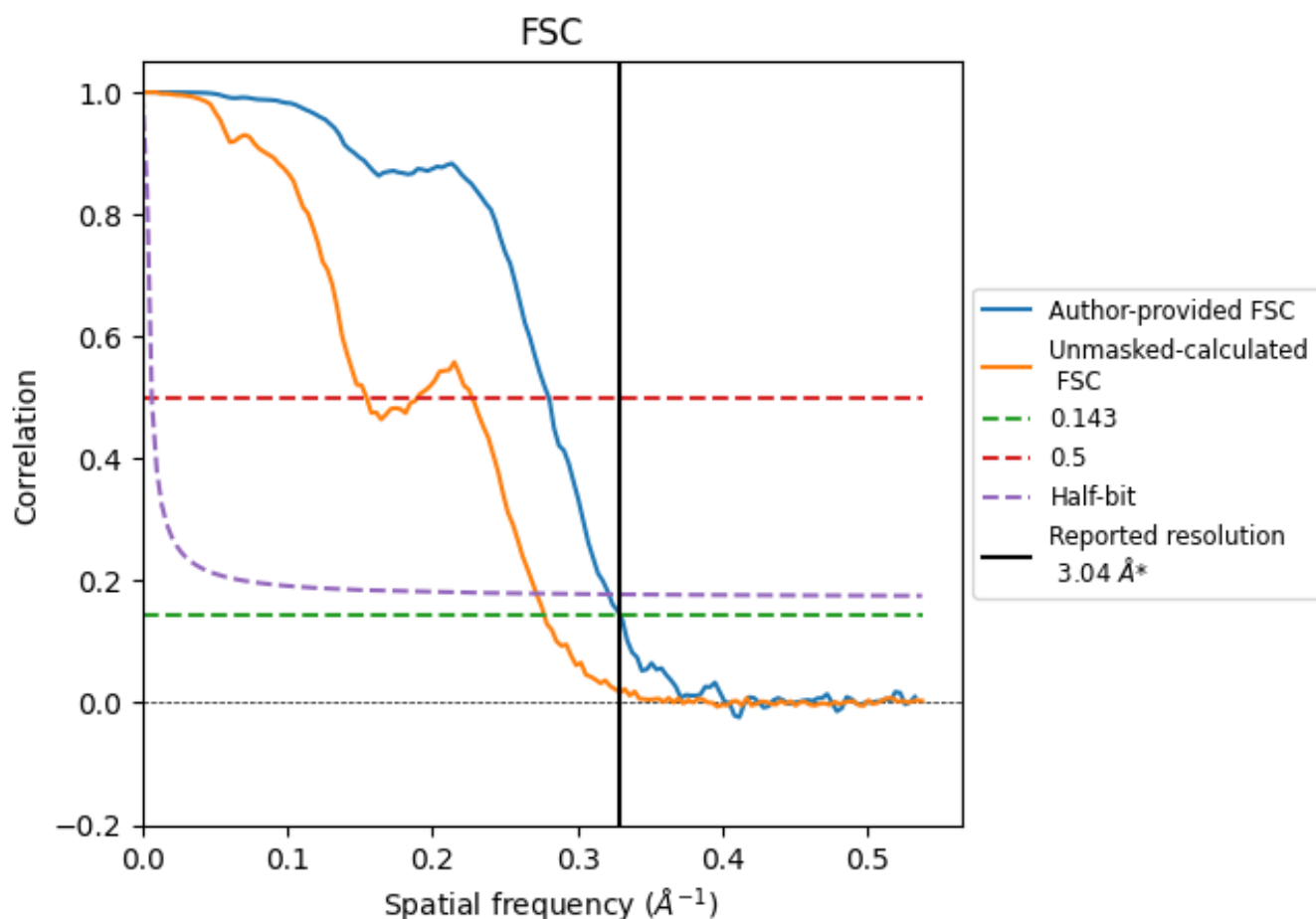


*Reported resolution corresponds to spatial frequency of 0.329 $\text{\AA}^{-1}$

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 $0.329 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

