



Full wwPDB EM Validation Report ⓘ

Jul 15, 2026 – 04:51 pm BST

PDB ID : 29TK / pdb_000029tk
EMDB ID : EMD-57364
Title : RNA polymerase II elongation complex with the +1 nucleosome
Authors : Zhan, Y.; Abril-Garrido, J.; Dienemann, C.; Cramer, P.
Deposited on : 2026-04-07
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

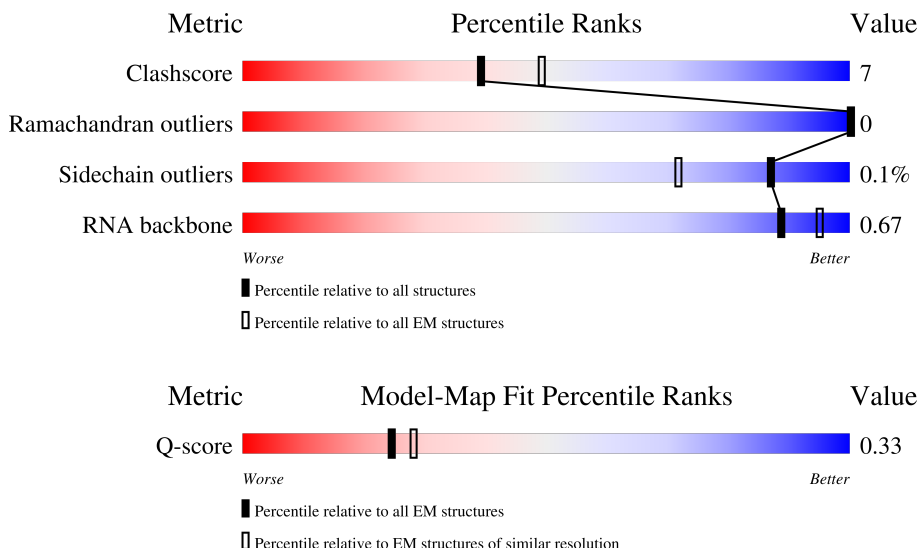
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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	C	275	
2	D	184	
3	E	210	

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Mol	Chain	Length	Quality of chain
4	F	127	
5	G	171	
6	H	150	
7	I	125	
8	J	67	
9	K	117	
10	L	58	
11	P	10	
12	Q	517	
13	R	249	
14	T	252	
15	W	439	
16	a	136	
16	e	136	
17	b	103	
17	f	103	
18	c	130	
18	g	130	
19	d	126	
19	h	126	
20	A	1970	
21	B	1300	
22	N	252	

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 94831 atoms, of which 45808 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	257	Total	C	H	N	O	S	0	0
			4071	1294	2012	351	408	6		

- Molecule 2 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	128	Total	C	H	N	O	S	0	0
			2084	656	1034	178	212	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	209	Total	C	H	N	O	S	0	0
			3458	1089	1738	300	323	8		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	82	Total	C	H	N	O	S	0	0
			1342	418	685	113	121	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	171	Total	C	H	N	O	S	0	0
			2709	875	1358	219	249	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	H	148	Total	C	H	N	O	S	0	0
			2334	750	1148	194	237	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	114	Total	C	H	N	O	S	0	0
			1795	571	868	166	179	11		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	67	Total	C	H	N	O	S	0	0
			1090	345	557	90	92	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	114	Total	C	H	N	O	S	0	0
			1855	591	939	151	172	2		

- Molecule 10 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	44	Total	C	H	N	O	S	0	0
			755	231	383	72	63	6		

- Molecule 11 is a RNA chain called RNA (5'-R(P*AP*CP*AP*CP*CP*CP*AP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
11	P	10	Total	C	H	N	O	P	0	0
			319	94	110	38	67	10		

- Molecule 12 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Q	138	Total	C	H	N	O	S	0	0
			2242	719	1104	208	208	3		

- Molecule 13 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	R	137	Total	C	H	N	O	S	0	0
			2158	666	1088	193	209	2		

- Molecule 14 is a DNA chain called DNA (199-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
14	T	199	Total	C	H	N	O	P	0	0
			6341	1943	2231	775	1193	199		

- Molecule 15 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	W	187	Total	C	H	N	O	S	0	0
			3079	964	1544	275	285	11		

- Molecule 16 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	a	97	Total	C	H	N	O	S	0	0
			1639	505	838	155	138	3		
16	e	98	Total	C	H	N	O	S	0	0
			1661	511	851	157	139	3		

- Molecule 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	b	82	Total	C	H	N	O	S	0	0
			1350	412	697	127	113	1		
17	f	82	Total	C	H	N	O	S	0	0
			1351	412	698	127	113	1		

- Molecule 18 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	c	109	Total	C	H	N	O	0	0
			1752	531	909	167	145		
18	g	106	Total	C	H	N	O	0	0
			1696	516	878	160	142		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	100	ARG	GLY	engineered mutation	UNP P06897
g	100	ARG	GLY	engineered mutation	UNP P06897

- Molecule 19 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	d	97	Total	C	H	N	O	S	0	0
			1564	480	798	142	142	2		
19	h	95	Total	C	H	N	O	S	0	0
			1516	468	772	134	140	2		

- Molecule 20 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	A	1417	Total	C	H	N	O	S	0	0
			22613	7070	11379	2010	2082	72		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2

- Molecule 21 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	B	1130	Total	C	H	N	O	S	0	0
			18110	5714	9080	1587	1665	64		

- Molecule 22 is a DNA chain called DNA (188-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
22	N	188	Total	C	H	N	O	P	0	0
			5937	1818	2109	693	1129	188		

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

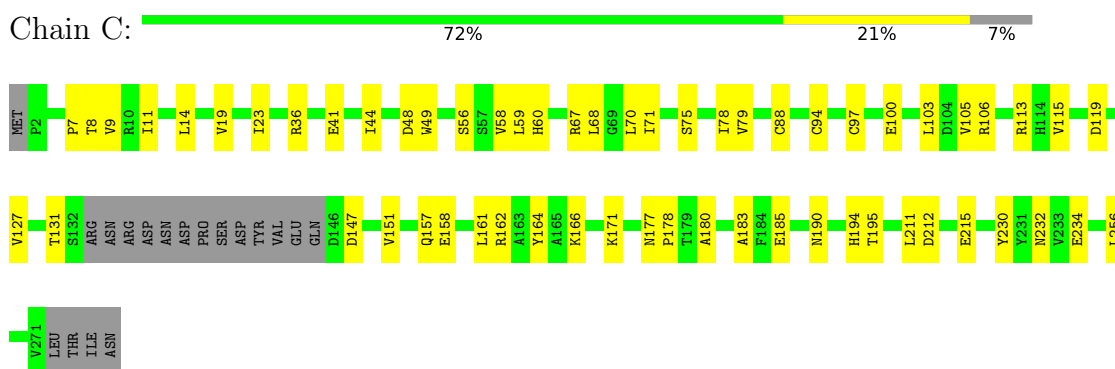
- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

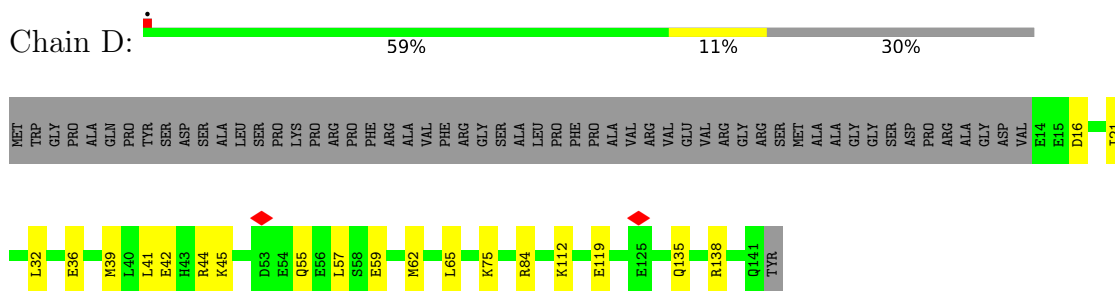
3 Residue-property plots

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.

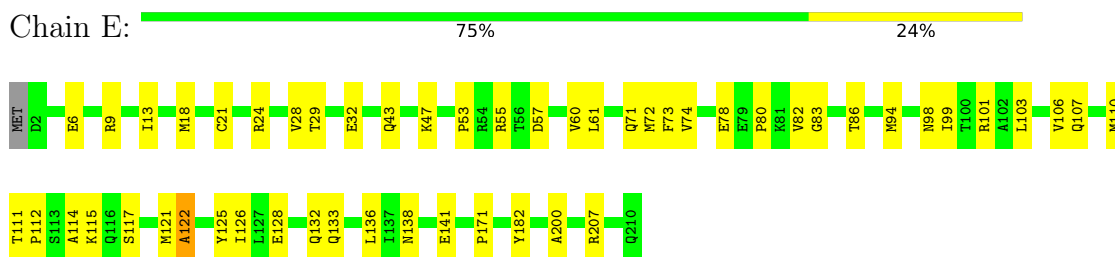
- Molecule 1: DNA-directed RNA polymerase II subunit RPB3



- Molecule 2: RNA polymerase II subunit D

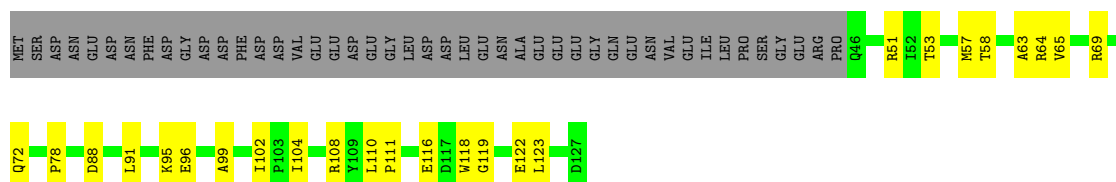


- Molecule 3: DNA-directed RNA polymerase II subunit E

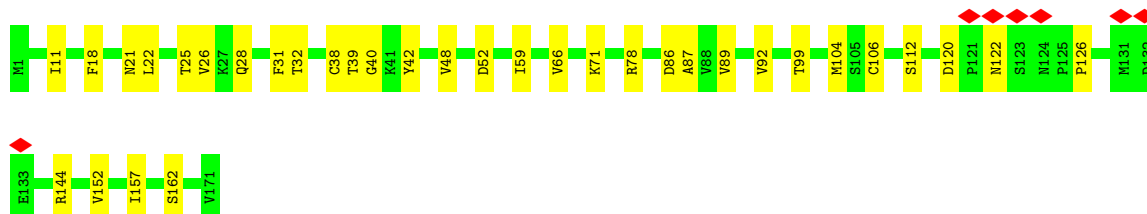
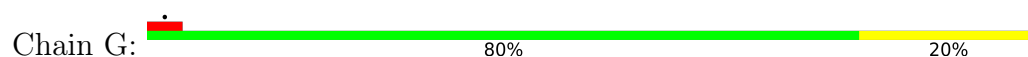


- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC2

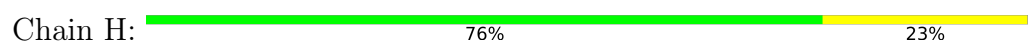




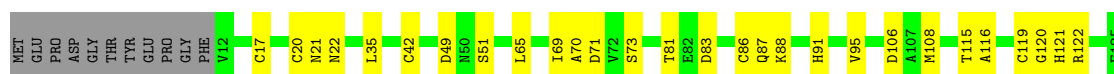
- Molecule 5: DNA-directed RNA polymerase subunit



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



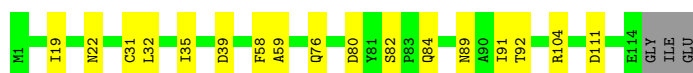
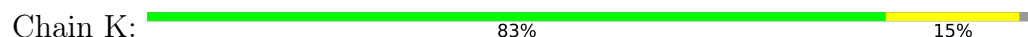
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



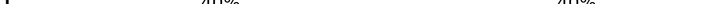
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11-a



- Molecule 10: RNA polymerase II subunit K

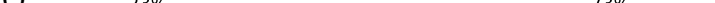


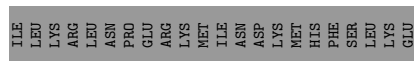
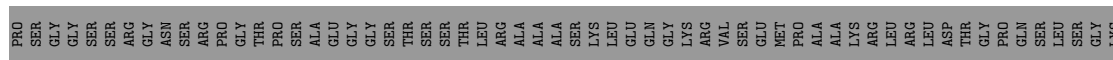
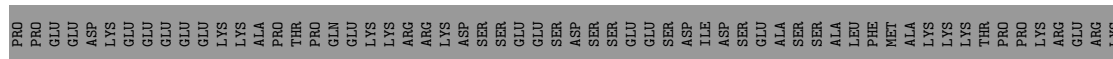
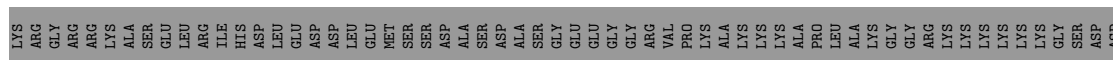
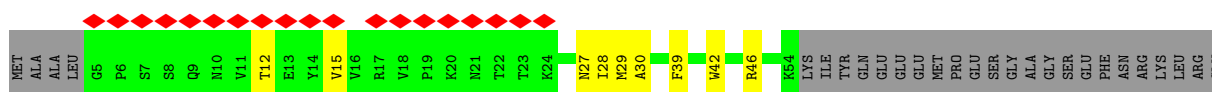
- Molecule 11: RNA (5'-R(P*AP*CP*AP*CP*CP*CP*AP*GP*CP*C)-3')

Chain P:  40% 40% 10% 10%

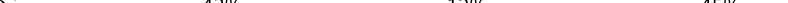


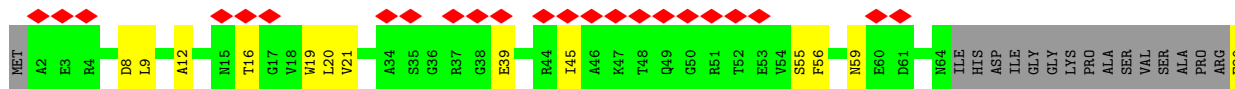
- Molecule 12: General transcription factor IIF subunit 1

