Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 02:36 am GMT

PDB ID	:	6TPS
EMDB ID	:	EMD-10544
Title	:	early intermediate RNA Polymerase I Pre-initiation complex - eiPIC
Authors	:	Pilsl, M.; Engel, C.
Deposited on	:	2019-12-14
Resolution	:	3.54 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:

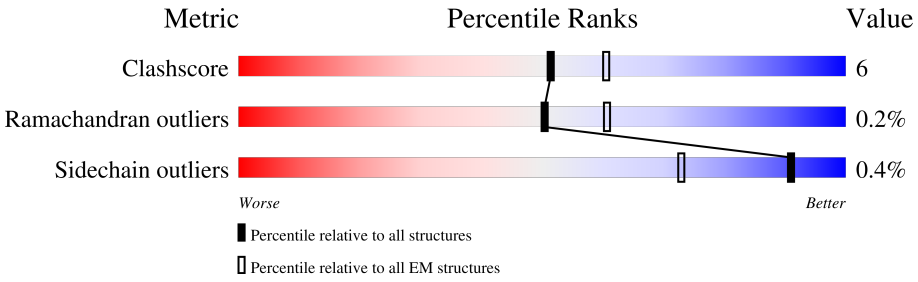
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.54 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1664	78% 11% 11%
2	B	1203	85% 13%
3	C	335	80% 11% 9%
4	D	137	36% 6% 58%
5	E	215	84% 15%
6	F	155	58% 6% 35%
7	G	326	50% 9% 41%
8	H	146	73% 17% 10%

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Mol	Chain	Length	Quality of chain
9	I	125	5% 48% 10% 42%
10	J	70	81% 17%
11	K	142	61% 11% 29%
12	L	70	51% 10% 39%
13	M	415	7% 20% 5% 75%
14	N	233	21% 52% 10% 38%
15	O	627	13% 64% 10% 26%
16	P	636	31% 70% 22% 6%
17	Q	514	22% 68% 21% 10%
18	R	507	9% 50% 14% 36%
19	S	27	48% 78% 22%
20	T	27	52% 74% 26%
21	U	12	67% 100%
22	V	12	67% 83% 17%

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 50070 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1475	11659	7364	2029	2205	61	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1177	9350	5913	1639	1747	51	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	305	2423	1539	416	460	8	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	58	459	289	78	92	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	212	1735	1102	306	316	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	100	823	522	144	154	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	193	Total	C	N	O	S	0	0
			1520	982	259	274	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	73	Total	C	N	O	S	0	0
			542	340	91	107	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	43	Total	C	N	O	S	0	0
			340	211	66	59	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	105	Total	C	N	O	0	0
			833	528	138	167		

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	145	Total	C	N	O	S	0	0
			1151	735	188	224	4		

- Molecule 15 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	463	Total	C	N	O	S	0	0
			3811	2473	623	694	21		

- Molecule 16 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	595	Total	C	N	O	S	0	0
			4840	3080	823	927	10		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	44	ARG	-	expression tag	UNP P32786
P	45	PRO	-	expression tag	UNP P32786
P	46	VAL	-	expression tag	UNP P32786
P	47	ASP	-	expression tag	UNP P32786
P	48	ASP	-	expression tag	UNP P32786
P	49	THR	-	expression tag	UNP P32786
P	50	LEU	-	expression tag	UNP P32786
P	51	ALA	-	expression tag	UNP P32786
P	52	GLU	-	expression tag	UNP P32786
P	53	ASP	-	expression tag	UNP P32786
P	54	ALA	-	expression tag	UNP P32786
P	55	LEU	-	expression tag	UNP P32786
P	56	ASP	-	expression tag	UNP P32786
P	57	LEU	-	expression tag	UNP P32786
P	58	HIS	-	expression tag	UNP P32786
P	59	ILE	-	expression tag	UNP P32786
P	60	VAL	-	expression tag	UNP P32786
P	61	VAL	-	expression tag	UNP P32786
P	62	LYS	-	expression tag	UNP P32786
P	63	SER	-	expression tag	UNP P32786
P	64	LEU	-	expression tag	UNP P32786
P	65	LEU	-	expression tag	UNP P32786
P	66	CYS	-	expression tag	UNP P32786

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Chain	Residue	Modelled	Actual	Comment	Reference
P	67	ASP	-	expression tag	UNP P32786
P	68	THR	-	expression tag	UNP P32786

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	461	Total	C	N	O	S	0	0
			3839	2473	658	688	20		

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	325	Total	C	N	O	S	0	0
			2725	1763	479	472	11		

- Molecule 19 is a DNA chain called NTS-DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	27	Total	C	N	O	P	0	0
			567	270	135	135	27		

- Molecule 20 is a DNA chain called TS-DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	27	Total	C	N	O	P	0	0
			539	269	55	188	27		

- Molecule 21 is a DNA chain called DNA foreign.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	12	Total	C	N	O	P	0	0
			264	120	60	72	12		

- Molecule 22 is a DNA chain called DNA foreign.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	12	Total	C	N	O	P	0	0
			228	108	36	72	12		

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

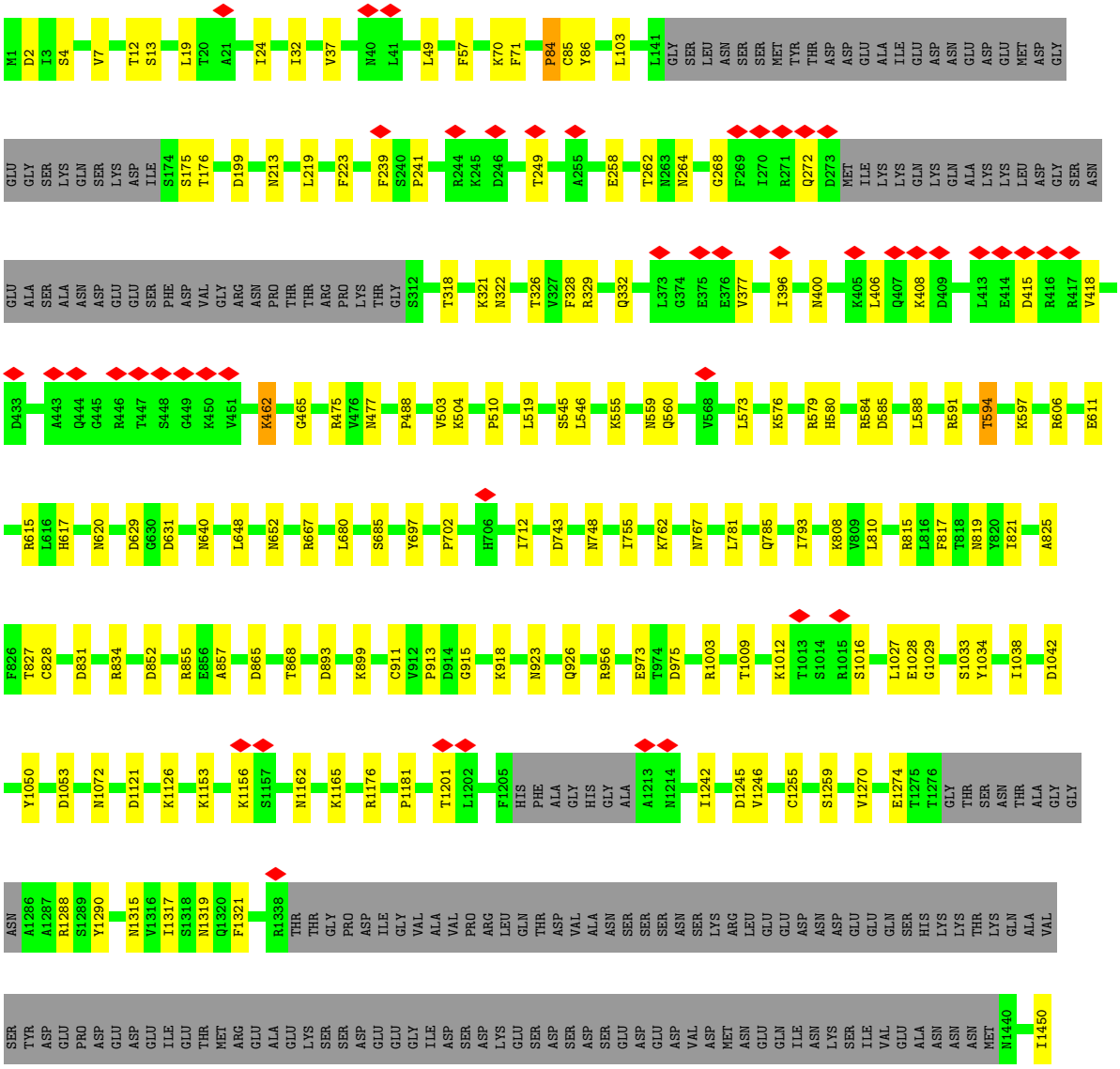
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total Mg 1 1	0

3 Residue-property plots (i)

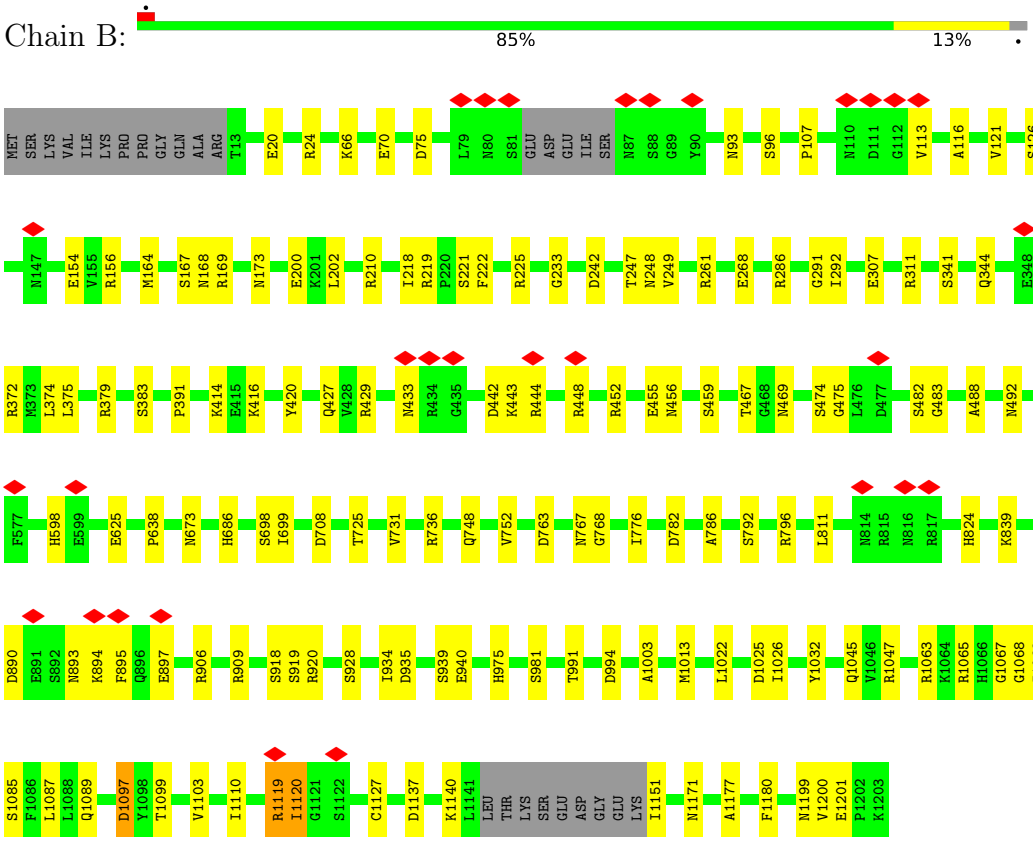
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 I subunit RPA190

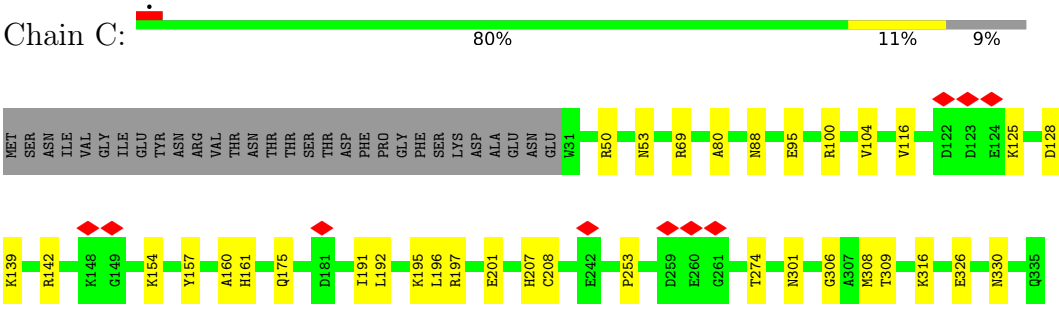
Chain A:



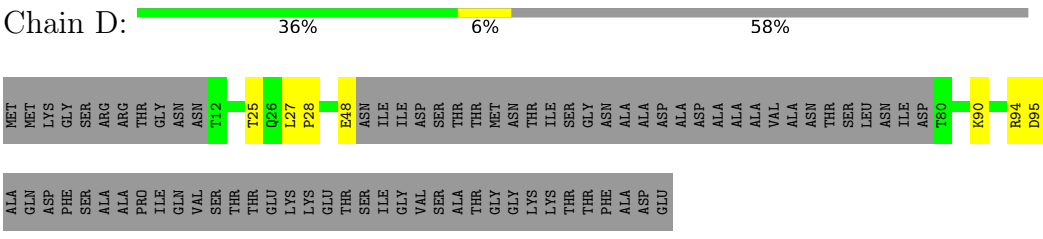
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135



• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

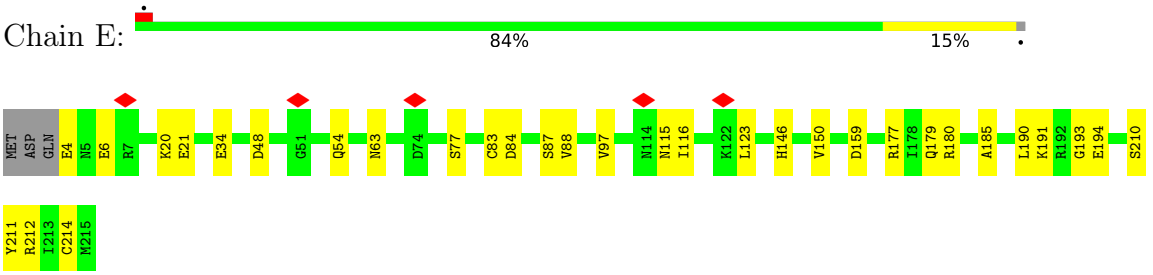


• Molecule 4: DNA-directed RNA polymerase I subunit RPA14



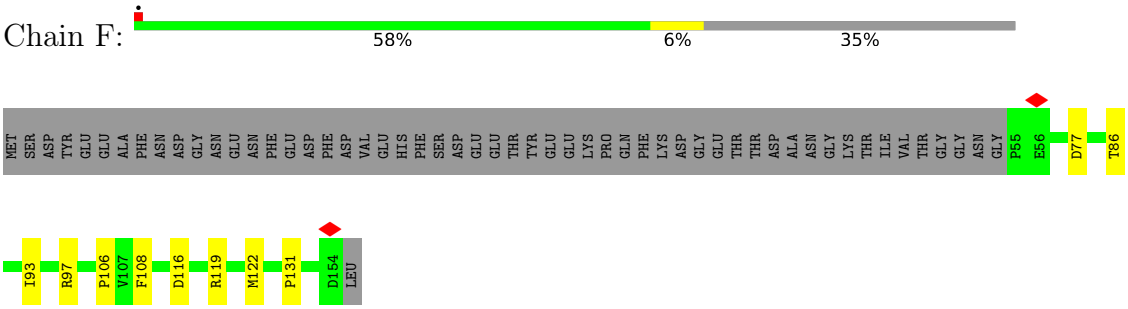
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



