



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:06 AM UTC

PDB ID : 5M5Y / pdb_00005m5y
EMDB ID : EMD-3448
Title : RNA Polymerase I elongation complex 2
Authors : Tafur, L.; Sadian, Y.; Hoffmann, N.A.; Jakobi, A.J.; Wetzel, R.; Hagen, W.J.H.; Sachse, C.; Muller, C.W.
Deposited on : 2016-10-23
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

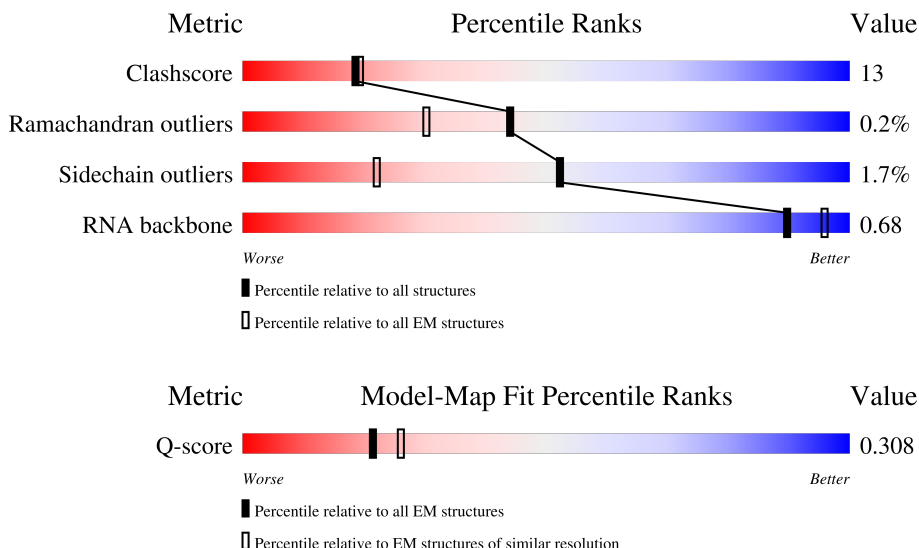
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1664	
2	B	1203	
3	C	335	

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Mol	Chain	Length	Quality of chain
4	D	137	
5	E	215	
6	F	155	
7	G	326	
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	R	10	
16	S	70	
17	T	70	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 34104 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
1	A	1466	Total	C	N	O	S	0	0
			11571	7309	2012	2188	62		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1170	Total	C	N	O	S	0	0
			9301	5888	1625	1737	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	304	Total	C	N	O	S	0	0
			2418	1536	414	460	8		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	59	Total	C	N	O	0	0
			467	293	80	94		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1751	1111	309	320	11		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	202	Total	C	N	O	S	0	0
			1600	1026	276	293	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	134	Total	C	N	O	S	0	0
			1075	677	182	212	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	64	Total	C	N	O	S	0	0
			472	295	78	95	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	100	Total	C	N	O	S	0	0
			784	491	128	160	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
			344	211	69	60	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	101	Total	C	N	O		0	0
			802	508	132	162			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	135	Total	C	N	O	S	0	0
			1070	685	175	206	4		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	7	Total	C	N	O	P	0	0
			145	65	22	51	7		

- Molecule 16 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	19	Total	C	N	O	P	0	0
			397	188	82	108	19		

- Molecule 17 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	25	Total	C	N	O	P	0	0
			509	244	86	154	25		

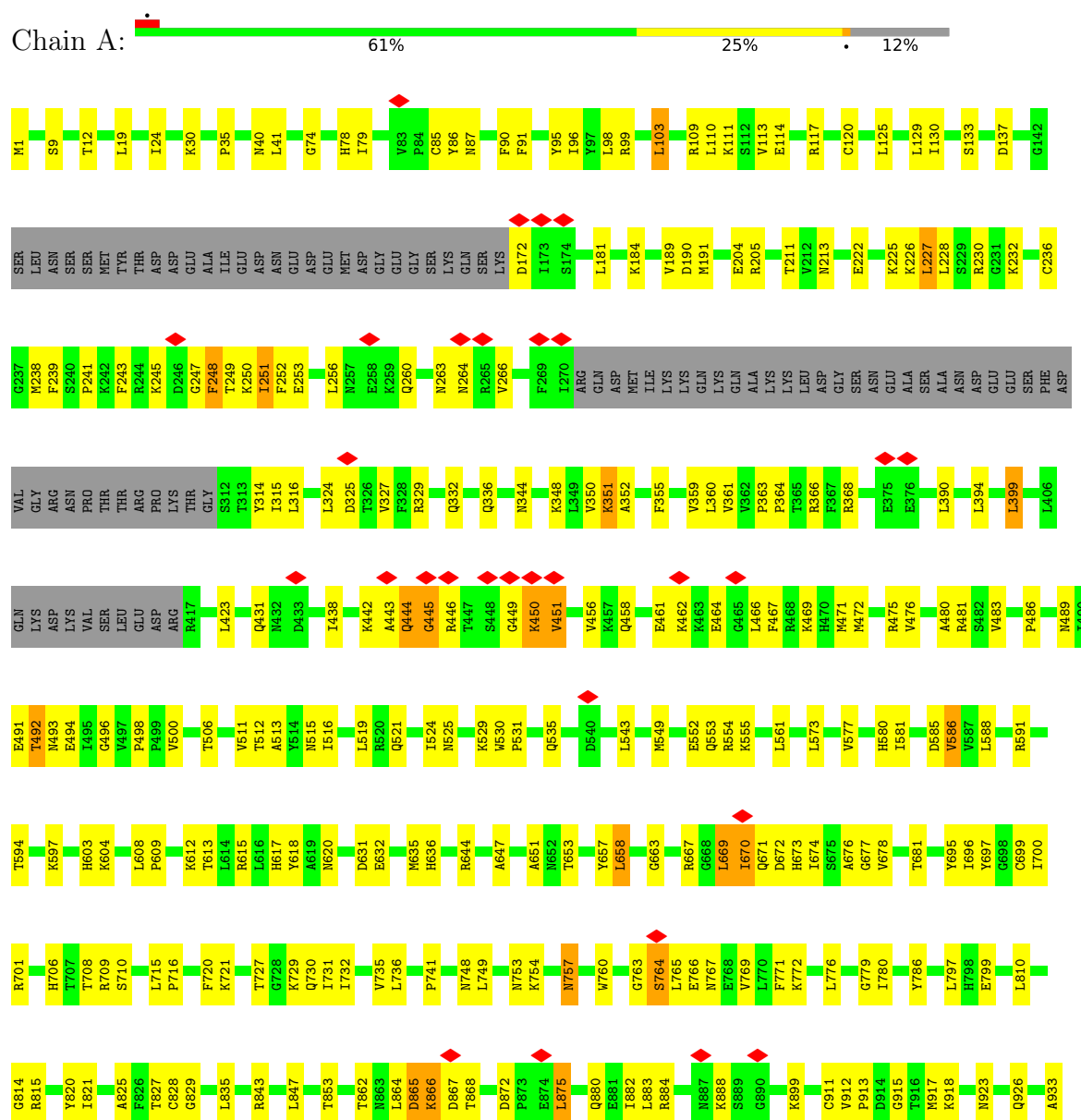
- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

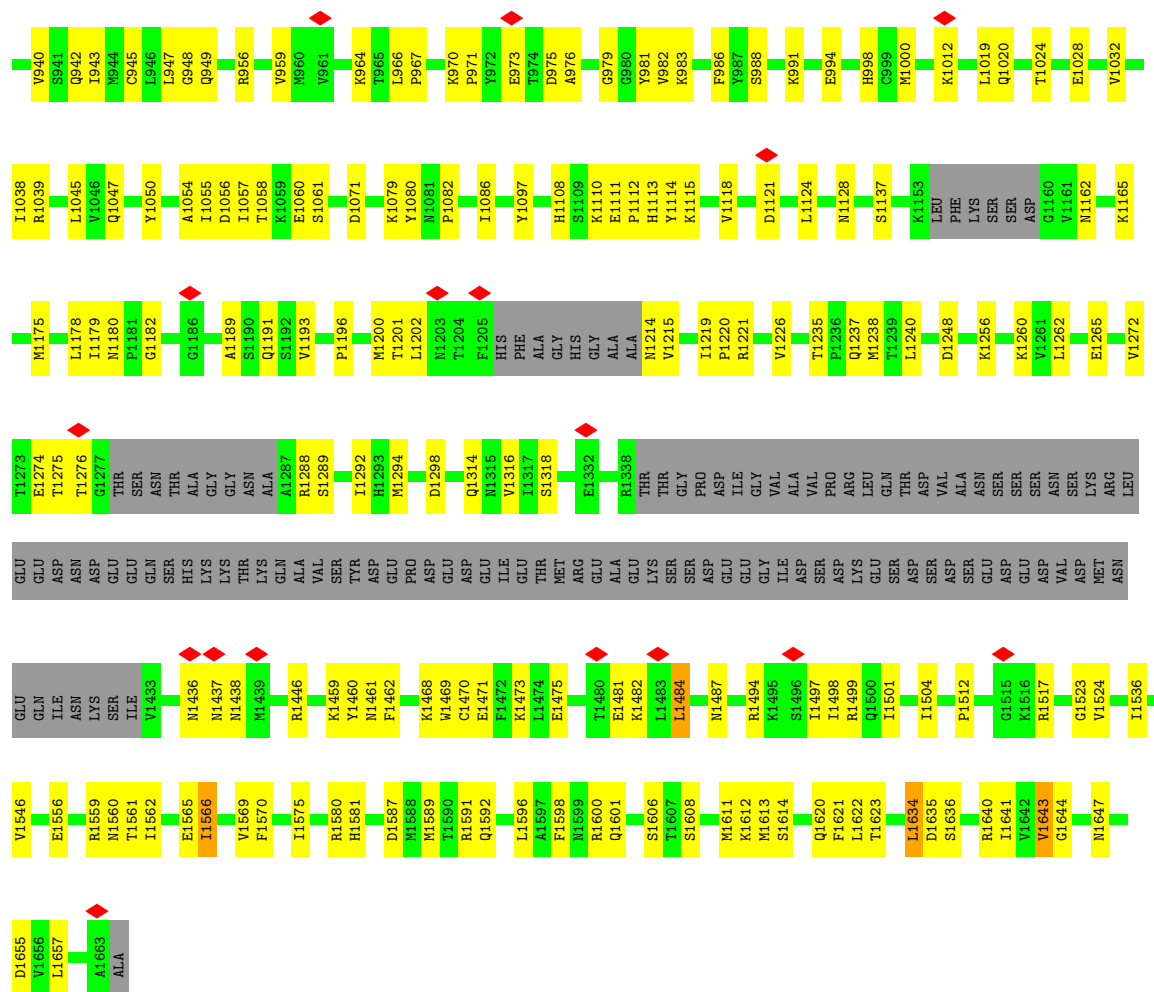
Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	
18	B	1	Total	Zn	0
			1	1	
18	I	1	Total	Zn	0
			1	1	
18	J	1	Total	Zn	0
			1	1	
18	L	1	Total	Zn	0
			1	1	

3 Residue-property plots

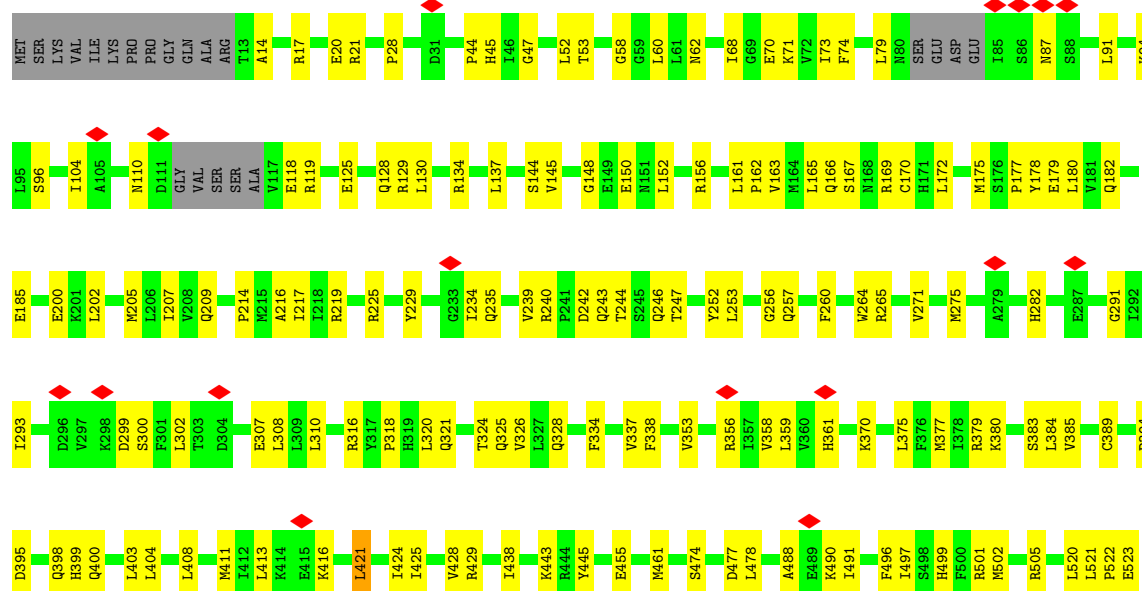
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

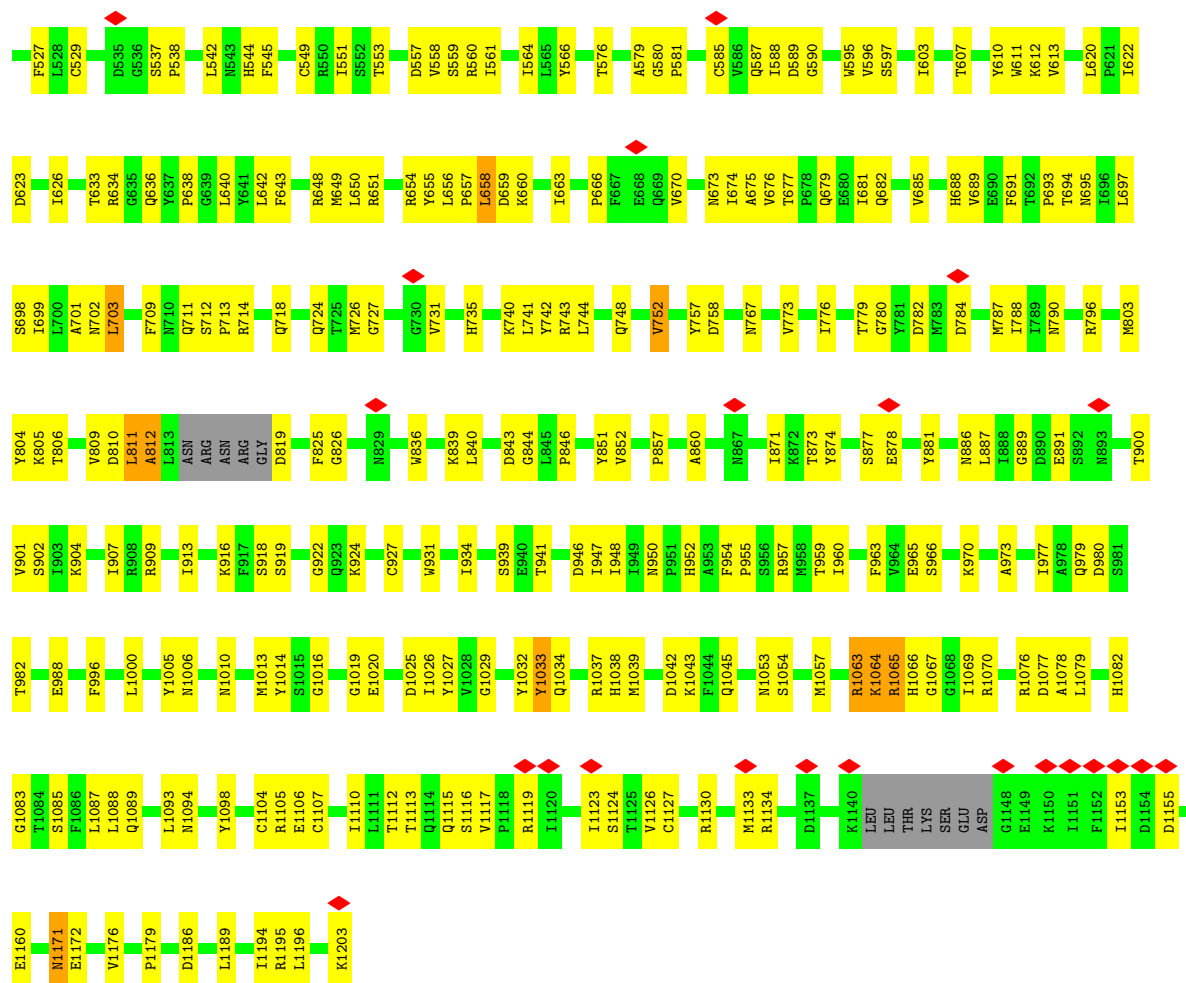
- Molecule 1: DNA-directed RNA polymerase I subunit RPA190