Chain Q:  6% 23% 73%

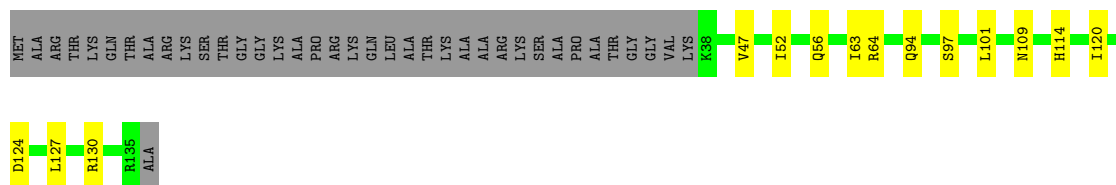


- Molecule 13: General transcription factor IIF subunit 2

Chain R: 

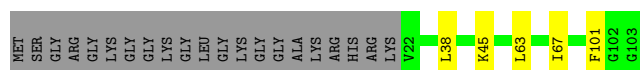


Chain e:  62% 10% 28%



- Molecule 17: Histone H4

Chain b:  75% 5% 20%



- Molecule 17: Histone H4

Chain f:  69% 11% 20%



- Molecule 18: Histone H2A type 1

Chain c:  74% 10% 16%



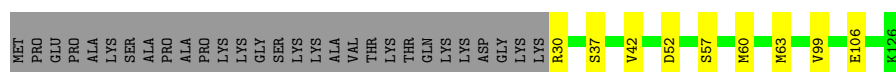
- Molecule 18: Histone H2A type 1

Chain g:  68% 14% 18%



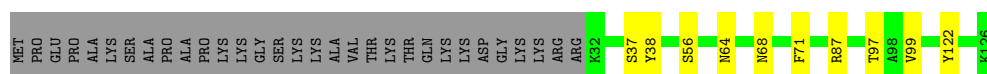
- Molecule 19: Histone H2B 1.1

Chain d:  70% 7% 23%



- Molecule 19: Histone H2B 1.1

Chain h:  67% 8% 25%

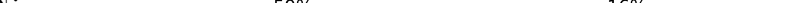


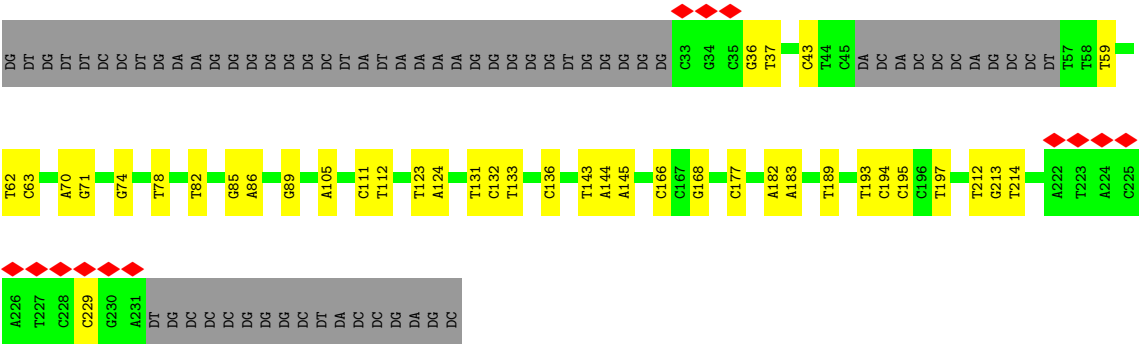
Chain A: 56% 15% 28%



- Molecule 21: DNA-directed RNA polymerase subunit beta

[illegible]

Chain N:  5% 59% 16% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62231	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size ($\text{\AA}$)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: 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	C	0.25	0/2102	0.45	0/2857
2	D	0.18	0/1064	0.46	0/1428
3	E	0.27	0/1751	0.57	1/2366 (0.0%)
4	F	0.26	0/667	0.66	0/901
5	G	0.20	0/1382	0.45	0/1874
6	H	0.29	0/1207	0.56	0/1628
7	I	0.22	0/948	0.53	0/1284
8	J	0.27	0/542	0.48	0/730
9	K	0.26	0/935	0.49	0/1266
10	L	0.28	0/377	0.73	0/500
11	P	0.46	0/232	1.05	1/358 (0.3%)
12	Q	0.15	0/1167	0.44	0/1576
13	R	0.14	0/1083	0.41	0/1459
14	T	0.25	0/4616	0.60	2/7127 (0.0%)
15	W	0.16	0/1560	0.48	0/2097
16	a	0.21	0/813	0.54	0/1090
16	e	0.23	0/822	0.55	0/1102
17	b	0.23	0/660	0.54	0/883
17	f	0.27	0/660	0.69	0/883
18	c	0.22	0/853	0.49	0/1149
18	g	0.21	0/828	0.51	0/1117
19	d	0.22	0/777	0.54	1/1041 (0.1%)
19	h	0.19	0/755	0.48	0/1013
20	A	0.27	1/11439 (0.0%)	0.61	6/15440 (0.0%)
21	B	0.25	0/9210	0.54	3/12431 (0.0%)
22	N	0.26	0/4287	0.88	9/6604 (0.1%)
All	All	0.25	1/50737 (0.0%)	0.60	23/70204 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
20	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1200	PRO	CG-CD	-5.36	1.32	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	62	DT	OP1-P-O3'	-23.46	37.62	108.00
22	N	71	DG	OP1-P-O3'	-21.93	42.22	108.00
22	N	43	DC	OP1-P-O3'	-21.84	42.49	108.00
22	N	59	DT	OP1-P-O3'	-21.54	43.38	108.00
22	N	37	DT	OP1-P-O3'	-21.53	43.42	108.00
22	N	36	DG	OP1-P-O3'	-21.32	44.03	108.00
20	A	1200	PRO	CA-N-CD	-13.95	92.47	112.00
20	A	1200	PRO	N-CD-CG	-8.74	90.09	103.20
14	T	59	DC	OP1-P-O3'	8.09	132.26	108.00
22	N	63	DC	OP1-P-OP2	-7.03	98.91	120.00
22	N	78	DT	OP1-P-O3'	7.02	129.07	108.00
20	A	1292	MET	CA-CB-CG	6.18	126.46	114.10
22	N	70	DA	OP1-P-O3'	5.53	124.59	108.00
20	A	660	MET	CB-CG-SD	5.50	129.20	112.70
21	B	226	GLU	CA-CB-CG	5.46	125.02	114.10
20	A	524	MET	CB-CA-C	5.43	121.22	110.42
21	B	347	MET	CB-CG-SD	5.27	128.52	112.70
21	B	109	MET	CB-CG-SD	5.26	128.48	112.70
20	A	467	MET	CB-CG-SD	5.22	128.35	112.70
11	P	2	C	OP1-P-O3'	5.21	123.62	108.00
14	T	60	DG	OP1-P-OP2	-5.08	104.77	120.00
19	d	60	MET	CB-CG-SD	5.05	127.85	112.70
3	E	122	ALA	N-CA-C	5.04	114.61	108.11

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	A	538	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2059	2012	2007	41	0
2	D	1050	1034	1033	15	0
3	E	1720	1738	1737	35	0
4	F	657	685	684	19	0
5	G	1351	1358	1358	23	0
6	H	1186	1148	1147	23	0
7	I	927	868	859	18	0
8	J	533	557	553	16	0
9	K	916	939	939	14	0
10	L	372	383	379	5	0
11	P	209	110	110	8	0
12	Q	1138	1104	1103	15	0
13	R	1070	1088	1086	21	0
14	T	4110	2231	2233	32	0
15	W	1535	1544	1540	9	0
16	a	801	838	839	11	0
16	e	810	851	851	13	0
17	b	653	697	696	4	0
17	f	653	698	696	11	0
18	c	843	909	908	11	0
18	g	818	878	877	15	0
19	d	766	798	797	8	0
19	h	744	772	771	9	0
20	A	11234	11379	11366	210	0
21	B	9030	9080	9073	176	0
22	N	3828	2109	2111	27	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	W	1	0	0	0	0
24	A	1	0	0	0	0
All	All	49023	45808	45753	661	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 7.

