



Full wwPDB EM Validation Report ⓘ

Dec 19, 2023 – 08:07 pm GMT

PDB ID : 8OEV
EMDB ID : EMD-16837
Title : Structure of the mammalian Pol II-SPT6-Elongin complex, lacking ELOA latch (composite structure, structure 3)
Authors : Chen, Y.; Kokic, G.; Dienemann, C.; Dybkov, O.; Urlaub, H.; Cramer, P.
Deposited on : 2023-03-13
Resolution : 2.86 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:

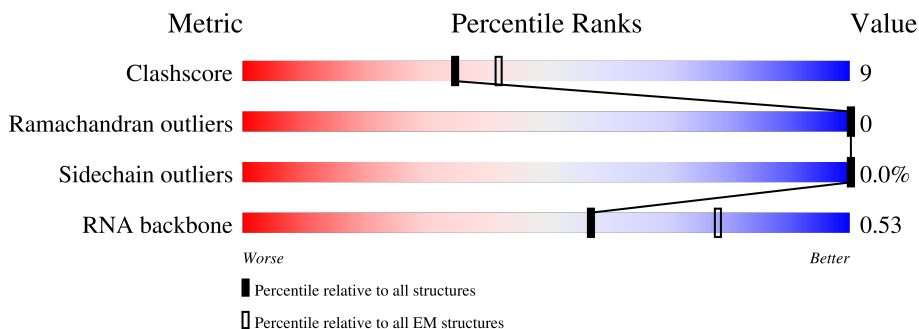
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.86 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.








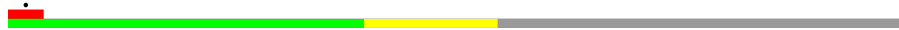




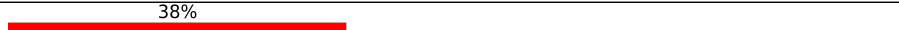

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1970	61% (green), 10% (yellow), 28% (grey)
2	B	1251	76% (green), 14% (yellow), 10% (grey)
3	C	275	79% (green), 15% (yellow), 6% (grey)
4	D	184	40% (green), 23% (yellow), 36% (grey)
5	E	210	87% (green), 12% (yellow)
6	F	127	54% (green), 7% (yellow), 39% (grey)
7	G	172	78% (green), 21% (yellow), .. (grey)

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Mol	Chain	Length	Quality of chain
8	H	150	 86% 13%
9	I	125	 80% 13% 7%
10	J	67	 87% 12%
11	K	117	 87% 11%
12	L	58	 59% 17% 24%
13	N	48	 40% 15% 46%
14	P	46	 22% 72%
15	T	48	 48% 31% 21%
16	M	801	 11% 84%
17	O	112	 29% 66% 24% 10%
18	Q	118	 38% 52% 22% 25%
19	S	1729	 31% 17% 52%

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 41781 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1409	11159	7024	2000	2064	71	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1131	9047	5721	1592	1670	64	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	258	2072	1300	356	410	6	0	0

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	118	967	608	167	188	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	78	626	401	106	114	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1347	872	218	249	8	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	116	932	577	165	179	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	66	524	339	88	91	6	0	0

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

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

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	44	367	228	69	64	6	0	0

- Molecule 13 is a DNA chain called Non-Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	N	26	549	255	117	151	26	0	0

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	P	13	280	125	54	88	13	0	0

- Molecule 15 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	T	38	769	365	130	236	38	0	0

- Molecule 16 is a protein called Elongin-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	M	128	1074	680	195	192	7	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q14241
M	-1	ASN	-	expression tag	UNP Q14241
M	0	ALA	-	expression tag	UNP Q14241

- Molecule 17 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	O	101	792	506	127	153	6	0	0

- Molecule 18 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Q	88	696	437	121	135	3	0	0

- Molecule 19 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	825	6744	4289	1168	1253	34	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	expression tag	UNP Q7KZ85
S	-1	ASN	-	expression tag	UNP Q7KZ85
S	0	ALA	-	expression tag	UNP Q7KZ85

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

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

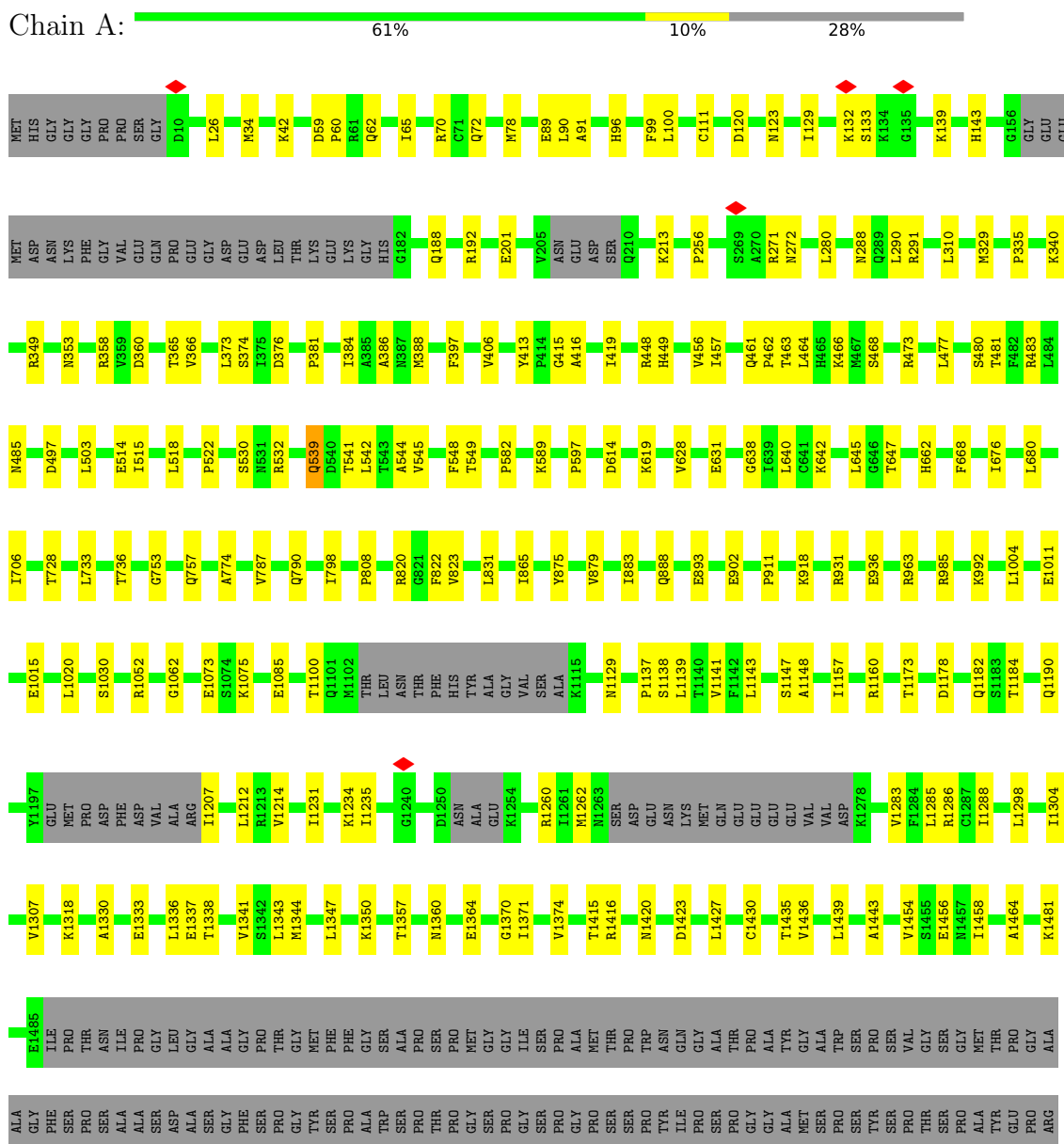
- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).


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

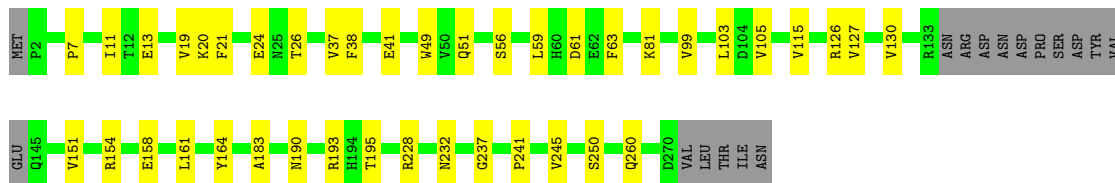
3 Residue-property plots [i](#)

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 II subunit RPB1

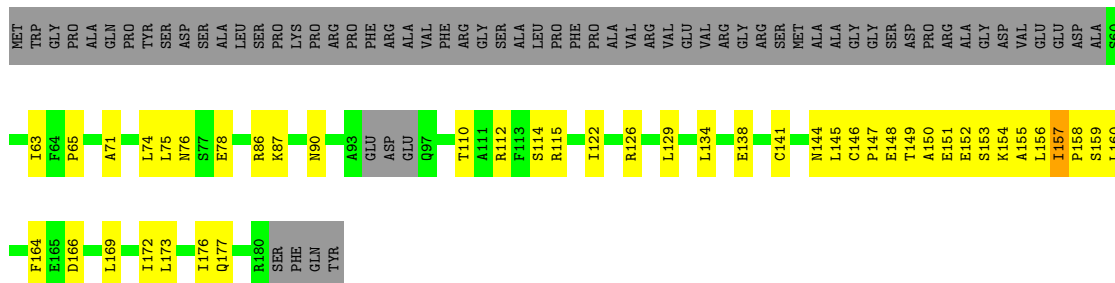


Chain C:  79% 15% 6%



• Molecule 4: RNA polymerase II subunit D

Chain D:  40% 23% 36%



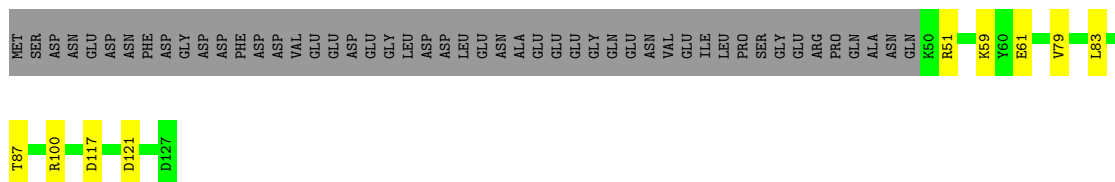
• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:  87% 12%




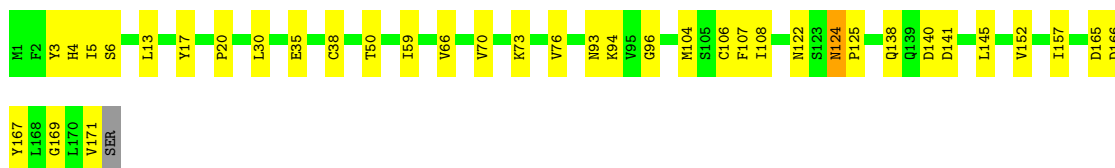
• Molecule 6: DNA-directed RNA polymerase II subunit F

Chain F:  54% 7% 39%

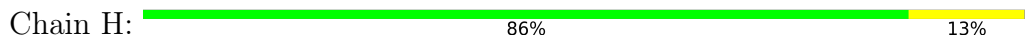


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

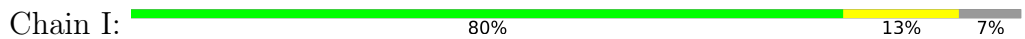
Chain G:  78% 21%



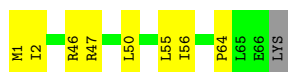
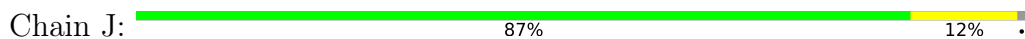
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



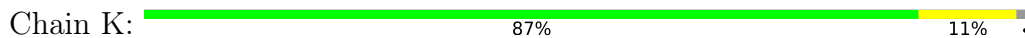
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



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



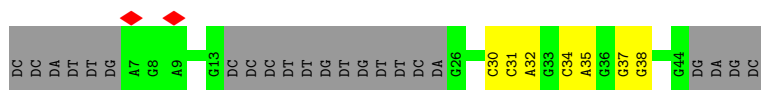
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



- Molecule 12: RNA polymerase II subunit K



- Molecule 13: Non-Template DNA



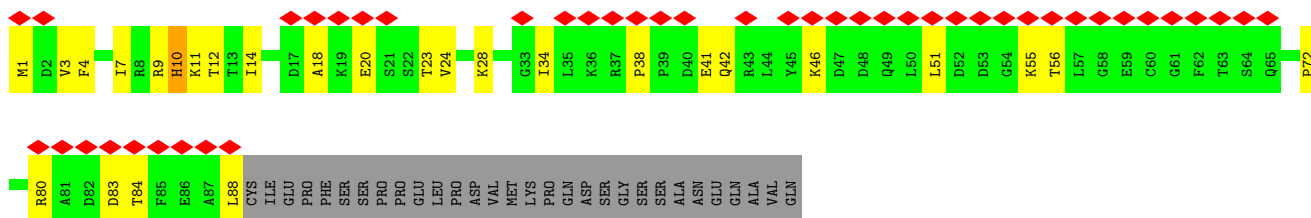
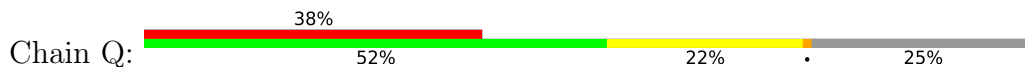
- Molecule 14: RNA