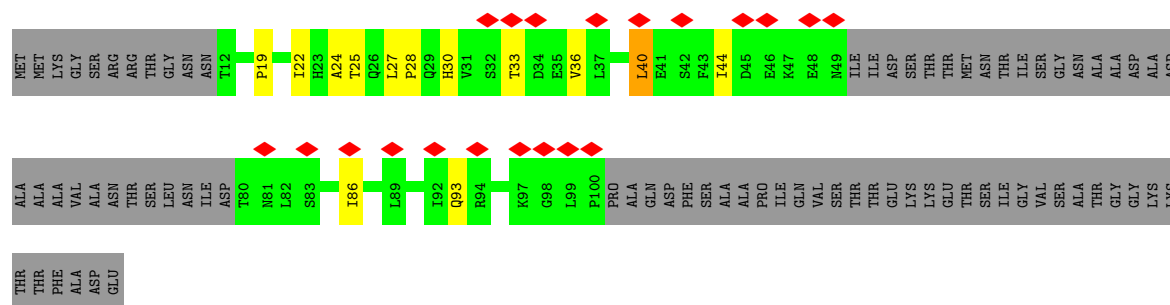




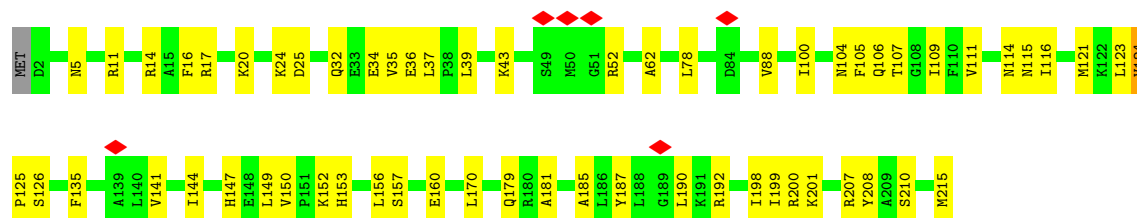
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135



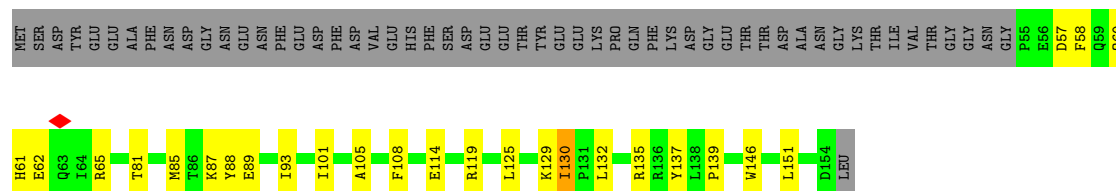




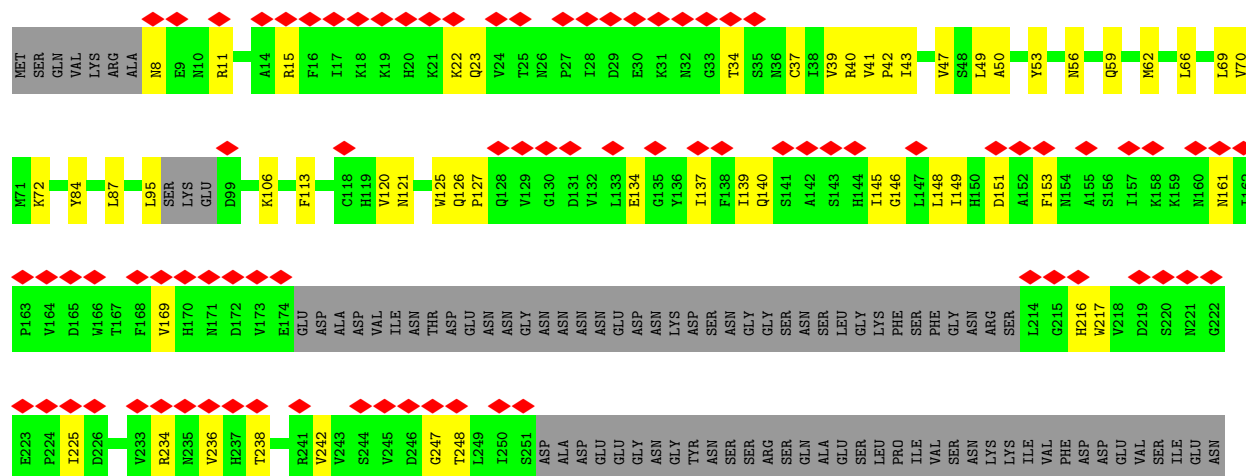
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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



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



LYS
GLU
SER
HIS
LYS
GLU
LEU
ASP
LEU
PRO
GLU
VAL
LYS
GLU
ASP
ASN
GLY
SER
SER
GLU
TLE
VAL
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ASN
ASP
GLY
GLU
SER
SER
SER
ASP
ASP

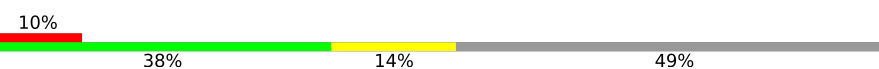
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 

MET SER N3 T4 L5 D8 I9 F10 Q11 P17 C24 A28 A29 S30 T31 T32 L38 S54 L55 T56 I59 N64 LEU GLU ASP THR PRO ALA ASN ASP SER A75 T76 R77 Y93 D94 Y95 Y96 Y97 Y98 V107 S108 L111 V114 Y115 Y116 S117

F118 G119 G120 L121 R124 L125 E126 G127 N128 N133 N139 A140 Y141 L142 L143 T144 R145 R146

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

Chain I: 

MET S2 G5 S6 L7 L11 G12 G13 G14 D15 L16 L17 L18 E19 A22 V23 L24 V28 E29 C30 S31 Q32 C33 K34 A35 I36 Y37 P38 K39 F42 L45 T49 S65 VAL LYS THR SER LEU LYS ASN LEU LYS ASP GLY ALA THR ILE LYS LYS

CYS PRO GLN CYS GLY ASN GLU MET ASN TYR HIS THR LEU GLN LEU ARG SER ASP ALA GLY THR VAL PHE THR CYS THR CYS I36 Y37 P38 K39 F42 L45 T49 S65 VAL LYS THR SER LEU LYS ASN LEU LYS ASP GLY ALA THR ILE LYS LYS

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

Chain J: 

M1 I2 V5 F8 S9 G10 G11 V14 G15 D16 K17 Y21 E27 D28 E29 L30 D31 E32 L36 L39 G40 L41 Y44 C45 M49 I50 L51 T52 H53 V54 D55 L56 F60 L61 R62 Y63 M64 P65 L66 R69 ASP

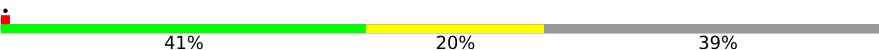
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K: 

MET THR ASP ASP ILE GLN LYS THR THR ALA ALA VAL THR PRO GLN GLU PRO LYS HIS ILE GLN GLU GLU GLN ASP VAL ASP MET THR GLY ASP GLU GLN GLU GLU PRO D43 T54 S55 E56 D57 G58 T59 S60 A61 S62 V66 E67 H70 T71

V79 I80 M81 K82 N83 V86 E87 F88 G89 G90 Y91 S92 I93 P94 N99 I103 R104 E110 G120 D123 L124 C128 V131 E132 K138 S141 M142

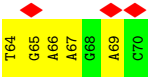
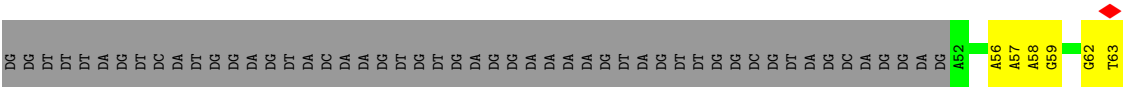
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 

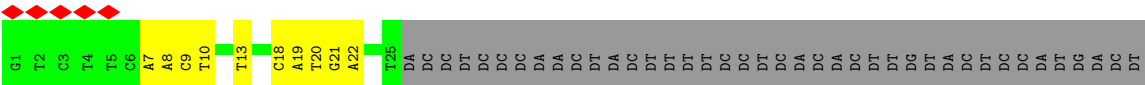
MET SER ARG GLU PHE GLN ILE PRO THR ASN LEU ASP ALA ALA ALA ALA GLY THR SER GLN ARG THR THR K28 Y29 I30 C31 A32 E33 L38 S41 S42 T43 R47 C48 K49 G52 H53 R54 I55 L56 R70

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





● Molecule 17: Template DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50784	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	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.231	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	237.6, 237.6, 237.6	wwPDB
Map dimensions	176, 176, 176	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	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

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	0.13	1/11782 (0.0%)	0.41	12/15913 (0.1%)
2	B	0.14	1/9506 (0.0%)	0.43	7/12847 (0.1%)
3	C	0.09	0/2469	0.28	0/3347
4	D	0.09	0/473	0.28	0/641
5	E	0.09	0/1787	0.27	0/2406
6	F	0.10	0/838	0.28	0/1129
7	G	0.09	0/1637	0.26	0/2226
8	H	0.09	0/1093	0.31	0/1480
9	I	0.09	0/478	0.31	0/647
10	J	0.11	0/578	0.33	0/775
11	K	0.64	2/794 (0.3%)	1.11	5/1070 (0.5%)
12	L	0.09	0/346	0.32	0/457
13	M	0.15	0/816	0.36	0/1095
14	N	0.14	0/1090	0.44	1/1466 (0.1%)
15	R	0.04	0/160	0.09	0/246
16	S	0.14	0/448	0.28	0/690
17	T	0.17	0/568	0.36	0/874
All	All	0.16	4/34863 (0.0%)	0.41	25/47309 (0.1%)

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
2	B	0	1
11	K	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	57	ASP	N-CA	16.07	1.66	1.46
2	B	1064	LYS	N-CA	8.00	1.56	1.46
11	K	57	ASP	CA-CB	7.28	1.65	1.53
1	A	763	GLY	N-CA	7.18	1.55	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	57	ASP	N-CA-C	-28.41	72.96	112.45
2	B	1064	LYS	N-CA-C	-27.75	78.58	113.55
1	A	445	GLY	N-CA-C	-15.18	77.20	113.18
1	A	764	SER	N-CA-C	-12.71	90.62	108.54
11	K	57	ASP	CB-CA-C	-12.22	87.02	110.11
1	A	867	ASP	N-CA-C	11.28	126.96	111.74
1	A	866	LYS	N-CA-C	10.17	125.56	109.50
11	K	57	ASP	N-CA-CB	-9.60	95.96	110.26
1	A	763	GLY	N-CA-C	-9.55	90.55	113.18
11	K	58	GLY	N-CA-C	-8.84	92.24	113.18
11	K	57	ASP	CA-CB-CG	-8.53	104.07	112.60
2	B	1064	LYS	CB-CA-C	-8.36	96.38	109.34
2	B	1065	ARG	N-CA-C	-7.19	104.59	113.15
1	A	450	LYS	N-CA-C	-7.17	103.60	113.56
1	A	445	GLY	CA-C-O	-6.53	109.21	120.57
14	N	147	ALA	N-CA-C	6.48	118.06	108.60
1	A	865	ASP	N-CA-C	6.18	118.99	111.82
2	B	1064	LYS	N-CA-CB	-5.70	102.14	110.40
1	A	444	GLN	N-CA-C	5.40	118.17	110.24
1	A	443	ALA	N-CA-C	5.37	117.01	110.41
2	B	1063	ARG	CA-C-N	-5.23	113.48	122.79
2	B	1063	ARG	C-N-CA	-5.23	113.48	122.79
1	A	866	LYS	CA-C-N	5.08	129.35	122.19
1	A	866	LYS	C-N-CA	5.08	129.35	122.19
2	B	811	LEU	N-CA-C	5.04	116.81	108.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	445	GLY	Mainchain
2	B	877	SER	Peptide
11	K	58	GLY	Mainchain

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	11571	0	11650	352	0
2	B	9301	0	9194	292	0
3	C	2418	0	2401	56	0
4	D	467	0	468	11	0
5	E	1751	0	1776	40	0
6	F	823	0	841	20	0
7	G	1600	0	1600	33	0
8	H	1075	0	1046	30	0
9	I	472	0	473	15	0
10	J	569	0	585	25	0
11	K	784	0	781	21	0
12	L	344	0	363	11	0
13	M	802	0	787	34	0
14	N	1070	0	1085	32	0
15	R	145	0	75	1	0
16	S	397	0	213	8	0
17	T	509	0	285	9	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	34104	0	33623	875	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 13.