All (661) 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)
20:A:539:GLN:HE22	21:B:791:GLU:HG2	1.49	0.76
12:Q:29:MET:HE3	12:Q:30:ALA:H	1.50	0.75
21:B:407:MET:HE1	21:B:440:ILE:HA	1.68	0.73
11:P:2:C:O2'	11:P:3:A:P	2.47	0.72
20:A:922:PHE:H	20:A:1052:ARG:HD2	1.55	0.71
20:A:11:SER:N	21:B:1135:TYR:HH	1.87	0.71
12:Q:127:PHE:HB2	13:R:19:TRP:HB2	1.73	0.70
6:H:96:VAL:HG12	6:H:116:VAL:HG22	1.74	0.70
21:B:108:MET:HE1	21:B:118:LEU:HG	1.75	0.69
21:B:1119:CYS:HB2	21:B:1137:CYS:SG	2.32	0.69
7:I:86:CYS:SG	7:I:87:GLN:N	2.66	0.68
3:E:112:PRO:HA	3:E:115:LYS:HB2	1.76	0.68
7:I:17:CYS:HB3	7:I:22:ASN:H	1.58	0.67
11:P:8:G:N2	14:T:46:DC:O2	2.27	0.67
20:A:33:ARG:HD2	21:B:1139:GLY:HA2	1.78	0.66
21:B:285:LEU:HD11	21:B:305:LEU:HD21	1.77	0.66
3:E:103:LEU:HG	3:E:128:GLU:HB2	1.78	0.65
8:J:1:MET:HB2	8:J:55:LEU:HB2	1.78	0.65
13:R:16:THR:HB	13:R:108:GLY:HA3	1.79	0.65
21:B:728:MET:HE1	21:B:942:LYS:HG2	1.79	0.64
4:F:57:MET:HB2	4:F:123:LEU:HB3	1.80	0.63
1:C:49:TRP:HB3	1:C:164:TYR:HB2	1.81	0.63
20:A:420:ILE:HB	20:A:445:LYS:HB2	1.81	0.62
8:J:10:CYS:SG	8:J:42:ARG:NH2	2.73	0.62
20:A:991:GLN:HG2	20:A:996:ILE:HD11	1.82	0.62
9:K:22:ASN:HB2	9:K:32:LEU:HB3	1.81	0.62
20:A:1216:LEU:HB2	20:A:1255:LEU:HB2	1.80	0.62
15:W:144:LEU:HD22	15:W:155:THR:H	1.63	0.62
20:A:515:ILE:HG23	20:A:519:ALA:HB3	1.82	0.61
21:B:255:ARG:HE	21:B:307:GLU:HG3	1.64	0.61
4:F:64:ARG:NH2	20:A:1468:THR:O	2.34	0.61
11:P:2:C:HO2'	11:P:3:A:P	2.23	0.61
20:A:890:ARG:HE	20:A:1023:VAL:HG22	1.66	0.61
20:A:335:PRO:HD3	21:B:460:HIS:HE1	1.65	0.61
3:E:6:GLU:HG2	3:E:9:ARG:HH11	1.66	0.60
22:N:143:DT:H4'	22:N:144:DA:H5'	1.84	0.60
10:L:38:GLU:OE1	10:L:38:GLU:N	2.35	0.60
16:e:109:ASN:HB2	17:f:44:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:289:ILE:HD12	21:B:297:MET:HG3	1.83	0.60
20:A:1206:ARG:NH1	20:A:1262:MET:SD	2.74	0.60
21:B:274:ARG:HG2	21:B:279:VAL:HA	1.82	0.60
7:I:21:ASN:HD21	21:B:282:ARG:HD2	1.66	0.60
6:H:103:GLU:OE2	20:A:999:ARG:NH1	2.34	0.60
12:Q:46:ARG:HB2	12:Q:101:ARG:HB2	1.82	0.60
21:B:270:ILE:HG23	21:B:284:ILE:HG21	1.82	0.60
21:B:1016:SER:HB2	21:B:1022:LEU:HB3	1.84	0.60
20:A:279:LYS:HZ1	20:A:336:LEU:HG	1.66	0.59
21:B:331:THR:HG23	21:B:334:LYS:H	1.67	0.59
20:A:1141:VAL:HB	20:A:1336:LEU:HB2	1.83	0.59
20:A:1180:ASN:HB3	20:A:1183:SER:HB3	1.83	0.59
20:A:114:CYS:SG	20:A:184:CYS:HB3	2.42	0.59
20:A:1189:ASP:OD2	20:A:1258:ARG:NH1	2.35	0.59
1:C:59:LEU:HD23	1:C:151:VAL:HG23	1.83	0.59
14:T:25:DC:H42	22:N:74:DG:H1	1.50	0.59
5:G:52:ASP:HB3	5:G:71:LYS:HG3	1.85	0.59
20:A:26:LEU:HG	21:B:1168:ALA:HB2	1.84	0.59
20:A:54:LEU:HD13	20:A:60:PRO:HD2	1.85	0.59
19:d:30:ARG:NH1	22:N:189:DT:O2	2.36	0.59
20:A:1232:ALA:O	20:A:1236:ASN:ND2	2.36	0.59
20:A:1368:VAL:HG13	20:A:1369:LEU:HG	1.83	0.59
20:A:31:LEU:HD11	20:A:254:PRO:HG3	1.83	0.59
20:A:359:VAL:HG21	21:B:1106:ARG:HD3	1.84	0.59
21:B:288:ILE:HD13	21:B:366:GLY:HA2	1.85	0.59
7:I:70:ALA:HB2	7:I:122:ARG:HH11	1.68	0.58
9:K:111:ASP:OD1	9:K:111:ASP:N	2.35	0.58
20:A:1343:LEU:HD22	20:A:1368:VAL:HG11	1.84	0.58
21:B:725:GLN:HA	21:B:728:MET:HG2	1.85	0.58
22:N:132:DC:H4'	22:N:133:DT:H5'	1.86	0.58
16:a:42:TYR:HA	22:N:229:DC:H5''	1.84	0.58
20:A:29:ASP:OD1	20:A:33:ARG:NH1	2.37	0.58
6:H:14:ASP:HB2	6:H:29:HIS:HB2	1.86	0.58
20:A:831:LEU:H	21:B:715:ASP:HB2	1.68	0.58
5:G:112:SER:HB2	5:G:162:SER:HA	1.84	0.58
1:C:58:VAL:HG21	8:J:59:LEU:HB3	1.85	0.58
20:A:727:PRO:HA	20:A:736:THR:HG21	1.85	0.58
21:B:273:PHE:HB3	21:B:284:ILE:HD12	1.85	0.58
1:C:9:VAL:HG12	1:C:23:ILE:HG12	1.84	0.58
21:B:566:LYS:HA	21:B:576:ILE:HG22	1.86	0.58
20:A:1017:SER:OG	20:A:1042:ASN:ND2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:18:DG:N2	22:N:82:DT:O2	2.36	0.58
20:A:373:LEU:O	20:A:485:ASN:ND2	2.37	0.58
12:Q:27:ASN:ND2	13:R:98:GLU:OE2	2.37	0.57
14:T:13:DT:H5"	22:N:89:DG:H5"	1.84	0.57
15:W:48:MET:HE1	15:W:63:LEU:HD21	1.86	0.57
20:A:369:PRO:HB3	20:A:486:LEU:HD21	1.86	0.57
21:B:1142:ASN:ND2	21:B:1145:GLN:O	2.37	0.57
1:C:78:ILE:HD11	1:C:127:VAL:HG23	1.86	0.57
5:G:40:GLY:HA2	5:G:152:VAL:HG21	1.86	0.57
20:A:352:GLY:HA2	21:B:1085:ARG:HH12	1.69	0.57
20:A:883:ILE:HG13	20:A:885:GLN:HG3	1.85	0.57
20:A:1139:LEU:HD21	20:A:1346:VAL:HG11	1.85	0.57
20:A:384:ILE:HG12	21:B:1061:SER:HB3	1.86	0.57
21:B:218:THR:HA	21:B:238:SER:HA	1.85	0.57
21:B:784:SER:HA	21:B:789:ASN:HD21	1.68	0.57
20:A:481:THR:OG1	20:A:483:ARG:NH2	2.37	0.57
1:C:9:VAL:HG22	9:K:104:ARG:HG2	1.87	0.57
20:A:549:THR:HG21	20:A:640:LEU:HG	1.86	0.57
21:B:758:LEU:H	21:B:777:ASN:HD21	1.52	0.57
1:C:194:HIS:HB3	21:B:1036:LYS:HB2	1.87	0.57
12:Q:39:PHE:HA	12:Q:42:TRP:HD1	1.69	0.57
1:C:183:ALA:HB3	1:C:232:ASN:HB3	1.87	0.56
3:E:80:PRO:HA	3:E:107:GLN:HB2	1.87	0.56
14:T:-103:DA:H5"	18:g:17:THR:HA	1.86	0.56
20:A:42:LYS:O	20:A:288:ASN:ND2	2.38	0.56
20:A:389:THR:O	20:A:507:GLN:NE2	2.38	0.56
18:g:16:LYS:O	18:g:21:ARG:NH2	2.38	0.56
21:B:715:ASP:N	21:B:715:ASP:OD1	2.37	0.56
1:C:113:ARG:NH1	1:C:119:ASP:OD1	2.37	0.56
12:Q:100:LEU:HB3	12:Q:110:PHE:HB2	1.86	0.56
2:D:59:GLU:HA	2:D:62:MET:HE1	1.87	0.56
18:c:55:VAL:HG21	19:d:99:VAL:HG21	1.86	0.56
20:A:1301:ILE:HB	20:A:1304:ILE:HD12	1.87	0.56
1:C:70:LEU:HD21	21:B:803:ARG:HA	1.87	0.56
8:J:17:LYS:HB3	8:J:38:LEU:HD13	1.88	0.56
14:T:-104:DG:OP1	18:g:33:ARG:NH2	2.39	0.56
3:E:110:MET:HE1	3:E:115:LYS:HG3	1.87	0.56
20:A:659:GLU:OE2	20:A:985:ARG:NH2	2.38	0.56
20:A:1201:ASP:OD1	20:A:1201:ASP:N	2.32	0.56
20:A:1408:ARG:HG3	20:A:1422:GLN:HE22	1.71	0.56
4:F:58:THR:HG21	20:A:1083:PRO:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:96:VAL:HA	6:H:116:VAL:HA	1.86	0.55
20:A:1221:MET:SD	20:A:1221:MET:N	2.75	0.55
20:A:791:GLN:OE1	20:A:839:HIS:ND1	2.38	0.55
13:R:129:ARG:NH2	21:B:595:ASP:OD1	2.38	0.55
5:G:59:ILE:HG12	5:G:66:VAL:HG22	1.88	0.55
21:B:89:GLU:OE2	21:B:127:ASP:N	2.39	0.55
12:Q:28:ILE:HD11	13:R:93:LEU:HD23	1.89	0.55
13:R:149:VAL:HG21	21:B:146:LYS:HD3	1.88	0.55
21:B:1115:GLN:HB3	21:B:1148:LEU:HD11	1.88	0.55
5:G:21:ASN:O	5:G:25:THR:OG1	2.25	0.55
18:c:82:ARG:NH1	16:e:56:GLN:O	2.39	0.55
20:A:1099:ALA:HA	20:A:1102:MET:HE1	1.89	0.55
21:B:792:ASP:OD2	21:B:975:ARG:NH2	2.40	0.55
8:J:1:MET:H1	21:B:754:PRO:HD2	1.72	0.55
18:c:116:LEU:HB3	17:f:45:LYS:HD3	1.89	0.55
3:E:60:VAL:H	3:E:74:VAL:HG12	1.72	0.54
4:F:53:THR:OG1	4:F:116:GLU:OE1	2.24	0.54
1:C:211:LEU:HD13	1:C:215:GLU:HG3	1.90	0.54
12:Q:12:THR:HB	13:R:45:ILE:HB	1.89	0.54
14:T:-102:DG:OP1	18:g:21:ARG:NH2	2.41	0.54
20:A:589:LYS:HZ3	20:A:637:MET:HA	1.73	0.54
14:T:-104:DG:H3'	18:g:29:GLY:HA3	1.90	0.54
20:A:76:GLY:HA2	20:A:81:CYS:HB2	1.89	0.54
20:A:1027:ASP:OD1	20:A:1027:ASP:N	2.39	0.54
21:B:369:VAL:O	21:B:373:LEU:N	2.39	0.54
1:C:14:LEU:HD12	1:C:19:VAL:HG22	1.90	0.54
20:A:1002:SER:HB3	20:A:1059:ARG:HG3	1.89	0.54
20:A:1296:MET:SD	20:A:1296:MET:N	2.81	0.54
21:B:796:MET:HG2	21:B:965:ILE:HG12	1.90	0.54
20:A:693:ILE:HD13	20:A:828:LEU:HD21	1.89	0.53
20:A:1032:GLN:O	20:A:1036:ASN:ND2	2.39	0.53
20:A:1279:MET:HE1	20:A:1284:PHE:HB2	1.90	0.53
21:B:929:PRO:O	21:B:948:GLN:NE2	2.40	0.53
3:E:94:MET:SD	3:E:94:MET:N	2.82	0.53
20:A:940:LYS:NZ	20:A:941:ASP:OD1	2.41	0.53
20:A:1292:MET:HA	20:A:1296:MET:SD	2.48	0.53
20:A:1294:THR:OG1	20:A:1295:ASP:OD1	2.25	0.53
16:a:130:ARG:O	16:a:130:ARG:NH2	2.37	0.53
20:A:535:MET:O	20:A:669:TYR:OH	2.25	0.53
20:A:1054:MET:HA	20:A:1058:PHE:HB2	1.91	0.53
21:B:617:ASP:O	21:B:620:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:55:ARG:HB2	3:E:78:GLU:HG3	1.89	0.53
6:H:92:MET:HB2	6:H:143:LEU:HB3	1.90	0.53
9:K:82:SER:OG	9:K:84:GLN:OE1	2.26	0.53
21:B:175:ASN:HB3	21:B:742:VAL:HG11	1.91	0.53
21:B:237:VAL:HG13	21:B:372:LEU:HD13	1.89	0.53
6:H:28:LEU:N	6:H:41:LEU:O	2.42	0.53
20:A:419:ILE:HB	20:A:427:ILE:HB	1.89	0.53
20:A:550:LYS:NZ	20:A:762:GLU:OE2	2.42	0.53
16:e:64:ARG:HH11	22:N:177:DC:H5"	1.74	0.53
19:h:64:ASN:O	19:h:68:ASN:ND2	2.40	0.53
20:A:59:ASP:HB3	20:A:62:GLN:HB2	1.91	0.53
20:A:526:VAL:HA	20:A:533:PRO:HA	1.91	0.52
1:C:190:ASN:ND2	1:C:195:THR:O	2.39	0.52
2:D:45:LYS:HZ3	2:D:57:LEU:HD12	1.74	0.52
7:I:65:LEU:HD12	7:I:122:ARG:HG3	1.92	0.52
14:T:-73:DA:OP1	17:f:37:ARG:NH1	2.39	0.52
3:E:106:VAL:HG11	3:E:110:MET:HB2	1.90	0.52
20:A:364:ARG:NH2	20:A:502:ASN:OD1	2.42	0.52
21:B:699:HIS:HD2	21:B:701:SER:H	1.55	0.52
9:K:59:ALA:H	20:A:561:MET:HE2	1.73	0.52
13:R:86:GLN:NE2	21:B:551:GLU:OE2	2.42	0.52
20:A:70:ARG:NH2	20:A:77:ASN:OD1	2.43	0.52
20:A:100:LEU:HD11	20:A:198:LEU:HD21	1.92	0.52
16:e:130:ARG:O	16:e:130:ARG:NH2	2.38	0.52
20:A:790:GLN:NE2	20:A:791:GLN:O	2.42	0.52
14:T:-93:DG:OP2	19:h:87:ARG:NH1	2.43	0.52
18:g:56:LEU:HD11	19:h:71:PHE:HB2	1.92	0.52
20:A:495:ASP:OD1	20:A:495:ASP:N	2.41	0.52
1:C:180:ALA:N	1:C:234:GLU:O	2.43	0.52
18:c:82:ARG:NH2	18:c:108:VAL:O	2.43	0.52
20:A:1192:TRP:HA	20:A:1195:VAL:HB	1.92	0.52
21:B:726:SER:O	21:B:730:LYS:NZ	2.43	0.52
20:A:862:ARG:NH2	21:B:1088:GLU:OE1	2.42	0.52
20:A:35:SER:O	21:B:1138:ARG:NH1	2.43	0.51
18:g:45:GLY:HA2	22:N:197:DT:H5"	1.93	0.51
6:H:59:VAL:HB	6:H:144:LEU:HB2	1.92	0.51
12:Q:100:LEU:HD22	12:Q:110:PHE:HD2	1.75	0.51
21:B:598:VAL:HG12	21:B:600:GLU:H	1.75	0.51
21:B:1172:MET:SD	21:B:1172:MET:N	2.84	0.51
1:C:7:PRO:O	9:K:104:ARG:NH2	2.43	0.51
5:G:120:ASP:OD1	5:G:122:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:g:22:ALA:HB2	19:h:122:TYR:HB2	1.92	0.51
20:A:496:PHE:H	21:B:791:GLU:HB3	1.75	0.51
20:A:612:ASP:OD1	20:A:612:ASP:N	2.44	0.51
21:B:237:VAL:HG23	21:B:258:ALA:HB2	1.91	0.51
3:E:57:ASP:N	3:E:57:ASP:OD1	2.40	0.51
3:E:117:SER:O	3:E:121:MET:HB2	2.11	0.51
8:J:2:ILE:HD13	8:J:56:ILE:HG13	1.92	0.51
14:T:-107:DC:H2''	14:T:-106:DT:C5	2.46	0.51
20:A:1167:ARG:NH2	20:A:1293:LEU:O	2.44	0.51
21:B:44:LEU:HD23	21:B:155:MET:HE3	1.92	0.51
3:E:171:PRO:HB2	3:E:207:ARG:HD3	1.92	0.51
8:J:10:CYS:SG	8:J:11:GLY:N	2.84	0.51
20:A:841:MET:HE1	21:B:503:ASN:HD22	1.76	0.51
12:Q:30:ALA:HB2	12:Q:143:TRP:HE1	1.75	0.51
20:A:686:THR:OG1	20:A:687:ILE:N	2.43	0.51
20:A:760:LEU:HD11	20:A:781:ILE:HG21	1.92	0.51
21:B:270:ILE:HA	21:B:273:PHE:HB2	1.92	0.51
2:D:44:ARG:NH2	5:G:48:VAL:O	2.44	0.51
21:B:161:CYS:SG	21:B:162:LEU:N	2.84	0.51
20:A:539:GLN:O	21:B:970:HIS:ND1	2.44	0.50
20:A:901:VAL:HA	20:A:980:PRO:HA	1.92	0.50
20:A:1093:GLN:HE22	21:B:1093:CYS:HA	1.77	0.50
21:B:90:GLN:NE2	21:B:92:TYR:OH	2.43	0.50
21:B:294:ASP:OD2	21:B:379:ARG:NH2	2.43	0.50
13:R:8:ASP:HB3	13:R:105:SER:HA	1.93	0.50
20:A:1020:LEU:O	20:A:1034:GLN:NE2	2.45	0.50
21:B:271:ILE:HD12	21:B:311:ILE:HG13	1.94	0.50
14:T:-97:DG:N2	22:N:197:DT:O2	2.44	0.50
21:B:217:TYR:H	21:B:239:MET:HB3	1.77	0.50
8:J:9:THR:OG1	8:J:10:CYS:N	2.45	0.50
20:A:367:ILE:HD13	20:A:501:MET:HE3	1.93	0.50
21:B:206:TYR:HB2	21:B:220:GLU:HB2	1.93	0.50
7:I:81:THR:OG1	7:I:83:ASP:OD1	2.28	0.50
21:B:1111:SER:OG	21:B:1112:ASP:OD1	2.28	0.50
3:E:82:VAL:HG22	3:E:110:MET:HG2	1.93	0.50
21:B:82:PRO:HB3	21:B:134:LYS:HA	1.92	0.50
4:F:51:ARG:NH1	4:F:122:GLU:OE2	2.39	0.50
