



Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 10:49 pm BST

PDB ID : 9FYX / pdb_00009fyx
EMDB ID : EMD-50892
Title : Influenza A/H7N9 polymerase pre-cleavage cap-snatching complex
Authors : Rotsch, A.H.; Li, D.; Dienemann, C.; Cusack, S.; Cramer, P.
Deposited on : 2024-07-04
Resolution : 3.30 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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

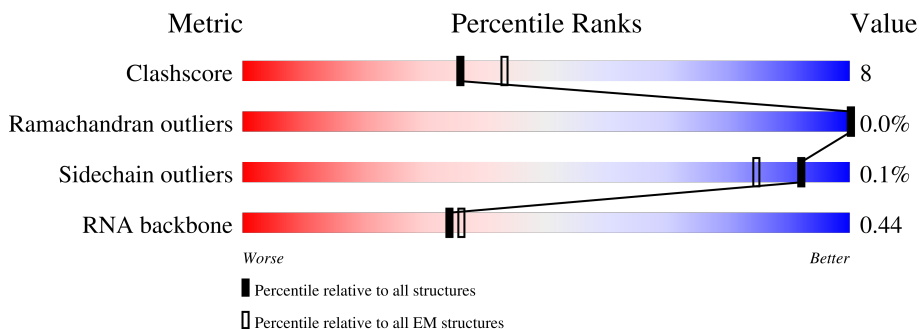
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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




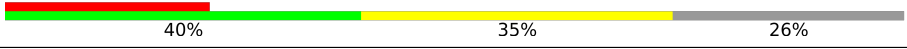

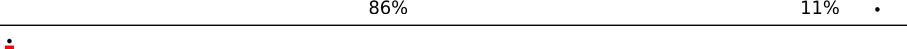
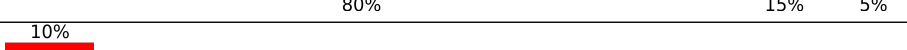
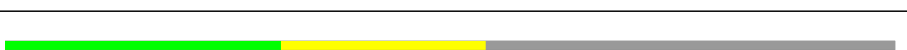
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	D	184	
2	E	210	
3	F	127	
4	G	171	
5	H	150	
6	I	125	
7	J	67	

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Mol	Chain	Length	Quality of chain
8	K	117	
9	L	58	
10	N	43	
11	P	35	
12	T	43	
13	Y	117	
14	Z	1087	
15	A	1641	
16	B	1160	
17	C	275	
18	a	717	
19	b	757	
20	c	759	
21	r	13	
22	v	14	
23	X	17	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 56176 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 RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	126	Total	C	N	O	S	0	0
			1030	642	175	209	4		

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

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

- Molecule 3 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	67	Total	C	N	O	S	0	0
			534	345	90	93	6		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 9 is a protein called RNA polymerase II, I and III subunit K.

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

- Molecule 10 is a DNA chain called non-template DNA (43-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	32	Total	C	N	O	P	0	0
			658	315	123	189	31		

- Molecule 11 is a RNA chain called cap(1)-RNA (35-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	26	Total	C	N	O	P	0	0
			568	254	118	170	26		

- Molecule 12 is a DNA chain called Template DNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	43	Total	C	N	O	P	0	0
			874	419	157	256	42		

- Molecule 13 is a protein called Transcription elongation factor SPT4.

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

- Molecule 14 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	470	Total	C	N	O	S	1	0
			3775	2408	663	688	16		

- Molecule 15 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	A	1435	Total	C	N	O	P	S	0	0
			11367	7143	2031	2121	2	70		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	527	THR	-	insertion	UNP I3LJR4
A	1300	GLY	-	insertion	UNP I3LJR4

- Molecule 16 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B	1131	Total	C	N	O	S	0	0
			9053	5727	1592	1670	64		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	C	261	Total	C	N	O	S	0	0
			2096	1314	360	416	6		

- Molecule 18 is a protein called Polymerase acidic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	702	Total	C	N	O	S	10	0
			5775	3652	981	1101	41		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	0	GLY	-	expression tag	UNP M9TI86
a	119	ASP	GLU	engineered mutation	UNP M9TI86

- Molecule 19 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	741	Total	C	N	O	S	0	0
			5911	3718	1035	1112	46		

- Molecule 20 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	736	Total	C	N	O	S	0	0
			5836	3667	1052	1077	40		

- Molecule 21 is a RNA chain called 3' vRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	r	7	Total	C	N	O	P	0	0
			143	64	20	52	7		

- Molecule 22 is a RNA chain called 5'-vRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	v	14	Total	C	N	O	P	0	0
			306	137	62	93	14		

- Molecule 23 is a protein called Likely SPT5 KOWx4-KOW5 linker, register unclear.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	17	Total	C	N	O	0	0
			90	56	17	17		

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

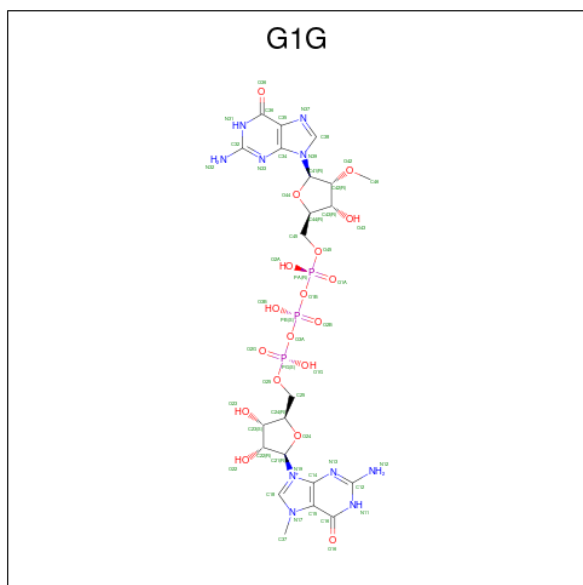
Mol	Chain	Residues	Atoms		AltConf
24	I	2	Total	Zn	0
			2	2	
24	J	1	Total	Zn	0
			1	1	
24	L	1	Total	Zn	0
			1	1	
24	Y	1	Total	Zn	0
			1	1	
24	A	2	Total	Zn	0
			2	2	
24	B	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
24	C	1	Total	Zn	0
			1	1	

- Molecule 25 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-(2'-O-METHYL)-GUANOSINE (CCD ID: G1G) (formula: $C_{22}H_{32}N_{10}O_{18}P_3$) (labeled as "Ligand of Interest" by depositor).

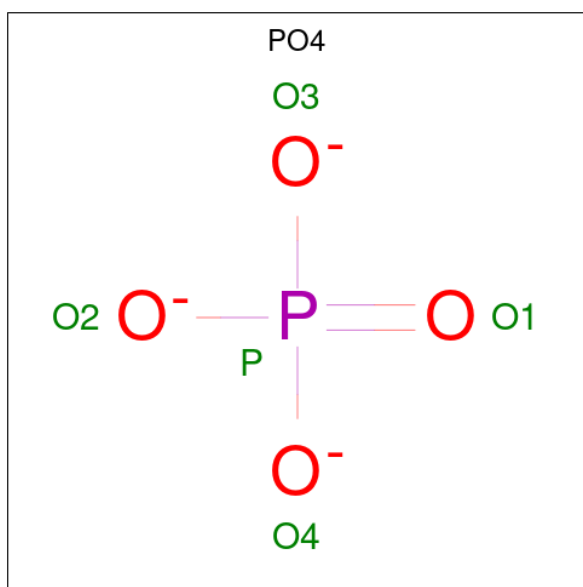


Mol	Chain	Residues	Atoms					AltConf
25	P	1	Total	C	N	O	P	0
			53	22	10	18	3	

- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	Mg	0
			1	1	
26	a	1	Total	Mg	0
			1	1	

- Molecule 27 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

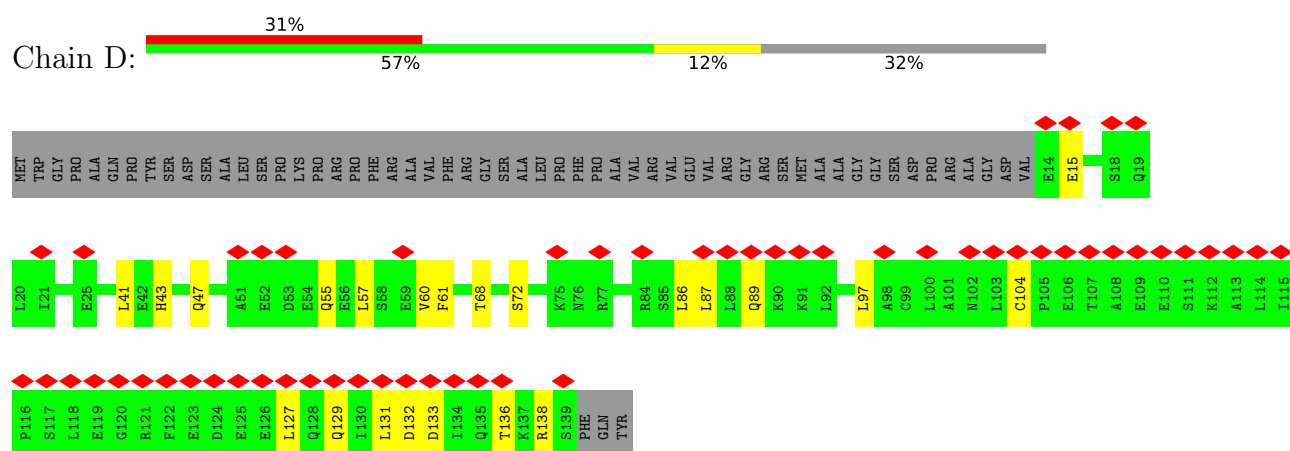


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
27	a	1	5	4	1	0
27	c	1	5	4	1	0

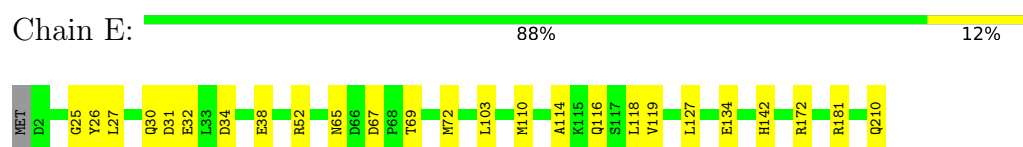
3 Residue-property plots

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.

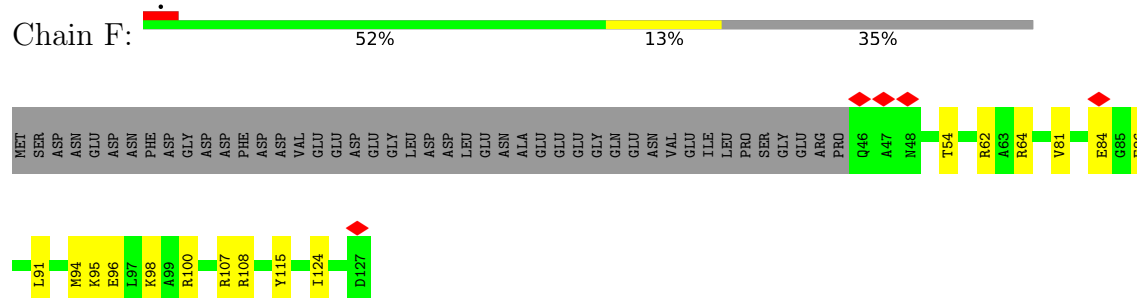
• Molecule 1: RNA polymerase II subunit D



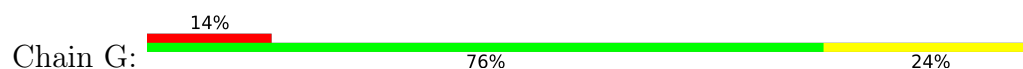
• Molecule 2: DNA-directed RNA polymerase II subunit E

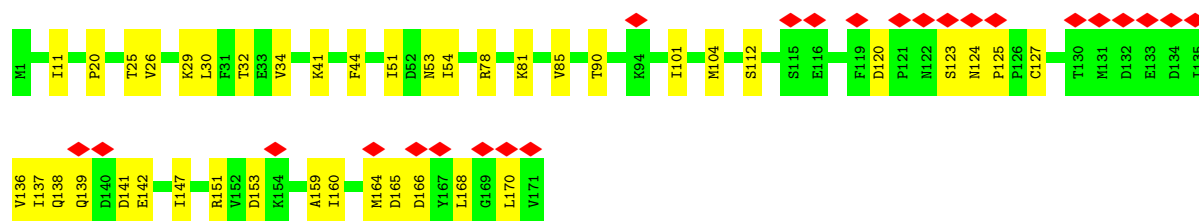


• Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC2

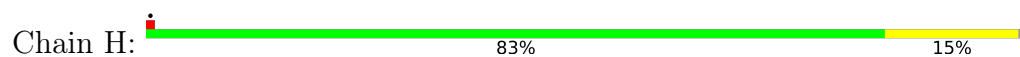


• Molecule 4: DNA-directed RNA polymerase subunit

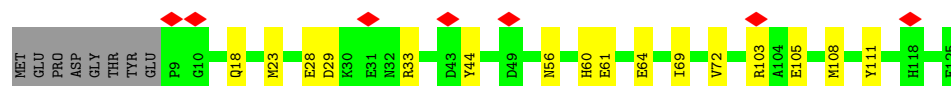
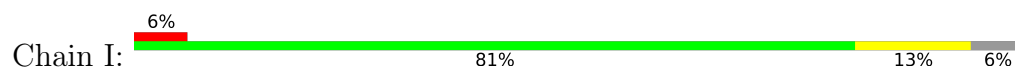




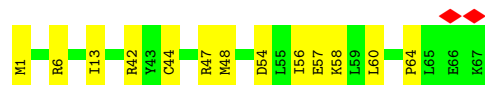
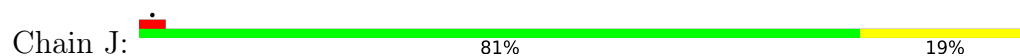
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC3



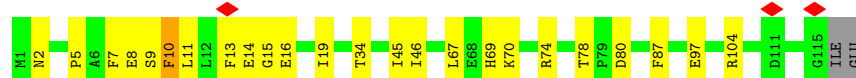
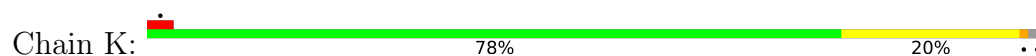
- Molecule 6: DNA-directed RNA polymerase II subunit RPB9



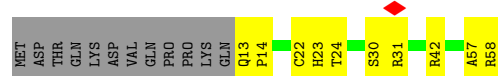
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC5



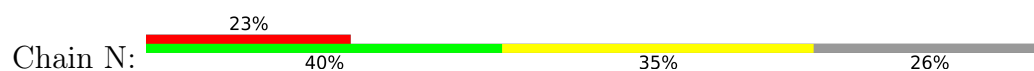
- Molecule 8: DNA-directed RNA polymerase II subunit RPB11-a

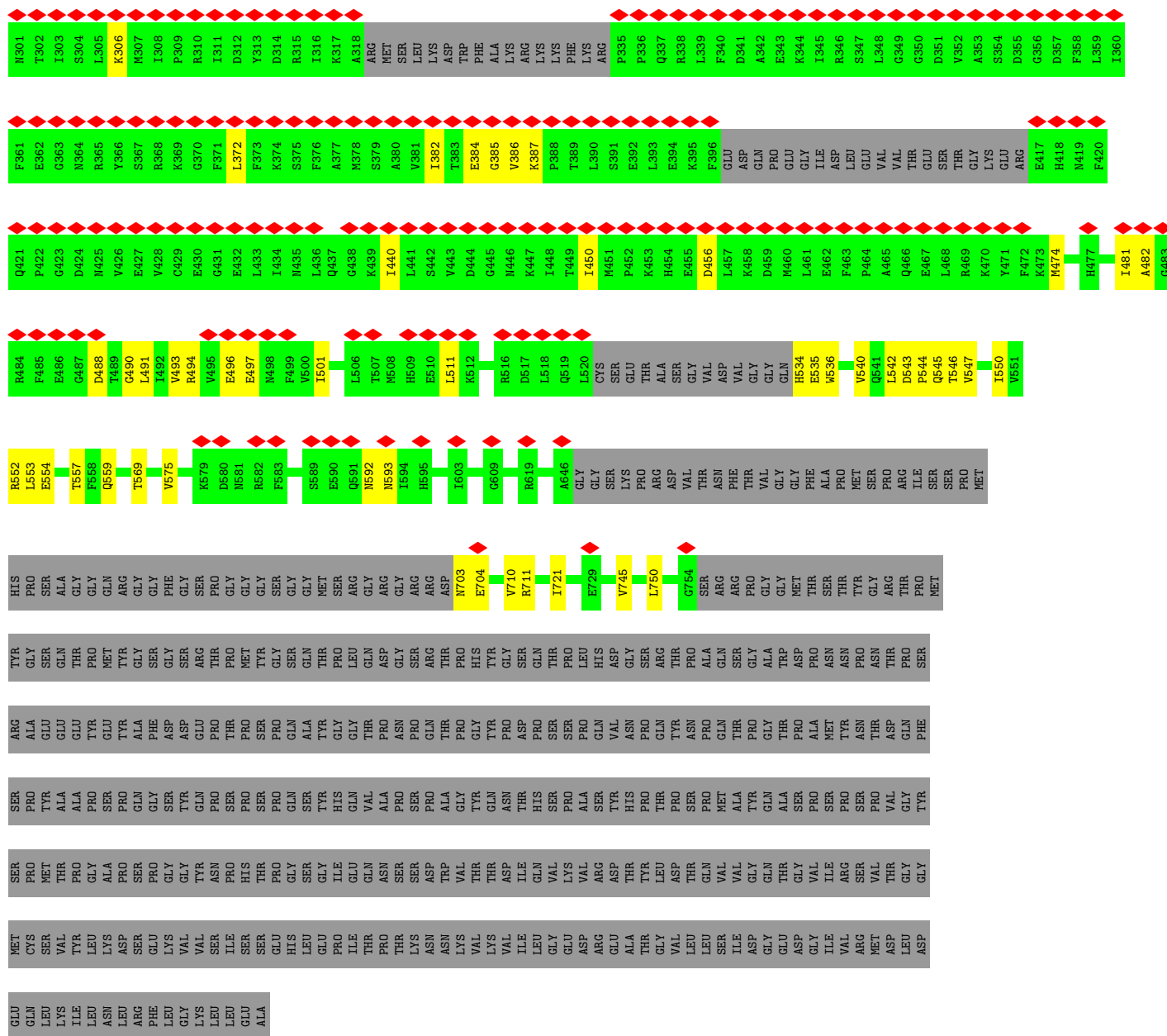


- Molecule 9: RNA polymerase II, I and III subunit K



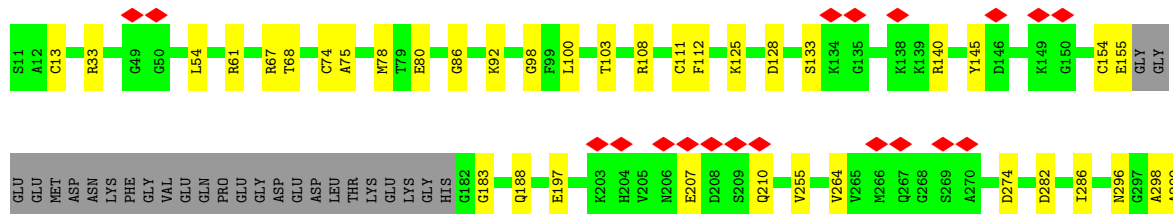
- Molecule 10: non-template DNA (43-mer)