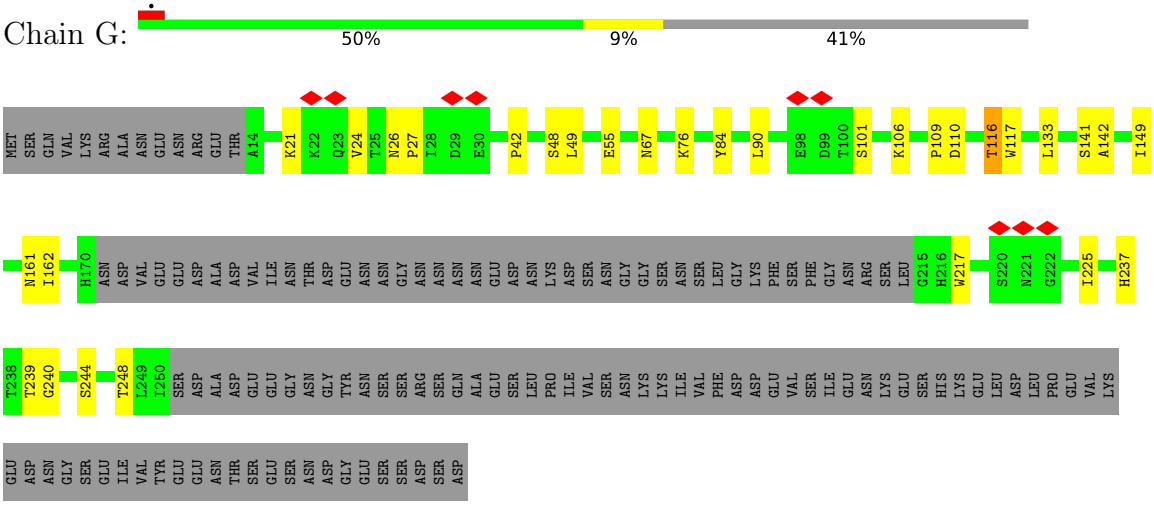
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



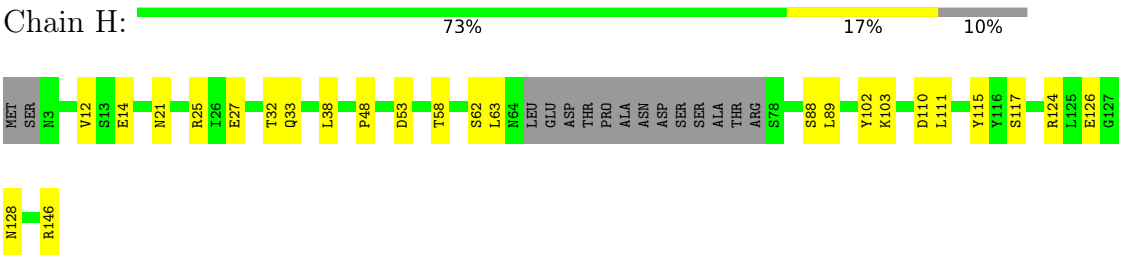
• Molecule 7: DNA-directed RNA polymerase I subunit RPA43

Chain G:



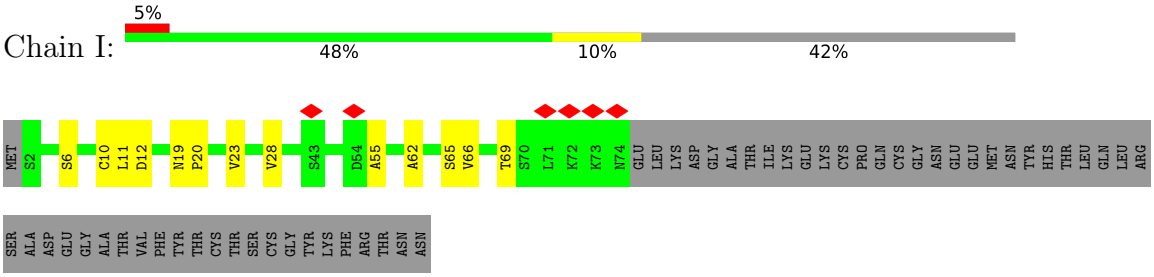
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



• Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain I:

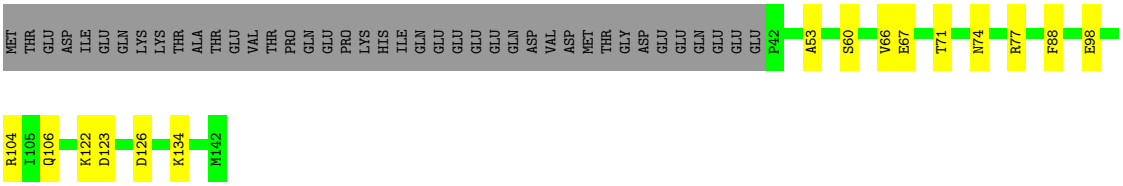


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

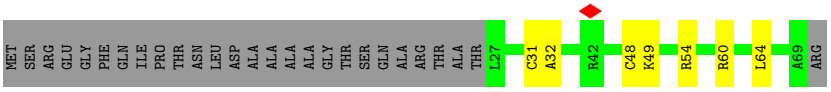
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:



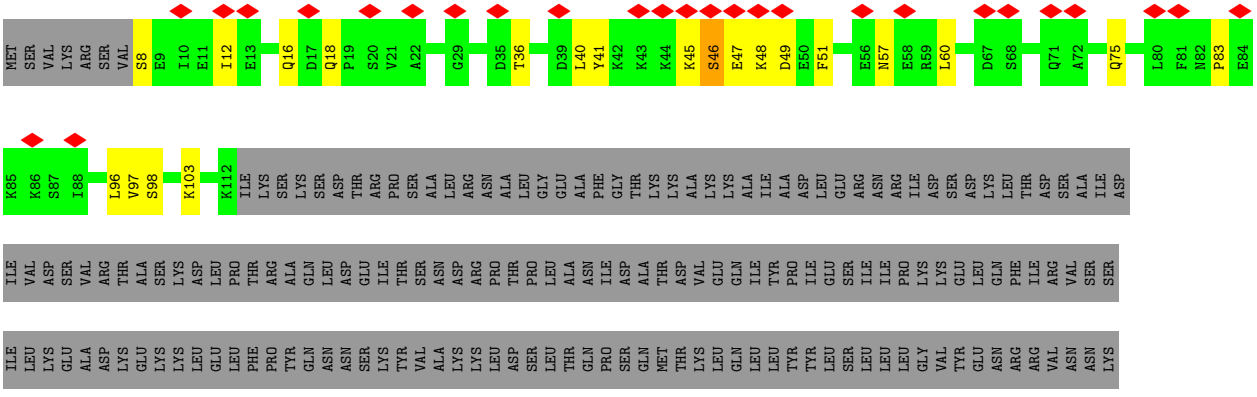
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

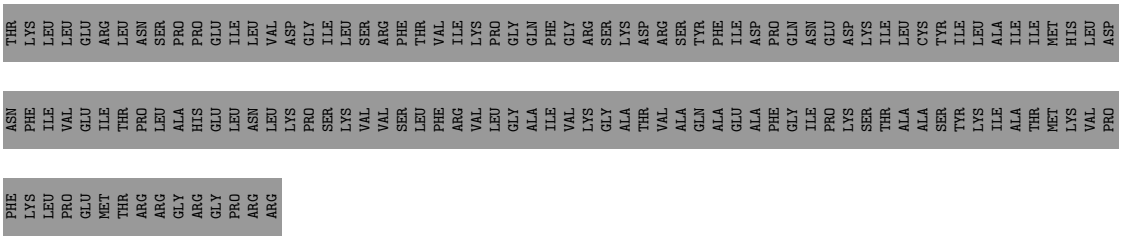
Chain L:



• Molecule 13: DNA-directed RNA polymerase I subunit RPA49

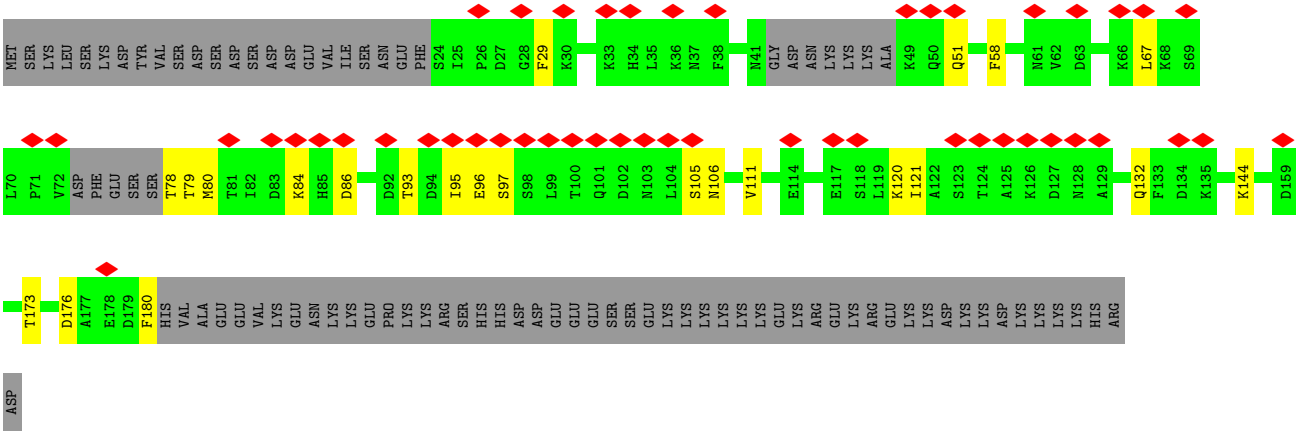
Chain M:





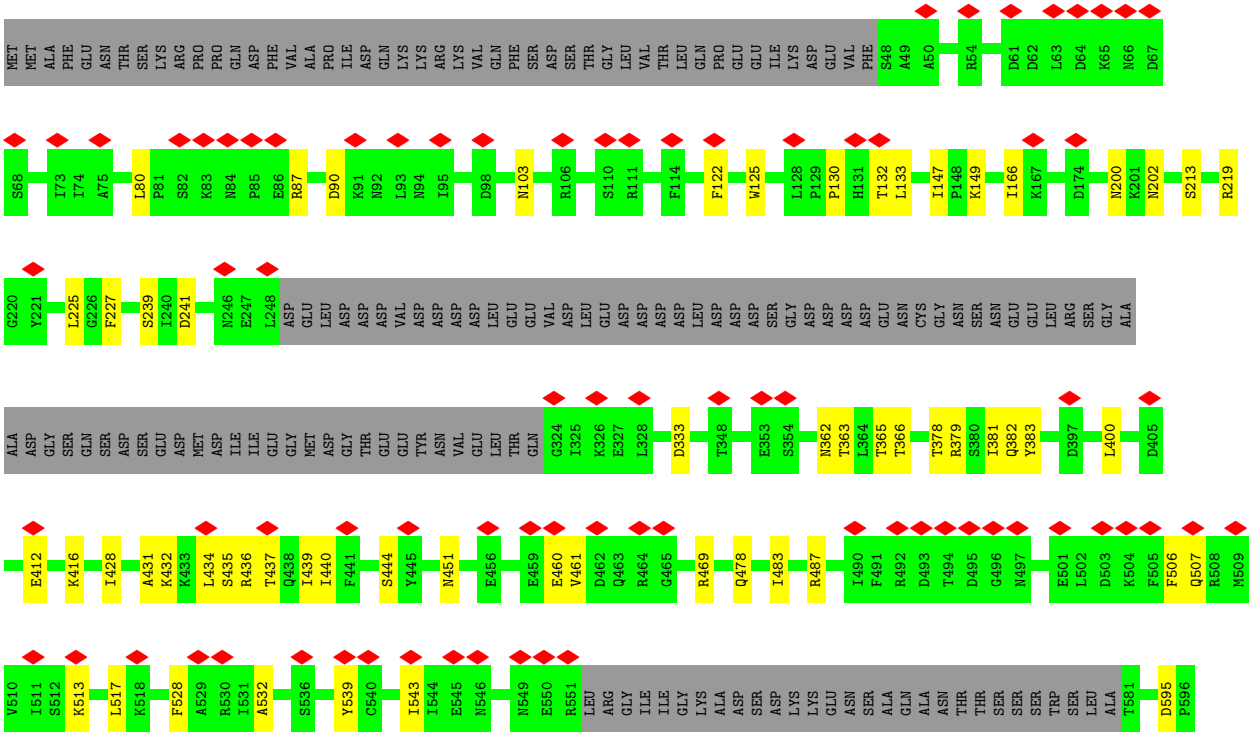
• Molecule 14: DNA-directed RNA polymerase I subunit RPA34

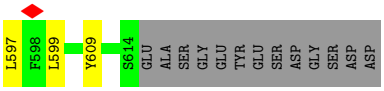
Chain N:



• Molecule 15: RNA polymerase I-specific transcription initiation factor RRN3

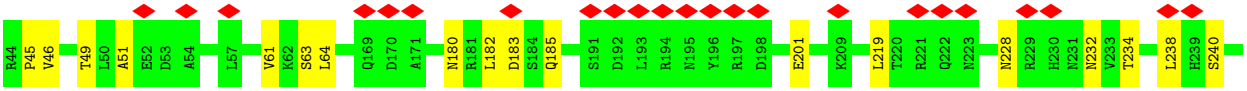
Chain O:

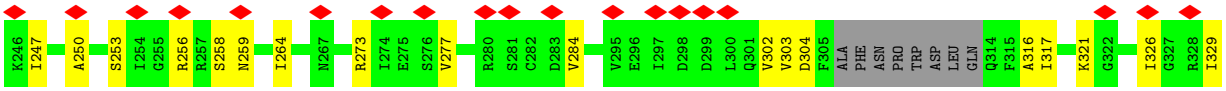


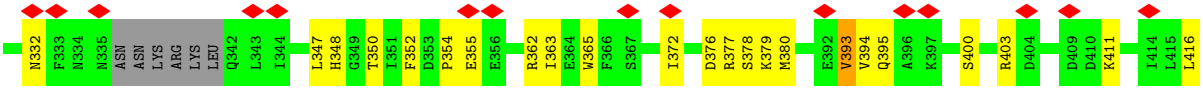


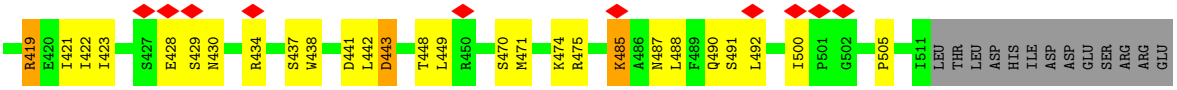
• Molecule 16: RNA polymerase I-specific transcription initiation factor RRN6