7:I:69:ILE:HG22	7:I:71:ASP:H	1.77	0.50
20:A:406:VAL:HG23	20:A:429:LEU:HD11	1.93	0.50
20:A:1307:VAL:HG13	20:A:1338:THR:HG22	1.92	0.50
4:F:51:ARG:HH11	4:F:118:TRP:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:111:PRO:O	20:A:884:ASN:ND2	2.45	0.50
21:B:477:SER:HA	21:B:730:LYS:HG2	1.92	0.50
21:B:934:LYS:HB3	21:B:1051:LEU:HB2	1.94	0.50
21:B:751:LEU:HD21	21:B:776:ILE:HD11	1.93	0.49
17:b:45:LYS:HD2	18:g:116:LEU:HB3	1.94	0.49
3:E:111:THR:HG23	3:E:114:ALA:H	1.76	0.49
18:c:30:ARG:NH2	19:d:37:SER:O	2.45	0.49
20:A:422:ASP:OD1	20:A:422:ASP:N	2.45	0.49
21:B:783:ALA:O	21:B:789:ASN:ND2	2.46	0.49
18:c:86:LEU:O	18:c:90:ASN:ND2	2.41	0.49
20:A:356:GLY:O	21:B:1085:ARG:NH2	2.46	0.49
20:A:801:GLY:HA3	21:B:503:ASN:HB2	1.93	0.49
21:B:606:ASP:OD2	21:B:613:ARG:NH1	2.45	0.49
3:E:136:LEU:HD22	20:A:1348:SER:HB2	1.94	0.49
15:W:125:ALA:O	15:W:128:LYS:NZ	2.45	0.49
16:e:52:ILE:HG13	17:f:40:ARG:HD2	1.94	0.49
20:A:1172:ASN:ND2	20:A:1215:GLU:OE2	2.40	0.49
21:B:604:ILE:HD11	21:B:668:LEU:HB3	1.95	0.49
14:T:13:DT:H2''	14:T:14:DC:H2'	1.94	0.49
20:A:58:MET:HG3	20:A:258:LEU:HD21	1.95	0.49
21:B:66:ASP:OD1	21:B:66:ASP:N	2.44	0.49
7:I:119:CYS:SG	7:I:120:GLY:N	2.84	0.49
10:L:17:TYR:HB3	10:L:44:MET:SD	2.53	0.49
11:P:10:C:OP1	21:B:942:LYS:NZ	2.45	0.49
21:B:115:LEU:HB3	21:B:908:MET:HE1	1.95	0.49
21:B:207:VAL:HG23	21:B:383:ASP:H	1.78	0.49
13:R:86:GLN:OE1	21:B:578:LYS:NZ	2.45	0.49
13:R:90:GLY:HA3	21:B:557:SER:HB2	1.95	0.49
14:T:-31:DG:N2	22:N:131:DT:O2	2.46	0.49
20:A:514:GLU:OE2	21:B:1102:PHE:N	2.44	0.49
20:A:1004:LEU:HD13	20:A:1062:GLY:HA2	1.95	0.49
6:H:84:ARG:NH1	6:H:85:ALA:O	2.46	0.49
14:T:-26:DC:H2''	14:T:-25:DT:C5	2.48	0.49
21:B:699:HIS:CD2	21:B:701:SER:H	2.30	0.49
1:C:11:ILE:HG21	1:C:14:LEU:HD13	1.95	0.48
4:F:53:THR:HG21	4:F:108:ARG:HD3	1.94	0.48
20:A:879:VAL:HB	20:A:888:GLN:HB2	1.95	0.48
21:B:728:MET:HA	21:B:731:GLN:HG3	1.95	0.48
1:C:185:GLU:HB3	1:C:230:TYR:HB2	1.95	0.48
14:T:-73:DA:H5''	17:f:31:THR:HG21	1.94	0.48
16:e:47:VAL:HG21	22:N:168:DG:H3'	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:18:ILE:HA	21:B:1173:SER:HA	1.94	0.48
21:B:41:ARG:NH1	21:B:45:ASP:OD1	2.47	0.48
21:B:1122:CYS:HB3	21:B:1140:CYS:SG	2.53	0.48
14:T:-93:DG:N2	22:N:193:DT:O2	2.46	0.48
3:E:13:ILE:HD11	3:E:132:GLN:HG3	1.96	0.48
11:P:8:G:O3'	21:B:731:GLN:NE2	2.46	0.48
21:B:570:ASN:HD21	21:B:616:THR:HB	1.77	0.48
14:T:-114:DC:H5''	19:h:56:SER:HA	1.95	0.48
21:B:789:ASN:OD1	21:B:789:ASN:N	2.44	0.48
4:F:88:ASP:HB3	4:F:91:LEU:HB2	1.95	0.48
20:A:1428:MET:HE1	20:A:1455:SER:H	1.78	0.48
15:W:114:ILE:HG23	15:W:177:LEU:HD22	1.96	0.48
1:C:48:ASP:HB3	1:C:166:LYS:HG3	1.96	0.48
20:A:62:GLN:HG3	20:A:257:PRO:HA	1.96	0.48
3:E:18:MET:HA	3:E:21:CYS:HB2	1.96	0.48
20:A:1032:GLN:HE21	20:A:1036:ASN:HD21	1.61	0.48
21:B:780:VAL:HG22	21:B:965:ILE:HB	1.95	0.48
1:C:60:HIS:CE1	21:B:809:VAL:HG21	2.49	0.48
2:D:55:GLN:NE2	5:G:32:THR:OG1	2.47	0.48
6:H:9:ILE:HA	6:H:57:ARG:HA	1.94	0.48
20:A:406:VAL:HG21	20:A:419:ILE:HD11	1.96	0.48
21:B:126:VAL:O	21:B:147:THR:N	2.38	0.48
21:B:1134:THR:O	21:B:1134:THR:OG1	2.32	0.48
20:A:1087:VAL:HG12	20:A:1400:LEU:HD22	1.95	0.47
21:B:758:LEU:H	21:B:777:ASN:ND2	2.12	0.47
1:C:212:ASP:OD1	1:C:212:ASP:N	2.44	0.47
2:D:39:MET:HA	2:D:42:GLU:HB2	1.97	0.47
3:E:138:ASN:HB3	3:E:141:GLU:HB2	1.96	0.47
5:G:92:VAL:HB	5:G:126:PRO:HB2	1.96	0.47
20:A:1212:LEU:HB2	20:A:1285:LEU:HD11	1.95	0.47
21:B:764:MET:HE3	21:B:769:PHE:HD2	1.79	0.47
21:B:834:ARG:NH2	21:B:840:MET:SD	2.87	0.47
20:A:96:HIS:HB3	20:A:99:PHE:HB2	1.95	0.47
20:A:400:ASP:OD1	20:A:400:ASP:N	2.43	0.47
20:A:937:ASP:OD1	20:A:937:ASP:N	2.42	0.47
7:I:106:ASP:OD1	20:A:734:ARG:NH2	2.47	0.47
15:W:36:ILE:HG22	15:W:43:VAL:HG21	1.96	0.47
20:A:1242:ASP:HA	20:A:1262:MET:HG2	1.96	0.47
1:C:88:CYS:SG	1:C:97:CYS:HB3	2.54	0.47
6:H:51:ASP:OD1	6:H:51:ASP:N	2.45	0.47
21:B:420:GLN:HA	21:B:423:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:905:ASP:HB2	21:B:924:ARG:HG2	1.97	0.47
3:E:133:GLN:HA	3:E:136:LEU:HD13	1.96	0.47
6:H:80:ASP:OD1	6:H:80:ASP:N	2.47	0.47
14:T:-66:DG:N2	22:N:166:DC:O2	2.48	0.47
14:T:48:DG:H2'	14:T:49:DG:C8	2.49	0.47
7:I:73:SER:HA	7:I:95:VAL:HG11	1.97	0.47
18:g:55:VAL:HG21	19:h:99:VAL:HG21	1.97	0.47
21:B:1105:GLU:OE1	21:B:1106:ARG:NH1	2.47	0.47
8:J:30:THR:HG23	8:J:33:ASP:H	1.80	0.47
20:A:833:PRO:HG3	21:B:1002:PHE:CG	2.50	0.47
21:B:310:VAL:HG23	21:B:311:ILE:HG12	1.97	0.47
5:G:104:MET:HE1	5:G:106:CYS:HB2	1.97	0.47
20:A:108:ARG:NE	20:A:145:TYR:OH	2.44	0.47
20:A:1426:PRO:HA	20:A:1429:LYS:HE2	1.96	0.47
21:B:237:VAL:HG21	21:B:369:VAL:HG12	1.96	0.47
1:C:56:SER:OG	1:C:158:GLU:N	2.41	0.47
2:D:112:LYS:HD2	2:D:119:GLU:HG3	1.96	0.47
3:E:200:ALA:HB2	20:A:894:ASP:HB3	1.95	0.47
20:A:99:PHE:O	20:A:103:THR:N	2.45	0.47
20:A:1206:ARG:HG2	20:A:1263:ASN:HA	1.97	0.47
1:C:94:CYS:N	1:C:97:CYS:SG	2.86	0.46
18:g:25:GLN:N	18:g:57:GLU:OE1	2.47	0.46
20:A:986:MET:HA	20:A:989:ASN:HB2	1.97	0.46
16:a:62:LEU:HD12	17:b:38:LEU:HD23	1.97	0.46
20:A:22:GLN:HB3	21:B:1170:ARG:HB2	1.96	0.46
1:C:75:SER:HB2	1:C:79:VAL:HB	1.96	0.46
14:T:48:DG:H2'	14:T:49:DG:H8	1.81	0.46
20:A:1218:ARG:HD3	20:A:1255:LEU:HD11	1.98	0.46
7:I:49:ASP:OD1	7:I:49:ASP:N	2.45	0.46
21:B:931:ILE:HA	21:B:945:CYS:HB3	1.98	0.46
1:C:68:LEU:HD23	1:C:71:ILE:HD12	1.97	0.46
1:C:147:ASP:OD1	1:C:147:ASP:N	2.47	0.46
5:G:38:CYS:SG	5:G:39:THR:N	2.88	0.46
22:N:85:DG:H1'	22:N:86:DA:H5'	1.97	0.46
5:G:11:ILE:HG21	5:G:26:VAL:HG13	1.97	0.46
13:R:55:SER:OG	13:R:80:GLU:OE2	2.27	0.46
20:A:663:ASP:OD1	20:A:666:ARG:NH2	2.41	0.46
20:A:823:VAL:HG22	20:A:835:GLU:HB2	1.98	0.46
21:B:1112:ASP:OD1	21:B:1112:ASP:N	2.47	0.46
7:I:116:ALA:HB3	7:I:119:CYS:HB3	1.97	0.46
21:B:836:THR:O	21:B:888:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ARG:NH2	21:B:952:GLU:O	2.49	0.46
4:F:96:GLU:HA	4:F:99:ALA:HB3	1.98	0.46
20:A:1003:ASP:OD1	20:A:1003:ASP:N	2.47	0.46
21:B:329:GLY:O	21:B:335:ARG:NH2	2.44	0.46
3:E:18:MET:SD	3:E:18:MET:N	2.86	0.46
21:B:824:ASP:O	21:B:872:THR:OG1	2.30	0.46
4:F:119:GLY:N	4:F:122:GLU:OE2	2.45	0.45
7:I:35:LEU:HD21	7:I:51:SER:HA	1.97	0.45
7:I:108:MET:HE2	20:A:734:ARG:HG2	1.97	0.45
20:A:1097:GLU:HG3	20:A:1098:PRO:HD3	1.98	0.45
21:B:131:THR:HG22	21:B:141:GLN:HB3	1.98	0.45
21:B:834:ARG:HA	21:B:840:MET:HE3	1.97	0.45
3:E:18:MET:HB2	3:E:28:VAL:HG11	1.98	0.45
21:B:564:ALA:HB3	21:B:576:ILE:HD12	1.98	0.45
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.99	0.45
10:L:16:ILE:HD12	10:L:47:LYS:HD3	1.98	0.45
15:W:15:LYS:HE2	15:W:38:ILE:HG23	1.99	0.45
17:f:76:HIS:HB2	19:h:97:THR:HG21	1.97	0.45
20:A:626:THR:OG1	20:A:627:LYS:N	2.48	0.45
22:N:123:DT:H2"	22:N:124:DA:N7	2.31	0.45
2:D:32:LEU:HD12	2:D:36:GLU:HG2	1.98	0.45
14:T:-108:DC:H2"	14:T:-107:DC:C5	2.51	0.45
20:A:1301:ILE:HD12	20:A:1345:ARG:HE	1.81	0.45
21:B:294:ASP:HB3	21:B:297:MET:HB2	1.97	0.45
1:C:131:THR:HG22	1:C:147:ASP:HB3	1.99	0.45
5:G:18:PHE:HA	5:G:22:LEU:HD12	1.98	0.45
18:c:93:GLU:OE2	19:d:106:GLU:N	2.47	0.45
21:B:479:LEU:HB3	21:B:706:VAL:HG11	1.98	0.45
6:H:81:ARG:NH2	6:H:82:PRO:HG3	2.31	0.45
17:b:63:LEU:O	17:b:67:ILE:HB	2.16	0.45
20:A:244:ARG:NH1	20:A:246:GLU:OE2	2.48	0.45
20:A:539:GLN:HA	20:A:774:ALA:HB1	1.98	0.45
20:A:1442:ALA:HA	20:A:1447:GLU:HG2	1.99	0.45
21:B:384:ASP:HB3	21:B:387:HIS:HB2	1.98	0.45
8:J:35:LEU:HD22	8:J:40:LEU:HD12	1.97	0.45
20:A:998:PRO:O	20:A:1059:ARG:NH2	2.50	0.45
21:B:782:ILE:HD12	21:B:1042:PHE:HD2	1.80	0.45
22:N:131:DT:H2"	22:N:132:DC:C6	2.52	0.45
20:A:34:MET:HE1	21:B:1139:GLY:HA3	1.99	0.45
2:D:44:ARG:HH22	5:G:48:VAL:H	1.65	0.45
13:R:99:SER:HB3	13:R:103:LYS:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:108:ARG:HA	12:Q:151:ARG:HD2	1.98	0.44
14:T:-13:DA:H2''	14:T:-12:DG:C8	2.52	0.44
20:A:959:MET:HA	20:A:962:ASP:HB2	1.99	0.44
20:A:1131:SER:OG	20:A:1133:LYS:O	2.35	0.44
22:N:111:DC:H2''	22:N:112:DT:C5	2.52	0.44
1:C:70:LEU:O	8:J:6:ARG:NH2	2.47	0.44
21:B:298:MET:HA	21:B:301:VAL:HG12	1.99	0.44
6:H:90:TYR:HB3	6:H:145:MET:HB3	1.99	0.44
8:J:43:TYR:HA	8:J:46:ARG:HB2	1.98	0.44
14:T:45:DG:OP1	21:B:1085:ARG:NE	2.44	0.44
16:e:63:ILE:O	16:e:94:GLN:NE2	2.51	0.44
16:e:97:SER:HB3	17:f:59:LEU:HD11	1.99	0.44
21:B:677:MET:H	21:B:682:LEU:HD23	1.81	0.44
1:C:256:LEU:HD12	9:K:91:ILE:HG23	2.00	0.44
14:T:-46:DT:H3	22:N:145:DA:H61	1.64	0.44
14:T:-22:DG:H5''	18:c:45:GLY:HA2	1.98	0.44
21:B:388:TYR:HE2	21:B:524:LYS:HE3	1.82	0.44
21:B:910:THR:OG1	21:B:911:LEU:N	2.50	0.44
21:B:1161:GLU:O	21:B:1164:SER:OG	2.26	0.44
7:I:20:CYS:HB3	7:I:42:CYS:SG	2.57	0.44
20:A:1053:ARG:HH11	20:A:1058:PHE:HZ	1.64	0.44
20:A:1198:GLU:HG2	20:A:1199:MET:HE3	1.99	0.44
21:B:665:ILE:HG23	21:B:669:GLU:HB2	2.00	0.44
1:C:56:SER:O	1:C:157:GLN:NE2	2.43	0.44
2:D:41:LEU:HB2	2:D:65:LEU:HD13	2.00	0.44
5:G:87:ALA:HB1	5:G:99:THR:HB	1.98	0.44
6:H:30:CYS:O	6:H:39:LEU:N	2.48	0.44
11:P:2:C:O2'	11:P:3:A:OP1	2.31	0.44
20:A:714:ILE:HD13	20:A:714:ILE:HA	1.92	0.44
20:A:807:LEU:HB3	20:A:809:HIS:HD2	1.82	0.44
21:B:92:TYR:HB2	21:B:125:TYR:HB2	1.99	0.44
21:B:990:SER:OG	21:B:995:GLU:O	2.30	0.44
2:D:32:LEU:HA	2:D:84:ARG:HH12	1.83	0.44
3:E:121:MET:HE3	3:E:121:MET:HB3	1.74	0.44
12:Q:42:TRP:HB3	13:R:9:LEU:HD13	2.00	0.44
13:R:20:LEU:HD23	13:R:113:ARG:HG2	2.00	0.44
13:R:56:PHE:HB3	13:R:81:HIS:HB2	1.99	0.44
16:e:120:ILE:HD11	17:f:47:ILE:HG23	1.99	0.44
20:A:1134:PRO:HG2	20:A:1137:PRO:HB3	2.00	0.44
21:B:872:THR:HG22	21:B:889:LYS:HG2	2.00	0.44
1:C:44:ILE:HD12	1:C:178:PRO:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:29:THR:HG23	3:E:32:GLU:H	1.83	0.44
16:a:100:TYR:OH	16:a:134:GLU:OE1	2.34	0.44
21:B:636:LYS:H	21:B:639:HIS:HD2	1.65	0.44
21:B:678:THR:HB	21:B:681:ASP:HB2	2.00	0.44
21:B:739:ASN:HB2	21:B:742:VAL:HB	1.98	0.44
6:H:39:LEU:HD21	6:H:41:LEU:HB2	1.99	0.44
16:a:91:MET:HG3	17:b:101:PHE:HE1	1.83	0.44
20:A:979:LEU:HD12	20:A:1041:PHE:HD1	1.82	0.44
20:A:1176:TYR:HE2	20:A:1213:ARG:HD3	1.83	0.44
21:B:281:ASP:OD1	21:B:281:ASP:N	2.48	0.44
5:G:152:VAL:HG22	5:G:157:ILE:HG12	2.00	0.43
6:H:12:VAL:HG13	6:H:56:PHE:HE1	1.81	0.43
6:H:38:ASP:OD1	6:H:38:ASP:N	2.44	0.43
6:H:145:MET:HE3	6:H:146:LYS:N	2.33	0.43
9:K:19:ILE:HD12	9:K:35:ILE:HG12	2.00	0.43
9:K:80:ASP:OD1	9:K:80:ASP:N	2.51	0.43
11:P:6:C:O3'	21:B:468:GLN:NE2	2.51	0.43
20:A:329:MET:HE3	20:A:330:GLN:N	2.33	0.43
22:N:213:DG:H2''	22:N:214:DT:C5	2.53	0.43
5:G:42:TYR:HA	5:G:78:ARG:HH12	1.82	0.43
6:H:115:TYR:HE2	20:A:621:ILE:HG12	1.83	0.43
12:Q:29:MET:HE1	12:Q:146:PHE:CD1	2.52	0.43
20:A:344:LYS:HD3	20:A:344:LYS:HA	1.78	0.43
20:A:1423:ASP:OD1	20:A:1423:ASP:N	2.38	0.43
21:B:50:PHE:HB2	21:B:397:GLY:HA2	2.00	0.43
21:B:223:SER:OG	21:B:350:HIS:ND1	2.38	0.43
22:N:182:DA:H1'	22:N:183:DA:H5'	1.99	0.43
3:E:47:LYS:O	3:E:53:PRO:HD2	2.18	0.43
14:T:-117:DT:H2''	14:T:-116:DG:N7	2.32	0.43
20:A:788:VAL:HG23	20:A:826:SER:HA	1.99	0.43
20:A:1163:HIS:CE1	20:A:1297:THR:HG22	2.53	0.43
4:F:78:PRO:HD2	5:G:18:PHE:HB2	1.98	0.43