All (875) 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:450:LYS:O	1:A:451:VAL:HG22	1.31	1.26
1:A:865:ASP:C	1:A:866:LYS:HD2	1.63	1.22
1:A:865:ASP:HB3	1:A:866:LYS:NZ	1.59	1.16
1:A:450:LYS:O	1:A:451:VAL:CG2	2.04	1.05
1:A:865:ASP:CB	1:A:866:LYS:NZ	2.29	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:ASP:HB3	1:A:866:LYS:HZ2	1.17	0.91
1:A:450:LYS:O	1:A:451:VAL:HG13	1.71	0.90
2:B:1063:ARG:HA	2:B:1067:GLY:H	1.35	0.87
1:A:450:LYS:C	1:A:451:VAL:HG22	1.99	0.86
1:A:462:LYS:HE2	1:A:469:LYS:HB2	1.62	0.82
1:A:865:ASP:CB	1:A:866:LYS:HZ2	1.94	0.79
1:A:450:LYS:O	1:A:451:VAL:CG1	2.31	0.78
7:G:149:ILE:HB	7:G:153:PHE:HB2	1.66	0.78
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.67	0.77
1:A:865:ASP:HB3	1:A:866:LYS:CE	2.14	0.77
2:B:17:ARG:HG3	2:B:20:GLU:HB3	1.67	0.76
1:A:760:TRP:HB2	1:A:764:SER:CB	2.16	0.75
1:A:506:THR:HA	1:A:580:HIS:HA	1.70	0.74
2:B:784:ASP:H	2:B:950:ASN:HD22	1.36	0.74
1:A:1012:LYS:HG3	1:A:1201:THR:HB	1.69	0.74
1:A:757:ASN:CG	1:A:764:SER:O	2.30	0.73
1:A:1498:ILE:HG23	1:A:1499:ARG:HD3	1.68	0.73
9:I:13:CYS:SG	9:I:32:GLN:NE2	2.62	0.72
1:A:865:ASP:CB	1:A:866:LYS:HD2	2.19	0.72
1:A:249:THR:HG21	1:A:431:GLN:HG3	1.71	0.72
1:A:450:LYS:O	1:A:451:VAL:CB	2.37	0.71
2:B:675:ALA:HB3	2:B:689:VAL:HG12	1.71	0.71
1:A:1272:VAL:HG12	1:A:1292:ILE:HA	1.73	0.71
2:B:53:THR:HG21	2:B:169:ARG:HH12	1.55	0.71
10:J:10:CYS:HB3	10:J:45:CYS:SG	2.31	0.71
3:C:91:VAL:HG11	10:J:60:PHE:HB3	1.71	0.70
1:A:865:ASP:CB	1:A:866:LYS:HZ3	2.00	0.70
2:B:741:LEU:HB3	2:B:804:TYR:HB2	1.73	0.70
1:A:222:GLU:HG2	1:A:225:LYS:HE3	1.72	0.70
13:M:44:LYS:HD3	13:M:48:LYS:HA	1.73	0.70
1:A:1556:GLU:OE2	5:E:153:HIS:NE2	2.26	0.69
1:A:749:LEU:H	1:A:771:PHE:HB2	1.57	0.69
1:A:1118:VAL:HG11	5:E:199:ILE:HG21	1.74	0.69
13:M:38:PHE:HB2	14:N:119:LEU:HD21	1.73	0.69
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.75	0.69
1:A:866:LYS:HD2	1:A:866:LYS:N	2.06	0.69
5:E:124:VAL:HG23	5:E:125:PRO:HD3	1.74	0.69
2:B:163:VAL:HG11	2:B:169:ARG:HB2	1.75	0.69
7:G:37:CYS:SG	7:G:125:TRP:NE1	2.65	0.69
1:A:19:LEU:HD22	2:B:1195:ARG:HB2	1.75	0.68
2:B:811:LEU:HD13	2:B:825:PHE:CZ	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:234:ARG:HB2	7:G:248:THR:HG23	1.76	0.68
14:N:82:ILE:HG22	14:N:83:ASP:H	1.59	0.68
1:A:669:LEU:HD21	1:A:814:GLY:HA2	1.74	0.68
2:B:310:LEU:HD22	9:I:16:LEU:HD23	1.75	0.68
14:N:56:ILE:HG22	14:N:137:PHE:HB2	1.76	0.68
1:A:827:THR:HB	2:B:776:ILE:HD12	1.75	0.68
1:A:461:GLU:HB3	1:A:464:GLU:HA	1.76	0.68
8:H:98:TYR:OH	8:H:139:ASN:OD1	2.05	0.67
8:H:146:ARG:OXT	8:H:146:ARG:NH1	2.27	0.67
2:B:682:GLN:HE22	2:B:685:VAL:H	1.42	0.67
17:T:20:DT:H2''	17:T:21:DG:H5'	1.77	0.67
1:A:85:CYS:SG	1:A:86:TYR:N	2.67	0.67
1:A:597:LYS:HE2	2:B:1082:HIS:HA	1.76	0.67
1:A:970:LYS:HA	2:B:673:ASN:HD22	1.58	0.67
3:C:114:THR:OG1	3:C:130:ASN:ND2	2.28	0.67
2:B:404:LEU:HD11	2:B:551:ILE:HG21	1.76	0.67
17:T:18:DC:H2''	17:T:19:DA:H5'	1.77	0.67
1:A:325:ASP:OD2	1:A:329:ARG:NH1	2.28	0.66
2:B:947:ILE:HG21	2:B:1033:TYR:HE2	1.60	0.66
2:B:650:LEU:HB3	2:B:663:ILE:HD11	1.77	0.65
1:A:344:ASN:HD21	1:A:348:LYS:H	1.45	0.65
1:A:658:LEU:HD12	1:A:1058:THR:HA	1.77	0.65
2:B:612:LYS:NZ	2:B:622:ILE:O	2.27	0.65
1:A:865:ASP:C	1:A:866:LYS:CD	2.57	0.65
1:A:1318:SER:HB3	1:A:1446:ARG:HH22	1.61	0.65
1:A:843:ARG:NH1	1:A:945:CYS:O	2.30	0.65
1:A:248:PHE:HB3	1:A:442:LYS:NZ	2.12	0.65
1:A:658:LEU:HD11	1:A:663:GLY:HA2	1.79	0.65
2:B:878:GLU:HG2	2:B:907:ILE:HG12	1.79	0.65
2:B:1039:MET:HG2	2:B:1042:ASP:H	1.60	0.64
2:B:811:LEU:HD12	2:B:811:LEU:N	2.11	0.64
1:A:760:TRP:HB2	1:A:764:SER:HB3	1.80	0.64
5:E:17:ARG:NH1	5:E:35:VAL:O	2.30	0.64
1:A:709:ARG:H	1:A:709:ARG:HD2	1.62	0.64
1:A:585:ASP:HA	1:A:644:ARG:HH21	1.63	0.64
1:A:243:PHE:HB3	1:A:251:ILE:HD11	1.79	0.64
1:A:250:LYS:O	1:A:251:ILE:C	2.38	0.64
1:A:1314:GLN:HG3	1:A:1446:ARG:HH21	1.62	0.64
1:A:1221:ARG:NH2	1:A:1565:GLU:OE1	2.31	0.64
2:B:318:PRO:O	2:B:321:GLN:NE2	2.30	0.64
2:B:501:ARG:NH1	2:B:549:CYS:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1647:ASN:HB2	2:B:1085:SER:HB2	1.80	0.63
1:A:647:ALA:HA	1:A:651:ALA:HB3	1.80	0.63
2:B:767:ASN:HB3	2:B:1034:GLN:HE21	1.63	0.63
1:A:966:LEU:HD12	1:A:967:PRO:HD2	1.79	0.63
2:B:703:LEU:HD21	2:B:757:TYR:HD2	1.63	0.63
1:A:130:ILE:O	5:E:192:ARG:NH1	2.30	0.63
13:M:20:SER:HG	13:M:91:TYR:HH	1.44	0.63
13:M:41:TYR:HB3	13:M:52:VAL:HG23	1.80	0.63
1:A:483:VAL:HG13	1:A:613:THR:HG23	1.81	0.62
2:B:585:CYS:HA	2:B:595:TRP:HB3	1.80	0.62
3:C:55:ASP:OD1	3:C:271:ARG:NH2	2.32	0.62
17:T:7:DA:H2"	17:T:8:DA:H5"	1.79	0.62
1:A:880:GLN:HB2	2:B:633:THR:HG21	1.79	0.62
2:B:694:THR:O	2:B:702:ASN:ND2	2.32	0.62
1:A:24:ILE:HD12	1:A:359:VAL:HG22	1.80	0.62
1:A:613:THR:O	1:A:615:ARG:NH2	2.33	0.62
2:B:970:LYS:HE3	2:B:1029:GLY:HA2	1.81	0.62
1:A:865:ASP:CB	1:A:866:LYS:CD	2.77	0.61
12:L:47:ARG:NH1	12:L:48:CYS:O	2.33	0.61
1:A:1000:MET:HA	2:B:520:LEU:HD13	1.82	0.61
7:G:161:ASN:ND2	7:G:247:GLY:O	2.33	0.61
2:B:275:MET:SD	2:B:316:ARG:NH2	2.74	0.61
2:B:119:ARG:NH1	12:L:52:GLY:O	2.33	0.61
1:A:681:THR:HG23	1:A:780:ILE:HD12	1.83	0.61
1:A:1655:ASP:HB2	6:F:137:TYR:HE2	1.66	0.61
1:A:248:PHE:CD1	1:A:442:LYS:HG2	2.35	0.61
2:B:73:ILE:HD12	2:B:425:ILE:HG23	1.83	0.61
2:B:1016:GLY:O	3:C:69:ARG:NH2	2.34	0.61
2:B:1116:SER:OG	2:B:1160:GLU:O	2.19	0.61
1:A:911:CYS:O	1:A:915:GLY:N	2.29	0.61
2:B:358:VAL:O	2:B:370:LYS:NZ	2.33	0.61
1:A:964:LYS:NZ	1:A:973:GLU:OE1	2.33	0.60
1:A:248:PHE:HB3	1:A:442:LYS:HZ3	1.66	0.60
2:B:58:GLY:HA3	2:B:62:ASN:HD22	1.66	0.60
2:B:779:THR:OG1	2:B:931:TRP:NE1	2.35	0.60
2:B:1006:ASN:ND2	2:B:1010:ASN:O	2.34	0.60
4:D:28:PRO:HB3	7:G:41:VAL:HG22	1.82	0.60
1:A:263:ASN:HA	1:A:266:VAL:HG22	1.83	0.60
2:B:73:ILE:HD11	2:B:429:ARG:HB3	1.83	0.60
14:N:57:LYS:HB2	14:N:138:SER:HA	1.82	0.60
2:B:724:GLN:HE21	2:B:1037:ARG:HE	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:811:LEU:O	2:B:812:ALA:CB	2.49	0.60
1:A:865:ASP:HB3	1:A:866:LYS:CD	2.31	0.60
2:B:216:ALA:HA	2:B:234:ILE:HG12	1.82	0.60
3:C:65:ASN:ND2	3:C:227:TYR:OH	2.34	0.60
13:M:26:PHE:HB3	13:M:98:SER:HB3	1.83	0.60
1:A:462:LYS:H	1:A:466:LEU:HB2	1.67	0.60
1:A:964:LYS:HD3	1:A:971:PRO:HA	1.83	0.60
2:B:588:ILE:HG12	2:B:642:LEU:HD12	1.84	0.60
1:A:1436:ASN:HD22	1:A:1469:TRP:HZ2	1.48	0.60
14:N:148:ILE:O	14:N:148:ILE:HG22	2.02	0.60
1:A:1260:LYS:HZ1	1:A:1497:ILE:HG22	1.66	0.59
13:M:14:SER:HB3	13:M:89:GLN:HB2	1.82	0.59
2:B:1039:MET:HG3	2:B:1043:LYS:HG2	1.84	0.59
1:A:1050:TYR:HB3	1:A:1054:ALA:HA	1.84	0.59
2:B:110:ASN:HB2	2:B:119:ARG:H	1.66	0.59
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.85	0.59
1:A:444:GLN:OE1	1:A:444:GLN:N	2.22	0.59
1:A:757:ASN:HD21	1:A:767:ASN:H	1.51	0.59
3:C:39:ASP:O	3:C:58:ASN:ND2	2.32	0.59
1:A:74:GLY:HA3	1:A:364:PRO:HB3	1.84	0.59
2:B:1133:MET:SD	2:B:1134:ARG:N	2.75	0.59
1:A:612:LYS:H	2:B:913:ILE:HG21	1.68	0.59
1:A:1657:LEU:HG	7:G:106:LYS:HA	1.84	0.59
3:C:240:LYS:HD2	3:C:262:SER:HA	1.84	0.59
14:N:92:ASP:HB3	14:N:136:VAL:HG23	1.83	0.59
2:B:924:LYS:NZ	15:R:10:C:OP1	2.36	0.59
2:B:225:ARG:HH12	2:B:229:TYR:HD2	1.51	0.59
2:B:811:LEU:O	2:B:812:ALA:HB2	2.02	0.59
1:A:450:LYS:C	1:A:451:VAL:HG13	2.27	0.59
9:I:33:CYS:SG	13:M:59:ARG:NH1	2.75	0.59
1:A:994:GLU:OE1	1:A:994:GLU:N	2.36	0.58
5:E:200:ARG:HH21	5:E:208:TYR:HE2	1.51	0.58
1:A:1459:LYS:NZ	1:A:1471:GLU:OE1	2.34	0.58
2:B:1065:ARG:O	2:B:1066:HIS:HB2	2.04	0.58
14:N:110:LEU:HD12	14:N:112:PRO:HD3	1.86	0.58
1:A:515:ASN:HB3	1:A:519:LEU:HD13	1.86	0.58
2:B:963:PHE:O	2:B:1027:TYR:OH	2.21	0.58
3:C:69:ARG:HH12	11:K:70:HIS:HB2	1.68	0.58
1:A:103:LEU:HD21	1:A:241:PRO:HD2	1.86	0.58
5:E:157:SER:OG	5:E:160:GLU:OE1	2.22	0.58
1:A:1055:ILE:HD11	1:A:1580:ARG:HH12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.85	0.58
11:K:67:GLU:HA	11:K:99:ASN:HB2	1.85	0.58
1:A:1039:ARG:HB3	1:A:1045:LEU:HD13	1.86	0.58
2:B:1093:LEU:HD13	2:B:1179:PRO:HG3	1.86	0.58
1:A:865:ASP:CA	1:A:866:LYS:HD2	2.33	0.57
2:B:293:ILE:HA	2:B:579:ALA:HB3	1.86	0.57
2:B:740:LYS:HB2	2:B:805:LYS:HZ3	1.69	0.57
2:B:836:TRP:O	2:B:839:LYS:NZ	2.26	0.57
5:E:88:VAL:HB	5:E:116:ILE:HG13	1.86	0.57
1:A:964:LYS:HZ2	1:A:973:GLU:HB2	1.67	0.57
2:B:502:MET:SD	2:B:544:HIS:NE2	2.78	0.57
1:A:947:LEU:HB3	1:A:982:VAL:HG21	1.87	0.57
2:B:156:ARG:HH12	2:B:455:GLU:HG3	1.68	0.57
2:B:175:MET:HG2	2:B:180:LEU:HD12	1.86	0.57
1:A:1643:VAL:HG13	1:A:1644:GLY:H	1.69	0.57
2:B:1042:ASP:O	2:B:1063:ARG:NH2	2.32	0.57
5:E:24:LYS:NZ	5:E:32:GLN:OE1	2.36	0.57
10:J:64:ASN:HD22	10:J:66:LEU:H	1.52	0.57
1:A:117:ARG:NH2	1:A:137:ASP:OD1	2.34	0.57
1:A:853:THR:HB	1:A:899:LYS:HD3	1.87	0.57
6:F:130:ILE:HG13	6:F:132:LEU:HD23	1.86	0.57
9:I:39:LYS:H	9:I:39:LYS:HD3	1.69	0.57
2:B:253:LEU:HD12	2:B:257:GLN:HB3	1.87	0.57
2:B:843:ASP:OD2	12:L:28:LYS:NZ	2.38	0.57
7:G:22:LYS:H	7:G:22:LYS:HD3	1.68	0.57
1:A:494:GLU:HG2	1:A:604:LYS:HB3	1.86	0.57
2:B:752:VAL:HG11	2:B:965:GLU:HG2	1.87	0.57
13:M:82:ASN:OD1	13:M:85:LYS:N	2.34	0.57
2:B:743:ARG:NH2	2:B:804:TYR:OH	2.38	0.56
5:E:201:LYS:HE3	5:E:207:ARG:HG2	1.87	0.56
2:B:886:ASN:HB2	2:B:902:SER:HB3	1.87	0.56
2:B:566:TYR:HD2	13:M:73:SER:HB3	1.70	0.56
5:E:17:ARG:NH2	5:E:37:LEU:O	2.37	0.56
11:K:62:SER:OG	11:K:104:ARG:NH1	2.34	0.56
2:B:320:LEU:HD11	2:B:326:VAL:HG12	1.87	0.56
5:E:62:ALA:HB3	5:E:78:LEU:HB3	1.85	0.56
1:A:1047:GLN:NE2	1:A:1587:ASP:OD2	2.39	0.56
1:A:1589:MET:O	1:A:1596:LEU:N	2.39	0.56
13:M:20:SER:OG	13:M:91:TYR:OH	2.16	0.56
16:S:62:DG:N2	17:T:10:DT:O2	2.38	0.56
13:M:40:LEU:HD21	14:N:119:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:PRO:O	1:A:368:ARG:NE	2.36	0.56
2:B:214:PRO:O	2:B:380:LYS:NZ	2.39	0.56
1:A:1240:LEU:HB3	1:A:1536:ILE:HD12	1.88	0.56
2:B:17:ARG:NH1	2:B:758:ASP:OD2	2.39	0.56
2:B:182:GLN:O	10:J:69:ARG:NH1	2.39	0.56
13:M:38:PHE:HD2	14:N:119:LEU:HD11	1.71	0.56
1:A:450:LYS:C	1:A:451:VAL:CG2	2.70	0.55
1:A:480:ALA:HB3	1:A:635:MET:HB3	1.87	0.55
1:A:1175:MET:HA	1:A:1178:LEU:HD23	1.88	0.55
1:A:1473:LYS:NZ	1:A:1475:GLU:OE2	2.38	0.55
2:B:47:GLY:HA3	2:B:553:THR:HG21	1.88	0.55
7:G:34:THR:HG21	7:G:134:GLU:HB2	1.88	0.55
2:B:811:LEU:HD13	2:B:825:PHE:CE1	2.40	0.55
6:F:85:MET:HG3	6:F:151:LEU:HD23	1.88	0.55
1:A:721:LYS:NZ	8:H:93:TYR:O	2.38	0.55
3:C:80:ALA:HA	3:C:208:CYS:HA	1.89	0.55
7:G:62:MET:HA	7:G:66:LEU:HB3	1.88	0.55
1:A:720:PHE:HE1	8:H:98:TYR:HB2	1.70	0.55
1:A:865:ASP:HB3	1:A:866:LYS:HD2	1.88	0.55
2:B:71:LYS:HD2	2:B:421:LEU:HD12	1.89	0.55
16:S:63:DT:H2''	16:S:64:DT:H3'	1.89	0.55
1:A:12:THR:HA	1:A:1634:LEU:HD11	1.88	0.55
2:B:68:ILE:O	2:B:356:ARG:NH2	2.31	0.55
1:A:444:GLN:H	1:A:444:GLN:CD	2.13	0.55
1:A:753:ASN:ND2	1:A:780:ILE:O	2.40	0.55
2:B:246:GLN:NE2	2:B:356:ARG:O	2.40	0.55
1:A:336:GLN:NE2	1:A:348:LYS:O	2.39	0.54
3:C:190:ASP:HB3	10:J:16:ASP:HB2	1.90	0.54
5:E:198:ILE:HD11	5:E:210:SER:HB3	1.88	0.54
7:G:127:PRO:HG2	7:G:236:VAL:HG21	1.89	0.54
1:A:332:GLN:HE22	1:A:350:VAL:HG22	1.72	0.54
1:A:764:SER:C	1:A:766:GLU:H	2.15	0.54
1:A:1097:TYR:OH	1:A:1121:ASP:OD1	2.22	0.54
1:A:1274:GLU:OE2	1:A:1288:ARG:NH2	2.40	0.54
1:A:1484:LEU:HD13	1:A:1487:ASN:HB3	1.88	0.54
8:H:107:VAL:HG12	8:H:108:SER:H	1.72	0.54
1:A:862:THR:HG23	1:A:864:LEU:H	1.71	0.54
2:B:177:PRO:HA	2:B:180:LEU:HD13	1.88	0.54
2:B:779:THR:HG21	2:B:788:ILE:HG13	1.89	0.54
2:B:803:MET:HB2	2:B:907:ILE:HB	1.89	0.54
1:A:700:ILE:O	1:A:706:HIS:ND1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:ASP:HA	1:A:1468:LYS:HE3	1.89	0.54
2:B:44:PRO:HG3	2:B:551:ILE:HB	1.90	0.54
2:B:490:LYS:HA	2:B:496:PHE:HE2	1.72	0.54
1:A:701:ARG:NH1	11:K:93:ILE:O	2.41	0.54
2:B:658:LEU:HD12	2:B:660:LYS:HE2	1.89	0.54
1:A:1:MET:SD	2:B:1094:ASN:ND2	2.81	0.53
1:A:95:TYR:CZ	1:A:245:LYS:HB2	2.43	0.53
2:B:416:LYS:HG3	2:B:461:MET:HE1	1.90	0.53
8:H:59:ILE:HG12	8:H:142:LEU:HG	1.89	0.53
8:H:28:ALA:HB3	8:H:38:LEU:HB3	1.90	0.53
1:A:998:HIS:HE1	2:B:712:SER:H	1.54	0.53
2:B:321:GLN:HE21	9:I:31:SER:HB3	1.72	0.53
2:B:796:ARG:NH1	10:J:8:PHE:O	2.41	0.53
2:B:979:GLN:HG2	2:B:996:PHE:HE1	1.73	0.53
8:H:56:THR:HB	8:H:145:ARG:HB2	1.90	0.53
1:A:366:ARG:NH2	2:B:1057:MET:SD	2.81	0.53
2:B:167:SER:N	2:B:170:CYS:SG	2.74	0.53
2:B:239:VAL:H	2:B:361:HIS:HB2	1.74	0.53
2:B:916:LYS:HD3	2:B:1038:HIS:CG	2.44	0.53
1:A:486:PRO:HB2	1:A:618:TYR:HE1	1.74	0.53
3:C:61:THR:HG22	3:C:298:PHE:HZ	1.74	0.53
4:D:24:ALA:HA	7:G:43:ILE:HG22	1.91	0.53
13:M:67:ASP:HB2	13:M:71:GLN:HB2	1.90	0.53
1:A:245:LYS:HG2	1:A:247:GLY:H	1.74	0.53
1:A:865:ASP:O	1:A:866:LYS:HD2	2.06	0.53
2:B:731:VAL:HG13	10:J:60:PHE:HD1	1.74	0.53
8:H:55:LEU:HD23	8:H:146:ARG:HH22	1.74	0.53
1:A:250:LYS:O	1:A:250:LYS:HG3	2.09	0.53
1:A:697:TYR:CZ	11:K:104:ARG:HB2	2.44	0.53
1:A:799:GLU:OE2	1:A:1061:SER:OG	2.26	0.53
1:A:956:ARG:NH1	1:A:979:GLY:O	2.41	0.53
2:B:626:ILE:HD11	2:B:640:LEU:HD11	1.91	0.53
2:B:677:THR:OG1	2:B:679:GLN:OE1	2.26	0.53
2:B:806:THR:OG1	2:B:904:LYS:NZ	2.34	0.53
11:K:83:ASN:HB3	11:K:86:VAL:HG23	1.90	0.53
2:B:782:ASP:O	2:B:950:ASN:ND2	2.42	0.52
4:D:22:ILE:HD11	7:G:43:ILE:HD12	1.90	0.52
9:I:39:LYS:HE2	9:I:42:PHE:HA	1.91	0.52
1:A:87:ASN:O	1:A:91:PHE:N	2.36	0.52
1:A:1256:LYS:O	1:A:1499:ARG:NH2	2.42	0.52
3:C:82:TYR:OH	3:C:125:LYS:NZ	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:TYR:HE2	1:A:316:LEU:HD23	1.74	0.52
2:B:134:ARG:HA	2:B:162:PRO:HA	1.89	0.52
2:B:300:SER:HB3	9:I:49:THR:HG22	1.91	0.52
2:B:851:TYR:HD1	2:B:881:TYR:HE1	1.56	0.52
4:D:25:THR:N	7:G:42:PRO:O	2.38	0.52