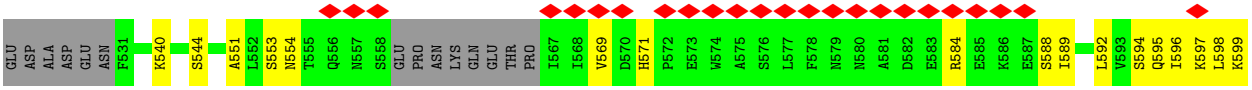
Chain P:

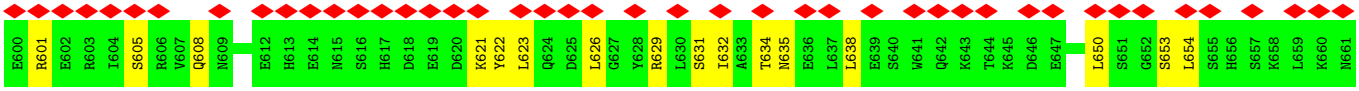


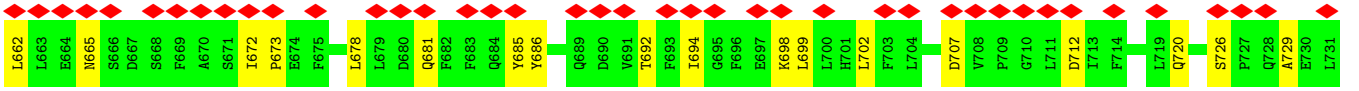


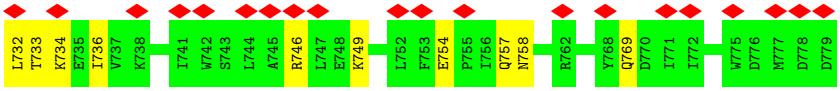






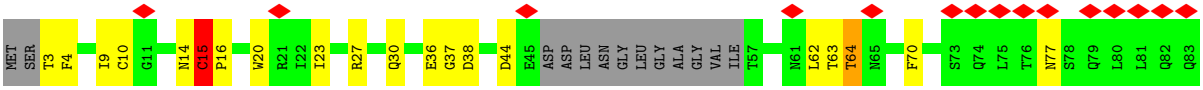


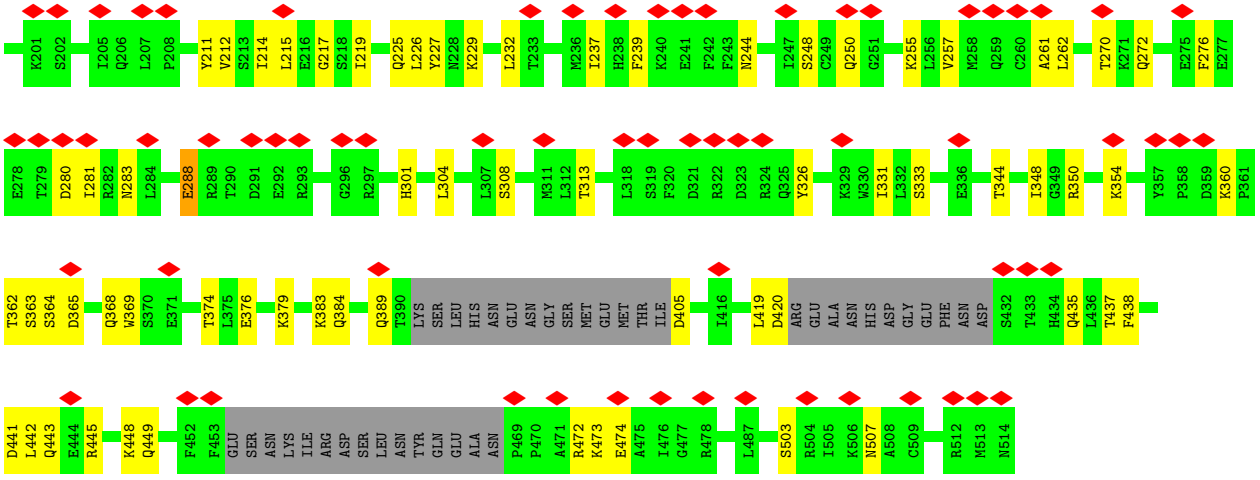




• Molecule 17: RNA polymerase I-specific transcription initiation factor RRN7

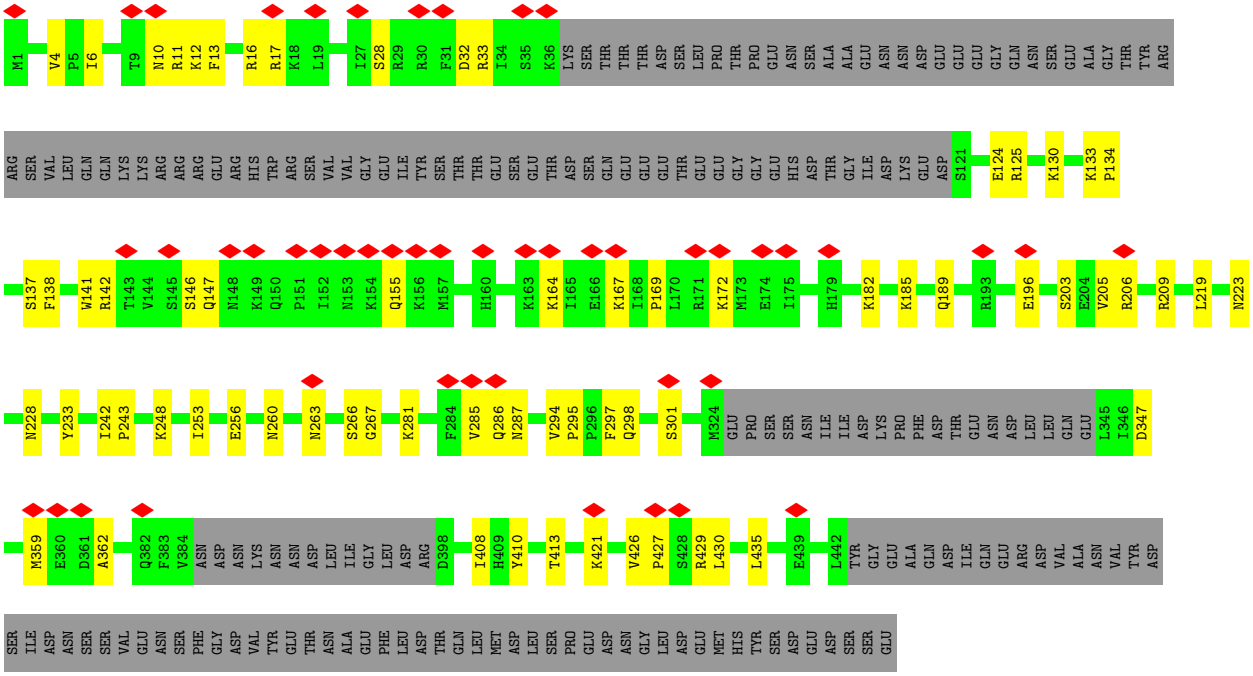
Chain Q:





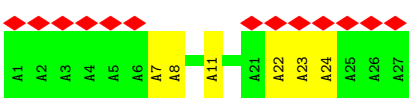
• Molecule 18: RNA polymerase I-specific transcription initiation factor RRN11

Chain R:



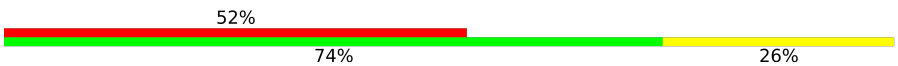
• Molecule 19: NTS-DNA (27-MER)

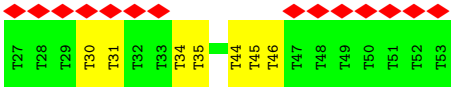
Chain S:



• Molecule 20: TS-DNA (27-MER)

Chain T:





• Molecule 21: DNA foreign

Chain U:

• Molecule 22: DNA foreign

Chain V:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	122099	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.4	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	457.80002, 457.80002, 457.80002	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.51	0/11873	0.57	1/16035 (0.0%)
2	B	0.55	1/9557 (0.0%)	0.58	0/12918
3	C	0.50	0/2475	0.55	0/3354
4	D	0.35	0/465	0.62	1/630 (0.2%)
5	E	0.44	0/1771	0.52	0/2383
6	F	0.52	0/838	0.53	0/1129
7	G	0.39	0/1558	0.54	0/2120
8	H	0.50	0/1070	0.59	1/1449 (0.1%)
9	I	0.36	0/548	0.56	0/740
10	J	0.59	0/578	0.55	0/775
11	K	0.47	0/804	0.53	0/1083
12	L	0.48	0/342	0.63	0/454
13	M	0.32	0/849	0.51	0/1140
14	N	0.33	0/1172	0.52	0/1580
15	O	0.36	0/3897	0.52	0/5268
16	P	0.33	0/4939	0.61	1/6689 (0.0%)
17	Q	0.34	0/3928	0.60	3/5302 (0.1%)
18	R	0.38	0/2789	0.57	0/3755
19	S	0.66	0/647	0.87	0/995
20	T	0.71	0/592	1.34	0/912
21	U	0.68	0/299	0.89	0/464
22	V	0.65	0/251	0.85	0/380
All	All	0.47	1/51242 (0.0%)	0.59	7/69555 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3
3	C	0	1
13	M	0	1
16	P	0	6
17	Q	0	7
18	R	0	4
All	All	0	25

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	121	VAL	C-N	-5.99	1.20	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	15	CYS	C-N-CD	-11.98	94.24	120.60
17	Q	15	CYS	C-N-CA	7.41	153.10	122.00
17	Q	154	LEU	CA-CB-CG	5.47	127.88	115.30
16	P	654	LEU	CA-CB-CG	5.46	127.86	115.30
4	D	95	ASP	CB-CG-OD2	5.34	123.11	118.30
8	H	111	LEU	CA-CB-CG	5.10	127.02	115.30
1	A	406	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1616	GLU	Peptide
1	A	57	PHE	Peptide
1	A	84	PRO	Peptide
2	B	116	ALA	Peptide
2	B	893	ASN	Peptide
2	B	895	PHE	Peptide
3	C	274	THR	Peptide
13	M	46	SER	Peptide
16	P	393	VAL	Peptide
16	P	443	ASP	Peptide
16	P	45	PRO	Peptide
16	P	46	VAL	Peptide
16	P	485	LYS	Peptide

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Mol	Chain	Res	Type	Group
16	P	500	ILE	Peptide
17	Q	15	CYS	Peptide
17	Q	20	TRP	Peptide
17	Q	219	ILE	Peptide
17	Q	23	ILE	Peptide
17	Q	280	ASP	Peptide
17	Q	288	GLU	Peptide
17	Q	77	ASN	Peptide
18	R	134	PRO	Peptide
18	R	285	VAL	Peptide
18	R	294	VAL	Peptide
18	R	426	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11659	0	11753	121	0
2	B	9350	0	9241	106	0
3	C	2423	0	2412	26	0
4	D	459	0	462	5	0
5	E	1735	0	1764	17	0
6	F	823	0	841	8	0
7	G	1520	0	1529	22	0
8	H	1052	0	1021	13	0
9	I	542	0	557	9	0
10	J	569	0	586	9	0
11	K	793	0	790	9	0
12	L	340	0	362	5	0
13	M	833	0	826	16	0
14	N	1151	0	1169	19	0
15	O	3811	0	3804	36	0
16	P	4840	0	4773	99	0
17	Q	3839	0	3861	70	0
18	R	2725	0	2798	43	0
19	S	567	0	298	4	0
20	T	539	0	324	6	0
21	U	264	0	133	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	V	228	0	133	1	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	I	1	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	Q	1	0	0	0	0
24	A	1	0	0	0	0
All	All	50070	0	49437	576	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 6.