5:G:28:GLN:O	5:G:32:THR:OG1	2.27	0.43
13:R:125:MET:HA	13:R:128:LYS:HB2	2.01	0.43
16:a:91:MET:H	16:a:91:MET:HG2	1.69	0.43
18:c:63:ILE:HD13	18:c:94:LEU:HD13	2.00	0.43
20:A:186:ARG:HD2	20:A:186:ARG:HA	1.79	0.43
4:F:69:ARG:NH1	4:F:72:GLN:OE1	2.51	0.43
9:K:31:CYS:SG	9:K:32:LEU:N	2.91	0.43
20:A:871:VAL:HG11	20:A:1400:LEU:HD21	2.00	0.43
21:B:298:MET:SD	21:B:298:MET:N	2.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:556:ILE:HD12	21:B:556:ILE:HA	1.90	0.43
22:N:123:DT:H2"	22:N:124:DA:C8	2.53	0.43
1:C:100:GLU:OE2	1:C:162:ARG:NH2	2.51	0.43
7:I:91:HIS:HE1	7:I:115:THR:HG23	1.82	0.43
13:R:12:ALA:HB2	13:R:106:LEU:HD23	1.99	0.43
13:R:94:THR:HG22	13:R:109:ILE:HA	2.00	0.43
20:A:299:ALA:HB3	20:A:302:VAL:HG23	2.01	0.43
20:A:452:ASP:N	20:A:452:ASP:OD1	2.50	0.43
20:A:875:TYR:HA	20:A:1083:PRO:HB3	2.00	0.43
20:A:923:ASP:N	20:A:923:ASP:OD1	2.48	0.43
20:A:1171:ALA:HB3	20:A:1215:GLU:HG3	2.01	0.43
21:B:808:SER:OG	21:B:1050:ARG:NH2	2.52	0.43
4:F:102:ILE:HG22	4:F:104:ILE:HG12	1.99	0.43
12:Q:125:TYR:HB2	13:R:21:VAL:HB	2.01	0.43
14:T:-103:DA:OP2	18:g:18:ARG:NH1	2.46	0.43
20:A:660:MET:HE3	20:A:660:MET:HA	1.99	0.43
3:E:71:GLN:HB2	3:E:99:ILE:HG22	2.00	0.43
5:G:28:GLN:HA	5:G:31:PHE:HB2	2.01	0.43
9:K:39:ASP:OD2	21:B:950:ARG:NH1	2.52	0.43
18:c:104:ALA:HB2	17:f:98:LEU:HD11	1.99	0.43
20:A:849:ASP:HA	20:A:852:VAL:HG12	1.99	0.43
20:A:1443:ALA:HB2	21:B:1167:ILE:HG23	2.01	0.43
21:B:224:CYS:HB3	21:B:232:THR:HA	2.00	0.43
21:B:313:GLU:HB3	21:B:316:VAL:HG12	2.01	0.43
21:B:622:CYS:HA	21:B:666:ASP:HA	2.00	0.43
2:D:135:GLN:OE1	2:D:138:ARG:NH2	2.52	0.43
9:K:89:ASN:HA	9:K:92:THR:HG22	2.01	0.43
19:d:57:SER:N	22:N:105:DA:OP1	2.51	0.43
20:A:728:THR:HB	20:A:731:ASN:HB2	2.00	0.43
21:B:814:TYR:HD2	21:B:921:ILE:HD11	1.84	0.43
1:C:41:GLU:OE2	1:C:171:LYS:NZ	2.52	0.43
1:C:177:ASN:HD22	21:B:803:ARG:HH11	1.67	0.43
14:T:-118:DC:H2"	14:T:-117:DT:C5	2.54	0.43
20:A:606:HIS:CE1	20:A:641:CYS:HB3	2.54	0.43
21:B:347:MET:HA	21:B:347:MET:HE2	1.99	0.43
1:C:8:THR:HA	9:K:104:ARG:HD2	2.01	0.42
1:C:103:LEU:HD23	1:C:161:LEU:HD21	2.01	0.42
3:E:122:ALA:HB3	3:E:125:TYR:HB2	2.00	0.42
4:F:63:ALA:HB1	20:A:514:GLU:HA	2.01	0.42
20:A:713:VAL:HA	20:A:716:VAL:HG12	2.01	0.42
21:B:311:ILE:HG23	21:B:316:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:89:VAL:HG22	5:G:99:THR:HG22	2.01	0.42
14:T:46:DC:OP2	20:A:358:ARG:NH1	2.50	0.42
16:a:114:HIS:CG	16:e:127:LEU:HD22	2.54	0.42
21:B:219:GLY:N	21:B:237:VAL:O	2.38	0.42
5:G:86:ASP:HA	5:G:144:ARG:HE	1.84	0.42
8:J:25:LEU:HD23	8:J:25:LEU:HA	1.93	0.42
20:A:379:GLY:N	20:A:483:ARG:O	2.39	0.42
20:A:610:PRO:HB2	20:A:613:GLU:HG3	2.00	0.42
21:B:955:PRO:HB2	21:B:1028:LEU:HD13	2.01	0.42
20:A:538:VAL:HG22	20:A:539:GLN:HB3	2.00	0.42
21:B:343:LEU:HD13	21:B:347:MET:HG2	2.02	0.42
21:B:617:ASP:N	21:B:617:ASP:OD1	2.51	0.42
21:B:814:TYR:HB2	21:B:921:ILE:HG12	2.01	0.42
7:I:88:LYS:HE3	7:I:121:HIS:HB2	2.02	0.42
20:A:684:GLY:HA3	21:B:1037:ILE:HG23	2.01	0.42
21:B:1128:ALA:HB1	21:B:1135:TYR:HD1	1.85	0.42
12:Q:15:VAL:O	12:Q:135:PHE:N	2.52	0.42
20:A:629:VAL:HG13	20:A:636:ILE:HB	2.01	0.42
6:H:6:PHE:HZ	6:H:37:MET:HG2	1.85	0.42
6:H:71:ASP:OD2	6:H:142:TYR:OH	2.29	0.42
17:f:39:ALA:HB1	17:f:44:VAL:HB	2.01	0.42
20:A:940:LYS:HE2	20:A:940:LYS:HB2	1.84	0.42
20:A:1295:ASP:OD1	20:A:1295:ASP:N	2.52	0.42
20:A:1358:THR:OG1	20:A:1359:SER:N	2.53	0.42
18:c:60:THR:HG21	19:d:42:VAL:HG22	2.01	0.42
20:A:67:ARG:HG2	20:A:67:ARG:HH21	1.83	0.42
20:A:560:VAL:HG22	20:A:564:LEU:HD23	2.02	0.42
1:C:105:VAL:HG21	1:C:115:VAL:HG22	2.01	0.42
15:W:70:LYS:HA	15:W:70:LYS:HD3	1.86	0.42
20:A:286:ILE:HG22	20:A:310:LEU:HD12	2.02	0.42
20:A:833:PRO:HA	20:A:836:PHE:HB3	2.01	0.42
21:B:26:CYS:O	21:B:30:ILE:HG12	2.20	0.42
3:E:61:LEU:HB2	3:E:73:PHE:HD1	1.85	0.41
8:J:47:ARG:NH2	21:B:777:ASN:O	2.53	0.41
20:A:464:LEU:HB2	20:A:465:HIS:CD2	2.55	0.41
20:A:606:HIS:ND1	20:A:639:ILE:O	2.39	0.41
2:D:16:ASP:H	2:D:21:ILE:HB	1.85	0.41
2:D:55:GLN:HE22	5:G:28:GLN:HB2	1.84	0.41
14:T:51:DT:H5"	21:B:449:ALA:HB1	2.02	0.41
16:a:73:ARG:NH1	22:N:136:DC:OP2	2.53	0.41
18:g:80:ILE:HG12	18:g:83:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:785:TYR:CZ	21:B:955:PRO:HD3	2.55	0.41
2:D:75:LYS:HA	2:D:75:LYS:HD3	1.91	0.41
4:F:110:LEU:HD23	4:F:110:LEU:HA	1.94	0.41
6:H:112:LEU:HD23	6:H:112:LEU:HA	1.90	0.41
8:J:5:VAL:H	8:J:5:VAL:HG22	1.63	0.41
11:P:6:C:H2'	11:P:7:A:C8	2.55	0.41
15:W:70:LYS:O	15:W:73:LYS:NZ	2.51	0.41
19:d:63:MET:HE3	19:d:63:MET:HA	2.02	0.41
20:A:260:VAL:O	20:A:342:ARG:NH1	2.52	0.41
20:A:768:SER:HA	20:A:771:VAL:HG12	2.02	0.41
20:A:917:GLU:OE2	20:A:921:ARG:NH1	2.53	0.41
20:A:972:THR:HA	20:A:1320:ILE:HG13	2.03	0.41
20:A:1087:VAL:O	20:A:1091:ALA:N	2.51	0.41
17:f:49:GLY:N	22:N:166:DC:OP2	2.53	0.41
20:A:432:HIS:HA	20:A:433:PRO:HD3	1.94	0.41
20:A:459:ASN:HB3	20:A:502:ASN:HB2	2.01	0.41
20:A:756:ALA:HB2	20:A:786:ALA:HB2	2.03	0.41
20:A:1224:ARG:HB3	20:A:1226:LEU:HD22	2.01	0.41
21:B:626:LEU:HD23	21:B:662:VAL:HG22	2.02	0.41
2:D:62:MET:SD	2:D:62:MET:N	2.90	0.41
3:E:24:ARG:NH1	3:E:182:TYR:O	2.40	0.41
3:E:61:LEU:HD11	3:E:71:GLN:HB3	2.02	0.41
20:A:1053:ARG:NE	20:A:1057:GLU:OE2	2.53	0.41
1:C:48:ASP:OD1	10:L:58:ARG:NE	2.50	0.41
16:a:114:HIS:NE2	16:e:124:ASP:OD1	2.42	0.41
18:g:30:ARG:NH2	19:h:37:SER:O	2.53	0.41
20:A:379:GLY:HA3	20:A:483:ARG:HB2	2.02	0.41
20:A:1005:HIS:ND1	20:A:1007:ILE:HG12	2.35	0.41
21:B:89:GLU:HG2	21:B:127:ASP:HB2	2.03	0.41
21:B:506:TRP:NE1	21:B:697:GLU:OE2	2.42	0.41
10:L:51:ARG:HD3	21:B:858:VAL:HG12	2.02	0.41
15:W:118:GLU:HA	15:W:174:ARG:HH22	1.84	0.41
20:A:706:ILE:HD11	20:A:787:VAL:HG21	2.03	0.41
20:A:841:MET:HG3	21:B:501:LEU:HD23	2.02	0.41
20:A:948:ILE:HD12	20:A:1007:ILE:HG21	2.02	0.41
20:A:1027:ASP:OD1	20:A:1030:SER:OG	2.35	0.41
21:B:526:LEU:HD11	21:B:532:ILE:HD11	2.02	0.41
21:B:761:THR:HG23	21:B:764:MET:H	1.86	0.41
1:C:106:ARG:HE	1:C:158:GLU:CD	2.29	0.41
3:E:94:MET:O	3:E:98:ASN:N	2.53	0.41
4:F:108:ARG:HD2	4:F:118:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:127:LEU:HD22	16:e:114:HIS:CG	2.55	0.41
18:g:63:ILE:HD11	18:g:94:LEU:HD22	2.03	0.41
20:A:544:ALA:HB2	20:A:680:LEU:HD22	2.01	0.41
20:A:611:ASP:N	20:A:611:ASP:OD1	2.51	0.41
20:A:902:GLU:OE2	20:A:985:ARG:NH1	2.47	0.41
20:A:997:ASN:HD22	20:A:1000:LEU:HG	1.86	0.41
21:B:794:VAL:HG12	21:B:967:ILE:HG22	2.01	0.41
4:F:95:LYS:HE2	4:F:95:LYS:HB2	1.81	0.41
6:H:27:ARG:HH11	20:A:621:ILE:HG23	1.85	0.41
7:I:69:ILE:HD13	21:B:608:ARG:HA	2.02	0.41
14:T:-88:DC:H2"	14:T:-87:DC:C6	2.55	0.41
19:h:37:SER:OG	19:h:38:TYR:N	2.54	0.41
20:A:808:PRO:HB2	21:B:675:LEU:HD23	2.02	0.41
20:A:1206:ARG:NE	20:A:1262:MET:O	2.43	0.41
21:B:242:ARG:HE	21:B:242:ARG:HB3	1.71	0.41
21:B:817:GLN:NE2	21:B:912:ASN:HD22	2.18	0.41
21:B:1120:ASN:HB2	21:B:1145:GLN:HB3	2.02	0.41
22:N:212:DT:H2"	22:N:213:DG:C8	2.55	0.41
20:A:423:ASN:OD1	20:A:423:ASN:N	2.51	0.41
20:A:873:VAL:HG12	20:A:1083:PRO:HA	2.03	0.41
20:A:992:LYS:HD3	20:A:992:LYS:HA	1.85	0.41
1:C:67:ARG:HE	8:J:5:VAL:HG13	1.86	0.40
3:E:72:MET:HE3	3:E:73:PHE:N	2.36	0.40
3:E:101:ARG:HD2	3:E:126:ILE:HB	2.02	0.40
20:A:306:ASP:O	20:A:310:LEU:N	2.45	0.40
21:B:743:ARG:O	21:B:922:ARG:NH2	2.54	0.40
13:R:39:GLU:HG2	13:R:59:ASN:HD21	1.86	0.40
16:e:101:LEU:HD23	16:e:101:LEU:HA	1.89	0.40
20:A:988:TRP:HE1	20:A:992:LYS:NZ	2.19	0.40
20:A:1242:ASP:N	20:A:1242:ASP:OD1	2.52	0.40
20:A:1307:VAL:HA	20:A:1338:THR:HA	2.03	0.40
4:F:65:VAL:HG13	4:F:104:ILE:HD11	2.02	0.40
20:A:331:LYS:HD2	20:A:331:LYS:HA	1.90	0.40
20:A:381:PRO:HB3	20:A:480:SER:HA	2.03	0.40
21:B:747:LEU:HD13	21:B:810:PHE:HE1	1.86	0.40
3:E:83:GLY:N	3:E:86:THR:OG1	2.54	0.40
16:a:129:ARG:HD3	16:a:135:ARG:HH21	1.86	0.40
19:d:52:ASP:OD1	19:d:52:ASP:N	2.46	0.40
20:A:1262:MET:H	20:A:1262:MET:HG3	1.55	0.40
20:A:1486:ILE:H	20:A:1486:ILE:HG13	1.67	0.40
21:B:256:ILE:H	21:B:304:SER:HG	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:951:GLN:HG3	21:B:962:THR:HG21	2.03	0.40
21:B:1116:VAL:HG11	21:B:1125:MET:HE1	2.03	0.40
22:N:194:DC:H2"	22:N:195:DC:C5	2.57	0.40
3:E:43:GLN:H	3:E:43:GLN:HG3	1.72	0.40
20:A:103:THR:HA	20:A:106:VAL:HG12	2.02	0.40
20:A:104:MET:HE1	20:A:191:ILE:HG22	2.03	0.40
20:A:738:GLU:OE1	20:A:797:ARG:NH2	2.44	0.40
21:B:841:ARG:NH2	21:B:863:ASP:OD1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	253/275 (92%)	241 (95%)	12 (5%)	0	100	100
2	D	126/184 (68%)	123 (98%)	3 (2%)	0	100	100
3	E	207/210 (99%)	199 (96%)	8 (4%)	0	100	100
4	F	80/127 (63%)	78 (98%)	2 (2%)	0	100	100
5	G	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
6	H	146/150 (97%)	138 (94%)	8 (6%)	0	100	100
7	I	112/125 (90%)	98 (88%)	14 (12%)	0	100	100
8	J	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
9	K	112/117 (96%)	107 (96%)	5 (4%)	0	100	100
10	L	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
12	Q	134/517 (26%)	132 (98%)	2 (2%)	0	100	100
13	R	133/249 (53%)	132 (99%)	1 (1%)	0	100	100
15	W	185/439 (42%)	184 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	a	95/136 (70%)	95 (100%)	0	0	100	100
16	e	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
17	b	80/103 (78%)	80 (100%)	0	0	100	100
17	f	80/103 (78%)	80 (100%)	0	0	100	100
18	c	107/130 (82%)	107 (100%)	0	0	100	100
18	g	104/130 (80%)	103 (99%)	1 (1%)	0	100	100
19	d	95/126 (75%)	94 (99%)	1 (1%)	0	100	100
19	h	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
20	A	1405/1970 (71%)	1320 (94%)	85 (6%)	0	100	100
21	B	1122/1300 (86%)	1070 (95%)	52 (5%)	0	100	100
All	All	5041/6949 (72%)	4832 (96%)	209 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	C	234/252 (93%)	234 (100%)	0	100	100
2	D	118/160 (74%)	118 (100%)	0	100	100
3	E	191/192 (100%)	191 (100%)	0	100	100
4	F	71/111 (64%)	71 (100%)	0	100	100
5	G	152/152 (100%)	152 (100%)	0	100	100
6	H	129/131 (98%)	129 (100%)	0	100	100
7	I	103/112 (92%)	103 (100%)	0	100	100
8	J	56/56 (100%)	56 (100%)	0	100	100
9	K	104/106 (98%)	104 (100%)	0	100	100
10	L	41/55 (74%)	41 (100%)	0	100	100
12	Q	121/448 (27%)	121 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	R	118/218 (54%)	118 (100%)	0	100	100
15	W	169/373 (45%)	169 (100%)	0	100	100
16	a	85/111 (77%)	85 (100%)	0	100	100
16	e	86/111 (78%)	86 (100%)	0	100	100
17	b	67/79 (85%)	67 (100%)	0	100	100
17	f	67/79 (85%)	67 (100%)	0	100	100
18	c	86/101 (85%)	86 (100%)	0	100	100
18	g	84/101 (83%)	84 (100%)	0	100	100
19	d	83/106 (78%)	83 (100%)	0	100	100
19	h	81/106 (76%)	81 (100%)	0	100	100
20	A	1249/1749 (71%)	1247 (100%)	2 (0%)	87	87
21	B	990/1127 (88%)	989 (100%)	1 (0%)	88	89
All	All	4485/6036 (74%)	4482 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	A	526	VAL
20	A	1341	VAL
21	B	1022	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	217	GLN
2	D	48	ASN
2	D	55	GLN
2	D	93	HIS
3	E	64	HIS
3	E	65	ASN
3	E	116	GLN
4	F	49	GLN
5	G	122	ASN
6	H	131	ASN
7	I	45	GLN
7	I	91	HIS
9	K	2	ASN