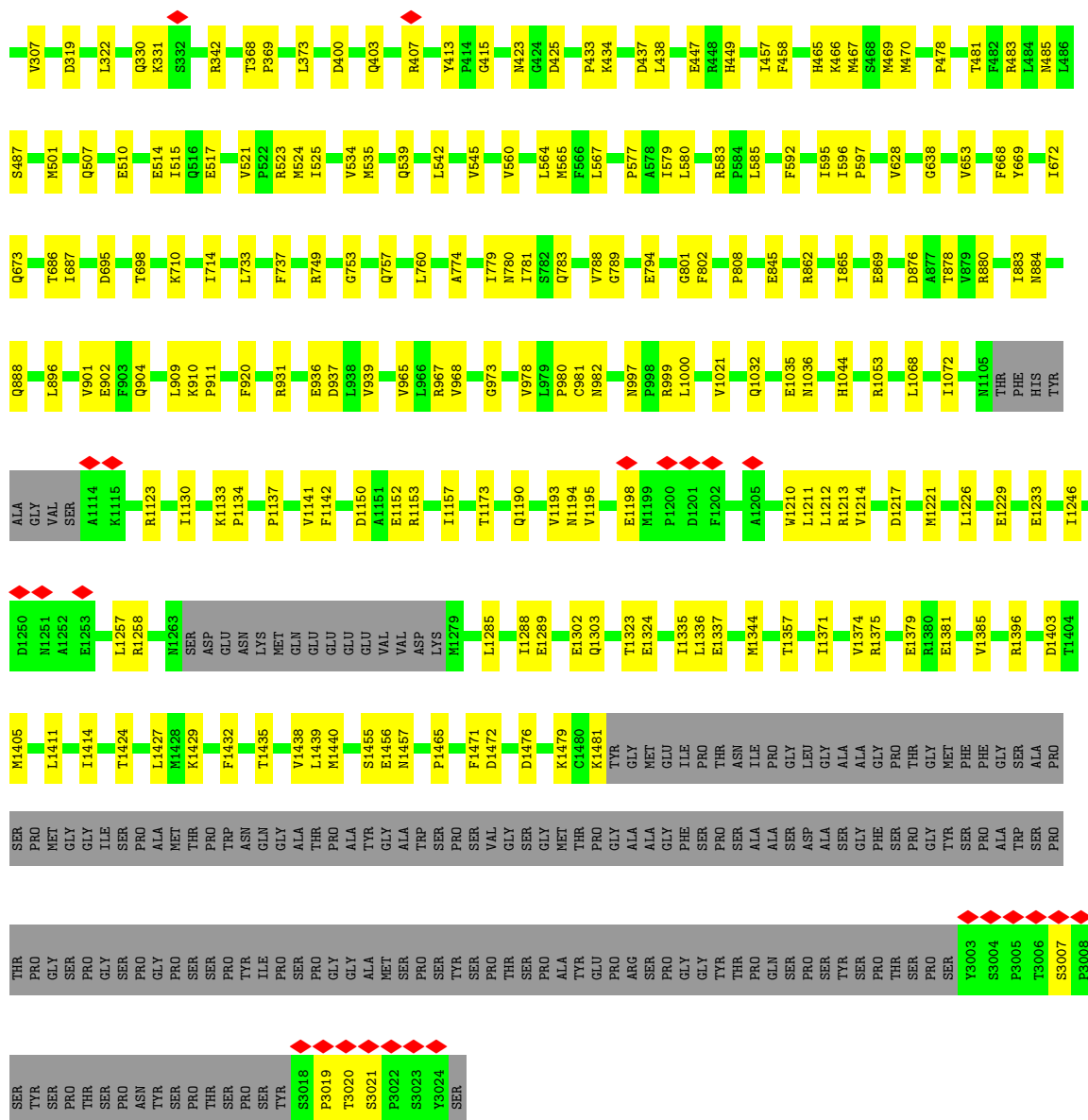




• Molecule 15: DNA-directed RNA polymerase subunit

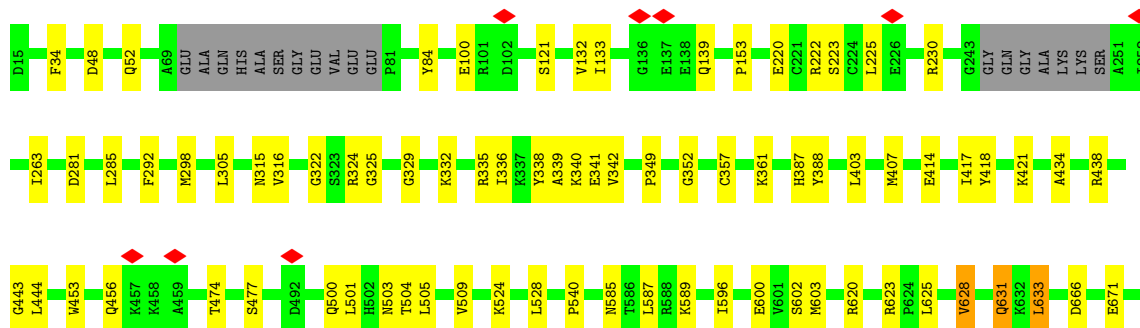
Chain A:

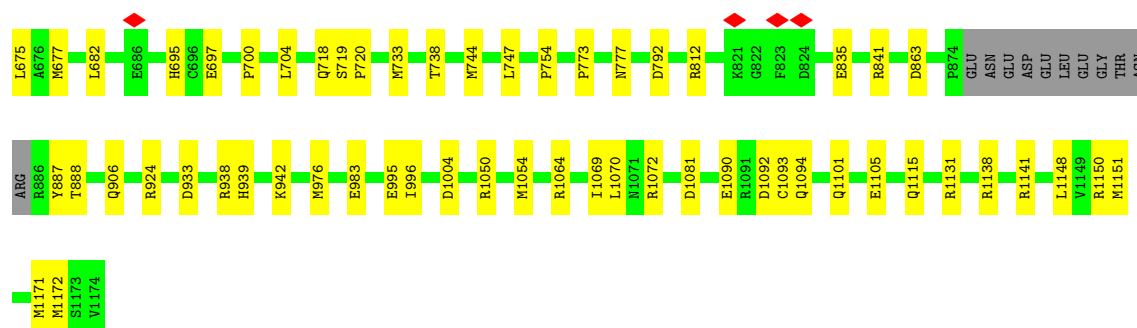




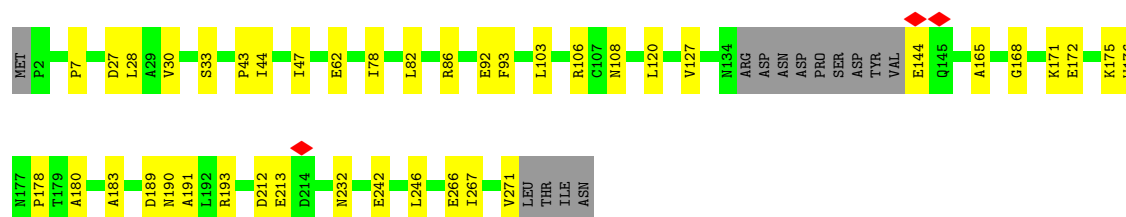
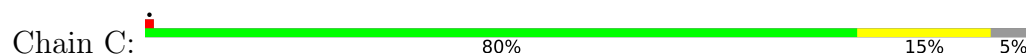
● Molecule 16: DNA-directed RNA polymerase subunit beta

Chain B: 86% 11%

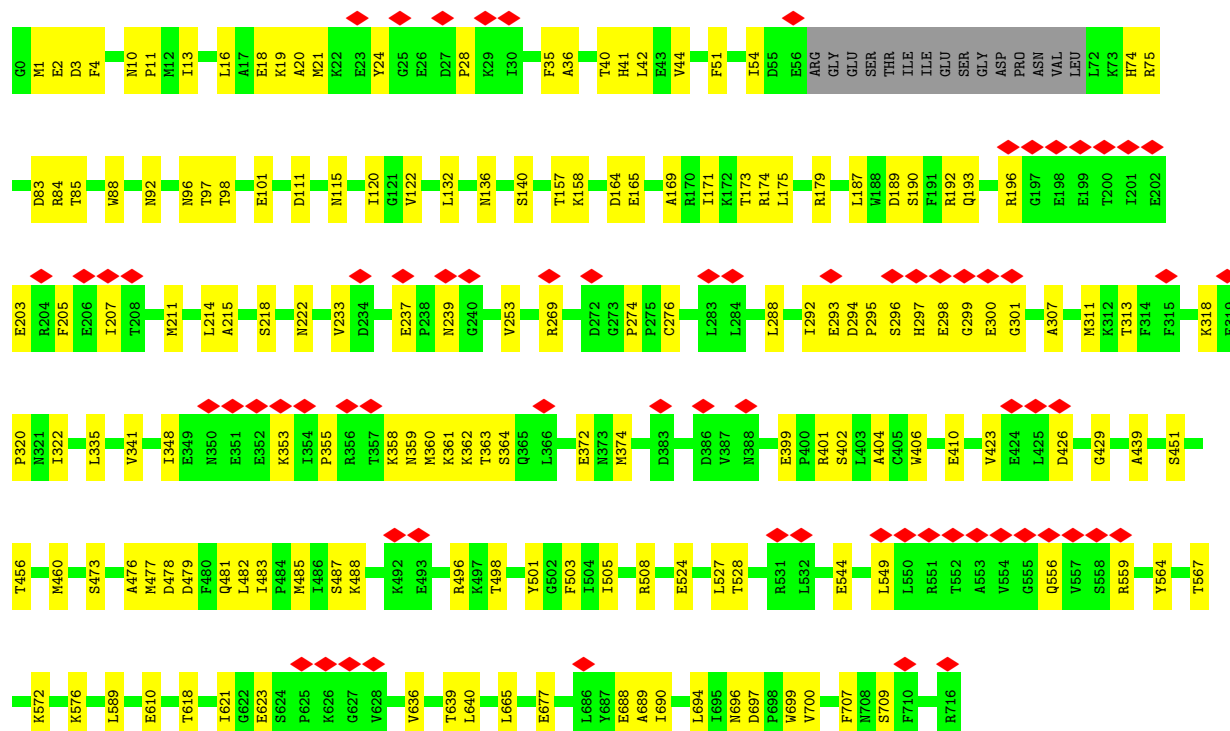
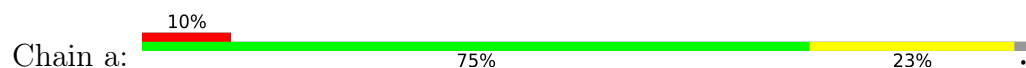




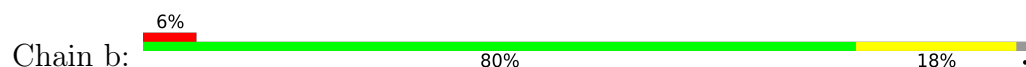
- Molecule 17: DNA-directed RNA polymerase II subunit RPB3

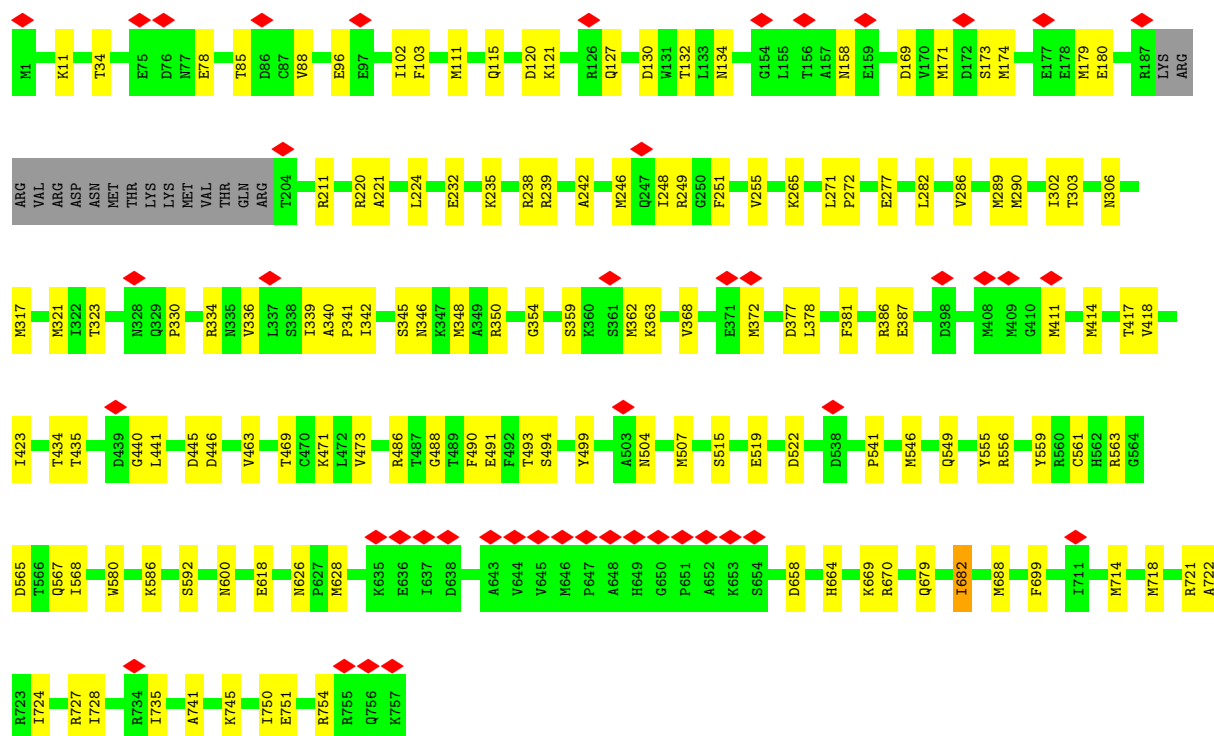


- Molecule 18: Polymerase acidic protein

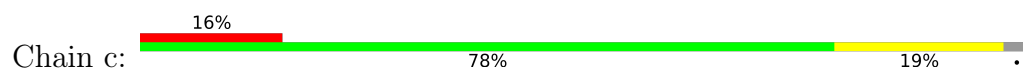


- Molecule 19: RNA-directed RNA polymerase catalytic subunit

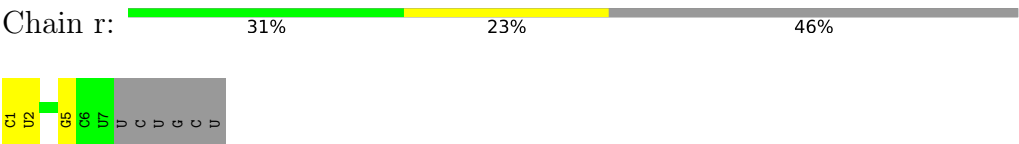




• Molecule 20: Polymerase basic protein 2



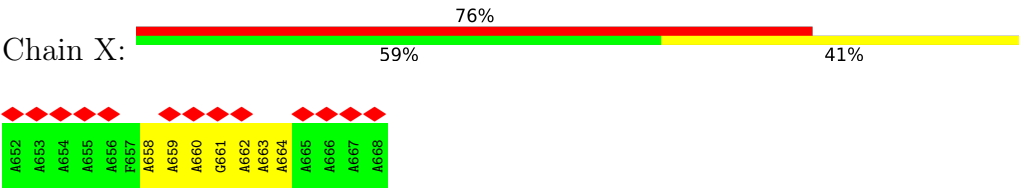
• Molecule 21: 3' vRNA



• Molecule 22: 5'-vRNA



• Molecule 23: Likely SPT5 KOWx4-KOW5 linker, register unclear



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	369858	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 ($e^-/\text{\AA}^2$)	39.94	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	470.39996, 470.39996, 470.39996	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, SEP, G1G, 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	D	0.13	0/1043	0.35	0/1400
2	E	0.19	0/1752	0.32	0/2366
3	F	0.22	0/668	0.35	0/901
4	G	0.19	0/1382	0.49	0/1874
5	H	0.25	0/1207	0.40	0/1628
6	I	0.18	0/973	0.34	0/1316
7	J	0.27	0/543	0.41	0/730
8	K	0.31	0/939	0.42	0/1271
9	L	0.19	0/395	0.35	0/524
10	N	0.30	0/738	0.59	0/1136
11	P	0.40	0/638	0.60	0/992
12	T	0.33	0/979	0.62	0/1508
13	Y	0.15	0/927	0.33	0/1250
14	Z	0.17	0/3845	0.39	0/5176
15	A	0.21	0/11554	0.38	0/15598
16	B	0.24	0/9234	0.41	1/12463 (0.0%)
17	C	0.28	0/2139	0.44	0/2906
18	a	0.14	0/5899	0.34	0/7952
19	b	0.13	0/6027	0.31	0/8126
20	c	0.13	0/5932	0.32	0/7997
21	r	0.21	0/157	0.42	0/241
22	v	0.24	0/344	0.43	0/535
23	X	0.13	0/90	0.44	0/123
All	All	0.20	0/57405	0.39	1/78013 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	631	GLN	N-CA-C	-6.98	102.03	111.87

