



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 11:28 PM UTC

PDB ID : 8W8F / pdb_00008w8f
EMDB ID : EMD-37353
Title : human co-transcriptional RNA capping enzyme RNGTT-CMTR1
Authors : Li, Y.; Wang, Q.; Xu, Y.; Li, Z.
Deposited on : 2023-09-02
Resolution : 4.00 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

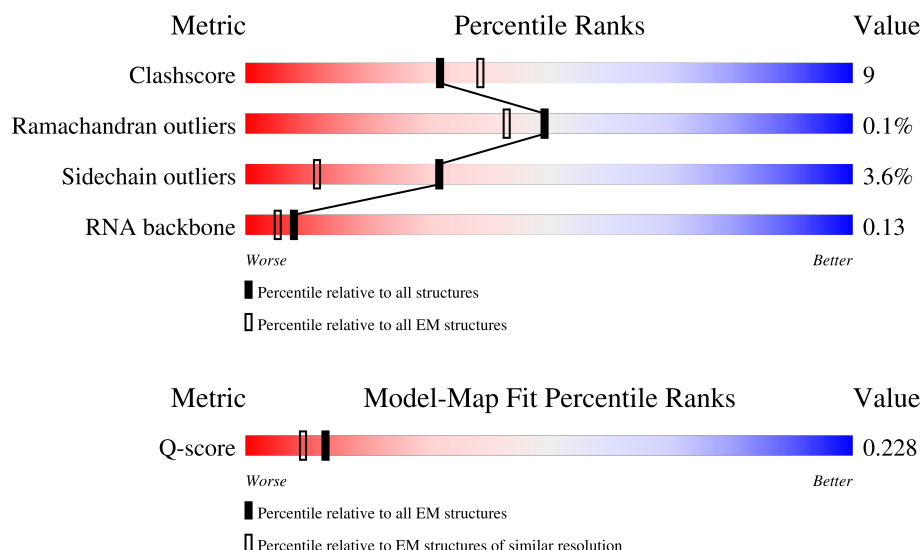
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.



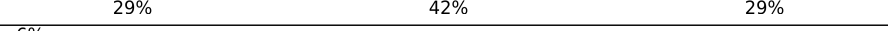
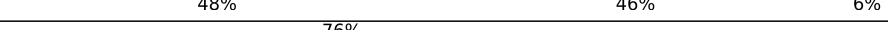
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	597	
2	b	835	
3	A	1970	

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Mol	Chain	Length	Quality of chain
4	B	1174	
5	C	271	
6	D	142	
7	E	210	
8	F	127	
9	G	172	
10	H	150	
11	I	125	
12	J	67	
13	K	117	
14	L	58	
15	N	48	
16	P	17	
17	T	48	
18	Y	121	
19	Z	1087	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 46667 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 mRNA-capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	517	Total	C	N	O	S	6	0
			4203	2684	726	759	34		

- Molecule 2 is a protein called Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	693	Total	C	N	O	S	0	0
			5584	3574	951	1024	35		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1426	Total	C	N	O	S	0	0
			11299	7111	2020	2099	69		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	1133	Total	C	N	O	S	0	0
			9046	5723	1594	1665	64		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	258	Total	C	N	O	S	0	0
			2072	1301	353	412	6		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	129	Total	C	N	O	S	0	1
			998	629	170	195	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	82	Total	C	N	O	S	0	0
			658	418	113	122	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	171	Total	C	N	O	S	0	0
			1305	852	205	240	8		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	117	Total	C	N	O	S	0	0
			950	587	169	183	11		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 14 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	46	Total	C	N	O	S	0	0
			389	241	75	67	6		

- Molecule 15 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	34	Total	C	N	O	P	0	0
			714	333	147	200	34		

- Molecule 16 is a RNA chain called RNA (5'-R(P*GP*AP*GP*AP*GP*AP*GP*GP*GP*A P*AP*CP*CP*CP*AP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	16	Total	C	N	O	P	0	0
			347	155	69	107	16		

- Molecule 17 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	45	Total	C	N	O	P	0	0
			910	432	156	277	45		

- Molecule 18 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 19 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	360	Total	C	N	O	S	0	0
			2880	1835	495	537	13		

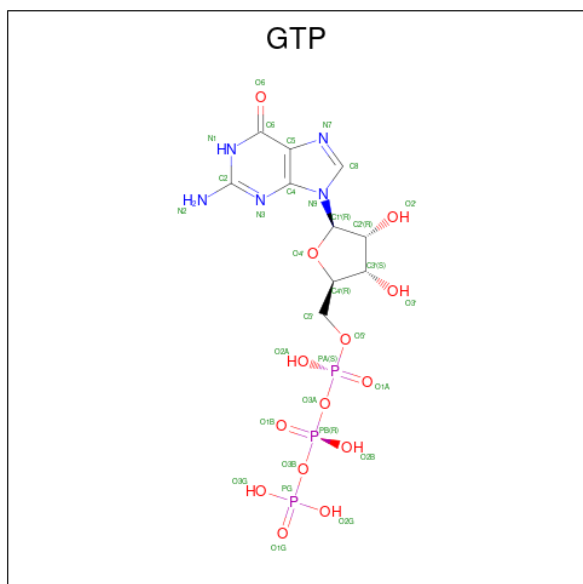
- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total 1	Mg 1	0

- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
21	A	2	Total 2	Zn 2	0
21	B	1	Total 1	Zn 1	0
21	C	1	Total 1	Zn 1	0
21	I	2	Total 2	Zn 2	0
21	L	1	Total 1	Zn 1	0
21	Y	1	Total 1	Zn 1	0

- Molecule 22 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).

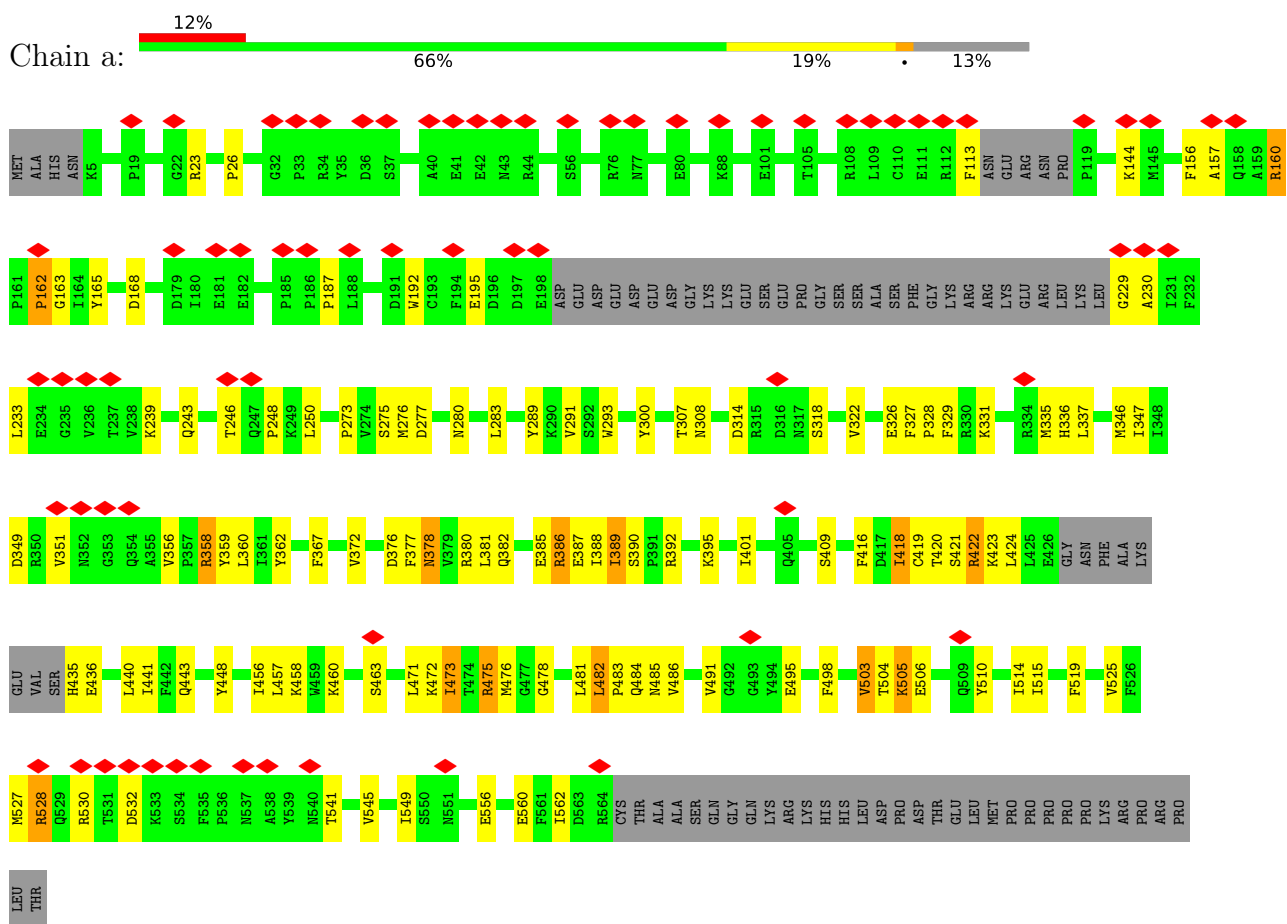


Mol	Chain	Residues	Atoms					AltConf
22	P	1	Total	C	N	O	P	0
			32	10	5	14	3	

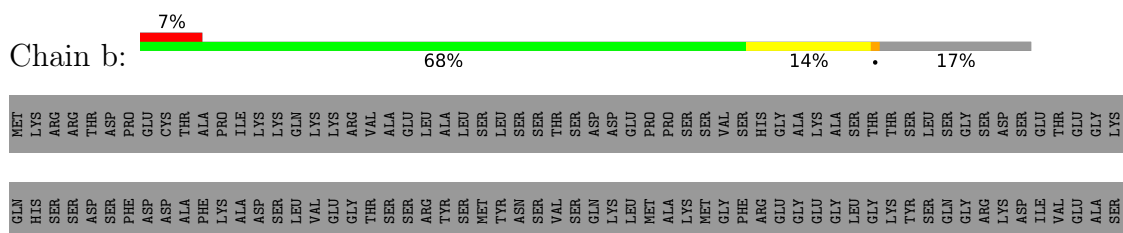
3 Residue-property plots

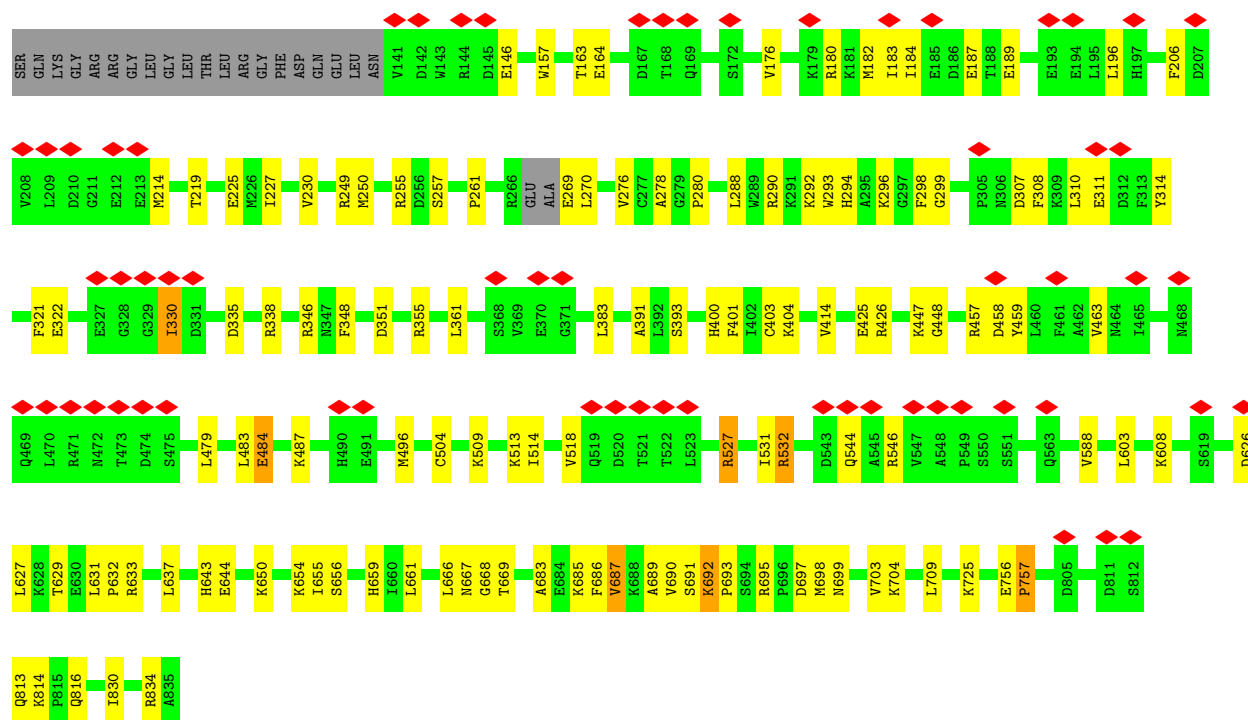
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: mRNA-capping enzyme



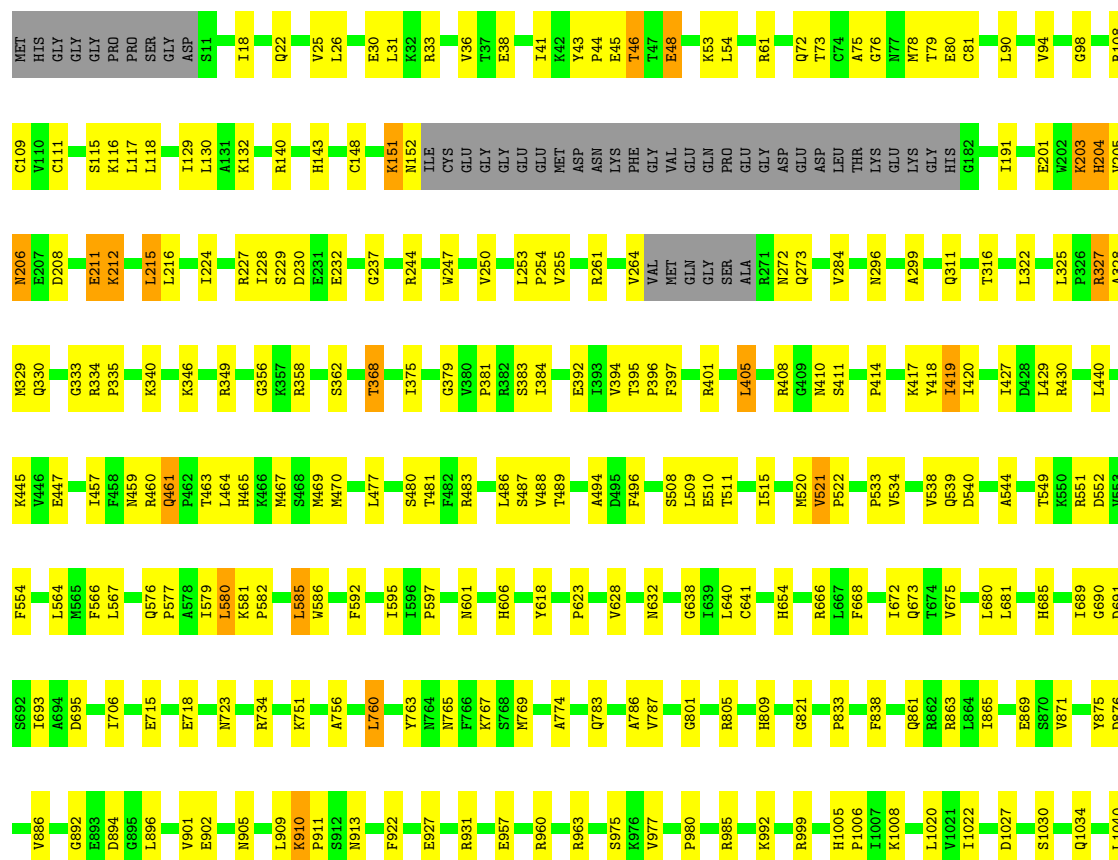
- Molecule 2: Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase 1