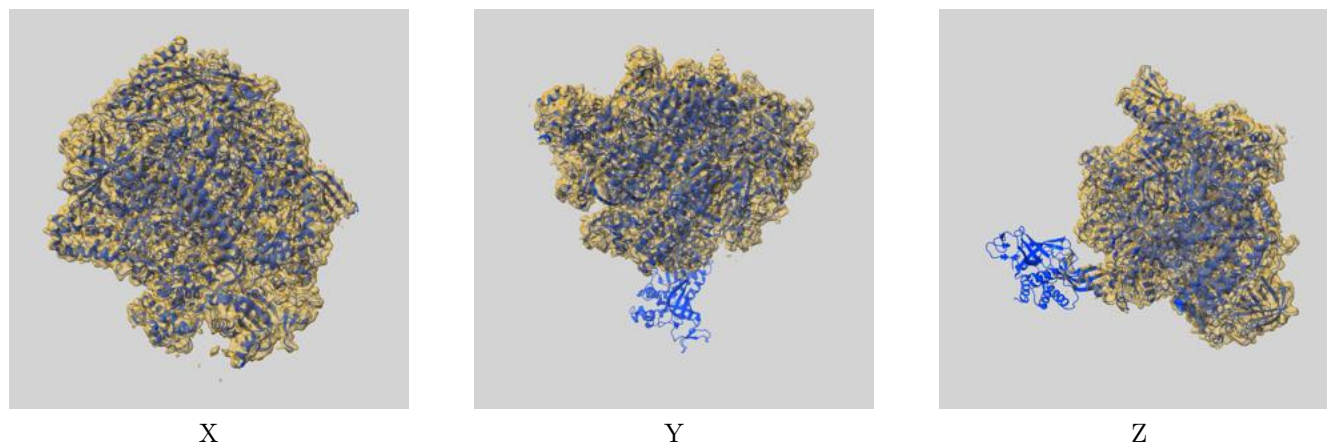
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.57	3.11
Unmasked-calculated*	3.61	6.47	3.68

*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 3.61 differs from the reported value 3.04 by more than 10 %

9 Map-model fit [i](#)

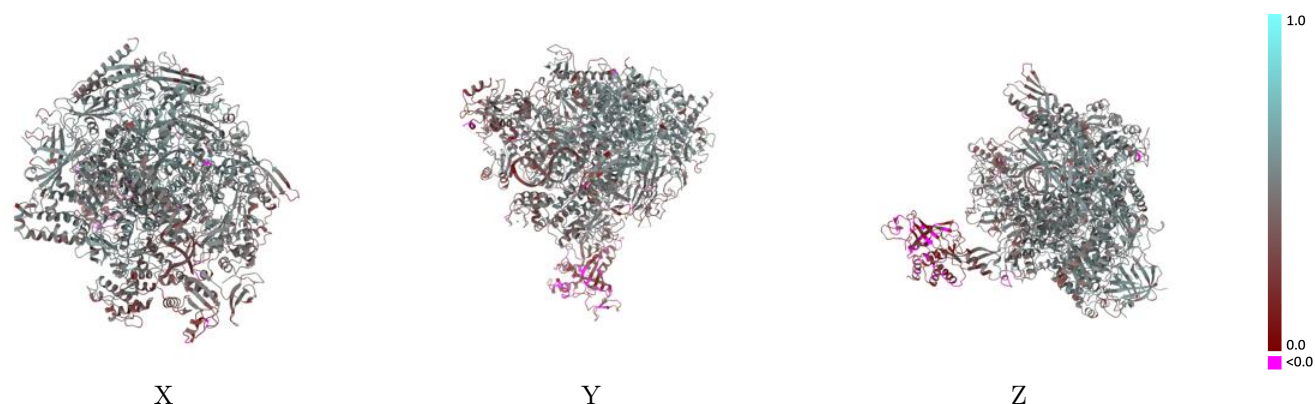
This section contains information regarding the fit between EMDB map EMD-65750 and PDB model 9W8S. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



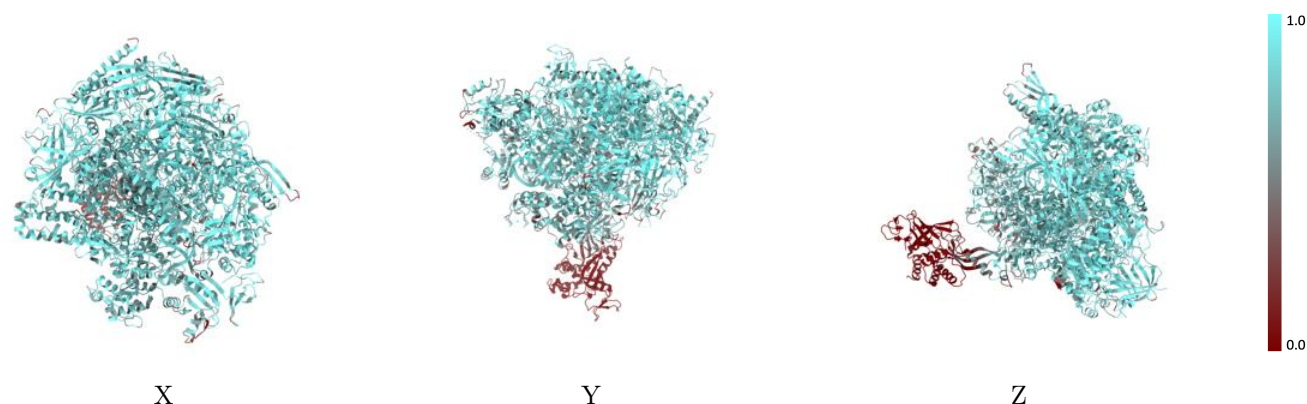
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