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	D	1030	0	1016	15	0
2	E	1721	0	1737	19	0
3	F	658	0	684	12	0
4	G	1351	0	1358	28	0
5	H	1186	0	1147	16	0
6	I	950	0	879	11	0
7	J	534	0	553	11	0
8	K	920	0	942	20	0
9	L	389	0	393	9	0
10	N	658	0	364	13	0
11	P	568	0	288	27	0
12	T	874	0	487	25	0
13	Y	911	0	904	9	0
14	Z	3775	0	3849	60	0
15	A	11367	0	11469	176	0
16	B	9053	0	9087	116	0
17	C	2096	0	2040	30	0
18	a	5775	0	5687	144	0
19	b	5911	0	5901	117	0
20	c	5836	0	5972	116	0
21	r	143	0	75	4	0
22	v	306	0	153	3	0
23	X	90	0	86	7	0
24	A	2	0	0	0	0
24	B	1	0	0	0	0
24	C	1	0	0	0	0
24	I	2	0	0	0	0
24	J	1	0	0	0	0
24	L	1	0	0	0	0
24	Y	1	0	0	0	0
25	P	53	0	28	1	0
26	A	1	0	0	0	0
26	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	a	5	0	0	0	0
27	c	5	0	0	0	0
All	All	56176	0	55099	847	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (847) 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)
16:B:835:GLU:OE2	18:a:193:GLN:HG3	1.63	0.98
19:b:282:LEU:HD22	19:b:441:LEU:HD13	1.63	0.78
14:Z:536:TRP:CD1	18:a:136:ASN:HD22	2.05	0.74
14:Z:552:ARG:HB2	14:Z:559:GLN:HB2	1.70	0.74
16:B:387:HIS:NE2	16:B:671:GLU:OE2	2.26	0.69
19:b:246:MET:HA	19:b:246:MET:HE2	1.73	0.69
11:P:25:G:H8	16:B:1069:ILE:HG21	1.58	0.68
19:b:248:ILE:HD12	19:b:248:ILE:H	1.59	0.68
18:a:83:ASP:OD1	18:a:85:THR:HG22	1.94	0.67
20:c:370:ALA:HB2	20:c:393:SER:OG	1.94	0.67
19:b:751:GLU:OE1	19:b:754:ARG:NH2	2.27	0.67
18:a:88:TRP:O	18:a:92:ASN:ND2	2.28	0.67
20:c:717:ALA:N	20:c:720:GLU:OE2	2.28	0.66
15:A:274:ASP:OD2	15:A:342:ARG:NH2	2.28	0.66
16:B:995:GLU:HG2	16:B:996:ILE:H	1.60	0.65
18:a:697:ASP:OD1	18:a:699:TRP:N	2.28	0.65
19:b:669:LYS:N	20:c:56:PRO:O	2.29	0.65
20:c:267:VAL:O	20:c:271:THR:HG23	1.96	0.65
15:A:749:ARG:NH1	15:A:789:GLY:HA3	2.12	0.64
12:T:40:DT:H1'	12:T:41:DG:C8	2.32	0.64
14:Z:536:TRP:HD1	18:a:136:ASN:ND2	1.96	0.64
18:a:348:ILE:HD11	18:a:358:LYS:HD3	1.79	0.64
16:B:835:GLU:OE2	18:a:193:GLN:CG	2.42	0.64
14:Z:536:TRP:HD1	18:a:136:ASN:HD22	1.46	0.64
19:b:724:ILE:O	19:b:728:ILE:HD12	1.98	0.64
18:a:101:GLU:OE2	18:a:101:GLU:N	2.31	0.63
16:B:1090:GLU:OE1	16:B:1090:GLU:N	2.32	0.63
11:P:25:G:O3'	11:P:26:A:H4'	1.99	0.63
15:A:413:TYR:O	15:A:449:HIS:ND1	2.32	0.63
12:T:34:DT:H2'	12:T:35:DA:C8	2.34	0.63
1:D:133:ASP:O	1:D:136:THR:OG1	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b:423:ILE:HD12	19:b:469:THR:HG22	1.80	0.63
15:A:910:LYS:HD3	15:A:973:GLY:O	1.99	0.62
17:C:106:ARG:NH1	17:C:108:ASN:OD1	2.31	0.62
14:Z:553:LEU:O	18:a:132:LEU:HD13	1.98	0.62
19:b:180:GLU:OE2	19:b:211:ARG:NE	2.32	0.62
20:c:114:VAL:HG11	20:c:198:ILE:HD13	1.81	0.62
7:J:1:MET:N	16:B:754:PRO:HD2	2.14	0.62
18:a:203:GLU:OE1	19:b:115:GLN:NE2	2.30	0.62
16:B:357:CYS:SG	16:B:361:LYS:NZ	2.72	0.62
20:c:419:ASN:O	20:c:433:GLN:NE2	2.33	0.62
7:J:42:ARG:NH2	17:C:180:ALA:O	2.33	0.61
18:a:215:ALA:HB2	19:b:342:ILE:HD13	1.82	0.61
19:b:618:GLU:OE2	19:b:618:GLU:N	2.25	0.61
18:a:299[A]:GLY:O	19:b:568:ILE:HG23	2.00	0.61
19:b:580:TRP:O	19:b:586:LYS:NZ	2.32	0.61
20:c:143:ARG:HE	20:c:524:THR:HG21	1.65	0.61
3:F:100:ARG:NH2	3:F:124:ILE:HA	2.16	0.61
11:P:26:A:H3'	11:P:27:A:H8	1.66	0.61
18:a:211:MET:HE3	18:a:211:MET:HA	1.82	0.61
18:a:372:GLU:OE2	18:a:508:ARG:NH1	2.34	0.60
18:a:187:LEU:HD23	18:a:187:LEU:H	1.66	0.60
18:a:269:ARG:HB3	18:a:269:ARG:NH1	2.16	0.60
15:A:845:GLU:OE2	16:B:500:GLN:NE2	2.33	0.60
12:T:21:DG:H2'	12:T:22:DC:C6	2.36	0.60
16:B:1172:MET:HA	16:B:1172:MET:HE3	1.83	0.60
19:b:515:SER:N	19:b:522:ASP:OD1	2.34	0.60
15:A:904:GLN:NE2	15:A:981:CYS:O	2.33	0.60
16:B:1138:ARG:O	16:B:1141:ARG:NH1	2.35	0.59
18:a:288:LEU:HD22	18:a:527:LEU:HG	1.84	0.59
6:I:56:ASN:ND2	15:A:1289:GLU:OE2	2.34	0.59
20:c:143:ARG:HH11	20:c:143:ARG:HB3	1.66	0.59
11:P:13:A:OP1	18:a:122:VAL:N	2.35	0.59
15:A:487:SER:OG	15:A:673:GLN:NE2	2.34	0.59
8:K:5:PRO:HD2	8:K:8:GLU:OE2	2.01	0.59
18:a:41:HIS:NE2	18:a:120:ILE:O	2.36	0.59
19:b:323:THR:O	19:b:334:ARG:NH2	2.35	0.59
15:A:74:CYS:O	16:B:1131:ARG:NH2	2.36	0.59
18:a:10:ASN:O	18:a:13:ILE:HG22	2.01	0.59
16:B:1151:MET:HE1	16:B:1171:MET:SD	2.43	0.59
18:a:476:ALA:HB1	18:a:479:ASP:OD1	2.03	0.58
17:C:190:ASN:O	17:C:193:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:a:473:SER:O	18:a:477:MET:HG2	2.03	0.58
20:c:691:LEU:HD12	20:c:696:ILE:HD11	1.84	0.58
20:c:202:MET:HE2	20:c:202:MET:HA	1.85	0.58
20:c:697:LEU:HD21	20:c:735:MET:HG2	1.84	0.58
3:F:64:ARG:NH1	15:A:1471:PHE:O	2.36	0.58
18:a:51:PHE:CD1	18:a:51:PHE:O	2.56	0.58
18:a:164:ASP:OD1	18:a:165:GLU:N	2.37	0.58
18:a:399:GLU:O	18:a:696:ASN:ND2	2.36	0.58
19:b:679:GLN:O	19:b:682:ILE:HG22	2.04	0.57
16:B:933:ASP:OD2	16:B:1050:ARG:NH2	2.37	0.57
16:B:995:GLU:HG2	16:B:996:ILE:N	2.20	0.57
18:a:477:MET:HE1	21:r:5:G:C5	2.40	0.57
19:b:563:ARG:NH2	19:b:565:ASP:OD2	2.38	0.57
18:a:426:ASP:O	19:b:549:GLN:NE2	2.37	0.57
19:b:362:MET:HE3	19:b:362:MET:HA	1.86	0.57
3:F:54:THR:O	3:F:108:ARG:NH1	2.34	0.57
11:P:27:A:H2'	11:P:28:G:C8	2.39	0.57
19:b:282:LEU:HD23	19:b:441:LEU:HD22	1.86	0.57
11:P:10:A:O4'	18:a:84:ARG:NH2	2.37	0.57
18:a:423:VAL:HG12	18:a:460:MET:HE3	1.85	0.57
18:a:527:LEU:O	18:a:559:ARG:NH2	2.37	0.56
8:K:7:PHE:HB2	8:K:11:LEU:HD12	1.87	0.56
6:I:64:GLU:OE1	6:I:111:TYR:OH	2.23	0.56
7:J:1:MET:H2	16:B:754:PRO:HD2	1.71	0.56
13:Y:62:ALA:HB1	14:Z:197:MET:SD	2.44	0.56
15:A:67:ARG:HG3	15:A:68:THR:HG23	1.87	0.56
11:P:12:A:H4'	18:a:41:HIS:ND1	2.20	0.56
18:a:439:ALA:HB2	19:b:541:PRO:HB2	1.87	0.56
15:A:133:SER:O	15:A:140:ARG:NH2	2.37	0.56
18:a:318:LYS:NZ	18:a:544:GLU:OE2	2.30	0.56
7:J:47:ARG:NH1	16:B:777:ASN:O	2.34	0.56
14:Z:386:VAL:HG12	14:Z:387:LYS:H	1.71	0.56
16:B:48:ASP:O	16:B:52:GLN:OE1	2.24	0.56
15:A:78:MET:O	16:B:1072:ARG:NH2	2.37	0.56
14:Z:535:GLU:OE2	18:a:158:LYS:HA	2.06	0.56
16:B:628:VAL:HG13	16:B:695:HIS:CA	2.36	0.56
19:b:88:VAL:HG21	19:b:317:MET:SD	2.45	0.56
19:b:158:ASN:HB3	19:b:169:ASP:OD1	2.06	0.56
20:c:256:ASP:OD1	20:c:301:ASN:ND2	2.36	0.56
20:c:657:ASN:O	20:c:665:LEU:HD12	2.05	0.56
15:A:1190:GLN:O	15:A:1194:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:691:LEU:HB2	20:c:694:PHE:HB2	1.86	0.55
16:B:924:ARG:NH1	17:C:62:GLU:OE1	2.39	0.55
18:a:171:ILE:O	18:a:175:LEU:HD23	2.06	0.55
19:b:699:PHE:HE2	19:b:722:ALA:HB2	1.71	0.55
9:L:42:ARG:NE	16:B:100:GLU:OE2	2.40	0.55
14:Z:284:GLY:C	14:Z:286:TYR:H	2.14	0.55
19:b:434:THR:HG22	19:b:435:THR:H	1.72	0.55
6:I:29:ASP:O	6:I:33:ARG:N	2.36	0.55
17:C:172:GLU:HG2	17:C:176:TRP:CZ3	2.41	0.55
18:a:21:MET:HE3	18:a:28:PRO:HB3	1.88	0.55
16:B:744:MET:SD	16:B:906:GLN:NE2	2.76	0.55
17:C:78:ILE:HG12	17:C:82:LEU:HD13	1.89	0.55
18:a:322:ILE:HD11	18:a:335:LEU:HB2	1.88	0.55
20:c:725:LEU:HD23	20:c:731:VAL:HG22	1.89	0.55
15:A:3019:PRO:O	18:a:527:LEU:HD12	2.07	0.55
14:Z:703:ASN:OD1	14:Z:704:GLU:N	2.38	0.55
15:A:282:ASP:O	15:A:286:ILE:HD12	2.07	0.55
16:B:587:LEU:HB3	16:B:603:MET:SD	2.47	0.55
16:B:220:GLU:OE2	16:B:222:ARG:NH1	2.40	0.54
4:G:90:THR:O	4:G:139:GLN:NE2	2.36	0.54
4:G:124:ASN:HB2	4:G:125:PRO:HD3	1.89	0.54
18:a:353:LYS:C	18:a:355:PRO:HD3	2.32	0.54
19:b:411:MET:O	19:b:411:MET:HG3	2.07	0.54
8:K:104:ARG:NH1	17:C:7:PRO:O	2.34	0.54
4:G:41:LYS:O	4:G:78:ARG:NH1	2.40	0.54
18:a:214:LEU:HD22	19:b:346:ASN:HD22	1.71	0.54
18:a:610:GLU:OE1	18:a:610:GLU:N	2.37	0.54
19:b:559:TYR:CE1	20:c:47:MET:HE3	2.43	0.54
11:P:25:G:C8	16:B:1069:ILE:HG21	2.42	0.54
4:G:138:GLN:N	4:G:141:ASP:OD2	2.39	0.54
18:a:359:ASN:ND2	18:a:479:ASP:OD2	2.41	0.54
19:b:372:MET:CG	19:b:372:MET:O	2.55	0.54
15:A:783:GLN:NE2	15:A:788:VAL:O	2.38	0.54
11:P:34:G:C2	12:T:23:DC:O2	2.61	0.54
20:c:570:MET:HE2	20:c:570:MET:HA	1.89	0.54
19:b:519:GLU:OE1	19:b:664:HIS:ND1	2.42	0.54
9:L:22:CYS:SG	9:L:24:THR:OG1	2.61	0.53
11:P:34:G:C2	11:P:35:C:C2	2.96	0.53
13:Y:61:ILE:N	13:Y:85:TYR:O	2.33	0.53
20:c:114:VAL:HG11	20:c:198:ILE:CD1	2.37	0.53
5:H:103:GLU:OE2	15:A:999:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:54:LEU:O	15:A:61:ARG:NH2	2.41	0.53
15:A:469:MET:HE3	16:B:1094:GLN:HG2	1.90	0.53
2:E:26:TYR:CE2	2:E:72:MET:SD	3.02	0.53
20:c:180:GLU:HA	20:c:183:LEU:HD23	1.91	0.53
15:A:749:ARG:HH11	15:A:789:GLY:HA3	1.74	0.53
17:C:212:ASP:OD1	17:C:213:GLU:N	2.41	0.53
15:A:1142:PHE:CD1	15:A:1335:ILE:HD12	2.44	0.53
18:a:677:GLU:OE2	19:b:486:ARG:NH2	2.37	0.53
20:c:146:ASP:OD1	20:c:146:ASP:O	2.27	0.53
12:T:32:DA:H2''	12:T:33:DC:OP2	2.08	0.53
18:a:488:LYS:NZ	18:a:498:THR:OG1	2.24	0.53
19:b:34:THR:HG21	19:b:354:GLY:O	2.09	0.53
15:A:780:ASN:HA	16:B:976:MET:CE	2.39	0.53
18:a:97:THR:HG23	18:a:98:THR:HG23	1.91	0.53
18:a:360:MET:HE3	18:a:482:LEU:HB2	1.90	0.53
14:Z:745:VAL:HG13	14:Z:750:LEU:HD11	1.90	0.52
15:A:780:ASN:HA	16:B:976:MET:HE2	1.90	0.52
19:b:78:GLU:O	19:b:471:LYS:NZ	2.42	0.52
20:c:185:ILE:HA	20:c:188:GLU:OE1	2.09	0.52
14:Z:592:ASN:OD1	14:Z:593:ASN:N	2.43	0.52
16:B:338:TYR:O	16:B:341:GLU:HG3	2.08	0.52
20:c:279:SER:O	20:c:283:MET:HE3	2.09	0.52
18:a:169:ALA:O	18:a:173:THR:HG23	2.09	0.52
19:b:317:MET:O	19:b:321:MET:HG3	2.08	0.52
11:P:24:A:H2'	11:P:25:G:N2	2.23	0.52
3:F:86:GLU:OE1	3:F:86:GLU:N	2.30	0.52
15:A:1198:GLU:OE1	15:A:1198:GLU:N	2.43	0.52
20:c:327:GLY:HA2	23:X:658:ALA:HA	1.92	0.52
16:B:230:ARG:N	16:B:230:ARG:HD2	2.25	0.52
12:T:31:DT:OP1	16:B:456:GLN:NE2	2.43	0.52
14:Z:496:GLU:HG2	14:Z:497:GLU:H	1.74	0.52
15:A:628:VAL:HA	15:A:638:GLY:HA3	1.91	0.52
1:D:55:GLN:NE2	14:Z:545:GLN:OE1	2.42	0.52
14:Z:553:LEU:HB2	18:a:132:LEU:HB2	1.91	0.52
15:A:1214:VAL:CG2	15:A:1257:LEU:HG	2.40	0.52
18:a:524:GLU:OE1	18:a:524:GLU:N	2.43	0.52
20:c:181:SER:O	20:c:185:ILE:HG23	2.10	0.52
1:D:132:ASP:OD1	1:D:133:ASP:N	2.43	0.51
15:A:862:ARG:NH2	15:A:1432:PHE:O	2.42	0.51
12:T:31:DT:H2''	12:T:32:DA:H5'	1.91	0.51
15:A:465:HIS:CD2	15:A:467:MET:HB2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:528:LEU:HD23	16:B:704:LEU:O	2.10	0.51
19:b:491:GLU:OE2	19:b:494:SER:N	2.43	0.51
20:c:506:ASP:OD1	20:c:507:GLN:N	2.40	0.51
6:I:61:GLU:O	6:I:61:GLU:HG2	2.09	0.51
19:b:289:MET:HE3	19:b:440:GLY:HA2	1.93	0.51
2:E:38:GLU:OE1	2:E:38:GLU:N	2.39	0.51
14:Z:456:ASP:CG	14:Z:456:ASP:O	2.54	0.51
15:A:1133:LYS:HD2	15:A:1133:LYS:O	2.10	0.51
19:b:377:ASP:OD1	19:b:378:LEU:N	2.43	0.51
20:c:614:GLN:NE2	20:c:649:VAL:O	2.40	0.51
15:A:577:PRO:HG2	15:A:580:LEU:HD23	1.93	0.51
17:C:183:ALA:HB3	17:C:232:ASN:HB3	1.92	0.51
11:P:23:C:HO2'	11:P:24:A:H8	1.55	0.51
15:A:1152:GLU:HG2	15:A:1153:ARG:HD2	1.93	0.51
15:A:901:VAL:HB	15:A:978:VAL:HG12	1.92	0.51
16:B:407:MET:HE1	16:B:444:LEU:HG	1.92	0.51
19:b:224:LEU:N	19:b:348:MET:O	2.43	0.51
18:a:322:ILE:CD1	18:a:335:LEU:HD22	2.41	0.51
18:a:697:ASP:O	18:a:700:VAL:HG12	2.10	0.51
19:b:248:ILE:HD12	19:b:248:ILE:N	2.26	0.51
4:G:104:MET:HE2	4:G:159:ALA:HB2	1.92	0.51
5:H:92:MET:HB2	5:H:143:LEU:HB2	1.93	0.51
10:N:37:DC:H2''	10:N:38:DT:OP2	2.10	0.50
18:a:363:THR:HG22	18:a:364:SER:N	2.25	0.50
20:c:179:SER:O	20:c:183:LEU:HD22	2.10	0.50
14:Z:199:LYS:NZ	14:Z:240:GLU:O	2.44	0.50
6:I:28:GLU:OE1	6:I:28:GLU:N	2.43	0.50
15:A:125:LYS:O	15:A:128:ASP:OD1	2.29	0.50
16:B:1069:ILE:HG13	16:B:1070:LEU:N	2.26	0.50
18:a:320:PRO:HG2	18:a:335:LEU:HD11	1.94	0.50
19:b:555:TYR:OH	19:b:592:SER:OG	2.29	0.50
8:K:14:GLU:O	8:K:15:GLY:C	2.54	0.50
11:P:27:A:H2'	11:P:28:G:H8	1.77	0.50
19:b:387:GLU:N	19:b:387:GLU:OE1	2.44	0.50
20:c:11:MET:HE3	20:c:17:ARG:HG3	1.94	0.50
16:B:628:VAL:HG13	16:B:695:HIS:N	2.26	0.50
14:Z:490:GLY:O	14:Z:491:LEU:HD12	2.12	0.50
18:a:21:MET:HE1	18:a:35:PHE:HD1	1.76	0.50
18:a:36:ALA:O	18:a:40:THR:HG22	2.12	0.50
15:A:403:GLN:O	15:A:407:ARG:HG3	2.11	0.50
18:a:298[A]:GLU:HA	18:a:488:LYS:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b:340:ALA:HB3	19:b:341:PRO:HD3	1.93	0.50
7:J:6:ARG:HD3	7:J:13:ILE:HD13	1.93	0.50
9:L:57:ALA:O	17:C:175:LYS:NZ	2.44	0.50
15:A:896:LEU:HD13	15:A:980:PRO:HG3	1.94	0.50
16:B:339:ALA:O	16:B:342:VAL:N	2.45	0.50
18:a:75:ARG:NH2	18:a:111:ASP:OD2	2.45	0.50
20:c:653:SER:O	20:c:657:ASN:OD1	2.30	0.50
14:Z:553:LEU:H	18:a:136:ASN:HD21	1.60	0.49
15:A:407:ARG:NH1	20:c:469:PRO:O	2.45	0.49
18:a:192:ARG:CZ	18:a:192:ARG:O	2.60	0.49
18:a:211:MET:SD	19:b:174:MET:HE1	2.52	0.49
20:c:279:SER:C	20:c:283:MET:HE3	2.37	0.49
15:A:507:GLN:N	16:B:1105:GLU:OE2	2.33	0.49
15:A:567:LEU:HD21	15:A:595:ILE:HG12	1.93	0.49
19:b:735:ILE:HD12	19:b:735:ILE:C	2.37	0.49
2:E:110:MET:HG2	2:E:114:ALA:HB3	1.94	0.49
4:G:11:ILE:HD11	4:G:26:VAL:HG13	1.94	0.49
19:b:224:LEU:HG	19:b:242:ALA:HB1	1.94	0.49
20:c:461:ILE:HD12	20:c:462:GLY:O	2.12	0.49
6:I:108:MET:HE1	15:A:737:PHE:CD2	2.48	0.49
15:A:197:GLU:N	15:A:197:GLU:OE1	2.44	0.49
15:A:467:MET:SD	15:A:524:MET:HB3	2.52	0.49
16:B:324:ARG:HG2	16:B:324:ARG:HH11	1.78	0.49
16:B:747:LEU:HD21	16:B:812:ARG:CZ	2.42	0.49
18:a:429:GLY:O	19:b:600:ASN:ND2	2.46	0.49
20:c:327:GLY:CA	23:X:658:ALA:HA	2.42	0.49
15:A:1032:GLN:OE1	15:A:1036:ASN:ND2	2.45	0.49
15:A:1035:GLU:OE1	15:A:1036:ASN:ND2	2.44	0.49
18:a:292:ILE:HD12	18:a:294[A]:ASP:HB2	1.94	0.49
20:c:60:ASP:OD1	20:c:88:ARG:NH1	2.45	0.49
2:E:72:MET:HE2	2:E:103:LEU:CD1	2.42	0.49
8:K:10:PHE:HZ	17:C:172:GLU:CD	2.21	0.49
15:A:1130:ILE:HD13	15:A:1411:LEU:HB3	1.95	0.49
16:B:938:ARG:NH2	16:B:983:GLU:OE2	2.39	0.49
19:b:688:MET:HE1	20:c:15:ARG:CG	2.43	0.49
20:c:571:LEU:CD2	20:c:619:LEU:HD11	2.43	0.49
12:T:35:DA:H8	12:T:35:DA:OP2	1.96	0.49
19:b:488:GLY:HA3	19:b:499:TYR:CE2	2.48	0.49
20:c:412:LYS:O	20:c:415:ARG:NH1	2.35	0.49
15:A:937:ASP:OD1	15:A:937:ASP:N	2.44	0.49
16:B:388:TYR:OH	16:B:524:LYS:HE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:a:174:ARG:HD2	18:a:174:ARG:O	2.13	0.49
18:a:341:VAL:CG2	18:a:505:ILE:HD11	2.43	0.49
19:b:111:MET:HE1	19:b:330:PRO:HG2	1.95	0.49
1:D:127:LEU:O	1:D:131:LEU:HG	2.13	0.49
13:Y:63:MET:SD	13:Y:66:PRO:HD3	2.53	0.49
14:Z:284:GLY:C	14:Z:286:TYR:N	2.70	0.49
15:A:80:GLU:OE2	16:B:1131:ARG:NH1	2.45	0.49
18:a:423:VAL:HG22	18:a:451:SER:OG	2.13	0.49
19:b:134:ASN:OD1	19:b:220:ARG:HD2	2.13	0.49
10:N:4:DA:H2''	10:N:5:DG:OP2	2.11	0.49
15:A:155:GLU:O	15:A:183:GLY:N	2.43	0.49
15:A:469:MET:HE2	16:B:1093:CYS:HB3	1.95	0.49
20:c:554:ILE:HD11	20:c:665:LEU:HD23	1.95	0.49
10:N:12:DT:H2''	10:N:13:DA:C8	2.48	0.48
15:A:521:VAL:HG13	15:A:535:MET:HE1	1.94	0.48
17:C:144:GLU:OE1	17:C:144:GLU:N	2.46	0.48
12:T:35:DA:H2'	12:T:36:DG:C8	2.49	0.48
16:B:1081:ASP:OD1	16:B:1081:ASP:O	2.31	0.48
19:b:235:LYS:O	19:b:238:ARG:NH2	2.46	0.48
18:a:576:LYS:HB2	20:c:45:LEU:HD13	1.95	0.48
19:b:368:VAL:O	19:b:368:VAL:HG13	2.13	0.48
19:b:381:PHE:O	19:b:386:ARG:NH2	2.45	0.48
15:A:111:CYS:SG	15:A:188:GLN:NE2	2.87	0.48
18:a:92:ASN:O	18:a:96:ASN:ND2	2.45	0.48
15:A:207:GLU:HB3	15:A:210:GLN:HG3	1.95	0.48
15:A:801:GLY:HA3	16:B:503:ASN:HB2	1.95	0.48
18:a:1:MET:SD	18:a:1:MET:C	2.96	0.48
18:a:205:PHE:CD2	19:b:336:VAL:HG23	2.48	0.48
16:B:719:SER:OG	16:B:720:PRO:HD3	2.13	0.48
19:b:423:ILE:HD11	19:b:473:VAL:HG21	1.95	0.48
19:b:721:ARG:NH1	20:c:171:GLU:OE2	2.44	0.48
20:c:581:GLN:OE1	20:c:581:GLN:HA	2.13	0.48
4:G:141:ASP:C	4:G:141:ASP:OD1	2.56	0.48
11:P:34:G:H2'	11:P:35:C:O4'	2.14	0.48
15:A:1141:VAL:HB	15:A:1336:LEU:HB2	1.96	0.48
16:B:633:LEU:HD12	16:B:682:LEU:CD1	2.44	0.48
16:B:995:GLU:CG	16:B:996:ILE:H	2.27	0.48
14:Z:384:GLU:HG2	14:Z:385:GLY:H	1.79	0.48
15:A:1150:ASP:OD2	15:A:1153:ARG:HD3	2.13	0.48
19:b:96:GLU:OE1	19:b:96:GLU:HA	2.13	0.48
20:c:553:ILE:HG22	20:c:616:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:661:GLY:O	23:X:662:ALA:HB3	2.13	0.48
10:N:36:DG:H2''	10:N:37:DC:OP2	2.14	0.48
15:A:13:CYS:SG	16:B:1148:LEU:HB2	2.54	0.48
20:c:402:MET:HE2	20:c:449:TRP:CD2	2.49	0.48
2:E:142:HIS:NE2	15:A:1357:THR:O	2.42	0.48
15:A:753:GLY:O	15:A:757:GLN:OE1	2.31	0.48
19:b:302:ILE:HD11	19:b:463:VAL:HG22	1.96	0.48
2:E:31:ASP:OD1	2:E:32:GLU:N	2.45	0.47
9:L:58:ARG:HH22	17:C:172:GLU:CG	2.26	0.47
12:T:41:DG:H2''	12:T:42:DC:H5'	1.95	0.47
13:Y:62:ALA:HB3	14:Z:215:VAL:HG23	1.96	0.47
15:A:542:LEU:O	15:A:545:VAL:HG12	2.14	0.47
13:Y:97:ILE:O	13:Y:100:GLU:HG3	2.14	0.47
15:A:802:PHE:CE2	15:A:808:PRO:HD3	2.49	0.47
15:A:1427:LEU:HB2	15:A:1456:GLU:HG3	1.95	0.47
20:c:659:ASN:O	20:c:663:LYS:N	2.47	0.47
20:c:19:ILE:O	20:c:23:THR:HG22	2.13	0.47
20:c:146:ASP:OD1	20:c:146:ASP:C	2.56	0.47
15:A:904:GLN:OE1	15:A:1044:HIS:NE2	2.47	0.47
20:c:650:ARG:NH1	20:c:730:ASP:OD2	2.44	0.47
4:G:112:SER:O	4:G:164:MET:SD	2.72	0.47
5:H:141:VAL:HG12	5:H:142:TYR:N	2.28	0.47
14:Z:288:ASP:C	14:Z:288:ASP:OD1	2.58	0.47
15:A:373:LEU:O	15:A:485:ASN:ND2	2.45	0.47
18:a:207:ILE:HG23	18:a:211:MET:HB3	1.95	0.47
19:b:688:MET:HE1	20:c:15:ARG:HG3	1.96	0.47
20:c:451:ILE:HD11	20:c:465:PRO:HD3	1.95	0.47
14:Z:225:ILE:HG22	14:Z:226:TYR:N	2.30	0.47
19:b:306:ASN:ND2	19:b:445:ASP:O	2.48	0.47
19:b:658:ASP:OD2	20:c:121:LYS:NZ	2.48	0.47
8:K:2:ASN:HB3	15:A:478:PRO:O	2.15	0.47
14:Z:552:ARG:HB2	14:Z:559:GLN:CB	2.42	0.47
15:A:485:ASN:ND2	15:A:673:GLN:OE1	2.47	0.47
17:C:189:ASP:O	17:C:191:ALA:N	2.46	0.47
20:c:566:GLN:N	20:c:566:GLN:OE1	2.47	0.47
2:E:52:ARG:HG3	2:E:52:ARG:O	2.14	0.47
11:P:24:A:OP2	16:B:841:ARG:HG2	2.14	0.47
15:A:1375:ARG:NH1	15:A:1379:GLU:OE2	2.42	0.47
16:B:939:HIS:NE2	16:B:983:GLU:OE1	2.42	0.47
7:J:64:PRO:O	9:L:23:HIS:NE2	2.47	0.47
12:T:41:DG:OP2	12:T:41:DG:H8	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:a:21:MET:HE1	18:a:35:PHE:CD1	2.49	0.47
18:a:404:ALA:HB3	18:a:406:TRP:CD1	2.49	0.47
18:a:97:THR:HG21	19:b:728:ILE:HG23	1.96	0.47
20:c:565:SER:HB2	20:c:566:GLN:OE1	2.14	0.47
8:K:9:SER:HB2	17:C:171:LYS:NZ	2.30	0.46
10:N:11:DG:H2''	10:N:12:DT:OP2	2.14	0.46
15:A:458:PHE:CD2	15:A:501:MET:HE2	2.50	0.46
15:A:1190:GLN:HA	15:A:1193:VAL:HG12	1.96	0.46
16:B:263:ILE:HG12	16:B:325:GLY:HA2	1.97	0.46
18:a:239:ASN:C	18:a:239:ASN:OD1	2.58	0.46
20:c:398:ILE:O	20:c:402:MET:HG3	2.14	0.46
18:a:481:GLN:O	18:a:483:ILE:HD12	2.15	0.46
19:b:359:SER:O	19:b:363:LYS:N	2.48	0.46
19:b:434:THR:HG22	19:b:435:THR:N	2.30	0.46
3:F:91:LEU:O	3:F:95:LYS:HG3	2.15	0.46
8:K:7:PHE:HA	8:K:10:PHE:CE2	2.50	0.46
15:A:458:PHE:CE2	15:A:501:MET:HE2	2.51	0.46
15:A:597:PRO:HD3	15:A:668:PHE:CD1	2.51	0.46
20:c:255:VAL:HG22	20:c:297:ILE:HD11	1.97	0.46
8:K:78:THR:OG1	8:K:80:ASP:OD1	2.30	0.46
15:A:1229:GLU:O	15:A:1233:GLU:HG2	2.15	0.46
18:a:482:LEU:HD11	18:a:503:PHE:HB3	1.97	0.46
20:c:249:GLU:HA	20:c:249:GLU:OE2	2.15	0.46
5:H:76:ASN:CG	5:H:76:ASN:O	2.58	0.46
12:T:39:DC:C6	12:T:40:DT:C7	2.99	0.46
18:a:16:LEU:HA	18:a:19:LYS:HG2	1.96	0.46
18:a:374:MET:HE2	22:v:1:A:N7	2.31	0.46
1:D:132:ASP:O	1:D:136:THR:HG23	2.15	0.46
4:G:153:ASP:OD1	4:G:153:ASP:O	2.34	0.46
5:H:92:MET:SD	15:A:579:ILE:HG12	2.55	0.46
7:J:58:LYS:HG3	16:B:738:THR:HG21	1.97	0.46
18:a:24:TYR:CG	18:a:24:TYR:O	2.69	0.46
18:a:74:HIS:O	19:b:727:ARG:NH1	2.49	0.46
18:a:189:ASP:OD1	18:a:190:SER:N	2.48	0.46
5:H:76:ASN:O	5:H:76:ASN:OD1	2.33	0.46
12:T:22:DC:H2'	12:T:23:DC:C6	2.51	0.46
15:A:108:ARG:HB2	15:A:145:TYR:HE1	1.81	0.46
15:A:514:GLU:OE1	16:B:1101:GLN:HB2	2.16	0.46
15:A:1429:LYS:HB2	15:A:1438:VAL:HG11	1.97	0.46
16:B:505:LEU:HD22	16:B:509:VAL:HB	1.96	0.46
18:a:10:ASN:OD1	18:a:11:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:a:41:HIS:O	18:a:44:VAL:HG12	2.15	0.46
18:a:528:THR:O	18:a:564:TYR:OH	2.28	0.46
19:b:85:THR:HG22	19:b:317:MET:HE1	1.98	0.46
4:G:53:ASN:OD1	4:G:54:ILE:N	2.49	0.46
12:T:33:DC:H3'	16:B:421:LYS:NZ	2.31	0.46
15:A:539:GLN:HA	15:A:774:ALA:HB1	1.98	0.46
16:B:863:ASP:OD1	16:B:863:ASP:O	2.34	0.46
19:b:628:MET:O	19:b:628:MET:SD	2.74	0.46
19:b:699:PHE:CG	19:b:718:MET:HG2	2.51	0.46
20:c:143:ARG:HA	20:c:217:PHE:CE2	2.51	0.46
20:c:451:ILE:HG22	20:c:473:MET:SD	2.55	0.46
14:Z:536:TRP:CD1	18:a:136:ASN:ND2	2.74	0.46
16:B:407:MET:SD	16:B:443:GLY:HA3	2.56	0.46
19:b:626:ASN:ND2	20:c:104:PRO:O	2.48	0.46
4:G:101:ILE:N	4:G:104:MET:O	2.47	0.46
15:A:413:TYR:O	15:A:415:GLY:N	2.48	0.46
18:a:269:ARG:HB3	18:a:269:ARG:HH11	1.81	0.46
18:a:623:GLU:OE2	18:a:709:SER:OG	2.32	0.46
18:a:688:GLU:OE2	18:a:689:ALA:N	2.49	0.46
21:r:1:C:H2'	21:r:2:U:H6	1.80	0.46
8:K:74:ARG:HB3	15:A:565:MET:SD	2.56	0.45
11:P:14:C:O3'	18:a:192:ARG:NH2	2.49	0.45
13:Y:63:MET:HE3	13:Y:85:TYR:CE1	2.52	0.45
18:a:18:GLU:HA	18:a:21:MET:HE2	1.98	0.45
19:b:96:GLU:OE1	19:b:102:ILE:HG22	2.16	0.45
19:b:670:ARG:NH2	20:c:36:SER:OG	2.46	0.45
15:A:1153:ARG:O	15:A:1157:ILE:HG12	2.16	0.45
15:A:1211:LEU:CD1	15:A:1258:ARG:NH2	2.79	0.45
18:a:322:ILE:N	18:a:322:ILE:HD12	2.30	0.45
1:D:15:GLU:OE2	4:G:81:LYS:N	2.45	0.45
15:A:400:ASP:OD2	20:c:461:ILE:HG21	2.16	0.45
15:A:466:LYS:HA	16:B:1093:CYS:SG	2.56	0.45
15:A:1212:LEU:HD11	15:A:1289:GLU:HB2	1.98	0.45
16:B:84:TYR:CE1	16:B:132:VAL:HG22	2.51	0.45
17:C:267:ILE:O	17:C:271:VAL:HG23	2.15	0.45
19:b:120:ASP:OD1	19:b:121:LYS:N	2.49	0.45
19:b:277:GLU:OE1	20:c:217:PHE:CD1	2.69	0.45
9:L:13:GLN:N	9:L:14:PRO:CD	2.79	0.45
16:B:133:ILE:CD1	16:B:139:GLN:HB2	2.47	0.45
16:B:388:TYR:CE2	16:B:505:LEU:HD21	2.52	0.45
20:c:467:MET:HA	20:c:467:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:HIS:O	1:D:47:GLN:HG3	2.16	0.45
11:P:26:A:H2'	11:P:26:A:N3	2.30	0.45
15:A:514:GLU:CD	16:B:1101:GLN:HB2	2.40	0.45
15:A:910:LYS:HZ2	15:A:973:GLY:HA3	1.81	0.45
20:c:652:ASN:OD1	20:c:657:ASN:HA	2.17	0.45
1:D:104:CYS:SG	1:D:138:ARG:NE	2.81	0.45
5:H:2:ALA:N	5:H:66:GLU:O	2.49	0.45
5:H:84:ARG:HD2	5:H:144:LEU:CD1	2.46	0.45
12:T:21:DG:H2'	12:T:22:DC:O4'	2.16	0.45
19:b:724:ILE:O	19:b:728:ILE:CD1	2.64	0.45
4:G:136:VAL:O	4:G:170:LEU:HD12	2.17	0.45
16:B:501:LEU:HD12	16:B:505:LEU:HD12	1.98	0.45
18:a:3:ASP:OD1	18:a:4:PHE:N	2.49	0.45
18:a:636:VAL:O	18:a:640:LEU:HD13	2.17	0.45
19:b:282:LEU:CD2	19:b:441:LEU:HD22	2.47	0.45
20:c:599:LEU:O	20:c:602:GLN:HG2	2.17	0.45
2:E:72:MET:HE2	2:E:103:LEU:HD11	1.98	0.45
3:F:107:ARG:HB3	15:A:1472:ASP:OD1	2.17	0.45
11:P:4:G:N7	20:c:213:ARG:NH1	2.65	0.45
18:a:423:VAL:HG13	18:a:456:THR:HG21	1.98	0.45
20:c:342:GLU:OE2	20:c:344:VAL:HG13	2.17	0.45
2:E:110:MET:HE1	2:E:118:LEU:HD11	1.98	0.45
4:G:165:ASP:HB3	4:G:168:LEU:HD11	1.99	0.45
11:P:5:C:O2	11:P:5:C:O2'	2.32	0.45
14:Z:488:ASP:HB3	14:Z:511:LEU:HD11	1.99	0.45
14:Z:536:TRP:HB3	18:a:140:SER:HB3	1.99	0.45
15:A:523:ARG:O	15:A:524:MET:HE2	2.16	0.45
14:Z:193:ALA:O	14:Z:197:MET:SD	2.75	0.45
15:A:425:ASP:N	15:A:425:ASP:OD1	2.49	0.45
15:A:865:ILE:HG21	16:B:1092:ASP:CG	2.42	0.45
15:A:910:LYS:HD3	15:A:973:GLY:C	2.41	0.45
16:B:315:ASN:OD1	16:B:316:VAL:N	2.50	0.45
18:a:295[B]:PRO:HB3	18:a:297[B]:HIS:HE1	1.82	0.45
18:a:589:LEU:CD1	19:b:546:MET:HE2	2.47	0.45
20:c:59:ALA:HB3	20:c:91:VAL:HG21	1.99	0.45
20:c:516:GLU:N	20:c:516:GLU:OE1	2.48	0.45
11:P:25:G:C8	15:A:264:VAL:HG23	2.52	0.44
14:Z:543:ASP:O	14:Z:544:PRO:C	2.60	0.44
15:A:592:PHE:O	15:A:596:ILE:HG13	2.17	0.44
19:b:372:MET:O	19:b:372:MET:HG2	2.16	0.44
20:c:163:ILE:HD13	20:c:208:GLU:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:339:LYS:HD3	20:c:355:ARG:HD3	2.00	0.44
9:L:30:SER:O	9:L:31:ARG:HG3	2.16	0.44
14:Z:711:ARG:NH2	17:C:92:GLU:HB2	2.32	0.44
15:A:883:ILE:HD11	15:A:1424:THR:HA	1.99	0.44
16:B:540:PRO:HB2	16:B:596:ILE:HG23	1.99	0.44
16:B:623:ARG:NH2	16:B:697:GLU:OE2	2.38	0.44
18:a:179:ARG:HD2	18:a:179:ARG:O	2.17	0.44
15:A:510:GLU:HB3	16:B:1101:GLN:OE1	2.17	0.44
15:A:902:GLU:OE2	15:A:982:ASN:HB2	2.17	0.44
15:A:1021:VAL:O	15:A:1021:VAL:HG23	2.17	0.44
15:A:1221:MET:HE1	15:A:1226:LEU:HB3	1.99	0.44
15:A:3020:THR:O	18:a:288:LEU:HD12	2.18	0.44
16:B:585:ASN:O	16:B:589:LYS:HG2	2.17	0.44
18:a:295[B]:PRO:HB2	18:a:300[B]:GLU:HG3	1.98	0.44
18:a:621:ILE:HD11	18:a:639:THR:HG21	1.98	0.44
5:H:59:VAL:O	5:H:144:LEU:HB2	2.17	0.44
9:L:30:SER:C	9:L:31:ARG:HG3	2.42	0.44
14:Z:542:LEU:HD23	14:Z:575:VAL:HG12	1.99	0.44
18:a:293[A]:GLU:O	18:a:294[A]:ASP:C	2.61	0.44
2:E:67:ASP:OD1	2:E:69:THR:HG22	2.17	0.44
5:H:51:ASP:O	5:H:54:ASP:OD2	2.35	0.44
8:K:97:GLU:OE2	17:C:30:VAL:HG11	2.17	0.44
10:N:39:DT:H2"	10:N:40:DG:OP2	2.18	0.44
15:A:1123:ARG:NH2	15:A:1381:GLU:OE1	2.41	0.44
15:A:1210:TRP:HB3	15:A:1285:LEU:CD1	2.47	0.44
16:B:1004:ASP:OD1	16:B:1004:ASP:N	2.51	0.44
18:a:618:THR:O	19:b:11:LYS:NZ	2.42	0.44
19:b:567:GLN:HA	19:b:567:GLN:OE1	2.17	0.44
4:G:30:LEU:O	4:G:34:VAL:HG22	2.18	0.44
6:I:18:GLN:OE1	6:I:44:TYR:CZ	2.71	0.44
15:A:668:PHE:CZ	15:A:672:ILE:HD11	2.53	0.44
17:C:86:ARG:HH22	17:C:172:GLU:CD	2.26	0.44
18:a:205:PHE:CZ	19:b:171:MET:HE3	2.52	0.44
18:a:406:TRP:O	18:a:410:GLU:HG2	2.18	0.44
19:b:272:PRO:CA	19:b:414:MET:HE1	2.48	0.44
19:b:741:ALA:O	19:b:745:LYS:HG2	2.18	0.44
20:c:154:LEU:HD21	20:c:181:SER:OG	2.17	0.44
2:E:25:GLY:O	2:E:65:ASN:ND2	2.49	0.44
5:H:60:ILE:CG2	5:H:141:VAL:HG11	2.47	0.44
8:K:13:PHE:CE1	8:K:16:GLU:HB2	2.53	0.44
14:Z:547:VAL:HG23	14:Z:547:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:802:PHE:CE1	16:B:504:THR:HG22	2.53	0.44
16:B:281:ASP:O	16:B:285:LEU:HD23	2.17	0.44
18:a:307:ALA:O	18:a:311:MET:HG2	2.17	0.44
20:c:143:ARG:HB3	20:c:143:ARG:NH1	2.32	0.44
20:c:392:GLN:HE21	23:X:663:ALA:HA	1.82	0.44
6:I:69:ILE:O	6:I:72:VAL:HG12	2.18	0.44
11:P:5:C:O2	11:P:5:C:C2'	2.65	0.44
15:A:1210:TRP:HB3	15:A:1285:LEU:HD12	1.99	0.44
16:B:754:PRO:HB2	16:B:773:PRO:HG2	2.00	0.44
19:b:303:THR:HG22	19:b:490:PHE:HB2	1.99	0.44
23:X:659:ALA:O	23:X:660:ALA:HB3	2.18	0.44
3:F:62:ARG:NH1	15:A:517:GLU:OE1	2.51	0.44
15:A:368:THR:HG23	15:A:369:PRO:HD2	2.00	0.44
16:B:1138:ARG:O	16:B:1141:ARG:HD2	2.18	0.44
18:a:233:VAL:HG11	19:b:323:THR:CG2	2.47	0.44
19:b:130:ASP:OD1	19:b:132:THR:OG1	2.29	0.44
19:b:499:TYR:CD1	20:c:657:ASN:ND2	2.86	0.44
20:c:91:VAL:CG1	20:c:95:ALA:HB3	2.48	0.44
20:c:137:ASN:ND2	20:c:551:GLN:OE1	2.43	0.44
3:F:100:ARG:HH21	3:F:124:ILE:HA	1.81	0.43
14:Z:280:ARG:HB2	14:Z:382:ILE:HG22	1.98	0.43
15:A:457:ILE:HD11	15:A:515:ILE:HG23	2.00	0.43
15:A:1371:ILE:O	15:A:1374:VAL:HG12	2.17	0.43
16:B:285:LEU:HD21	16:B:305:LEU:HD11	2.00	0.43
16:B:887:TYR:O	16:B:888:THR:HG22	2.17	0.43
18:a:97:THR:HG23	18:a:98:THR:N	2.33	0.43
19:b:134:ASN:O	19:b:350:ARG:NH1	2.51	0.43
19:b:251:PHE:CE1	19:b:339:ILE:HG21	2.52	0.43
1:D:86:LEU:O	1:D:89:GLN:HG2	2.18	0.43
15:A:457:ILE:HD11	15:A:515:ILE:HD12	2.00	0.43
19:b:271:LEU:HD23	19:b:417:THR:HG21	2.00	0.43
19:b:714:MET:HB3	19:b:718:MET:HE2	1.99	0.43
9:L:58:ARG:HH22	17:C:172:GLU:CD	2.26	0.43
12:T:33:DC:H2''	12:T:34:DT:C6	2.52	0.43
14:Z:386:VAL:HG12	14:Z:387:LYS:N	2.33	0.43
15:A:686:THR:OG1	15:A:687:ILE:N	2.52	0.43
15:A:931:ARG:NH1	15:A:936:GLU:OE1	2.52	0.43
15:A:1142:PHE:HD1	15:A:1335:ILE:HD12	1.82	0.43
15:A:1302:GLU:O	15:A:1303:GLN:HB2	2.18	0.43
19:b:255:VAL:HG21	19:b:340:ALA:HB3	2.00	0.43
19:b:414:MET:O	19:b:417:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:134:GLU:HB3	15:A:1344:MET:HE1	1.99	0.43
16:B:34:PHE:HZ	16:B:528:LEU:HB3	1.82	0.43
16:B:339:ALA:O	16:B:340:LYS:C	2.60	0.43
16:B:600:GLU:OE1	16:B:620:ARG:NH2	2.51	0.43
16:B:677:MET:SD	16:B:700:PRO:HG3	2.59	0.43
17:C:27:ASP:OD1	17:C:28:LEU:N	2.52	0.43
18:a:294[B]:ASP:OD2	18:a:296[B]:SER:OG	2.36	0.43
18:a:296[A]:SER:O	18:a:496:ARG:NH2	2.52	0.43
20:c:177:LEU:HB3	20:c:183:LEU:HD13	2.01	0.43
13:Y:41:GLN:OE1	13:Y:41:GLN:HA	2.18	0.43
19:b:220:ARG:O	19:b:220:ARG:HG3	2.18	0.43
20:c:581:GLN:OE1	20:c:584:VAL:HG21	2.17	0.43
20:c:664:ARG:NH1	20:c:674:ALA:HB2	2.34	0.43
4:G:166:ASP:C	4:G:166:ASP:OD1	2.61	0.43
19:b:221:ALA:O	19:b:248:ILE:HD11	2.18	0.43
20:c:461:ILE:HD12	20:c:461:ILE:C	2.43	0.43
20:c:603:MET:HE3	20:c:689:ALA:CB	2.48	0.43
20:c:608:GLY:O	20:c:609:THR:OG1	2.33	0.43
2:E:134:GLU:OE2	2:E:181:ARG:NH2	2.51	0.43
17:C:103:LEU:HD12	17:C:120:LEU:HD12	2.00	0.43
18:a:274:PRO:O	18:a:401:ARG:HB3	2.18	0.43
19:b:414:MET:O	19:b:418:VAL:HG23	2.18	0.43
5:H:39:LEU:HD21	5:H:41:LEU:HB2	2.00	0.43
15:A:910:LYS:N	15:A:911:PRO:CD	2.82	0.43
15:A:1194:ASN:OD1	15:A:1195:VAL:N	2.52	0.43
18:a:362:LYS:NZ	18:a:478:ASP:O	2.38	0.43
18:a:665:LEU:HD22	18:a:690:ILE:CD1	2.49	0.43
18:a:697:ASP:OD1	18:a:697:ASP:C	2.62	0.43
19:b:499:TYR:CE1	20:c:657:ASN:ND2	2.87	0.43
20:c:83:ASP:OD1	20:c:84:ALA:N	2.52	0.43
20:c:648:VAL:CG1	20:c:650:ARG:O	2.67	0.43
4:G:137:ILE:HA	4:G:141:ASP:OD2	2.19	0.43
4:G:159:ALA:O	4:G:160:ILE:HD13	2.19	0.43
11:P:26:A:O2'	15:A:264:VAL:HG21	2.19	0.43
14:Z:542:LEU:HD12	14:Z:546:THR:HG22	2.00	0.43
15:A:86:GLY:C	15:A:255:VAL:HG22	2.44	0.43
15:A:98:GLY:HA3	15:A:1440:MET:HE3	2.01	0.43
15:A:802:PHE:HE1	16:B:504:THR:HA	1.84	0.43
16:B:625:LEU:HD13	16:B:675:LEU:HD21	2.01	0.43
16:B:631:GLN:O	16:B:682:LEU:HB3	2.19	0.43
18:a:222:ASN:OD1	18:a:222:ASN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:a:276:CYS:N	18:a:402:SER:O	2.50	0.43
18:a:694:LEU:HD23	18:a:700:VAL:HG22	2.01	0.43
19:b:750:ILE:HG23	20:c:11:MET:HG3	2.01	0.43
4:G:85:VAL:CG2	4:G:147:ILE:HD11	2.49	0.43
14:Z:282:LYS:O	14:Z:283:ARG:HG2	2.19	0.43
15:A:653:VAL:HG11	15:A:669:TYR:OH	2.19	0.43
15:A:896:LEU:O	15:A:1396:ARG:NH1	2.52	0.43
15:A:1134:PRO:O	15:A:1137:PRO:HD3	2.18	0.43
16:B:352:GLY:O	16:B:361:LYS:NZ	2.42	0.43
18:a:485:MET:HB3	18:a:501:TYR:HB2	2.01	0.43
18:a:549:LEU:HG	18:a:556:GLN:HG2	2.01	0.43
20:c:725:LEU:HD13	20:c:725:LEU:C	2.44	0.43
1:D:57:LEU:HD13	1:D:61:PHE:CD1	2.54	0.42
2:E:172:ARG:HD3	2:E:210:GLN:HG3	2.00	0.42
15:A:108:ARG:HD2	15:A:145:TYR:OH	2.19	0.42
15:A:433:PRO:HB2	15:A:438:LEU:HD21	2.01	0.42
15:A:749:ARG:HH21	15:A:779:ILE:HG23	1.84	0.42
15:A:1173:THR:HG21	15:A:1289:GLU:HG3	2.01	0.42
17:C:92:GLU:HG2	17:C:93:PHE:N	2.35	0.42
14:Z:282:LYS:O	14:Z:283:ARG:CG	2.67	0.42
15:A:330:GLN:O	15:A:331:LYS:C	2.62	0.42
18:a:423:VAL:HG13	18:a:456:THR:CG2	2.49	0.42
19:b:446:ASP:OD2	19:b:493:THR:N	2.45	0.42
19:b:504:ASN:ND2	19:b:507:MET:HG2	2.34	0.42
4:G:151:ARG:HB2	14:Z:491:LEU:CD1	2.50	0.42
8:K:34:THR:CG2	8:K:70:LYS:HD2	2.50	0.42
15:A:92:LYS:HD3	15:A:307:VAL:HG21	2.01	0.42
15:A:112:PHE:CD1	15:A:112:PHE:O	2.72	0.42
15:A:583:ARG:HE	15:A:585:LEU:HD21	1.84	0.42
15:A:710:LYS:O	15:A:714:ILE:HG13	2.19	0.42
16:B:329:GLY:HA3	16:B:335:ARG:HG3	2.00	0.42
18:a:665:LEU:HD23	18:a:707:PHE:CZ	2.55	0.42
4:G:142:GLU:CD	4:G:142:GLU:N	2.78	0.42
13:Y:62:ALA:HB3	14:Z:215:VAL:CG2	2.49	0.42
16:B:121:SER:HA	16:B:153:PRO:HA	2.01	0.42
17:C:47:ILE:HA	17:C:165:ALA:HA	2.01	0.42
20:c:17:ARG:NH2	20:c:18:GLU:OE2	2.50	0.42
20:c:694:PHE:CD1	20:c:736:LYS:HA	2.54	0.42
2:E:110:MET:HE1	2:E:118:LEU:CD1	2.49	0.42
3:F:115:TYR:CD1	3:F:115:TYR:C	2.97	0.42
13:Y:116:LYS:O	13:Y:117:THR:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:494:ARG:HB3	14:Z:501:ILE:HG22	2.01	0.42
15:A:481:THR:O	15:A:483:ARG:NE	2.52	0.42
15:A:876:ASP:OD1	15:A:878:THR:HG22	2.19	0.42
15:A:997:ASN:ND2	15:A:1000:LEU:HD23	2.35	0.42
19:b:173:SER:HB2	19:b:179:MET:HE1	2.00	0.42
20:c:361:GLU:HG3	20:c:363:PHE:CE2	2.55	0.42
2:E:27:LEU:HD13	2:E:65:ASN:OD1	2.20	0.42
2:E:116:GLN:HA	2:E:119:VAL:HG22	2.01	0.42
7:J:6:ARG:CD	7:J:13:ILE:HD13	2.49	0.42
10:N:2:DG:H2''	10:N:3:DC:OP2	2.18	0.42
14:Z:382:ILE:HG23	14:Z:382:ILE:O	2.19	0.42
16:B:418:TYR:CD1	16:B:434:ALA:HB2	2.54	0.42
16:B:438:ARG:HG3	16:B:438:ARG:HH11	1.84	0.42
19:b:265:LYS:HE3	20:c:417:ASP:OD2	2.20	0.42
20:c:252:ASN:O	20:c:255:VAL:HG12	2.20	0.42
20:c:392:GLN:NE2	23:X:663:ALA:HA	2.35	0.42
20:c:598:VAL:HG11	20:c:692:ARG:HD3	2.00	0.42
4:G:120:ASP:OD1	4:G:127:CYS:O	2.38	0.42
10:N:30:DA:C2	12:T:15:DA:C2	3.08	0.42
14:Z:259:GLU:O	14:Z:259:GLU:HG2	2.19	0.42
14:Z:285:ILE:O	14:Z:285:ILE:HG22	2.20	0.42
14:Z:474:MET:HE1	14:Z:493:VAL:C	2.45	0.42
18:a:19:LYS:HG3	18:a:20:ALA:N	2.35	0.42
18:a:567:THR:HG23	18:a:567:THR:O	2.19	0.42
19:b:317:MET:HE2	19:b:317:MET:HA	2.01	0.42
1:D:60:VAL:HG11	4:G:44:PHE:CE1	2.54	0.42
4:G:32:THR:HG21	14:Z:545:GLN:HG3	2.02	0.42
14:Z:306:LYS:HA	14:Z:372:LEU:O	2.20	0.42
16:B:338:TYR:O	16:B:342:VAL:HG23	2.20	0.42
16:B:602:SER:OG	16:B:620:ARG:NH1	2.53	0.42
19:b:721:ARG:NH2	20:c:171:GLU:OE2	2.48	0.42
10:N:37:DC:H1'	10:N:38:DT:O5'	2.19	0.42
11:P:10:A:N3	11:P:10:A:H2'	2.35	0.42
15:A:1214:VAL:HG23	15:A:1257:LEU:HG	2.02	0.42
15:A:1337:GLU:N	15:A:1337:GLU:OE1	2.52	0.42
18:a:115:ASN:OD1	18:a:115:ASN:O	2.37	0.42
18:a:360:MET:HE3	18:a:482:LEU:HD22	2.02	0.42
19:b:445:ASP:C	19:b:445:ASP:OD1	2.62	0.42
8:K:7:PHE:HB2	8:K:11:LEU:CD1	2.49	0.42
15:A:909:LEU:O	15:A:967:ARG:NE	2.48	0.42
16:B:388:TYR:CZ	16:B:505:LEU:HD21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:675:LEU:HD23	16:B:695:HIS:HB2	2.01	0.42
16:B:718:GLN:HG2	16:B:720:PRO:HD2	2.01	0.42
19:b:679:GLN:O	19:b:682:ILE:CG2	2.67	0.42
20:c:407:GLU:OE1	20:c:476:ARG:NH2	2.53	0.42
5:H:12:VAL:HG11	5:H:15:ILE:HD11	2.02	0.41
8:K:10:PHE:CD2	8:K:10:PHE:N	2.87	0.41
15:A:33:ARG:HB3	16:B:1141:ARG:HH12	1.85	0.41
15:A:75:ALA:O	16:B:1131:ARG:CZ	2.68	0.41
15:A:154:CYS:O	15:A:155:GLU:C	2.63	0.41
15:A:319:ASP:O	15:A:322:LEU:CD1	2.68	0.41
15:A:749:ARG:HH22	15:A:783:GLN:NE2	2.18	0.41
15:A:880:ARG:NE	15:A:884:ASN:OD1	2.53	0.41
16:B:225:LEU:HD22	16:B:349:PRO:HB2	2.02	0.41
16:B:292:PHE:O	16:B:298:MET:HE1	2.20	0.41
18:a:44:VAL:HG11	18:a:122:VAL:CG2	2.50	0.41
18:a:253:VAL:O	18:a:253:VAL:HG13	2.20	0.41
18:a:572:LYS:HG2	20:c:45:LEU:HD11	2.02	0.41
20:c:346:THR:HA	20:c:411:ILE:HG22	2.02	0.41
21:r:1:C:H2'	21:r:2:U:C6	2.54	0.41
1:D:87:LEU:HD23	1:D:97:LEU:HA	2.02	0.41
10:N:37:DC:C2'	10:N:38:DT:H72	2.50	0.41
14:Z:193:ALA:O	14:Z:197:MET:CE	2.68	0.41
14:Z:278:TRP:O	14:Z:386:VAL:HG21	2.20	0.41
15:A:100:LEU:O	15:A:103:THR:HG22	2.20	0.41
15:A:469:MET:HG2	16:B:1093:CYS:SG	2.60	0.41
15:A:1405:MET:HG2	15:A:1414:ILE:HD11	2.02	0.41
15:A:1476:ASP:OD1	15:A:1479:LYS:N	2.48	0.41
16:B:602:SER:OG	16:B:666:ASP:CG	2.63	0.41
18:a:295[A]:PRO:O	18:a:296[A]:SER:C	2.63	0.41
19:b:286:VAL:HG22	19:b:290:MET:CE	2.50	0.41
20:c:342:GLU:OE2	20:c:342:GLU:C	2.63	0.41
20:c:462:GLY:HA3	20:c:474:SER:HB2	2.02	0.41
1:D:129:GLN:HA	1:D:132:ASP:OD2	2.20	0.41
11:P:9:A:H4'	11:P:10:A:OP1	2.20	0.41
14:Z:540:VAL:HG11	14:Z:550:ILE:HD11	2.01	0.41
15:A:434:LYS:O	15:A:437:ASP:OD1	2.39	0.41
15:A:888:GLN:NE2	15:A:1403:ASP:OD2	2.40	0.41
15:A:1323:THR:HG22	15:A:1324:GLU:N	2.35	0.41
20:c:294:MET:HA	20:c:297:ILE:HG22	2.02	0.41
3:F:94:MET:O	3:F:98:LYS:HD3	2.20	0.41
4:G:25:THR:O	4:G:29:LYS:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:33:G:O2'	11:P:34:G:H5'	2.19	0.41
14:Z:552:ARG:HB2	14:Z:559:GLN:CG	2.49	0.41
15:A:1211:LEU:HD21	15:A:1213:ARG:HB2	2.03	0.41
15:A:1381:GLU:O	15:A:1385:VAL:HG23	2.19	0.41
18:a:360:MET:O	18:a:361:LYS:C	2.63	0.41
18:a:487:SER:HB3	18:a:501:TYR:HE2	1.86	0.41
20:c:535:MET:HE3	20:c:538:GLU:HG2	2.02	0.41
20:c:564:TRP:HB2	20:c:571:LEU:HD22	2.02	0.41
2:E:127:LEU:HD23	2:E:127:LEU:H	1.86	0.41
3:F:84:GLU:N	3:F:84:GLU:OE1	2.52	0.41
4:G:51:ILE:HG13	4:G:51:ILE:O	2.21	0.41
6:I:23:MET:CE	16:B:305:LEU:HB3	2.50	0.41
14:Z:569:THR:HB	15:A:423:ASN:OD1	2.20	0.41
15:A:1285:LEU:HD23	15:A:1288:ILE:HD11	2.02	0.41
19:b:277:GLU:OE1	20:c:217:PHE:HD1	2.03	0.41
3:F:81:VAL:HG22	3:F:96:GLU:HG2	2.00	0.41
6:I:105:GLU:OE2	15:A:733:LEU:HB3	2.21	0.41
10:N:40:DG:H2''	10:N:41:DA:C8	2.56	0.41
10:N:41:DA:H2''	10:N:42:DT:H72	2.03	0.41
14:Z:440:ILE:HG12	14:Z:450:ILE:HD11	2.02	0.41
14:Z:554:GLU:HB2	14:Z:557:THR:O	2.21	0.41
15:A:296:ASN:OD1	15:A:296:ASN:O	2.38	0.41
15:A:525:ILE:O	15:A:534:VAL:HG12	2.21	0.41
15:A:794:GLU:OE2	16:B:500:GLN:NE2	2.54	0.41
15:A:1246:ILE:HD11	15:A:1258:ARG:HH11	1.85	0.41
17:C:43:PRO:HA	17:C:168:GLY:O	2.21	0.41
18:a:237:GLU:OE1	18:a:237:GLU:HA	2.21	0.41
19:b:555:TYR:HH	19:b:592:SER:HG	1.66	0.41
20:c:40:GLU:OE2	20:c:42:ASN:OD1	2.39	0.41
1:D:41:LEU:HG	1:D:61:PHE:CZ	2.56	0.41
8:K:45:ILE:HG23	17:C:33:SER:OG	2.21	0.41
14:Z:534:HIS:HA	14:Z:550:ILE:CD1	2.50	0.41
17:C:44:ILE:HG21	17:C:178:PRO:HB3	2.02	0.41
18:a:360:MET:CE	18:a:482:LEU:HD22	2.51	0.41
19:b:271:LEU:N	19:b:272:PRO:HD2	2.36	0.41
5:H:56:PHE:CD1	5:H:145:MET:HG3	2.55	0.41
12:T:31:DT:C2'	12:T:32:DA:C8	3.04	0.41
15:A:298:ALA:O	15:A:299:ALA:HB3	2.21	0.41
15:A:695:ASP:OD1	15:A:698:THR:OG1	2.35	0.41
15:A:869:GLU:OE2	15:A:1455:SER:OG	2.34	0.41
15:A:931:ARG:HA	15:A:939:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:a:196:ARG:HA	18:a:196:ARG:NE	2.35	0.41
2:E:30:GLN:O	2:E:34:ASP:OD1	2.39	0.41
5:H:37:MET:HE1	5:H:131:ASN:CB	2.50	0.41
7:J:44:CYS:O	7:J:48:MET:HG2	2.21	0.41
8:K:46:ILE:HG21	8:K:87:PHE:CE1	2.56	0.41
12:T:31:DT:H3'	16:B:438:ARG:HH12	1.85	0.41
12:T:39:DC:C6	12:T:40:DT:H73	2.56	0.41
14:Z:535:GLU:HG2	18:a:157:THR:HG23	2.03	0.41
15:A:1435:THR:O	15:A:1439:LEU:HD23	2.20	0.41
15:A:1457:ASN:OD1	15:A:1465:PRO:HD3	2.21	0.41
16:B:322:GLY:C	16:B:335:ARG:HG2	2.45	0.41
16:B:403:LEU:HD13	16:B:453:TRP:NE1	2.36	0.41
16:B:995:GLU:CG	16:B:996:ILE:N	2.84	0.41
18:a:13:ILE:HD11	18:a:42:LEU:C	2.45	0.41
19:b:232:GLU:OE2	19:b:239:ARG:NE	2.36	0.41
19:b:363:LYS:HD3	19:b:363:LYS:O	2.21	0.41
20:c:161:ASP:OD2	20:c:175:ARG:NH2	2.54	0.41
20:c:439:GLN:O	23:X:664:ALA:HA	2.21	0.41
20:c:533:SER:O	20:c:536:MET:HE2	2.20	0.41
20:c:573:ASN:O	20:c:574:LYS:C	2.64	0.41
18:a:1:MET:SD	18:a:2:GLU:N	2.93	0.41
18:a:218:SER:HB2	19:b:345:SER:HB2	2.01	0.41
19:b:246:MET:HE1	19:b:249:ARG:HH11	1.86	0.41
19:b:556:ARG:HA	19:b:561:CYS:SG	2.61	0.41
21:r:5:G:OP2	21:r:5:G:N2	2.45	0.41
5:H:6:PHE:CE1	5:H:37:MET:SD	3.14	0.40
7:J:56:ILE:O	7:J:60:LEU:HG	2.21	0.40
10:N:4:DA:C2	12:T:41:DG:C2	3.10	0.40
14:Z:227:VAL:HG11	14:Z:235:VAL:HG13	2.02	0.40
15:A:1068:LEU:O	15:A:1072:ILE:HG13	2.21	0.40
16:B:1115:GLN:CG	16:B:1150:ARG:HD2	2.51	0.40
18:a:567:THR:OG1	22:v:1:A:H2	2.04	0.40
19:b:102:ILE:HG23	19:b:103:PHE:N	2.36	0.40
19:b:127:GLN:OE1	19:b:127:GLN:HA	2.20	0.40
20:c:506:ASP:CG	20:c:507:GLN:H	2.29	0.40
20:c:508:ARG:HA	20:c:508:ARG:NH1	2.36	0.40
1:D:68:THR:O	1:D:72:SER:OG	2.35	0.40
4:G:123:SER:O	4:G:124:ASN:C	2.64	0.40
8:K:9:SER:HA	8:K:69:HIS:CG	2.55	0.40
12:T:31:DT:C2'	12:T:32:DA:H5'	2.51	0.40
12:T:40:DT:H2''	12:T:41:DG:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:447:GLU:OE2	16:B:1064:ARG:NH2	2.54	0.40
15:A:470:MET:HE3	15:A:521:VAL:HG22	2.03	0.40
15:A:760:LEU:HD11	15:A:781:ILE:HG21	2.02	0.40
15:A:920:PHE:CE1	15:A:1053:ARG:HD2	2.56	0.40
15:A:965:VAL:O	15:A:968:VAL:HG22	2.21	0.40
16:B:223:SER:OG	16:B:349:PRO:HD2	2.21	0.40
16:B:414:GLU:HA	16:B:417:ILE:HG12	2.02	0.40
16:B:733:MET:CE	16:B:1054:MET:SD	3.09	0.40
20:c:725:LEU:HD23	20:c:731:VAL:CG2	2.50	0.40
8:K:19:ILE:HG23	17:C:266:GLU:HG3	2.02	0.40
8:K:67:LEU:HD13	15:A:478:PRO:HD2	2.03	0.40
11:P:9:A:H1'	11:P:10:A:C2	2.56	0.40
25:P:101:G1G:O3B	20:c:264:ARG:NH2	2.55	0.40
12:T:32:DA:OP2	16:B:438:ARG:NH2	2.46	0.40
14:Z:710:VAL:HG11	14:Z:750:LEU:HD23	2.03	0.40
15:A:1217:ASP:OD1	15:A:1217:ASP:N	2.53	0.40
16:B:332:LYS:O	16:B:336:ILE:HG13	2.21	0.40
16:B:792:ASP:OD1	16:B:942:LYS:O	2.38	0.40
17:C:78:ILE:HG21	17:C:127:VAL:CG2	2.52	0.40
17:C:242:GLU:O	17:C:246:LEU:HD23	2.21	0.40
19:b:714:MET:HE2	20:c:28:MET:HB2	2.02	0.40
20:c:50:MET:O	20:c:56:PRO:HB3	2.21	0.40
20:c:163:ILE:HG12	20:c:207:LEU:HB3	2.03	0.40
22:v:4:A:O2'	22:v:5:G:H5'	2.21	0.40
4:G:20:PRO:HA	15:A:1481:LYS:HD3	2.02	0.40
7:J:54:ASP:OD2	7:J:57:GLU:HG2	2.22	0.40
11:P:34:G:C6	11:P:35:C:N3	2.90	0.40
12:T:35:DA:H2'	12:T:36:DG:H8	1.87	0.40
14:Z:481:ILE:HG13	14:Z:482:ALA:N	2.36	0.40
15:A:1130:ILE:HG21	15:A:1411:LEU:HB3	2.03	0.40
6:I:60:HIS:CE1	6:I:103:ARG:HB3	2.57	0.40
14:Z:711:ARG:HD2	14:Z:721:ILE:HD11	2.03	0.40
15:A:560:VAL:O	15:A:564:LEU:HG	2.21	0.40
16:B:474:THR:HG23	16:B:477:SER:H	1.86	0.40
18:a:54:ILE:O	18:a:54:ILE:HG23	2.21	0.40
18:a:313:THR:O	18:a:313:THR:HG22	2.22	0.40
18:a:401:ARG:HH11	18:a:401:ARG:HG2	1.85	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	D	124/184 (67%)	120 (97%)	4 (3%)	0	100	100
2	E	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
3	F	80/127 (63%)	76 (95%)	4 (5%)	0	100	100
4	G	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
5	H	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
6	I	115/125 (92%)	111 (96%)	4 (4%)	0	100	100
7	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
8	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
9	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100
13	Y	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
14	Z	459/1087 (42%)	427 (93%)	32 (7%)	0	100	100
15	A	1421/1641 (87%)	1373 (97%)	48 (3%)	0	100	100
16	B	1123/1160 (97%)	1086 (97%)	37 (3%)	0	100	100
17	C	257/275 (94%)	252 (98%)	5 (2%)	0	100	100
18	a	708/717 (99%)	681 (96%)	25 (4%)	2 (0%)	37	66
19	b	737/757 (97%)	721 (98%)	16 (2%)	0	100	100
20	c	732/759 (96%)	705 (96%)	27 (4%)	0	100	100
23	X	15/17 (88%)	11 (73%)	4 (27%)	0	100	100
All	All	6629/7739 (86%)	6400 (96%)	227 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	a	301[A]	GLY
18	a	301[B]	GLY