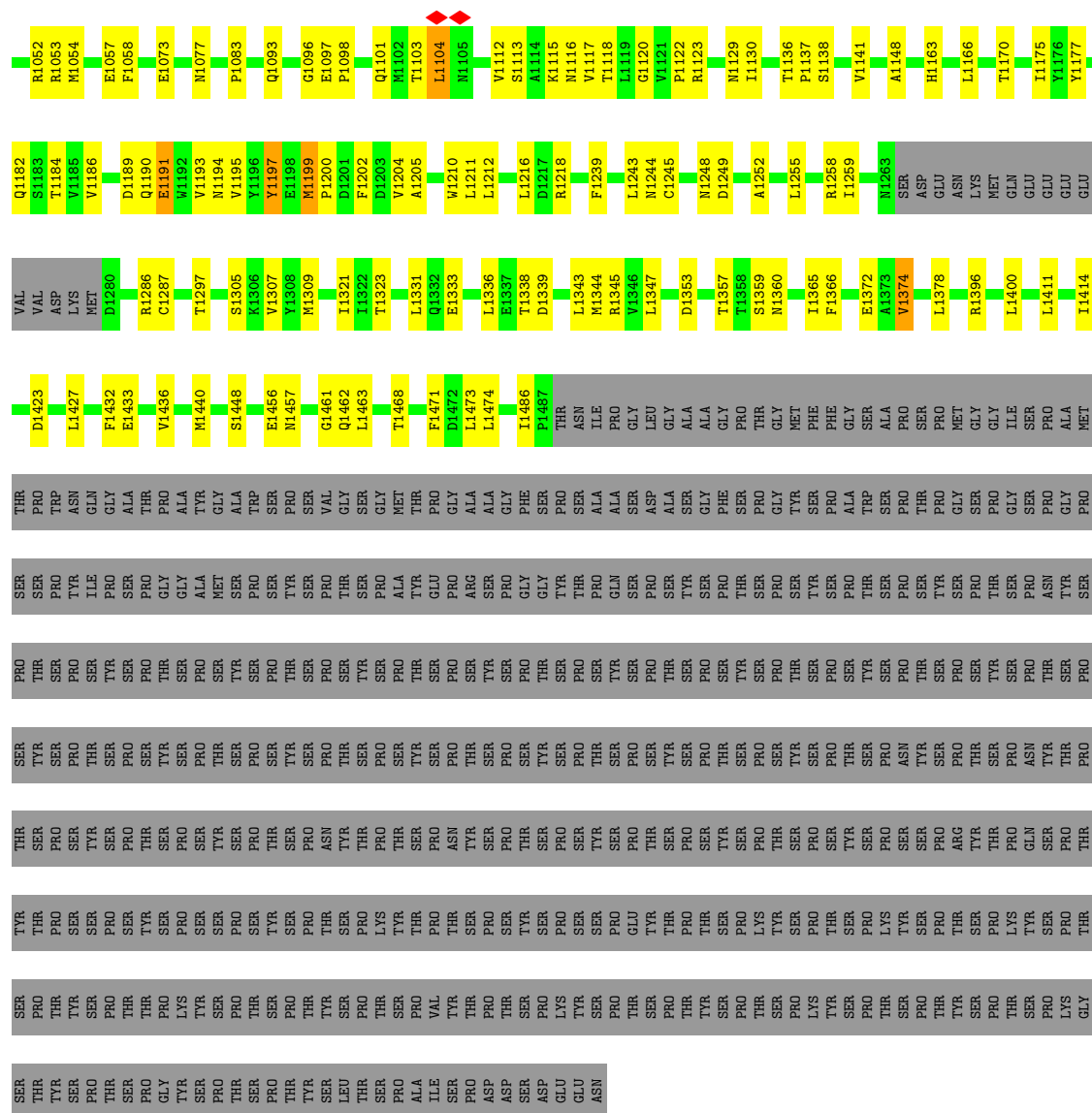




• Molecule 3: DNA-directed RNA polymerase subunit

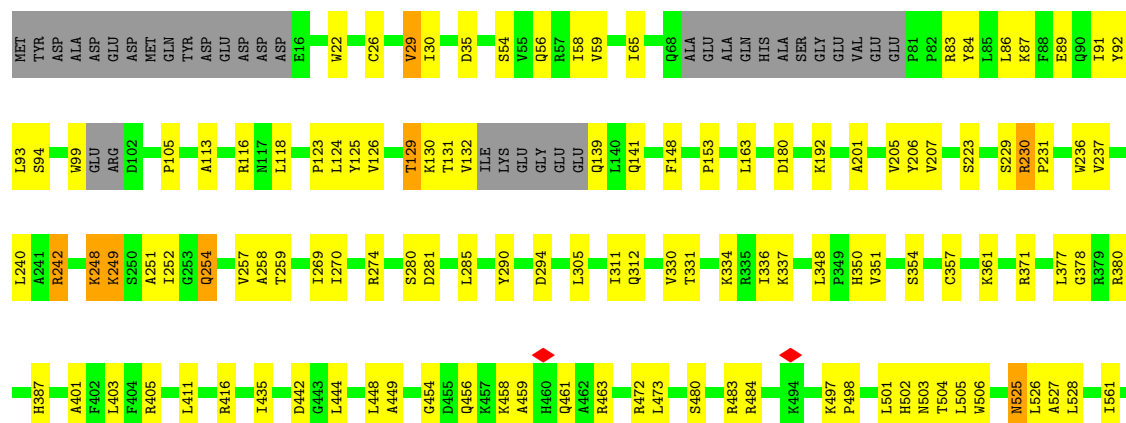
Chain A: 54% 17% 28%

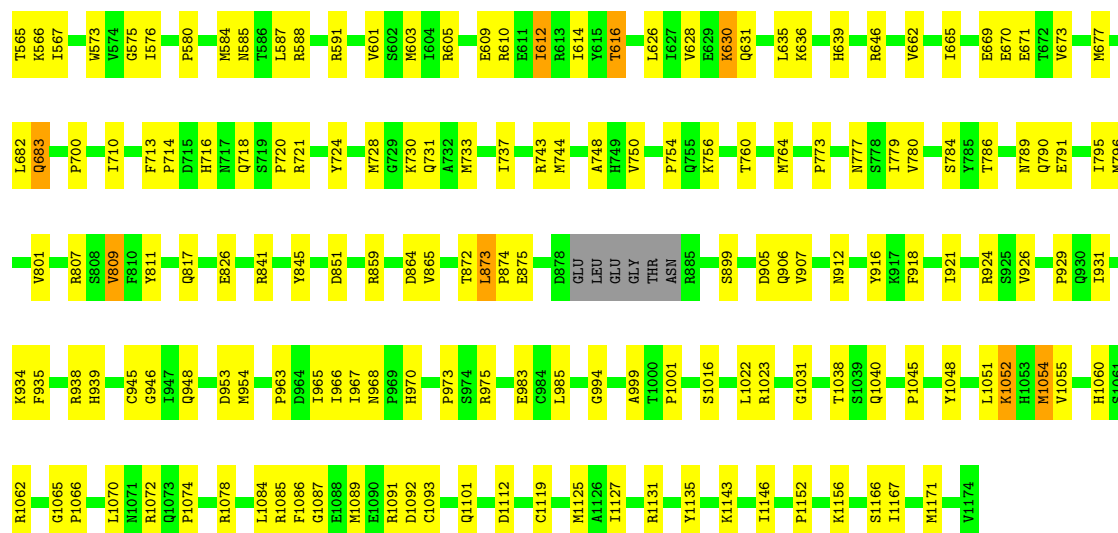




• Molecule 4: DNA-directed RNA polymerase subunit beta

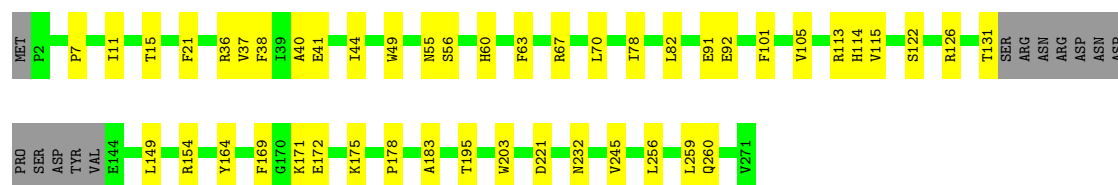
Chain B: 72% 23%





• Molecule 5: DNA-directed RNA polymerase II subunit RPB3

Chain C: 78% 17% 5%



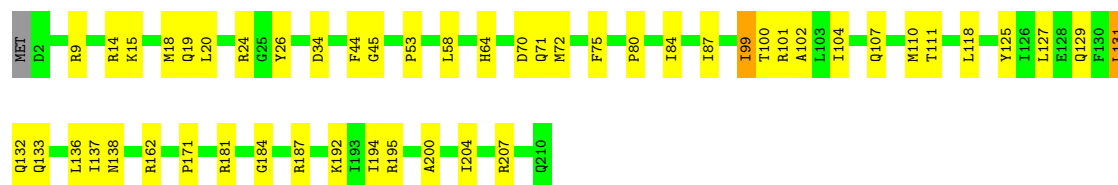
• Molecule 6: DNA-directed RNA polymerase II subunit RPB4

Chain D: 80% 11% 9%



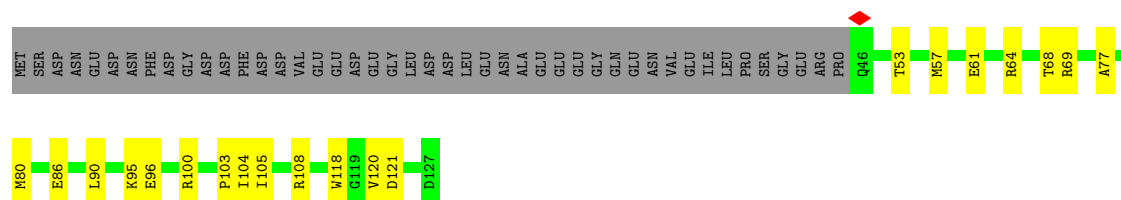
• Molecule 7: DNA-directed RNA polymerase II subunit E

Chain E: 76% 23%



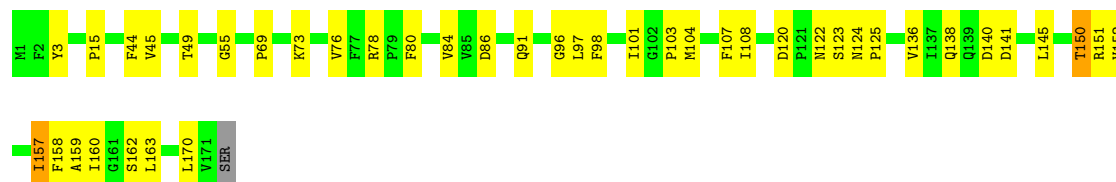
• Molecule 8: DNA-directed RNA polymerase II subunit F

Chain F: 49% 16% 35%



- Molecule 9: DNA-directed RNA polymerase II subunit RPB7

Chain G: 75% 23% ..



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 68% 29% ..



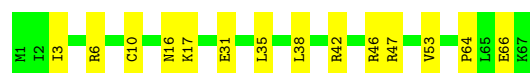
- Molecule 11: DNA-directed RNA polymerase II subunit RPB9

Chain I: 75% 18% 6%



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 79% 21%

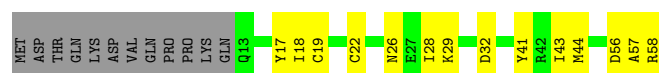


- Molecule 13: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 79% 18% ..



- Molecule 14: RPB12



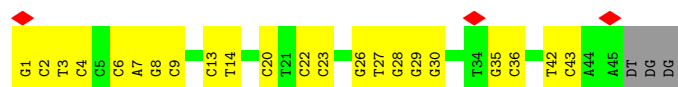
Chain N: 6% 29% 42% 29%



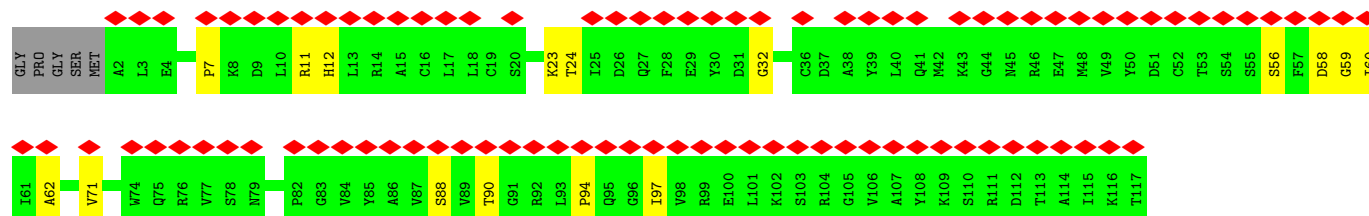
Chain P: 6% 6% 59% 29% 6%



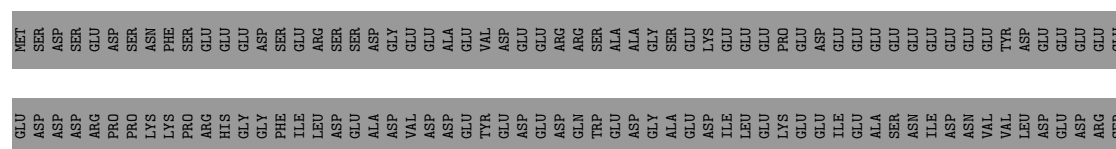
Chain T:



Chain Y: 76% 83% 13%



Chain Z: 13% 28% 6% 67%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.604	Depositor
Minimum map value	-1.299	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.26	Depositor
Map size (Å)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.14	0/4322	0.38	0/5831
2	b	0.17	0/5715	0.39	0/7708
3	A	0.09	0/11509	0.29	2/15542 (0.0%)
4	B	0.08	0/9226	0.28	0/12451
5	C	0.08	0/2115	0.27	0/2873
6	D	0.07	0/1012	0.21	0/1366
7	E	0.09	0/1752	0.27	0/2366
8	F	0.07	0/668	0.23	0/901
9	G	0.10	0/1336	0.29	0/1820
10	H	0.08	0/1207	0.25	0/1628
11	I	0.07	0/973	0.25	0/1316
12	J	0.08	0/542	0.27	0/730
13	K	0.09	0/939	0.25	0/1271
14	L	0.09	0/395	0.27	0/524
15	N	0.16	0/804	0.38	0/1240
16	P	0.10	0/389	0.30	0/605
17	T	0.20	0/1015	0.46	0/1562
18	Y	0.05	0/927	0.20	0/1250
19	Z	0.06	0/2928	0.23	0/3940
All	All	0.11	0/47774	0.31	2/64924 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1120	GLY	CA-C-N	5.02	123.40	120.24
3	A	1120	GLY	C-N-CA	5.02	123.40	120.24

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	4203	0	4182	62	0
2	b	5584	0	5509	98	0
3	A	11299	0	11416	244	0
4	B	9046	0	9078	196	0
5	C	2072	0	2016	37	0
6	D	998	0	953	12	0
7	E	1721	0	1737	34	0
8	F	658	0	684	14	0
9	G	1305	0	1267	33	0
10	H	1186	0	1147	34	0
11	I	950	0	880	17	0
12	J	533	0	557	10	0
13	K	920	0	942	16	0
14	L	389	0	395	11	0
15	N	714	0	379	23	0
16	P	347	0	175	11	0
17	T	910	0	507	20	0
18	Y	911	0	905	12	0
19	Z	2880	0	2925	40	0
20	A	1	0	0	0	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	C	1	0	0	0	0
21	I	2	0	0	0	0
21	L	1	0	0	0	0
21	Y	1	0	0	0	0
22	P	32	0	11	0	0
All	All	46667	0	45665	791	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 9.