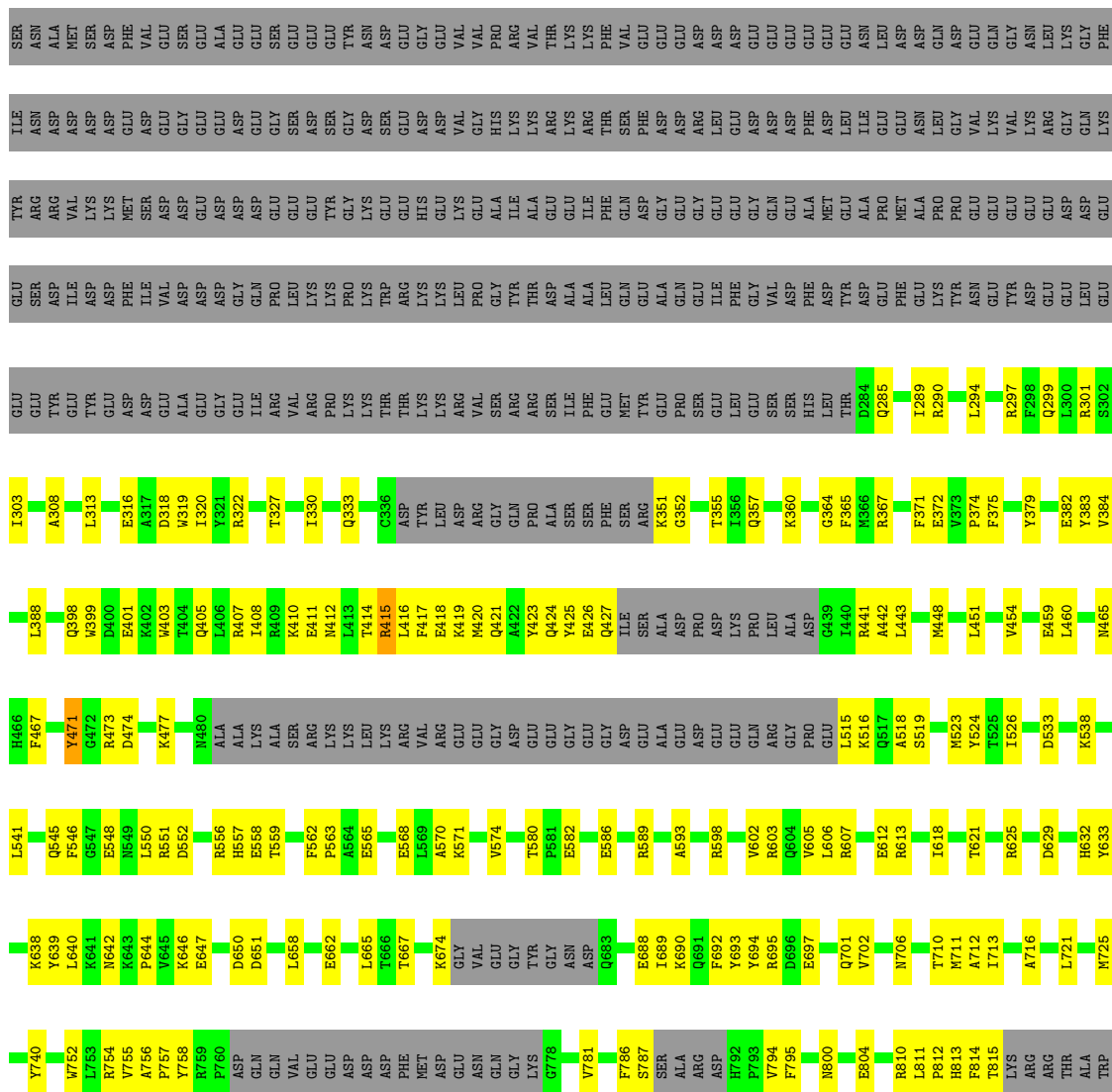
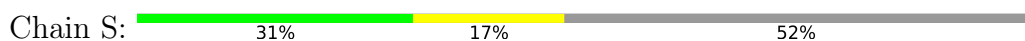
- Molecule 15: Template DNA