1:A:248:PHE:CD1	1:A:442:LYS:CG	2.93	0.52
1:A:1316:VAL:HG21	1:A:1498:ILE:HA	1.91	0.52
2:B:17:ARG:H	2:B:17:ARG:HD2	1.75	0.52
7:G:169:VAL:HG23	7:G:216:HIS:HB3	1.92	0.52
1:A:461:GLU:HA	1:A:466:LEU:H	1.74	0.52
1:A:911:CYS:SG	1:A:912:VAL:N	2.83	0.52
1:A:1019:LEU:HD11	1:A:1193:VAL:HG13	1.91	0.52
10:J:5:VAL:HG22	10:J:15:GLY:HA3	1.91	0.52
1:A:670:ILE:HD12	1:A:671:GLN:H	1.75	0.52
1:A:1655:ASP:HB3	6:F:135:ARG:HB3	1.92	0.52
6:F:62:GLU:OE2	6:F:65:ARG:NH2	2.43	0.52
1:A:475:ARG:HD3	2:B:1070:ARG:HB2	1.91	0.52
1:A:828:CYS:SG	1:A:829:GLY:N	2.75	0.52
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.92	0.52
1:A:883:LEU:HD13	1:A:959:VAL:HG11	1.91	0.52
1:A:1032:VAL:HG21	1:A:1179:ILE:HG21	1.92	0.52
3:C:85:PHE:HE2	3:C:98:ALA:HB2	1.75	0.52
13:M:75:GLN:HE21	13:M:92:LYS:HG3	1.74	0.52
1:A:552:GLU:OE1	1:A:555:LYS:NZ	2.43	0.52
1:A:481:ARG:HB3	2:B:1045:GLN:HB2	1.92	0.51
2:B:421:LEU:HD22	2:B:424:ILE:HD11	1.92	0.51
7:G:137:ILE:HG23	7:G:140:GLN:HE21	1.74	0.51
14:N:62:VAL:HG23	14:N:64:ILE:HG23	1.92	0.51
1:A:9:SER:HB2	2:B:1176:VAL:HG12	1.91	0.51
1:A:1057:ILE:HG12	1:A:1581:HIS:CE1	2.46	0.51
1:A:1128:ASN:OD1	1:A:1128:ASN:N	2.43	0.51
1:A:535:GLN:HB3	1:A:543:LEU:HD11	1.93	0.51
1:A:1612:LYS:HB3	1:A:1621:PHE:CD2	2.45	0.51
2:B:247:THR:OG1	2:B:477:ASP:OD1	2.26	0.51
2:B:581:PRO:HB3	2:B:638:PRO:HG2	1.92	0.51
1:A:227:LEU:O	1:A:230:ARG:N	2.42	0.51
1:A:496:GLY:H	1:A:615:ARG:HB2	1.75	0.51
1:A:1262:LEU:HD13	1:A:1494:ARG:HG2	1.91	0.51
2:B:1153:ILE:HG13	2:B:1155:ASP:H	1.76	0.51
1:A:653:THR:O	1:A:667:ARG:NH2	2.41	0.51
1:A:757:ASN:ND2	1:A:767:ASN:H	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:HIS:CE1	2:B:712:SER:H	2.28	0.51
4:D:30:HIS:HA	7:G:39:VAL:HG23	1.93	0.51
5:E:147:HIS:CD2	5:E:149:LEU:H	2.28	0.51
7:G:40:ARG:HD2	7:G:121:ASN:HB3	1.93	0.51
1:A:716:PRO:O	1:A:730:GLN:NE2	2.32	0.51
2:B:585:CYS:SG	2:B:587:GLN:NE2	2.84	0.51
2:B:857:PRO:HB3	2:B:871:ILE:HG23	1.92	0.51
5:E:78:LEU:HD11	5:E:109:ILE:HG12	1.93	0.51
8:H:95:TYR:HD2	8:H:144:ILE:HD13	1.76	0.51
16:S:59:DG:N2	17:T:13:DT:O2	2.44	0.51
1:A:771:PHE:HE1	1:A:776:LEU:HD13	1.76	0.51
2:B:200:GLU:HB2	2:B:488:ALA:HB3	1.93	0.51
1:A:1057:ILE:H	1:A:1057:ILE:HD12	1.76	0.51
6:F:101:ILE:HD12	6:F:105:ALA:HB3	1.91	0.51
1:A:472:MET:SD	1:A:1614:SER:OG	2.64	0.50
1:A:678:VAL:HA	1:A:780:ILE:HD11	1.93	0.50
1:A:1288:ARG:NH1	1:A:1481:GLU:OE2	2.45	0.50
2:B:596:VAL:HG22	2:B:597:SER:H	1.75	0.50
1:A:580:HIS:CG	1:A:581:ILE:H	2.28	0.50
2:B:1189:LEU:HG	2:B:1194:ILE:HD11	1.92	0.50
3:C:41:GLU:OE1	3:C:58:ASN:ND2	2.44	0.50
1:A:618:TYR:OH	2:B:780:GLY:O	2.21	0.50
1:A:827:THR:HG21	2:B:1026:ILE:HA	1.92	0.50
3:C:117:ASP:HB3	3:C:120:LEU:HD23	1.93	0.50
8:H:111:LEU:HD23	8:H:128:ASN:HB3	1.92	0.50
1:A:872:ASP:HB3	1:A:875:LEU:HG	1.92	0.50
1:A:1275:THR:HG23	1:A:1289:SER:HB2	1.92	0.50
1:A:253:GLU:HB2	1:A:315:ILE:HD11	1.93	0.50
13:M:15:VAL:HG11	14:N:65:SER:HA	1.93	0.50
1:A:250:LYS:HG3	1:A:252:PHE:CE1	2.47	0.50
1:A:1608:SER:HB3	1:A:1611:MET:HG2	1.92	0.50
1:A:444:GLN:C	1:A:446:ARG:N	2.68	0.50
1:A:591:ARG:HH22	1:A:631:ASP:HB3	1.77	0.50
1:A:1248:ASP:OD1	1:A:1517:ARG:NH2	2.45	0.50
1:A:95:TYR:CE2	1:A:99:ARG:HD2	2.47	0.50
2:B:545:PHE:HB3	2:B:549:CYS:SG	2.52	0.50
2:B:655:TYR:O	2:B:659:ASP:HA	2.12	0.50
1:A:79:ILE:HD12	1:A:390:LEU:HD21	1.93	0.49
2:B:217:ILE:HD13	2:B:219:ARG:HE	1.77	0.49
2:B:576:THR:HG1	2:B:595:TRP:CD1	2.30	0.49
2:B:811:LEU:N	2:B:811:LEU:CD1	2.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:819:ASP:OD1	2:B:819:ASP:N	2.44	0.49
5:E:123:LEU:O	5:E:126:SER:OG	2.29	0.49
1:A:438:ILE:HA	1:A:456:VAL:HG12	1.94	0.49
1:A:672:ASP:HA	2:B:952:HIS:CE1	2.47	0.49
1:A:1047:GLN:HE22	1:A:1559:ARG:HH22	1.58	0.49
2:B:1020:GLU:OE2	3:C:295:ARG:NH1	2.45	0.49
3:C:54:PHE:HB3	3:C:300:PHE:HB2	1.93	0.49
5:E:116:ILE:HD13	5:E:121:MET:HE3	1.93	0.49
1:A:1647:ASN:HD21	2:B:1088:LEU:HD23	1.77	0.49
5:E:100:ILE:HA	5:E:105:PHE:HD2	1.77	0.49
16:S:57:DA:H2''	16:S:58:DA:C8	2.47	0.49
1:A:1113:HIS:NE2	5:E:150:VAL:O	2.46	0.49
1:A:1265:GLU:OE1	1:A:1265:GLU:N	2.46	0.49
2:B:545:PHE:HE1	2:B:649:MET:HE3	1.77	0.49
5:E:147:HIS:HB3	5:E:150:VAL:HG22	1.94	0.49
6:F:108:PHE:HB2	6:F:129:LYS:HD3	1.93	0.49
10:J:10:CYS:SG	10:J:11:GLY:N	2.86	0.49
14:N:114:GLU:OE1	14:N:115:SER:N	2.46	0.49
2:B:939:SER:HA	2:B:1013:MET:HG2	1.93	0.49
1:A:494:GLU:HG2	1:A:604:LYS:HD2	1.94	0.49
1:A:709:ARG:HG2	1:A:710:SER:H	1.77	0.49
1:A:1437:ASN:HD22	1:A:1438:ASN:H	1.61	0.49
2:B:144:SER:HB3	2:B:148:GLY:HA2	1.94	0.49
2:B:161:LEU:HD21	2:B:413:LEU:HD11	1.94	0.49
1:A:865:ASP:HB2	1:A:866:LYS:HZ3	1.76	0.49
1:A:866:LYS:N	1:A:866:LYS:CD	2.73	0.49
2:B:325:GLN:HG2	13:M:107:ASN:HD21	1.77	0.49
5:E:20:LYS:NZ	5:E:34:GLU:O	2.43	0.49
1:A:489:ASN:ND2	11:K:94:PRO:O	2.46	0.49
1:A:715:LEU:HB3	1:A:730:GLN:HE21	1.77	0.49
2:B:265:ARG:HD3	2:B:474:SER:HA	1.95	0.49
2:B:681:ILE:HG22	14:N:154:ARG:HH21	1.78	0.49
1:A:1501:ILE:HG23	1:A:1504:ILE:HB	1.94	0.48
2:B:674:ILE:HG22	2:B:688:HIS:HB2	1.96	0.48
6:F:57:ASP:OD1	6:F:57:ASP:N	2.44	0.48
7:G:69:LEU:HA	7:G:72:LYS:HD2	1.95	0.48
7:G:217:TRP:HE1	7:G:225:ILE:HG12	1.78	0.48
10:J:36:LEU:HD12	10:J:41:LEU:HD12	1.94	0.48
16:S:66:DA:H2''	16:S:67:DA:C8	2.48	0.48
2:B:244:THR:HA	2:B:411:MET:HE3	1.94	0.48
2:B:361:HIS:CD2	2:B:590:GLY:HA3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1186:ASP:HB3	2:B:1196:LEU:HD21	1.94	0.48
8:H:5:LEU:O	8:H:133:ASN:ND2	2.46	0.48
7:G:139:ILE:HB	7:G:146:GLY:HA3	1.94	0.48
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.95	0.48
1:A:986:PHE:O	2:B:960:ILE:HG21	2.13	0.48
1:A:1024:THR:O	1:A:1028:GLU:HG3	2.13	0.48
1:A:1562:ILE:O	1:A:1566:ILE:HG13	2.13	0.48
1:A:1591:ARG:HE	1:A:1592:GLN:HG2	1.77	0.48
8:H:114:VAL:HG22	8:H:125:LEU:HB2	1.94	0.48
1:A:466:LEU:HD22	1:A:469:LYS:HB3	1.96	0.48
1:A:720:PHE:HB2	8:H:96:VAL:HB	1.94	0.48
2:B:1064:LYS:C	2:B:1066:HIS:H	2.20	0.48
2:B:1089:GLN:HE21	2:B:1093:LEU:HD23	1.77	0.48
8:H:17:PRO:HA	8:H:24:CYS:HA	1.95	0.48
1:A:109:ARG:HB2	1:A:227:LEU:HD13	1.96	0.48
1:A:247:GLY:O	1:A:248:PHE:HB2	2.12	0.48
2:B:558:VAL:HG13	2:B:561:ILE:HB	1.95	0.48
16:S:65:DG:H2"	16:S:66:DA:C8	2.48	0.48
1:A:942:GLN:HA	1:A:947:LEU:HA	1.96	0.48
9:I:15:ASP:HB2	9:I:32:GLN:HE22	1.79	0.48
14:N:170:HIS:CG	14:N:171:PHE:H	2.31	0.48
2:B:214:PRO:HB3	2:B:377:MET:HG2	1.95	0.48
4:D:44:ILE:HD12	4:D:86:ILE:HG23	1.96	0.48
7:G:50:ALA:HB3	7:G:53:TYR:HD2	1.78	0.48
2:B:156:ARG:NH2	2:B:455:GLU:OE2	2.43	0.48
2:B:973:ALA:HB1	10:J:44:TYR:HB2	1.96	0.48
2:B:1104:CYS:HB3	2:B:1107:CYS:SG	2.53	0.48
4:D:27:LEU:HD23	7:G:23:GLN:HE21	1.78	0.48
1:A:964:LYS:NZ	1:A:970:LYS:O	2.46	0.48
2:B:28:PRO:HB2	2:B:178:TYR:HA	1.94	0.48
2:B:839:LYS:HE2	2:B:840:LEU:HD13	1.95	0.48
2:B:918:SER:HB2	2:B:924:LYS:HA	1.96	0.48
1:A:588:LEU:HB3	1:A:636:HIS:HB2	1.96	0.47
1:A:760:TRP:CB	1:A:764:SER:HB3	2.43	0.47
1:A:913:PRO:HB3	1:A:926:GLN:HE22	1.79	0.47
2:B:73:ILE:HD13	2:B:428:VAL:HG23	1.95	0.47
2:B:307:GLU:HG3	9:I:7:LEU:HD11	1.94	0.47
11:K:80:ILE:HG12	11:K:120:GLY:HA3	1.96	0.47
1:A:493:ASN:HA	1:A:653:THR:HG21	1.96	0.47
2:B:840:LEU:HD21	2:B:860:ALA:H	1.78	0.47
5:E:5:ASN:OD1	5:E:52:ARG:NH2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:HB3	1:A:355:PHE:HD1	1.78	0.47
1:A:1316:VAL:HG21	1:A:1498:ILE:HD12	1.95	0.47
2:B:229:TYR:CD1	2:B:253:LEU:HD22	2.49	0.47
2:B:839:LYS:HE2	2:B:840:LEU:HB2	1.96	0.47
2:B:1083:GLY:HA3	6:F:88:TYR:HE2	1.78	0.47
5:E:114:ASN:OD1	5:E:115:ASN:N	2.46	0.47
8:H:116:TYR:OH	8:H:140:ALA:O	2.24	0.47
1:A:172:ASP:OD1	1:A:172:ASP:N	2.47	0.47
1:A:1560:ASN:ND2	5:E:149:LEU:O	2.40	0.47
2:B:478:LEU:H	2:B:478:LEU:HD23	1.79	0.47
1:A:498:PRO:HB2	1:A:500:VAL:HG22	1.96	0.47
7:G:56:ASN:ND2	7:G:59:GLN:OE1	2.47	0.47
13:M:83:PRO:HB3	14:N:49:LYS:N	2.30	0.47
1:A:110:LEU:HG	1:A:227:LEU:HB3	1.96	0.47
1:A:603:HIS:CE1	1:A:620:ASN:HD21	2.33	0.47
1:A:729:LYS:HZ2	8:H:120:GLY:HA2	1.80	0.47
1:A:757:ASN:O	1:A:760:TRP:N	2.48	0.47
1:A:1038:ILE:HD11	1:A:1047:GLN:HB2	1.97	0.47
1:A:1162:ASN:OD1	1:A:1165:LYS:NZ	2.35	0.47
2:B:52:LEU:HA	2:B:60:LEU:H	1.79	0.47
2:B:209:GLN:HE22	2:B:235:GLN:HG3	1.79	0.47
2:B:673:ASN:ND2	2:B:685:VAL:O	2.47	0.47
3:C:90:SER:HA	3:C:200:GLN:HG2	1.96	0.47
3:C:107:LYS:HE3	3:C:187:ALA:HA	1.96	0.47
1:A:35:PRO:HD3	1:A:394:LEU:HD12	1.96	0.47
1:A:458:GLN:CD	1:A:458:GLN:H	2.22	0.47
1:A:697:TYR:HB2	11:K:88:PHE:CE2	2.50	0.47
1:A:727:THR:HG23	1:A:730:GLN:H	1.79	0.47
2:B:980:ASP:OD1	2:B:982:THR:OG1	2.32	0.47
2:B:1014:TYR:OH	3:C:293:ARG:NH1	2.44	0.47
11:K:79:VAL:HG21	11:K:124:LEU:HD23	1.97	0.47
1:A:1459:LYS:HB3	1:A:1473:LYS:HB3	1.95	0.47
3:C:54:PHE:HE2	3:C:56:LEU:HD12	1.80	0.47
13:M:52:VAL:HG12	13:M:65:TYR:HA	1.96	0.47
17:T:20:DT:C2'	17:T:21:DG:H5'	2.45	0.47
1:A:239:PHE:CD2	1:A:260:GLN:HG3	2.50	0.46
1:A:918:LYS:O	1:A:923:ASN:ND2	2.49	0.46
1:A:949:GLN:HG2	1:A:981:TYR:HB2	1.96	0.46
2:B:809:VAL:HG13	2:B:901:VAL:HB	1.97	0.46
3:C:136:LEU:HD23	3:C:204:LEU:HD21	1.97	0.46
10:J:14:VAL:HG13	10:J:50:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:78:VAL:HA	14:N:54:TRP:O	2.15	0.46
16:S:69:DA:H5'	16:S:69:DA:C8	2.49	0.46
1:A:125:LEU:HD11	1:A:133:SER:HB3	1.96	0.46
1:A:521:GLN:HA	1:A:524:ILE:HG22	1.97	0.46
1:A:1226:VAL:HG13	1:A:1598:PHE:HD2	1.81	0.46
2:B:166:GLN:N	2:B:170:CYS:SG	2.88	0.46
2:B:1077:ASP:OD1	2:B:1078:ALA:N	2.48	0.46
3:C:69:ARG:HD2	11:K:71:THR:HG22	1.98	0.46
1:A:695:TYR:HE1	1:A:820:TYR:HA	1.80	0.46
1:A:706:HIS:CE1	1:A:815:ARG:HH22	2.33	0.46
2:B:1019:GLY:HA3	3:C:65:ASN:OD1	2.15	0.46
13:M:82:ASN:HB2	13:M:83:PRO:HD2	1.97	0.46
14:N:80:MET:HB2	14:N:87:TYR:HB2	1.96	0.46
1:A:1180:ASN:ND2	6:F:87:LYS:HG2	2.30	0.46
2:B:656:LEU:HD21	2:B:689:VAL:HG13	1.96	0.46
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.98	0.46
12:L:31:CYS:SG	12:L:32:ALA:N	2.88	0.46
14:N:35:LEU:HD11	14:N:112:PRO:HB2	1.97	0.46
1:A:835:LEU:HA	1:A:917:MET:H	1.80	0.46
2:B:282:HIS:HB2	13:M:99:LYS:HD3	1.97	0.46
2:B:941:THR:HG22	14:N:171:PHE:CE1	2.51	0.46
2:B:1123:ILE:HG22	2:B:1124:SER:H	1.80	0.46
2:B:394:PRO:O	2:B:505:ARG:NH2	2.48	0.46
2:B:654:ARG:HB2	2:B:691:PHE:HD1	1.81	0.46
1:A:249:THR:HB	1:A:431:GLN:HG2	1.97	0.46
2:B:165:LEU:HD12	2:B:172:LEU:HD12	1.97	0.46
2:B:979:GLN:HG2	2:B:996:PHE:CE1	2.51	0.46
2:B:1105:ARG:NH1	2:B:1172:GLU:OE2	2.49	0.46
1:A:764:SER:O	1:A:766:GLU:N	2.43	0.46
6:F:93:ILE:HD11	6:F:125:LEU:HD12	1.97	0.46
11:K:54:THR:HG22	11:K:61:ALA:HA	1.97	0.46
1:A:111:LYS:HG2	1:A:113:VAL:H	1.81	0.46
1:A:991:LYS:HB3	1:A:994:GLU:OE1	2.16	0.46
1:A:1613:MET:HE1	1:A:1622:LEU:HA	1.98	0.46
8:H:56:THR:HG21	8:H:145:ARG:HD2	1.97	0.46
1:A:78:HIS:HB2	1:A:359:VAL:HB	1.98	0.46
1:A:940:VAL:HA	1:A:943:ILE:HG22	1.98	0.46
2:B:110:ASN:N	2:B:118:GLU:OE2	2.49	0.46
3:C:82:TYR:HB2	3:C:207:HIS:HB2	1.98	0.46
5:E:25:ASP:OD2	5:E:187:TYR:OH	2.32	0.46
13:M:74:ASN:HA	14:N:59:PRO:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:ASN:HD22	6:F:87:LYS:HG2	1.81	0.45
2:B:185:GLU:O	10:J:63:TYR:OH	2.20	0.45
2:B:383:SER:OG	2:B:389:CYS:SG	2.68	0.45
2:B:558:VAL:O	2:B:560:ARG:N	2.46	0.45
7:G:66:LEU:HD21	7:G:84:TYR:CZ	2.51	0.45
10:J:21:TYR:OH	10:J:32:GLU:OE1	2.33	0.45
1:A:696:ILE:HD11	1:A:731:ILE:HG23	1.98	0.45
2:B:1186:ASP:OD1	2:B:1186:ASP:N	2.50	0.45
6:F:85:MET:HG2	6:F:89:GLU:OE2	2.16	0.45
1:A:211:THR:HG21	5:E:215:MET:HE1	1.98	0.45
1:A:449:GLY:C	1:A:451:VAL:N	2.73	0.45
1:A:821:ILE:HG23	1:A:825:ALA:HA	1.97	0.45
1:A:332:GLN:HE21	1:A:336:GLN:HE21	1.64	0.45
2:B:242:ASP:O	2:B:243:GLN:HG2	2.17	0.45
1:A:948:GLY:O	1:A:982:VAL:HG22	2.17	0.45
1:A:1219:ILE:HG22	1:A:1220:PRO:HD3	1.98	0.45
2:B:260:PHE:HB3	2:B:271:VAL:HG13	1.98	0.45
2:B:324:THR:O	2:B:328:GLN:HG2	2.17	0.45
7:G:148:LEU:HB3	7:G:151:ASP:HA	1.98	0.45
1:A:467:PHE:HA	1:A:471:MET:HE2	1.97	0.45
1:A:732:ILE:HA	1:A:735:VAL:HG12	1.99	0.45
1:A:1238:MET:HE3	1:A:1524:VAL:HA	1.99	0.45
1:A:1276:THR:HB	9:I:45:LEU:HB3	1.99	0.45
2:B:1119:ARG:HH12	2:B:1160:GLU:HB3	1.82	0.45
7:G:87:LEU:HA	7:G:120:VAL:HG12	1.98	0.45
2:B:502:MET:HE1	2:B:542:LEU:HD13	1.98	0.45
2:B:1127:CYS:SG	2:B:1171:ASN:ND2	2.89	0.45
3:C:87:ASN:ND2	3:C:201:GLU:OE2	2.50	0.45
3:C:100:ARG:HH22	10:J:2:ILE:HG23	1.81	0.45
5:E:185:ALA:HA	5:E:190:LEU:HD12	1.99	0.45
1:A:213:ASN:ND2	1:A:1606:SER:O	2.49	0.45
1:A:709:ARG:HG2	1:A:710:SER:N	2.32	0.45
1:A:982:VAL:HA	1:A:994:GLU:HG2	1.98	0.45
2:B:1189:LEU:HD23	2:B:1196:LEU:HD23	1.97	0.45
3:C:319:ARG:NH2	11:K:132:GLU:OE2	2.49	0.45
2:B:74:PHE:CE2	2:B:94:LYS:HB3	2.52	0.45
2:B:137:LEU:HB2	2:B:161:LEU:HD13	1.97	0.45
2:B:497:ILE:HG23	2:B:699:ILE:HG21	1.99	0.45
1:A:449:GLY:C	1:A:451:VAL:H	2.24	0.44
2:B:537:SER:OG	2:B:538:PRO:HD3	2.17	0.44
2:B:810:ASP:HB3	2:B:900:THR:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:889:GLY:O	12:L:54:ARG:HD2	2.16	0.44
2:B:919:SER:HB2	2:B:1032:TYR:CE1	2.51	0.44
5:E:16:PHE:CE2	5:E:20:LYS:HE3	2.52	0.44
2:B:557:ASP:OD1	2:B:557:ASP:N	2.49	0.44
13:M:74:ASN:OD1	13:M:75:GLN:N	2.50	0.44
1:A:580:HIS:CG	1:A:581:ILE:N	2.84	0.44
2:B:252:TYR:CD1	2:B:385:VAL:HG11	2.51	0.44
2:B:558:VAL:C	2:B:560:ARG:H	2.25	0.44
2:B:1112:THR:OG1	2:B:1130:ARG:HB2	2.17	0.44
8:H:8:ASP:OD2	8:H:30:SER:OG	2.32	0.44
16:S:56:DA:H2''	16:S:57:DA:C8	2.52	0.44
1:A:561:LEU:HD11	1:A:577:VAL:HG21	1.98	0.44
1:A:1196:PRO:O	1:A:1200:MET:N	2.51	0.44
2:B:129:ARG:HG2	12:L:54:ARG:HH21	1.83	0.44
2:B:803:MET:SD	2:B:909:ARG:NE	2.84	0.44