All (791) 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)
3:A:1115:LYS:HE3	3:A:1339:ASP:HA	1.48	0.92
15:N:43:DG:N2	17:T:6:DC:N3	2.18	0.92
2:b:270:LEU:HA	2:b:685:LYS:HE3	1.51	0.91
1:a:157:ALA:HA	1:a:163:GLY:H	1.37	0.88
2:b:687:VAL:HA	2:b:690:VAL:HG22	1.58	0.83
2:b:725:LYS:NZ	9:G:136:VAL:O	2.11	0.83
2:b:692:LYS:HG3	2:b:695:ARG:HB2	1.63	0.81
15:N:43:DG:H1	17:T:6:DC:H42	1.25	0.81
2:b:294:HIS:HA	2:b:685:LYS:HE2	1.63	0.80
2:b:683:ALA:O	2:b:687:VAL:HB	1.81	0.80
5:C:37:VAL:HG13	5:C:41:GLU:HB2	1.65	0.78
2:b:348:PHE:HE1	2:b:693:PRO:HB2	1.51	0.75
3:A:327:ARG:NH2	3:A:329:MET:SD	2.60	0.74
3:A:1141:VAL:HB	3:A:1336:LEU:HB2	1.69	0.73
4:B:83:ARG:HH22	4:B:139:GLN:HB3	1.54	0.73
4:B:750:VAL:HG23	4:B:809:VAL:HG13	1.70	0.73
4:B:754:PRO:HB2	4:B:773:PRO:HG2	1.72	0.72
4:B:859:ARG:HH22	19:Z:740:CYS:HA	1.54	0.71
2:b:293:TRP:CZ3	2:b:669:THR:HB	2.25	0.71
3:A:411:SER:OG	19:Z:733:ARG:NH1	2.23	0.71
3:A:486:LEU:HB3	3:A:538:VAL:HG21	1.73	0.71
2:b:288:LEU:HD11	2:b:321:PHE:HB2	1.72	0.70
19:Z:450:ILE:HG23	19:Z:452:PRO:HD3	1.73	0.69
3:A:894:ASP:HB3	7:E:200:ALA:HB2	1.75	0.69
1:a:478:GLY:HA3	1:a:484:GLN:HB3	1.75	0.69
2:b:322:GLU:HG3	2:b:692:LYS:HE3	1.74	0.69
2:b:644:GLU:HB2	2:b:655:ILE:HG22	1.73	0.69
6:D:60:VAL:HG13	9:G:103:PRO:HG3	1.75	0.69
19:Z:444:ASP:HB3	19:Z:448:ILE:HA	1.73	0.69
2:b:293:TRP:HB2	2:b:686:PHE:CD1	2.27	0.69
4:B:748:ALA:HB3	4:B:811:TYR:HB2	1.74	0.68
3:A:94:VAL:HG13	3:A:311:GLN:HG2	1.75	0.68
15:N:29:DG:H2"	15:N:30:DC:C5	2.28	0.68
3:A:132:LYS:HG2	7:E:187:ARG:HH12	1.59	0.68
3:A:206:ASN:HB3	3:A:211:GLU:HB3	1.74	0.68
4:B:1085:ARG:NH1	17:T:26:DG:OP1	2.26	0.68
4:B:459:ALA:HB3	4:B:461:GLN:HE22	1.57	0.68
3:A:1287:CYS:SG	4:B:249:LYS:NZ	2.68	0.67
3:A:1468:THR:HG23	8:F:64:ARG:HB2	1.75	0.67
3:A:420:ILE:HB	3:A:445:LYS:HB2	1.77	0.67
4:B:274:ARG:NH2	4:B:281:ASP:OD1	2.28	0.67
3:A:481:THR:OG1	3:A:483:ARG:NH1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:355:ASP:HB3	19:Z:358:PHE:HB3	1.76	0.67
2:b:588:VAL:HA	2:b:709:LEU:HD23	1.76	0.67
7:E:20:LEU:HD21	7:E:24:ARG:HH21	1.61	0.66
19:Z:199:LYS:NZ	19:Z:240:GLU:O	2.27	0.66
4:B:65:ILE:HD11	4:B:86:LEU:HD12	1.78	0.66
4:B:473:LEU:HD21	4:B:1052:LYS:HD2	1.77	0.66
10:H:14:ASP:HB2	10:H:29:HIS:HB2	1.77	0.65
2:b:346:ARG:HD2	2:b:393:SER:HB3	1.77	0.65
15:N:42:DT:H2''	15:N:43:DG:C8	2.31	0.65
3:A:334:ARG:HH11	3:A:335:PRO:HD2	1.60	0.65
3:A:375:ILE:HG12	3:A:666:ARG:HG3	1.79	0.65
4:B:760:THR:OG1	4:B:764:MET:SD	2.55	0.65
3:A:111:CYS:HB3	3:A:116:LYS:H	1.62	0.64
8:F:100:ARG:NH2	8:F:121:ASP:O	2.30	0.64
3:A:419:ILE:HG23	3:A:427:ILE:HB	1.80	0.64
11:I:80:ARG:HG3	11:I:95:VAL:HG12	1.80	0.64
4:B:864:ASP:OD1	19:Z:725:LYS:NZ	2.31	0.63
2:b:293:TRP:CD1	2:b:686:PHE:HB2	2.32	0.63
4:B:780:VAL:HG12	4:B:965:ILE:HB	1.80	0.63
5:C:78:ILE:HD11	5:C:126:ARG:HD2	1.81	0.63
2:b:296:LYS:HD3	2:b:689:ALA:HA	1.80	0.63
3:A:467:MET:HG2	3:A:534:VAL:HG21	1.81	0.63
3:A:1239:PHE:HB3	3:A:1243:LEU:HD23	1.81	0.63
3:A:48:GLU:HG2	3:A:53:LYS:HD3	1.81	0.63
4:B:501:LEU:HD12	4:B:505:LEU:HD13	1.78	0.63
4:B:636:LYS:H	4:B:639:HIS:HD2	1.47	0.63
3:A:78:MET:O	4:B:1072:ARG:NH2	2.32	0.63
1:a:230:ALA:HA	1:a:243:GLN:HE22	1.63	0.62
4:B:873:LEU:HD22	4:B:874:PRO:HD2	1.80	0.62
2:b:348:PHE:CE1	2:b:693:PRO:HB2	2.33	0.62
3:A:886:VAL:HG23	7:E:171:PRO:HD3	1.81	0.62
3:A:520:MET:HB3	3:A:522:PRO:HD2	1.80	0.62
3:A:869:GLU:OE1	4:B:1091:ARG:NH1	2.27	0.62
15:N:27:DG:H2'	15:N:28:DA:C5	2.34	0.62
2:b:666:LEU:HD22	2:b:686:PHE:HD2	1.64	0.62
3:A:1093:GLN:HE22	4:B:1093:CYS:HA	1.63	0.62
3:A:1005:HIS:HD2	3:A:1006:PRO:HD2	1.64	0.62
3:A:1163:HIS:HE1	3:A:1297:THR:HG22	1.65	0.62
4:B:677:MET:HE2	4:B:700:PRO:HB3	1.82	0.62
15:N:27:DG:H2'	15:N:28:DA:C4	2.35	0.62
4:B:483:ARG:HH12	4:B:528:LEU:HA	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:873:LEU:HD13	4:B:875:GLU:H	1.64	0.62
7:E:129:GLN:O	7:E:181:ARG:NH2	2.32	0.62
11:I:68:ILE:O	11:I:122:ARG:NH1	2.33	0.62
5:C:7:PRO:O	13:K:104:ARG:NH1	2.33	0.61
1:a:420:THR:HG23	1:a:423:LYS:HD2	1.82	0.61
8:F:53:THR:OG1	8:F:118:TRP:NE1	2.33	0.61
3:A:922:PHE:HA	3:A:1052:ARG:HD3	1.81	0.61
17:T:27:DT:H2'	17:T:28:DG:C8	2.34	0.61
3:A:228:ILE:O	3:A:244:ARG:NH2	2.33	0.61
3:A:477:LEU:HB2	3:A:483:ARG:HH21	1.65	0.60
5:C:175:LYS:HZ2	14:L:57:ALA:HB3	1.66	0.60
4:B:223:SER:OG	4:B:350:HIS:ND1	2.27	0.60
4:B:851:ASP:OD2	14:L:17:TYR:OH	2.19	0.60
9:G:45:VAL:HA	9:G:76:VAL:HG12	1.83	0.60
19:Z:427:GLU:OE2	19:Z:469:ARG:NH2	2.34	0.60
3:A:539:GLN:HA	3:A:774:ALA:HB1	1.83	0.60
3:A:801:GLY:HA3	4:B:503:ASN:HB2	1.83	0.60
6:D:67:TYR:OH	9:G:86:ASP:O	2.19	0.60
4:B:718:GLN:HG2	4:B:720:PRO:HD2	1.82	0.60
3:A:623:PRO:HA	10:H:27:ARG:HH21	1.67	0.60
2:b:176:VAL:HB	2:b:479:LEU:HB2	1.83	0.60
15:N:42:DT:H3	17:T:7:DA:H61	1.50	0.59
19:Z:367:SER:HB2	19:Z:372:LEU:HD23	1.82	0.59
1:a:229:GLY:N	1:a:318:SER:HG	2.00	0.59
3:A:383:SER:H	13:K:2:ASN:HD21	1.49	0.59
5:C:260:GLN:HB2	13:K:91:ILE:HG21	1.84	0.59
1:a:335:MET:HE3	1:a:336:HIS:H	1.66	0.59
7:E:14:ARG:HE	7:E:18:MET:HE2	1.66	0.59
3:A:115:SER:HB3	3:A:227:ARG:HD3	1.84	0.59
2:b:294:HIS:CA	2:b:685:LYS:HE2	2.29	0.59
3:A:581:LYS:HB2	10:H:91:VAL:HG23	1.84	0.59
3:A:680:LEU:HD21	4:B:784:SER:HB3	1.85	0.59
3:A:977:VAL:HG21	3:A:1040:LEU:HD21	1.85	0.59
4:B:334:LYS:HZ3	4:B:337:LYS:HD2	1.68	0.59
18:Y:7:PRO:HG3	18:Y:23:LYS:HA	1.84	0.59
2:b:695:ARG:NE	2:b:697:ASP:OD1	2.33	0.58
3:A:628:VAL:HA	3:A:638:GLY:HA3	1.85	0.58
19:Z:440:ILE:HG23	19:Z:450:ILE:HD11	1.84	0.58
3:A:539:GLN:NE2	4:B:790:GLN:O	2.35	0.58
3:A:905:ASN:ND2	3:A:975:SER:OG	2.36	0.58
4:B:796:MET:HB2	4:B:948:GLN:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:458:LYS:NZ	4:B:459:ALA:O	2.29	0.58
4:B:1119:CYS:HA	4:B:1146:ILE:HA	1.84	0.58
2:b:632:PRO:HD2	2:b:686:PHE:HZ	1.67	0.58
4:B:192:LYS:HE3	4:B:449:ALA:HA	1.85	0.58
2:b:269:GLU:O	2:b:685:LYS:NZ	2.28	0.58
6:D:135:GLN:HE22	6:D:138:ARG:HH11	1.48	0.58
19:Z:364:ASN:O	19:Z:374:LYS:NZ	2.34	0.58
3:A:44:PRO:HB3	3:A:284:VAL:HG23	1.86	0.58
3:A:894:ASP:OD2	3:A:1396:ARG:NH2	2.37	0.58
8:F:53:THR:HG1	8:F:118:TRP:HE1	1.50	0.58
4:B:1062:ARG:NH2	4:B:1066:PRO:O	2.30	0.58
4:B:86:LEU:HD23	4:B:130:LYS:HB3	1.84	0.58
11:I:97:PHE:HB2	11:I:100:HIS:HE2	1.69	0.58
4:B:483:ARG:NH2	4:B:527:ALA:O	2.37	0.58
3:A:395:THR:HG23	3:A:397:PHE:H	1.68	0.57
2:b:655:ILE:HA	9:G:125:PRO:HD3	1.86	0.57
4:B:380:ARG:HH21	4:B:609:GLU:HG2	1.69	0.57
7:E:192:LYS:HE2	7:E:194:ILE:HD11	1.86	0.57
3:A:508:SER:HB3	3:A:511:THR:HG22	1.87	0.57
4:B:677:MET:H	4:B:682:LEU:HD12	1.69	0.57
4:B:817:GLN:HB3	4:B:918:PHE:HD1	1.69	0.57
7:E:80:PRO:HA	7:E:107:GLN:HB2	1.87	0.57
18:Y:94:PRO:HD2	18:Y:97:ILE:HD12	1.86	0.57
2:b:351:ASP:OD1	2:b:355:ARG:NH1	2.37	0.57
1:a:327:PHE:CD1	1:a:392:ARG:HD2	2.39	0.57
2:b:666:LEU:HD22	2:b:686:PHE:CD2	2.39	0.57
2:b:686:PHE:O	2:b:690:VAL:N	2.36	0.57
7:E:9:ARG:HG3	7:E:136:LEU:HD21	1.86	0.57
1:a:23:ARG:NH2	1:a:113:PHE:O	2.33	0.57
1:a:372:VAL:HG12	1:a:380:ARG:HG2	1.85	0.57
4:B:387:HIS:NE2	4:B:671:GLU:OE2	2.37	0.57
4:B:790:GLN:O	4:B:968:ASN:ND2	2.37	0.57
11:I:119:CYS:SG	11:I:120:GLY:N	2.77	0.57
1:a:358:ARG:HG3	1:a:409:SER:HB3	1.87	0.57
1:a:514:ILE:HG22	1:a:530:ARG:HB3	1.87	0.57
9:G:108:ILE:HD11	9:G:145:LEU:HD22	1.86	0.57
15:N:36:DG:H2"	15:N:37:DG:C8	2.40	0.57
2:b:293:TRP:HZ3	2:b:669:THR:HB	1.70	0.57
3:A:1212:LEU:HB3	3:A:1259:ILE:HB	1.88	0.56
4:B:1135:TYR:HB3	4:B:1146:ILE:HD13	1.86	0.56
15:N:39:DA:H2"	15:N:40:DG:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:3:DT:H2''	17:T:4:DC:C5	2.40	0.56
3:A:521:VAL:HG22	3:A:522:PRO:HD3	1.86	0.56
4:B:721:ARG:HD2	4:B:975:ARG:HB3	1.88	0.56
17:T:42:DT:H4'	17:T:43:DC:H5'	1.87	0.56
3:A:480:SER:HB3	13:K:2:ASN:HB2	1.85	0.56
15:N:45:DG:H2''	15:N:46:DA:C8	2.40	0.56
4:B:585:ASN:OD1	4:B:588:ARG:NH2	2.39	0.56
3:A:98:GLY:HA3	3:A:1440:MET:HE2	1.88	0.56
3:A:833:PRO:HB2	4:B:506:TRP:HH2	1.71	0.56
4:B:153:PRO:HG2	4:B:448:LEU:HD12	1.88	0.56
3:A:1309:MET:HB3	3:A:1336:LEU:HD23	1.87	0.56
4:B:403:LEU:HD23	4:B:444:LEU:HD13	1.86	0.56
4:B:1038:THR:HA	5:C:195:THR:HA	1.88	0.56
3:A:322:LEU:HG	3:A:325:LEU:HD12	1.87	0.56
9:G:150:THR:HA	9:G:159:ALA:HA	1.87	0.56
19:Z:352:VAL:HG23	19:Z:359:LEU:HD21	1.88	0.56
3:A:394:VAL:HG21	3:A:440:LEU:HD22	1.88	0.56
18:Y:7:PRO:HB3	18:Y:24:THR:HG23	1.88	0.56
1:a:377:PHE:HD1	1:a:380:ARG:HH21	1.54	0.55
4:B:94:SER:HB3	4:B:123:PRO:HG2	1.88	0.55
6:D:114:LEU:HD22	9:G:84:VAL:HG11	1.87	0.55
7:E:44:PHE:HB3	7:E:53:PRO:HB3	1.88	0.55
2:b:756:GLU:HB3	2:b:757:PRO:HD2	1.89	0.55
6:D:17:ALA:HB2	9:G:80:PHE:HB3	1.88	0.55
3:A:552:ASP:HB2	10:H:24:ARG:HB2	1.88	0.55
19:Z:184:CYS:SG	19:Z:185:LYS:N	2.80	0.55
1:a:329:PHE:HD1	1:a:331:LYS:H	1.54	0.55
2:b:270:LEU:HD13	2:b:685:LYS:HG3	1.89	0.55
19:Z:479:LYS:HD3	19:Z:521:CYS:HB2	1.88	0.55
7:E:24:ARG:HH12	7:E:184:GLY:HA3	1.70	0.55
3:A:461:GLN:HG2	17:T:26:DG:H1'	1.88	0.55
4:B:779:ILE:HD13	4:B:1045:PRO:HB3	1.89	0.55
1:a:26:PRO:HB2	1:a:160:ARG:HD3	1.88	0.55
4:B:59:VAL:HG21	4:B:91:ILE:HD12	1.87	0.55
13:K:56:VAL:HG22	13:K:77:THR:HG22	1.89	0.55
2:b:250:MET:HE3	2:b:447:LYS:HB3	1.89	0.55
3:A:805:ARG:NH2	4:B:670:GLU:O	2.40	0.55
3:A:496:PHE:HD2	4:B:791:GLU:HB3	1.72	0.54
5:C:183:ALA:HB3	5:C:232:ASN:HB3	1.87	0.54
2:b:314:TYR:HA	2:b:546:ARG:HE	1.72	0.54
3:A:76:GLY:HA3	3:A:81:CYS:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:913:ASN:OD1	3:A:963:ARG:NH1	2.40	0.54
4:B:205:VAL:O	4:B:371:ARG:NH1	2.41	0.54
4:B:480:SER:OG	4:B:525:ASN:OD1	2.18	0.54
4:B:737:ILE:HG21	4:B:743:ARG:HD3	1.90	0.54
4:B:1031:GLY:O	5:C:36:ARG:NH1	2.40	0.54
3:A:1115:LYS:NZ	3:A:1138:SER:OG	2.29	0.54
3:A:1175:ILE:HG12	11:I:54:TYR:HB3	1.89	0.54
4:B:378:GLY:HA3	11:I:102:ALA:HB3	1.88	0.54
10:H:7:GLU:HG3	10:H:59:VAL:HG22	1.89	0.54
3:A:296:ASN:HB2	19:Z:267:VAL:HG21	1.89	0.54
4:B:229:SER:HA	4:B:405:ARG:HD3	1.88	0.54
4:B:610:ARG:NH1	11:I:71:ASP:OD2	2.40	0.54
3:A:1427:LEU:HB2	3:A:1456:GLU:HG3	1.90	0.54
3:A:1372:GLU:OE2	7:E:195:ARG:NH1	2.41	0.54
4:B:56:GLN:NE2	4:B:89:GLU:O	2.37	0.54
1:a:230:ALA:HA	1:a:243:GLN:NE2	2.23	0.54
2:b:527:ARG:HD3	2:b:531:ILE:HD11	1.90	0.54
3:A:457:ILE:HD11	3:A:515:ILE:HD12	1.90	0.54
2:b:335:ASP:HB3	2:b:338:ARG:HG3	1.90	0.54
3:A:734:ARG:NE	11:I:105:GLU:O	2.28	0.54
3:A:909:LEU:HG	3:A:910:LYS:HD3	1.89	0.54
3:A:1194:ASN:HA	3:A:1197:TYR:HB2	1.89	0.54
4:B:665:ILE:HG23	4:B:669:GLU:HB3	1.89	0.54
4:B:939:HIS:NE2	4:B:983:GLU:OE1	2.37	0.54
3:A:1286:ARG:HD2	4:B:252:ILE:HD13	1.90	0.53
8:F:77:ALA:HB2	9:G:15:PRO:HB3	1.89	0.53
16:P:37:G:H3'	16:P:38:G:H8	1.73	0.53
3:A:723:ASN:OD1	11:I:109:ARG:NE	2.41	0.53
5:C:49:TRP:HB3	5:C:164:TYR:HB2	1.90	0.53
16:P:43:C:N4	17:T:29:DG:O6	2.41	0.53
1:a:424:LEU:HD13	1:a:440:LEU:HD21	1.90	0.53
4:B:497:LYS:HG3	4:B:498:PRO:HD3	1.89	0.53
1:a:291:VAL:HG11	1:a:421:SER:HB3	1.91	0.53
2:b:687:VAL:HG11	2:b:703:VAL:HG23	1.90	0.53
2:b:293:TRP:CH2	2:b:669:THR:HB	2.44	0.53
2:b:687:VAL:HA	2:b:690:VAL:CG2	2.33	0.53
4:B:1016:SER:HB2	4:B:1022:LEU:HD23	1.90	0.53
1:a:276:MET:HA	1:a:280:ASN:HD22	1.74	0.53
2:b:830:ILE:HG22	2:b:834:ARG:HE	1.73	0.53
3:A:896:LEU:HB2	3:A:1396:ARG:HH21	1.72	0.53
4:B:1143:LYS:NZ	19:Z:522:SER:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:280:ARG:HB3	19:Z:288:ASP:HA	1.89	0.53
2:b:314:TYR:CE1	2:b:546:ARG:HA	2.44	0.53
2:b:457:ARG:NH2	2:b:458:ASP:OD1	2.41	0.53
3:A:30:GLU:HA	3:A:33:ARG:HG2	1.90	0.52
1:a:156:PHE:CD2	1:a:163:GLY:HA3	2.44	0.52
3:A:340:LYS:HG2	3:A:1436:VAL:HG21	1.92	0.52
19:Z:479:LYS:HG3	19:Z:489:THR:HG22	1.90	0.52
2:b:293:TRP:CD2	2:b:666:LEU:HB2	2.44	0.52
3:A:760:LEU:HG	3:A:767:LYS:HB2	1.90	0.52
7:E:107:GLN:HA	7:E:132:GLN:HG3	1.90	0.52
13:K:7:PHE:HB2	13:K:11:LEU:HD12	1.92	0.52
2:b:692:LYS:HG2	2:b:698:MET:HB2	1.90	0.52
3:A:61:ARG:HA	3:A:72:GLN:HB3	1.91	0.52
19:Z:450:ILE:HG21	19:Z:468:LEU:HD11	1.91	0.52
3:A:957:GLU:OE2	3:A:960:ARG:NH2	2.42	0.52
4:B:954:MET:HG3	4:B:963:PRO:HD2	1.92	0.52
1:a:327:PHE:HB3	1:a:337:LEU:HD12	1.92	0.52
3:A:690:GLY:HA2	4:B:1023:ARG:HG2	1.90	0.52
3:A:1193:VAL:O	3:A:1197:TYR:N	2.42	0.52
3:A:1461:GLY:HA3	4:B:1152:PRO:HD3	1.91	0.52
4:B:826:GLU:H	4:B:872:THR:HG22	1.75	0.52
4:B:934:LYS:HG2	4:B:1051:LEU:HD12	1.92	0.52
10:H:32:SER:OG	10:H:36:LYS:N	2.43	0.52
2:b:633:ARG:O	2:b:667:ASN:HA	2.09	0.52
3:A:549:THR:HG21	3:A:640:LEU:H	1.75	0.52
13:K:63:VAL:HG12	13:K:71:ILE:HG22	1.92	0.52
3:A:1118:THR:HG22	3:A:1136:THR:HB	1.91	0.52
12:J:10:CYS:SG	12:J:42:ARG:NE	2.82	0.52
2:b:627:LEU:HD22	2:b:699:ASN:ND2	2.25	0.52
15:N:40:DG:H2"	15:N:41:DC:C5	2.45	0.52
1:a:471:LEU:HD22	1:a:515:ILE:HD13	1.92	0.51
3:A:1138:SER:H	3:A:1360:ASN:HB3	1.75	0.51
3:A:1170:THR:HA	3:A:1216:LEU:HD13	1.91	0.51
5:C:44:ILE:HG21	5:C:178:PRO:HB3	1.92	0.51
5:C:70:LEU:HD12	12:J:6:ARG:HD2	1.92	0.51
7:E:26:TYR:HD1	7:E:64:HIS:HA	1.75	0.51
10:H:60:ILE:HG21	10:H:135:PHE:HE1	1.74	0.51
2:b:401:PHE:CZ	2:b:403:CYS:HB2	2.46	0.51
3:A:76:GLY:HA2	3:A:80:GLU:HG3	1.92	0.51
3:A:1473:LEU:HD23	8:F:104:ILE:HG21	1.91	0.51
4:B:236:TRP:HB2	4:B:259:THR:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:277:ASP:H	1:a:280:ASN:HB2	1.75	0.51
2:b:627:LEU:HD22	2:b:699:ASN:HD21	1.76	0.51
4:B:354:SER:OG	4:B:357:CYS:SG	2.57	0.51
6:D:31:THR:HG22	9:G:3:TYR:HE1	1.75	0.51
2:b:725:LYS:NZ	9:G:170:LEU:HD22	2.24	0.51
13:K:5:PRO:HG2	13:K:8:GLU:HG2	1.92	0.51
1:a:349:ASP:OD2	1:a:358:ARG:NH1	2.44	0.51
4:B:26:CYS:O	4:B:29:VAL:HG12	2.10	0.51
4:B:1125:MET:HE1	4:B:1156:LYS:HG2	1.93	0.51
7:E:131:LEU:HD23	7:E:133:GLN:H	1.75	0.51
19:Z:292:GLN:HB3	19:Z:306:LYS:HB3	1.92	0.51
4:B:601:VAL:HG22	4:B:616:THR:HG23	1.93	0.51
5:C:105:VAL:HG11	5:C:115:VAL:HG22	1.92	0.51
3:A:465:HIS:CD2	3:A:467:MET:HB2	2.46	0.51
3:A:459:ASN:HB3	3:A:469:MET:HG3	1.93	0.51
3:A:691:ASP:OD2	3:A:765:ASN:ND2	2.44	0.51
4:B:626:LEU:HD23	4:B:662:VAL:HG12	1.93	0.51
8:F:86:GLU:OE2	8:F:95:LYS:NZ	2.43	0.51
10:H:49:PRO:O	10:H:147:LYS:NZ	2.44	0.51
3:A:592:PHE:HA	3:A:595:ILE:HD12	1.93	0.50
4:B:1062:ARG:HE	4:B:1065:GLY:H	1.59	0.50
3:A:1005:HIS:CD2	3:A:1006:PRO:HD2	2.44	0.50
10:H:96:VAL:HA	10:H:116:VAL:HA	1.94	0.50
3:A:756:ALA:HB2	3:A:786:ALA:HB2	1.93	0.50
5:C:38:PHE:HE1	5:C:245:VAL:HA	1.77	0.50
17:T:13:DC:H2'	17:T:14:DT:C6	2.46	0.50
19:Z:506:LEU:HD21	19:Z:527:GLY:HA2	1.94	0.50
3:A:892:GLY:HA3	3:A:1396:ARG:HG3	1.94	0.50
11:I:11:PHE:HA	11:I:55:VAL:HG11	1.94	0.50
16:P:42:C:H2'	16:P:43:C:C6	2.46	0.50
1:a:289:TYR:HB3	1:a:418:ILE:HD11	1.93	0.50
3:A:1305:SER:OG	3:A:1339:ASP:HB3	2.11	0.50
4:B:237:VAL:HG13	4:B:269:ILE:HD11	1.92	0.50
18:Y:60:ILE:HD13	19:Z:190:ARG:HG3	1.93	0.50
1:a:346:MET:SD	1:a:359:TYR:HB2	2.52	0.50
3:A:875:TYR:HA	3:A:1083:PRO:HB3	1.94	0.50
3:A:901:VAL:HA	3:A:980:PRO:HA	1.93	0.50
4:B:561:ILE:HD11	4:B:566:LYS:HG2	1.93	0.50
18:Y:59:GLY:H	19:Z:219:GLU:HB2	1.76	0.50
19:Z:472:PHE:HE1	19:Z:520:LEU:HB2	1.76	0.50
2:b:666:LEU:O	2:b:668:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:180:ARG:HD3	2:b:182:MET:HE2	1.94	0.49
2:b:414:VAL:HG22	2:b:496:MET:HE2	1.94	0.49
4:B:454:GLY:HA3	4:B:458:LYS:HD3	1.93	0.49
1:a:380:ARG:HH12	1:a:448:TYR:N	2.11	0.49
2:b:643:HIS:CG	2:b:654:LYS:HE3	2.47	0.49
5:C:60:HIS:CE1	5:C:63:PHE:HB2	2.48	0.49
19:Z:306:LYS:HA	19:Z:372:LEU:O	2.12	0.49
1:a:545:VAL:O	1:a:549:ILE:HG23	2.12	0.49
3:A:129:ILE:HD13	3:A:143:HIS:HB3	1.94	0.49
3:A:863:ARG:HH12	3:A:1129:ASN:ND2	2.10	0.49
1:a:328:PRO:HD2	1:a:392:ARG:HG2	1.94	0.49
3:A:554:PHE:HB3	3:A:585:LEU:HG	1.93	0.49
3:A:327:ARG:HH21	3:A:329:MET:HB3	1.78	0.49
4:B:116:ARG:NH1	4:B:118:LEU:HD11	2.28	0.49
8:F:80:MET:HG3	8:F:103:PRO:HD3	1.93	0.49
1:a:556:GLU:O	1:a:560:GLU:HG3	2.13	0.49
3:A:999:ARG:NH1	10:H:103:GLU:OE1	2.46	0.49
3:A:1115:LYS:HZ3	3:A:1136:THR:HG22	1.78	0.49
4:B:525:ASN:HD22	4:B:526:LEU:N	2.10	0.49
17:T:2:DC:H2''	17:T:3:DT:C6	2.48	0.49
3:A:510:GLU:OE2	4:B:1101:GLN:NE2	2.46	0.48
15:N:30:DC:H2''	15:N:31:DC:H5'	1.95	0.48
2:b:293:TRP:HB2	2:b:686:PHE:CG	2.48	0.48
2:b:654:LYS:HB3	9:G:138:GLN:OE1	2.13	0.48
2:b:656:SER:H	9:G:124:ASN:CB	2.26	0.48
3:A:1321:ILE:HG12	3:A:1331:LEU:HD13	1.95	0.48
3:A:1423:ASP:OD1	3:A:1423:ASP:N	2.46	0.48
3:A:90:LEU:HD23	3:A:90:LEU:H	1.78	0.48
4:B:242:ARG:HD2	4:B:242:ARG:HA	1.60	0.48
4:B:330:VAL:HG12	4:B:331:THR:HG23	1.96	0.48
5:C:91:GLU:O	5:C:92:GLU:HG3	2.13	0.48
10:H:39:LEU:HD12	10:H:125:LEU:HD13	1.95	0.48
12:J:35:LEU:HD13	12:J:46:ARG:HB3	1.95	0.48
16:P:38:G:H2'	16:P:39:A:C8	2.48	0.48
2:b:146:GLU:OE2	2:b:513:LYS:NZ	2.36	0.48
3:A:392:GLU:OE2	3:A:401:ARG:NH2	2.41	0.48
3:A:606:HIS:CE1	3:A:641:CYS:HB3	2.48	0.48
7:E:110:MET:HE1	7:E:118:LEU:HD11	1.94	0.48
18:Y:23:LYS:NZ	18:Y:32:GLY:O	2.40	0.48
4:B:99:TRP:HE1	4:B:105:PRO:HG3	1.78	0.48
18:Y:71:VAL:HG13	19:Z:264:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:92:TYR:HB2	4:B:125:TYR:HB2	1.95	0.48
10:H:100:GLU:HG2	10:H:115:TYR:HE1	1.78	0.48
1:a:476:MET:H	1:a:485:ASN:HA	1.77	0.48
3:A:1211:LEU:HD22	3:A:1258:ARG:HH21	1.78	0.48
4:B:826:GLU:N	4:B:872:THR:HG22	2.29	0.48
7:E:24:ARG:NH1	7:E:184:GLY:HA3	2.29	0.48
2:b:697:ASP:HB2	9:G:122:ASN:CG	2.38	0.48
3:A:540:ASP:HB3	4:B:790:GLN:HE22	1.79	0.48
3:A:1097:GLU:O	3:A:1101:GLN:NE2	2.47	0.48
3:A:1343:LEU:C	3:A:1345:ARG:H	2.22	0.48
4:B:899:SER:OG	4:B:1078:ARG:NH2	2.47	0.48
6:D:42:GLU:HG2	6:D:65:LEU:HD11	1.95	0.48
6:D:70:ARG:NH1	9:G:140:ASP:OD1	2.43	0.48
3:A:18:ILE:HD12	4:B:1171:MET:HB2	1.96	0.48
4:B:744:MET:HE1	4:B:906:GLN:HG3	1.96	0.48
4:B:760:THR:O	4:B:999:ALA:N	2.46	0.48
15:N:29:DG:N2	17:T:20:DC:N3	2.62	0.48
2:b:626:ASP:O	2:b:627:LEU:HD23	2.14	0.47
2:b:695:ARG:HB3	2:b:697:ASP:OD1	2.14	0.47
4:B:710:ILE:HA	4:B:764:MET:HE2	1.96	0.47
7:E:75:PHE:HB2	7:E:104:ILE:HG22	1.95	0.47
14:L:26:ASN:HD21	14:L:44:MET:HE1	1.79	0.47
1:a:293:TRP:HA	1:a:440:LEU:HD23	1.96	0.47
2:b:293:TRP:HD1	2:b:686:PHE:HB2	1.75	0.47
2:b:484:GLU:CD	2:b:484:GLU:H	2.21	0.47
3:A:397:PHE:HZ	3:A:1486:ILE:HG12	1.78	0.47
3:A:1115:LYS:NZ	3:A:1137:PRO:O	2.43	0.47
4:B:807:ARG:HA	4:B:929:PRO:HD3	1.96	0.47
5:C:259:LEU:HG	13:K:42:LEU:HD21	1.96	0.47
1:a:505:LYS:HA	1:a:505:LYS:HD3	1.55	0.47
3:A:902:GLU:OE2	3:A:985:ARG:NH1	2.43	0.47
3:A:1366:PHE:HB2	3:A:1374:VAL:HG21	1.96	0.47
4:B:65:ILE:HB	4:B:416:ARG:HH11	1.80	0.47
19:Z:433:LEU:HD13	19:Z:461:LEU:HD13	1.96	0.47
1:a:162:PRO:HB3	1:a:187:PRO:HG3	1.96	0.47
3:A:417:LYS:HD3	3:A:430:ARG:HH21	1.79	0.47