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Mol	Chain	Res	Type
9	K	49	GLN
9	K	89	ASN
12	Q	32	ASN
12	Q	103	ASN
12	Q	129	GLN
12	Q	142	ASN
12	Q	172	ASN
12	Q	173	HIS
13	R	64	ASN
13	R	112	GLN
13	R	123	ASN
15	W	101	ASN
15	W	181	ASN
16	a	40	HIS
18	c	25	GLN
18	c	83	HIS
19	d	48	GLN
19	d	50	HIS
19	d	96	GLN
16	e	109	ASN
19	h	83	HIS
19	h	96	GLN
20	A	267	GLN
20	A	278	HIS
20	A	353	ASN
20	A	377	GLN
20	A	412	GLN
20	A	504	HIS
20	A	539	GLN
20	A	576	GLN
20	A	601	ASN
20	A	662	HIS
20	A	673	GLN
20	A	677	ASN
20	A	678	ASN
20	A	703	GLN
20	A	740	GLN
20	A	765	ASN
20	A	780	ASN
20	A	790	GLN
20	A	884	ASN
20	A	904	GLN

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Mol	Chain	Res	Type
20	A	1032	GLN
20	A	1042	ASN
20	A	1093	GLN
20	A	1146	GLN
20	A	1163	HIS
20	A	1236	ASN
20	A	1422	GLN
20	A	1462	GLN
21	B	43	GLN
21	B	90	GLN
21	B	164	ASN
21	B	265	GLN
21	B	315	ASN
21	B	370	HIS
21	B	460	HIS
21	B	631	GLN
21	B	639	HIS
21	B	642	GLN
21	B	654	GLN
21	B	683	GLN
21	B	717	ASN
21	B	817	GLN
21	B	930	GLN
21	B	1071	ASN
21	B	1097	HIS
21	B	1101	GLN
21	B	1117	HIS
21	B	1129	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	P	9/10 (90%)	2 (22%)	1 (11%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	P	2	C
11	P	3	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	P	2	C