All (576) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PHE:H	1:A:264:ASN:HD21	1.45	0.65
16:P:584:ARG:HH12	16:P:588:SER:HB3	1.60	0.65
2:B:467:THR:HG23	2:B:469:ASN:H	1.61	0.65
16:P:228:ASN:ND2	16:P:232:ASN:OD1	2.30	0.64
18:R:427:PRO:HD2	18:R:430:LEU:HB2	1.79	0.64
15:O:122:PHE:HB3	15:O:125:TRP:HB3	1.78	0.64
16:P:720:GLN:O	17:Q:443:GLN:NE2	2.30	0.64
13:M:16:GLN:HG3	13:M:18:GLN:H	1.63	0.64
16:P:626:LEU:HD22	16:P:665:ASN:HB2	1.80	0.63
16:P:726:SER:HB2	16:P:729:ALA:HB2	1.80	0.62
2:B:935:ASP:OD1	3:C:69:ARG:NH2	2.31	0.62
3:C:69:ARG:NH1	11:K:71:THR:OG1	2.33	0.62
2:B:249:VAL:HG21	2:B:261:ARG:HH21	1.64	0.62
3:C:100:ARG:NH2	10:J:3:VAL:O	2.33	0.62
16:P:474:LYS:HG3	16:P:505:PRO:HD3	1.81	0.61
16:P:180:ASN:ND2	16:P:182:LEU:O	2.34	0.61
15:O:435:SER:HG	15:O:437:THR:HG1	1.48	0.61
2:B:307:GLU:OE2	2:B:311:ARG:NH1	2.34	0.61
16:P:699:LEU:HD12	17:Q:175:PRO:HD2	1.83	0.61
17:Q:365:ASP:O	17:Q:369:TRP:NE1	2.33	0.61
15:O:166:ILE:HD11	15:O:213:SER:HB2	1.83	0.60
2:B:492:ASN:ND2	2:B:725:THR:OG1	2.34	0.60
13:M:12:ILE:HD13	14:N:67:LEU:HB2	1.84	0.60
15:O:434:LEU:HD12	15:O:439:ILE:HG13	1.83	0.60
2:B:429:ARG:O	2:B:433:ASN:ND2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:ARG:NH2	2:B:530:PRO:O	2.34	0.59
16:P:729:ALA:HA	16:P:732:LEU:HD12	1.84	0.59
18:R:281:LYS:HD3	18:R:301:SER:HB3	1.85	0.59
2:B:725:THR:OG1	2:B:767:ASN:ND2	2.36	0.59
16:P:673:PRO:HB3	16:P:712:ASP:HB3	1.85	0.59
2:B:1103:VAL:HG12	2:B:1110:ILE:HG22	1.84	0.59
1:A:477:ASN:OD1	2:B:1047:ARG:NH1	2.36	0.58
16:P:326:ILE:HB	16:P:347:LEU:HB2	1.85	0.58
13:M:57:ASN:HD21	13:M:60:LEU:HB2	1.67	0.58
1:A:318:THR:O	1:A:322:ASN:ND2	2.37	0.58
3:C:53:ASN:HD22	3:C:301:ASN:HD22	1.51	0.58
17:Q:120:ILE:HA	17:Q:125:PHE:H	1.69	0.58
8:H:25:ARG:NH2	8:H:27:GLU:OE2	2.36	0.58
18:R:219:LEU:O	18:R:223:ASN:ND2	2.37	0.58
1:A:815:ARG:O	1:A:819:ASN:ND2	2.36	0.58
16:P:443:ASP:N	16:P:443:ASP:OD1	2.33	0.58
2:B:763:ASP:N	2:B:763:ASP:OD1	2.37	0.58
6:F:119:ARG:NH1	6:F:122:MET:SD	2.77	0.58
1:A:973:GLU:HG3	1:A:975:ASP:H	1.67	0.57
1:A:620:ASN:OD1	1:A:667:ARG:NH2	2.37	0.57
5:E:177:ARG:O	5:E:212:ARG:NH1	2.35	0.57
16:P:629:ARG:O	16:P:629:ARG:NH1	2.37	0.57
1:A:13:SER:OG	2:B:1199:ASN:ND2	2.38	0.57
1:A:415:ASP:HA	1:A:418:VAL:HG22	1.87	0.57
7:G:116:THR:OG1	7:G:117:TRP:N	2.36	0.57
1:A:86:TYR:HD2	1:A:249:THR:HB	1.70	0.57
1:A:475:ARG:NH1	2:B:1069:ILE:O	2.37	0.57
2:B:1097:ASP:N	2:B:1097:ASP:OD1	2.34	0.57
17:Q:212:VAL:HA	17:Q:215:LEU:HB2	1.86	0.57
3:C:50:ARG:HH12	3:C:306:GLY:HA2	1.69	0.57
11:K:60:SER:HB2	11:K:106:GLN:HG2	1.86	0.57
2:B:219:ARG:HG2	2:B:221:SER:H	1.70	0.57
14:N:176:ASP:OD1	14:N:176:ASP:N	2.37	0.57
17:Q:333:SER:O	17:Q:448:LYS:NZ	2.38	0.57
1:A:591:ARG:NH2	1:A:631:ASP:OD1	2.38	0.56
1:A:1494:ARG:NH1	9:I:55:ALA:O	2.38	0.56
2:B:292:ILE:O	2:B:379:ARG:NH1	2.38	0.56
2:B:919:SER:OG	2:B:920:ARG:N	2.37	0.56
5:E:97:VAL:HG21	5:E:123:LEU:HB3	1.87	0.56
15:O:200:ASN:ND2	15:O:202:ASN:OD1	2.37	0.56
17:Q:389:GLN:H	18:R:209:ARG:HH12	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:THR:HG21	2:B:1075:GLU:HG3	1.87	0.56
1:A:1009:THR:HA	1:A:1012:LYS:HG3	1.87	0.56
2:B:698:SER:OG	2:B:699:ILE:N	2.38	0.56
2:B:1045:GLN:NE2	2:B:1067:GLY:O	2.38	0.56
17:Q:326:TYR:O	17:Q:472:ARG:NH2	2.37	0.56
1:A:1459:LYS:HB2	1:A:1473:LYS:HB2	1.87	0.56
16:P:238:LEU:HG	16:P:240:SER:H	1.70	0.56
17:Q:383:LYS:HG3	17:Q:384:GLN:HG2	1.88	0.56
15:O:460:GLU:O	15:O:469:ARG:NH2	2.38	0.56
1:A:1274:GLU:OE2	1:A:1288:ARG:NH1	2.39	0.56
16:P:584:ARG:O	16:P:584:ARG:NH1	2.39	0.56
3:C:88:ASN:O	12:L:60:ARG:NH1	2.38	0.56
15:O:333:ASP:HB3	15:O:599:LEU:HD13	1.87	0.56
17:Q:248:SER:OG	17:Q:250:GLN:NE2	2.39	0.56
18:R:13:PHE:HA	18:R:16:ARG:HB2	1.86	0.56
17:Q:442:LEU:HA	17:Q:445:ARG:HG2	1.88	0.56
16:P:183:ASP:HB2	16:P:247:ILE:HG22	1.88	0.55
15:O:130:PRO:HA	15:O:133:LEU:HB3	1.88	0.55
1:A:852:ASP:OD1	1:A:852:ASP:N	2.40	0.55
1:A:1242:ILE:HA	1:A:1536:ILE:HA	1.88	0.55
1:A:1600:ARG:NH1	1:A:1616:GLU:OE1	2.38	0.55
18:R:203:SER:O	18:R:206:ARG:NH2	2.39	0.55
2:B:731:VAL:HG21	10:J:59:LYS:HE2	1.89	0.55
18:R:32:ASP:OD1	18:R:33:ARG:NH2	2.40	0.55
2:B:369:ASP:OD1	2:B:372:ARG:NH1	2.40	0.55
16:P:393:VAL:HG23	18:R:142:ARG:H	1.71	0.55
1:A:555:LYS:O	1:A:559:ASN:ND2	2.40	0.55
2:B:20:GLU:OE2	2:B:24:ARG:NH2	2.40	0.55
1:A:1315:ASN:OD1	1:A:1319:ASN:ND2	2.40	0.55
16:P:434:ARG:HB2	18:R:141:TRP:HE1	1.72	0.55
16:P:769:GLN:NE2	17:Q:145:ASN:OD1	2.40	0.54
15:O:241:ASP:OD2	15:O:378:THR:OG1	2.23	0.54
16:P:51:ALA:HB3	16:P:492:LEU:HD13	1.90	0.54
1:A:1560:ASN:O	1:A:1564:ASN:ND2	2.40	0.54
16:P:256:ARG:HH22	16:P:259:ASN:HB2	1.73	0.54
2:B:890:ASP:O	12:L:54:ARG:NH1	2.41	0.54
2:B:1127:CYS:SG	2:B:1171:ASN:ND2	2.81	0.54
3:C:116:VAL:HG22	3:C:130:ASN:HB3	1.87	0.54
2:B:776:ILE:HD12	2:B:1026:ILE:HD13	1.88	0.54
16:P:594:SER:HA	16:P:597:LYS:HG2	1.88	0.54
16:P:698:LYS:HD2	17:Q:124:ARG:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:ASN:OD1	2:B:492:ASN:N	2.38	0.54
5:E:48:ASP:OD2	5:E:54:GLN:NE2	2.41	0.54
16:P:61:VAL:HB	16:P:551:ALA:HB3	1.90	0.54
18:R:362:ALA:H	18:R:421:LYS:HE3	1.71	0.54
16:P:733:THR:HA	16:P:736:ILE:HD12	1.90	0.54
2:B:225:ARG:NH2	2:B:268:GLU:OE1	2.41	0.54
1:A:652:ASN:OD1	1:A:652:ASN:N	2.40	0.53
11:K:66:VAL:HG12	11:K:67:GLU:HG2	1.89	0.53
15:O:517:LEU:HD21	15:O:543:ILE:HB	1.89	0.53
17:Q:364:SER:OG	17:Q:368:GLN:NE2	2.42	0.53
1:A:1121:ASP:OD2	1:A:1126:LYS:NZ	2.41	0.53
2:B:168:ASN:HA	2:B:173:ASN:HD22	1.73	0.53
3:C:196:LEU:O	3:C:197:ARG:NH1	2.39	0.53
17:Q:143:THR:HA	17:Q:146:ASP:HB2	1.90	0.53
2:B:792:SER:O	2:B:796:ARG:NH1	2.40	0.53
7:G:48:SER:OG	7:G:49:LEU:N	2.41	0.53
10:J:17:LYS:HB3	10:J:39:LEU:HD13	1.90	0.53
18:R:295:PRO:HB2	18:R:297:PHE:H	1.71	0.53
16:P:394:VAL:HG12	16:P:395:GLN:HB2	1.90	0.53
2:B:1137:ASP:HA	2:B:1140:LYS:HD2	1.90	0.53
16:P:553:SER:OG	16:P:554:ASN:N	2.41	0.53
1:A:1543:SER:OG	1:A:1544:ASN:N	2.41	0.53
2:B:939:SER:OG	2:B:940:GLU:N	2.42	0.53
16:P:681:GLN:O	16:P:685:TYR:N	2.39	0.53
18:R:185:LYS:O	18:R:189:GLN:NE2	2.42	0.53
7:G:141:SER:OG	7:G:142:ALA:N	2.42	0.53
8:H:62:SER:OG	8:H:63:LEU:N	2.42	0.53
16:P:253:SER:OG	16:P:411:LYS:NZ	2.42	0.53
3:C:128:ASP:O	3:C:175:GLN:NE2	2.40	0.52
17:Q:169:SER:HA	17:Q:174:LEU:HD12	1.90	0.52
17:Q:369:TRP:HE3	17:Q:374:THR:HG22	1.74	0.52
1:A:755:ILE:O	1:A:767:ASN:ND2	2.41	0.52
2:B:210:ARG:NH2	2:B:625:GLU:OE1	2.42	0.52
1:A:1053:ASP:N	1:A:1053:ASP:OD2	2.42	0.52
14:N:86:ASP:OD2	14:N:144:LYS:NZ	2.41	0.52
16:P:201:GLU:HB2	16:P:219:LEU:HB2	1.90	0.52
2:B:1103:VAL:HG21	2:B:1200:VAL:HG21	1.92	0.52
15:O:597:LEU:HG	15:O:599:LEU:H	1.74	0.52
1:A:488:PRO:HA	1:A:617:HIS:HD2	1.74	0.52
2:B:444:ARG:O	2:B:448:ARG:NH1	2.43	0.52
9:I:65:SER:OG	9:I:66:VAL:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1065:ARG:NH2	17:Q:44:ASP:OD1	2.41	0.52
13:M:40:LEU:HD11	13:M:51:PHE:HB3	1.91	0.52
17:Q:193:PHE:O	17:Q:389:GLN:NE2	2.43	0.52
8:H:12:VAL:HG22	8:H:53:ASP:H	1.74	0.52
2:B:200:GLU:OE2	2:B:736:ARG:NH2	2.43	0.52
2:B:474:SER:OG	2:B:475:GLY:N	2.42	0.52
15:O:440:ILE:O	15:O:444:SER:N	2.40	0.52
1:A:648:LEU:O	1:A:652:ASN:ND2	2.43	0.51
8:H:88:SER:OG	8:H:89:LEU:N	2.40	0.51
17:Q:239:PHE:HZ	17:Q:288:GLU:HG3	1.75	0.51
17:Q:473:LYS:NZ	17:Q:474:GLU:OE2	2.44	0.51
16:P:350:THR:HG22	16:P:352:PHE:H	1.76	0.51
16:P:623:LEU:HB2	16:P:678:LEU:HD22	1.92	0.51
16:P:672:ILE:HD13	16:P:734:LYS:HG3	1.91	0.51
7:G:141:SER:O	7:G:217:TRP:NE1	2.34	0.51
11:K:74:ASN:OD1	11:K:77:ARG:NH2	2.44	0.51
16:P:569:VAL:HG13	16:P:571:HIS:HD2	1.76	0.51
16:P:605:SER:HA	16:P:608:GLN:HB2	1.91	0.51
17:Q:331:ILE:HD11	17:Q:472:ARG:HH21	1.76	0.51
2:B:991:THR:OG1	2:B:994:ASP:OD2	2.28	0.51
4:D:48:GLU:OE2	4:D:90:LYS:NZ	2.41	0.51
2:B:906:ARG:NE	3:C:95:GLU:OE2	2.44	0.51
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.92	0.51
2:B:113:VAL:HG11	20:T:35:DT:H4'	1.93	0.51
2:B:918:SER:OG	2:B:919:SER:N	2.43	0.51
16:P:598:LEU:HA	16:P:601:ARG:HB2	1.92	0.51
18:R:133:LYS:HB2	18:R:286:GLN:HG2	1.93	0.51
2:B:427:GLN:OE1	2:B:452:ARG:NH1	2.44	0.50
1:A:893:ASP:OD1	1:A:956:ARG:NE	2.43	0.50
16:P:631:SER:O	16:P:635:ASN:ND2	2.43	0.50
9:I:10:CYS:SG	9:I:11:LEU:N	2.84	0.50
1:A:834:ARG:NH1	2:B:994:ASP:OD1	2.43	0.50
2:B:492:ASN:HD22	2:B:767:ASN:HD21	1.58	0.50
17:Q:90:LYS:NZ	17:Q:93:LYS:O	2.45	0.50
18:R:125:ARG:NH1	18:R:287:ASN:O	2.44	0.50
5:E:210:SER:OG	5:E:211:TYR:N	2.45	0.50
14:N:86:ASP:OD1	14:N:86:ASP:N	2.40	0.50
8:H:32:THR:OG1	8:H:33:GLN:N	2.44	0.50
16:P:376:ASP:N	16:P:376:ASP:OD1	2.43	0.50
9:I:62:ALA:HB1	9:I:69:THR:HG21	1.92	0.50
16:P:355:GLU:OE1	18:R:130:LYS:NZ	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:428:GLU:HG3	16:P:487:ASN:HD22	1.76	0.50
17:Q:437:THR:OG1	17:Q:438:PHE:N	2.43	0.50
1:A:1246:VAL:O	1:A:1517:ARG:NH2	2.45	0.50
5:E:4:GLU:HG3	5:E:6:GLU:H	1.76	0.50
14:N:111:VAL:O	14:N:120:LYS:N	2.41	0.50
15:O:412:GLU:HB3	15:O:416:LYS:HE3	1.92	0.50
1:A:258:GLU:O	1:A:262:THR:OG1	2.26	0.49
8:H:124:ARG:NH2	8:H:126:GLU:OE1	2.43	0.49
16:P:63:SER:OG	16:P:64:LEU:N	2.45	0.49
16:P:589:ILE:HA	16:P:592:LEU:HB3	1.94	0.49
17:Q:261:ALA:O	17:Q:449:GLN:NE2	2.38	0.49
2:B:70:GLU:OE2	2:B:96:SER:OG	2.30	0.49
5:E:191:LYS:N	5:E:194:GLU:OE1	2.44	0.49
17:Q:360:LYS:HA	17:Q:362:THR:H	1.77	0.49
1:A:1655:ASP:OD2	7:G:106:LYS:NZ	2.45	0.49
8:H:48:PRO:O	8:H:146:ARG:NH2	2.39	0.49
10:J:45:CYS:O	10:J:48:ARG:NH1	2.46	0.49
1:A:762:LYS:NZ	8:H:14:GLU:OE2	2.45	0.49
1:A:1290:TYR:HB2	1:A:1474:LEU:HB3	1.94	0.49
17:Q:9:ILE:HG13	17:Q:10:CYS:H	1.76	0.49
17:Q:133:ALA:HA	17:Q:136:ILE:HB	1.94	0.49
1:A:1016:SER:OG	1:A:1016:SER:O	2.31	0.49
14:N:105:SER:OG	14:N:106:ASN:N	2.46	0.49
14:N:111:VAL:N	14:N:120:LYS:O	2.46	0.49
15:O:431:ALA:O	15:O:487:ARG:NH2	2.46	0.49
1:A:611:GLU:OE1	1:A:615:ARG:NH1	2.42	0.49
1:A:1033:SER:OG	1:A:1034:TYR:N	2.44	0.49
22:V:5:DC:H2”	22:V:6:DC:H5”	1.94	0.48
16:P:588:SER:O	16:P:592:LEU:N	2.44	0.48
16:P:702:LEU:O	17:Q:255:LYS:NZ	2.37	0.48
16:P:185:GLN:HB3	16:P:247:ILE:HD13	1.96	0.48
17:Q:503:SER:O	17:Q:507:ASN:ND2	2.46	0.48
18:R:17:ARG:NH1	18:R:124:GLU:OE2	2.41	0.48
13:M:57:ASN:O	13:M:103:LYS:NZ	2.33	0.48
1:A:503:VAL:O	1:A:580:HIS:NE2	2.46	0.48
16:P:449:LEU:HD23	16:P:470:SER:HB2	1.95	0.48
18:R:137:SER:OG	18:R:138:PHE:N	2.46	0.48
1:A:175:SER:OG	1:A:176:THR:N	2.45	0.48
1:A:326:THR:HA	1:A:329:ARG:HH11	1.78	0.48
1:A:328:PHE:O	1:A:332:GLN:NE2	2.38	0.48
1:A:1592:GLN:O	5:E:179:GLN:NE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:482:SER:OG	2:B:483:GLY:N	2.47	0.48
2:B:878:GLU:OE1	2:B:909:ARG:NH1	2.46	0.48
8:H:21:ASN:N	8:H:21:ASN:OD1	2.46	0.48
17:Q:193:PHE:HD1	17:Q:217:GLY:HA3	1.79	0.48
7:G:239:THR:OG1	7:G:240:GLY:N	2.47	0.48
14:N:93:THR:O	14:N:97:SER:OG	2.28	0.48
16:P:302:VAL:HG21	16:P:362:ARG:HA	1.95	0.48
16:P:470:SER:OG	16:P:471:MET:N	2.47	0.48
16:P:634:THR:O	16:P:638:LEU:N	2.46	0.48
18:R:12:LYS:O	18:R:16:ARG:N	2.42	0.48
1:A:1255:CYS:O	1:A:1259:SER:OG	2.31	0.48
5:E:20:LYS:HE2	5:E:34:GLU:HG2	1.96	0.48
1:A:697:TYR:HE1	1:A:702:PRO:HD2	1.78	0.48
13:M:75:GLN:HB3	14:N:58:PHE:HB2	1.96	0.48
17:Q:405:ASP:N	17:Q:405:ASP:OD1	2.46	0.48
1:A:629:ASP:OD1	1:A:629:ASP:N	2.44	0.47
1:A:855:ARG:NH1	1:A:868:THR:O	2.47	0.47
2:B:708:ASP:OD1	2:B:708:ASP:N	2.38	0.47
2:B:786:ALA:HB1	2:B:928:SER:HB3	1.96	0.47
2:B:918:SER:OG	2:B:919:SER:O	2.30	0.47
14:N:95:ILE:HG22	14:N:96:GLU:HG2	1.95	0.47
3:C:253:PRO:HD2	14:N:180:PHE:HD1	1.80	0.47
16:P:378:SER:OG	16:P:379:LYS:NZ	2.38	0.47
15:O:200:ASN:ND2	17:Q:14:ASN:O	2.47	0.47
15:O:478:GLN:O	15:O:478:GLN:NE2	2.47	0.47
16:P:332:ASN:OD1	16:P:332:ASN:N	2.41	0.47
1:A:1027:LEU:O	1:A:1029:GLY:N	2.47	0.47
2:B:1089:GLN:NE2	7:G:110:ASP:OD2	2.46	0.47
20:T:34:DT:H2"	20:T:35:DT:H5"	1.97	0.47
2:B:126:SER:OG	2:B:132:SER:O	2.32	0.47
2:B:383:SER:O	2:B:383:SER:OG	2.31	0.47
2:B:575:HIS:HB3	13:M:97:VAL:HG22	1.97	0.47
2:B:939:SER:HA	2:B:1013:MET:HG2	1.97	0.47
7:G:76:LYS:HD2	7:G:76:LYS:HA	1.76	0.47
16:P:365:TRP:HA	16:P:372:ILE:HA	1.97	0.47
16:P:365:TRP:HB3	16:P:372:ILE:HG22	1.96	0.47
17:Q:4:PHE:HE1	17:Q:30:GLN:HG2	1.80	0.47
1:A:213:ASN:ND2	1:A:1605:THR:O	2.47	0.47
2:B:154:GLU:OE2	2:B:156:ARG:NH1	2.47	0.47
3:C:53:ASN:ND2	14:N:173:THR:O	2.48	0.47
6:F:77:ASP:OD1	6:F:77:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:48:CYS:SG	12:L:49:LYS:N	2.88	0.47
16:P:416:LEU:HD23	16:P:423:ILE:HD12	1.96	0.47
1:A:32:ILE:HG21	1:A:49:LEU:HD23	1.97	0.47
2:B:839:LYS:NZ	2:B:856:ASP:OD2	2.47	0.47
16:P:437:SER:OG	16:P:438:TRP:N	2.48	0.47
17:Q:211:TYR:HA	17:Q:214:ILE:HD12	1.96	0.47
17:Q:283:ASN:N	17:Q:283:ASN:OD1	2.46	0.47
17:Q:441:ASP:OD2	17:Q:441:ASP:N	2.48	0.47
1:A:827:THR:OG1	1:A:828:CYS:N	2.48	0.46
15:O:80:LEU:HB2	15:O:87:ARG:HG3	1.97	0.46
16:P:754:GLU:O	16:P:757:GLN:NE2	2.48	0.46
17:Q:244:ASN:OD1	17:Q:244:ASN:N	2.45	0.46
1:A:857:ALA:HB2	1:A:899:LYS:HD2	1.97	0.46
1:A:911:CYS:O	1:A:915:GLY:N	2.41	0.46
15:O:400:LEU:HD13	15:O:428:ILE:HD11	1.97	0.46
19:S:7:DA:H2'	19:S:8:DA:C8	2.50	0.46
13:M:49:ASP:OD1	13:M:49:ASP:N	2.49	0.46
16:P:316:ALA:HB2	16:P:329:ILE:HG23	1.97	0.46
17:Q:226:LEU:HA	17:Q:229:LYS:HB2	1.96	0.46
1:A:606:ARG:NH2	11:K:98:GLU:OE1	2.49	0.46
13:M:46:SER:OG	13:M:47:GLU:N	2.48	0.46
15:O:383:TYR:OH	15:O:595:ASP:O	2.33	0.46
16:P:258:SER:OG	16:P:259:ASN:N	2.48	0.46
1:A:1557:ALA:HB2	5:E:150:VAL:HG22	1.98	0.46
5:E:193:GLY:N	5:E:214:CYS:O	2.48	0.46
7:G:67:ASN:OD1	7:G:84:TYR:OH	2.33	0.46
16:P:422:ILE:HG13	16:P:442:LEU:HD23	1.97	0.46
2:B:202:LEU:HD22	2:B:488:ALA:HB2	1.98	0.46
16:P:429:SER:OG	16:P:430:ASN:N	2.47	0.46