3:A:418:TYR:HB2	3:A:447:GLU:HB2	1.96	0.47
3:A:689:ILE:HG21	4:B:985:LEU:HD22	1.95	0.47
3:A:1053:ARG:NE	3:A:1057:GLU:OE2	2.32	0.47
4:B:584:MET:HG3	4:B:605:ARG:HB2	1.96	0.47
10:H:97:TYR:CZ	10:H:115:TYR:HB3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:291:VAL:HG11	1:a:421:SER:CB	2.45	0.47
4:B:230:ARG:NH1	4:B:231:PRO:O	2.48	0.47
14:L:17:TYR:HB3	14:L:44:MET:HB3	1.95	0.47
3:A:909:LEU:C	3:A:911:PRO:HD3	2.40	0.47
3:A:1210:TRP:HZ3	11:I:28:GLU:HB3	1.80	0.47
4:B:130:LYS:O	4:B:141:GLN:HA	2.15	0.47
15:N:7:DA:H2''	15:N:8:DG:C8	2.50	0.47
19:Z:492:ILE:HG22	19:Z:502:LEU:HB3	1.97	0.47
3:A:618:TYR:HB3	3:A:623:PRO:HD3	1.97	0.47
4:B:565:THR:HG22	4:B:610:ARG:HB3	1.95	0.47
5:C:67:ARG:NH2	5:C:149:LEU:O	2.37	0.47
9:G:91:GLN:HB3	9:G:98:PHE:HB2	1.97	0.47
16:P:31:A:N3	16:P:31:A:H2'	2.30	0.47
3:A:1027:ASP:OD1	3:A:1027:ASP:N	2.44	0.47
3:A:1123:ARG:NH2	3:A:1360:ASN:OD1	2.48	0.47
3:A:1248:ASN:HD22	3:A:1249:ASP:N	2.13	0.47
9:G:44:PHE:CE2	9:G:104:MET:HB2	2.50	0.47
13:K:35:ILE:HB	13:K:71:ILE:HG12	1.96	0.47
3:A:299:ALA:HA	19:Z:262:ASP:HB3	1.97	0.47
3:A:577:PRO:HG3	3:A:586:TRP:CZ2	2.50	0.47
3:A:1005:HIS:HB3	3:A:1008:LYS:HG2	1.97	0.47
3:A:1177:TYR:H	11:I:51:SER:HB3	1.78	0.47
4:B:1040:GLN:NE2	5:C:195:THR:OG1	2.47	0.47
17:T:29:DG:H4'	17:T:30:DG:OP1	2.14	0.47
1:a:246:THR:HG22	1:a:248:PRO:HD2	1.97	0.47
3:A:272:ASN:HD22	3:A:273:GLN:N	2.13	0.47
4:B:967:ILE:HG21	4:B:1048:TYR:OH	2.15	0.47
15:N:28:DA:C5	15:N:29:DG:C6	3.03	0.47
19:Z:291:ALA:HB1	19:Z:305:LEU:HB3	1.96	0.47
1:a:347:ILE:HD13	1:a:360:LEU:HD11	1.97	0.46
1:a:471:LEU:HD11	1:a:473:ILE:HG13	1.97	0.46
3:A:1097:GLU:HB3	3:A:1098:PRO:HD3	1.97	0.46
4:B:733:MET:HE3	4:B:1051:LEU:O	2.16	0.46
4:B:931:ILE:HA	4:B:945:CYS:HB3	1.96	0.46
2:b:296:LYS:HE3	2:b:298:PHE:CE1	2.50	0.46
3:A:25:VAL:HG23	3:A:247:TRP:HE3	1.81	0.46
3:A:117:LEU:HD21	3:A:232:GLU:HB3	1.97	0.46
3:A:1344:MET:H	3:A:1347:LEU:HD12	1.80	0.46
7:E:100:THR:HB	7:E:125:TYR:HA	1.97	0.46
9:G:120:ASP:OD2	9:G:123:SER:N	2.37	0.46
10:H:59:VAL:O	10:H:144:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:314:TYR:HE1	2:b:546:ARG:HA	1.78	0.46
3:A:460:ARG:HD2	3:A:494:ALA:HB2	1.98	0.46
4:B:502:HIS:N	4:B:505:LEU:HD12	2.30	0.46
4:B:764:MET:HE1	4:B:938:ARG:NH1	2.30	0.46
5:C:131:THR:HG21	12:J:16:ASN:HD22	1.80	0.46
3:A:1244:ASN:HD22	3:A:1245:CYS:N	2.13	0.46
5:C:40:ALA:HB1	5:C:171:LYS:HG3	1.97	0.46
1:a:435:HIS:CG	1:a:436:GLU:N	2.83	0.46
3:A:533:PRO:HD3	3:A:654:HIS:CD2	2.50	0.46
3:A:1473:LEU:HD22	8:F:68:THR:HG21	1.97	0.46
4:B:87:LYS:HB3	4:B:129:THR:HG23	1.97	0.46
5:C:256:LEU:HD13	13:K:94:LEU:HB3	1.97	0.46
2:b:425:GLU:HG3	2:b:448:GLY:O	2.16	0.46
4:B:801:VAL:HG13	4:B:929:PRO:HD2	1.98	0.46
7:E:72:MET:HA	7:E:101:ARG:O	2.16	0.46
2:b:293:TRP:CE3	2:b:666:LEU:HB2	2.50	0.46
3:A:358:ARG:HH12	17:T:27:DT:P	2.39	0.46
3:A:693:ILE:HD12	4:B:1023:ARG:HE	1.80	0.46
5:C:40:ALA:O	5:C:169:PHE:HB2	2.15	0.46
5:C:101:PHE:CE1	5:C:122:SER:HB2	2.51	0.46
10:H:20:LYS:HE2	10:H:23:ASP:HA	1.98	0.46
19:Z:433:LEU:HB3	19:Z:436:LEU:HD12	1.96	0.46
3:A:1191:GLU:HG2	3:A:1195:VAL:HG23	1.97	0.46
4:B:274:ARG:NH1	4:B:312:GLN:HA	2.31	0.46
3:A:769:MET:SD	4:B:973:PRO:HG3	2.56	0.46
3:A:1182:GLN:H	3:A:1182:GLN:CD	2.22	0.46
1:a:378:ASN:O	1:a:382:GLN:HG3	2.16	0.46
1:a:495:GLU:CD	1:a:495:GLU:H	2.24	0.46
3:A:31:LEU:HD11	3:A:254:PRO:HB3	1.98	0.46
3:A:381:PRO:HB3	3:A:480:SER:HA	1.97	0.46
7:E:171:PRO:O	7:E:207:ARG:HA	2.16	0.46
8:F:61:GLU:OE2	8:F:108:ARG:NE	2.49	0.46
10:H:98:ARG:HB3	10:H:115:TYR:HB2	1.98	0.46
3:A:316:THR:HG21	3:A:328:ALA:HB3	1.97	0.45
4:B:809:VAL:HA	4:B:926:VAL:HA	1.98	0.45
19:Z:705:LEU:HG	19:Z:724:VAL:HG21	1.97	0.45
4:B:573:TRP:NE1	4:B:575:GLY:O	2.49	0.45
5:C:38:PHE:CE1	5:C:245:VAL:HA	2.51	0.45
5:C:259:LEU:HD21	13:K:35:ILE:HD12	1.96	0.45
7:E:15:LYS:HE2	7:E:34:ASP:HA	1.97	0.45
1:a:475:ARG:HA	1:a:485:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:491:VAL:HG22	1:a:498:PHE:HB2	1.98	0.45
2:b:654:LYS:HB3	9:G:138:GLN:CD	2.42	0.45
4:B:270:ILE:HG13	4:B:305:LEU:HA	1.97	0.45
4:B:587:LEU:HD13	4:B:603:MET:HG2	1.99	0.45
4:B:756:LYS:O	4:B:777:ASN:ND2	2.50	0.45
3:A:362:SER:HB2	4:B:1084:LEU:HD12	1.97	0.45
3:A:408:ARG:NH2	3:A:414:PRO:HD2	2.31	0.45
3:A:487:SER:OG	3:A:673:GLN:NE2	2.49	0.45
3:A:551:ARG:HG2	10:H:25:VAL:HG11	1.98	0.45
3:A:1073:GLU:OE2	3:A:1077:ASN:ND2	2.49	0.45
15:N:26:DG:H2''	15:N:27:DG:C8	2.52	0.45
2:b:189:GLU:OE1	2:b:487:LYS:NZ	2.49	0.45
2:b:206:PHE:CD1	2:b:214:MET:HG3	2.51	0.45
2:b:514:ILE:O	2:b:518:VAL:HG23	2.17	0.45
3:A:552:ASP:HB3	10:H:22:PHE:HB3	1.99	0.45
4:B:907:VAL:HG13	4:B:921:ILE:HG12	1.99	0.45
5:C:78:ILE:HG22	5:C:82:LEU:HG	1.98	0.45
5:C:154:ARG:HD3	12:J:64:PRO:HD3	1.98	0.45
3:A:349:ARG:HH22	4:B:1070:LEU:HD21	1.82	0.45
3:A:695:ASP:OD1	3:A:695:ASP:N	2.48	0.45
16:P:41:C:H2'	16:P:42:C:C6	2.51	0.45
19:Z:484:ARG:HH11	19:Z:485:PHE:HE1	1.63	0.45
3:A:821:GLY:HA2	3:A:838:PHE:CD2	2.51	0.45
4:B:26:CYS:O	4:B:30:ILE:HG12	2.16	0.45
15:N:41:DC:H2''	15:N:42:DT:C6	2.52	0.45
1:a:165:TYR:HA	1:a:187:PRO:HD2	1.99	0.45
3:A:1457:ASN:HD22	3:A:1462:GLN:HE21	1.65	0.45
4:B:401:ALA:O	4:B:405:ARG:HG3	2.16	0.45
13:K:17:LYS:O	13:K:36:ASN:ND2	2.40	0.45
1:a:273:PRO:HB2	1:a:458:LYS:HD3	1.99	0.44
2:b:691:SER:O	2:b:692:LYS:HD2	2.18	0.44
3:A:75:ALA:HB1	4:B:1131:ARG:HH11	1.82	0.44
3:A:1307:VAL:HG13	3:A:1338:THR:HA	1.98	0.44
3:A:1440:MET:SD	4:B:1167:ILE:HD11	2.57	0.44
6:D:16:ASP:OD2	6:D:18:SER:OG	2.23	0.44
10:H:41:LEU:HG	10:H:43:VAL:HG13	1.99	0.44
3:A:203:LYS:HD2	3:A:203:LYS:HA	1.66	0.44
4:B:603:MET:HE2	4:B:603:MET:HB2	1.93	0.44
9:G:151:ARG:HA	9:G:151:ARG:HD3	1.69	0.44
10:H:103:GLU:HB3	10:H:109:ALA:HB2	1.98	0.44
13:K:47:LYS:HD3	13:K:61:TYR:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:426:ARG:HD3	2:b:426:ARG:HA	1.75	0.44
3:A:496:PHE:HB2	4:B:791:GLU:O	2.16	0.44
4:B:924:ARG:NH1	5:C:60:HIS:HB2	2.32	0.44
4:B:1040:GLN:HG2	5:C:203:TRP:CZ2	2.53	0.44
14:L:56:ASP:CG	14:L:58:ARG:HH11	2.25	0.44
3:A:38:GLU:H	3:A:61:ARG:HH12	1.65	0.44
4:B:603:MET:HG3	4:B:614:ILE:HG12	1.98	0.44
15:N:26:DG:H1	17:T:23:DC:N4	2.15	0.44
3:A:922:PHE:HB2	3:A:1052:ARG:HB2	1.99	0.44
1:a:485:ASN:HB2	1:a:503:VAL:HG11	2.00	0.44
2:b:299:GLY:HA3	2:b:321:PHE:CZ	2.53	0.44
2:b:629:THR:HB	2:b:699:ASN:HB2	2.00	0.44
3:A:1104:LEU:O	3:A:1122:PRO:HD2	2.18	0.44
3:A:1248:ASN:HD22	3:A:1249:ASP:H	1.64	0.44
4:B:254:GLN:H	4:B:254:GLN:HG2	1.53	0.44
10:H:41:LEU:HD13	10:H:123:MET:HG3	2.00	0.44
10:H:116:VAL:HG13	10:H:123:MET:HB3	2.00	0.44
11:I:24:LEU:HB3	11:I:37:TYR:HB3	2.00	0.44
3:A:261:ARG:O	3:A:261:ARG:HG2	2.18	0.44
9:G:150:THR:OG1	9:G:157:ILE:O	2.32	0.44
15:N:26:DG:C2	15:N:27:DG:C6	3.06	0.44
15:N:32:DA:H2''	15:N:33:DG:C8	2.52	0.44
2:b:184:ILE:HD12	2:b:187:GLU:HG3	1.99	0.44
2:b:292:LYS:NZ	2:b:669:THR:OG1	2.30	0.44
3:A:668:PHE:CZ	3:A:672:ILE:HD11	2.53	0.44
4:B:628:VAL:HG12	4:B:630:LYS:O	2.17	0.44
3:A:1022:ILE:N	3:A:1034:GLN:OE1	2.49	0.44
3:A:1343:LEU:O	3:A:1344:MET:HG2	2.18	0.44
4:B:35:ASP:OD2	4:B:646:ARG:NH1	2.49	0.44
4:B:442:ASP:C	4:B:456:GLN:HE22	2.25	0.44
10:H:64:LEU:HB3	10:H:83:SER:HB2	2.00	0.44
17:T:22:DC:O3'	17:T:23:DC:H3'	2.18	0.44
3:A:140:ARG:HH11	3:A:237:GLY:HA2	1.83	0.43
3:A:1353:ASP:O	3:A:1357:THR:OG1	2.32	0.43
4:B:294:ASP:OD1	4:B:294:ASP:N	2.51	0.43
4:B:484:ARG:NH2	4:B:730:LYS:HE3	2.32	0.43
10:H:40:ILE:O	10:H:123:MET:HA	2.16	0.43
14:L:29:LYS:HB3	14:L:32:ASP:HB2	1.99	0.43
19:Z:214:SER:OG	19:Z:228:GLU:OE1	2.27	0.43
2:b:157:TRP:CE3	2:b:426:ARG:HG3	2.53	0.43
2:b:650:LYS:HA	9:G:170:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:725:LYS:HZ2	9:G:170:LEU:HD22	1.84	0.43
3:A:356:GLY:HA3	4:B:1087:GLY:HA2	2.00	0.43
3:A:809:HIS:HE1	4:B:506:TRP:CE2	2.35	0.43
4:B:93:LEU:HD23	4:B:124:LEU:HD13	1.99	0.43
7:E:45:GLY:HA3	7:E:53:PRO:HD3	2.00	0.43
14:L:19:CYS:HB2	14:L:22:CYS:HB2	1.99	0.43
3:A:212:LYS:H	3:A:212:LYS:HG2	1.54	0.43
3:A:693:ILE:HG21	4:B:1023:ARG:HH21	1.82	0.43
3:A:783:GLN:HA	3:A:787:VAL:O	2.18	0.43
4:B:1062:ARG:NH1	4:B:1074:PRO:HB3	2.33	0.43
7:E:194:ILE:HG13	7:E:204:ILE:HG12	2.00	0.43
10:H:35:PHE:HB3	10:H:37:MET:HE3	2.00	0.43
1:a:192:TRP:HA	1:a:195:GLU:HG3	1.99	0.43
1:a:530:ARG:HG3	1:a:532:ASP:OD1	2.18	0.43
3:A:579:ILE:HD13	10:H:92:MET:HG2	2.00	0.43
3:A:1163:HIS:CE1	3:A:1297:THR:HG22	2.51	0.43
7:E:24:ARG:HD2	7:E:26:TYR:CE2	2.53	0.43
9:G:97:LEU:HD23	9:G:108:ILE:HD12	1.99	0.43
19:Z:424:ASP:HB2	19:Z:440:ILE:HD12	1.98	0.43
1:a:389:ILE:HD12	1:a:389:ILE:HA	1.83	0.43
1:a:422:ARG:HB3	1:a:562:ILE:CG2	2.49	0.43
2:b:255:ARG:HA	2:b:261:PRO:HA	2.00	0.43
2:b:276:VAL:HG22	2:b:361:LEU:HD11	2.00	0.43
3:A:109:CYS:HA	3:A:148:CYS:SG	2.59	0.43
3:A:379:GLY:N	3:A:483:ARG:O	2.32	0.43
3:A:566:PHE:HB2	3:A:675:VAL:HG12	2.00	0.43
6:D:87:LEU:HB3	6:D:97:LEU:HG	2.01	0.43
7:E:71:GLN:HB2	7:E:99:ILE:HD12	2.00	0.43
9:G:55:GLY:HA3	9:G:69:PRO:HG2	2.01	0.43
1:a:519:PHE:CD1	1:a:549:ILE:HD12	2.54	0.43
3:A:36:VAL:HG21	3:A:73:THR:OG1	2.18	0.43
3:A:1216:LEU:HB2	3:A:1255:LEU:HB2	2.00	0.43
4:B:411:LEU:HD21	4:B:435:ILE:HG23	1.99	0.43
4:B:1054:MET:H	4:B:1054:MET:HG2	1.63	0.43
2:b:219:THR:HG23	2:b:225:GLU:HG2	2.00	0.43
3:A:215:LEU:H	3:A:215:LEU:HG	1.65	0.43
3:A:417:LYS:HA	3:A:429:LEU:HB2	1.99	0.43
3:A:681:LEU:HD11	4:B:786:THR:HA	2.00	0.43
4:B:180:ASP:OD1	4:B:472:ARG:NH2	2.52	0.43
4:B:789:ASN:ND2	4:B:966:ILE:HG22	2.34	0.43
9:G:150:THR:OG1	9:G:157:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:66:GLU:HA	14:L:18:ILE:HD13	1.99	0.43
17:T:1:DG:H2"	17:T:2:DC:C6	2.53	0.43
2:b:250:MET:HE2	2:b:400:HIS:HB3	2.01	0.43
3:A:876:ASP:OD1	3:A:876:ASP:N	2.44	0.43
1:a:527:MET:HG3	1:a:528:ARG:HG3	2.01	0.43
2:b:227:ILE:HA	2:b:532:ARG:HG3	2.01	0.43
3:A:46:THR:OG1	3:A:273:GLN:NE2	2.52	0.43
3:A:623:PRO:HA	10:H:27:ARG:NH2	2.34	0.43
3:A:871:VAL:HG11	3:A:1400:LEU:HD11	2.01	0.43
4:B:502:HIS:H	4:B:505:LEU:HD12	1.84	0.43
4:B:929:PRO:HB3	4:B:935:PHE:HZ	1.83	0.43
18:Y:58:ASP:HB2	18:Y:88:SER:HB3	1.99	0.43
2:b:249:ARG:HA	2:b:249:ARG:HD3	1.84	0.43
2:b:659:HIS:HB3	2:b:704:LYS:HE2	2.01	0.43
2:b:830:ILE:O	2:b:834:ARG:HG3	2.18	0.43
3:A:43:TYR:HA	3:A:44:PRO:HD3	1.88	0.43
3:A:1020:LEU:O	3:A:1034:GLN:NE2	2.52	0.43
3:A:1113:SER:C	3:A:1115:LYS:H	2.27	0.43
4:B:22:TRP:CZ3	4:B:635:LEU:HD23	2.54	0.43
4:B:845:TYR:CE1	4:B:865:VAL:HG11	2.54	0.43
9:G:101:ILE:HB	9:G:104:MET:HE2	2.01	0.43
3:A:151:LYS:HA	3:A:151:LYS:HD3	1.63	0.42
3:A:401:ARG:O	3:A:405:LEU:HD22	2.19	0.42
3:A:576:GLN:HE21	3:A:580:LEU:HD21	1.83	0.42
3:A:601:ASN:OD1	3:A:632:ASN:N	2.37	0.42
4:B:274:ARG:NH1	4:B:311:ILE:O	2.52	0.42
4:B:1060:HIS:HB3	4:B:1078:ARG:HE	1.85	0.42
5:C:7:PRO:HB2	13:K:101:LEU:HD13	2.01	0.42
7:E:75:PHE:HD2	7:E:104:ILE:HG22	1.84	0.42
10:H:89:GLU:OE2	10:H:147:LYS:HG2	2.19	0.42
18:Y:58:ASP:OD2	19:Z:268:LYS:NZ	2.32	0.42
4:B:84:TYR:HB3	4:B:132:VAL:HG23	2.01	0.42
4:B:258:ALA:HB2	4:B:269:ILE:HD13	2.00	0.42
4:B:631:GLN:O	4:B:683:GLN:HG2	2.19	0.42
6:D:26:PHE:HE2	9:G:78:ARG:HG2	1.84	0.42
9:G:138:GLN:HG2	9:G:141:ASP:OD2	2.19	0.42
10:H:106:THR:OG1	10:H:107:GLU:OE1	2.28	0.42
19:Z:498:ASN:O	19:Z:515:PRO:HD3	2.19	0.42
1:a:300:TYR:CE1	1:a:314:ASP:HB3	2.53	0.42
3:A:272:ASN:OD1	16:P:37:G:N2	2.52	0.42
4:B:201:ALA:HB3	4:B:206:TYR:OH	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:113:ARG:NH1	5:C:114:HIS:O	2.52	0.42
9:G:96:GLY:HA3	9:G:107:PHE:CE1	2.54	0.42
15:N:29:DG:H2''	15:N:30:DC:H5	1.78	0.42
3:A:79:THR:HA	4:B:1072:ARG:HH22	1.84	0.42
3:A:264:VAL:HG21	16:P:37:G:O2'	2.19	0.42
3:A:685:HIS:HB3	4:B:784:SER:HB2	2.01	0.42
3:A:1218:ARG:NH2	3:A:1252:ALA:O	2.52	0.42
3:A:1474:LEU:HB2	8:F:105:ILE:HB	2.02	0.42
4:B:348:LEU:HB3	4:B:351:VAL:HG22	2.02	0.42
4:B:565:THR:HG21	4:B:580:PRO:HB3	2.01	0.42
4:B:591:ARG:HD3	4:B:603:MET:HE1	2.01	0.42
4:B:994:GLY:O	12:J:31:GLU:HB2	2.19	0.42
2:b:661:LEU:HD23	2:b:704:LYS:HG3	2.01	0.42
3:A:469:MET:HE1	4:B:1086:PHE:CE1	2.54	0.42
4:B:714:PRO:HG2	4:B:1001:PRO:HB3	2.01	0.42
11:I:65:LEU:HD22	11:I:122:ARG:HG2	2.00	0.42
17:T:28:DG:H2''	17:T:29:DG:H5'	2.02	0.42
4:B:777:ASN:O	12:J:47:ARG:NH1	2.52	0.42
7:E:70:ASP:OD1	7:E:70:ASP:N	2.52	0.42
9:G:49:THR:N	9:G:73:LYS:O	2.52	0.42
2:b:632:PRO:HD2	2:b:686:PHE:CZ	2.51	0.42
2:b:692:LYS:CG	2:b:695:ARG:HB2	2.40	0.42
3:A:763:TYR:OH	10:H:23:ASP:OD2	2.37	0.42
4:B:54:SER:O	4:B:58:ILE:HG12	2.20	0.42
4:B:713:PHE:HB3	4:B:716:HIS:ND1	2.35	0.42
4:B:953:ASP:OD1	5:C:36:ARG:NH2	2.41	0.42
18:Y:62:ALA:HB3	19:Z:215:VAL:HB	2.02	0.42
2:b:603:LEU:HD22	2:b:637:LEU:HD12	2.01	0.42
3:A:715:GLU:HA	3:A:718:GLU:HG2	2.02	0.42
7:E:84:ILE:HA	7:E:87:ILE:HG12	2.01	0.42
10:H:8:ASP:OD1	10:H:9:ILE:N	2.51	0.42
17:T:35:DG:H2''	17:T:36:DC:C5	2.54	0.42
3:A:330:GLN:HE21	3:A:334:ARG:HB3	1.85	0.42
14:L:41:TYR:CE2	14:L:43:ILE:HB	2.54	0.42
3:A:927:GLU:O	3:A:931:ARG:HG2	2.20	0.42
1:a:273:PRO:HB3	1:a:456:ILE:HG22	2.01	0.41
2:b:278:ALA:HB3	2:b:308:PHE:HE1	1.84	0.41
3:A:381:PRO:HD2	3:A:384:ILE:HD12	2.02	0.41
3:A:395:THR:OG1	3:A:396:PRO:HD2	2.19	0.41
4:B:905:ASP:HB2	4:B:924:ARG:HB2	2.01	0.41
4:B:912:ASN:OD1	4:B:916:TYR:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:390:LEU:HD23	19:Z:393:LEU:HD12	2.00	0.41
1:a:386:ARG:HG2	1:a:387:GLU:HG2	2.02	0.41
3:A:108:ARG:HE	3:A:191:ILE:HB	1.85	0.41
3:A:203:LYS:HE3	3:A:204:HIS:ND1	2.34	0.41
3:A:1054:MET:HA	3:A:1058:PHE:HB2	2.02	0.41
4:B:841:ARG:HH12	16:P:35:A:H1'	1.84	0.41
7:E:111:THR:HG21	15:N:39:DA:OP1	2.19	0.41
8:F:69:ARG:NE	8:F:96:GLU:OE1	2.42	0.41
17:T:8:DG:H2''	17:T:9:DC:H5'	2.00	0.41
3:A:383:SER:N	13:K:2:ASN:HD21	2.18	0.41
4:B:113:ALA:HA	4:B:118:LEU:HB2	2.00	0.41
5:C:11:ILE:HG12	5:C:21:PHE:HB3	2.03	0.41
7:E:19:GLN:OE1	7:E:138:ASN:ND2	2.50	0.41
3:A:1148:ALA:HB1	3:A:1333:GLU:HB2	2.02	0.41
7:E:34:ASP:OD1	7:E:34:ASP:N	2.51	0.41
10:H:91:VAL:HG22	10:H:144:LEU:HD13	2.01	0.41
2:b:391:ALA:HB2	2:b:401:PHE:CE1	2.56	0.41
3:A:410:ASN:HD22	3:A:430:ARG:HB3	1.85	0.41
3:A:483:ARG:NH1	4:B:931:ILE:HD11	2.35	0.41
3:A:564:LEU:HA	3:A:567:LEU:HD13	2.01	0.41
4:B:280:SER:OG	11:I:21:ASN:O	2.35	0.41
4:B:968:ASN:ND2	4:B:970:HIS:HB2	2.36	0.41
5:C:67:ARG:NH1	12:J:3:ILE:O	2.49	0.41
5:C:221:ASP:OD1	5:C:221:ASP:N	2.54	0.41
12:J:17:LYS:HB3	12:J:38:LEU:HD13	2.02	0.41
2:b:293:TRP:CE2	2:b:666:LEU:HD12	2.55	0.41
3:A:229:SER:OG	3:A:230:ASP:N	2.53	0.41
3:A:581:LYS:HB3	3:A:582:PRO:HD3	2.03	0.41
3:A:1030:SER:OG	7:E:162:ARG:NE	2.52	0.41
3:A:1432:PHE:CD2	3:A:1433:GLU:HG2	2.55	0.41
4:B:290:TYR:HB3	4:B:561:ILE:HG23	2.02	0.41
4:B:631:GLN:NE2	4:B:683:GLN:HA	2.36	0.41
4:B:841:ARG:CZ	16:P:34:G:H21	2.33	0.41
5:C:55:ASN:HD22	5:C:56:SER:N	2.18	0.41
8:F:57:MET:HE1	8:F:120:VAL:HG13	2.00	0.41
1:a:168:ASP:OD1	1:a:168:ASP:N	2.53	0.41
1:a:395:LYS:HB2	1:a:401:ILE:HD12	2.03	0.41
2:b:690:VAL:HG23	2:b:690:VAL:O	2.20	0.41
3:A:329:MET:SD	3:A:333:GLY:HA2	2.61	0.41
3:A:1359:SER:HB3	3:A:1365:ILE:HD11	2.02	0.41
19:Z:367:SER:HA	19:Z:372:LEU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:280:ASN:HB3	1:a:457:LEU:HD13	2.02	0.41
2:b:307:ASP:OD1	2:b:308:PHE:N	2.49	0.41
3:A:863:ARG:HB3	3:A:1414:ILE:HG22	2.03	0.41
3:A:865:ILE:HG21	4:B:1092:ASP:HB3	2.03	0.41
3:A:992:LYS:HA	3:A:992:LYS:HD3	1.84	0.41
4:B:387:HIS:CD2	4:B:504:THR:HG21	2.56	0.41
5:C:172:GLU:CG	14:L:58:ARG:HH21	2.34	0.41
10:H:15:ILE:HG13	10:H:52:LEU:HD12	2.02	0.41
1:a:307:THR:HG23	1:a:336:HIS:ND1	2.36	0.41
1:a:377:PHE:CE2	1:a:443:GLN:HG2	2.56	0.41
1:a:541:THR:O	1:a:545:VAL:HG23	2.21	0.41
3:A:544:ALA:HB2	3:A:680:LEU:HD22	2.03	0.41
3:A:597:PRO:HD3	3:A:668:PHE:CD1	2.56	0.41
3:A:861:GLN:NE2	3:A:1096:GLY:O	2.49	0.41
4:B:84:TYR:HA	4:B:131:THR:O	2.21	0.41
4:B:285:LEU:HD12	4:B:285:LEU:HA	1.90	0.41
4:B:285:LEU:HD23	11:I:16:PHE:HZ	1.86	0.41
4:B:670:GLU:HA	4:B:673:VAL:HG12	2.03	0.41
4:B:795:ILE:HB	4:B:966:ILE:HB	2.03	0.41
6:D:18:SER:HB2	6:D:116:PRO:HG2	2.03	0.41
18:Y:56:SER:HB2	18:Y:90:THR:HB	2.02	0.41
3:A:253:LEU:HD12	3:A:254:PRO:HD2	2.03	0.41
3:A:552:ASP:HB3	10:H:25:VAL:HG12	2.03	0.41
3:A:1471:PHE:CZ	8:F:61:GLU:HA	2.56	0.41
4:B:724:TYR:HB3	4:B:728:MET:HE3	2.03	0.41
7:E:102:ALA:HB3	7:E:127:LEU:HD23	2.03	0.41
16:P:37:G:H3'	16:P:38:G:C8	2.55	0.41
1:a:367:PHE:CE2	1:a:387:GLU:HB3	2.56	0.40
3:A:22:GLN:HA	3:A:1448:SER:HA	2.03	0.40
3:A:470:MET:HB3	3:A:521:VAL:HG12	2.02	0.40
3:A:1130:ILE:HG13	3:A:1411:LEU:HB3	2.03	0.40
3:A:1199:MET:O	3:A:1200:PRO:C	2.63	0.40
4:B:125:TYR:HD1	4:B:148:PHE:HA	1.87	0.40
4:B:1112:ASP:OD1	4:B:1112:ASP:N	2.52	0.40
3:A:1244:ASN:O	3:A:1259:ILE:HA	2.22	0.40
4:B:473:LEU:CD2	4:B:1052:LYS:HD2	2.48	0.40
2:b:459:TYR:O	2:b:463:VAL:HG23	2.21	0.40
3:A:327:ARG:H	3:A:327:ARG:HG3	1.33	0.40
3:A:581:LYS:HA	3:A:581:LYS:HD2	1.81	0.40
4:B:248:LYS:HE2	4:B:251:ALA:HB2	2.02	0.40
2:b:311:GLU:HG2	2:b:608:LYS:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:654:LYS:HB3	9:G:138:GLN:NE2	2.37	0.40
3:A:26:LEU:HD12	4:B:1166:SER:HA	2.03	0.40
3:A:368:THR:OG1	4:B:946:GLY:HA2	2.21	0.40
3:A:481:THR:HG22	4:B:1055:VAL:HG21	2.02	0.40
4:B:567:ILE:HA	4:B:612:ILE:O	2.21	0.40
15:N:44:DG:H2''	15:N:45:DG:H5'	2.04	0.40
1:a:482:LEU:HA	1:a:483:PRO:HD3	1.97	0.40
2:b:330:ILE:HG21	2:b:695:ARG:HD2	2.03	0.40
11:I:92:LYS:H	11:I:92:LYS:HD3	1.86	0.40
14:L:28:ILE:HD12	14:L:28:ILE:HA	1.95	0.40
18:Y:11:ARG:HG2	18:Y:12:HIS:CD2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	515/597 (86%)	497 (96%)	17 (3%)	1 (0%)	43	75
2	b	689/835 (82%)	664 (96%)	22 (3%)	3 (0%)	30	65
3	A	1418/1970 (72%)	1320 (93%)	97 (7%)	1 (0%)	48	81
4	B	1123/1174 (96%)	1057 (94%)	66 (6%)	0	100	100
5	C	254/271 (94%)	248 (98%)	6 (2%)	0	100	100
6	D	127/142 (89%)	122 (96%)	5 (4%)	0	100	100
7	E	207/210 (99%)	200 (97%)	7 (3%)	0	100	100
8	F	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
9	G	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
10	H	146/150 (97%)	139 (95%)	7 (5%)	0	100	100
11	I	115/125 (92%)	108 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
13	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
14	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
18	Y	114/121 (94%)	112 (98%)	2 (2%)	0	100	100
19	Z	348/1087 (32%)	334 (96%)	14 (4%)	0	100	100
All	All	5527/7223 (76%)	5257 (95%)	265 (5%)	5 (0%)	49	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	162	PRO
2	b	280	PRO
2	b	757	PRO
3	A	1205	ALA
2	b	230	VAL