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, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	T	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	25:DC	O3'	26:DT	P	5.38

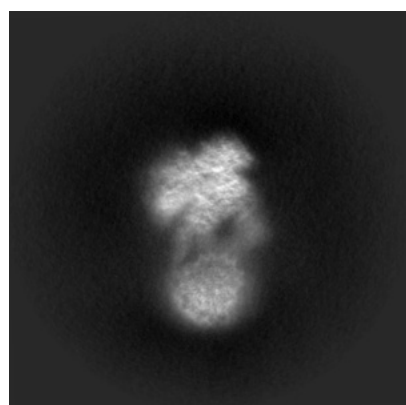
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57364. These allow visual inspection of the internal detail of the map and identification of artifacts.

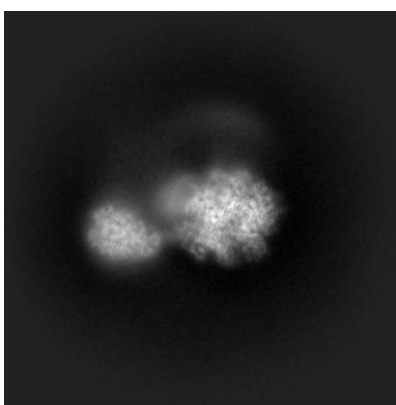
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

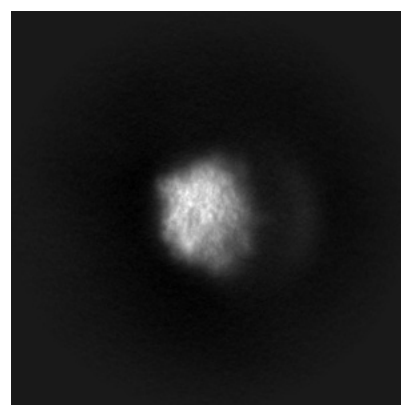
6.1.1 Primary map



X



Y

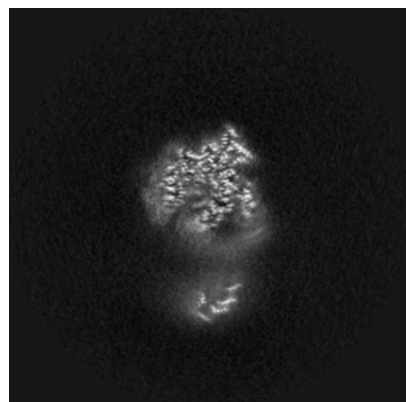


Z

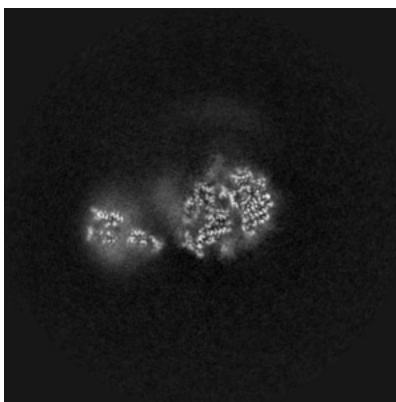
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

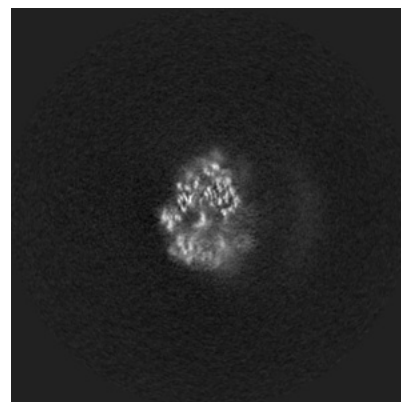
6.2.1 Primary map



X Index: 240



Y Index: 240

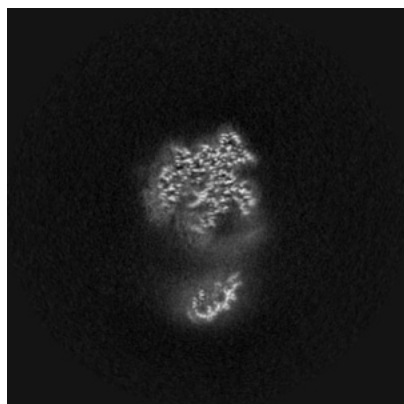


Z Index: 240

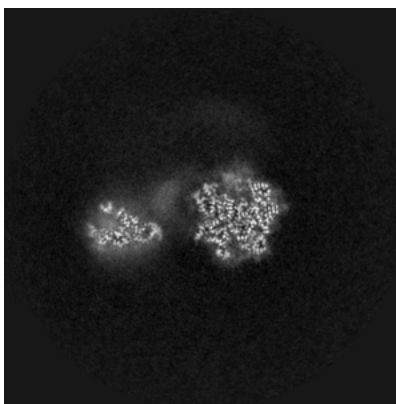
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

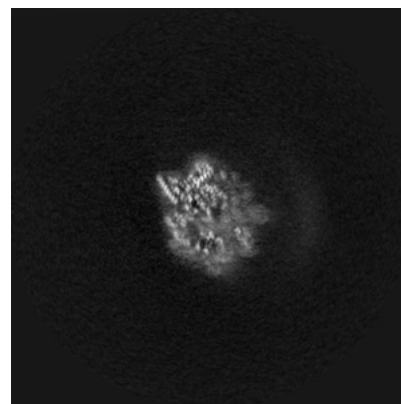
6.3.1 Primary map



X Index: 236



Y Index: 260



Z Index: 258

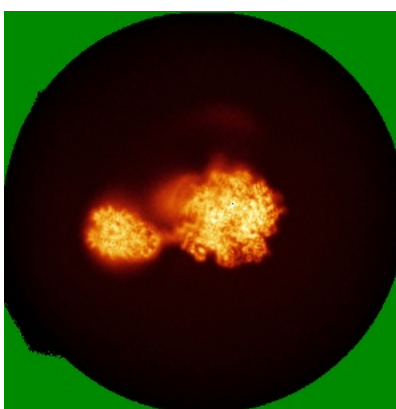
The images above show the largest variance slices of the map in three orthogonal directions.

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

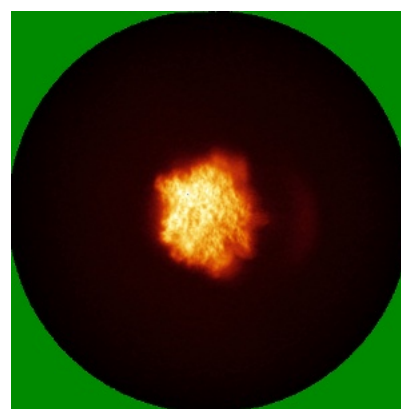
6.4.1 Primary map



X



Y

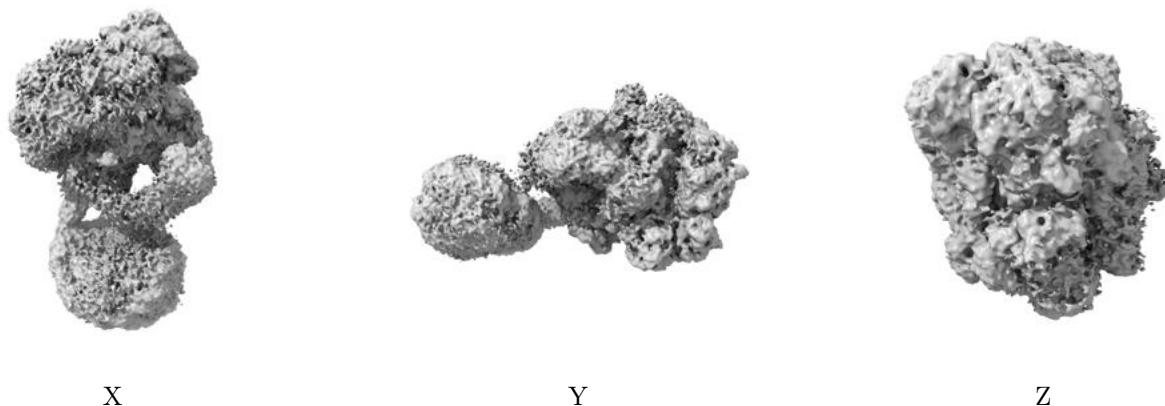


Z

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 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

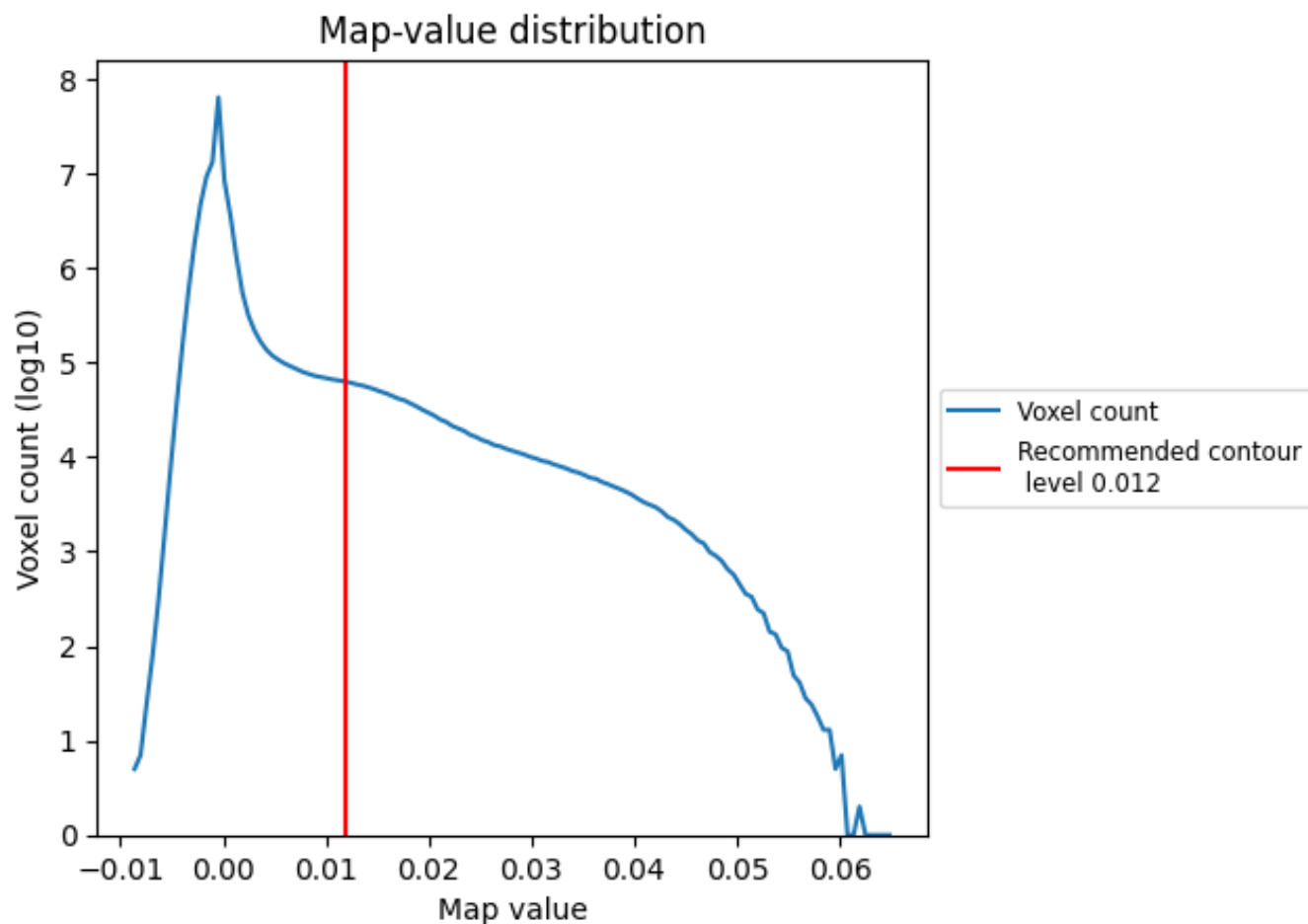
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

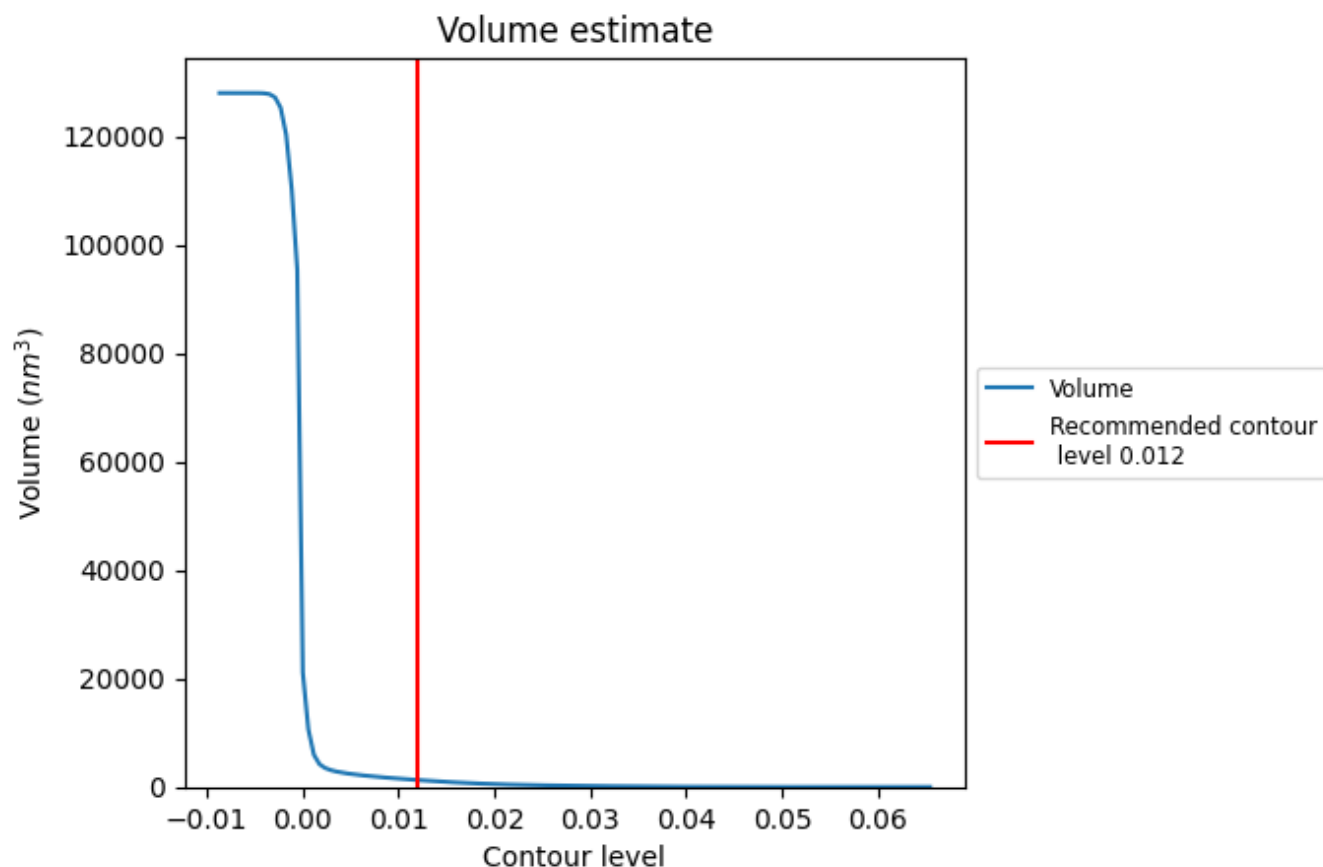
This section contains the results of statistical analysis of the map.