● Molecule 18: Elongin-B



● Molecule 19: Transcription elongation factor SPT6



ARG GLU	E924 E825	K829 I833	L836 K837	L840 V847	V848 W849	W850 A851	G852 E853	D856 A857	I861 E862	D863 V864	K865 R866	I867 V868	H869 E870	LEU GLN	GLN LEU	LEU SER	I880 G881	V882 V885	D886 N887	A890 G993	Y893 S896	S899 K1002					
P903	Y906	V909 R911	Q912 A913	S915 L916	A917 R918	R919 Q921	P923 L924	E926	V930	L938 C939	R940 K951	L954 L955	L958	Y971	N974	Y977	P980	Q983 A984	L985 I986	V989 C990	S991 L992	G993 P994	R995 H999	E1000 E1001			
I1003 L1004	N1007	L1011 L1017	M1020 C1021	G1033	K1036 S1041	LEU GLY	ASP SER	THR ASP	SER TYR	I1050 D1054	R1057 V1058	H1059 P1060	E1061 Y1062	Y1063 M1065	A1066 M1069	A1070	P980	I1074	GLU TYR	ASP GLU	SER ALA	ALA ASP	ASN ALA	E1088 L1089	E1090 E1091		
I1092 L1093	E1097 R1098	D1101 L1102	F1107 A1108	E1109 L1110	L1111 R1113	G1117 D1118	K1119 E1129	Y1134 K1135	D1136 L1137	R1138 T1139	A1140	M1145 E1148	T1149 M1152	T1157 T1160	T1167	A1175	HIS ARG	A984 L985	PRO GLU	GLN GLY	VAL GLU	VAL TYR	ASP TYR	ALA ILE	GLN SER		
ASP GLU	THR GLY	LEU GLN	TRP CYS	PRO PHE	CYS GLN	ASP ASN	ASN PHE	PRO TRP	VAL TRP	ASP GLY	HIS PHE	PHE GLY	GLN ALA	I1226 G1227	V1228	L1232	V1236	I1240 P1241	F1244 L1245	SER ASP	LYS VAL	VAL ILE	VAL PHE	VAL SER	ALA HIS	PRO GLY	
T1262 V1263	H1264 C1265	F1275 L1279	D1288	ASN MET	ASN GLU	THR PHE	LYS VAL	LEU TYR	VAL GLN	ILE PRO	ILE ARG	ARG GLU	ASN ALA	GLU SER	HIS LEU	GLN VAL	GLY ASP	ASP MET	LYS TYR	ARG GLN	MET ASN	GLY THR	ARG PHE	ILE SER	ALA MET	THR VAL	
ASN PHE	LYS GLN	ALA GLU	GLU LYS	MET MET	THR GLN	THR GLY	THR VAL	THR ALA	VAL VAL	ILE ILE	ARG PRO	GLY ASP	GLY SER	GLY SER	GLN GLY	ASP VAL	VAL LEU	THR VAL	THR GLU	ARG GLU	GLU GLY	ILE LEU	VAL GLY	GLY VAL	ASN PHE	ALA HIS	
TRP ILE	ASN SER	GLU GLU	PHE GLU	ASP ASP	ASP ASP	ASP ILE	ASP GLN	ASP PRO	ASP MET	ASP ALA	ASP ALA	ASP ARG	ASP GLY	ASP GLY	ASP TYR	ASP ARG	ASP MET	ASP PHE	ASP GLN	ASP THR	ASP MET	ASP THR	ASP ARG	ASP VAL	ASP PHE	ASP SER	
PRO TYR	PHE ILE	CYS ALA	ALA CYS	LYS PHE	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU	LEU LEU
VAL PRO	GLY THR	THR TRP	PRO SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	
ALA THR	PRO ALA	GLN TRP	ALA ALA	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	
GLN ALA	THR THR	PRO THR	THR GLN	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	ALA SER	
ARG PRO	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	SER SER	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118642	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.09	Depositor
Minimum defocus (nm)	350	Depositor
Maximum defocus (nm)	7500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	39.253	Depositor
Minimum map value	-16.528	Depositor
Average map value	0.015	Depositor
Map value standard deviation	1.086	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/11360	0.50	0/15328
2	B	0.30	0/9227	0.49	1/12454 (0.0%)
3	C	0.31	0/2115	0.47	0/2873
4	D	0.39	0/979	0.69	0/1312
5	E	0.28	0/1752	0.49	0/2366
6	F	0.29	0/636	0.51	0/859
7	G	0.33	0/1378	0.59	0/1870
8	H	0.29	0/1207	0.50	0/1628
9	I	0.28	0/954	0.49	0/1293
10	J	0.31	0/533	0.48	0/719
11	K	0.31	0/939	0.48	0/1271
12	L	0.30	0/372	0.58	0/493
13	N	0.54	0/619	0.77	0/954
14	P	0.25	0/313	0.83	0/486
15	T	0.57	0/857	0.99	0/1319
16	M	0.31	0/1098	0.58	1/1481 (0.1%)
17	O	0.33	0/810	0.63	0/1097
18	Q	0.30	0/707	0.73	1/952 (0.1%)
19	S	0.30	0/6868	0.47	0/9250
All	All	0.31	0/42724	0.53	3/58005 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	D	0	1
7	G	0	1
19	S	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	10	HIS	C-N-CA	5.99	136.66	121.70
16	M	585	LEU	CB-CG-CD1	-5.39	101.83	111.00
2	B	824	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	539	GLN	Mainchain
4	D	157	ILE	Mainchain
7	G	124	ASN	Peptide
19	S	415	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11159	0	11304	138	0
2	B	9047	0	9080	115	0
3	C	2072	0	2019	27	0
4	D	967	0	973	54	0
5	E	1721	0	1737	17	0
6	F	626	0	657	6	0
7	G	1347	0	1347	72	0
8	H	1186	0	1147	11	0
9	I	932	0	856	12	0
10	J	524	0	540	5	0
11	K	920	0	942	8	0
12	L	367	0	367	10	0
13	N	549	0	289	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	P	280	0	142	2	0
15	T	769	0	429	13	0
16	M	1074	0	1070	27	0
17	O	792	0	774	18	0
18	Q	696	0	694	15	0
19	S	6744	0	6723	266	0
20	A	1	0	0	0	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	C	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
All	All	41781	0	41090	712	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (712) 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)
7:G:171:VAL:HG22	19:S:518:ALA:CB	1.43	1.48
7:G:171:VAL:CG2	19:S:518:ALA:HB1	1.58	1.32
7:G:171:VAL:CG2	19:S:518:ALA:CB	2.07	1.32
19:S:815:THR:O	19:S:829:LYS:HD2	1.11	1.24
7:G:122:ASN:HB2	19:S:405:GLN:NE2	1.57	1.18
4:D:141:CYS:O	4:D:145:LEU:HD12	1.42	1.18
7:G:171:VAL:HG22	19:S:518:ALA:HB3	1.31	1.13
7:G:171:VAL:HG13	19:S:519:SER:O	1.51	1.08
19:S:815:THR:O	19:S:829:LYS:CD	2.00	1.07
7:G:122:ASN:CB	19:S:405:GLN:NE2	2.18	1.05
19:S:424:GLN:HE22	19:S:442:ALA:HA	1.19	1.03
7:G:171:VAL:HG22	19:S:518:ALA:HB1	1.06	0.98
4:D:152:GLU:HA	7:G:167:TYR:CE2	2.02	0.95
7:G:171:VAL:CG2	19:S:518:ALA:HB3	1.87	0.94
19:S:416:LEU:HA	19:S:419:LYS:HD2	1.47	0.93
7:G:122:ASN:HB2	19:S:405:GLN:HE22	1.18	0.93
7:G:122:ASN:CG	19:S:405:GLN:HE21	1.74	0.90
7:G:122:ASN:CG	19:S:405:GLN:NE2	2.27	0.89
7:G:122:ASN:ND2	19:S:303:ILE:CD1	2.38	0.87
4:D:75:LEU:HB3	4:D:144:ASN:OD1	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:925:ILE:HA	19:S:985:LEU:HD21	1.60	0.84
4:D:152:GLU:HA	7:G:167:TYR:CZ	2.12	0.83
19:S:420:MET:HG3	19:S:443:LEU:HD11	1.61	0.82
7:G:171:VAL:HG23	19:S:518:ALA:CB	2.07	0.82
19:S:424:GLN:NE2	19:S:442:ALA:HA	1.95	0.81
4:D:157:ILE:O	4:D:159:SER:N	2.14	0.81
19:S:415:ARG:HG2	19:S:419:LYS:HE3	1.60	0.80
7:G:167:TYR:HE1	19:S:516:LYS:HD3	1.46	0.80
19:S:1167:ILE:HD12	19:S:1232:LEU:HD11	1.62	0.80
4:D:149:THR:OG1	4:D:152:GLU:HB2	1.83	0.78
7:G:122:ASN:ND2	19:S:303:ILE:HD11	1.96	0.78
19:S:755:VAL:HG23	19:S:923:PRO:HG2	1.64	0.78
19:S:420:MET:HG2	19:S:467:PHE:HE1	1.47	0.77
19:S:414:THR:O	19:S:418:GLU:HG2	1.84	0.77
19:S:420:MET:CG	19:S:443:LEU:HD11	2.15	0.77
19:S:417:PHE:CD2	19:S:451:LEU:HD22	2.20	0.76
7:G:122:ASN:ND2	19:S:303:ILE:HD13	2.01	0.76
7:G:122:ASN:OD1	19:S:405:GLN:NE2	2.20	0.75
7:G:171:VAL:CG1	19:S:519:SER:O	2.33	0.75
19:S:414:THR:HA	19:S:451:LEU:CD2	2.16	0.75
7:G:122:ASN:O	19:S:405:GLN:NE2	2.22	0.73
19:S:586:GLU:HA	19:S:589:ARG:HE	1.54	0.73
19:S:441:ARG:NH1	19:S:471:TYR:OH	2.21	0.72
19:S:562:PHE:O	19:S:701:GLN:NE2	2.22	0.72
7:G:171:VAL:HG21	19:S:518:ALA:HB1	1.71	0.71
19:S:1228:VAL:HB	19:S:1240:ILE:HB	1.72	0.71
18:Q:7:ILE:HB	18:Q:14:ILE:HB	1.73	0.70
16:M:585:LEU:HG	16:M:606:VAL:HG21	1.74	0.70
4:D:152:GLU:O	4:D:156:LEU:HG	1.91	0.69
19:S:837:LYS:HG2	19:S:867:ILE:HG23	1.74	0.69
2:B:825:ALA:HB3	2:B:888:TYR:HB2	1.75	0.69
7:G:122:ASN:CB	19:S:405:GLN:HE21	1.97	0.69
17:O:104:LEU:O	17:O:107:ALA:HB3	1.92	0.69
19:S:1136:ASP:OD2	19:S:1138:ARG:NH2	2.24	0.69
19:S:421:GLN:HA	19:S:443:LEU:HD12	1.75	0.69
19:S:316:GLU:OE2	19:S:367:ARG:NH1	2.24	0.69
19:S:333:GLN:HE22	19:S:740:TYR:HB2	1.57	0.69
7:G:166:ASP:HB3	7:G:167:TYR:CE2	2.28	0.68
19:S:589:ARG:NH1	19:S:711:MET:SD	2.65	0.68
19:S:552:ASP:OD2	19:S:556:ARG:NE	2.26	0.68
19:S:598:ARG:HG3	19:S:598:ARG:HH11	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:GLU:HB3	3:C:20:LYS:HB2	1.75	0.68
19:S:1036:LYS:HG2	19:S:1134:TYR:CE2	2.28	0.68
19:S:593:ALA:HA	19:S:716:ALA:HB2	1.76	0.67
18:Q:9:ARG:HD3	18:Q:12:THR:OG1	1.93	0.67
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.77	0.66
8:H:95:LYS:HD3	8:H:138:ASP:HA	1.77	0.66
4:D:155:ALA:HB3	7:G:167:TYR:HE2	1.60	0.66
19:S:697:GLU:HB3	19:S:702:VAL:HG11	1.78	0.66
19:S:650:ASP:HB3	19:S:740:TYR:CZ	2.31	0.66
19:S:414:THR:HA	19:S:451:LEU:HD23	1.76	0.66
1:A:539:GLN:HA	1:A:774:ALA:HB1	1.78	0.65
19:S:1240:ILE:HG12	19:S:1279:LEU:HB2	1.77	0.65
19:S:565:GLU:HB3	19:S:568:GLU:HG2	1.78	0.65
19:S:1148:GLU:O	19:S:1152:MET:HG3	1.97	0.65
17:O:23:SER:HB2	17:O:65:ILE:HB	1.78	0.65
19:S:563:PRO:HA	19:S:701:GLN:HE22	1.61	0.65
4:D:78:GLU:HG3	4:D:122:ILE:HG21	1.78	0.64
19:S:810:ARG:HG2	19:S:812:PRO:HD3	1.79	0.64
7:G:122:ASN:O	19:S:405:GLN:CD	2.36	0.64
19:S:906:TYR:O	19:S:911:ARG:NH1	2.31	0.64
19:S:938:LEU:HD11	19:S:955:LEU:HD21	1.79	0.64
2:B:854:ASN:O	10:J:47:ARG:NH1	2.31	0.64
19:S:424:GLN:O	19:S:427:GLN:HB2	1.98	0.64
6:F:100:ARG:NH2	6:F:121:ASP:O	2.31	0.63
19:S:1054:ASP:OD1	19:S:1063:TYR:OH	2.15	0.63
7:G:122:ASN:CB	19:S:405:GLN:HE22	1.97	0.63
19:S:913:ALA:HA	19:S:916:LEU:HD12	1.79	0.63
1:A:902:GLU:OE1	1:A:985:ARG:NH2	2.31	0.63
3:C:24:GLU:HG2	3:C:228:ARG:HG3	1.81	0.63
1:A:514:GLU:O	1:A:518:LEU:HB2	1.99	0.63
19:S:695:ARG:HB3	19:S:706:ASN:HD21	1.63	0.63
19:S:580:THR:HG22	19:S:582:GLU:H	1.63	0.62
19:S:787:SER:HB2	19:S:909:VAL:HG11	1.80	0.62
19:S:318:ASP:OD1	19:S:319:TRP:N	2.32	0.62
19:S:322:ARG:O	19:S:327:THR:OG1	2.16	0.62
19:S:1265:CYS:SG	19:S:1279:LEU:HD23	2.39	0.62
16:M:586:LYS:HD3	16:M:609:ARG:HD2	1.82	0.61
19:S:352:GLY:O	19:S:355:THR:OG1	2.15	0.61
19:S:618:ILE:HD12	19:S:640:LEU:HD12	1.82	0.61
19:S:890:ALA:HB1	19:S:912:GLN:HG3	1.81	0.61
3:C:154:ARG:HD3	10:J:64:PRO:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:166:ASP:HA	4:D:169:LEU:HD12	1.83	0.61
19:S:420:MET:SD	19:S:477:LYS:HD3	2.40	0.61
1:A:728:THR:H	1:A:736:THR:HG21	1.66	0.61
7:G:122:ASN:HD21	19:S:303:ILE:HD13	1.65	0.61
16:M:619:GLU:OE1	16:M:653:ARG:NH1	2.32	0.60
8:H:98:ARG:HB3	8:H:115:TYR:HB2	1.82	0.60
1:A:1285:LEU:HA	1:A:1288:ILE:HG12	1.83	0.60
19:S:618:ILE:HG12	19:S:667:THR:HG22	1.83	0.60
19:S:1090:GLU:HA	19:S:1093:LEU:HB3	1.82	0.60
7:G:166:ASP:HB3	7:G:167:TYR:CD2	2.36	0.60
18:Q:46:LYS:HD3	18:Q:51:LEU:H	1.66	0.60
19:S:1017:LEU:O	19:S:1021:CYS:HB2	2.02	0.60
18:Q:4:PHE:HB3	18:Q:72:PRO:HB3	1.84	0.60
4:D:87:LYS:O	4:D:90:ASN:N	2.35	0.59
7:G:122:ASN:CG	19:S:303:ILE:HD11	2.22	0.59
19:S:414:THR:HA	19:S:451:LEU:HD21	1.83	0.59
19:S:853:GLU:HB2	19:S:887:ASN:HD21	1.67	0.59
1:A:59:ASP:HB3	1:A:62:GLN:HG3	1.84	0.59
19:S:420:MET:HG2	19:S:467:PHE:CE1	2.34	0.59
19:S:914:VAL:O	19:S:918:ARG:HG3	2.02	0.59
4:D:76:ASN:N	4:D:144:ASN:OD1	2.33	0.59
19:S:800:ASN:HB2	19:S:804:GLU:O	2.02	0.59
2:B:208:THR:HA	2:B:217:LEU:O	2.02	0.59
19:S:418:GLU:CD	19:S:448:MET:HE1	2.23	0.59
16:M:575:MET:SD	16:M:583:ARG:NH1	2.76	0.59
1:A:1212:LEU:HB2	1:A:1285:LEU:HD21	1.85	0.59
1:A:34:MET:HA	2:B:1215:ARG:HB2	1.85	0.59
7:G:122:ASN:OD1	19:S:405:GLN:HG2	2.03	0.59
12:L:29:LYS:HG3	12:L:32:ASP:HB2	1.85	0.59
1:A:1427:LEU:HB2	1:A:1456:GLU:HG3	1.85	0.58
5:E:82:VAL:HB	5:E:110:MET:HG2	1.83	0.58
2:B:831:PRO:HB2	2:B:850:PRO:HG2	1.85	0.58
5:E:26:TYR:HA	5:E:64:HIS:HA	1.84	0.58
2:B:834:PRO:HG2	2:B:841:MET:HE1	1.85	0.58
16:M:590:ASP:HA	16:M:617:ARG:HH22	1.67	0.58
4:D:76:ASN:O	4:D:110:THR:OG1	2.21	0.58
4:D:112:ARG:NH1	7:G:140:ASP:OD1	2.36	0.58
19:S:297:ARG:NH2	19:S:992:LEU:O	2.37	0.58
2:B:919:HIS:HB2	14:P:35:A:H61	1.68	0.58
1:A:1173:THR:H	9:I:56:ASN:HB2	1.69	0.57
18:Q:28:LYS:O	18:Q:42:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:167:TYR:O	7:G:169:GLY:N	2.38	0.57
1:A:1318:LYS:HD2	1:A:1330:ALA:HB1	1.86	0.57
4:D:152:GLU:HG3	7:G:167:TYR:CE1	2.40	0.57
7:G:122:ASN:HD21	19:S:303:ILE:CD1	2.16	0.57
1:A:544:ALA:O	1:A:548:PHE:HB2	2.05	0.57
1:A:129:ILE:HD13	1:A:143:HIS:HB3	1.87	0.57
1:A:192:ARG:NH1	1:A:201:GLU:OE2	2.37	0.57
19:S:408:ILE:O	19:S:412:ASN:ND2	2.38	0.57
19:S:424:GLN:HE22	19:S:442:ALA:CA	2.04	0.57
19:S:644:PRO:HG2	19:S:647:GLU:HB2	1.85	0.57
2:B:209:VAL:HB	2:B:217:LEU:HB3	1.87	0.57
19:S:1007:ASN:ND2	19:S:1020:MET:SD	2.78	0.57
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.87	0.56
19:S:420:MET:HG3	19:S:443:LEU:CD1	2.34	0.56
4:D:149:THR:O	4:D:152:GLU:N	2.38	0.56
1:A:1347:LEU:HB3	5:E:137:ILE:HD13	1.87	0.56
4:D:152:GLU:HG3	7:G:167:TYR:CD1	2.39	0.56
19:S:423:TYR:CD2	19:S:477:LYS:HG2	2.40	0.56
19:S:465:ASN:HD22	19:S:603:ARG:HH12	1.54	0.56
19:S:1110:GLU:HA	19:S:1113:ARG:HG2	1.87	0.56
16:M:582:ILE:O	16:M:586:LYS:HB2	2.05	0.56
19:S:829:LYS:HE3	19:S:863:ASP:OD2	2.06	0.56
19:S:548:GLU:OE1	19:S:557:HIS:NE2	2.39	0.56
19:S:786:PHE:CE1	19:S:857:ALA:HB2	2.40	0.56
1:A:1139:LEU:HD21	1:A:1343:LEU:HA	1.88	0.56
2:B:1112:ARG:NH1	2:B:1113:LYS:O	2.38	0.56
2:B:1186:GLU:HA	2:B:1190:PRO:HG3	1.86	0.56
7:G:122:ASN:HB2	19:S:405:GLN:HE21	1.56	0.56
4:D:147:PRO:O	4:D:177:GLN:NE2	2.39	0.56
19:S:1057:ARG:HG3	19:S:1134:TYR:CE1	2.40	0.56
19:S:893:TYR:CD2	19:S:915:SER:HB3	2.41	0.56
1:A:1234:LYS:NZ	1:A:1298:LEU:O	2.39	0.55
2:B:763:GLU:HG2	2:B:764:VAL:HG23	1.87	0.55
5:E:55:ARG:HA	5:E:58:LEU:HD12	1.86	0.55
7:G:6:SER:HB3	7:G:73:LYS:HD3	1.88	0.55
7:G:122:ASN:O	19:S:405:GLN:OE1	2.25	0.55
19:S:983:GLN:O	19:S:986:ILE:HG12	2.06	0.55
19:S:1098:ARG:NH2	19:S:1101:ASP:OD2	2.40	0.55
2:B:702:LEU:HD13	2:B:752:LEU:HD21	1.87	0.55
19:S:301:ARG:HD2	19:S:401:GLU:OE2	2.07	0.55