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	468/534 (88%)	426 (91%)	42 (9%)	9	31
2	b	610/741 (82%)	587 (96%)	23 (4%)	29	51
3	A	1255/1749 (72%)	1196 (95%)	59 (5%)	23	46
4	B	989/1027 (96%)	960 (97%)	29 (3%)	37	58
5	C	235/248 (95%)	234 (100%)	1 (0%)	84	84
6	D	104/126 (82%)	104 (100%)	0	100	100
7	E	191/192 (100%)	187 (98%)	4 (2%)	47	65
8	F	71/111 (64%)	70 (99%)	1 (1%)	59	71
9	G	138/153 (90%)	131 (95%)	7 (5%)	21	45
10	H	129/131 (98%)	125 (97%)	4 (3%)	35	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	I	105/112 (94%)	104 (99%)	1 (1%)	68	76
12	J	56/56 (100%)	55 (98%)	1 (2%)	51	68
13	K	104/106 (98%)	100 (96%)	4 (4%)	29	51
14	L	43/55 (78%)	43 (100%)	0	100	100
18	Y	102/105 (97%)	102 (100%)	0	100	100
19	Z	319/940 (34%)	318 (100%)	1 (0%)	86	85
All	All	4919/6386 (77%)	4742 (96%)	177 (4%)	32	53