1:A:408:LYS:HA	1:A:408:LYS:HD2	1.81	0.46
1:A:918:LYS:O	1:A:923:ASN:ND2	2.39	0.46
1:A:1609:SER:OG	1:A:1630:GLU:OE2	2.34	0.46
2:B:906:ARG:NH2	3:C:95:GLU:OE1	2.49	0.46
2:B:1119:ARG:HB3	2:B:1120:ILE:H	1.53	0.46
16:P:273:ARG:HD2	16:P:332:ASN:HB3	1.97	0.46
16:P:631:SER:O	16:P:686:TYR:OH	2.30	0.46
8:H:103:LYS:HB3	8:H:115:TYR:HD1	1.81	0.45
15:O:147:ILE:HG22	15:O:149:LYS:HG2	1.97	0.45
1:A:1012:LYS:HA	1:A:1201:THR:HG21	1.97	0.45
14:N:144:LYS:HD3	14:N:144:LYS:HA	1.79	0.45
16:P:692:THR:O	16:P:746:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HG12	1:A:49:LEU:HB2	1.99	0.45
4:D:28:PRO:HD2	7:G:24:VAL:HG21	1.98	0.45
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.98	0.45
17:Q:112:LEU:HD11	17:Q:164:ILE:HD11	1.98	0.45
20:T:30:DT:H2'	20:T:31:DT:C4	2.51	0.45
1:A:865:ASP:O	1:A:868:THR:OG1	2.35	0.45
5:E:21:GLU:OE2	5:E:146:HIS:NE2	2.43	0.45
9:I:10:CYS:SG	9:I:12:ASP:N	2.89	0.45
16:P:400:SER:HA	16:P:419:ARG:HD2	1.99	0.45
5:E:83:CYS:SG	5:E:84:ASP:N	2.89	0.45
13:M:8:SER:O	13:M:8:SER:OG	2.29	0.45
15:O:461:VAL:HG13	15:O:513:LYS:HD2	1.99	0.45
1:A:781:LEU:HD22	1:A:785:GLN:HG3	1.98	0.45
1:A:1647:ASN:HB3	2:B:1085:SER:HB2	1.97	0.45
2:B:420:TYR:OH	2:B:455:GLU:OE2	2.35	0.45
17:Q:194:GLN:HA	17:Q:389:GLN:HE21	1.81	0.45
11:K:53:ALA:HB1	11:K:104:ARG:HH12	1.81	0.45
16:P:348:HIS:HD2	18:R:155:GLN:HB3	1.82	0.45
1:A:702:PRO:HD3	1:A:712:ILE:HD11	1.98	0.45
1:A:1610:PHE:HD2	1:A:1632:GLU:HG2	1.82	0.45
8:H:110:ASP:O	8:H:128:ASN:ND2	2.44	0.45
15:O:362:ASN:HA	15:O:365:THR:HG22	1.98	0.45
1:A:831:ASP:N	1:A:831:ASP:OD1	2.49	0.45
1:A:1038:ILE:HD11	1:A:1050:TYR:HB2	1.99	0.45
2:B:442:ASP:OD1	2:B:442:ASP:N	2.44	0.45
3:C:308:MET:SD	3:C:316:LYS:NZ	2.80	0.45
8:H:117:SER:O	8:H:117:SER:OG	2.32	0.45
16:P:430:ASN:N	16:P:430:ASN:OD1	2.50	0.45
17:Q:63:THR:O	17:Q:63:THR:OG1	2.32	0.45
16:P:304:ASP:OD2	16:P:304:ASP:N	2.46	0.44
18:R:169:PRO:HA	18:R:172:LYS:HB2	1.98	0.44
1:A:1317:ILE:HA	1:A:1321:PHE:HB3	2.00	0.44
2:B:456:ASN:HB3	2:B:459:SER:HB3	1.99	0.44
13:M:36:THR:HG22	13:M:57:ASN:HB3	1.98	0.44
2:B:824:HIS:ND1	2:B:897:GLU:HG2	2.32	0.44
14:N:78:THR:OG1	14:N:79:THR:N	2.49	0.44
16:P:540:LYS:NZ	16:P:544:SER:O	2.46	0.44
18:R:347:ASP:N	18:R:347:ASP:OD1	2.50	0.44
1:A:1492:ILE:HD13	1:A:1492:ILE:HA	1.88	0.44
2:B:1119:ARG:HB3	2:B:1120:ILE:HD12	2.00	0.44
3:C:131:THR:HG21	3:C:207:HIS:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:41:TYR:HB3	14:N:29:PHE:HB3	2.00	0.44
13:M:45:LYS:HB2	13:M:45:LYS:HE3	1.75	0.44
14:N:79:THR:OG1	14:N:80:MET:N	2.51	0.44
16:P:653:SER:H	16:P:749:LYS:HG3	1.83	0.44
17:Q:64:THR:HB	17:Q:70:PHE:HA	1.99	0.44
1:A:680:LEU:HD22	1:A:817:PHE:HE1	1.83	0.44
14:N:121:ILE:H	14:N:121:ILE:HG13	1.60	0.44
15:O:440:ILE:HD13	15:O:440:ILE:HA	1.90	0.44
1:A:1153:LYS:HA	1:A:1156:LYS:HE2	1.99	0.44
1:A:1242:ILE:HD11	1:A:1517:ARG:HE	1.83	0.44
1:A:1450:ILE:O	1:A:1454:HIS:ND1	2.51	0.44
2:B:75:ASP:OD1	2:B:93:ASN:N	2.45	0.44
16:P:599:LYS:O	16:P:599:LYS:NZ	2.40	0.44
16:P:632:ILE:HA	16:P:635:ASN:HD22	1.82	0.44
20:T:46:DT:H6	20:T:46:DT:H2'	1.66	0.44
1:A:825:ALA:H	2:B:1022:LEU:HD22	1.82	0.44
3:C:125:LYS:O	3:C:130:ASN:ND2	2.51	0.44
18:R:164:LYS:HD2	18:R:164:LYS:HA	1.80	0.44
18:R:253:ILE:HA	18:R:256:GLU:HB2	2.00	0.44
1:A:70:LYS:HG3	1:A:71:PHE:HD2	1.83	0.44
3:C:154:LYS:HB2	3:C:154:LYS:HE2	1.85	0.44
17:Q:27:ARG:NH2	17:Q:38:ASP:OD1	2.51	0.44
19:S:23:DA:H1'	19:S:24:DA:C8	2.53	0.44
1:A:7:VAL:HG11	2:B:1177:ALA:HB2	1.99	0.43
5:E:88:VAL:HB	5:E:116:ILE:HD13	2.00	0.43
16:P:183:ASP:OD1	16:P:183:ASP:N	2.51	0.43
16:P:448:THR:OG1	16:P:470:SER:OG	2.36	0.43
16:P:491:SER:OG	16:P:492:LEU:N	2.51	0.43
1:A:268:GLY:O	1:A:272:GLN:NE2	2.51	0.43
1:A:462:LYS:H	1:A:462:LYS:HG2	1.54	0.43
2:B:1099:THR:HG21	2:B:1180:PHE:HD1	1.83	0.43
15:O:507:GLN:OE1	15:O:539:TYR:N	2.46	0.43
18:R:266:SER:OG	18:R:267:GLY:N	2.52	0.43
2:B:218:ILE:HG13	2:B:391:PRO:HB3	2.00	0.43
19:S:22:DA:H1'	19:S:23:DA:H5'	2.01	0.43
1:A:597:LYS:O	2:B:1082:HIS:NE2	2.51	0.43
2:B:286:ARG:HA	2:B:286:ARG:HD2	1.78	0.43
4:D:94:ARG:HG2	4:D:99:LEU:HB2	2.00	0.43
1:A:808:LYS:HA	1:A:808:LYS:HD2	1.78	0.43
2:B:748:GLN:OE1	10:J:52:THR:OG1	2.37	0.43
5:E:185:ALA:HA	5:E:190:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:225:LEU:O	15:O:227:PHE:N	2.50	0.43
1:A:321:LYS:HB3	1:A:321:LYS:HE3	1.82	0.43
2:B:934:ILE:H	2:B:934:ILE:HG12	1.64	0.43
1:A:584:ARG:NE	6:F:116:ASP:OD1	2.52	0.43
1:A:588:LEU:HD22	2:B:1087:LEU:HD22	2.00	0.43
1:A:640:ASN:OD1	1:A:640:ASN:N	2.52	0.43
1:A:1646:LEU:HD22	7:G:109:PRO:HB3	2.00	0.43
15:O:103:ASN:OD1	15:O:103:ASN:N	2.51	0.43
1:A:70:LYS:HD2	17:Q:38:ASP:HB3	2.01	0.43
3:C:161:HIS:HD2	3:C:195:LYS:HG2	1.83	0.43
16:P:250:ALA:HB2	16:P:258:SER:HB2	2.00	0.43
1:A:2:ASP:OD2	1:A:4:SER:OG	2.37	0.43
1:A:545:SER:OG	1:A:546:LEU:N	2.52	0.43
16:P:234:THR:O	16:P:234:THR:OG1	2.31	0.43
16:P:421:ILE:HA	16:P:441:ASP:HA	2.00	0.43
16:P:488:LEU:HD13	16:P:490:GLN:HE21	1.83	0.43
20:T:44:DT:H2'	20:T:45:DT:H72	2.01	0.43
1:A:1181:PRO:HD2	6:F:86:THR:HG21	2.01	0.43
6:F:108:PHE:HE2	6:F:131:PRO:HG3	1.84	0.43
15:O:528:PHE:O	15:O:532:ALA:N	2.50	0.43
17:Q:376:GLU:HA	17:Q:379:LYS:HB2	2.00	0.43
1:A:488:PRO:HA	1:A:617:HIS:CD2	2.53	0.42
2:B:975:HIS:CE1	2:B:1003:ALA:HB2	2.54	0.42
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.87	0.42
16:P:350:THR:OG1	18:R:155:GLN:O	2.37	0.42
18:R:242:ILE:HA	18:R:243:PRO:HD3	1.85	0.42
1:A:1653:SER:O	1:A:1653:SER:OG	2.37	0.42
2:B:981:SER:O	2:B:981:SER:OG	2.29	0.42
3:C:195:LYS:NZ	10:J:58:GLU:OE2	2.38	0.42
18:R:11:ARG:HD3	19:S:11:DA:H2'	2.01	0.42
1:A:462:LYS:O	1:A:465:GLY:N	2.47	0.42
1:A:1156:LYS:HB2	1:A:1156:LYS:HE3	1.74	0.42
2:B:242:ASP:OD2	2:B:414:LYS:NZ	2.41	0.42
2:B:1119:ARG:HD2	2:B:1119:ARG:HA	1.87	0.42
7:G:237:HIS:N	7:G:244:SER:O	2.48	0.42
9:I:23:VAL:HG11	9:I:28:VAL:HG23	2.00	0.42
16:P:429:SER:HG	16:P:430:ASN:H	1.67	0.42
18:R:248:LYS:NZ	18:R:298:GLN:HB3	2.35	0.42
1:A:12:THR:OG1	2:B:1201:GLU:OE1	2.27	0.42
2:B:136:LYS:HD2	2:B:138:LEU:HD21	2.01	0.42
2:B:247:THR:O	2:B:248:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:782:ASP:N	2:B:782:ASP:OD1	2.47	0.42
17:Q:225:GLN:NE2	20:T:46:DT:O3'	2.53	0.42
18:R:167:LYS:HA	18:R:167:LYS:HD2	1.79	0.42
18:R:408:ILE:HD12	18:R:435:LEU:HD22	2.02	0.42
16:P:707:ASP:N	16:P:707:ASP:OD1	2.50	0.42
18:R:4:VAL:HG22	18:R:6:ILE:HG12	2.01	0.42
1:A:913:PRO:HB3	1:A:926:GLN:HE22	1.84	0.42
2:B:565:LEU:HD23	2:B:565:LEU:HA	1.88	0.42
7:G:133:LEU:HD13	7:G:149:ILE:HD13	2.01	0.42
9:I:19:ASN:HA	9:I:20:PRO:HD3	1.94	0.42
16:P:485:LYS:HA	16:P:485:LYS:HD2	1.77	0.42
17:Q:272:GLN:O	17:Q:276:PHE:N	2.53	0.42
18:R:223:ASN:HB3	18:R:228:ASN:HB2	2.02	0.42
1:A:4:SER:HB2	1:A:573:LEU:HD13	2.02	0.42
1:A:396:ILE:O	1:A:400:ASN:N	2.51	0.42
1:A:810:LEU:HD12	1:A:810:LEU:HA	1.90	0.42
1:A:1176:ARG:HE	1:A:1176:ARG:HB3	1.69	0.42
15:O:241:ASP:HB2	15:O:381:ILE:HD11	2.00	0.42
15:O:363:THR:HA	15:O:366:THR:HG22	2.01	0.42
15:O:379:ARG:HA	15:O:382:GLN:HE22	1.85	0.42
15:O:432:LYS:HD2	15:O:609:TYR:HA	2.00	0.42
1:A:748:ASN:N	1:A:1072:ASN:OD1	2.49	0.42
2:B:598:HIS:HE1	2:B:638:PRO:HB2	1.85	0.42
11:K:134:LYS:HE2	11:K:134:LYS:HB2	1.91	0.42
16:P:448:THR:OG1	16:P:448:THR:O	2.38	0.42
17:Q:178:THR:HG21	17:Q:227:TYR:HE1	1.84	0.42
7:G:161:ASN:HB3	7:G:248:THR:HG23	2.00	0.42
11:K:122:LYS:NZ	11:K:126:ASP:OD2	2.41	0.42
16:P:621:LYS:HA	16:P:621:LYS:HD2	1.91	0.42
2:B:168:ASN:O	2:B:169:ARG:NH1	2.52	0.42
3:C:104:VAL:HG13	3:C:191:ILE:HD12	2.02	0.42
12:L:64:LEU:HA	12:L:64:LEU:HD12	1.82	0.42
13:M:46:SER:O	13:M:48:LYS:N	2.53	0.42
17:Q:3:THR:O	17:Q:3:THR:OG1	2.34	0.42
17:Q:270:THR:HG22	17:Q:313:THR:HG21	2.01	0.42
17:Q:363:SER:OG	17:Q:364:SER:N	2.53	0.42
18:R:408:ILE:HG23	18:R:435:LEU:HD22	2.01	0.42
2:B:443:LYS:HB2	2:B:443:LYS:HE2	1.84	0.41
2:B:768:GLY:N	2:B:1032:TYR:OH	2.53	0.41
2:B:1025:ASP:OD1	2:B:1025:ASP:N	2.52	0.41
16:P:49:THR:O	16:P:49:THR:OG1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:ASP:OD1	1:A:743:ASP:N	2.53	0.41
1:A:1162:ASN:HB3	1:A:1165:LYS:HG3	2.00	0.41
16:P:694:ILE:H	16:P:746:ARG:HD3	1.84	0.41
17:Q:182:ILE:HD13	17:Q:182:ILE:HA	1.90	0.41
18:R:146:SER:OG	18:R:147:GLN:N	2.50	0.41
1:A:377:VAL:HG11	17:Q:62:LEU:HB2	2.01	0.41
1:A:475:ARG:NH1	2:B:1068:GLY:O	2.53	0.41
7:G:26:ASN:HA	7:G:27:PRO:HD3	1.92	0.41
16:P:277:VAL:HA	16:P:284:VAL:HG12	2.02	0.41
16:P:317:ILE:HG22	16:P:363:ILE:HD12	2.02	0.41
16:P:650:LEU:O	16:P:758:ASN:ND2	2.53	0.41
17:Q:90:LYS:HZ3	17:Q:95:LEU:HB2	1.85	0.41
18:R:182:LYS:HA	18:R:185:LYS:HE3	2.03	0.41
3:C:326:GLU:O	3:C:330:ASN:ND2	2.54	0.41
5:E:63:ASN:OD1	5:E:77:SER:OG	2.34	0.41
6:F:106:PRO:HG2	7:G:55:GLU:HG2	2.03	0.41
10:J:42:LYS:HE2	10:J:42:LYS:HB3	1.90	0.41
13:M:96:LEU:O	13:M:98:SER:OG	2.32	0.41
16:P:596:ILE:HD12	17:Q:272:GLN:HB3	2.02	0.41
17:Q:10:CYS:HB2	17:Q:15:CYS:HB2	2.01	0.41
17:Q:237:ILE:HD13	17:Q:237:ILE:HA	1.91	0.41
17:Q:350:ARG:HG2	17:Q:354:LYS:HE2	2.01	0.41
2:B:164:MET:O	2:B:167:SER:OG	2.33	0.41
2:B:416:LYS:HA	2:B:416:LYS:HD3	1.87	0.41
2:B:1151:ILE:HD13	7:G:21:LYS:HD3	2.01	0.41
7:G:90:LEU:HD23	7:G:90:LEU:HA	1.91	0.41
13:M:83:PRO:HD3	14:N:51:GLN:HA	2.02	0.41
17:Q:90:LYS:HD2	17:Q:90:LYS:HA	1.72	0.41
18:R:435:LEU:HD23	18:R:435:LEU:HA	1.91	0.41
1:A:103:LEU:HD12	1:A:241:PRO:HD2	2.03	0.41
1:A:821:ILE:HD13	1:A:821:ILE:HA	1.94	0.41
2:B:673:ASN:HB3	2:B:686:HIS:HD2	1.85	0.41
12:L:31:CYS:SG	12:L:32:ALA:N	2.93	0.41
16:P:377:ARG:NH2	18:R:196:GLU:OE2	2.52	0.41
1:A:504:LYS:HE3	1:A:504:LYS:HB3	1.85	0.41
1:A:1042:ASP:OD1	1:A:1042:ASP:N	2.39	0.41
2:B:169:ARG:HD3	2:B:169:ARG:HA	1.86	0.41
2:B:291:GLY:HA3	2:B:375:LEU:HD13	2.03	0.41
3:C:139:LYS:HG2	3:C:201:GLU:HB3	2.03	0.41
6:F:93:ILE:HD13	6:F:93:ILE:HA	1.93	0.41
9:I:19:ASN:N	9:I:19:ASN:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:428:ILE:HB	15:O:483:ILE:HD11	2.02	0.41
17:Q:85:GLN:NE2	17:Q:88:SER:OG	2.54	0.41
3:C:80:ALA:HA	3:C:208:CYS:HA	2.01	0.41
3:C:142:ARG:NH2	10:J:67:GLU:OE2	2.54	0.41
3:C:157:TYR:HB2	3:C:160:ALA:HB2	2.02	0.41
5:E:84:ASP:N	5:E:84:ASP:OD1	2.48	0.41
15:O:451:ASN:HD22	15:O:451:ASN:HA	1.68	0.41
15:O:506:PHE:HD1	15:O:506:PHE:HA	1.76	0.41
16:P:380:MET:HB3	16:P:394:VAL:HG23	2.03	0.41
17:Q:232:LEU:HD23	17:Q:232:LEU:HA	1.94	0.41
1:A:219:LEU:O	1:A:223:PHE:N	2.49	0.41
1:A:1270:VAL:HG11	1:A:1489:VAL:HG11	2.02	0.41
2:B:341:SER:N	2:B:344:GLN:OE1	2.43	0.41
2:B:374:LEU:HD12	2:B:374:LEU:HA	1.89	0.41
4:D:27:LEU:HD23	4:D:27:LEU:HA	1.93	0.41
5:E:87:SER:HB3	5:E:115:ASN:HD22	1.84	0.41
7:G:101:SER:O	7:G:101:SER:OG	2.37	0.41
7:G:162:ILE:HD13	7:G:162:ILE:HA	1.89	0.41
16:P:592:LEU:HA	16:P:595:GLN:HB3	2.03	0.41
18:R:248:LYS:HD3	18:R:248:LYS:HA	1.84	0.41
18:R:427:PRO:HB2	18:R:429:ARG:HG2	2.03	0.41
1:A:510:PRO:HA	1:A:576:LYS:HA	2.02	0.41
1:A:519:LEU:HD23	1:A:519:LEU:HA	1.89	0.41
1:A:560:GLN:HE22	15:O:239:SER:HA	1.85	0.41
2:B:752:VAL:O	2:B:920:ARG:NH2	2.42	0.41
7:G:217:TRP:HB2	7:G:225:ILE:HD11	2.03	0.41
9:I:6:SER:O	9:I:6:SER:OG	2.32	0.41
10:J:7:CYS:SG	10:J:8:PHE:N	2.93	0.41
14:N:105:SER:HB2	14:N:132:GLN:HE21	1.85	0.41
16:P:264:ILE:HD11	16:P:303:VAL:HB	2.02	0.41
18:R:233:TYR:HB2	18:R:260:ASN:HD21	1.85	0.41
18:R:410:TYR:O	18:R:413:THR:OG1	2.30	0.41
2:B:107:PRO:HG2	2:B:133:TYR:CZ	2.55	0.40
2:B:222:PHE:HE2	2:B:233:GLY:HA3	1.86	0.40
17:Q:301:HIS:HB2	17:Q:304:LEU:HD13	2.03	0.40
17:Q:304:LEU:O	17:Q:308:SER:OG	2.34	0.40
1:A:19:LEU:HB3	1:A:24:ILE:HD11	2.02	0.40
1:A:199:ASP:OD1	1:A:199:ASP:N	2.37	0.40
2:B:66:LYS:HE3	2:B:66:LYS:HB2	1.85	0.40
15:O:90:ASP:HB3	15:O:132:THR:HG21	2.03	0.40
17:Q:348:ILE:HD13	17:Q:348:ILE:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1120:ILE:H	2:B:1120:ILE:HD12	1.87	0.40
16:P:584:ARG:HD2	16:P:584:ARG:HA	1.77	0.40
17:Q:36:GLU:HA	17:Q:37:GLY:HA2	1.82	0.40
1:A:579:ARG:NH2	1:A:585:ASP:OD1	2.51	0.40
3:C:100:ARG:NH1	3:C:192:LEU:O	2.48	0.40
8:H:102:TYR:HE2	8:H:117:SER:HB3	1.87	0.40
16:P:622:TYR:CZ	16:P:626:LEU:HD21	2.57	0.40
16:P:662:LEU:HD12	16:P:662:LEU:HA	1.89	0.40
17:Q:257:VAL:HG13	17:Q:262:LEU:HB2	2.03	0.40
17:Q:344:THR:HA	17:Q:435:GLN:HE21	1.86	0.40
17:Q:420:ASP:OD1	18:R:263:ASN:ND2	2.55	0.40
1:A:685:SER:O	1:A:685:SER:OG	2.39	0.40
1:A:1245:ASP:OD1	1:A:1245:ASP:N	2.55	0.40
2:B:1047:ARG:HE	2:B:1067:GLY:HA2	1.86	0.40
4:D:25:THR:OG1	7:G:42:PRO:O	2.36	0.40
16:P:354:PRO:HB2	18:R:28:SER:HA	2.04	0.40
16:P:403:ARG:HD3	16:P:403:ARG:HA	1.86	0.40
17:Q:229:LYS:HA	17:Q:229:LYS:HD3	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1463/1664 (88%)	1339 (92%)	120 (8%)	4 (0%)	41 75
2	B	1171/1203 (97%)	1083 (92%)	85 (7%)	3 (0%)	41 75
3	C	303/335 (90%)	281 (93%)	22 (7%)	0	100 100
4	D	54/137 (39%)	52 (96%)	2 (4%)	0	100 100
5	E	210/215 (98%)	193 (92%)	17 (8%)	0	100 100
6	F	98/155 (63%)	93 (95%)	5 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	189/326 (58%)	172 (91%)	17 (9%)	0	100	100
8	H	127/146 (87%)	115 (91%)	12 (9%)	0	100	100
9	I	71/125 (57%)	63 (89%)	8 (11%)	0	100	100
10	J	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
11	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
12	L	41/70 (59%)	35 (85%)	6 (15%)	0	100	100
13	M	103/415 (25%)	89 (86%)	14 (14%)	0	100	100
14	N	139/233 (60%)	121 (87%)	18 (13%)	0	100	100
15	O	457/627 (73%)	431 (94%)	26 (6%)	0	100	100
16	P	583/636 (92%)	515 (88%)	68 (12%)	0	100	100
17	Q	451/514 (88%)	402 (89%)	47 (10%)	2 (0%)	34	71
18	R	317/507 (62%)	273 (86%)	44 (14%)	0	100	100
All	All	5943/7520 (79%)	5414 (91%)	520 (9%)	9 (0%)	50	80