2:B:977:ILE:HD13	14:N:163:VAL:HG21	1.99	0.44
3:C:326:GLU:HG2	3:C:329:LYS:HE3	1.99	0.44
14:N:58:PHE:CD2	14:N:62:VAL:HG21	2.52	0.44
1:A:256:LEU:HD23	1:A:264:ASN:HD21	1.83	0.44
2:B:610:TYR:CE1	14:N:146:PRO:HG2	2.51	0.44
3:C:73:SER:O	3:C:214:GLY:N	2.50	0.44
8:H:95:TYR:HE2	8:H:97:MET:HE3	1.83	0.44
2:B:887:LEU:HD12	12:L:56:LEU:HD12	1.98	0.44
2:B:954:PHE:N	2:B:955:PRO:HD2	2.32	0.44
2:B:1079:LEU:HD11	2:B:1087:LEU:HB3	2.00	0.44
2:B:1104:CYS:CB	2:B:1107:CYS:SG	3.04	0.44
1:A:511:VAL:HG11	1:A:561:LEU:HD21	2.00	0.44
1:A:516:ILE:H	1:A:516:ILE:HG13	1.67	0.44
1:A:1504:ILE:HG12	1:A:1523:GLY:HA3	1.99	0.44
13:M:66:THR:HG23	13:M:95:VAL:O	2.18	0.44
1:A:79:ILE:H	1:A:360:LEU:H	1.64	0.44
1:A:232:LYS:HE2	1:A:239:PHE:CE2	2.53	0.44
1:A:260:GLN:N	1:A:260:GLN:OE1	2.51	0.44
1:A:351:LYS:HG2	1:A:352:ALA:H	1.83	0.44
1:A:1512:PRO:HB3	1:A:1517:ARG:HA	2.00	0.44
2:B:21:ARG:HH22	10:J:54:VAL:HA	1.82	0.44
2:B:727:GLY:HA2	2:B:744:LEU:HD22	1.98	0.44
2:B:891:GLU:H	12:L:54:ARG:HH11	1.64	0.44
6:F:58:PHE:HA	6:F:61:HIS:HD2	1.82	0.44
9:I:28:VAL:HG22	9:I:38:PRO:HD3	2.00	0.44
17:T:21:DG:OP2	17:T:21:DG:H3'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:GLN:HG2	2:B:670:VAL:HG11	2.00	0.44
2:B:499:HIS:HA	2:B:502:MET:HG2	2.00	0.44
4:D:19:PRO:HA	7:G:47:VAL:HG12	1.99	0.44
13:M:105:SER:OG	13:M:106:LYS:N	2.50	0.44
1:A:1113:HIS:O	5:E:152:LYS:NZ	2.38	0.43
2:B:256:GLY:HA3	2:B:308:LEU:HD13	1.99	0.43
2:B:338:PHE:CD2	2:B:353:VAL:HG12	2.52	0.43
2:B:1115:GLN:HG3	2:B:1126:VAL:HB	2.00	0.43
3:C:246:ARG:HH22	3:C:284:GLU:HB2	1.82	0.43
1:A:489:ASN:HD21	1:A:701:ARG:HH12	1.66	0.43
1:A:988:SER:HB2	2:B:988:GLU:HA	1.99	0.43
2:B:527:PHE:CE2	2:B:666:PRO:HA	2.53	0.43
3:C:246:ARG:NH2	3:C:284:GLU:OE1	2.51	0.43
14:N:41:ASN:OD1	14:N:42:GLY:N	2.51	0.43
1:A:1570:PHE:CG	1:A:1575:ILE:HD11	2.53	0.43
2:B:152:LEU:HD23	2:B:443:LYS:HD2	2.00	0.43
2:B:588:ILE:HA	2:B:642:LEU:HB2	2.01	0.43
2:B:1043:LYS:O	2:B:1063:ARG:NH2	2.50	0.43
4:D:40:LEU:HD11	4:D:93:GLN:HB2	2.01	0.43
8:H:124:ARG:NH1	8:H:126:GLU:OE2	2.51	0.43
11:K:128:CYS:HA	11:K:131:VAL:HG12	2.00	0.43
1:A:586:VAL:HG11	1:A:647:ALA:HB1	2.00	0.43
1:A:748:ASN:HD22	1:A:1071:ASP:HB3	1.83	0.43
3:C:275:VAL:HG13	3:C:291:LEU:HD23	2.01	0.43
14:N:111:VAL:O	14:N:120:LYS:HB2	2.18	0.43
1:A:757:ASN:OD1	1:A:767:ASN:N	2.51	0.43
1:A:1292:ILE:O	1:A:1471:GLU:HA	2.18	0.43
2:B:70:GLU:OE2	2:B:96:SER:OG	2.26	0.43
2:B:613:VAL:HG22	2:B:660:LYS:HE3	2.01	0.43
3:C:326:GLU:OE2	3:C:330:ASN:ND2	2.45	0.43
5:E:14:ARG:HB3	5:E:141:VAL:O	2.19	0.43
6:F:58:PHE:HA	6:F:61:HIS:CD2	2.54	0.43
7:G:126:GLN:OE1	7:G:126:GLN:N	2.51	0.43
1:A:111:LYS:H	1:A:111:LYS:HD2	1.83	0.43
1:A:204:GLU:HG2	1:A:205:ARG:HD3	2.00	0.43
1:A:670:ILE:H	1:A:670:ILE:HG13	1.54	0.43
1:A:975:ASP:OD1	1:A:976:ALA:N	2.50	0.43
1:A:1641:ILE:HG21	2:B:1076:ARG:HH11	1.83	0.43
2:B:293:ILE:HG23	2:B:302:LEU:HD22	1.99	0.43
2:B:622:ILE:HG13	2:B:663:ILE:HG22	2.00	0.43
2:B:1006:ASN:HD21	2:B:1010:ASN:N	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:LEU:HD21	3:C:167:LEU:HD13	2.00	0.43
4:D:25:THR:HA	6:F:58:PHE:HZ	1.84	0.43
8:H:95:TYR:HB3	8:H:144:ILE:HB	2.00	0.43
1:A:757:ASN:ND2	1:A:764:SER:O	2.51	0.43
1:A:884:ARG:NH2	2:B:634:ARG:HE	2.16	0.43
1:A:1461:ASN:OD1	1:A:1462:PHE:N	2.51	0.43
3:C:110:PRO:HB2	3:C:316:LYS:NZ	2.33	0.43
9:I:15:ASP:OD2	9:I:32:GLN:NE2	2.51	0.43
1:A:1020:GLN:HE22	1:A:1191:GLN:HA	1.84	0.43
1:A:1110:LYS:HD2	1:A:1111:GLU:HB2	2.00	0.43
2:B:299:ASP:OD1	2:B:299:ASP:N	2.51	0.43
2:B:651:ARG:HH11	2:B:695:ASN:ND2	2.17	0.43
2:B:1025:ASP:OD1	2:B:1025:ASP:N	2.50	0.43
9:I:23:VAL:HG12	9:I:24:LEU:H	1.84	0.43
13:M:103:LYS:HD2	13:M:103:LYS:HA	1.88	0.43
1:A:483:VAL:HA	1:A:632:GLU:HA	2.01	0.43
1:A:525:ASN:O	1:A:554:ARG:NH1	2.51	0.43
1:A:1060:GLU:OE1	1:A:1060:GLU:N	2.33	0.43
2:B:1000:LEU:HB3	2:B:1005:TYR:HB2	1.99	0.43
5:E:111:VAL:HG22	5:E:135:PHE:HB2	2.01	0.43
1:A:226:LYS:HD2	1:A:226:LYS:HA	1.80	0.43
1:A:525:ASN:HD21	1:A:529:LYS:HD3	1.83	0.43
2:B:395:ASP:OD1	2:B:395:ASP:N	2.52	0.43
3:C:142:ARG:HE	3:C:198:PRO:HG3	1.84	0.43
3:C:274:THR:OG1	14:N:170:HIS:NE2	2.50	0.43
8:H:77:ARG:HD2	8:H:77:ARG:H	1.84	0.43
9:I:34:LYS:HE2	9:I:34:LYS:HB3	1.90	0.43
1:A:462:LYS:N	1:A:466:LEU:HB2	2.34	0.42
1:A:674:ILE:HD13	1:A:933:ALA:HA	2.01	0.42
2:B:521:LEU:HD23	2:B:523:GLU:H	1.83	0.42
2:B:656:LEU:HB2	2:B:657:PRO:HD3	2.01	0.42
9:I:17:LEU:HD13	9:I:28:VAL:HG21	2.01	0.42
13:M:22:ALA:O	14:N:110:LEU:HG	2.19	0.42
1:A:555:LYS:HZ2	1:A:555:LYS:HB2	1.83	0.42
1:A:882:ILE:HG13	1:A:888:LYS:HB3	2.01	0.42
2:B:651:ARG:C	2:B:663:ILE:HD12	2.44	0.42
2:B:773:VAL:HG13	2:B:947:ILE:HD11	2.00	0.42
3:C:36:PHE:HZ	3:C:59:ILE:HG13	1.83	0.42
11:K:66:VAL:O	11:K:67:GLU:HG3	2.19	0.42
1:A:324:LEU:HA	1:A:327:VAL:HG22	2.00	0.42
1:A:764:SER:C	1:A:766:GLU:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1053:ASN:OD1	2:B:1054:SER:N	2.44	0.42
3:C:110:PRO:HD2	3:C:308:MET:HE3	2.02	0.42
3:C:239:ILE:H	3:C:239:ILE:HG13	1.72	0.42
10:J:1:MET:HA	10:J:56:LEU:HB3	2.01	0.42
1:A:573:LEU:HD11	7:G:113:PHE:HZ	1.83	0.42
2:B:497:ILE:HG21	2:B:699:ILE:HG12	2.01	0.42
2:B:966:SER:HB2	2:B:1027:TYR:OH	2.20	0.42
2:B:1063:ARG:C	2:B:1066:HIS:H	2.27	0.42
3:C:58:ASN:HA	3:C:296:ASN:CG	2.45	0.42
3:C:92:ILE:HD13	3:C:97:LEU:HD23	2.02	0.42
7:G:70:VAL:O	7:G:72:LYS:NZ	2.47	0.42
10:J:28:ASP:HB3	10:J:30:LEU:HD23	2.01	0.42
13:M:18:GLN:OE1	13:M:18:GLN:N	2.47	0.42
14:N:29:PHE:CD2	14:N:30:LYS:HG2	2.55	0.42
1:A:98:LEU:HD21	1:A:324:LEU:HD21	2.01	0.42
1:A:1054:ALA:O	1:A:1179:ILE:N	2.48	0.42
5:E:32:GLN:O	5:E:36:GLU:HG2	2.20	0.42
6:F:114:GLU:OE1	6:F:119:ARG:NH2	2.38	0.42
8:H:93:TYR:CE2	8:H:145:ARG:HG3	2.54	0.42
1:A:110:LEU:HB3	1:A:114:GLU:OE2	2.20	0.42
1:A:190:ASP:OD1	1:A:191:MET:N	2.52	0.42
1:A:248:PHE:HD1	1:A:442:LYS:HD2	1.83	0.42
1:A:899:LYS:HB3	1:A:899:LYS:HE3	1.78	0.42
1:A:1437:ASN:ND2	1:A:1438:ASN:H	2.16	0.42
2:B:438:ILE:HD11	2:B:445:TYR:HB2	2.01	0.42
2:B:643:PHE:CE2	2:B:648:ARG:HB3	2.54	0.42
2:B:1033:TYR:HD1	2:B:1033:TYR:HA	1.72	0.42
13:M:40:LEU:O	14:N:31:LYS:HG2	2.20	0.42
1:A:697:TYR:CE1	11:K:104:ARG:HB2	2.55	0.42
1:A:708:THR:HG21	1:A:741:PRO:HA	2.01	0.42
1:A:1314:GLN:HE22	1:A:1460:TYR:HE2	1.67	0.42
2:B:839:LYS:HE3	2:B:857:PRO:HG2	2.00	0.42
2:B:919:SER:HB2	2:B:1032:TYR:HE1	1.85	0.42
3:C:71:MET:HE1	3:C:313:ILE:HG23	2.01	0.42
8:H:28:ALA:O	8:H:38:LEU:N	2.52	0.42
12:L:38:LEU:HD22	12:L:49:LYS:HE2	2.02	0.42
1:A:120:CYS:HB3	1:A:189:VAL:HG21	2.00	0.42
1:A:769:VAL:HG12	1:A:779:GLY:HA3	2.01	0.42
2:B:45:HIS:NE2	2:B:205:MET:HE2	2.34	0.42
2:B:207:ILE:HD11	2:B:400:GLN:HB3	2.02	0.42
2:B:566:TYR:CZ	13:M:74:ASN:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:840:LEU:HA	2:B:846:PRO:HA	2.01	0.42
5:E:179:GLN:HG3	5:E:181:ALA:H	1.84	0.42
8:H:10:PHE:HB2	8:H:55:LEU:HB2	2.01	0.42
1:A:204:GLU:OE2	1:A:205:ARG:NH1	2.48	0.42
1:A:736:LEU:HD11	1:A:797:LEU:HD21	2.02	0.42
2:B:91:LEU:HD23	2:B:91:LEU:H	1.84	0.42
2:B:399:HIS:CE1	2:B:636:GLN:HE22	2.38	0.42
3:C:42:VAL:HB	11:K:138:LYS:HG3	2.02	0.42
5:E:121:MET:HE2	5:E:121:MET:HA	2.01	0.42
1:A:1189:ALA:HA	1:A:1581:HIS:HB3	2.02	0.42
2:B:643:PHE:HE2	2:B:648:ARG:HB3	1.84	0.42
2:B:697:LEU:HB3	2:B:701:ALA:HB3	2.02	0.42
2:B:714:ARG:HA	2:B:714:ARG:HD3	1.84	0.42
4:D:33:THR:O	4:D:36:VAL:HG22	2.19	0.42
13:M:53:LEU:HD22	13:M:96:LEU:HD13	2.01	0.42
13:M:81:PHE:O	14:N:51:GLN:HA	2.20	0.42
1:A:1:MET:HG3	2:B:1098:TYR:CZ	2.55	0.41
1:A:30:LYS:HE2	1:A:30:LYS:HB3	1.90	0.41
1:A:1032:VAL:O	1:A:1182:GLY:N	2.51	0.41
2:B:379:ARG:HH11	2:B:580:GLY:HA2	1.85	0.41
3:C:31:TRP:CG	11:K:82:LYS:HZ3	2.38	0.41
1:A:1260:LYS:NZ	1:A:1497:ILE:HG22	2.35	0.41
1:A:1640:ARG:O	1:A:1644:GLY:HA2	2.19	0.41
2:B:79:LEU:HD23	2:B:87:ASN:HD22	1.85	0.41
2:B:403:LEU:HD13	2:B:408:LEU:HD21	2.02	0.41
3:C:278:GLU:OE2	3:C:281:ARG:NH1	2.43	0.41
1:A:129:LEU:HD13	1:A:129:LEU:HA	1.87	0.41
1:A:677:GLY:O	1:A:681:THR:HG22	2.20	0.41
1:A:1079:LYS:HE3	1:A:1080:TYR:CE2	2.55	0.41
2:B:334:PHE:HD2	2:B:337:VAL:HG21	1.85	0.41
2:B:676:VAL:HG22	2:B:693:PRO:HB3	2.02	0.41
5:E:144:ILE:O	5:E:150:VAL:HG21	2.20	0.41
7:G:161:ASN:HB2	7:G:248:THR:HA	2.01	0.41
8:H:11:GLN:N	8:H:29:ALA:O	2.53	0.41
11:K:91:TYR:HA	11:K:103:ILE:HA	2.01	0.41
1:A:1635:ASP:OD1	1:A:1636:SER:N	2.53	0.41
2:B:709:PHE:HB3	2:B:960:ILE:HG23	2.02	0.41
3:C:308:MET:HE2	3:C:308:MET:HA	2.02	0.41
1:A:669:LEU:HD22	1:A:786:TYR:HE2	1.85	0.41
1:A:1561:THR:O	1:A:1565:GLU:HG2	2.20	0.41
2:B:14:ALA:HB2	2:B:980:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:GLU:HG2	12:L:55:ILE:HG13	2.03	0.41
2:B:240:ARG:NH2	2:B:356:ARG:O	2.53	0.41
2:B:529:CYS:HB2	2:B:698:SER:HB3	2.03	0.41
2:B:714:ARG:CZ	2:B:957:ARG:HG3	2.50	0.41
3:C:165:ARG:HD3	3:C:165:ARG:H	1.85	0.41
3:C:230:LEU:HD22	3:C:297:HIS:ND1	2.36	0.41
10:J:64:ASN:ND2	10:J:66:LEU:H	2.18	0.41
13:M:88:ILE:HG21	14:N:54:TRP:CD1	2.56	0.41
1:A:226:LYS:O	1:A:228:LEU:N	2.54	0.41
1:A:617:HIS:HB3	1:A:620:ASN:HB2	2.03	0.41
1:A:1214:ASN:OD1	1:A:1215:VAL:N	2.53	0.41
5:E:198:ILE:HG13	5:E:210:SER:O	2.20	0.41
8:H:10:PHE:O	8:H:54:SER:HA	2.20	0.41
1:A:40:ASN:O	1:A:41:LEU:HG	2.21	0.41
1:A:530:TRP:HA	1:A:531:PRO:HA	1.88	0.41
1:A:549:MET:HE2	1:A:553:GLN:HB3	2.02	0.41
1:A:669:LEU:HD23	1:A:673:HIS:HB2	2.02	0.41
2:B:520:LEU:HD12	2:B:520:LEU:H	1.86	0.41
2:B:564:ILE:HD11	2:B:620:LEU:HD21	2.02	0.41
3:C:294:VAL:HG12	3:C:296:ASN:H	1.86	0.41
5:E:106:GLN:OE1	5:E:107:THR:OG1	2.34	0.41
11:K:81:MET:SD	11:K:89:CYS:HB3	2.60	0.41
17:T:9:DC:H2"	17:T:10:DT:C6	2.55	0.41
1:A:670:ILE:HD12	1:A:671:GLN:N	2.36	0.41
1:A:699:CYS:O	1:A:815:ARG:NH2	2.54	0.41
1:A:847:LEU:HD12	1:A:983:LYS:HD2	2.02	0.41
1:A:1056:ASP:OD1	1:A:1056:ASP:N	2.54	0.41
1:A:1108:HIS:CE1	1:A:1110:LYS:HE3	2.56	0.41
1:A:1566:ILE:HG13	1:A:1566:ILE:H	1.61	0.41
2:B:779:THR:HG22	2:B:948:ILE:HG21	2.01	0.41
5:E:11:ARG:NH2	5:E:14:ARG:HG3	2.35	0.41
5:E:39:LEU:HG	5:E:43:LYS:HE3	2.02	0.41
6:F:151:LEU:HD12	6:F:151:LEU:HA	1.89	0.41
17:T:21:DG:OP2	17:T:22:DA:OP2	2.39	0.41
1:A:462:LYS:HG2	1:A:466:LEU:HD23	2.03	0.41
1:A:657:TYR:HD1	1:A:667:ARG:HD2	1.86	0.41
1:A:1124:LEU:HD23	1:A:1137:SER:HA	2.02	0.41
1:A:1235:THR:HG1	1:A:1237:GLN:HE21	1.65	0.41
1:A:1294:MET:HB3	1:A:1470:CYS:HB3	2.02	0.41
2:B:128:GLN:NE2	2:B:735:HIS:HA	2.36	0.41
2:B:216:ALA:HB1	2:B:384:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:VAL:O	2:B:361:HIS:ND1	2.51	0.41
3:C:38:LYS:HE2	3:C:38:LYS:HB3	1.87	0.41
3:C:103:LEU:HD23	3:C:218:LYS:HB3	2.03	0.41
7:G:11:ARG:O	7:G:15:ARG:NH1	2.54	0.41
8:H:8:ASP:OD1	8:H:32:THR:OG1	2.37	0.41
14:N:170:HIS:CD2	14:N:171:PHE:H	2.39	0.41
1:A:1112:PRO:HG2	1:A:1114:TYR:CE1	2.56	0.41
2:B:28:PRO:HD3	10:J:62:ARG:HH12	1.86	0.41
2:B:607:THR:O	2:B:611:TRP:HD1	2.04	0.41
2:B:623:ASP:OD1	2:B:623:ASP:N	2.53	0.41
2:B:748:GLN:HB3	10:J:52:THR:HG22	2.03	0.41
2:B:790:ASN:HB2	2:B:946:ASP:HA	2.03	0.41
3:C:239:ILE:O	3:C:243:SER:OG	2.33	0.41
11:K:57:ASP:HB3	11:K:59:THR:N	2.36	0.41
1:A:181:LEU:HA	1:A:184:LYS:HG2	2.03	0.40
1:A:236:CYS:HB2	1:A:238:MET:HE1	2.02	0.40
1:A:399:LEU:HD12	1:A:423:LEU:HD13	2.03	0.40
2:B:145:VAL:HG22	2:B:150:GLU:HG2	2.03	0.40
2:B:291:GLY:HA3	2:B:375:LEU:HD12	2.03	0.40
2:B:589:ASP:OD1	2:B:589:ASP:N	2.55	0.40
2:B:718:GLN:HE21	2:B:922:GLY:HA2	1.86	0.40
2:B:787:MET:O	2:B:927:CYS:HA	2.21	0.40
6:F:81:THR:OG1	6:F:146:TRP:NE1	2.54	0.40
1:A:444:GLN:N	1:A:444:GLN:CD	2.77	0.40
1:A:512:THR:OG1	1:A:513:ALA:N	2.52	0.40
2:B:699:ILE:O	2:B:703:LEU:HB2	2.22	0.40
2:B:1203:LYS:HB2	2:B:1203:LYS:HE2	1.87	0.40
3:C:322:LYS:HE3	3:C:322:LYS:HB2	1.87	0.40
10:J:14:VAL:HG11	10:J:49:MET:HG3	2.02	0.40
1:A:476:VAL:HB	2:B:1069:ILE:O	2.22	0.40
1:A:1039:ARG:HD2	6:F:139:PRO:HG2	2.04	0.40
1:A:1055:ILE:HG13	1:A:1580:ARG:HH22	1.86	0.40
2:B:264:TRP:CG	2:B:265:ARG:H	2.39	0.40
2:B:873:THR:OG1	2:B:874:TYR:N	2.55	0.40
10:J:31:ASP:OD1	10:J:31:ASP:N	2.55	0.40
12:L:33:GLU:H	12:L:33:GLU:CD	2.29	0.40
13:M:10:ILE:HD12	13:M:10:ILE:HA	1.95	0.40
1:A:491:GLU:O	1:A:492:THR:HG22	2.21	0.40
1:A:1600:ARG:HH11	1:A:1601:GLN:HG3	1.87	0.40
2:B:1106:GLU:CD	2:B:1106:GLU:H	2.28	0.40
2:B:1110:ILE:O	2:B:1113:THR:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:LEU:HA	1:A:609:PRO:HD3	1.88	0.40
1:A:676:ALA:HB2	1:A:821:ILE:HD11	2.04	0.40
1:A:1000:MET:HE1	2:B:522:PRO:HG3	2.03	0.40
1:A:1082:PRO:O	1:A:1086:ILE:HG13	2.22	0.40
1:A:1482:LYS:HD2	2:B:307:GLU:CD	2.46	0.40
1:A:1620:GLN:O	1:A:1623:THR:OG1	2.27	0.40
2:B:826:GLY:HA2	2:B:844:GLY:HA3	2.04	0.40
2:B:1079:LEU:HD11	2:B:1087:LEU:HD23	2.04	0.40
7:G:140:GLN:HE22	7:G:145:ILE:HG23	1.84	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	1450/1664 (87%)	1364 (94%)	80 (6%)	6 (0%)	30	65
2	B	1160/1203 (96%)	1094 (94%)	64 (6%)	2 (0%)	43	75
3	C	300/335 (90%)	289 (96%)	11 (4%)	0	100	100
4	D	55/137 (40%)	54 (98%)	1 (2%)	0	100	100
5	E	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
6	F	98/155 (63%)	94 (96%)	4 (4%)	0	100	100
7	G	196/326 (60%)	184 (94%)	12 (6%)	0	100	100
8	H	130/146 (89%)	125 (96%)	5 (4%)	0	100	100
9	I	62/125 (50%)	59 (95%)	3 (5%)	0	100	100
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
11	K	98/142 (69%)	92 (94%)	6 (6%)	0	100	100
12	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
13	M	97/415 (23%)	90 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	127/233 (54%)	105 (83%)	22 (17%)	0	100	100
All	All	4093/5236 (78%)	3860 (94%)	225 (6%)	8 (0%)	44	75