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	D	116/160 (72%)	116 (100%)	0	100	100
2	E	191/192 (100%)	191 (100%)	0	100	100
3	F	71/111 (64%)	71 (100%)	0	100	100
4	G	152/152 (100%)	152 (100%)	0	100	100
5	H	129/131 (98%)	129 (100%)	0	100	100
6	I	105/112 (94%)	105 (100%)	0	100	100
7	J	56/56 (100%)	56 (100%)	0	100	100
8	K	104/106 (98%)	103 (99%)	1 (1%)	73	84
9	L	43/55 (78%)	43 (100%)	0	100	100
13	Y	102/103 (99%)	102 (100%)	0	100	100
14	Z	417/940 (44%)	417 (100%)	0	100	100
15	A	1263/1425 (89%)	1263 (100%)	0	100	100
16	B	992/1014 (98%)	990 (100%)	2 (0%)	92	95
17	C	238/252 (94%)	238 (100%)	0	100	100
18	a	640/645 (99%)	640 (100%)	0	100	100
19	b	652/668 (98%)	651 (100%)	1 (0%)	92	95
20	c	645/666 (97%)	642 (100%)	3 (0%)	86	91
23	X	1/1 (100%)	1 (100%)	0	100	100
All	All	5917/6789 (87%)	5910 (100%)	7 (0%)	92	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	K	10	PHE
16	B	628	VAL
16	B	633	LEU
19	b	682	ILE
20	c	217	PHE
20	c	354	ILE