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	PRO
1	A	1028	GLU
1	A	85	CYS
2	B	1119	ARG
1	A	462	LYS
2	B	894	LYS
2	B	1120	ILE
17	Q	16	PRO
17	Q	281	ILE

5.3.2 Protein sidechains (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1304/1465 (89%)	1303 (100%)	1 (0%)	93 98
2	B	1030/1053 (98%)	1026 (100%)	4 (0%)	91 97
3	C	269/296 (91%)	267 (99%)	2 (1%)	84 93
4	D	55/116 (47%)	55 (100%)	0	100 100
5	E	194/197 (98%)	192 (99%)	2 (1%)	76 89
6	F	90/137 (66%)	90 (100%)	0	100 100
7	G	170/291 (58%)	169 (99%)	1 (1%)	86 94
8	H	115/128 (90%)	113 (98%)	2 (2%)	60 83
9	I	65/110 (59%)	65 (100%)	0	100 100
10	J	64/65 (98%)	64 (100%)	0	100 100
11	K	91/130 (70%)	90 (99%)	1 (1%)	73 88
12	L	38/57 (67%)	38 (100%)	0	100 100
13	M	95/371 (26%)	95 (100%)	0	100 100
14	N	135/220 (61%)	134 (99%)	1 (1%)	84 93
15	O	427/576 (74%)	425 (100%)	2 (0%)	88 95
16	P	551/590 (93%)	548 (100%)	3 (0%)	88 95
17	Q	430/476 (90%)	428 (100%)	2 (0%)	88 95
18	R	308/474 (65%)	305 (99%)	3 (1%)	76 89
All	All	5431/6752 (80%)	5407 (100%)	24 (0%)	91 97