19:S:829:LYS:CE	19:S:863:ASP:OD2	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:VAL:HG13	2:B:388:ILE:HD12	1.87	0.55
2:B:421:GLN:NE2	2:B:432:ASP:OD1	2.39	0.55
5:E:64:HIS:ND1	5:E:66:ASP:OD1	2.39	0.55
19:S:971:VAL:HG11	19:S:986:ILE:HG22	1.88	0.55
2:B:578:LEU:HD12	2:B:582:LEU:HD12	1.89	0.55
18:Q:24:VAL:HG12	18:Q:55:LYS:HA	1.87	0.55
17:O:40:GLY:HA3	17:O:111:ASP:HB2	1.88	0.55
1:A:1207:ILE:N	1:A:1262:MET:SD	2.80	0.55
2:B:994:LYS:HE2	12:L:34:ILE:HD11	1.88	0.55
7:G:167:TYR:CD1	19:S:516:LYS:HB2	2.42	0.55
19:S:410:LYS:O	19:S:414:THR:HG23	2.06	0.54
19:S:1148:GLU:N	19:S:1148:GLU:OE1	2.35	0.54
2:B:351:ARG:NH2	2:B:358:ASP:OD1	2.41	0.54
3:C:59:LEU:HD12	3:C:151:VAL:HG23	1.88	0.54
2:B:211:LYS:HB2	2:B:214:GLU:HB3	1.90	0.54
2:B:375:MET:HB3	9:I:14:ILE:HG12	1.89	0.54
5:E:134:GLU:OE1	5:E:181:ARG:NH2	2.41	0.54
2:B:664:LEU:HD22	2:B:674:ILE:HD11	1.90	0.54
1:A:96:HIS:HB3	1:A:99:PHE:HB2	1.89	0.54
4:D:149:THR:OG1	4:D:152:GLU:N	2.34	0.54
2:B:171:SER:HB3	2:B:200:PRO:HG2	1.90	0.54
2:B:563:ASN:OD1	2:B:568:ARG:NH2	2.40	0.54
19:S:316:GLU:HG2	19:S:403:TRP:CD1	2.43	0.54
19:S:896:SER:HB3	19:S:899:SER:HB3	1.89	0.54
1:A:329:MET:HA	1:A:335:PRO:HA	1.90	0.54
2:B:1192:GLN:HB3	2:B:1225:LEU:HD11	1.89	0.54
13:N:34:DC:H2'	13:N:35:DA:C8	2.43	0.54
19:S:546:PHE:HZ	19:S:689:ILE:HG23	1.73	0.54
1:A:256:PRO:HD2	1:A:280:LEU:HD11	1.90	0.53
1:A:798:ILE:O	1:A:820:ARG:NH1	2.41	0.53
19:S:833:ILE:HA	19:S:836:LEU:HD12	1.89	0.53
4:D:153:SER:HB3	4:D:173:LEU:HD21	1.90	0.53
7:G:167:TYR:CE1	19:S:516:LYS:HD3	2.35	0.53
19:S:757:PRO:HB2	19:S:758:TYR:HD1	1.73	0.53
19:S:995:ARG:HG3	19:S:995:ARG:HH11	1.73	0.53
1:A:42:LYS:O	1:A:288:ASN:ND2	2.33	0.53
1:A:1160:ARG:NH2	1:A:1350:LYS:O	2.41	0.53
2:B:461:ASP:HB3	2:B:464:HIS:HB2	1.90	0.53
1:A:1030:SER:OG	5:E:162:ARG:NE	2.40	0.53
17:O:18:TYR:HB2	18:Q:34:ILE:HG21	1.91	0.53
19:S:926:GLU:O	19:S:930:VAL:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1147:SER:HB3	1:A:1157:ILE:HD11	1.91	0.53
4:D:86:ARG:NH1	7:G:35:GLU:OE2	2.37	0.53
4:D:149:THR:O	4:D:150:ALA:C	2.45	0.53
19:S:866:ARG:HG3	19:S:867:ILE:HD12	1.91	0.53
19:S:971:VAL:O	19:S:1036:LYS:N	2.42	0.53
2:B:1117:GLN:NE2	3:C:195:THR:OG1	2.34	0.53
18:Q:1:MET:N	18:Q:20:GLU:OE2	2.42	0.53
3:C:190:ASN:O	3:C:193:ARG:NH1	2.43	0.52
7:G:167:TYR:HD1	19:S:516:LYS:HB2	1.73	0.52
16:M:647:GLU:HG2	16:M:650:GLU:HG3	1.92	0.52
17:O:100:ALA:O	17:O:104:LEU:N	2.41	0.52
19:S:621:THR:O	19:S:625:ARG:N	2.42	0.52
19:S:642:ASN:HD21	19:S:674:LYS:H	1.56	0.52
1:A:120:ASP:O	1:A:123:ASN:ND2	2.43	0.52
7:G:165:ASP:OD1	7:G:166:ASP:N	2.41	0.52
11:K:42:LEU:HD23	11:K:45:ILE:HD11	1.91	0.52
12:L:17:TYR:HB2	12:L:44:MET:HE2	1.92	0.52
17:O:96:ALA:HB3	17:O:99:ILE:HG12	1.92	0.52
19:S:294:LEU:O	19:S:299:GLN:NE2	2.42	0.52
19:S:795:PHE:HB2	19:S:909:VAL:HG23	1.91	0.52
1:A:358:ARG:NH1	15:T:27:DT:OP1	2.43	0.52
2:B:300:SER:OG	2:B:427:HIS:ND1	2.33	0.52
2:B:944:ILE:HB	2:B:971:THR:HB	1.92	0.52
7:G:50:THR:HG22	7:G:73:LYS:HB2	1.92	0.52
1:A:374:SER:OG	1:A:376:ASP:OD1	2.26	0.52
4:D:157:ILE:O	4:D:160:LEU:N	2.38	0.52
19:S:559:THR:O	19:S:695:ARG:NH2	2.36	0.52
19:S:850:VAL:HG21	19:S:861:ILE:HG22	1.92	0.52
19:S:903:PHE:CE2	19:S:914:VAL:HG11	2.44	0.52
1:A:272:ASN:HB3	15:T:35:DG:H22	1.75	0.52
19:S:365:PHE:HB3	19:S:371:PHE:HB2	1.92	0.52
1:A:1129:ASN:OD1	1:A:1415:THR:OG1	2.27	0.52
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.92	0.52
17:O:105:MET:O	17:O:108:ASN:HB2	2.09	0.52
7:G:96:GLY:HA3	7:G:108:ILE:O	2.10	0.51
7:G:108:ILE:HD11	7:G:145:LEU:HD22	1.92	0.51
16:M:594:GLU:HA	16:M:622:ASN:HD21	1.75	0.51
10:J:1:MET:HA	10:J:55:LEU:HB2	1.92	0.51
16:M:577:LEU:HD11	17:O:103:LEU:HD21	1.93	0.51
1:A:1143:LEU:HD22	1:A:1157:ILE:HD13	1.91	0.51
2:B:171:SER:OG	2:B:172:LYS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:GLN:NE2	12:L:52:LEU:HD22	2.25	0.51
19:S:814:PHE:HE1	19:S:825:GLU:HB3	1.74	0.51
17:O:18:TYR:HB3	17:O:30:ILE:HD11	1.92	0.51
19:S:541:LEU:HB2	19:S:693:TYR:CE1	2.45	0.51
3:C:56:SER:HB2	3:C:158:GLU:H	1.76	0.51
7:G:152:VAL:HG22	7:G:157:ILE:HD12	1.92	0.51
3:C:19:VAL:HG12	3:C:241:PRO:HB2	1.93	0.51
19:S:1236:VAL:HG12	19:S:1275:PHE:HD2	1.76	0.51
5:E:172:ARG:NH1	5:E:210:GLN:OE1	2.43	0.51
1:A:477:LEU:HB2	1:A:483:ARG:HH21	1.76	0.51
2:B:871:VAL:HG12	2:B:1044:ILE:HG22	1.92	0.51
2:B:123:SER:HB3	2:B:474:GLY:H	1.76	0.50
2:B:470:LEU:HD22	2:B:562:LEU:HD22	1.93	0.50
18:Q:23:THR:HA	18:Q:56:THR:HA	1.92	0.50
2:B:722:GLU:HB3	2:B:725:TYR:HB2	1.93	0.50
3:C:81:LYS:HZ1	3:C:126:ARG:HH22	1.60	0.50
13:N:31:DC:H2'	13:N:32:DA:C8	2.45	0.50
16:M:690:ALA:HB1	16:M:692:VAL:HG23	1.93	0.50
17:O:35:HIS:HA	17:O:81:VAL:HG11	1.92	0.50
19:S:589:ARG:HG2	19:S:712:ALA:HB2	1.93	0.50
12:L:18:ILE:HD11	12:L:47:LYS:HD2	1.91	0.50
1:A:461:GLN:NE2	2:B:1167:GLU:OE2	2.42	0.50
2:B:1016:HIS:NE2	2:B:1060:GLU:OE1	2.34	0.50
4:D:151:GLU:OE2	4:D:155:ALA:HB2	2.11	0.50
11:K:12:LEU:HD11	11:K:18:LYS:HD3	1.93	0.50
19:S:414:THR:CA	19:S:451:LEU:HD21	2.42	0.50
1:A:911:PRO:O	1:A:963:ARG:NH2	2.40	0.50
4:D:152:GLU:HG3	7:G:167:TYR:CZ	2.47	0.50
4:D:157:ILE:O	4:D:158:PRO:C	2.50	0.50
15:T:13:DC:H2''	15:T:14:DT:H5''	1.94	0.50
1:A:466:LYS:O	2:B:1174:HIS:NE2	2.45	0.50
1:A:753:GLY:O	1:A:757:GLN:OE1	2.29	0.50
8:H:90:TYR:HB3	8:H:145:MET:HB3	1.94	0.50
11:K:40:HIS:O	11:K:44:ASN:HB2	2.11	0.50
1:A:893:GLU:OE1	5:E:197:SER:OG	2.27	0.49
2:B:924:LYS:NZ	2:B:941:ASP:OD2	2.40	0.49
19:S:421:GLN:HA	19:S:443:LEU:CD1	2.41	0.49
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.93	0.49
4:D:152:GLU:HG3	7:G:167:TYR:CG	2.46	0.49
16:M:585:LEU:HD11	16:M:592:ILE:HD11	1.93	0.49
9:I:57:LYS:HB3	9:I:60:HIS:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:ILE:HA	1:A:1374:VAL:HG12	1.94	0.49
2:B:1018:GLN:NE2	2:B:1054:THR:OG1	2.46	0.49
7:G:171:VAL:HG23	19:S:518:ALA:HB3	1.77	0.49
19:S:638:LYS:HE2	19:S:639:TYR:HE1	1.78	0.49
19:S:710:THR:HA	19:S:713:ILE:HG22	1.94	0.49
19:S:814:PHE:CE1	19:S:825:GLU:HB3	2.48	0.49
8:H:40:ILE:O	8:H:123:MET:HA	2.12	0.49
1:A:60:PRO:HB2	1:A:72:GLN:HG3	1.95	0.49
1:A:78:MET:O	2:B:1149:ARG:NH2	2.46	0.49
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.95	0.49
3:C:61:ASP:OD2	12:L:48:ARG:NH2	2.40	0.49
2:B:145:GLN:OE1	2:B:160:ARG:NH1	2.45	0.49
1:A:1458:ILE:HD13	2:B:1168:ARG:HD3	1.95	0.49
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.78	0.49
4:D:110:THR:O	4:D:114:SER:OG	2.26	0.49
19:S:556:ARG:HG2	19:S:557:HIS:CD2	2.48	0.49
19:S:598:ARG:HA	19:S:603:ARG:HH21	1.77	0.49
19:S:992:LEU:HD23	19:S:993:GLY:N	2.28	0.49
2:B:690:ARG:NH1	2:B:692:TYR:OH	2.46	0.49
1:A:65:ILE:O	1:A:271:ARG:NH2	2.46	0.49
1:A:129:ILE:O	1:A:133:SER:N	2.42	0.49
1:A:1178:ASP:HB3	1:A:1260:ARG:HH22	1.78	0.49
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.81	0.48
19:S:974:ASN:O	19:S:977:ILE:HG22	2.13	0.48
19:S:980:PRO:HA	19:S:983:GLN:HG3	1.95	0.48
2:B:1196:CYS:HB3	2:B:1199:CYS:SG	2.53	0.48
3:C:250:SER:OG	11:K:102:GLU:OE2	2.29	0.48
4:D:150:ALA:C	4:D:154:LYS:HZ3	2.16	0.48
10:J:2:ILE:HD12	10:J:56:ILE:HD13	1.95	0.48
19:S:297:ARG:NH2	19:S:989:VAL:O	2.46	0.48
19:S:840:LEU:HD12	19:S:867:ILE:HG22	1.95	0.48
19:S:849:THR:HG21	19:S:920:ILE:HG21	1.96	0.48
19:S:1112:GLU:HA	19:S:1117:GLY:HA2	1.94	0.48
16:M:578:HIS:HD2	17:O:107:ALA:HB1	1.78	0.48
19:S:786:PHE:HE1	19:S:857:ALA:HB2	1.78	0.48
1:A:373:LEU:O	1:A:485:ASN:ND2	2.45	0.48
1:A:733:LEU:HD23	9:I:107:ALA:HA	1.96	0.48
2:B:706:GLU:HB2	2:B:711:LEU:HD21	1.95	0.48
19:S:1241:PRO:HG2	19:S:1244:PHE:HB2	1.94	0.48
1:A:1020:LEU:HD21	1:A:1073:GLU:HA	1.94	0.48
2:B:137:GLU:OE2	16:M:685:ARG:NH1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:34:DT:H3'	15:T:35:DG:H3'	1.95	0.48
19:S:800:ASN:O	19:S:921:GLN:NE2	2.44	0.48
1:A:416:ALA:HA	1:A:448:ARG:HA	1.95	0.48
16:M:578:HIS:CD2	17:O:107:ALA:HB1	2.48	0.48
1:A:481:THR:H	1:A:483:ARG:HH12	1.61	0.48
1:A:132:LYS:HG2	1:A:139:LYS:HZ1	1.77	0.48
7:G:3:TYR:N	7:G:76:VAL:O	2.43	0.48
19:S:546:PHE:CZ	19:S:713:ILE:HD11	2.49	0.48
9:I:73:SER:HB2	9:I:115:THR:HA	1.94	0.48
1:A:1141:VAL:HA	1:A:1357:THR:HG23	1.96	0.48
1:A:1430:CYS:HB2	1:A:1435:THR:HG23	1.94	0.48
2:B:160:ARG:HB3	2:B:210:ILE:HB	1.96	0.48
2:B:644:ILE:HD11	2:B:654:HIS:HB2	1.95	0.48
4:D:74:LEU:HD13	7:G:4:HIS:HB2	1.95	0.48
17:O:79:TYR:OH	17:O:92:GLU:O	2.26	0.48
19:S:421:GLN:NE2	19:S:443:LEU:O	2.47	0.48
19:S:454:VAL:HG11	19:S:460:LEU:HB2	1.96	0.48
1:A:360:ASP:OD1	2:B:1139:ARG:NE	2.40	0.47
9:I:29:ASP:O	9:I:33:ARG:N	2.47	0.47
19:S:556:ARG:HG2	19:S:557:HIS:HD2	1.77	0.47
1:A:545:VAL:HG11	1:A:645:LEU:HD12	1.96	0.47
4:D:151:GLU:HG3	7:G:167:TYR:OH	2.13	0.47
4:D:149:THR:C	4:D:151:GLU:N	2.66	0.47
19:S:426:GLU:O	19:S:427:GLN:C	2.52	0.47
1:A:26:LEU:HG	2:B:1245:ALA:HB2	1.96	0.47
1:A:1173:THR:HG22	1:A:1214:VAL:HG13	1.96	0.47
1:A:1184:THR:N	1:A:1190:GLN:OE1	2.45	0.47
2:B:627:MET:HG3	2:B:644:ILE:HD12	1.96	0.47
4:D:172:ILE:O	4:D:176:ILE:HD12	2.15	0.47
7:G:93:ASN:OD1	7:G:94:LYS:N	2.47	0.47
1:A:808:PRO:HG2	2:B:752:LEU:HD12	1.96	0.47
2:B:360:ASP:O	2:B:364:HIS:ND1	2.37	0.47
4:D:153:SER:O	4:D:156:LEU:HB2	2.14	0.47
19:S:474:ASP:O	19:S:477:LYS:HE2	2.15	0.47
1:A:90:LEU:HD22	1:A:310:LEU:HD11	1.96	0.47
7:G:13:LEU:HD21	7:G:17:TYR:HB2	1.96	0.47
16:M:600:TYR:CD2	16:M:628:GLU:HB3	2.50	0.47
19:S:418:GLU:HA	19:S:448:MET:HE1	1.97	0.47
19:S:833:ILE:HG22	19:S:837:LYS:NZ	2.29	0.47
1:A:522:PRO:HB2	1:A:662:HIS:HB2	1.97	0.47
1:A:614:ASP:HA	1:A:619:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1182:GLN:O	1:A:1190:GLN:NE2	2.48	0.47
4:D:138:GLU:OE1	4:D:157:ILE:HG21	2.15	0.47
4:D:157:ILE:HB	4:D:160:LEU:HB3	1.97	0.47
6:F:79:VAL:HG11	6:F:83:LEU:HD23	1.96	0.47
7:G:124:ASN:OD1	7:G:125:PRO:HD3	2.14	0.47
19:S:425:TYR:O	19:S:426:GLU:C	2.53	0.47
4:D:150:ALA:CB	4:D:169:LEU:HB3	2.45	0.47
1:A:42:LYS:HE3	1:A:42:LYS:HB2	1.79	0.47
9:I:29:ASP:O	9:I:33:ARG:HA	2.14	0.47
16:M:605:PRO:O	16:M:608:GLU:HG3	2.14	0.47
19:S:757:PRO:HB3	19:S:921:GLN:O	2.15	0.47
4:D:154:LYS:HD3	4:D:169:LEU:CD1	2.45	0.46
4:D:156:LEU:O	4:D:158:PRO:HD3	2.15	0.46
1:A:549:THR:HG21	1:A:640:LEU:HD12	1.97	0.46
19:S:374:PRO:HG2	19:S:990:CYS:HB3	1.96	0.46
19:S:1059:HIS:ND1	19:S:1061:GLU:HG2	2.29	0.46
1:A:1231:ILE:O	1:A:1235:ILE:HG12	2.15	0.46
7:G:122:ASN:OD1	19:S:405:GLN:CD	2.54	0.46
19:S:398:GLN:HA	19:S:401:GLU:OE1	2.14	0.46
2:B:812:VAL:HG23	2:B:831:PRO:HG3	1.97	0.46
1:A:1148:ALA:HB1	1:A:1333:GLU:HB3	1.98	0.46
2:B:994:LYS:HG3	12:L:34:ILE:HD11	1.98	0.46
17:O:74:CYS:HA	17:O:77:PHE:HD2	1.81	0.46
19:S:316:GLU:HG2	19:S:403:TRP:NE1	2.31	0.46
19:S:473:ARG:HH22	19:S:524:TYR:HE1	1.62	0.46
1:A:89:GLU:O	1:A:291:ARG:NH2	2.47	0.46
8:H:96:VAL:HG22	8:H:116:VAL:HG22	1.97	0.46
3:C:260:GLN:HB2	11:K:91:ILE:HG21	1.98	0.46
19:S:297:ARG:NE	19:S:372:GLU:OE2	2.38	0.46
19:S:412:ASN:HA	19:S:415:ARG:CZ	2.46	0.46
1:A:497:ASP:HB2	2:B:1019:LYS:HG3	1.97	0.46
2:B:127:PHE:HB2	2:B:474:GLY:HA2	1.96	0.46
4:D:152:GLU:HG3	7:G:167:TYR:CD2	2.51	0.46
8:H:103:GLU:HB3	8:H:109:ALA:HB2	1.98	0.46
19:S:410:LYS:HD2	19:S:454:VAL:HB	1.98	0.46
19:S:568:GLU:HA	19:S:571:LYS:HE2	1.97	0.46
19:S:688:GLU:OE1	19:S:688:GLU:N	2.44	0.46
19:S:1002:LYS:HA	19:S:1002:LYS:HD3	1.76	0.46
2:B:177:GLU:HG2	2:B:179:ASP:H	1.81	0.46
2:B:568:ARG:HG3	2:B:599:LEU:HD12	1.98	0.46
2:B:712:LEU:HD21	2:B:717:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:VAL:HG21	3:C:127:VAL:HG21	1.98	0.46
16:M:655:MET:HG3	16:M:659:LEU:HD13	1.97	0.46
19:S:285:GLN:O	19:S:289:ILE:HG12	2.16	0.46
3:C:11:ILE:HD13	3:C:21:PHE:HB3	1.98	0.46
19:S:1119:LYS:HD3	19:S:1119:LYS:HA	1.73	0.46
1:A:70:ARG:HH12	2:B:1208:ARG:HH21	1.64	0.45
1:A:481:THR:HG22	2:B:1132:VAL:HG21	1.98	0.45
4:D:75:LEU:HD12	4:D:122:ILE:HG23	1.98	0.45
19:S:1228:VAL:HG23	19:S:1245:LEU:HD11	1.98	0.45
7:G:167:TYR:H	19:S:515:LEU:HA	1.81	0.45
19:S:1088:ALA:HA	19:S:1091:GLU:HG2	1.98	0.45
19:S:1149:ILE:HA	19:S:1152:MET:HE3	1.99	0.45
1:A:544:ALA:HB2	1:A:680:LEU:HD13	1.98	0.45
4:D:75:LEU:CB	4:D:144:ASN:OD1	2.56	0.45
16:M:608:GLU:HA	16:M:632:LEU:HD11	1.98	0.45
16:M:622:ASN:HB3	16:M:625:LEU:HD13	1.99	0.45
19:S:1258:LYS:HB2	19:S:1261:MET:HE1	1.98	0.45
1:A:133:SER:OG	1:A:139:LYS:NZ	2.43	0.45
4:D:141:CYS:C	4:D:145:LEU:HD12	2.26	0.45
4:D:146:CYS:O	4:D:148:GLU:OE2	2.34	0.45
1:A:481:THR:OG1	1:A:483:ARG:NH1	2.48	0.45
1:A:1443:ALA:HB2	2:B:1244:ILE:HG23	1.99	0.45
19:S:320:ILE:HG12	19:S:399:TRP:HB3	1.98	0.45
1:A:413:TYR:O	1:A:449:HIS:ND1	2.49	0.45
17:O:46:LEU:HD12	17:O:55:ASN:HA	1.97	0.45
18:Q:10:HIS:O	18:Q:11:LYS:HG2	2.16	0.45
19:S:633:TYR:OH	19:S:662:GLU:OE2	2.35	0.45
1:A:1439:LEU:HD13	2:B:1239:LEU:HD21	1.99	0.45
2:B:664:LEU:HB3	2:B:680:MET:SD	2.57	0.45
2:B:1065:LYS:O	2:B:1069:ASN:ND2	2.49	0.45
19:S:308:ALA:HB3	19:S:313:LEU:HD12	1.98	0.45
19:S:606:LEU:HD23	19:S:721:LEU:HD22	1.99	0.45
19:S:867:ILE:HD12	19:S:867:ILE:H	1.82	0.45
1:A:931:ARG:NE	1:A:936:GLU:OE2	2.44	0.45
2:B:569:ASP:OD1	2:B:569:ASP:N	2.44	0.45
9:I:29:ASP:O	9:I:33:ARG:CA	2.64	0.45
15:T:22:DC:H2'	15:T:23:DC:C6	2.52	0.45
16:M:629:THR:O	16:M:632:LEU:HB3	2.16	0.45