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Mol	Chain	Res	Type
20	c	427	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	35	GLN
4	G	28	GLN
6	I	22	ASN
6	I	32	ASN
6	I	67	GLN
7	J	61	ASN
8	K	29	ASN
9	L	26	ASN
13	Y	12	HIS
13	Y	75	GLN
14	Z	477	HIS
15	A	504	HIS
15	A	740	GLN
15	A	780	ASN
15	A	792	ASN
15	A	905	ASN
15	A	1190	GLN
15	A	1394	ASN
16	B	430	ASN
16	B	460	HIS
16	B	986	GLN
16	B	1117	HIS
16	B	1133	HIS
16	B	1160	GLN
17	C	114	HIS
17	C	265	HIS
18	a	52	HIS
18	a	136	ASN
18	a	278	GLN
18	a	331	ASN
18	a	346	GLN
18	a	556	GLN
19	b	346	ASN
19	b	504	ASN
20	c	194	GLN
20	c	447	GLN
20	c	507	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	P	24/35 (68%)	9 (37%)	1 (4%)
21	r	6/13 (46%)	0	0
22	v	13/14 (92%)	3 (23%)	0
All	All	43/62 (69%)	12 (27%)	1 (2%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	P	5	C
11	P	6	G
11	P	7	A
11	P	8	G
11	P	10	A
11	P	11	G
11	P	14	C
11	P	24	A
11	P	26	A
22	v	7	A
22	v	11	A
22	v	14	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	P	9	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
15	SEP	A	3021	15	8,9,10	1.53	1 (12%)	8,12,14	1.51	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	SEP	A	3007	15	8,9,10	1.53	1 (12%)	8,12,14	1.53	2 (25%)