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	144	LYS
1	a	160	ARG
1	a	233	LEU
1	a	239	LYS
1	a	250	LEU
1	a	275	SER
1	a	283	LEU
1	a	308	ASN
1	a	322	VAL
1	a	326	GLU
1	a	351	VAL
1	a	356	VAL
1	a	358	ARG
1	a	362	TYR
1	a	376	ASP
1	a	378	ASN
1	a	381	LEU
1	a	385	GLU
1	a	386	ARG
1	a	388	ILE
1	a	389	ILE
1	a	390	SER
1	a	416	PHE
1	a	418	ILE
1	a	419	CYS
1	a	422	ARG
1	a	441	ILE
1	a	460	LYS
1	a	463	SER

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Mol	Chain	Res	Type
1	a	472	LYS
1	a	473	ILE
1	a	475	ARG
1	a	481	LEU
1	a	482	LEU
1	a	486	VAL
1	a	503	VAL
1	a	504	THR
1	a	505	LYS
1	a	506	GLU
1	a	510	TYR
1	a	525	VAL
1	a	528	ARG
2	b	163	THR
2	b	164	GLU
2	b	183	ILE
2	b	196	LEU
2	b	257	SER
2	b	290	ARG
2	b	310	LEU
2	b	330	ILE
2	b	383	LEU
2	b	404	LYS
2	b	483	LEU
2	b	484	GLU
2	b	504	CYS
2	b	509	LYS
2	b	527	ARG
2	b	532	ARG
2	b	544	GLN
2	b	631	LEU
2	b	687	VAL
2	b	692	LYS
2	b	813	GLN
2	b	814	LYS
2	b	816	GLN
3	A	41	ILE
3	A	45	GLU
3	A	46	THR
3	A	48	GLU
3	A	54	LEU
3	A	118	LEU

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Mol	Chain	Res	Type
3	A	130	LEU
3	A	151	LYS
3	A	152	ASN
3	A	201	GLU
3	A	203	LYS
3	A	204	HIS
3	A	205	VAL
3	A	206	ASN
3	A	208	ASP
3	A	211	GLU
3	A	212	LYS
3	A	215	LEU
3	A	216	LEU
3	A	224	ILE
3	A	250	VAL
3	A	255	VAL
3	A	327	ARG
3	A	346	LYS
3	A	368	THR
3	A	405	LEU
3	A	419	ILE
3	A	461	GLN
3	A	463	THR
3	A	464	LEU
3	A	488	VAL
3	A	489	THR
3	A	509	LEU
3	A	521	VAL
3	A	580	LEU
3	A	585	LEU
3	A	706	ILE
3	A	751	LYS
3	A	760	LEU
3	A	910	LYS
3	A	1103	THR
3	A	1104	LEU
3	A	1112	VAL
3	A	1116	ASN
3	A	1117	VAL
3	A	1166	LEU
3	A	1184	THR
3	A	1186	VAL

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Mol	Chain	Res	Type
3	A	1189	ASP
3	A	1190	GLN
3	A	1191	GLU
3	A	1197	TYR
3	A	1199	MET
3	A	1202	PHE
3	A	1204	VAL
3	A	1323	THR
3	A	1374	VAL
3	A	1378	LEU
3	A	1463	LEU
4	B	29	VAL
4	B	126	VAL
4	B	129	THR
4	B	163	LEU
4	B	207	VAL
4	B	230	ARG
4	B	240	LEU
4	B	242	ARG
4	B	248	LYS
4	B	249	LYS
4	B	254	GLN
4	B	257	VAL
4	B	336	ILE
4	B	361	LYS
4	B	377	LEU
4	B	463	ARG
4	B	525	ASN
4	B	576	ILE
4	B	612	ILE
4	B	616	THR
4	B	630	LYS
4	B	683	GLN
4	B	731	GLN
4	B	809	VAL
4	B	873	LEU
4	B	1052	LYS
4	B	1054	MET
4	B	1089	MET
4	B	1127	ILE
5	C	15	THR
7	E	58	LEU

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Mol	Chain	Res	Type
7	E	99	ILE
7	E	131	LEU
7	E	137	ILE
8	F	90	LEU
9	G	150	THR
9	G	152	VAL
9	G	157	ILE
9	G	158	PHE
9	G	160	ILE
9	G	162	SER
9	G	163	LEU
10	H	60	ILE
10	H	96	VAL
10	H	143	LEU
10	H	148	LEU
11	I	119	CYS
12	J	53	VAL
13	K	41	THR
13	K	45	ILE
13	K	80	ASP
13	K	94	LEU
19	Z	481	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	102	ASN
1	a	243	GLN
1	a	258	HIS
1	a	272	GLN
1	a	280	ASN
1	a	324	ASN
1	a	405	GLN
1	a	435	HIS
1	a	485	ASN
1	a	521	ASN
1	a	537	ASN
1	a	540	ASN
2	b	382	GLN
2	b	490	HIS
2	b	677	ASN
2	b	678	GLN

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Mol	Chain	Res	Type
2	b	699	ASN
3	A	123	ASN
3	A	136	GLN
3	A	188	GLN
3	A	206	ASN
3	A	210	GLN
3	A	272	ASN
3	A	273	GLN
3	A	278	HIS
3	A	311	GLN
3	A	330	GLN
3	A	377	GLN
3	A	472	HIS
3	A	504	HIS
3	A	576	GLN
3	A	654	HIS
3	A	711	GLN
3	A	809	HIS
3	A	905	ASN
3	A	989	ASN
3	A	1005	HIS
3	A	1032	GLN
3	A	1093	GLN
3	A	1101	GLN
3	A	1105	ASN
3	A	1129	ASN
3	A	1163	HIS
3	A	1194	ASN
3	A	1244	ASN
3	A	1248	ASN
3	A	1299	GLN
3	A	1332	GLN
3	A	1457	ASN
4	B	43	GLN
4	B	111	ASN
4	B	164	ASN
4	B	245	GLN
4	B	420	GLN
4	B	456	GLN
4	B	461	GLN
4	B	486	ASN
4	B	518	HIS

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Mol	Chain	Res	Type
4	B	577	HIS
4	B	639	HIS
4	B	650	ASN
4	B	683	GLN
4	B	699	HIS
4	B	717	ASN
4	B	731	GLN
4	B	749	HIS
4	B	1003	ASN
4	B	1021	HIS
4	B	1025	ASN
4	B	1053	HIS
4	B	1094	GLN
4	B	1145	GLN
5	C	55	ASN
5	C	66	HIS
6	D	66	ASN
6	D	129	GLN
6	D	135	GLN
7	E	95	GLN
7	E	107	GLN
7	E	132	GLN
7	E	169	GLN
8	F	49	GLN
10	H	44	ASN
11	I	22	ASN
11	I	41	ASN
11	I	45	GLN
12	J	61	ASN
13	K	49	GLN
18	Y	12	HIS
18	Y	45	ASN
19	Z	232	GLN
19	Z	509	HIS
19	Z	737	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	15/17 (88%)	11 (73%)	0

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	32	G
16	P	33	A
16	P	34	G
16	P	35	A
16	P	36	G
16	P	37	G
16	P	38	G
16	P	42	C
16	P	44	A
16	P	45	C
16	P	46	U

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
22	GTP	P	101	16	33,34,34	0.96	1 (3%)	50,54,54	1.56	9 (18%)

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
22	GTP	P	101	16	-	5/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	101	GTP	C2-N3	2.17	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	101	GTP	C5-C4-N3	-4.88	120.62	128.39
22	P	101	GTP	C2-N3-C4	4.59	120.21	112.30
22	P	101	GTP	N9-C4-N3	3.12	132.19	125.95
22	P	101	GTP	C2-N1-C6	-2.87	119.91	125.11
22	P	101	GTP	N9-C8-N7	-2.69	108.42	113.40
22	P	101	GTP	C5-C6-N1	2.52	119.66	113.25
22	P	101	GTP	C8-N7-C5	2.50	108.71	104.26
22	P	101	GTP	O6-C6-C5	-2.41	120.17	126.53
22	P	101	GTP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (5) torsion outliers are listed below:

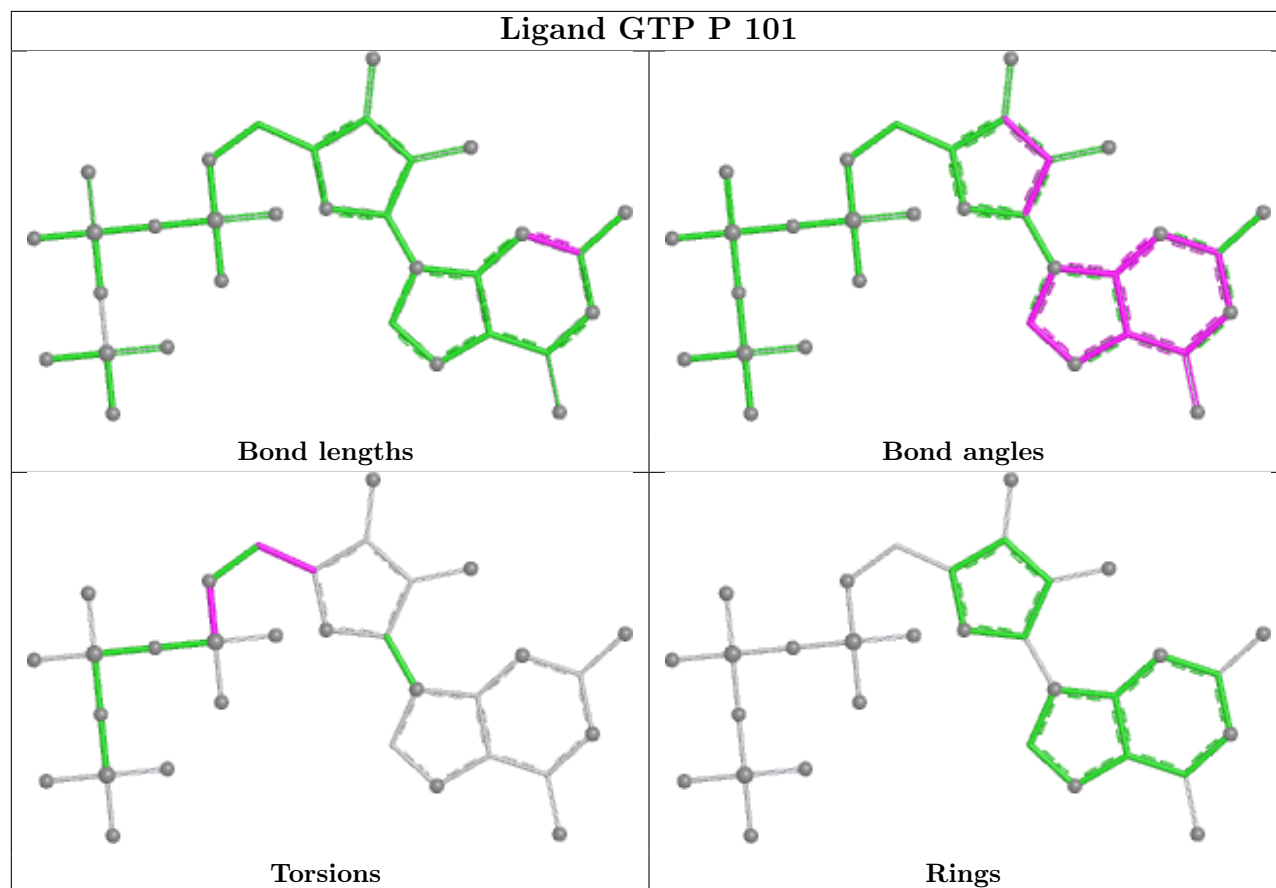
Mol	Chain	Res	Type	Atoms
22	P	101	GTP	C5'-O5'-PA-O3A
22	P	101	GTP	C5'-O5'-PA-O1A
22	P	101	GTP	C5'-O5'-PA-O2A
22	P	101	GTP	O4'-C4'-C5'-O5'
22	P	101	GTP	C3'-C4'-C5'-O5'

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.

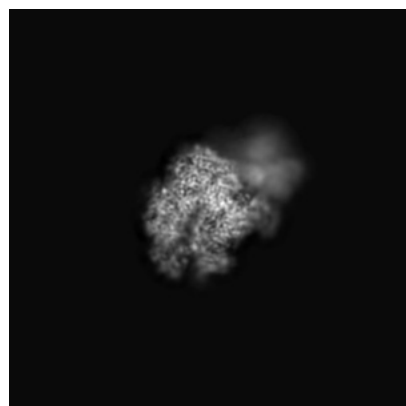
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37353. These allow visual inspection of the internal detail of the map and identification of artifacts.

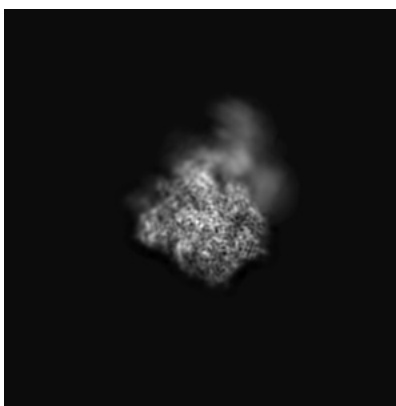
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

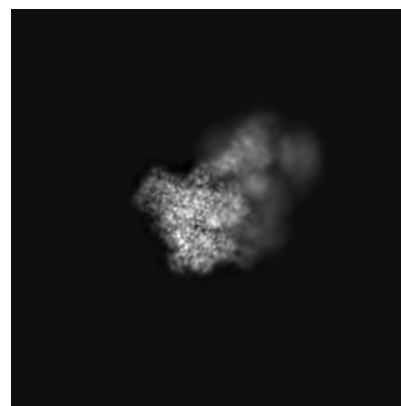
6.1.1 Primary map



X

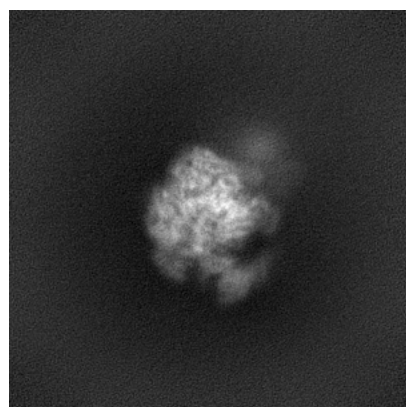


Y

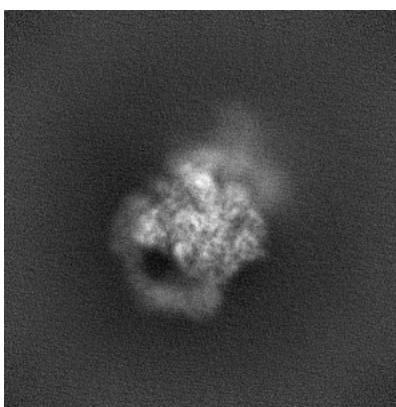


Z

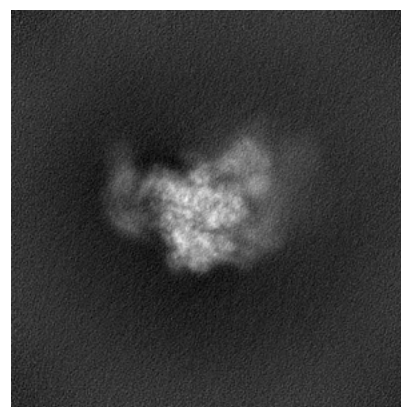
6.1.2 Raw map



X



Y

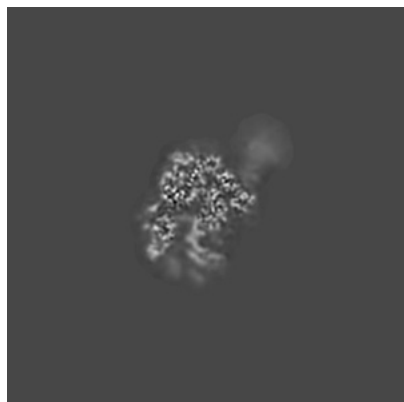


Z

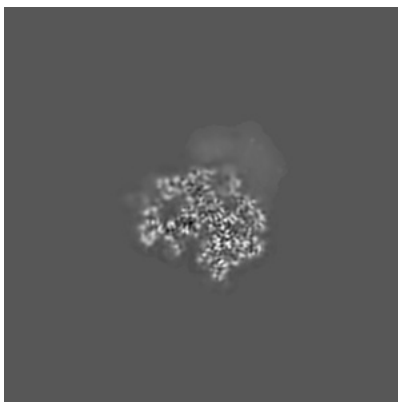
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