19:S:786:PHE:CE2	19:S:856:ASP:HB2	2.52	0.45
1:A:1138:SER:N	1:A:1360:ASN:OD1	2.49	0.45
1:A:1283:VAL:O	1:A:1286:ARG:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:LEU:HB3	3:C:161:LEU:HG	1.98	0.45
7:G:122:ASN:OD1	19:S:405:GLN:CG	2.65	0.45
19:S:403:TRP:NE1	19:S:407:ARG:HD2	2.32	0.45
19:S:418:GLU:OE1	19:S:448:MET:HE1	2.17	0.45
19:S:658:LEU:O	19:S:662:GLU:HG3	2.16	0.45
1:A:1085:GLU:OE2	6:F:59:LYS:NZ	2.49	0.44
4:D:152:GLU:HG3	7:G:167:TYR:CE2	2.53	0.44
19:S:411:GLU:O	19:S:414:THR:OG1	2.35	0.44
19:S:1102:LEU:HG	19:S:1107:PHE:CE2	2.52	0.44
2:B:894:GLN:HB3	2:B:995:PHE:HD1	1.81	0.44
13:N:37:DG:H2'	13:N:38:DG:C8	2.53	0.44
1:A:589:LYS:HD2	8:H:120:GLY:HA3	1.98	0.44
1:A:823:VAL:HG11	1:A:831:LEU:HD22	2.00	0.44
2:B:252:ASN:HB3	2:B:819:VAL:HG21	1.98	0.44
2:B:526:ALA:HB1	15:T:32:DT:H5''	1.99	0.44
19:S:754:ARG:O	19:S:1139:THR:OG1	2.35	0.44
19:S:1108:ALA:O	19:S:1112:GLU:HG3	2.18	0.44
4:D:134:LEU:HB3	4:D:164:PHE:HE2	1.82	0.44
6:F:51:ARG:NH1	6:F:117:ASP:O	2.51	0.44
15:T:30:DG:H2'	15:T:31:DT:C6	2.52	0.44
16:M:600:TYR:HD2	16:M:628:GLU:HB3	1.83	0.44
16:M:620:GLU:OE2	16:M:653:ARG:NH2	2.51	0.44
19:S:415:ARG:HB3	19:S:419:LYS:HZ1	1.82	0.44
19:S:690:LYS:O	19:S:694:TYR:HB2	2.17	0.44
1:A:381:PRO:HG2	1:A:384:ILE:HD12	1.98	0.44
2:B:341:LYS:NZ	2:B:403:ALA:O	2.51	0.44
1:A:406:VAL:HG11	1:A:419:ILE:HD11	2.00	0.44
4:D:78:GLU:OE1	4:D:126:ARG:NH2	2.43	0.44
5:E:15:LYS:NZ	5:E:33:LEU:O	2.47	0.44
5:E:104:ILE:HD11	5:E:127:LEU:HD23	1.99	0.44
8:H:88:PHE:CG	8:H:144:LEU:HB3	2.53	0.44
18:Q:38:PRO:HD2	18:Q:41:GLU:HG3	2.00	0.44
2:B:234:ARG:NH2	2:B:254:CYS:O	2.51	0.44
19:S:813:HIS:HE1	19:S:836:LEU:HD11	1.81	0.44
19:S:885:VAL:HG13	19:S:916:LEU:HD22	1.99	0.44
1:A:388:MET:HA	2:B:1140:ALA:HB2	1.99	0.44
2:B:146:ALA:HB3	2:B:158:PRO:HB3	1.98	0.44
12:L:26:ASN:HB2	12:L:44:MET:HE1	1.99	0.44
16:M:589:ILE:HD12	16:M:589:ILE:H	1.81	0.44
19:S:986:ILE:O	19:S:992:LEU:HD22	2.18	0.44
19:S:999:HIS:O	19:S:1003:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:1066:ALA:O	19:S:1069:MET:HB2	2.18	0.44
1:A:462:PRO:HG3	15:T:24:DG:H21	1.83	0.43
2:B:234:ARG:HH21	2:B:248:LEU:HD13	1.82	0.43
2:B:313:TRP:HB2	2:B:336:THR:HB	1.99	0.43
2:B:763:GLU:HG3	16:M:571:LEU:HG	1.99	0.43
7:G:104:MET:HG3	7:G:157:ILE:O	2.18	0.43
19:S:533:ASP:N	19:S:533:ASP:OD1	2.51	0.43
19:S:752:TRP:HZ3	19:S:940:LEU:HD23	1.83	0.43
19:S:794:VAL:HB	19:S:811:LEU:O	2.18	0.43
19:S:1145:ASN:HB3	19:S:1148:GLU:OE1	2.18	0.43
1:A:349:ARG:O	1:A:353:ASN:HB2	2.17	0.43
1:A:1137:PRO:HB2	1:A:1341:VAL:HG13	2.00	0.43
2:B:670:GLN:NE2	2:B:672:ASP:OD2	2.33	0.43
19:S:848:VAL:HG13	19:S:882:VAL:HG23	2.00	0.43
16:M:600:TYR:O	16:M:604:GLU:N	2.51	0.43
1:A:376:ASP:HB3	1:A:522:PRO:HD3	2.00	0.43
1:A:397:PHE:HB3	6:F:87:THR:HG23	2.00	0.43
1:A:413:TYR:O	1:A:415:GLY:N	2.52	0.43
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	2.00	0.43
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.53	0.43
4:D:115:ARG:HD2	4:D:146:CYS:SG	2.58	0.43
15:T:24:DG:H2'	15:T:25:DA:H8	1.84	0.43
19:S:558:GLU:HB3	19:S:695:ARG:HH22	1.83	0.43
2:B:805:MET:SD	2:B:1019:LYS:HB3	2.59	0.43
2:B:1171:GLN:HB2	2:B:1180:LEU:HD13	2.00	0.43
3:C:130:VAL:HG11	3:C:237:GLY:HA3	2.01	0.43
4:D:148:GLU:HA	4:D:177:GLN:NE2	2.34	0.43
18:Q:10:HIS:HB2	18:Q:88:LEU:H	1.83	0.43
19:S:833:ILE:O	19:S:836:LEU:HB2	2.18	0.43
2:B:1189:ASP:N	2:B:1189:ASP:OD1	2.51	0.43
11:K:61:TYR:HA	11:K:72:ILE:O	2.19	0.43
19:S:330:ILE:O	19:S:646:LYS:HA	2.18	0.43
1:A:457:ILE:HD11	1:A:515:ILE:HD12	2.00	0.43
1:A:875:TYR:OH	6:F:61:GLU:OE2	2.28	0.43
1:A:1307:VAL:HA	1:A:1337:GLU:O	2.19	0.43
2:B:176:TRP:HE1	2:B:182:PRO:HG3	1.84	0.43
2:B:169:TYR:HB2	2:B:202:TYR:HB2	2.01	0.43
2:B:791:PRO:HG2	2:B:1078:PRO:HG3	2.00	0.43
19:S:548:GLU:HA	19:S:551:ARG:HG2	2.00	0.43
19:S:1157:THR:H	19:S:1160:THR:HG1	1.66	0.43
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:86:SER:OG	17:O:87:SER:N	2.51	0.42
19:S:523:MET:HB2	19:S:526:ILE:HD12	2.00	0.42
19:S:910:LEU:O	19:S:914:VAL:HG23	2.19	0.42
2:B:175:HIS:HB2	2:B:185:MET:HB2	2.01	0.42
2:B:347:ILE:HB	2:B:385:ALA:HB3	2.01	0.42
2:B:928:ASP:OD2	12:L:17:TYR:OH	2.33	0.42
16:M:670:LEU:HD23	16:M:670:LEU:HA	1.73	0.42
19:S:333:GLN:NE2	19:S:740:TYR:HB2	2.30	0.42
19:S:550:LEU:HD23	19:S:692:PHE:HD2	1.84	0.42
19:S:1004:LEU:HD11	19:S:1011:LEU:HG	2.01	0.42
2:B:1115:THR:HA	3:C:195:THR:HA	2.01	0.42
5:E:77:PRO:HG3	5:E:90:TYR:HE2	1.83	0.42
19:S:290:ARG:NE	19:S:999:HIS:HB2	2.34	0.42
1:A:879:VAL:HB	1:A:888:GLN:HB2	2.02	0.42
4:D:155:ALA:CB	7:G:167:TYR:HE2	2.31	0.42
9:I:118:HIS:O	9:I:118:HIS:ND1	2.45	0.42
13:N:30:DC:H2'	13:N:31:DC:C6	2.54	0.42
18:Q:80:ARG:HG2	18:Q:83:ASP:HB2	2.01	0.42
19:S:541:LEU:HB2	19:S:693:TYR:HE1	1.83	0.42
19:S:1107:PHE:O	19:S:1111:LEU:HG	2.19	0.42
2:B:1032:PRO:HB2	2:B:1105:LEU:HD23	2.01	0.42
2:B:1139:ARG:NH1	2:B:1158:ASP:O	2.52	0.42
19:S:721:LEU:O	19:S:725:MET:HG2	2.20	0.42
1:A:464:LEU:HD13	1:A:1100:THR:HG21	2.00	0.42
1:A:1011:GLU:O	1:A:1015:GLU:HG2	2.19	0.42
2:B:194:ASN:HA	2:B:266:GLY:HA3	2.01	0.42
9:I:65:LEU:HD23	9:I:68:ILE:HD12	2.02	0.42
19:S:550:LEU:HB3	19:S:605:VAL:HG11	2.01	0.42
19:S:607:ARG:HB2	19:S:725:MET:HE1	2.01	0.42
19:S:756:ALA:HB3	19:S:1140:ALA:HA	2.02	0.42
2:B:629:ASN:HB2	2:B:632:GLU:HG2	2.02	0.42
9:I:91:HIS:CG	9:I:116:ALA:HB2	2.55	0.42
19:S:375:PHE:CE1	19:S:379:TYR:HD2	2.38	0.42
19:S:550:LEU:HD12	19:S:602:VAL:HG13	2.01	0.42
19:S:1057:ARG:H	19:S:1129:GLU:CD	2.22	0.42
1:A:192:ARG:HH22	1:A:213:LYS:HZ1	1.68	0.42
2:B:897:LYS:HB3	2:B:897:LYS:HE2	1.94	0.42
5:E:9:ARG:O	5:E:13:ILE:HG12	2.20	0.42
19:S:414:THR:N	19:S:451:LEU:HD21	2.34	0.42
19:S:570:ALA:O	19:S:574:VAL:HG13	2.19	0.42
1:A:883:ILE:HD13	1:A:1423:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:SER:HB3	2:B:269:LYS:HE2	2.01	0.42
2:B:1197:ASN:HB2	2:B:1222:GLN:HB3	2.00	0.42
4:D:129:LEU:HD12	4:D:134:LEU:HD21	2.01	0.42
4:D:138:GLU:HA	4:D:141:CYS:SG	2.60	0.42
5:E:192:LYS:HE3	5:E:194:ILE:HD11	2.00	0.42
17:O:32:LYS:HE2	17:O:32:LYS:HB2	1.96	0.42
1:A:376:ASP:OD2	1:A:473:ARG:NE	2.48	0.42
1:A:542:LEU:HD23	1:A:774:ALA:HA	2.01	0.42
1:A:918:LYS:O	1:A:1052:ARG:NH1	2.53	0.42
1:A:1416:ARG:O	1:A:1420:ASN:HB2	2.20	0.42
9:I:17:CYS:SG	9:I:18:GLN:N	2.93	0.42
17:O:39:SER:HB3	17:O:42:ILE:HB	2.02	0.42
19:S:1070:ALA:HB1	19:S:1088:ALA:HB1	2.02	0.42
1:A:541:THR:HG23	1:A:676:ILE:HB	2.02	0.41
2:B:893:GLU:OE1	2:B:971:THR:OG1	2.37	0.41
3:C:59:LEU:HD13	3:C:63:PHE:CE1	2.55	0.41
18:Q:80:ARG:HB3	18:Q:84:THR:O	2.20	0.41
19:S:612:GLU:HG3	19:S:613:ARG:N	2.35	0.41
1:A:132:LYS:HB3	1:A:132:LYS:HE2	1.80	0.41
1:A:456:VAL:HG11	1:A:503:LEU:HD21	2.01	0.41
1:A:831:LEU:H	2:B:792:ASP:HB2	1.85	0.41
2:B:438:LYS:HB2	2:B:438:LYS:HE2	1.76	0.41
2:B:458:GLU:OE1	2:B:458:GLU:N	2.50	0.41
19:S:851:ALA:HB2	19:S:916:LEU:CD1	2.50	0.41
19:S:951:LYS:O	19:S:955:LEU:HD23	2.20	0.41
1:A:340:LYS:HD2	1:A:1436:VAL:HG11	2.02	0.41
2:B:371:ASP:OD2	2:B:456:ARG:NH1	2.42	0.41
2:B:703:LEU:HG	2:B:775:ILE:HG12	2.01	0.41
19:S:308:ALA:HB1	19:S:313:LEU:HB2	2.02	0.41
19:S:781:VAL:HG13	19:S:847:VAL:O	2.20	0.41
1:A:91:ALA:HB3	1:A:290:LEU:HD22	2.02	0.41
1:A:91:ALA:HB2	1:A:291:ARG:HE	1.85	0.41
1:A:365:THR:OG1	1:A:366:VAL:N	2.53	0.41
1:A:1075:LYS:HD3	1:A:1075:LYS:HA	1.87	0.41
2:B:918:ARG:O	14:P:35:A:N6	2.53	0.41
3:C:7:PRO:HB3	3:C:26:THR:HB	2.02	0.41
10:J:46:ARG:O	10:J:50:LEU:HB2	2.20	0.41
15:T:36:DC:H6	15:T:36:DC:H2'	1.71	0.41
19:S:618:ILE:HG21	19:S:665:LEU:HD13	2.02	0.41
19:S:1263:VAL:HG13	19:S:1265:CYS:SG	2.61	0.41
1:A:100:LEU:HD12	1:A:100:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:THR:HG23	1:A:468:SER:HB2	2.02	0.41
1:A:1357:THR:O	5:E:142:HIS:NE2	2.41	0.41
3:C:38:PHE:CE1	3:C:245:VAL:HA	2.55	0.41
19:S:379:TYR:OH	19:S:1033:GLY:O	2.38	0.41
19:S:650:ASP:HB3	19:S:740:TYR:CE2	2.55	0.41
19:S:954:LEU:O	19:S:958:LEU:HG	2.20	0.41
1:A:1344:MET:HE2	5:E:134:GLU:HA	2.02	0.41
2:B:226:ILE:HG22	2:B:512:ILE:HG21	2.03	0.41
2:B:551:THR:OG1	2:B:809:ALA:O	2.30	0.41
2:B:810:MET:SD	2:B:826:HIS:ND1	2.94	0.41
2:B:823:THR:HG21	15:T:30:DG:H5''	2.03	0.41
19:S:313:LEU:HD11	19:S:364:GLY:HA2	2.01	0.41
19:S:586:GLU:HB2	19:S:589:ARG:HH21	1.85	0.41
1:A:532:ARG:HD2	1:A:647:THR:O	2.20	0.41
1:A:865:ILE:HD12	2:B:1169:ASP:HB3	2.03	0.41
2:B:346:ILE:HD11	2:B:442:LEU:HD11	2.02	0.41
3:C:37:VAL:HG13	3:C:41:GLU:HB2	2.03	0.41
7:G:59:ILE:HG12	7:G:66:VAL:HG22	2.02	0.41
18:Q:3:VAL:HG12	18:Q:18:ALA:H	1.85	0.41
1:A:386:ALA:HB2	1:A:413:TYR:HD1	1.84	0.41
2:B:623:GLU:OE2	2:B:629:ASN:ND2	2.47	0.41
7:G:138:GLN:N	7:G:141:ASP:OD2	2.54	0.41
15:T:24:DG:H2''	15:T:25:DA:C8	2.56	0.41
19:S:629:ASP:OD1	19:S:632:HIS:N	2.44	0.41
19:S:651:ASP:HB3	19:S:740:TYR:CD2	2.56	0.41
1:A:381:PRO:HB3	1:A:480:SER:HA	2.03	0.41
1:A:631:GLU:HG2	1:A:992:LYS:HD2	2.02	0.41
1:A:1304:ILE:HG23	1:A:1338:THR:HB	2.03	0.41
2:B:699:CYS:HA	2:B:743:ASP:HA	2.03	0.41
4:D:71:ALA:HB2	7:G:5:ILE:HD13	2.02	0.41
11:K:9:SER:HA	11:K:69:HIS:CG	2.55	0.41
11:K:41:THR:O	11:K:45:ILE:HG12	2.21	0.41
15:T:41:DC:H2''	15:T:42:DT:H5''	2.03	0.41
19:S:357:GLN:O	19:S:360:LYS:HB3	2.21	0.41
19:S:829:LYS:NZ	19:S:863:ASP:OD2	2.54	0.41
19:S:864:VAL:HA	19:S:867:ILE:HD13	2.03	0.41
19:S:1098:ARG:HB2	19:S:1101:ASP:HB2	2.03	0.41
1:A:530:SER:HB2	1:A:532:ARG:HG2	2.03	0.41
1:A:706:ILE:HD13	1:A:706:ILE:HA	1.91	0.41
1:A:1370:GLY:HA2	5:E:178:PRO:HD2	2.02	0.41
2:B:190:ALA:HA	2:B:195:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:63:ILE:HG13	4:D:65:PRO:HD2	2.03	0.41
7:G:106:CYS:SG	7:G:107:PHE:N	2.94	0.41
19:S:351:LYS:HA	19:S:351:LYS:HD2	1.87	0.41
19:S:384:VAL:HB	19:S:388:LEU:HB2	2.03	0.41
19:S:1232:LEU:HB2	19:S:1236:VAL:HG22	2.03	0.41
1:A:597:PRO:HD3	1:A:668:PHE:CD1	2.56	0.40
1:A:790:GLN:HA	1:A:822:PHE:HA	2.01	0.40
2:B:301:CYS:HB2	2:B:309:THR:HG22	2.03	0.40
7:G:30:LEU:HD22	7:G:70:VAL:HG11	2.03	0.40
19:S:319:TRP:CZ3	19:S:403:TRP:HB2	2.56	0.40
19:S:538:LYS:HD3	19:S:538:LYS:HA	1.76	0.40
1:A:642:LYS:HE2	1:A:642:LYS:HB3	1.84	0.40
2:B:162:LEU:HB3	2:B:208:THR:OG1	2.21	0.40
3:C:51:GLN:HE21	12:L:52:LEU:HD22	1.86	0.40
19:S:382:GLU:HG2	19:S:383:TYR:CD1	2.56	0.40
19:S:411:GLU:C	19:S:411:GLU:CD	2.79	0.40
19:S:454:VAL:HG22	19:S:459:GLU:HG2	2.02	0.40
19:S:865:LYS:O	19:S:868:VAL:HB	2.21	0.40
19:S:1097:GLU:HG2	19:S:1098:ARG:N	2.36	0.40
1:A:706:ILE:HD11	1:A:787:VAL:HG21	2.02	0.40
1:A:1343:LEU:N	1:A:1364:GLU:OE2	2.54	0.40
2:B:916:GLY:O	2:B:918:ARG:NH2	2.53	0.40
16:M:612:PRO:HB3	16:M:633:TRP:HZ3	1.86	0.40
19:S:851:ALA:HB2	19:S:916:LEU:HD11	2.03	0.40
2:B:950:LEU:HD23	2:B:950:LEU:HA	1.97	0.40
19:S:301:ARG:HH21	19:S:303:ILE:HB	1.86	0.40
19:S:1057:ARG:HG3	19:S:1134:TYR:HE1	1.83	0.40
1:A:1454:VAL:HG13	1:A:1464:ALA:HB1	2.04	0.40
1:A:1481:LYS:HA	7:G:20:PRO:HA	2.03	0.40
2:B:127:PHE:HA	2:B:131:SER:HB2	2.03	0.40
2:B:860:ALA:O	2:B:866:ASN:ND2	2.54	0.40
7:G:38:CYS:HB3	7:G:157:ILE:HG12	2.04	0.40
8:H:111:ARG:HD2	8:H:127:GLY:O	2.21	0.40
19:S:545:GLN:HG2	19:S:557:HIS:ND1	2.37	0.40
19:S:995:ARG:HG3	19:S:995:ARG:NH1	2.36	0.40
19:S:1062:THR:HA	19:S:1065:TRP:CE3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1395/1970 (71%)	1365 (98%)	30 (2%)	0	100	100
2	B	1123/1251 (90%)	1088 (97%)	35 (3%)	0	100	100
3	C	254/275 (92%)	247 (97%)	7 (3%)	0	100	100
4	D	114/184 (62%)	106 (93%)	8 (7%)	0	100	100
5	E	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
6	F	76/127 (60%)	76 (100%)	0	0	100	100
7	G	169/172 (98%)	156 (92%)	13 (8%)	0	100	100
8	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
9	I	114/125 (91%)	111 (97%)	3 (3%)	0	100	100
10	J	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
16	M	126/801 (16%)	119 (94%)	7 (6%)	0	100	100
17	O	99/112 (88%)	90 (91%)	9 (9%)	0	100	100
18	Q	86/118 (73%)	73 (85%)	13 (15%)	0	100	100
19	S	799/1729 (46%)	770 (96%)	29 (4%)	0	100	100
All	All	4927/7466 (66%)	4757 (96%)	170 (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	A	1239/1749 (71%)	1239 (100%)	0	100	100
2	B	991/1084 (91%)	991 (100%)	0	100	100
3	C	235/252 (93%)	235 (100%)	0	100	100
4	D	109/160 (68%)	109 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	68 (100%)	0	100	100
7	G	151/153 (99%)	151 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	102/112 (91%)	102 (100%)	0	100	100
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	40/55 (73%)	40 (100%)	0	100	100
16	M	118/706 (17%)	118 (100%)	0	100	100
17	O	88/96 (92%)	88 (100%)	0	100	100
18	Q	75/103 (73%)	75 (100%)	0	100	100
19	S	731/1524 (48%)	730 (100%)	1 (0%)	93	98
All	All	4426/6590 (67%)	4425 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	S	471	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	538	GLN
11	K	89	ASN
12	L	26	ASN
19	S	405	GLN
19	S	465	ASN
19	S	701	GLN
19	S	813	HIS
19	S	887	ASN
19	S	1007	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	12/46 (26%)	3 (25%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	35	A
14	P	36	G
14	P	37	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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