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
15	SEP	A	3021	15	-	0/5/8/10	-
15	SEP	A	3007	15	-	2/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	3007	SEP	P-O1P	3.36	1.61	1.50
15	A	3021	SEP	P-O1P	3.35	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	3021	SEP	P-OG-CB	-2.93	110.23	118.30
15	A	3007	SEP	P-OG-CB	-2.91	110.27	118.30
15	A	3007	SEP	OG-CB-CA	2.61	110.68	108.14
15	A	3021	SEP	OG-CB-CA	2.49	110.56	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	3007	SEP	N-CA-CB-OG
15	A	3007	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PO4	c	801	-	4,4,4	0.95	0	6,6,6	0.41	0
25	G1G	P	101	11	46,58,58	1.74	7 (15%)	47,91,91	2.01	12 (25%)
27	PO4	a	1002	-	4,4,4	0.93	0	6,6,6	0.43	0

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
25	G1G	P	101	11	-	11/26/66/66	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	101	G1G	C35-C36	-7.09	1.33	1.47
25	P	101	G1G	C15-C16	-4.88	1.33	1.45
25	P	101	G1G	C35-C34	-3.85	1.33	1.43
25	P	101	G1G	O44-C41	2.98	1.45	1.41
25	P	101	G1G	C22-C21	-2.93	1.49	1.53
25	P	101	G1G	C15-C14	-2.69	1.33	1.39
25	P	101	G1G	C43-C42	-2.12	1.48	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	101	G1G	O24-C21-C22	-7.60	95.82	106.93
25	P	101	G1G	C12-N11-C16	-3.77	118.16	125.10
25	P	101	G1G	C32-N31-C36	-3.70	118.28	125.10
25	P	101	G1G	C35-C36-N31	3.27	119.72	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	101	G1G	PG-O3A-PB	-3.21	121.80	132.83
25	P	101	G1G	C43-C42-C41	-3.13	97.00	102.89
25	P	101	G1G	PB-O1B-PA	-2.92	122.82	132.83
25	P	101	G1G	C38-N37-C35	2.70	108.13	102.99
25	P	101	G1G	C23-C22-C21	-2.53	97.17	100.98
25	P	101	G1G	C42-C43-C44	-2.33	96.93	101.99
25	P	101	G1G	N31-C32-N33	-2.13	119.34	123.32
25	P	101	G1G	N11-C12-N13	-2.02	119.55	123.32

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	P	101	G1G	C43-C42-O42-C46
25	P	101	G1G	C45-O45-PA-O1A
25	P	101	G1G	C45-O45-PA-O2A
25	P	101	G1G	O44-C44-C45-O45
25	P	101	G1G	C43-C44-C45-O45
25	P	101	G1G	C44-C45-O45-PA
25	P	101	G1G	PB-O1B-PA-O45
25	P	101	G1G	PG-O3A-PB-O2B
25	P	101	G1G	C45-O45-PA-O1B
25	P	101	G1G	PG-O3A-PB-O3B
25	P	101	G1G	C25-O25-PG-O2G

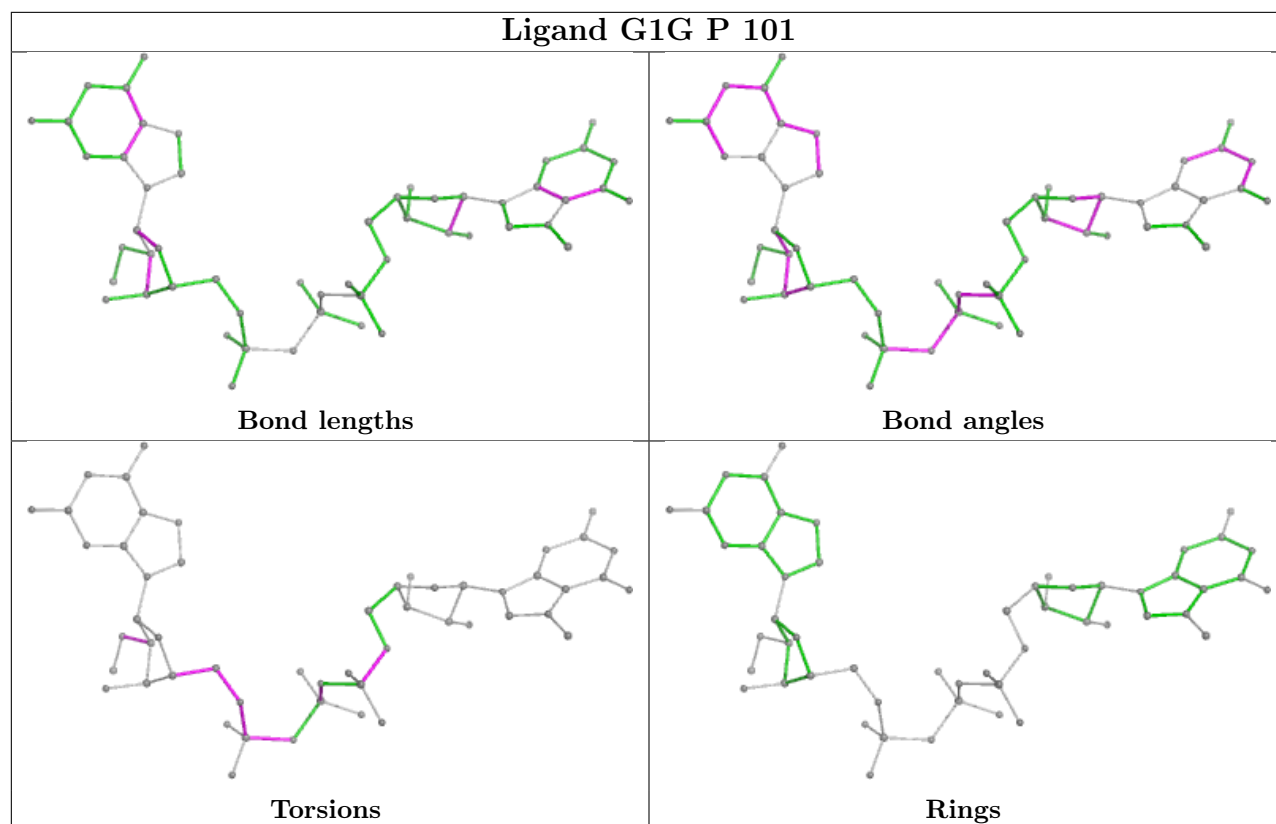
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	101	G1G	1	0

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

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

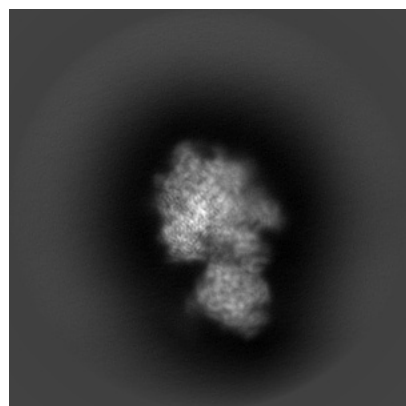
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50892. These allow visual inspection of the internal detail of the map and identification of artifacts.

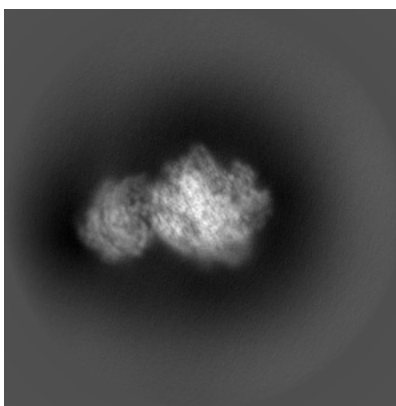
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

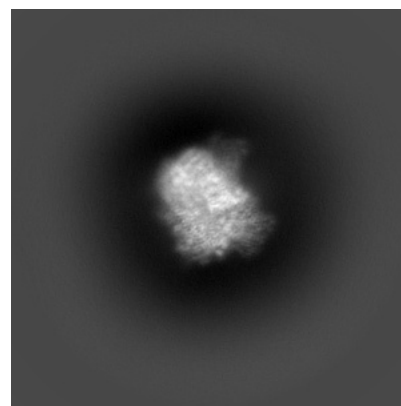
6.1.1 Primary map



X

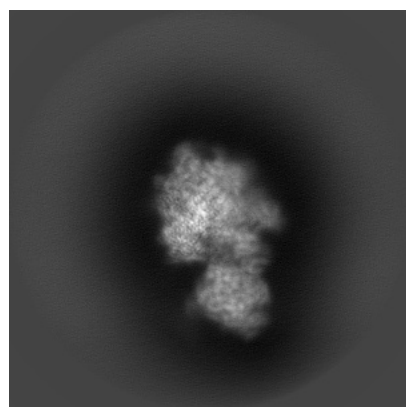


Y

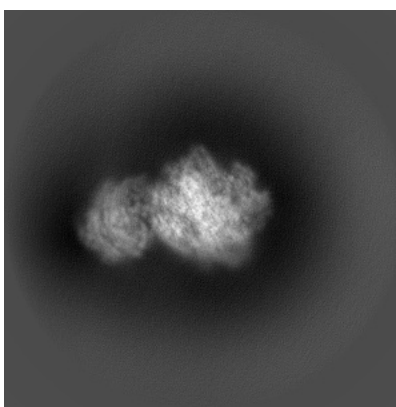


Z

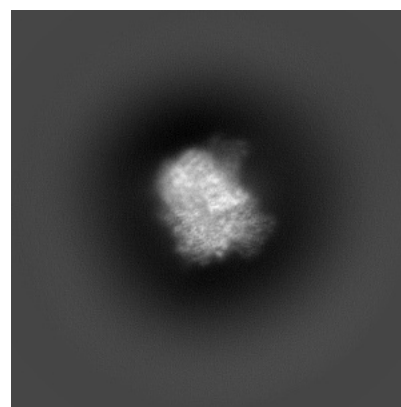
6.1.2 Raw map



X



Y

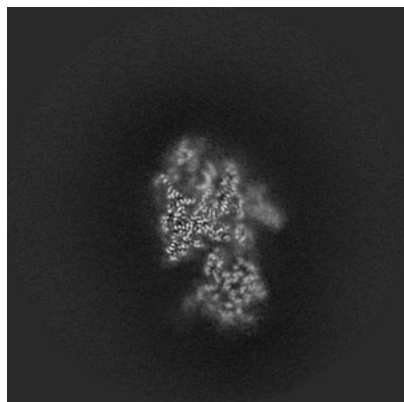


Z

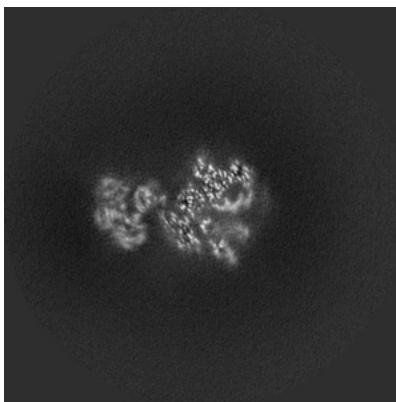
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