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	VAL
2	B	812	ALA
1	A	227	LEU
1	A	248	PHE
1	A	765	LEU
2	B	559	SER
1	A	251	ILE
1	A	757	ASN

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	1293/1465 (88%)	1269 (98%)	24 (2%)	50	67
2	B	1025/1053 (97%)	1008 (98%)	17 (2%)	53	68
3	C	269/296 (91%)	267 (99%)	2 (1%)	76	79
4	D	56/116 (48%)	55 (98%)	1 (2%)	51	68
5	E	196/197 (100%)	192 (98%)	4 (2%)	48	66
6	F	90/137 (66%)	88 (98%)	2 (2%)	45	65
7	G	180/291 (62%)	175 (97%)	5 (3%)	38	60
8	H	117/128 (91%)	117 (100%)	0	100	100
9	I	56/110 (51%)	56 (100%)	0	100	100
10	J	64/65 (98%)	62 (97%)	2 (3%)	35	56
11	K	89/130 (68%)	89 (100%)	0	100	100
12	L	38/57 (67%)	36 (95%)	2 (5%)	20	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	91/371 (24%)	90 (99%)	1 (1%)	65	74
14	N	125/220 (57%)	124 (99%)	1 (1%)	73	77
All	All	3689/4636 (80%)	3628 (98%)	61 (2%)	52	68