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	594	THR
2	B	811	LEU
2	B	873	THR
2	B	1063	ARG
2	B	1097	ASP
3	C	131	THR
3	C	309	THR
5	E	159	ASP
5	E	180	ARG
7	G	116	THR
8	H	38	LEU

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Mol	Chain	Res	Type
8	H	58	THR
11	K	123	ASP
14	N	84	LYS
15	O	219	ARG
15	O	436	ARG
16	P	321	LYS
16	P	419	ARG
16	P	475	ARG
17	Q	64	THR
17	Q	419	LEU
18	R	10	ASN
18	R	205	VAL
18	R	359	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	A	322	ASN
1	A	610	ASN
1	A	656	GLN
1	A	767	ASN
1	A	1319	ASN
1	A	1514	ASN
1	A	1567	ASN
2	B	50	ASN
2	B	80	ASN
2	B	166	GLN
2	B	248	ASN
2	B	282	HIS
2	B	321	GLN
2	B	422	GLN
2	B	433	ASN
2	B	469	ASN
2	B	543	ASN
2	B	598	HIS
2	B	669	GLN
2	B	683	ASN
2	B	767	ASN
2	B	893	ASN
2	B	1171	ASN
2	B	1199	ASN

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Mol	Chain	Res	Type
3	C	161	HIS
3	C	207	HIS
3	C	301	ASN
3	C	323	ASN
3	C	330	ASN
4	D	81	ASN
5	E	115	ASN
7	G	59	GLN
7	G	65	HIS
8	H	52	GLN
8	H	139	ASN
14	N	52	GLN
14	N	101	GLN
15	O	94	ASN
15	O	362	ASN
15	O	422	GLN
15	O	451	ASN
16	P	348	HIS
16	P	401	ASN
16	P	487	ASN
16	P	554	ASN
16	P	571	HIS
16	P	635	ASN
17	Q	77	ASN
17	Q	85	GLN
17	Q	194	GLN
17	Q	250	GLN
17	Q	368	GLN
17	Q	389	GLN
17	Q	507	ASN
18	R	189	GLN
18	R	223	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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
16	P	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	68:THR	C	169:GLN	N	23.31
1	B	121:VAL	C	122:TYR	N	1.20

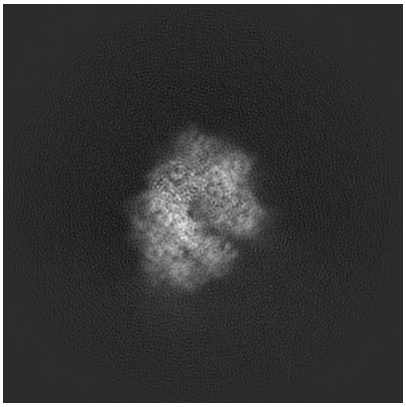
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10544. These allow visual inspection of the internal detail of the map and identification of artifacts.

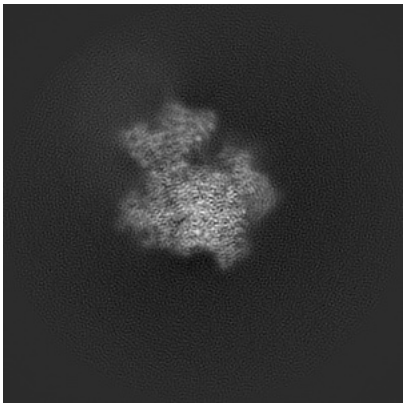
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

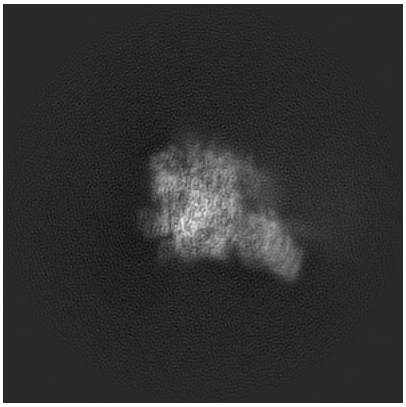
6.1.1 Primary map



X



Y

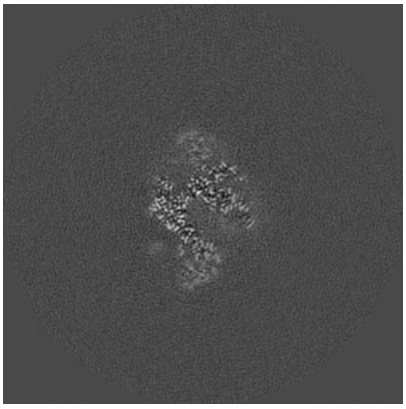


Z

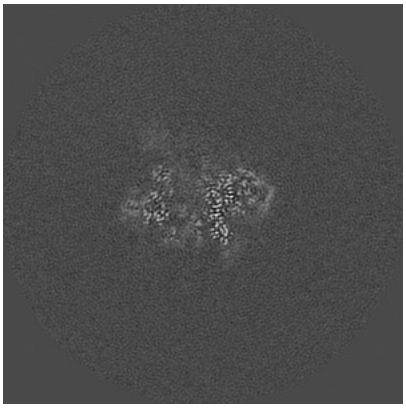
The images above show the map projected in three orthogonal directions.

6.2 Central slices

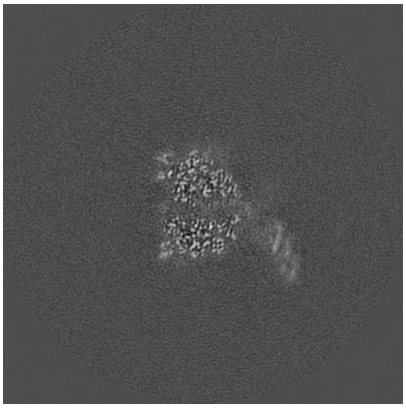
6.2.1 Primary map



X Index: 210



Y Index: 210

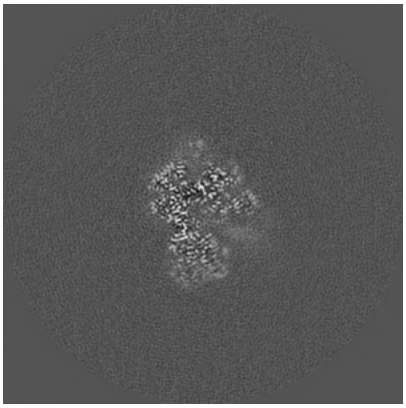


Z Index: 210

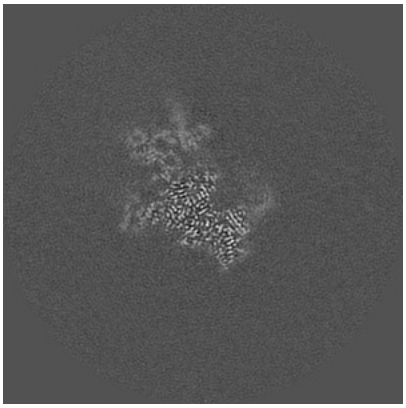
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

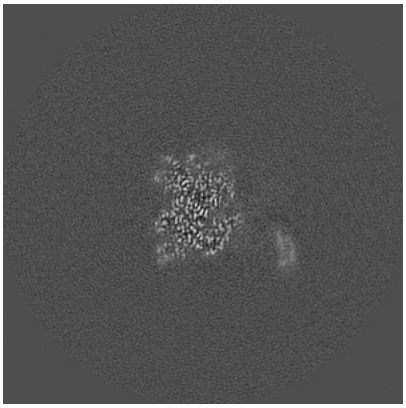
6.3.1 Primary map



X Index: 199



Y Index: 186



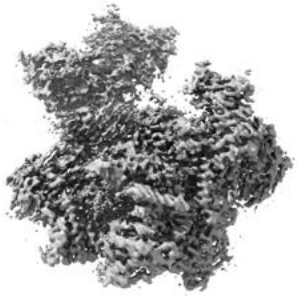
Z Index: 219

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

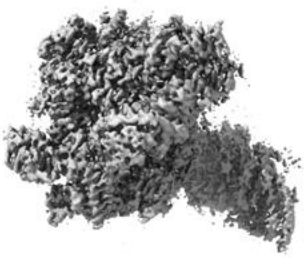
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

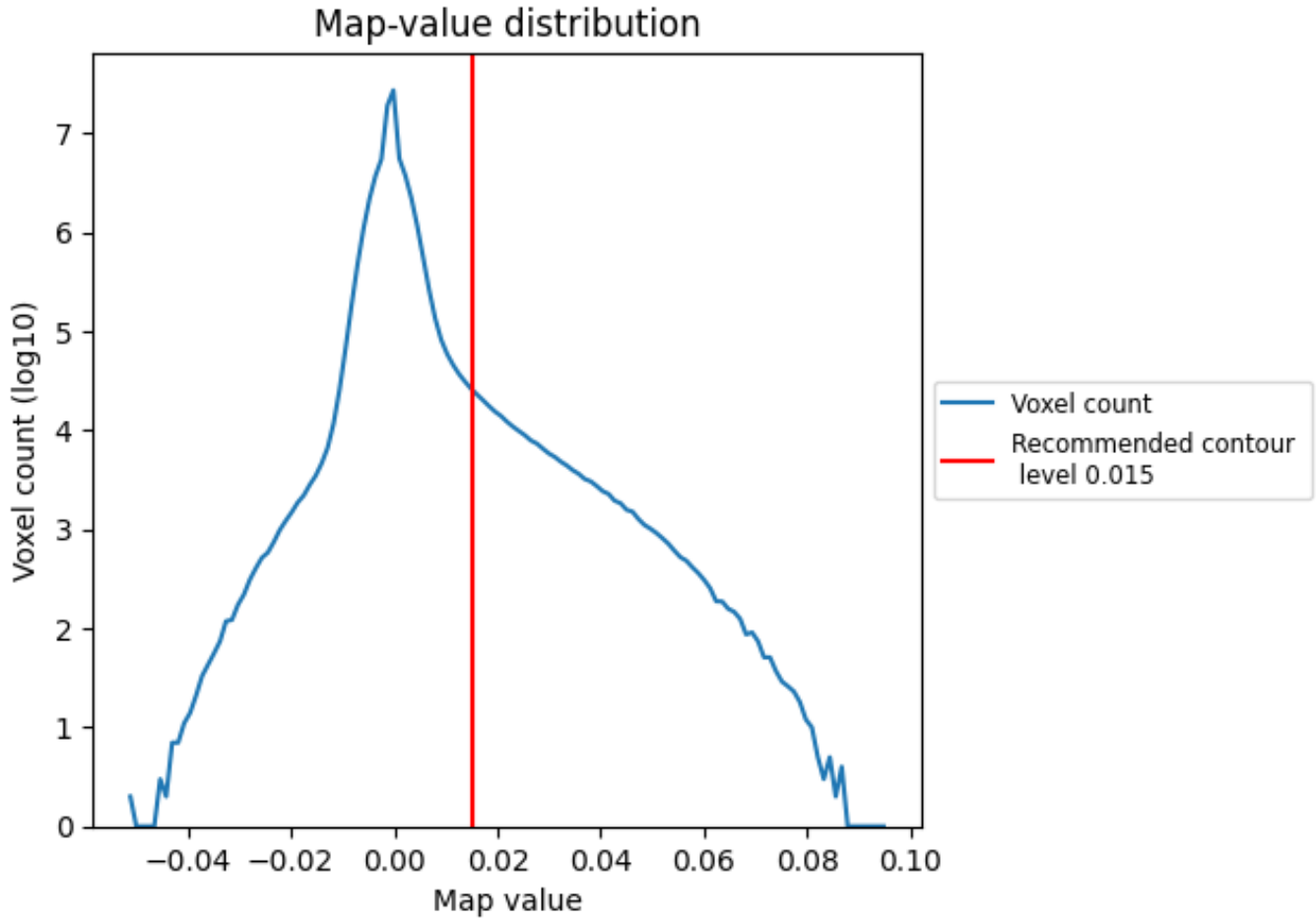
6.5 Mask visualisation (i)