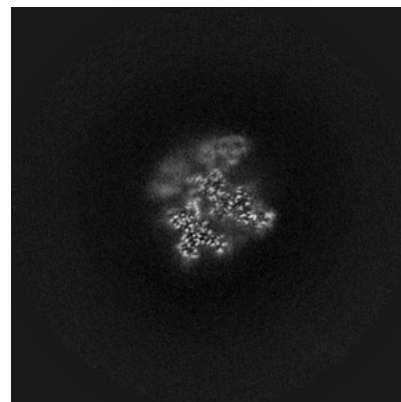
6.2.1 Primary map



X Index: 224

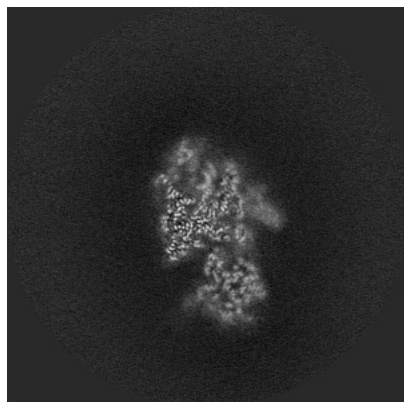


Y Index: 224

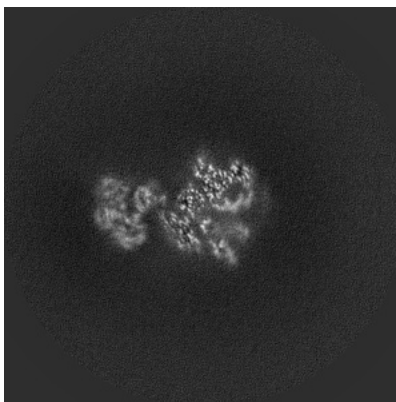


Z Index: 224

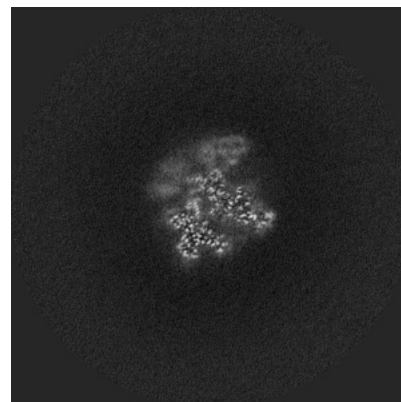
6.2.2 Raw map



X Index: 224



Y Index: 224

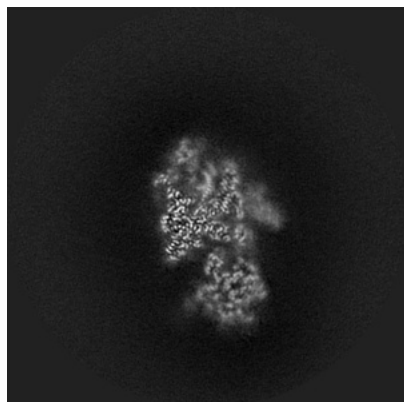


Z Index: 224

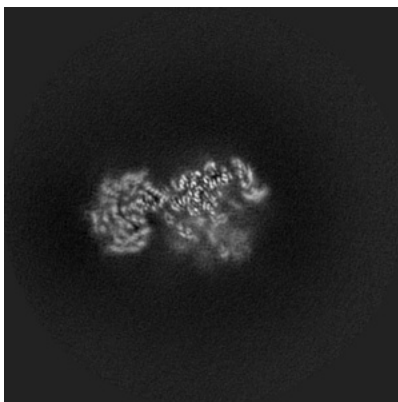
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

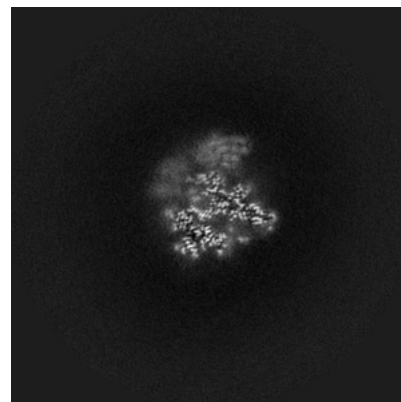
6.3.1 Primary map



X Index: 223

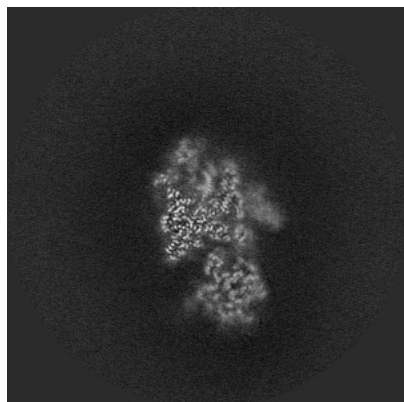


Y Index: 234

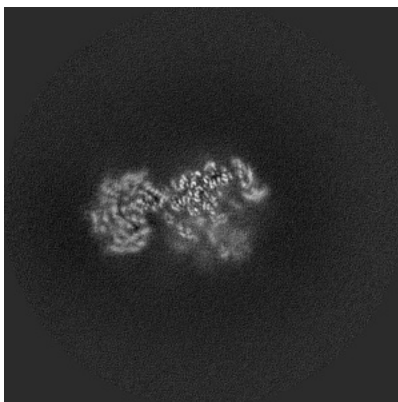


Z Index: 220

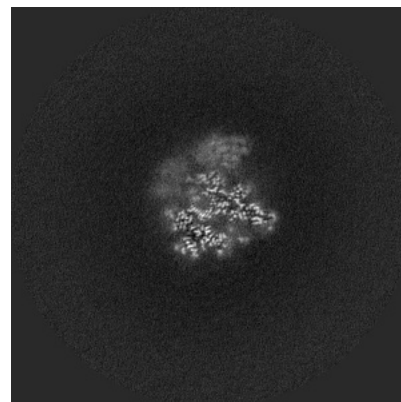
6.3.2 Raw map



X Index: 223



Y Index: 234

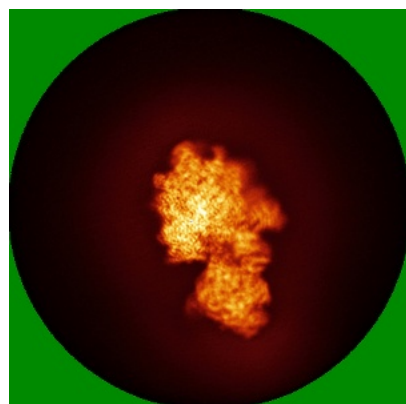


Z Index: 220

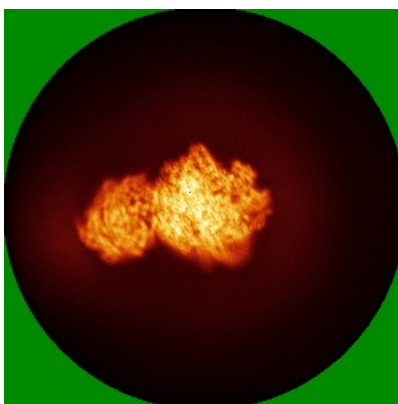
The images above show the largest variance slices of the map in three orthogonal directions.

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

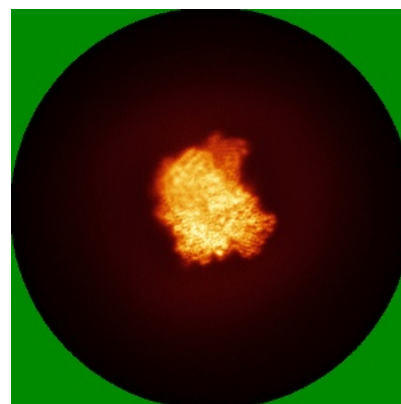
6.4.1 Primary map



X

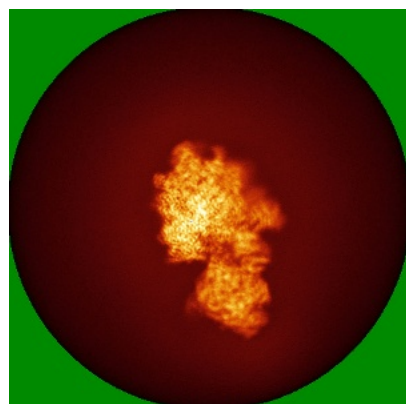


Y

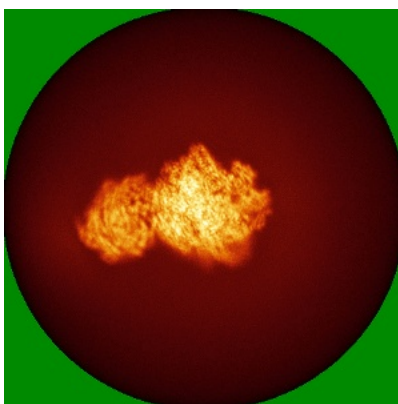


Z

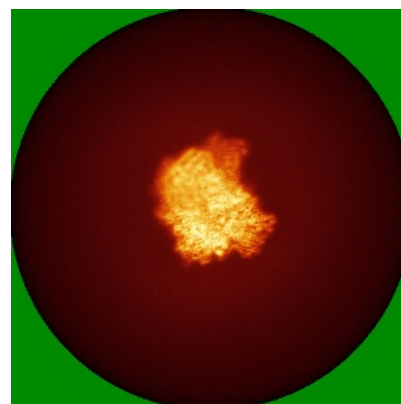
6.4.2 Raw map



X



Y

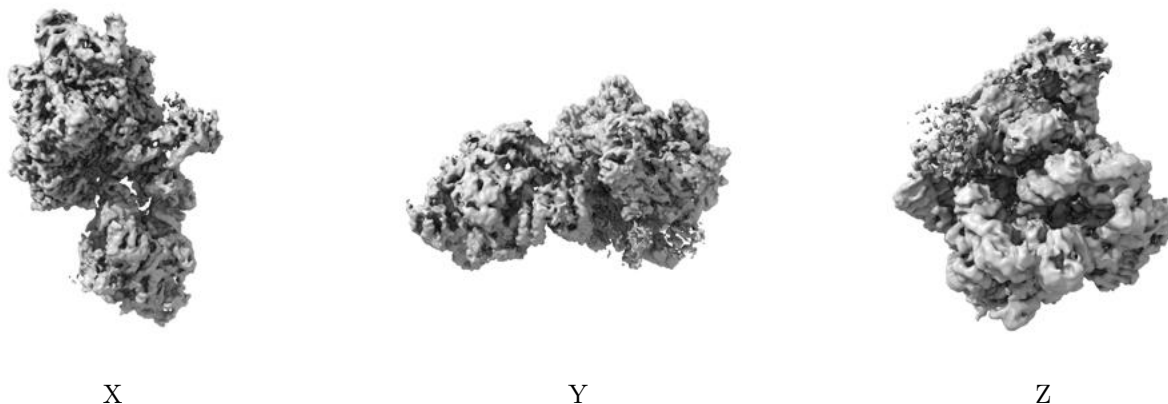


Z

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.

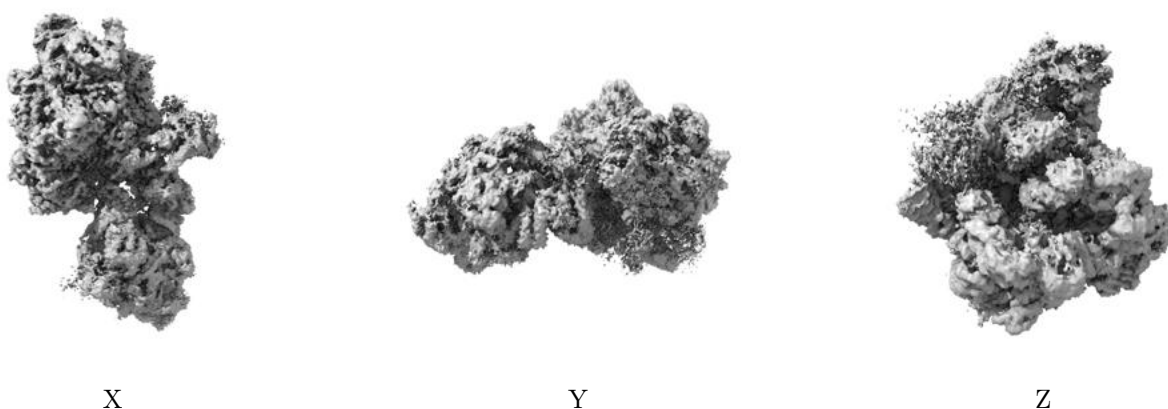
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. 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.

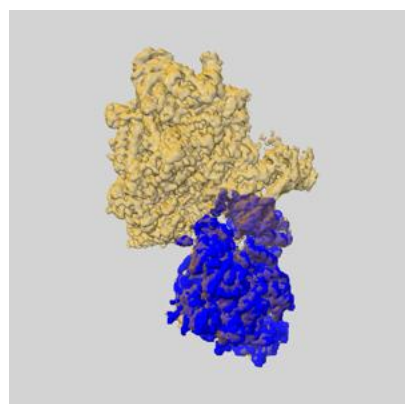
6.6 Mask visualisation [i](#)

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

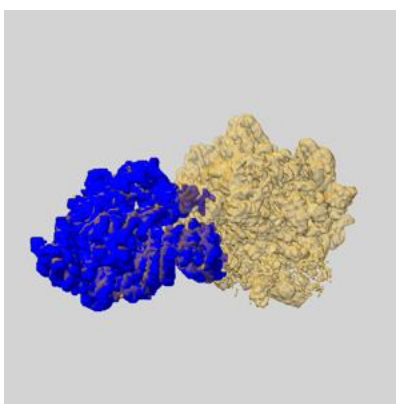
A mask typically either:

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

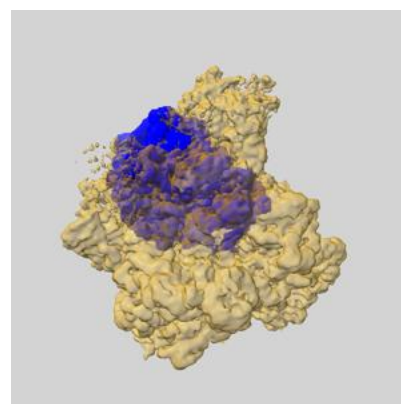
6.6.1 emd_50892_msk_1.map [i](#)



X

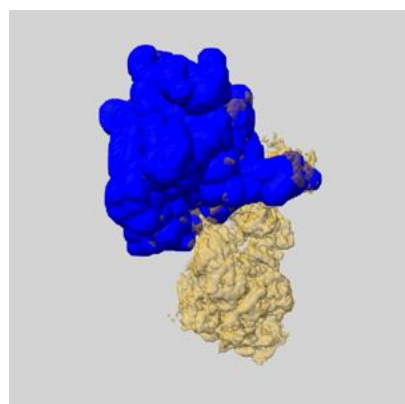


Y

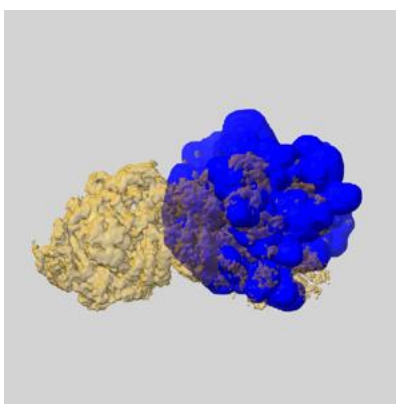


Z

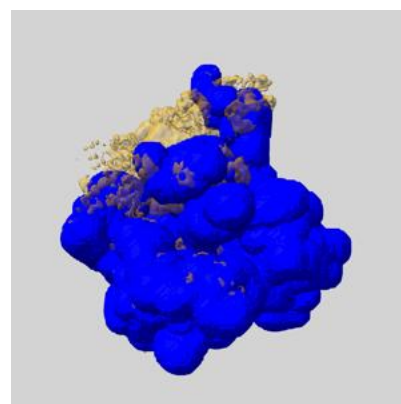
6.6.2 emd_50892_msk_2.map [i](#)



X

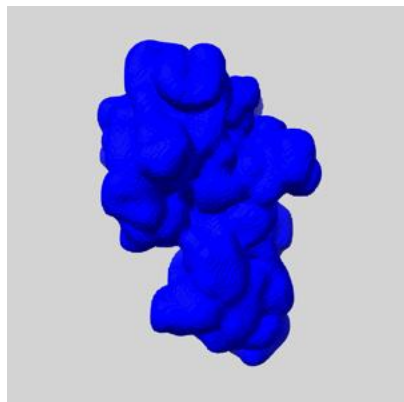


Y

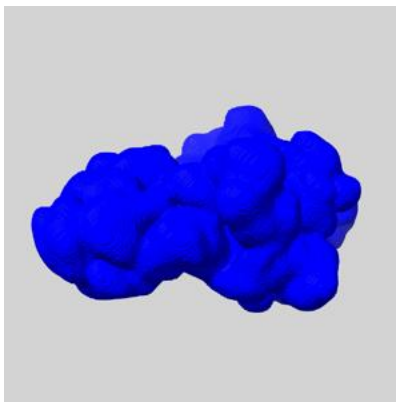


Z

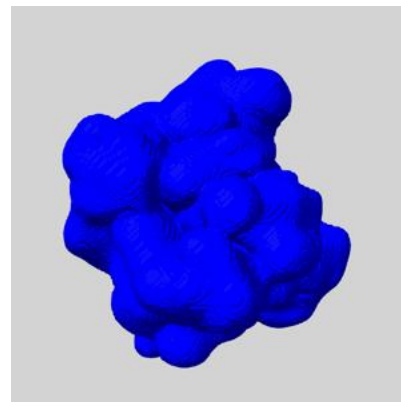
6.6.3 emd_50892_msk_3.map [i](#)