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ILE
1	A	103	LEU
1	A	351	LYS
1	A	361	VAL
1	A	399	LEU
1	A	492	THR
1	A	586	VAL
1	A	594	THR
1	A	658	LEU
1	A	669	LEU
1	A	670	ILE
1	A	754	LYS
1	A	772	LYS
1	A	810	LEU
1	A	868	THR
1	A	875	LEU
1	A	1115	LYS
1	A	1202	LEU
1	A	1484	LEU
1	A	1546	VAL
1	A	1566	ILE
1	A	1569	VAL
1	A	1634	LEU
1	A	1643	VAL
2	B	104	ILE
2	B	130	LEU
2	B	179	GLU
2	B	202	LEU
2	B	359	LEU
2	B	421	LEU
2	B	491	ILE
2	B	603	ILE
2	B	658	LEU
2	B	703	LEU

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Mol	Chain	Res	Type
2	B	752	VAL
2	B	852	VAL
2	B	934	ILE
2	B	959	THR
2	B	1033	TYR
2	B	1117	VAL
2	B	1171	ASN
3	C	97	LEU
3	C	258	ILE
4	D	40	LEU
5	E	104	ASN
5	E	124	VAL
5	E	156	LEU
5	E	170	LEU
6	F	60	GLN
6	F	130	ILE
7	G	8	ASN
7	G	49	LEU
7	G	95	LEU
7	G	238	THR
7	G	242	VAL
10	J	30	LEU
10	J	56	LEU
12	L	30	ILE
12	L	43	THR
13	M	95	VAL
14	N	117	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	A	264	ASN
1	A	332	GLN
1	A	344	ASN
1	A	574	ASN
1	A	620	ASN
1	A	748	ASN
1	A	798	HIS
1	A	923	ASN
1	A	926	GLN
1	A	998	HIS

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Mol	Chain	Res	Type
1	A	1020	GLN
1	A	1072	ASN
1	A	1314	GLN
1	A	1436	ASN
1	A	1437	ASN
1	A	1453	HIS
1	A	1564	ASN
1	A	1601	GLN
1	A	1647	ASN
2	B	62	ASN
2	B	87	ASN
2	B	128	GLN
2	B	231	HIS
2	B	321	GLN
2	B	547	HIS
2	B	587	GLN
2	B	636	GLN
2	B	682	GLN
2	B	686	HIS
2	B	718	GLN
2	B	724	GLN
2	B	755	ASN
2	B	912	GLN
2	B	1034	GLN
2	B	1066	HIS
2	B	1100	GLN
2	B	1115	GLN
2	B	1163	GLN
2	B	1171	ASN
3	C	65	ASN
3	C	130	ASN
3	C	216	HIS
3	C	296	ASN
5	E	8	ASN
5	E	104	ASN
6	F	60	GLN
6	F	61	HIS
7	G	26	ASN
7	G	140	GLN
7	G	160	ASN
7	G	161	ASN
7	G	171	ASN

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Mol	Chain	Res	Type
8	H	11	GLN
10	J	64	ASN
11	K	102	ASN
13	M	54	HIS
13	M	75	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	6/10 (60%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

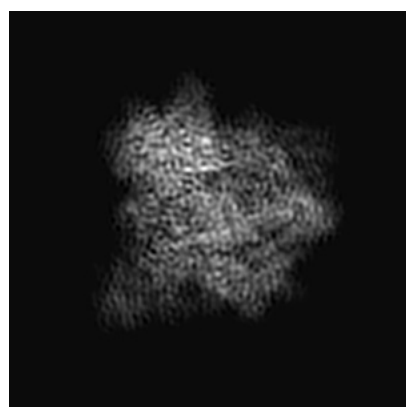
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3448. These allow visual inspection of the internal detail of the map and identification of artifacts.

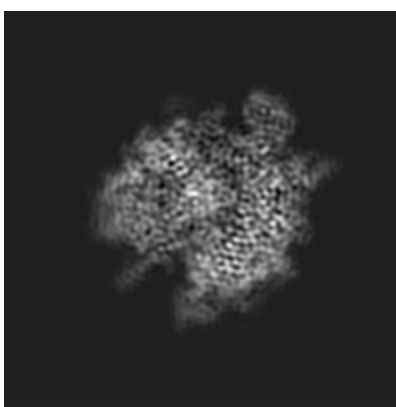
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

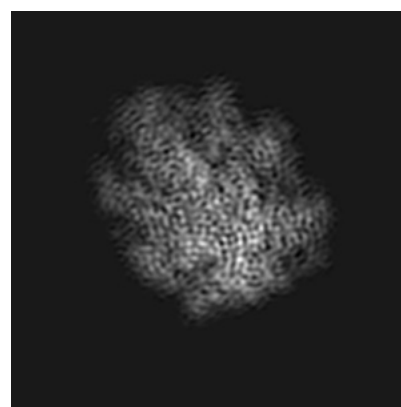
6.1.1 Primary map



X



Y

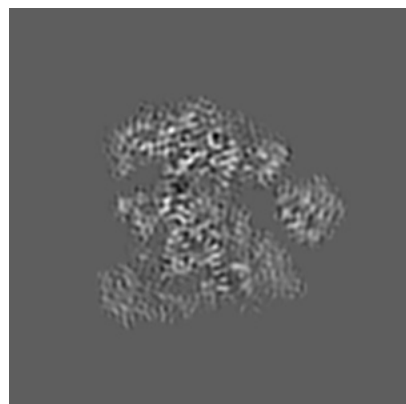


Z

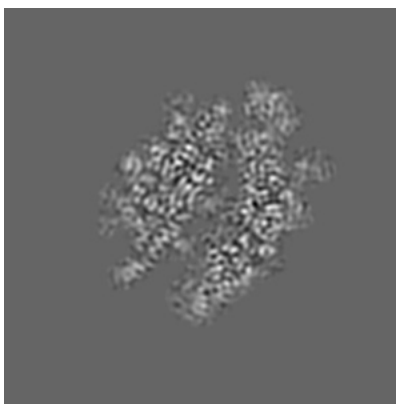
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

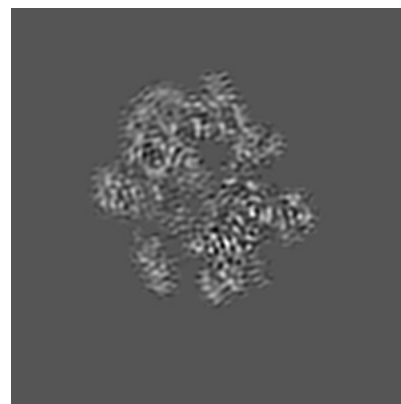
6.2.1 Primary map



X Index: 88



Y Index: 88

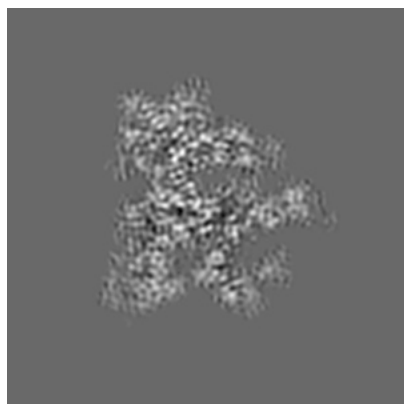


Z Index: 88

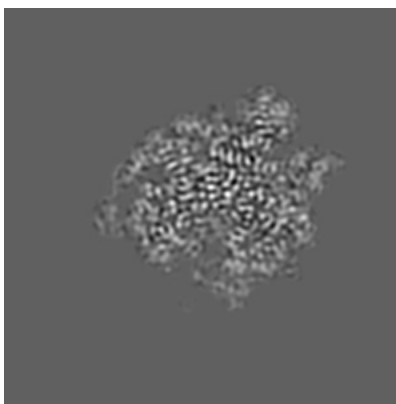
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

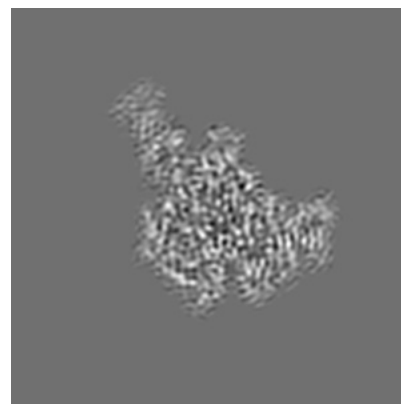
6.3.1 Primary map



X Index: 100



Y Index: 75

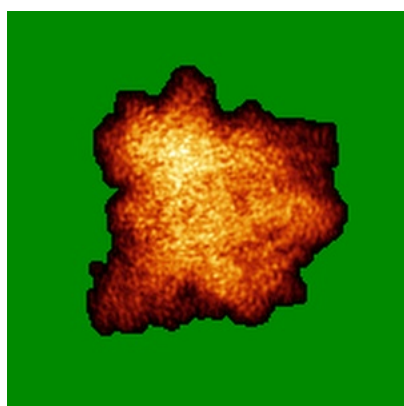


Z Index: 113

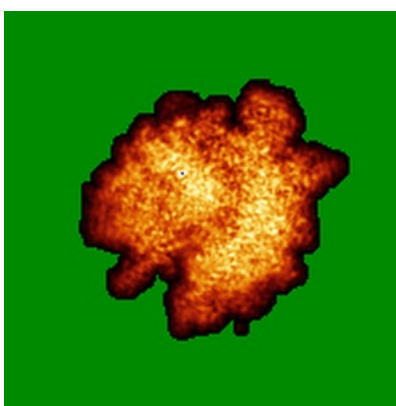
The images above show the largest variance slices of the map in three orthogonal directions.

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

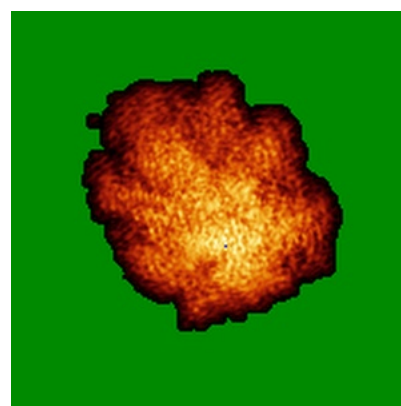
6.4.1 Primary map



X



Y

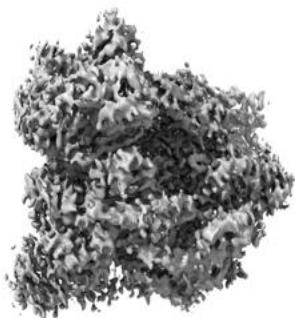


Z

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](#)

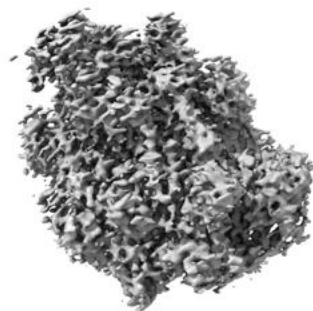
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

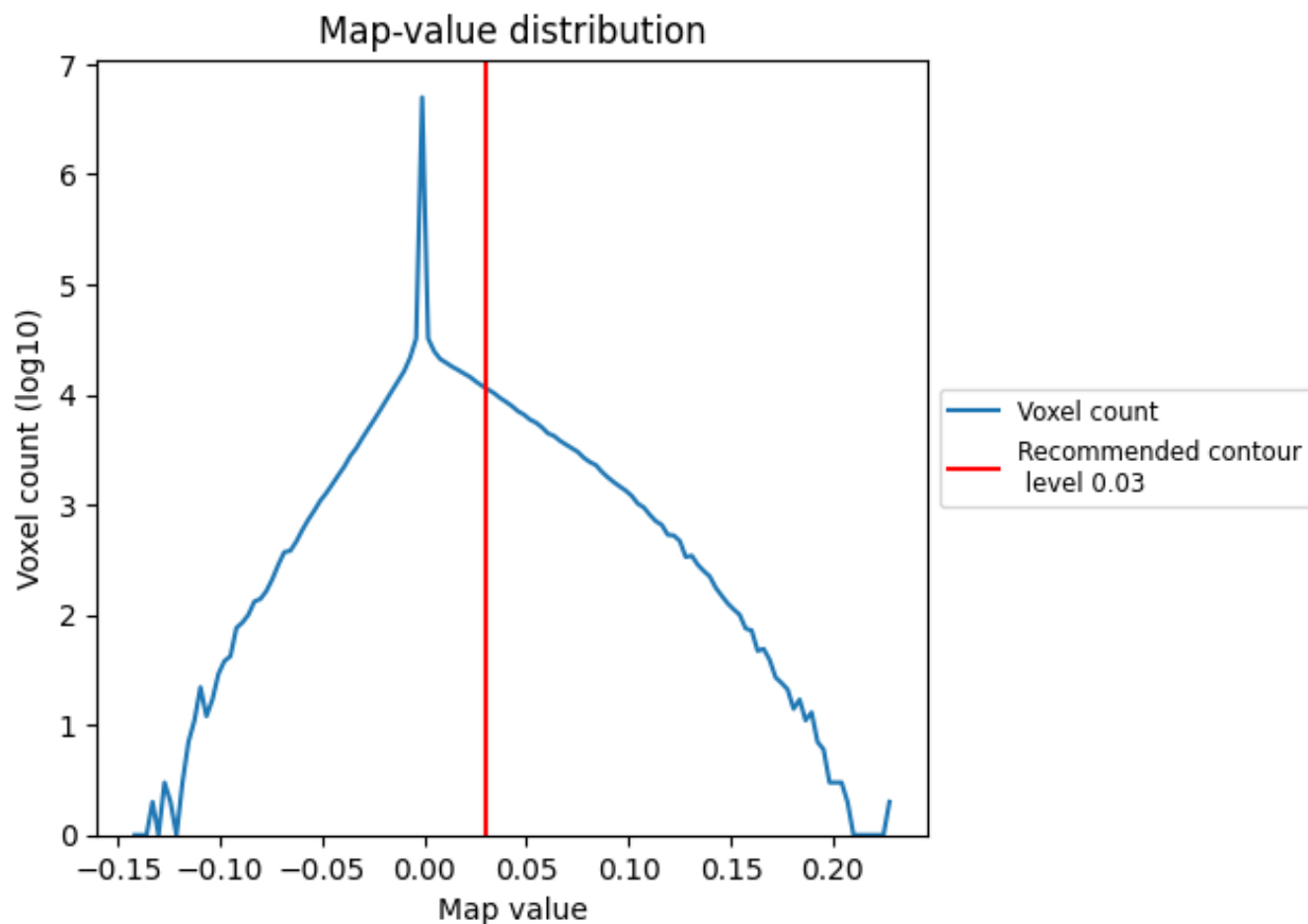
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

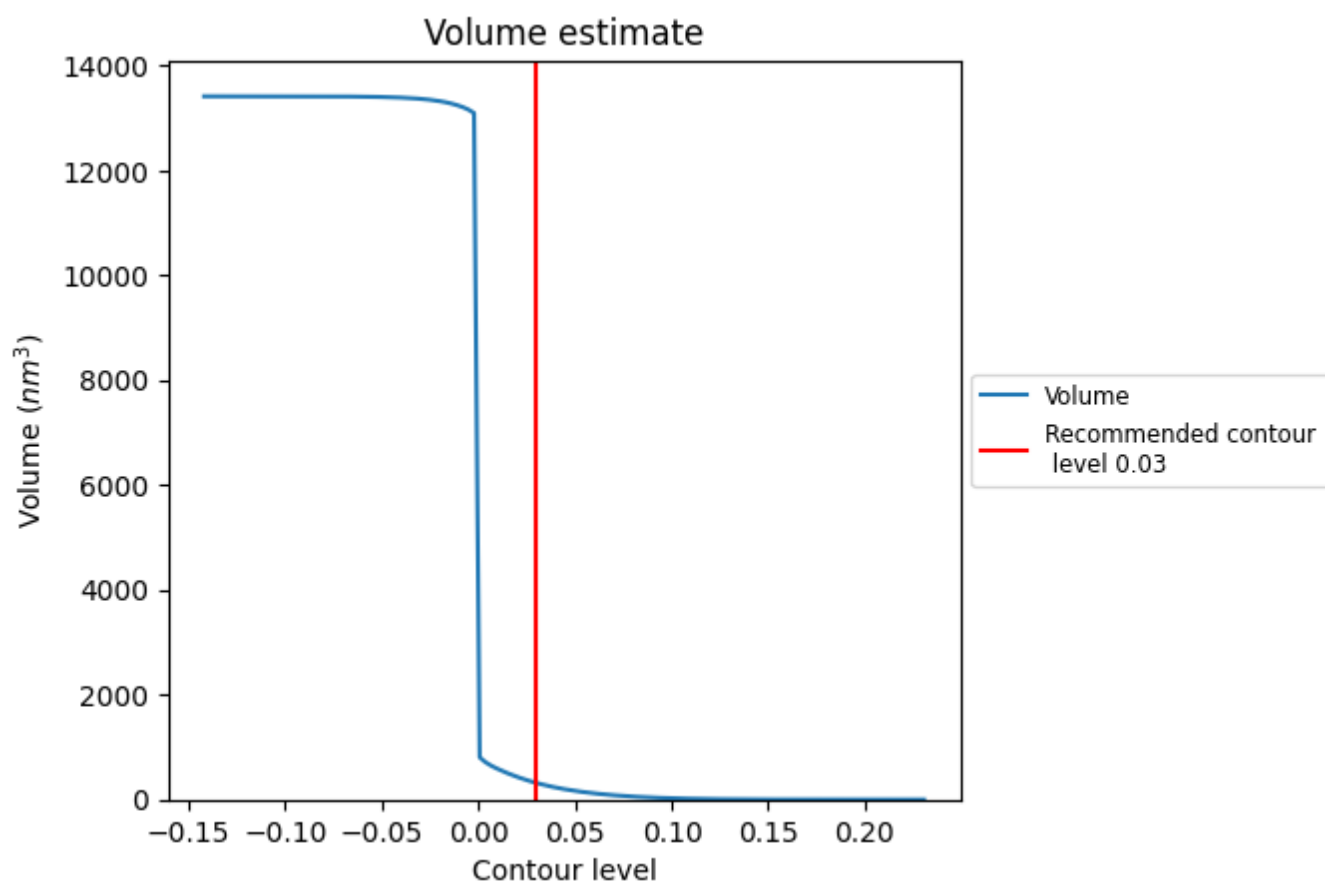
This section contains the results of statistical analysis of the map.