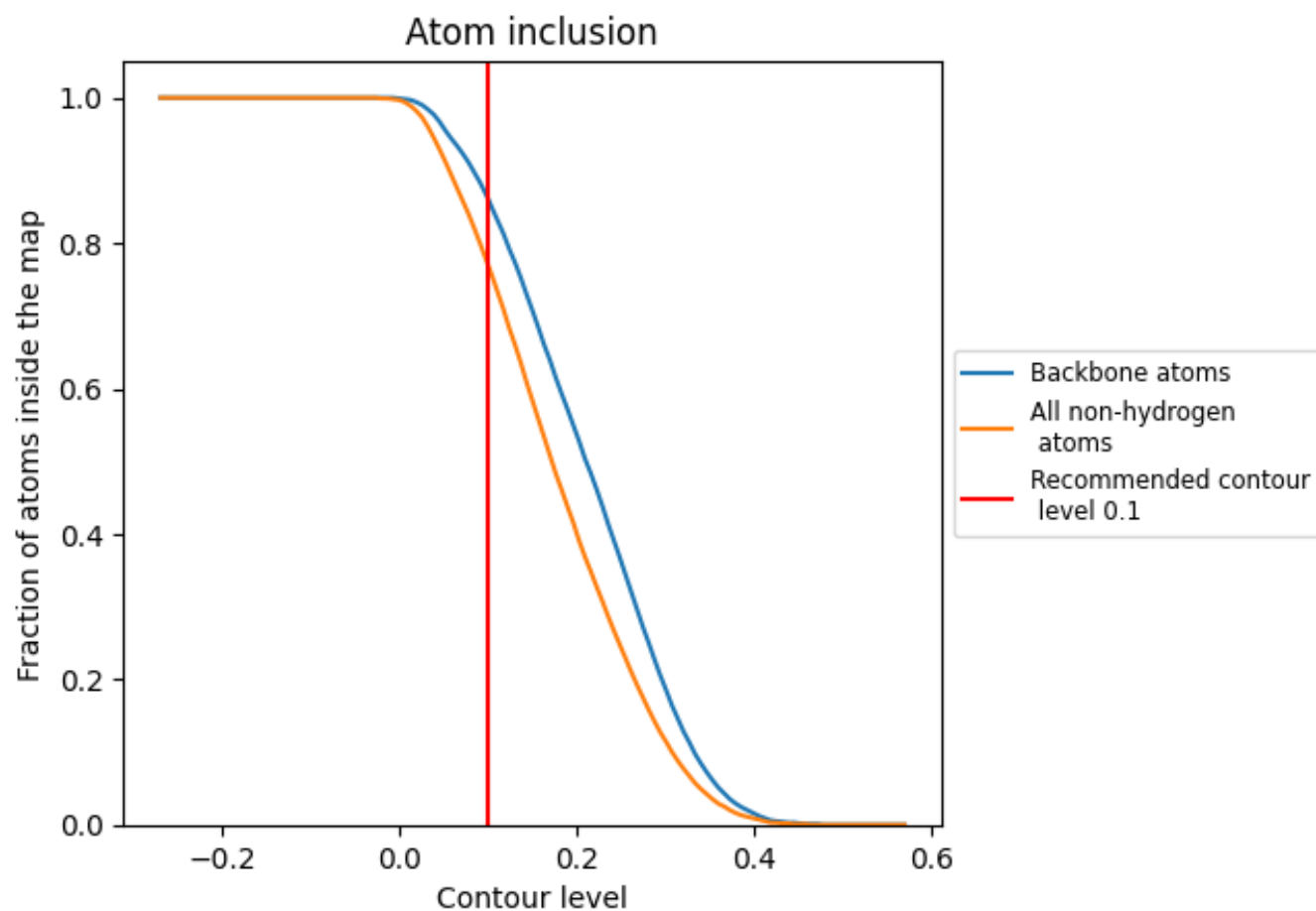
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 77% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7680	 0.4480
A	 0.7980	 0.4640
B	 0.8390	 0.4820
C	 0.8440	 0.4860
D	 0.0040	 0.1340
E	 0.8120	 0.4390
F	 0.7540	 0.4430
G	 0.1810	 0.2300
H	 0.8110	 0.4780
I	 0.7950	 0.4130
J	 0.8910	 0.5160
K	 0.8290	 0.4850
L	 0.8200	 0.4630
N	 0.8690	 0.3020
P	 0.9680	 0.5330
T	 0.9400	 0.4610