X



Y

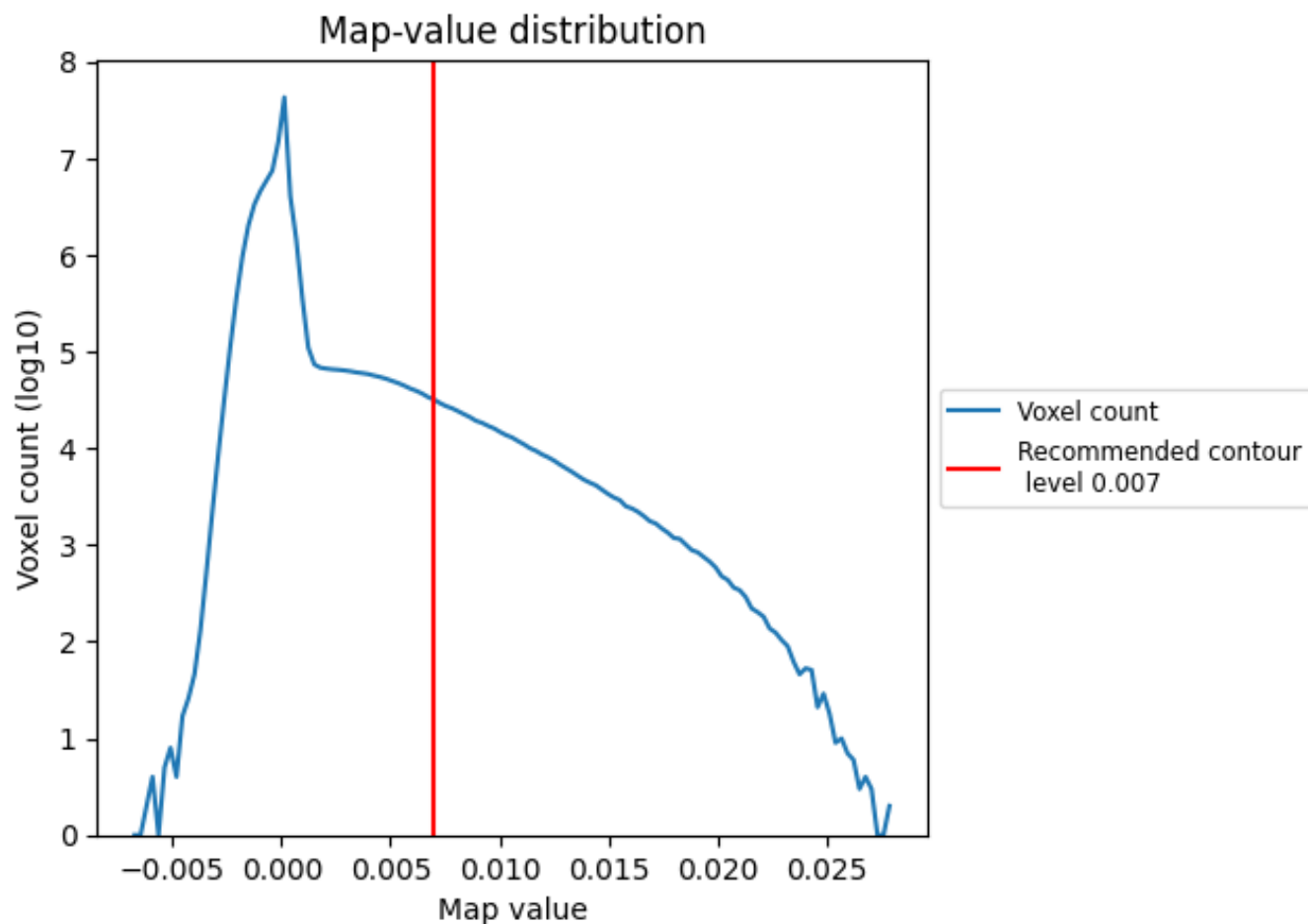


Z

7 Map analysis [i](#)

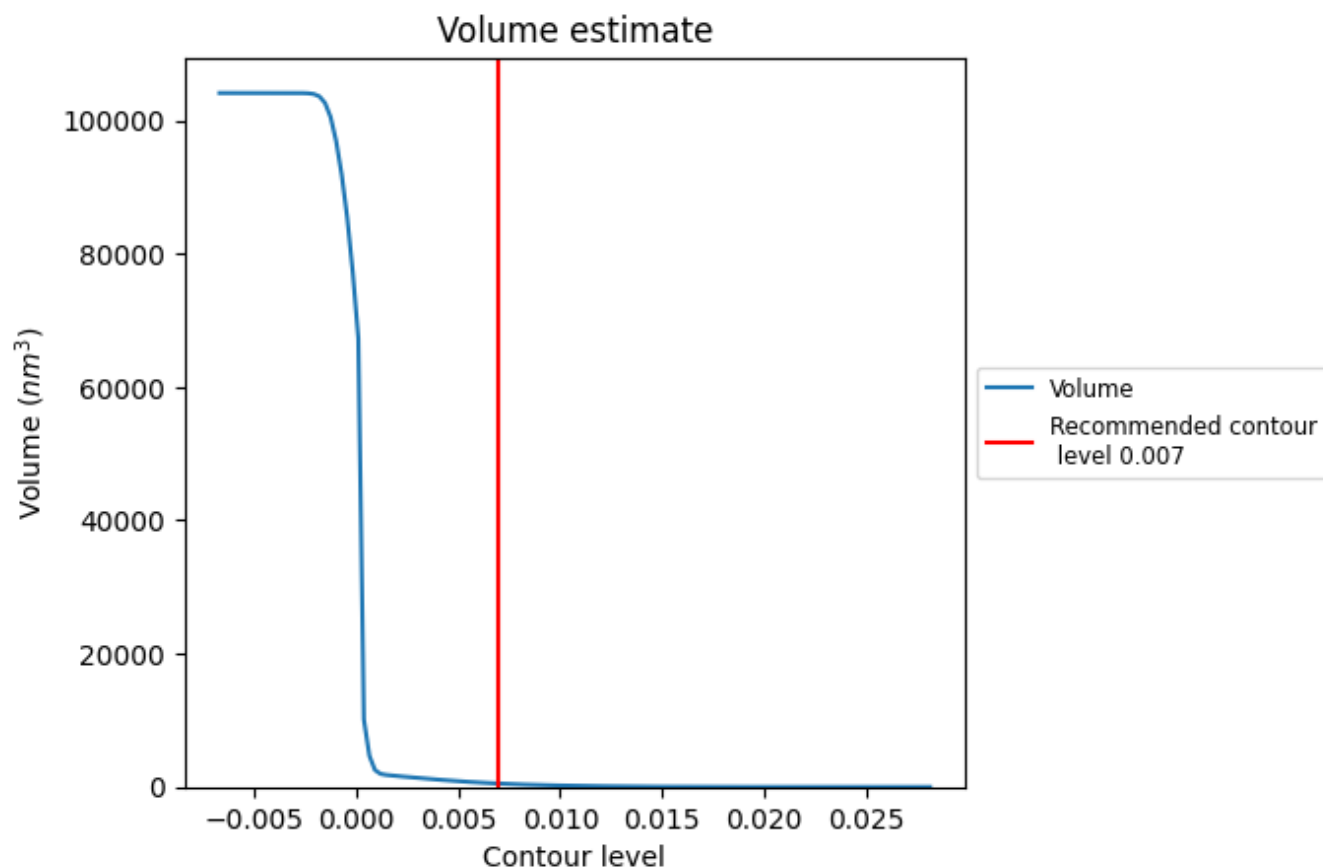
This section contains the results of statistical analysis of the map.

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.

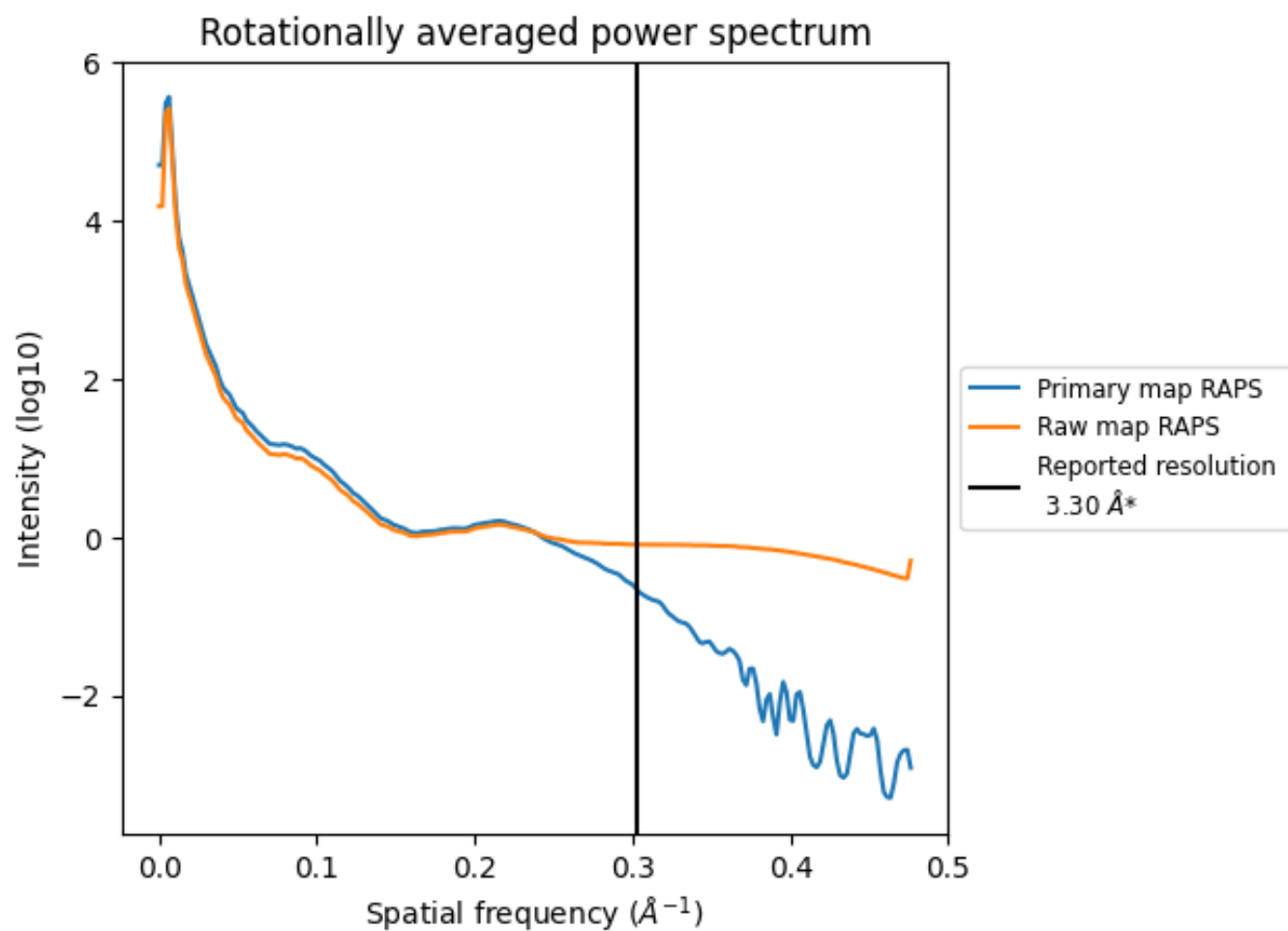
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 507 nm^3 ; this corresponds to an approximate mass of 458 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 ⓘ

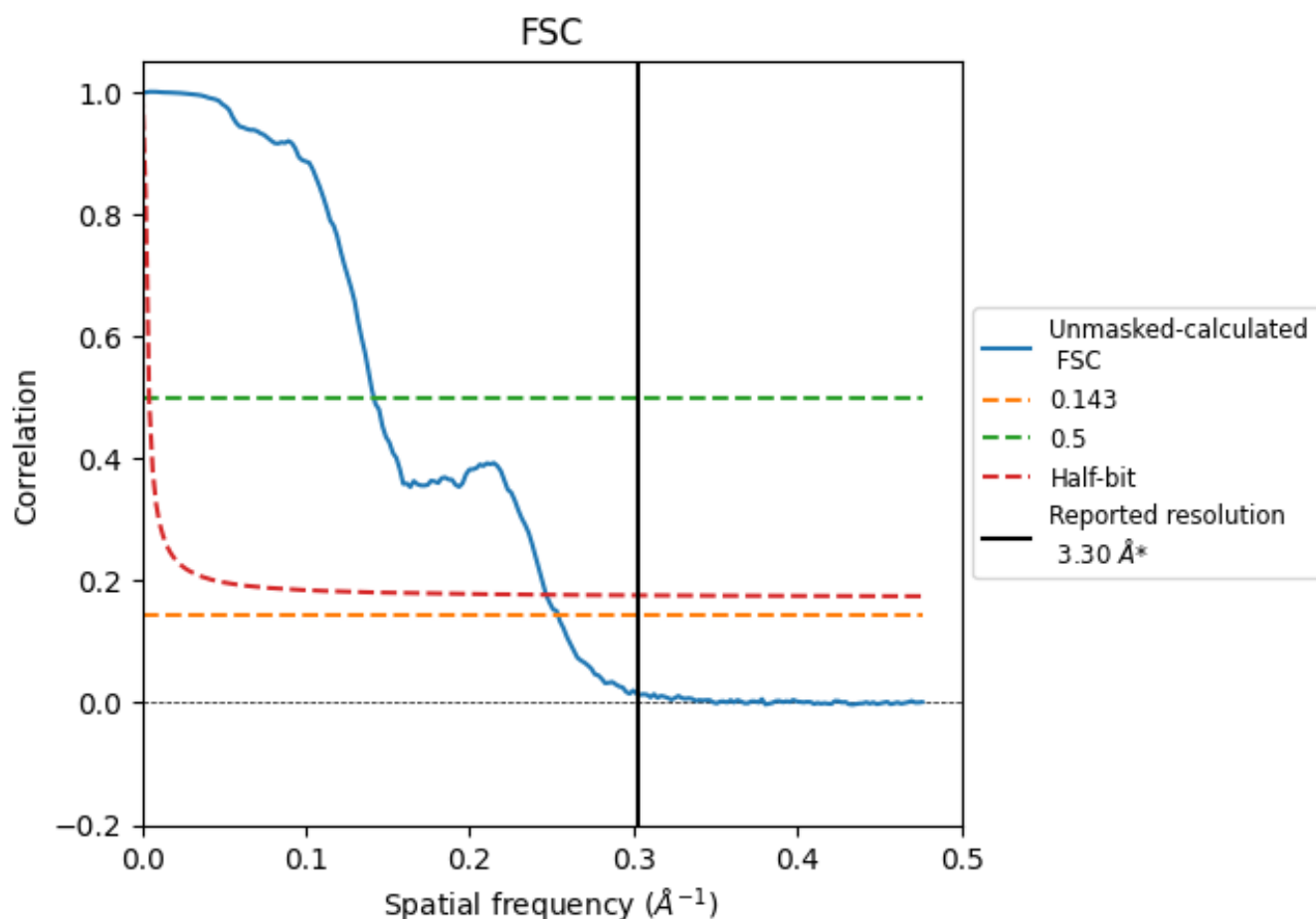


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

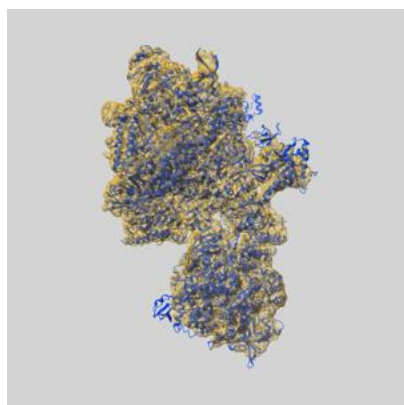
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	7.07	4.06

*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 3.94 differs from the reported value 3.3 by more than 10 %

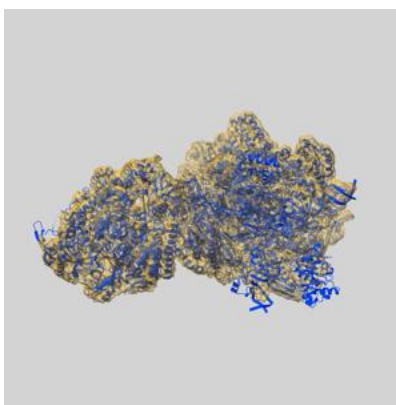
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50892 and PDB model 9FYX. Per-residue inclusion information can be found in section 3 on page 10.

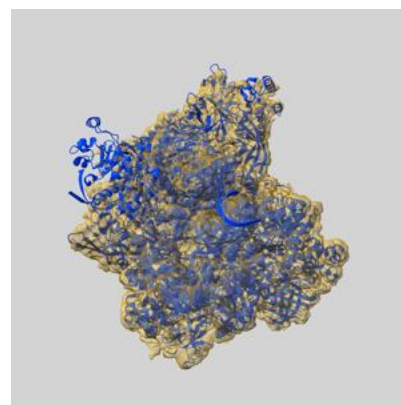
9.1 Map-model overlay [i](#)



X



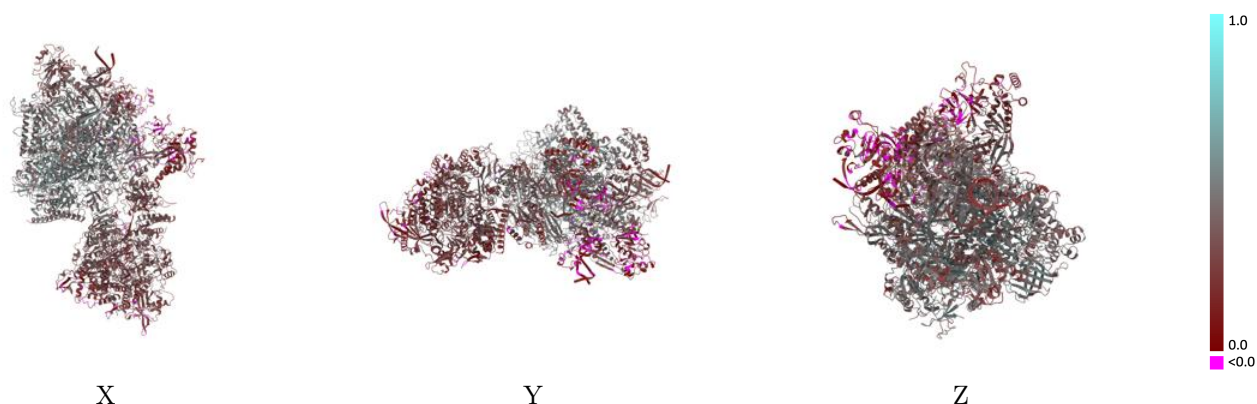
Y



Z

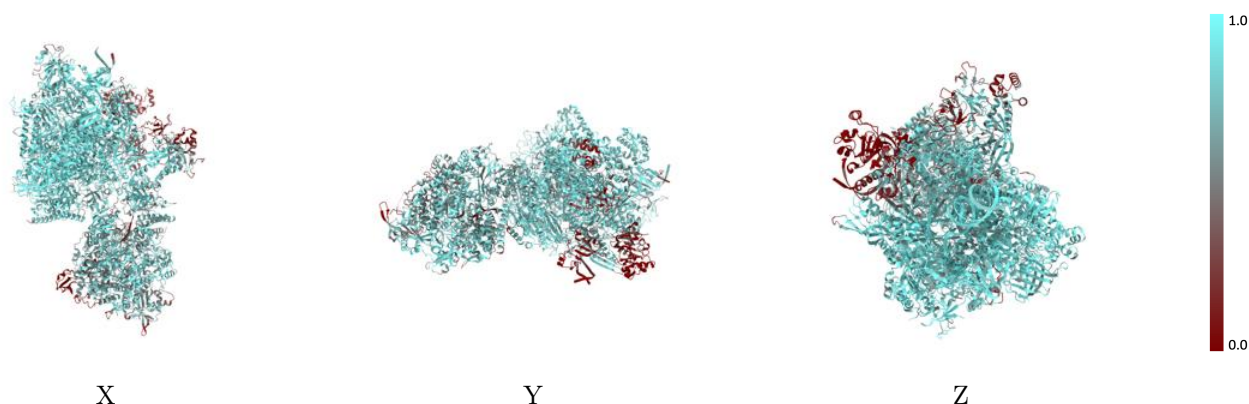
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



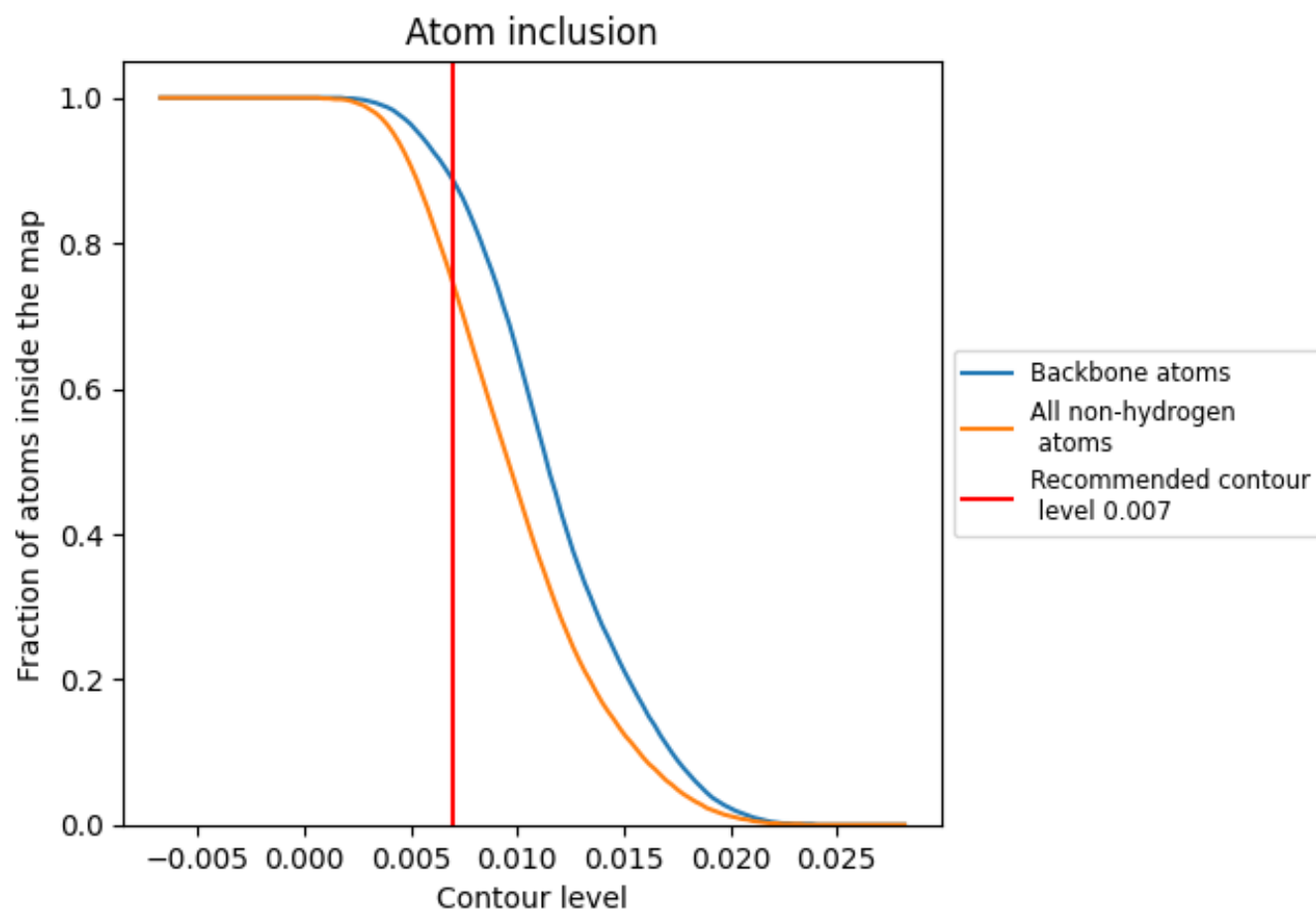
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 74% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7440	 0.3490
A	 0.8540	 0.4300
B	 0.8820	 0.4520
C	 0.8420	 0.4560
D	 0.4690	 0.2100
E	 0.8540	 0.4130
F	 0.8340	 0.4630
G	 0.7310	 0.2790
H	 0.8380	 0.4620
I	 0.7890	 0.3810
J	 0.8770	 0.4630
K	 0.8290	 0.4630
L	 0.8500	 0.4210
N	 0.7140	 0.2060
P	 0.8280	 0.3500
T	 0.7870	 0.2720
X	 0.2560	 0.1430
Y	 0.0280	 0.1020
Z	 0.3480	 0.1860
a	 0.6900	 0.2330
b	 0.7220	 0.2820
c	 0.6480	 0.3020
r	 0.8880	 0.3090
v	 0.9900	 0.2880