There are no chain breaks in this entry.

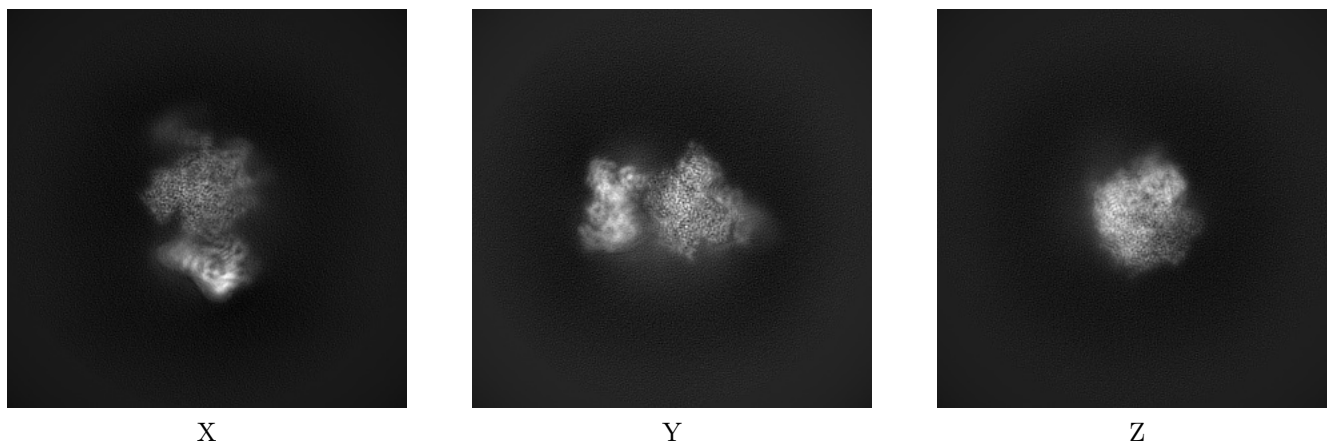
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16837. 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](#)