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.

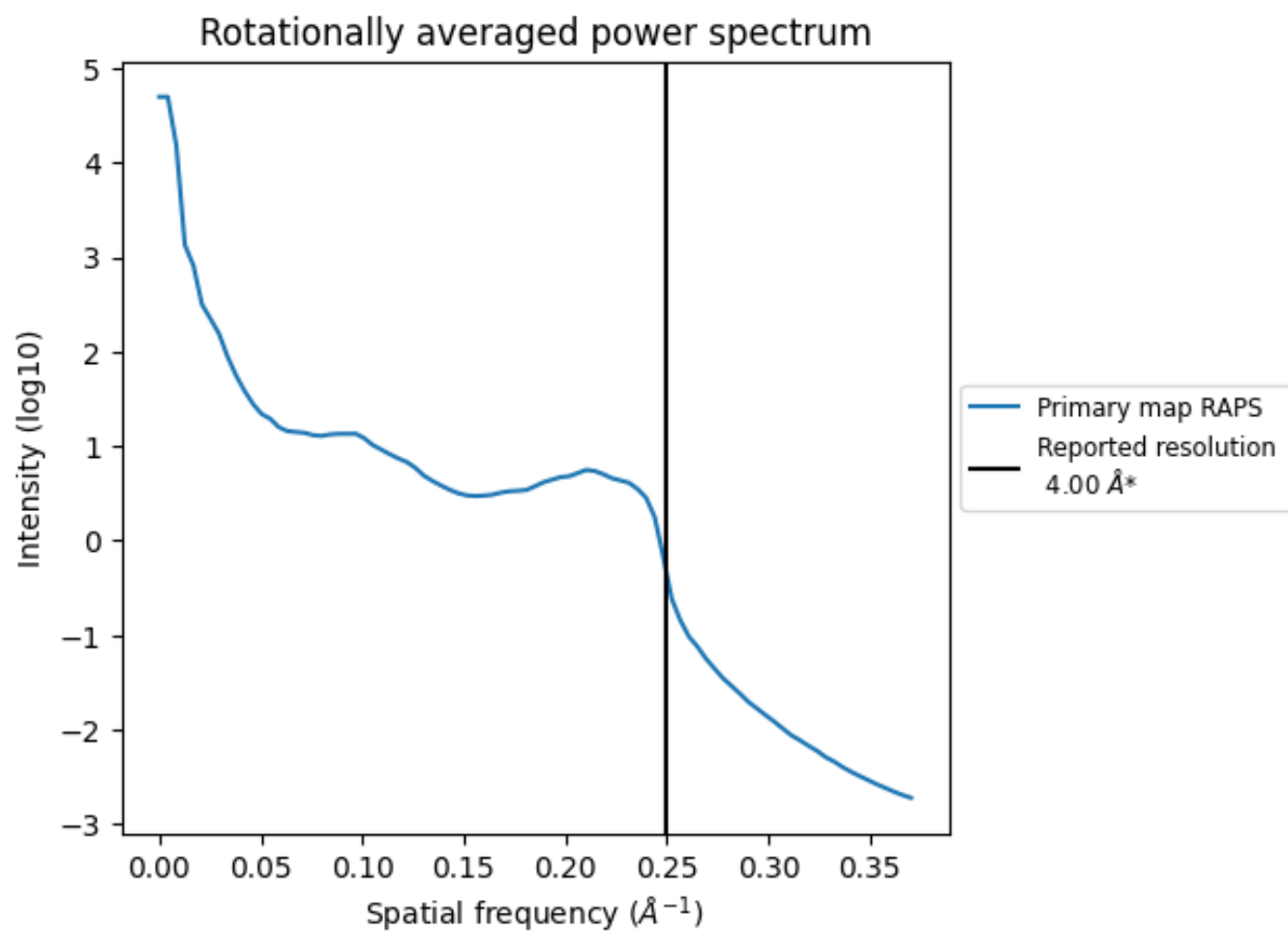
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 317 nm³; this corresponds to an approximate mass of 287 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

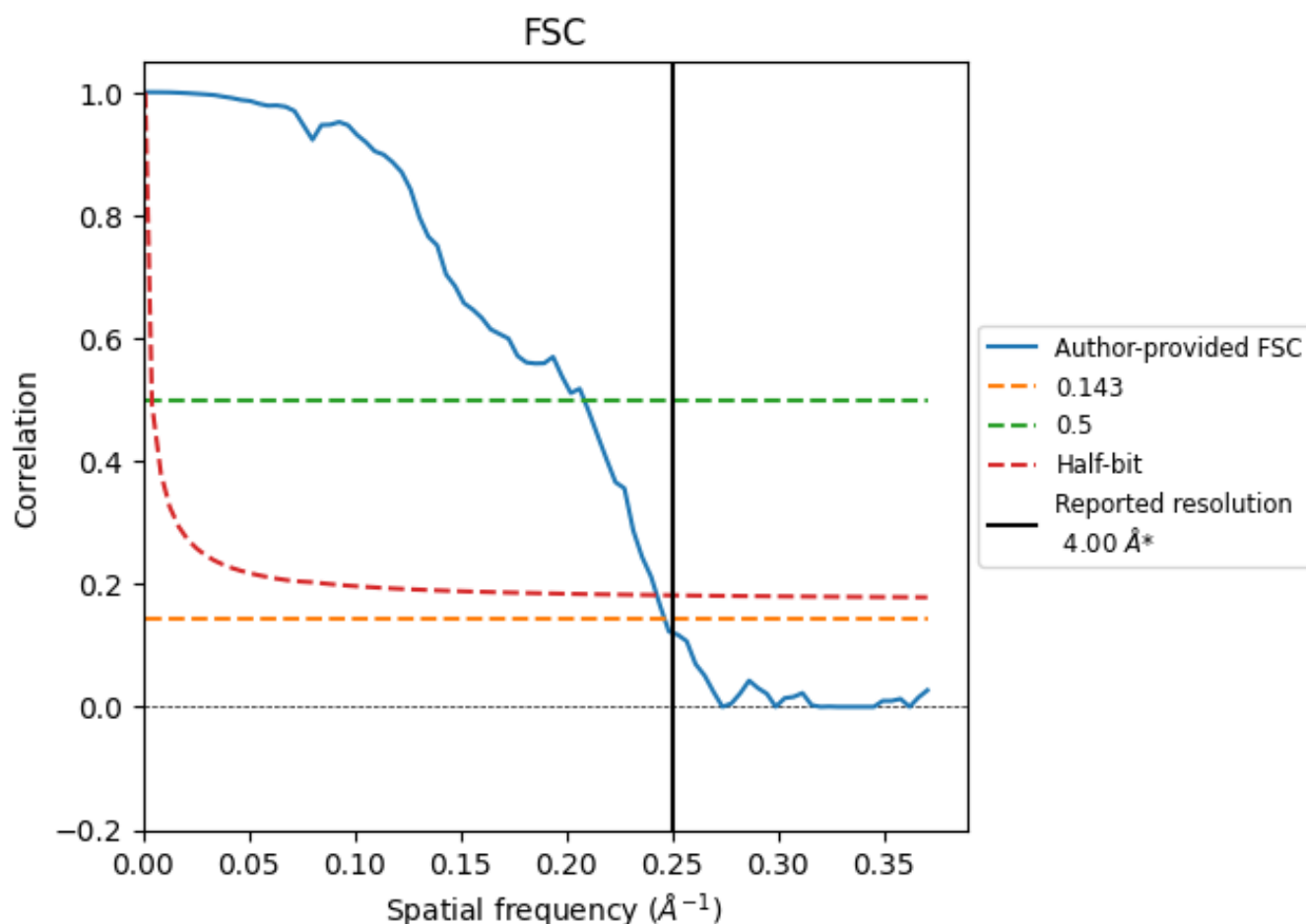


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

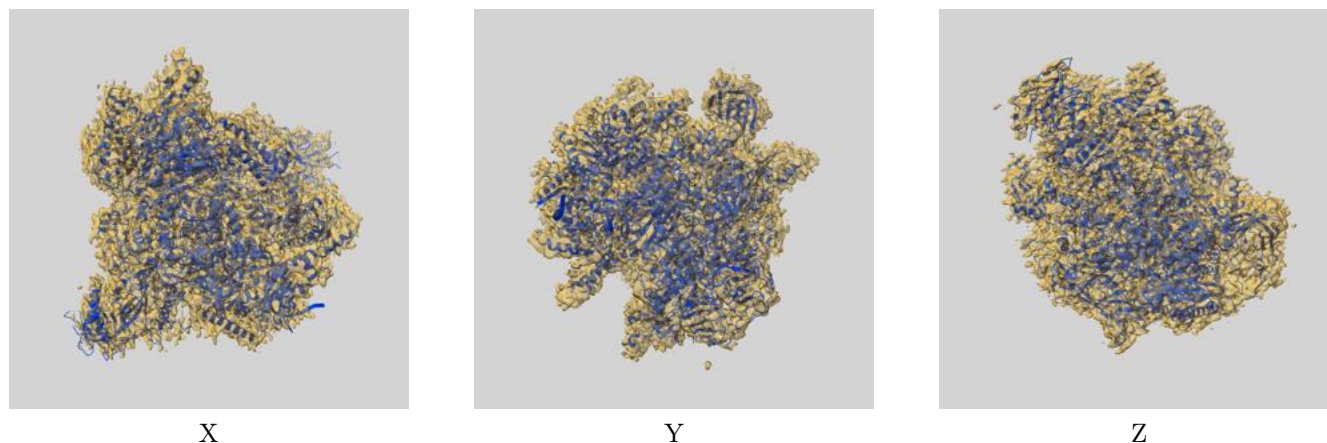
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.06	4.80	4.12
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

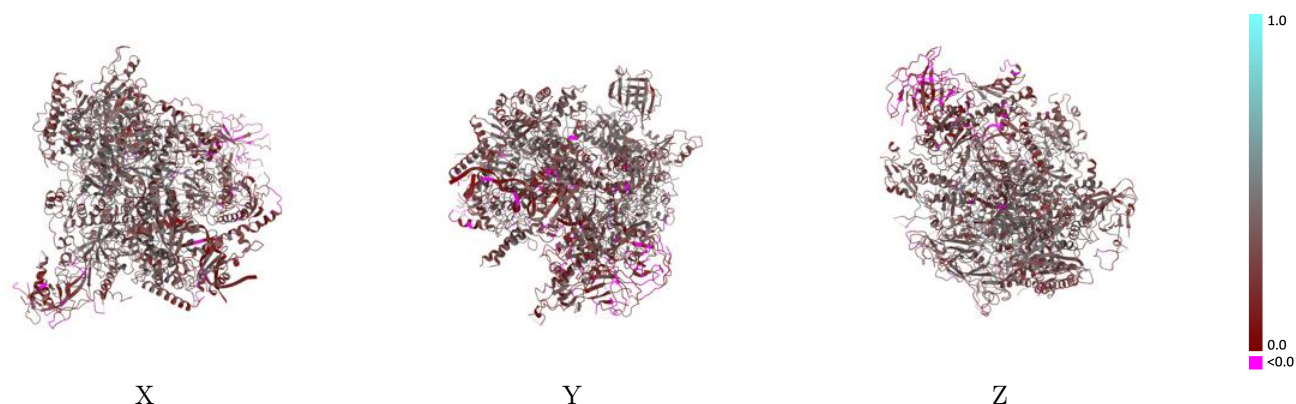
This section contains information regarding the fit between EMDB map EMD-3448 and PDB model 5M5Y. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



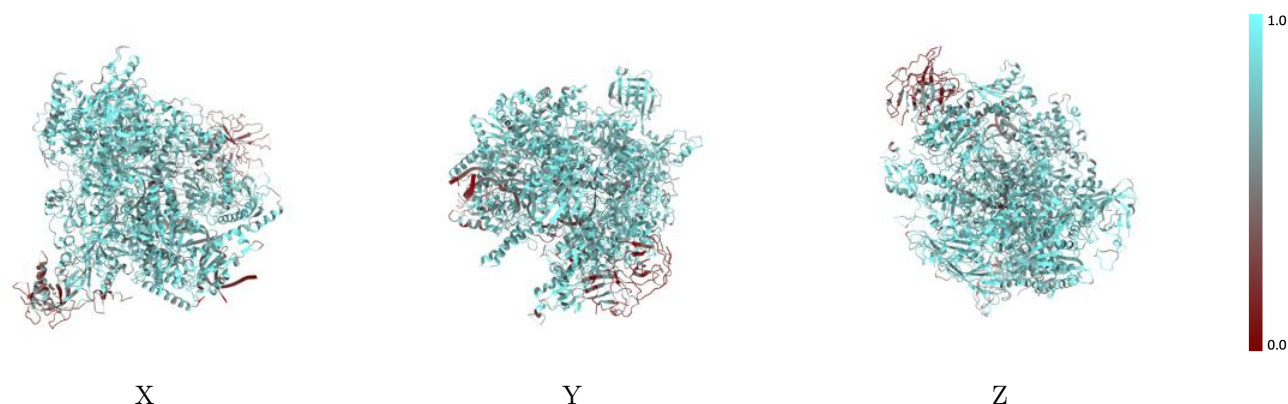
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



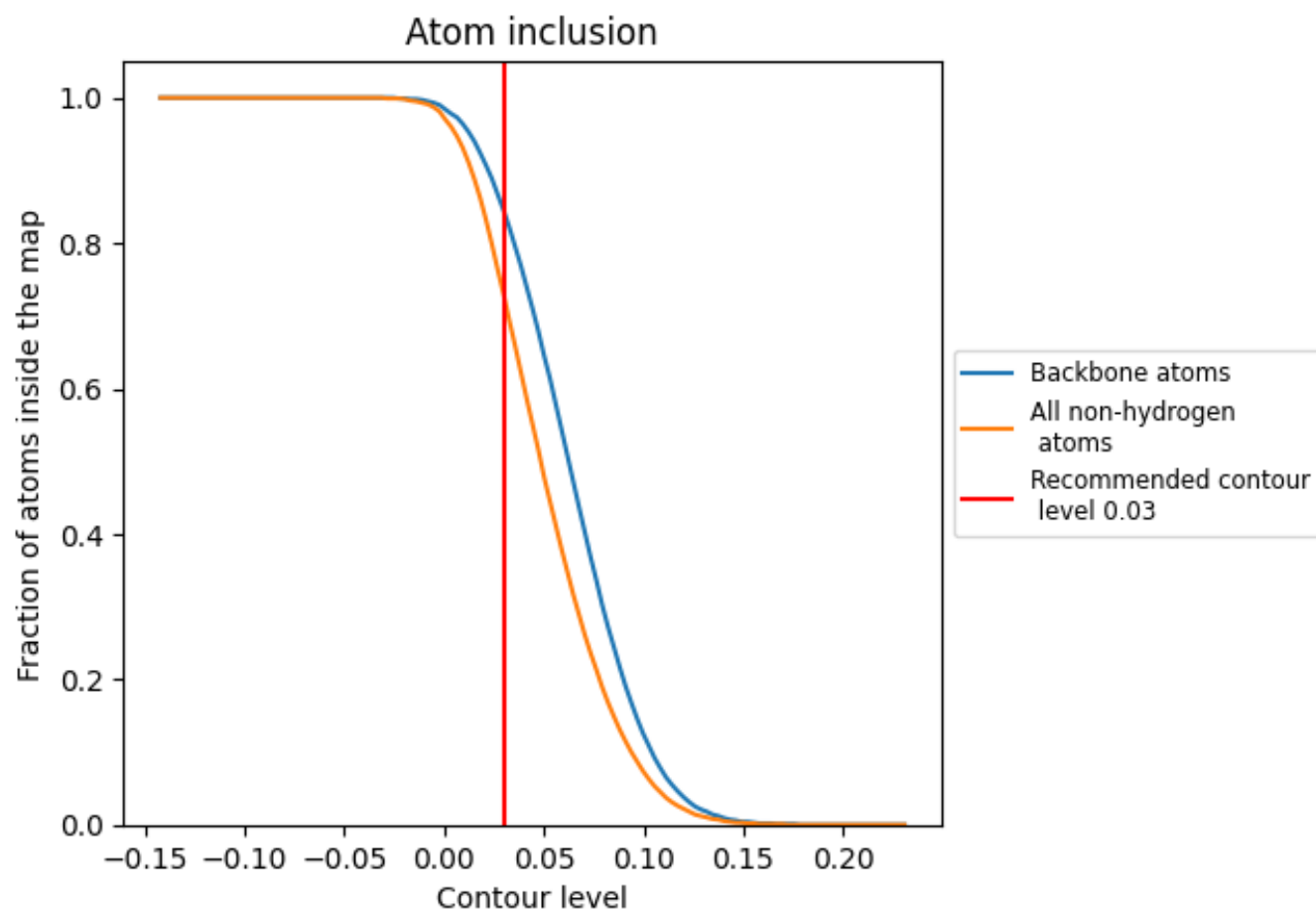
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7280	 0.3080
A	 0.7780	 0.3290
B	 0.7770	 0.3320
C	 0.7980	 0.3360
D	 0.4900	 0.2350
E	 0.7840	 0.3240
F	 0.7900	 0.3400
G	 0.4910	 0.2520
H	 0.7830	 0.3260
I	 0.6490	 0.1970
J	 0.8480	 0.3980
K	 0.7680	 0.3310
L	 0.7380	 0.3060
M	 0.3670	 0.1350
N	 0.3100	 0.1440
R	 0.3720	 0.1200
S	 0.5390	 0.1180
T	 0.5030	 0.1660