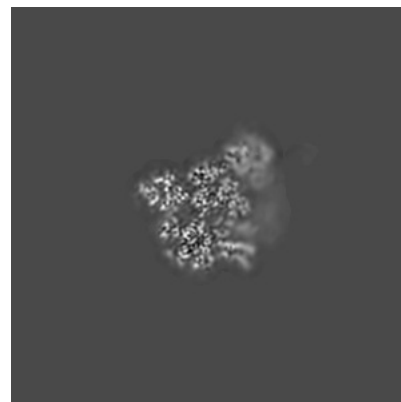
6.2.1 Primary map



X Index: 160

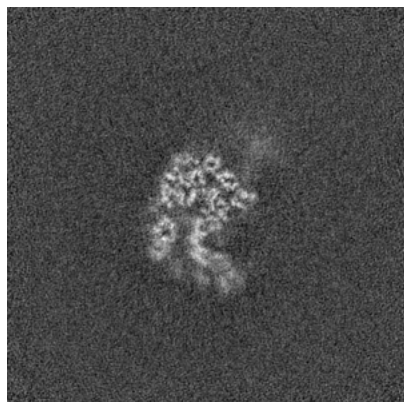


Y Index: 160

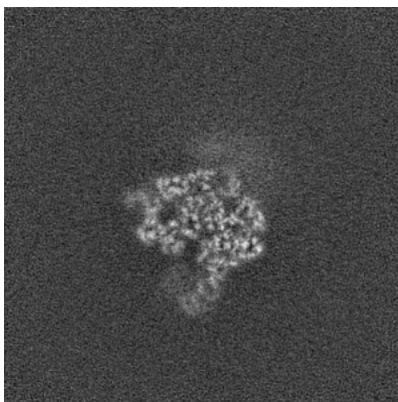


Z Index: 160

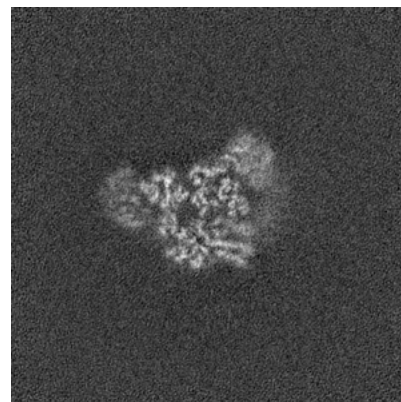
6.2.2 Raw map



X Index: 160



Y Index: 160

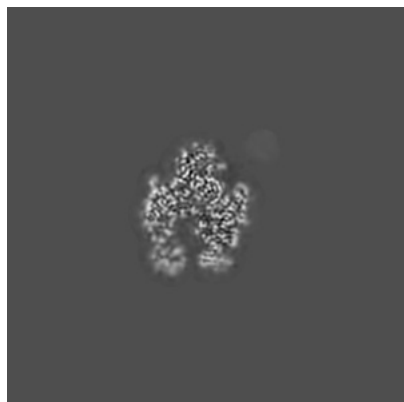


Z Index: 160

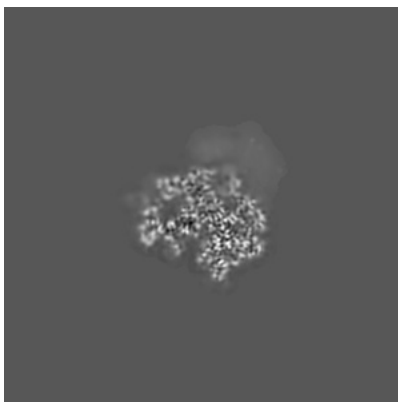
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

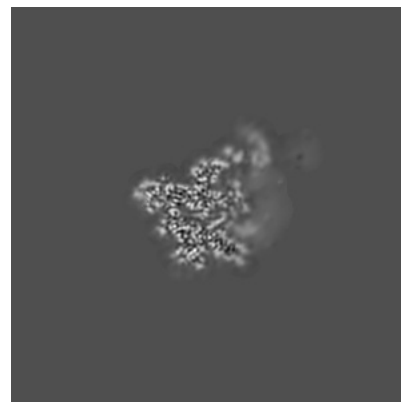
6.3.1 Primary map



X Index: 148

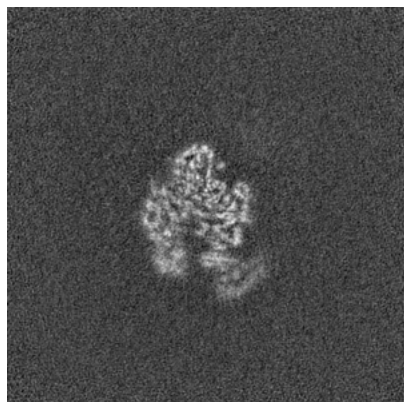


Y Index: 160

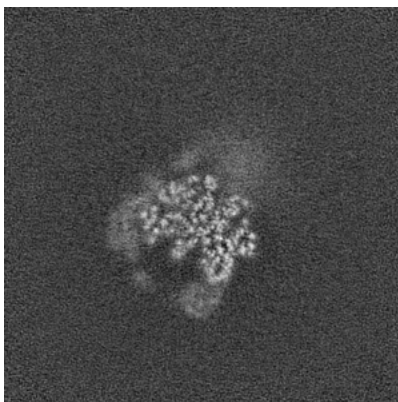


Z Index: 165

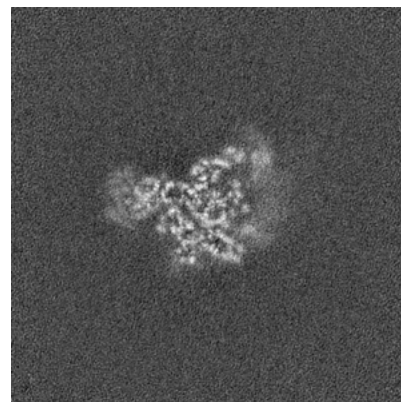
6.3.2 Raw map



X Index: 149



Y Index: 170

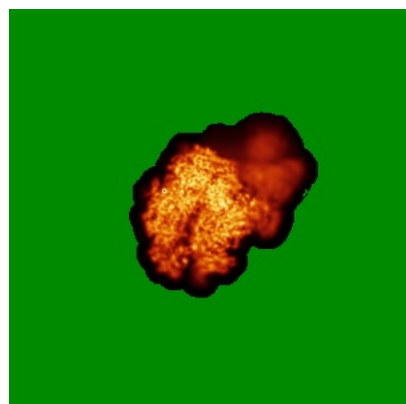


Z Index: 166

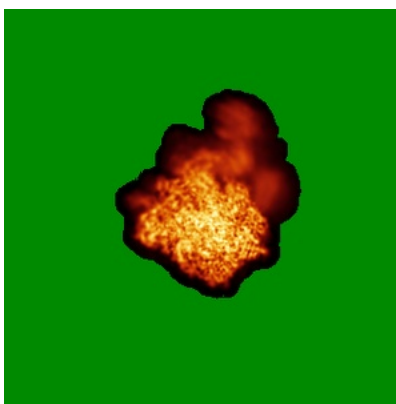
The images above show the largest variance slices of the map in three orthogonal directions.

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

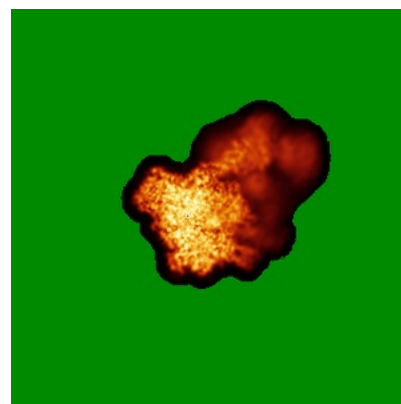
6.4.1 Primary map



X

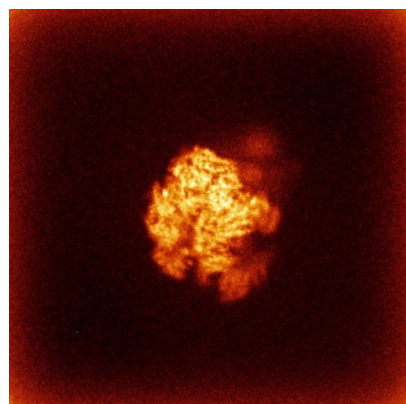


Y

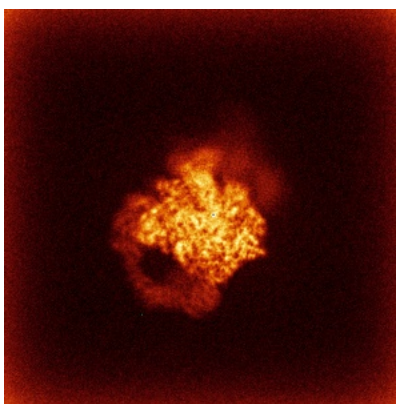


Z

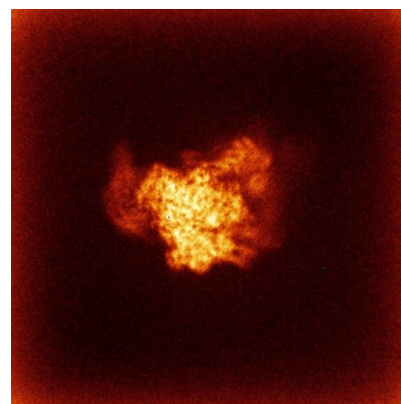
6.4.2 Raw map



X



Y

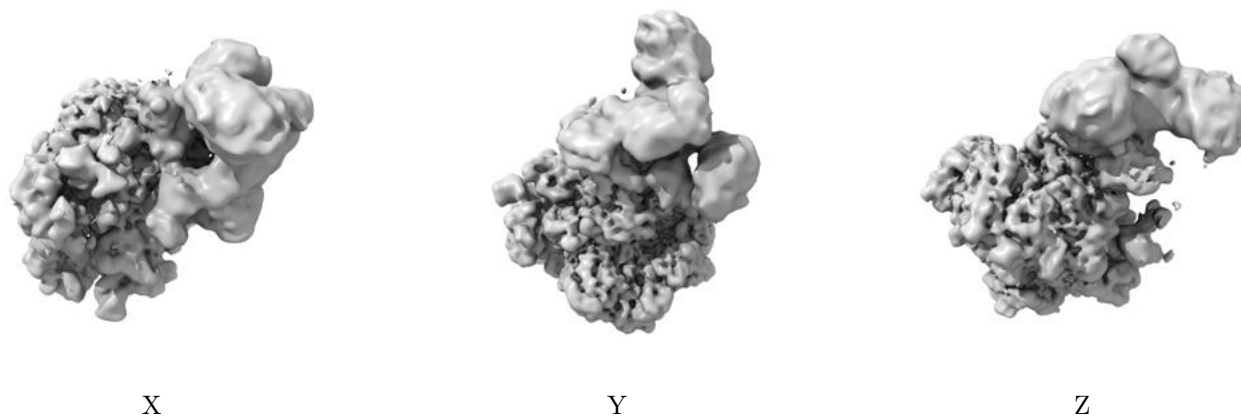


Z

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.

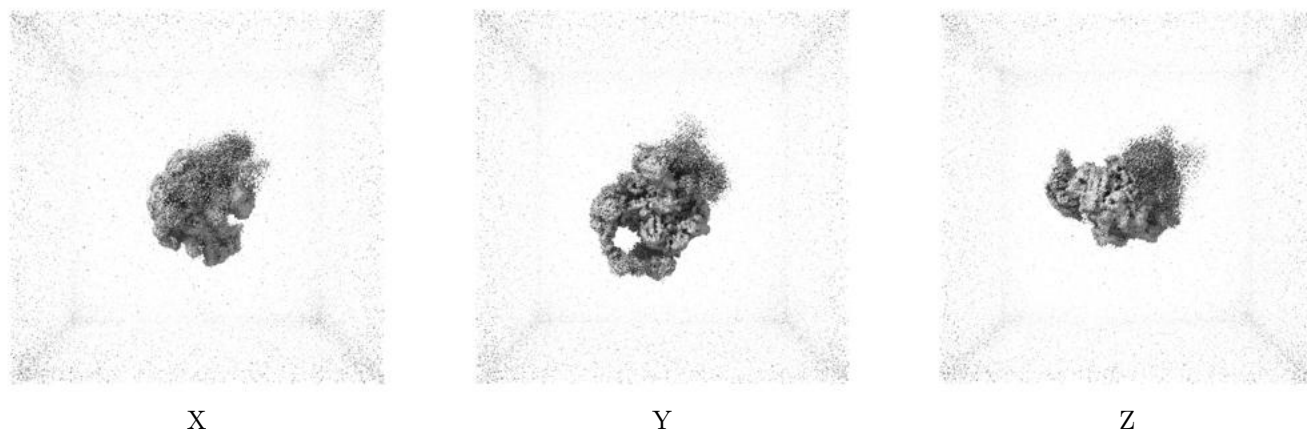
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.26. 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.

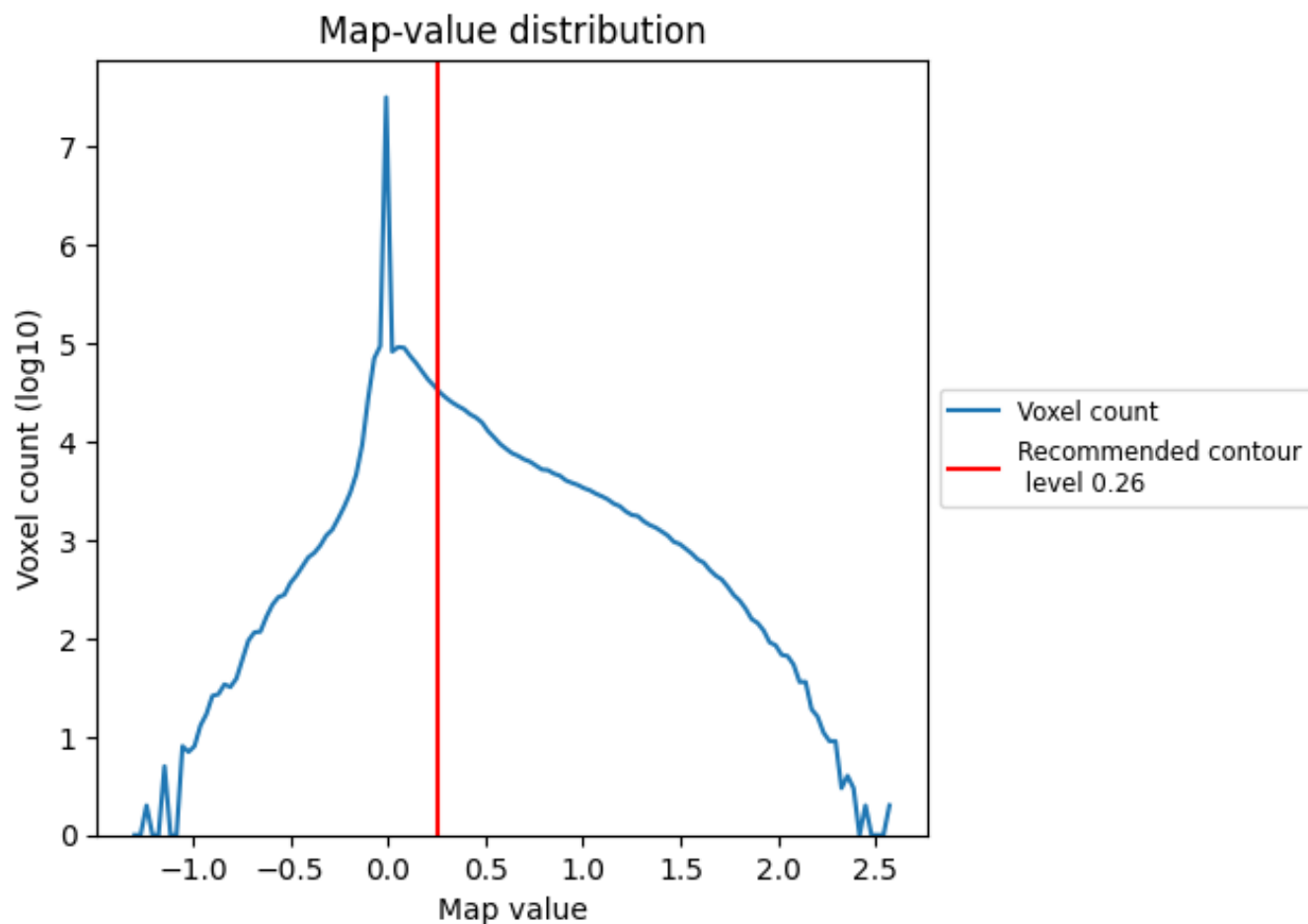
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

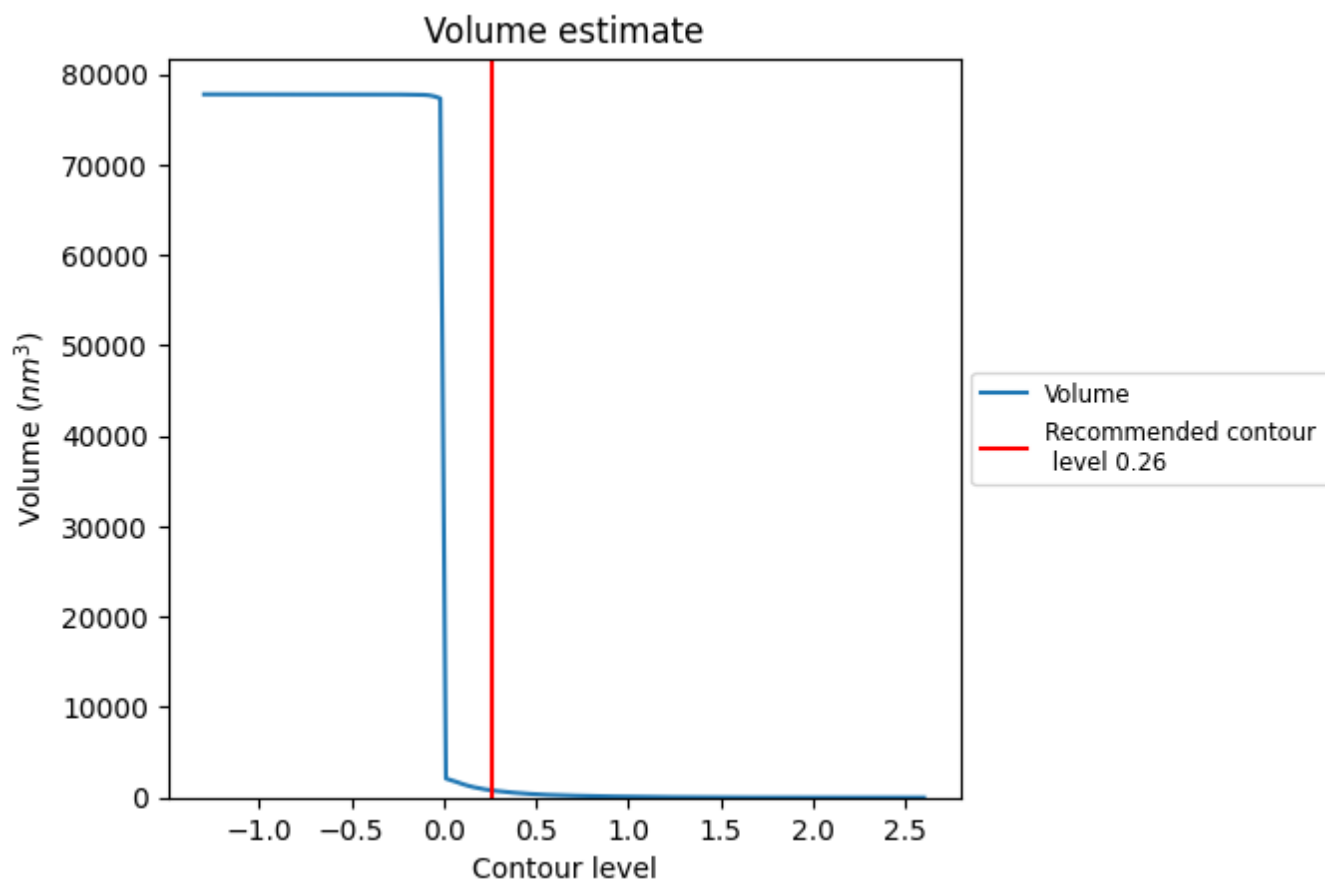
This section contains the results of statistical analysis of the map.