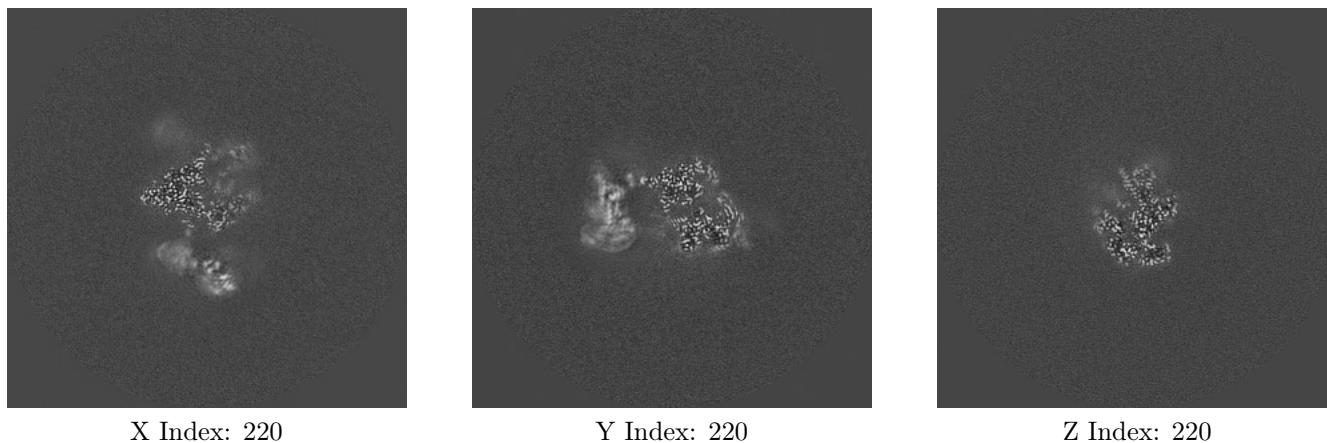
6.1.1 Primary map



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

6.2 Central slices [i](#)

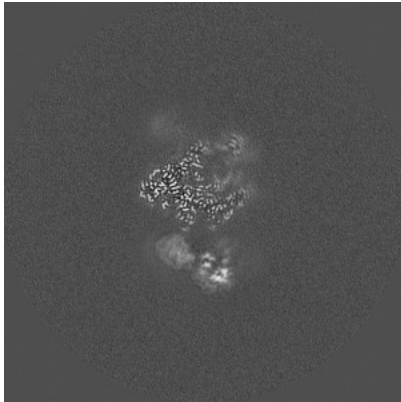
6.2.1 Primary map



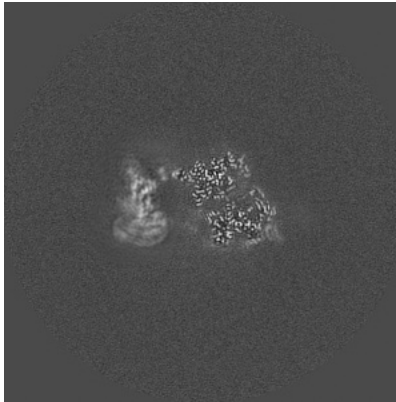
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

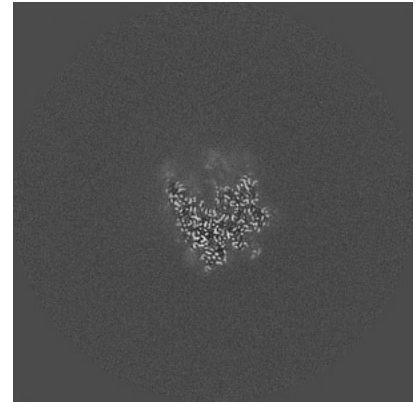
6.3.1 Primary map



X Index: 223



Y Index: 219

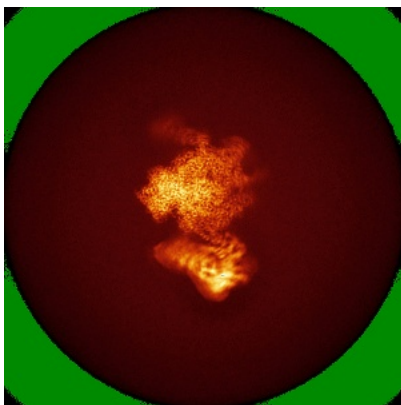


Z Index: 235

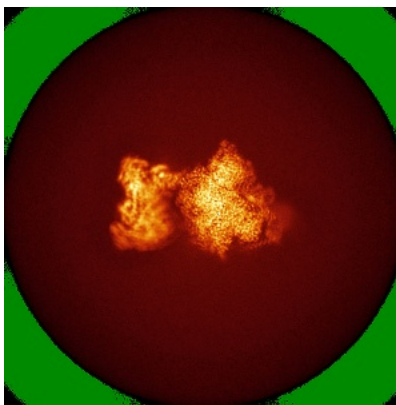
The images above show the largest variance slices of the map in three orthogonal directions.

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

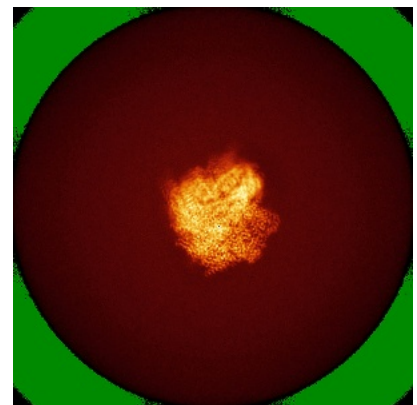
6.4.1 Primary map



X



Y

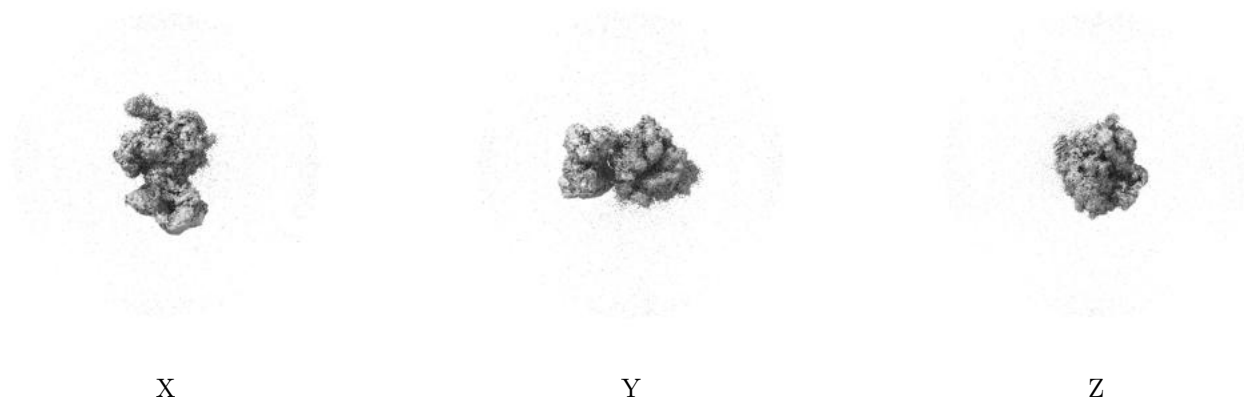


Z

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

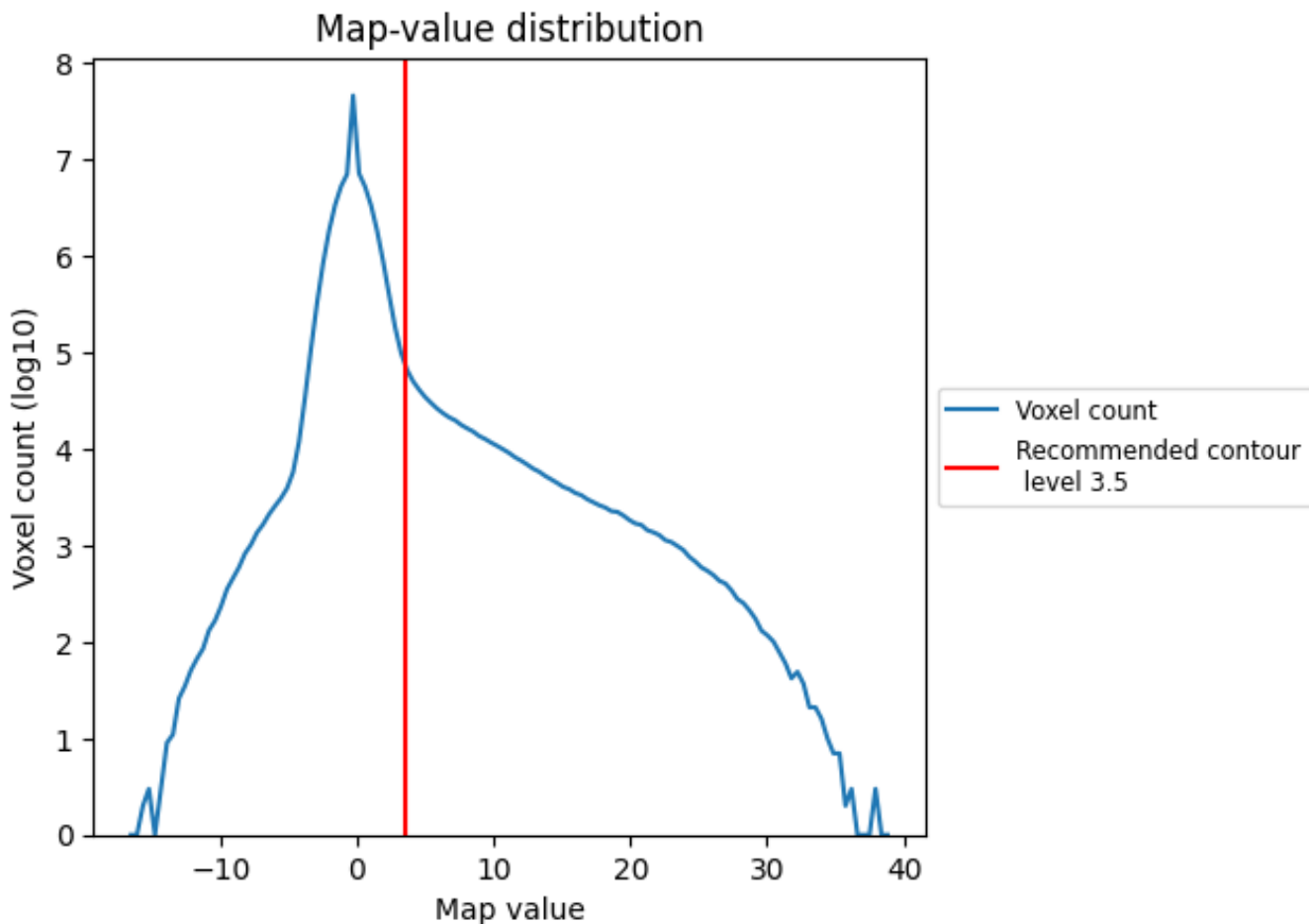
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

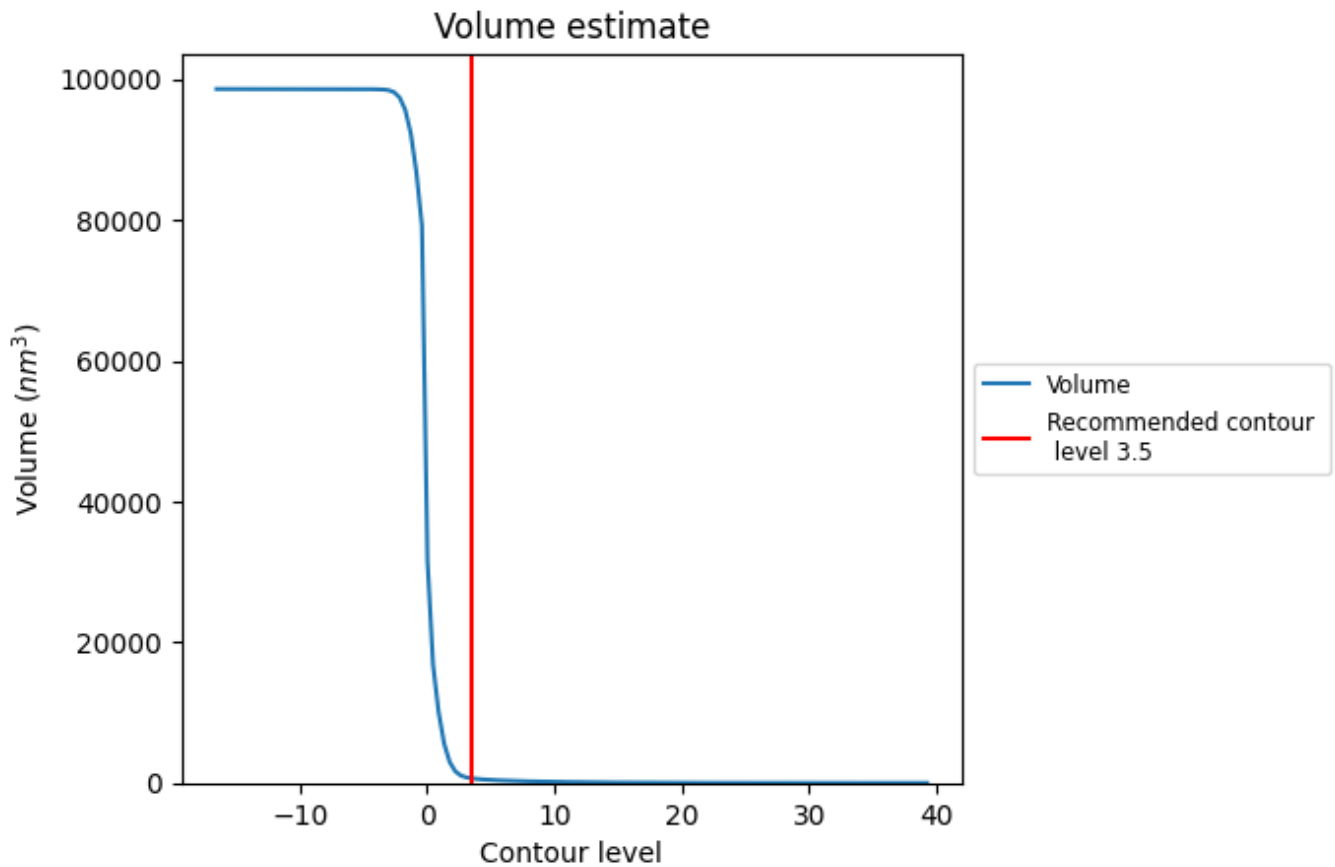
This section contains the results of statistical analysis of the map.