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.

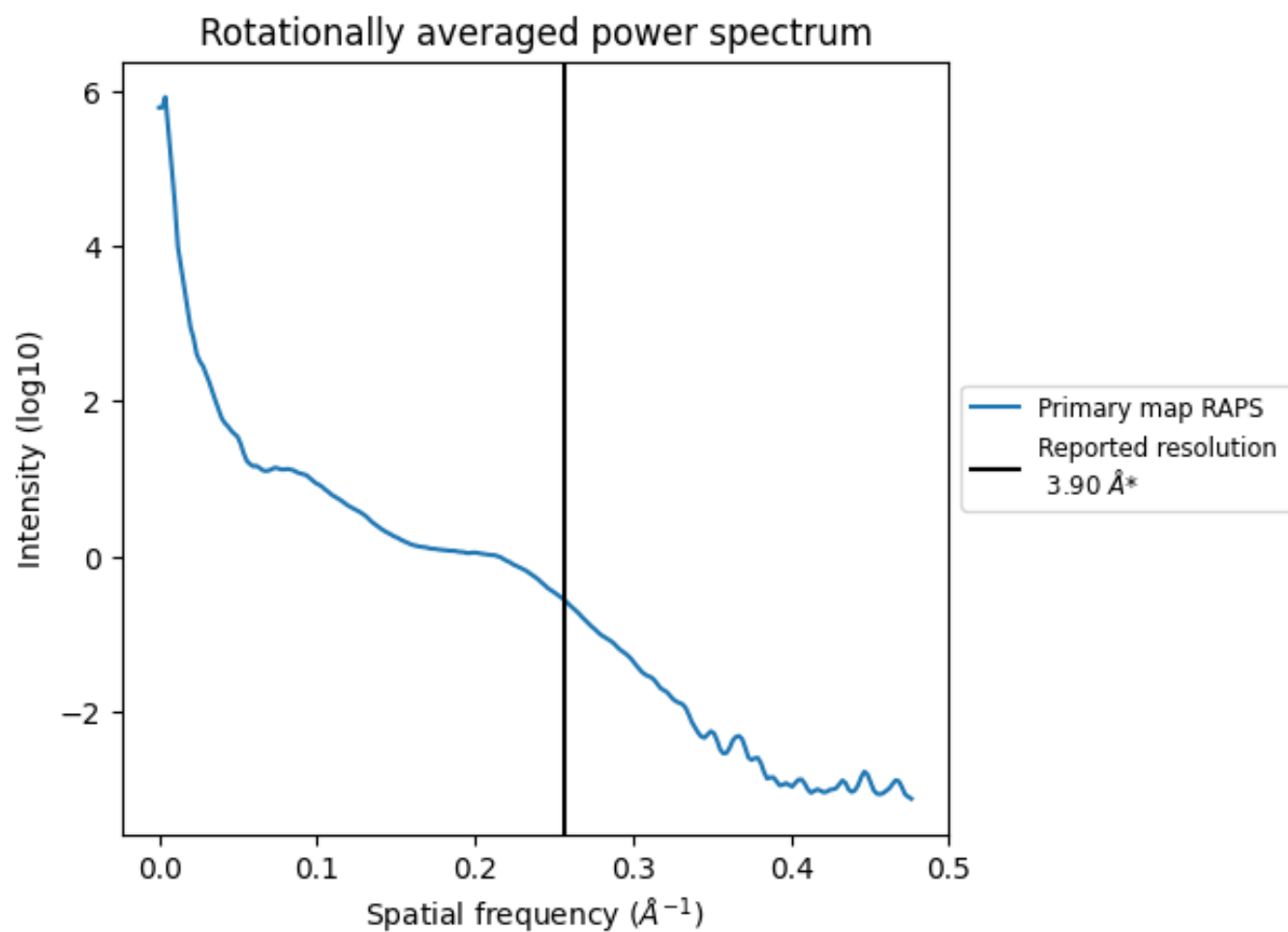
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1281 nm^3 ; this corresponds to an approximate mass of 1157 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 0.256 Å⁻¹

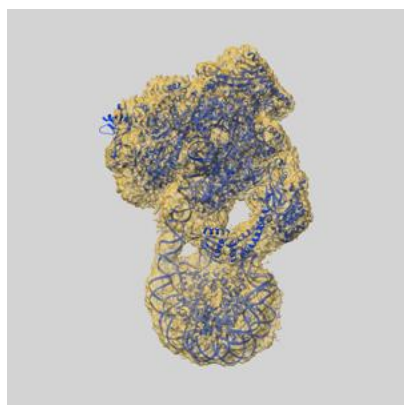
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

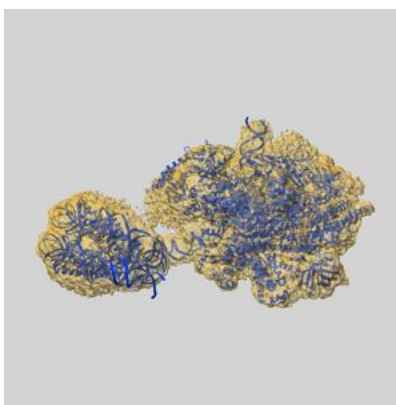
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57364 and PDB model 29TK. Per-residue inclusion information can be found in section [3](#) on page [9](#).

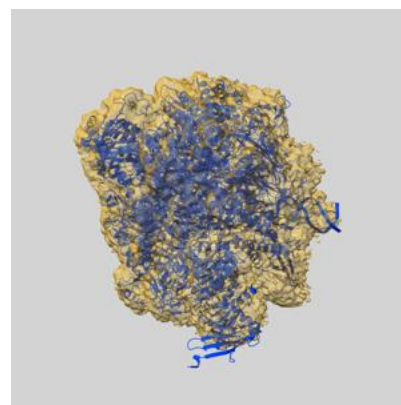
9.1 Map-model overlay [i](#)



X



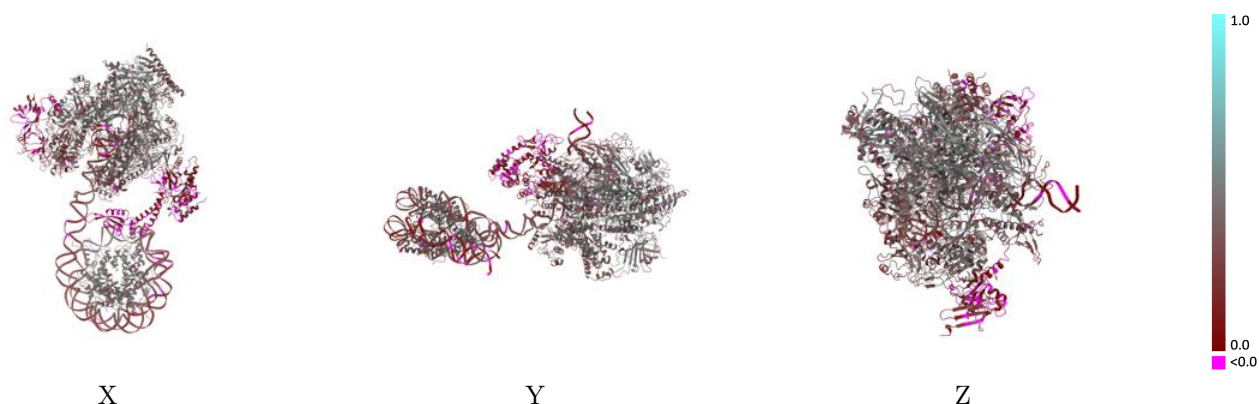
Y



Z

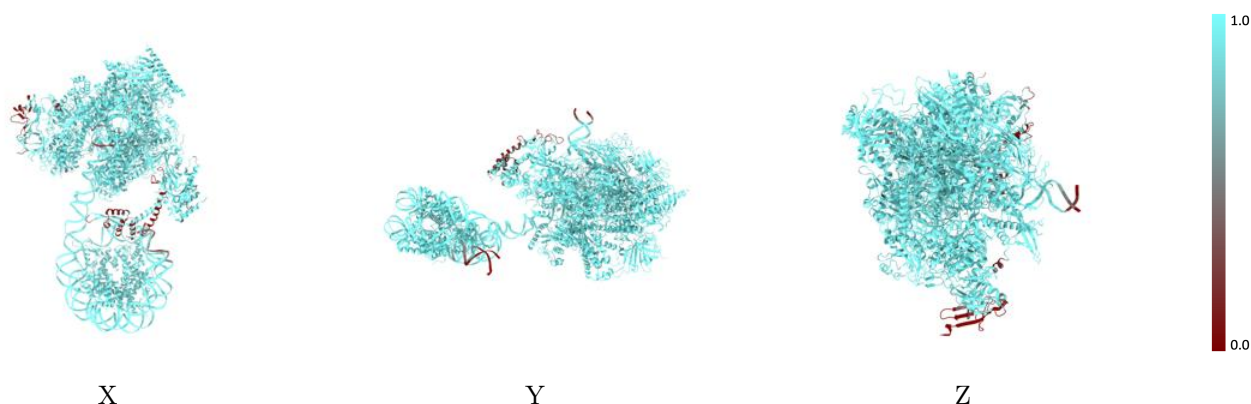
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



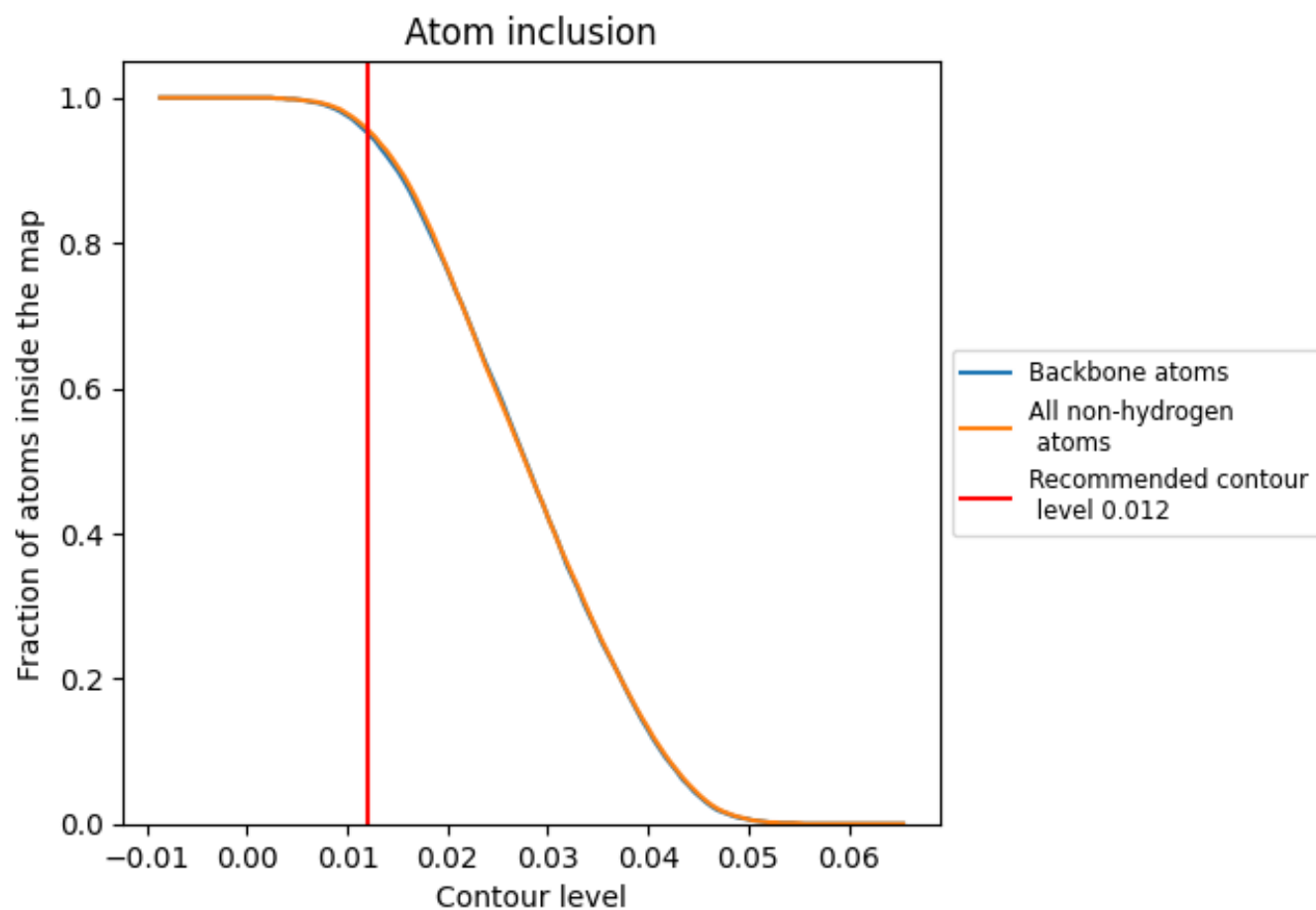
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9570	 0.3300
A	 0.9880	 0.3840
B	 0.9940	 0.3990
C	 0.9960	 0.4310
D	 0.9520	 0.1360
E	 0.9800	 0.3620
F	 1.0000	 0.3950
G	 0.9440	 0.1750
H	 0.9890	 0.4000
I	 0.9920	 0.3580
J	 0.9920	 0.4230
K	 0.9910	 0.4230
L	 0.9800	 0.3220
N	 0.9180	 0.2230
P	 1.0000	 0.4220
Q	 0.7800	 0.1130
R	 0.7170	 0.0900
T	 0.9430	 0.2360
W	 0.5700	 0.0390
a	 0.9690	 0.3870
b	 0.9950	 0.4210
c	 0.9790	 0.3850
d	 0.9970	 0.3800
e	 0.9940	 0.3960
f	 1.0000	 0.4240
g	 0.9900	 0.3830
h	 1.0000	 0.3590