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

7 Map analysis

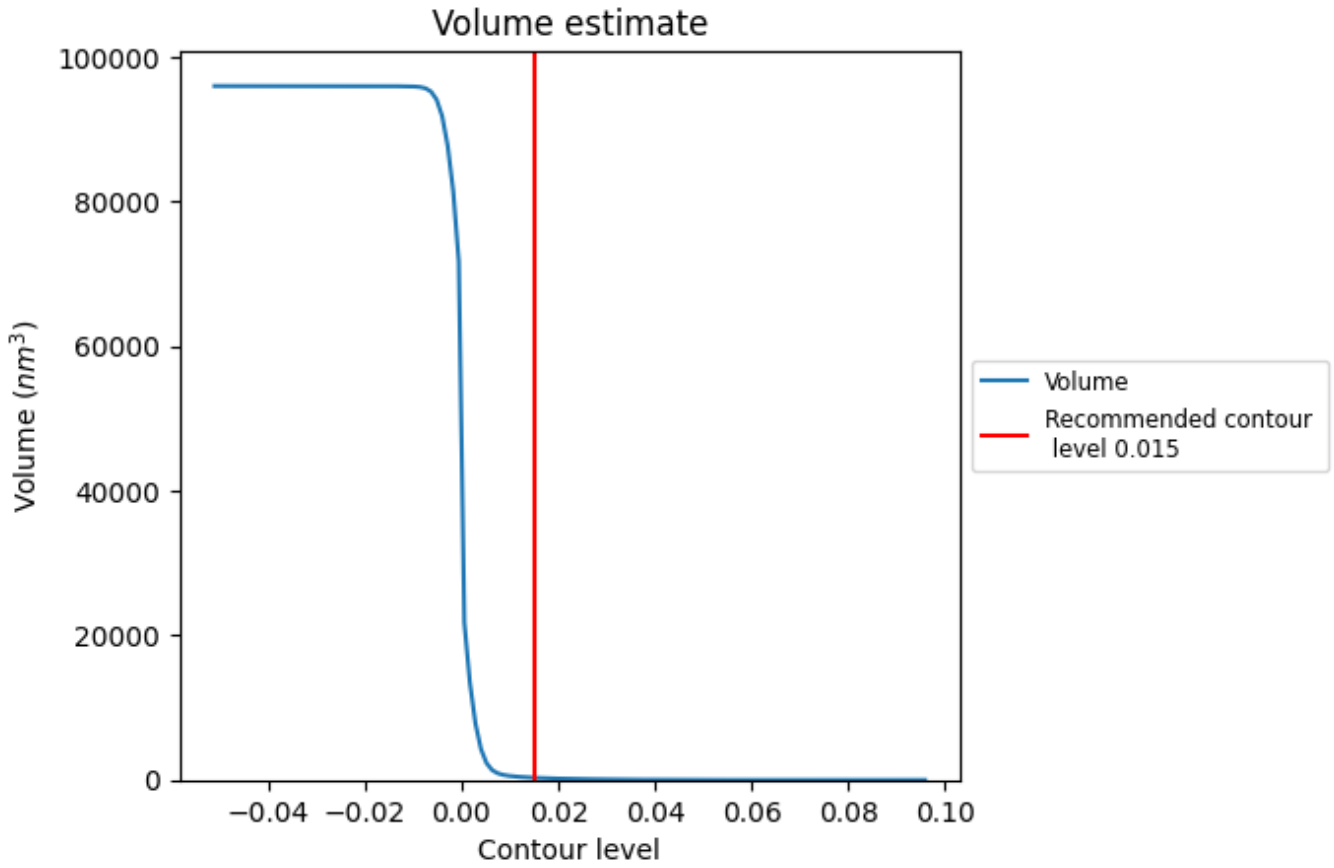
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

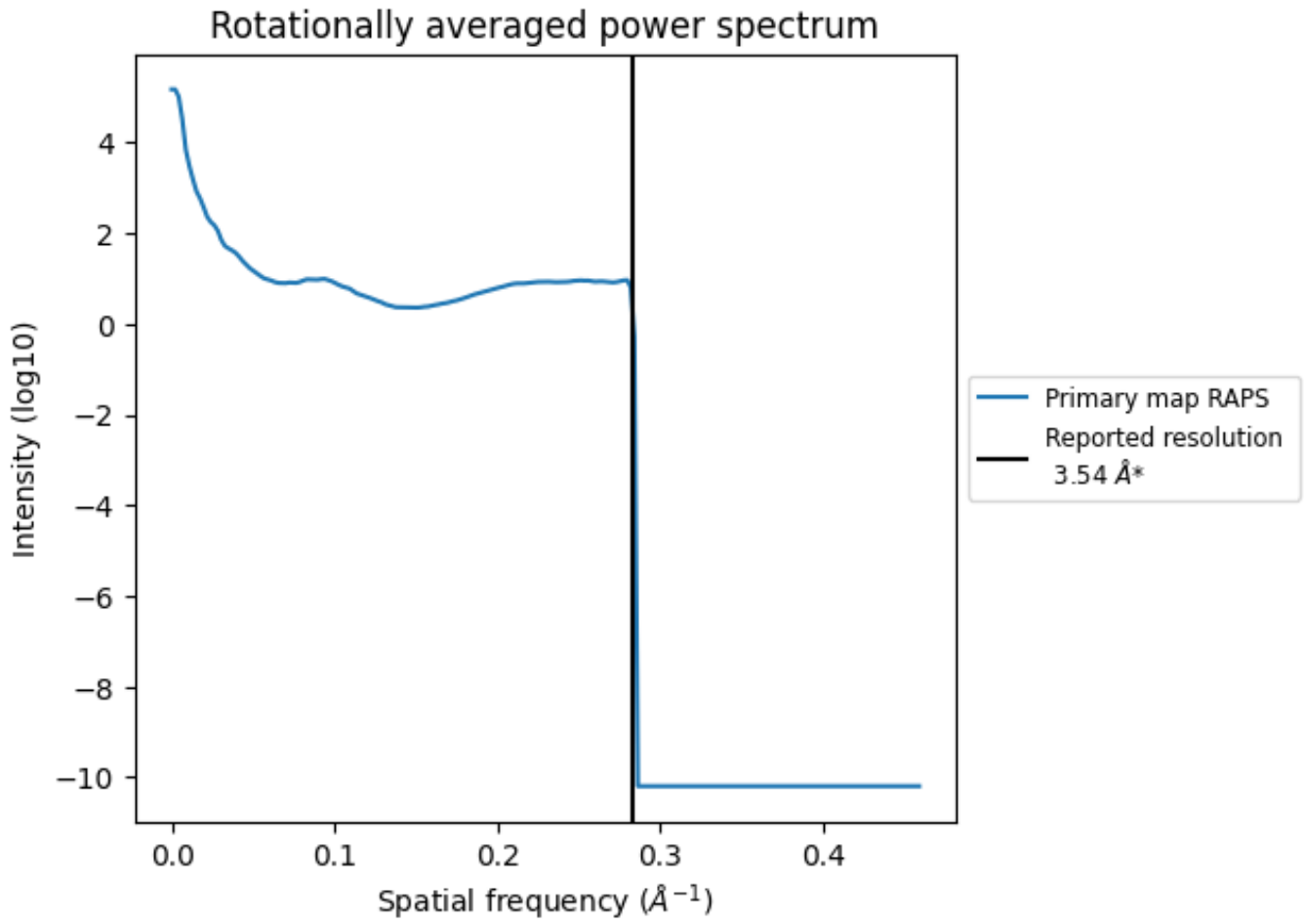
7.2 Volume estimate



The volume at the recommended contour level is 308 nm^3; this corresponds to an approximate mass of 278 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.282 Å^{-1}

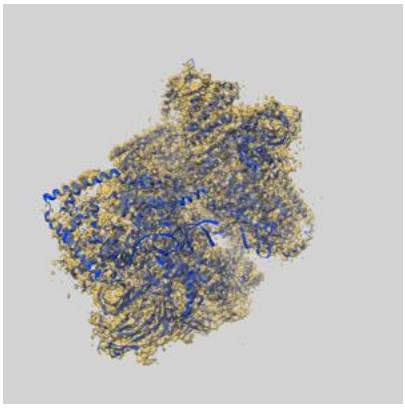
8 Fourier-Shell correlation (i)

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

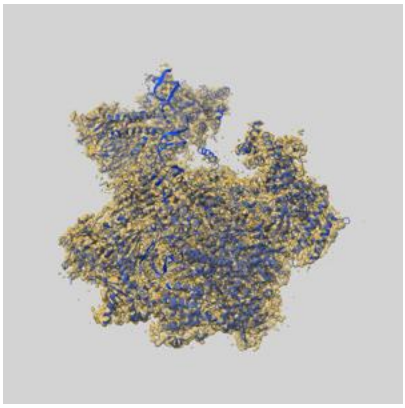
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10544 and PDB model 6TPS. Per-residue inclusion information can be found in section 3 on page 9.

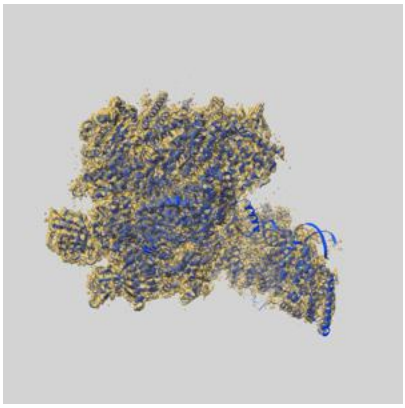
9.1 Map-model overlay



X



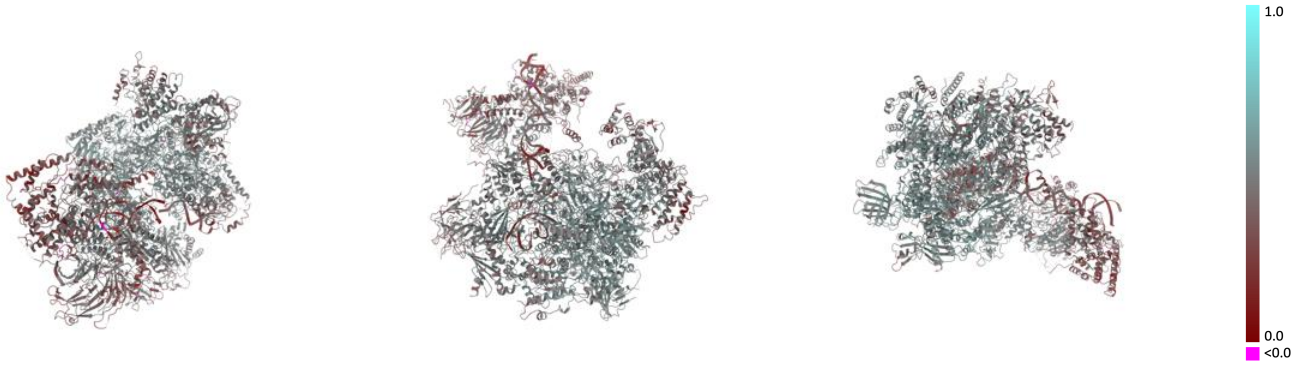
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

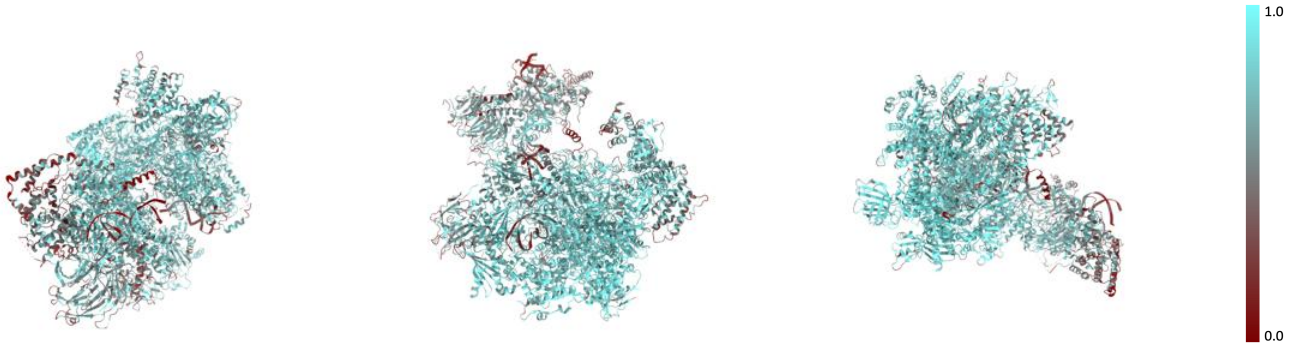
9.2 Q-score mapped to coordinate model



X Y Z

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.

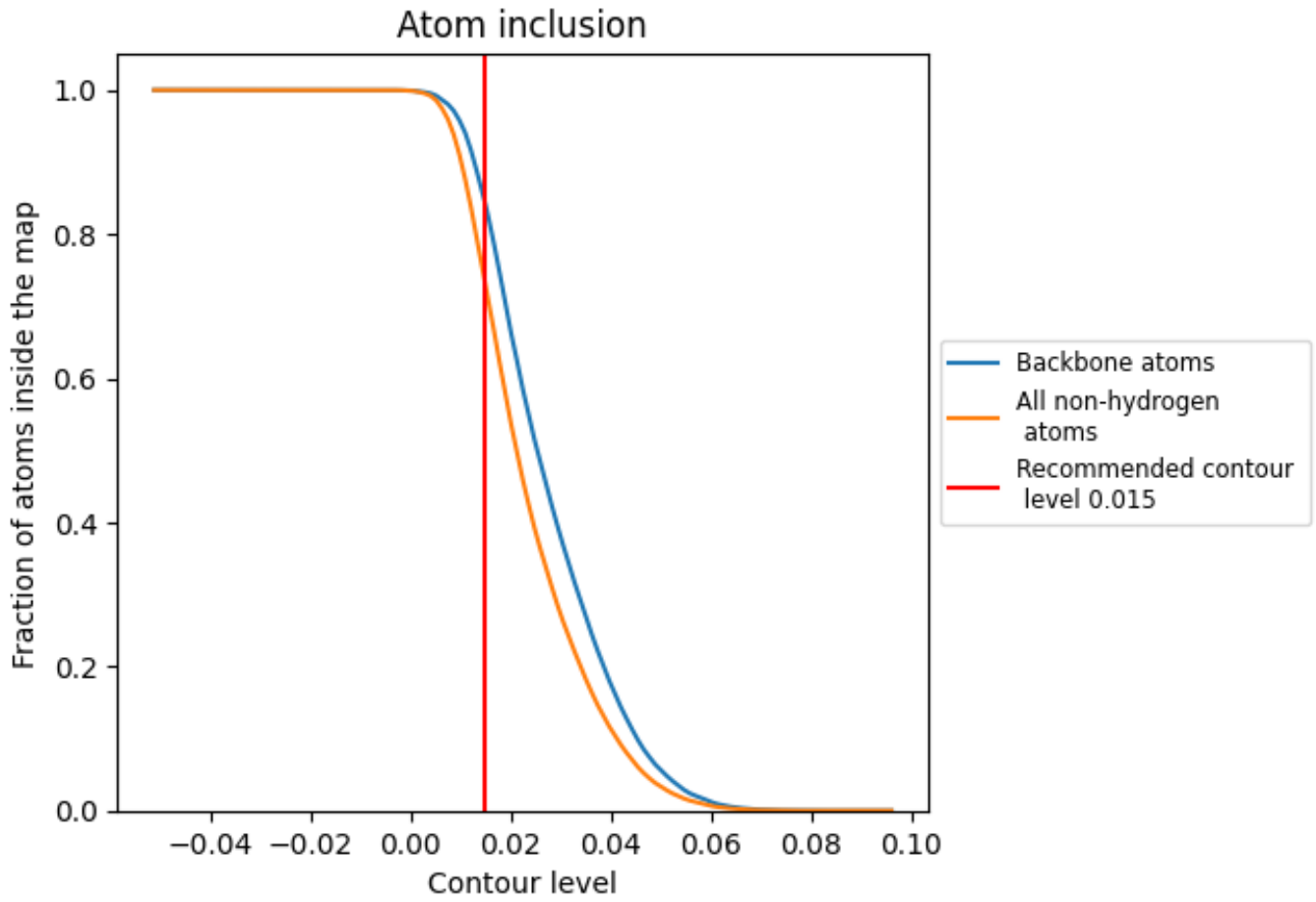
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 73% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7289	0.4700
A	0.8237	0.5190
B	0.8368	0.5300
C	0.8377	0.5240
D	0.7824	0.4860
E	0.8079	0.4930
F	0.8340	0.5350
G	0.7690	0.4810
H	0.8343	0.5230
I	0.7185	0.4400
J	0.8967	0.5470
K	0.8610	0.5260
L	0.8667	0.5250
M	0.5596	0.4260
N	0.5083	0.4250
O	0.6514	0.4250
P	0.5196	0.3670
Q	0.5633	0.3860
R	0.6714	0.4270
S	0.4392	0.2710
T	0.4267	0.2650
U	0.3068	0.2440
V	0.3246	0.2830