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.

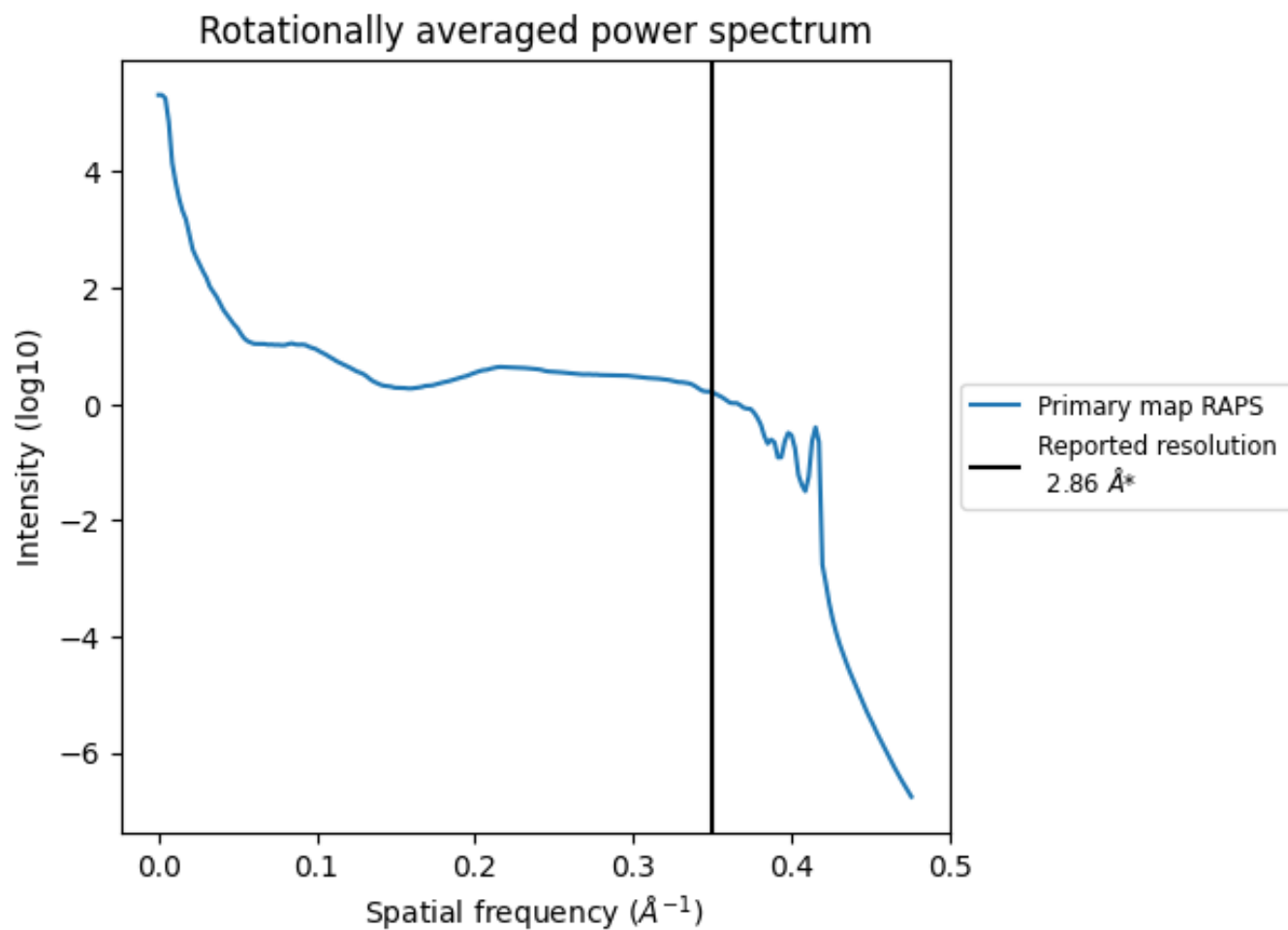
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 656 nm³; this corresponds to an approximate mass of 593 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 0.350 Å⁻¹

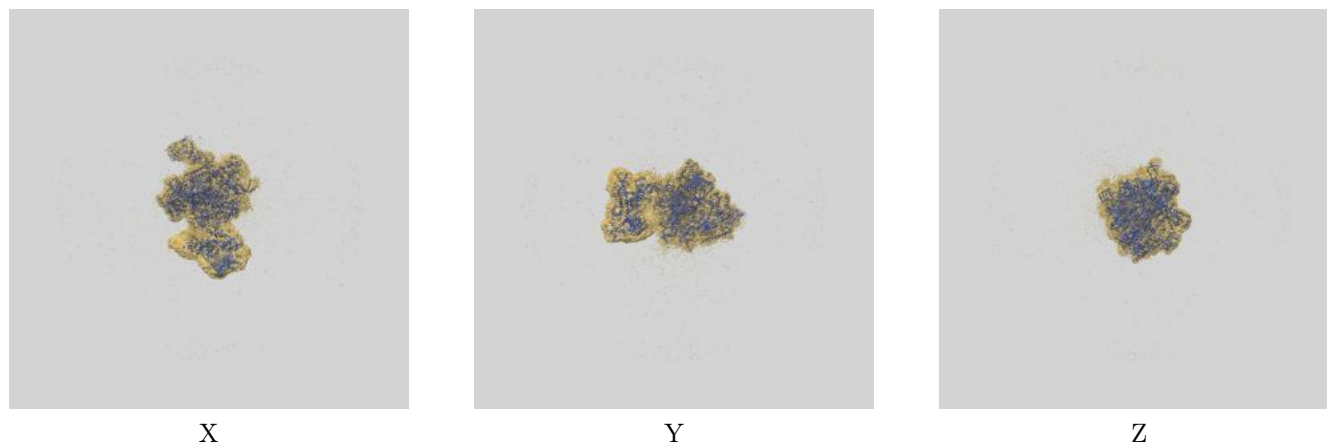
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

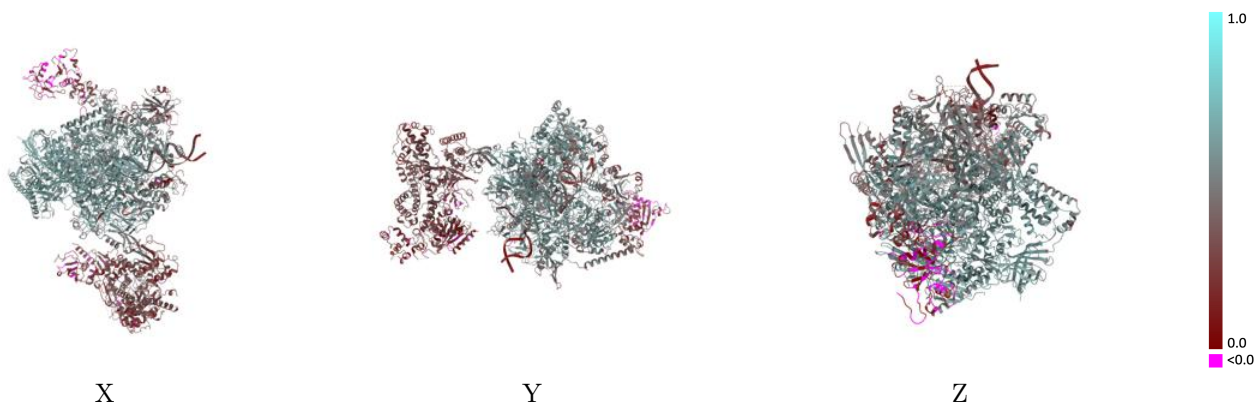
This section contains information regarding the fit between EMDB map EMD-16837 and PDB model 80EV. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



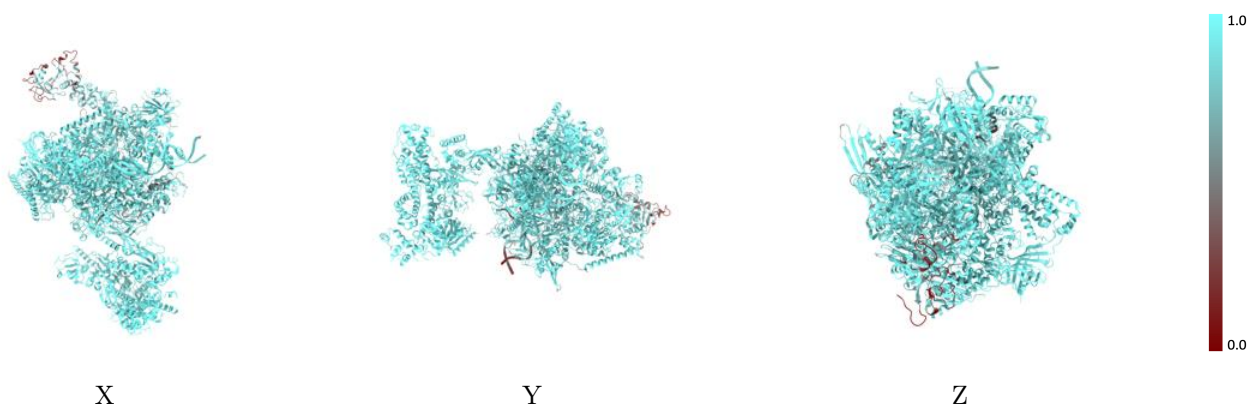
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



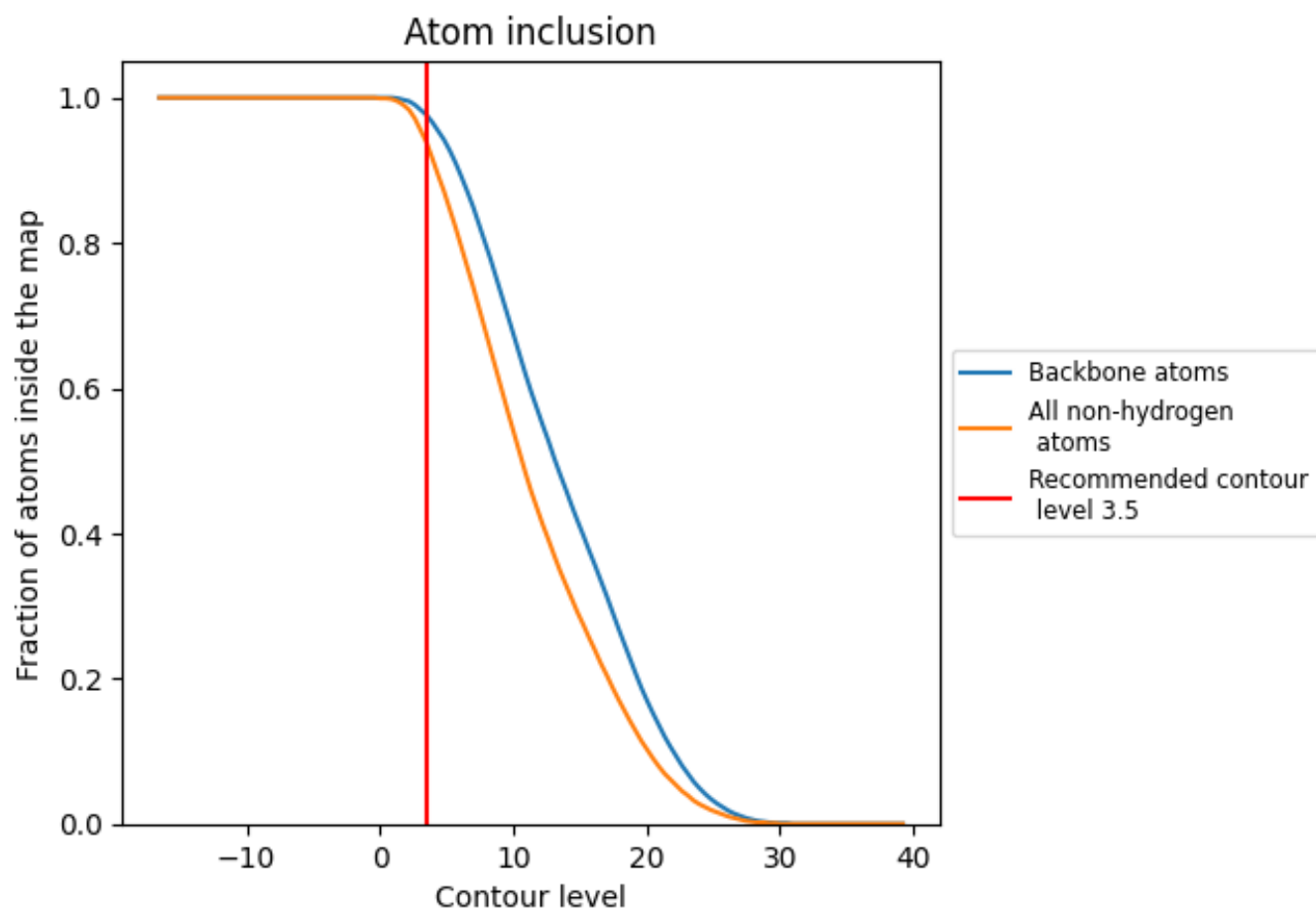
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9390	 0.4680
A	 0.9550	 0.5510
B	 0.9600	 0.5650
C	 0.9690	 0.5950
D	 0.9610	 0.3040
E	 0.9520	 0.5160
F	 0.9620	 0.5790
G	 0.9500	 0.4070
H	 0.9650	 0.5760
I	 0.9310	 0.4670
J	 0.9750	 0.6040
K	 0.9670	 0.5950
L	 0.9410	 0.5120
M	 0.8590	 0.3090
N	 0.8140	 0.2840
O	 0.5700	 0.1210
P	 0.8820	 0.4980
Q	 0.4420	 0.0670
S	 0.9830	 0.2530
T	 0.8450	 0.3850