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.

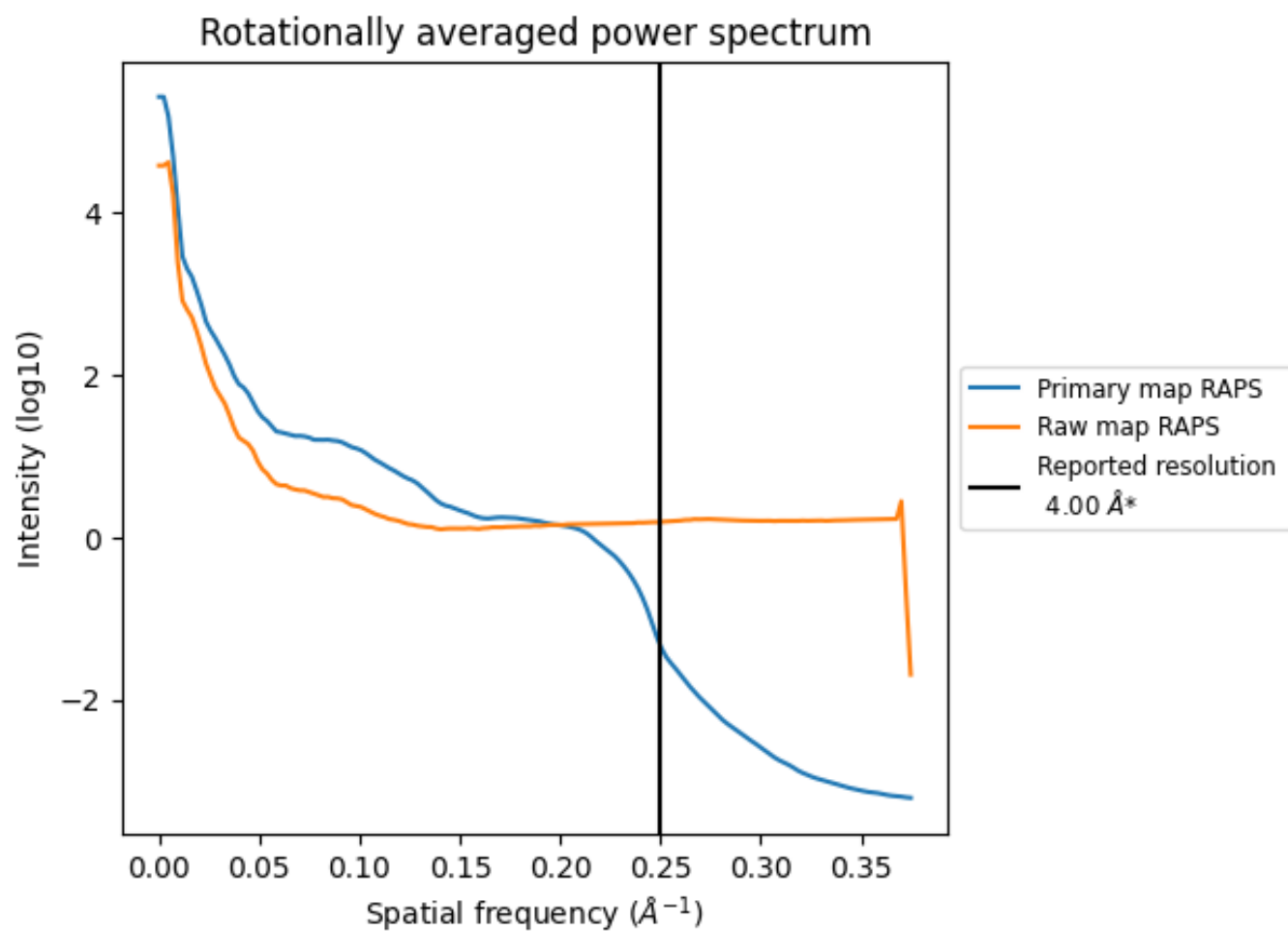
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 798 nm^3 ; this corresponds to an approximate mass of 720 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 ⓘ

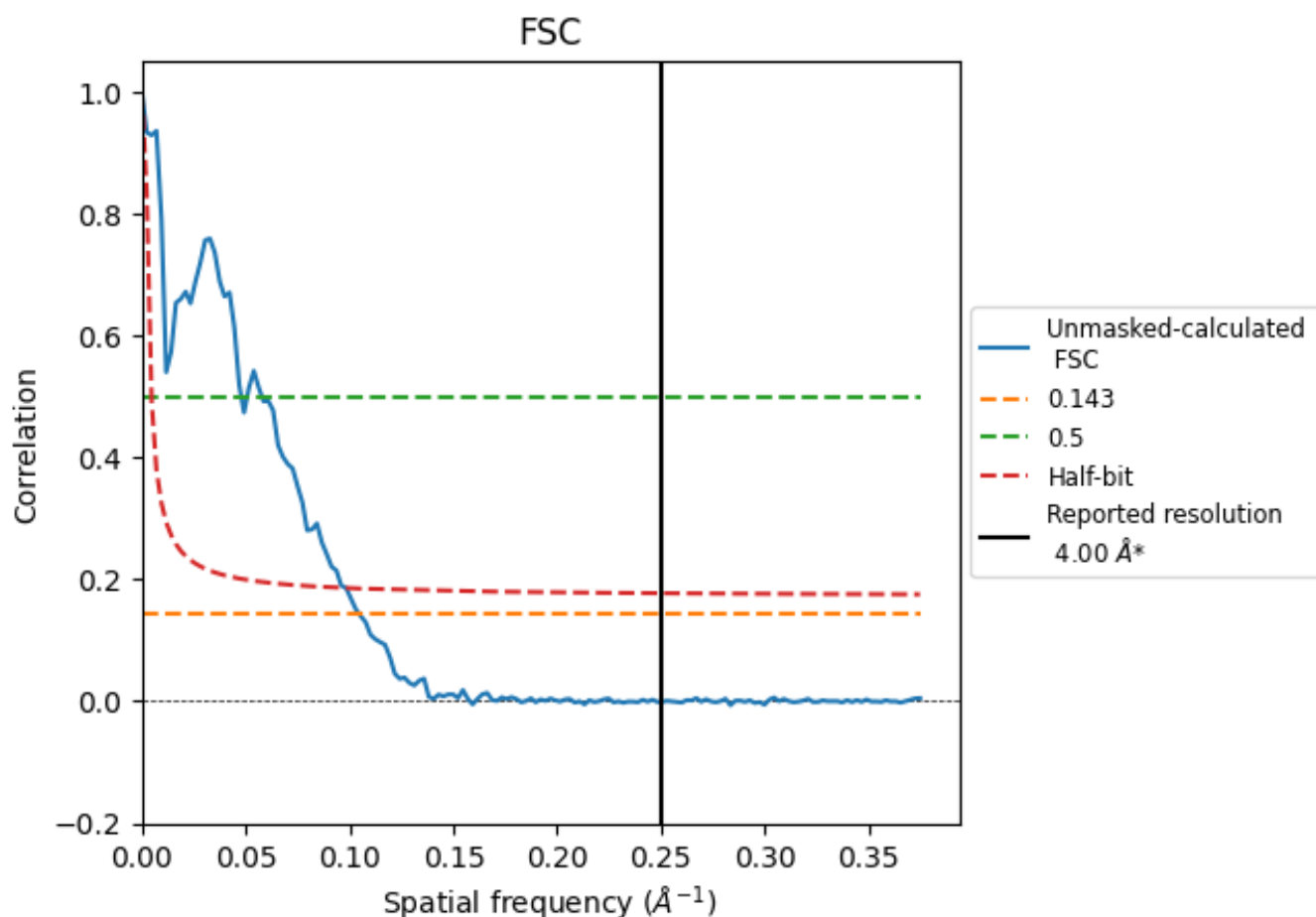


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

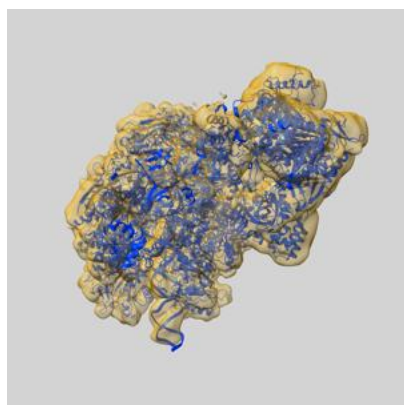
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.55	20.92	10.17

*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 9.55 differs from the reported value 4.0 by more than 10 %

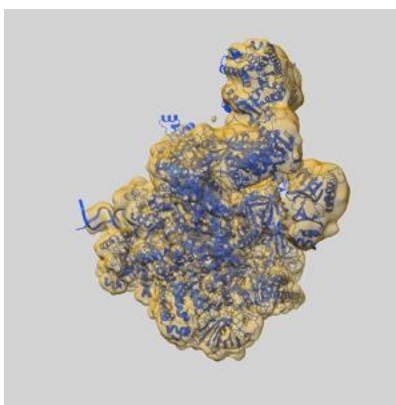
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37353 and PDB model 8W8F. Per-residue inclusion information can be found in section [3](#) on page [9](#).

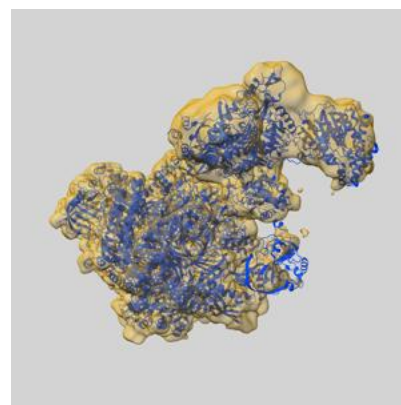
9.1 Map-model overlay [i](#)



X



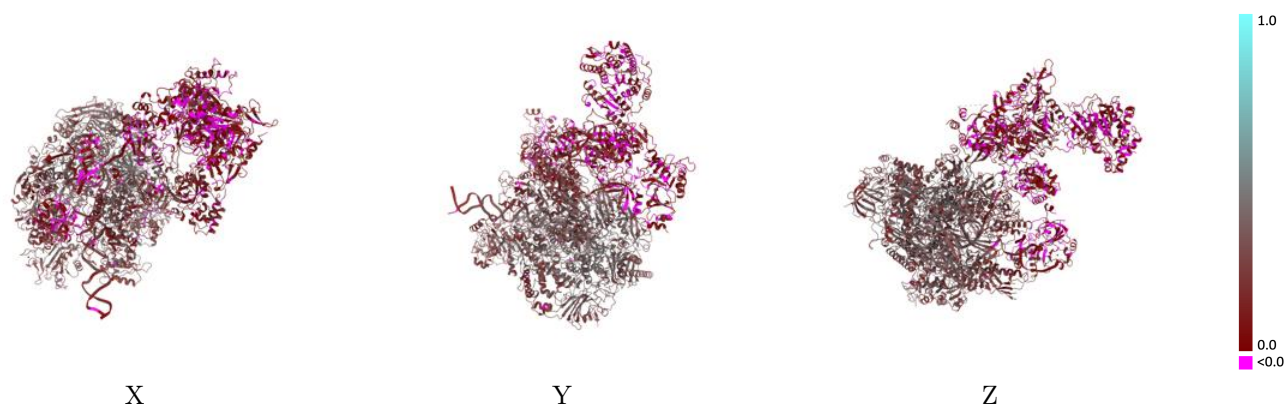
Y



Z

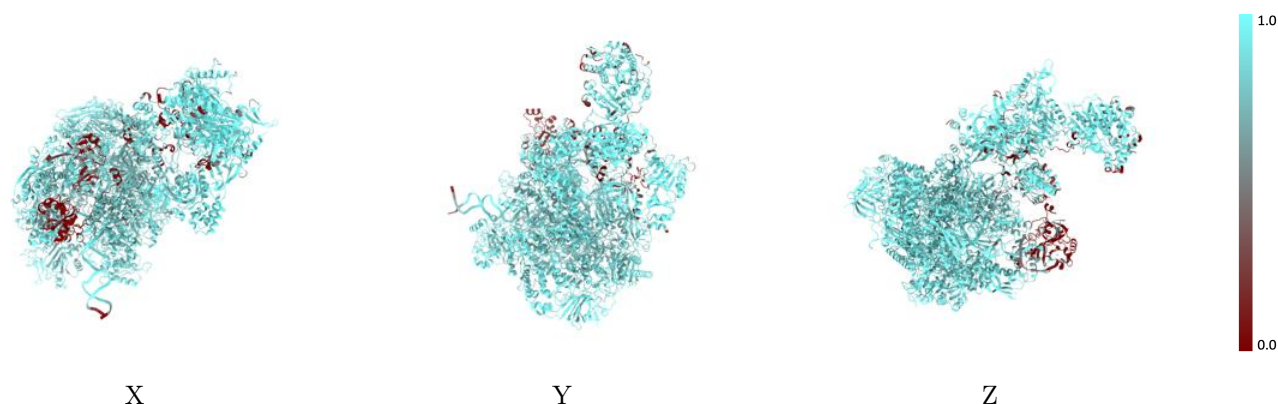
The images above show the 3D surface view of the map at the recommended contour level 0.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



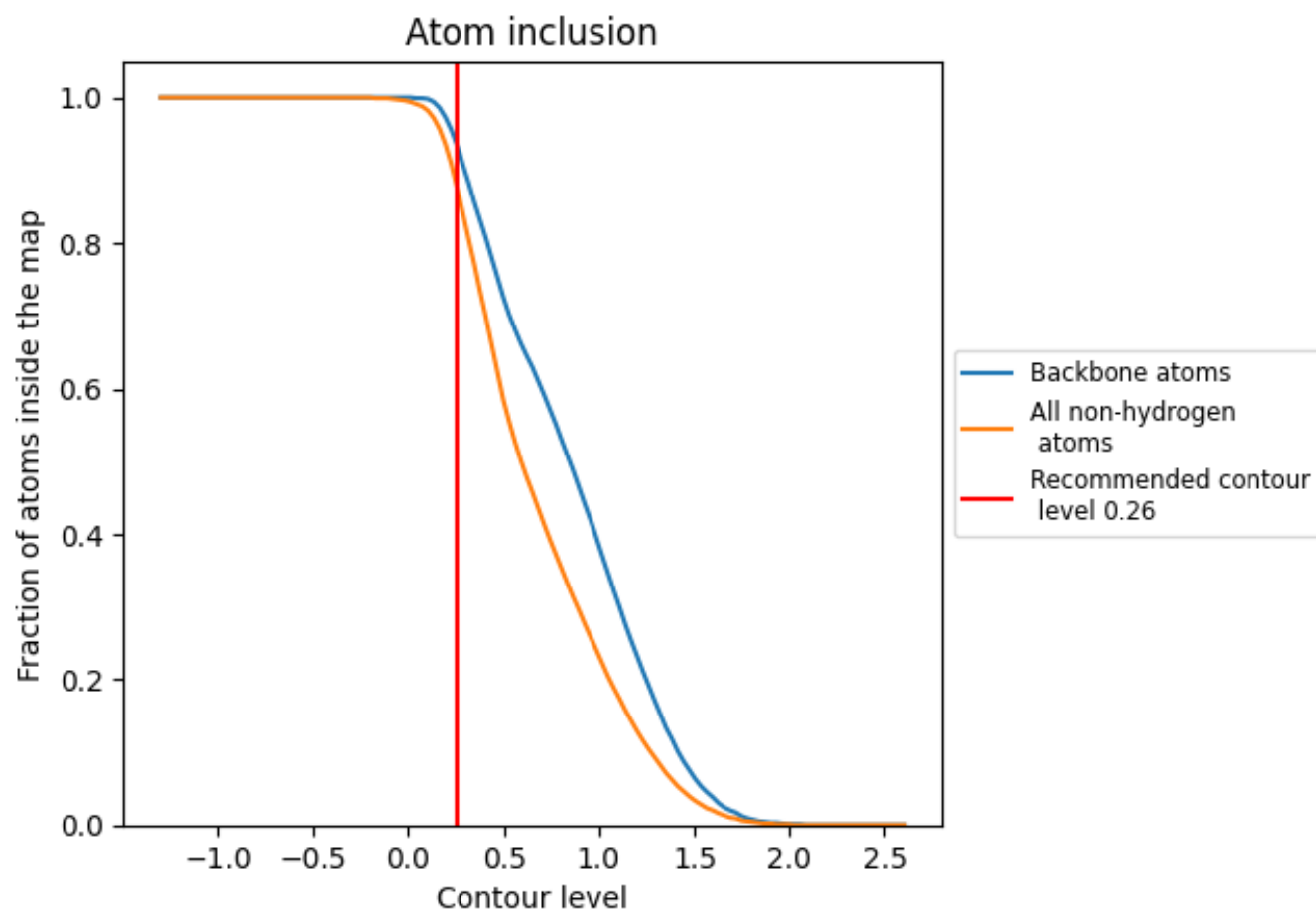
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.26).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (0.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8720	 0.2280
A	 0.9200	 0.3030
B	 0.9220	 0.3120
C	 0.9420	 0.3220
D	 0.9420	 0.1550
E	 0.9390	 0.2660
F	 0.8970	 0.3140
G	 0.9390	 0.1880
H	 0.9500	 0.3190
I	 0.9530	 0.2680
J	 0.9230	 0.3270
K	 0.9280	 0.3420
L	 0.9440	 0.2890
N	 0.8040	 0.1780
P	 0.8260	 0.2170
T	 0.8900	 0.2210
Y	 0.2110	 0.0700
Z	 0.5460	 0.0970
a	 0.8270	 0.0530
b	 0.8850	 0.0820

