



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:22 AM UTC

PDB ID : 6RQT / pdb_00006rqt
EMDB ID : EMD-4985
Title : RNA Polymerase I-tWH-Rrn3-DNA
Authors : Mueller, C.W.; Sadian, Y.; Tafur, L.
Deposited on : 2019-05-16
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:

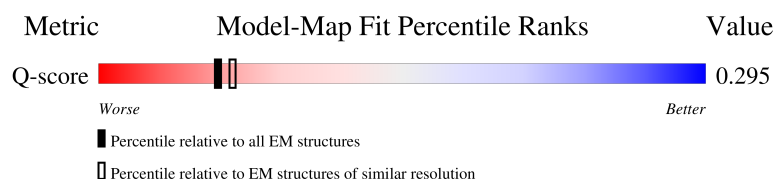
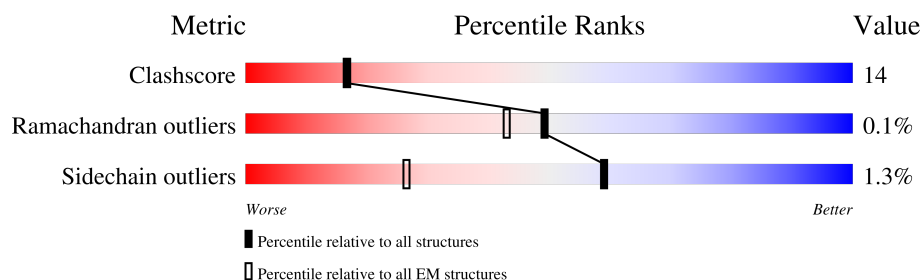
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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	-
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	T	70	13% 14% 10% 74%
2	U	70	11% 14% 80%
3	A	1664	17% 62% 25% 12%
4	B	1203	16% 63% 33%

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Mol	Chain	Length	Quality of chain
5	C	335	
6	D	137	
7	E	215	
8	F	155	
9	G	326	
10	H	146	
11	I	125	
12	J	70	
13	K	142	
14	L	70	
15	M	415	
16	N	233	
17	O	627	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 39820 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 DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	18	Total	C	N	O	P	0	0
			364	175	59	112	18		

- Molecule 2 is a DNA chain called Nontemplate strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	14	Total	C	N	O	P	0	0
			293	139	59	81	14		

- Molecule 3 is a protein called DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1466	Total	C	N	O	S	0	0
			11571	7309	2012	2188	62		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA135.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerase I subunit RPA14.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	202	Total	C	N	O	S	0	0
			1600	1026	276	293	5		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	134	Total	C	N	O	S	0	0
			1075	677	182	212	4		

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	64	Total	C	N	O	S	0	0
			472	295	78	95	4		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	100	Total	C	N	O	S	0	0
			785	491	129	160	5		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	43	Total	C	N	O	S	0	0
			344	211	69	60	4		

- Molecule 15 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	392	Total	C	N	O	S	0	0
			3100	1978	526	592	4		

- Molecule 16 is a protein called DNA-directed RNA polymerase I subunit RPA34.

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

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

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

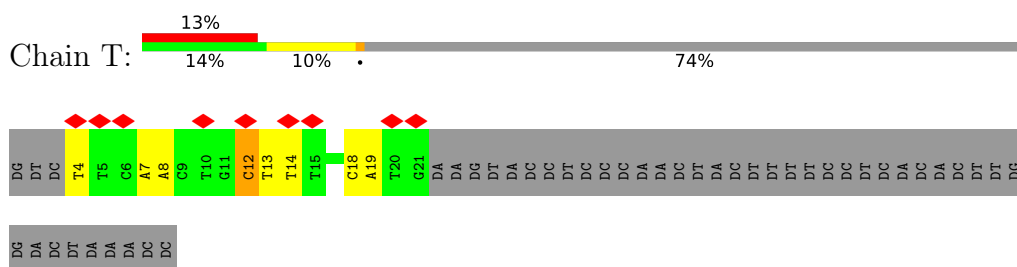
- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	

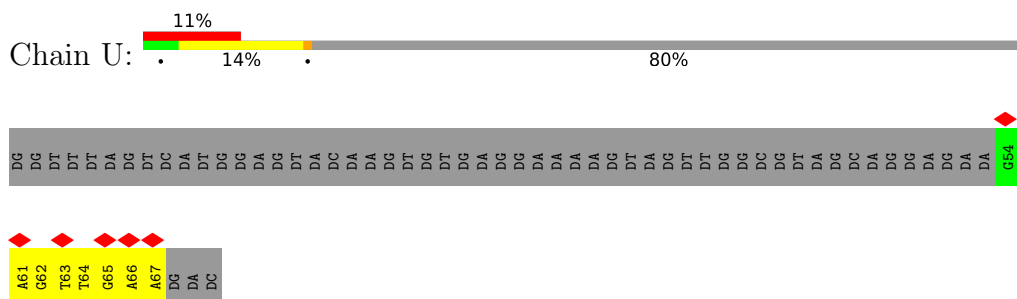
3 Residue-property plots [i](#)

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.

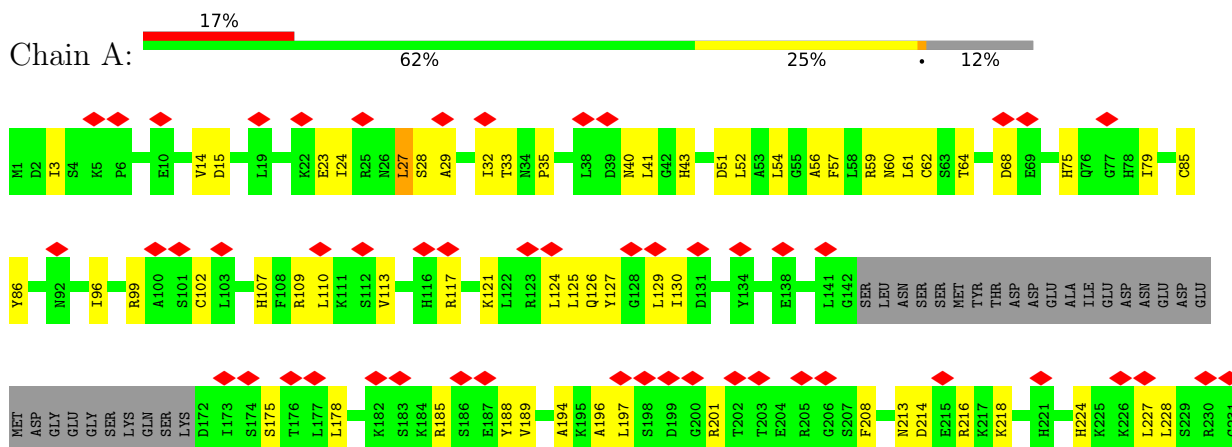
- Molecule 1: Template strand



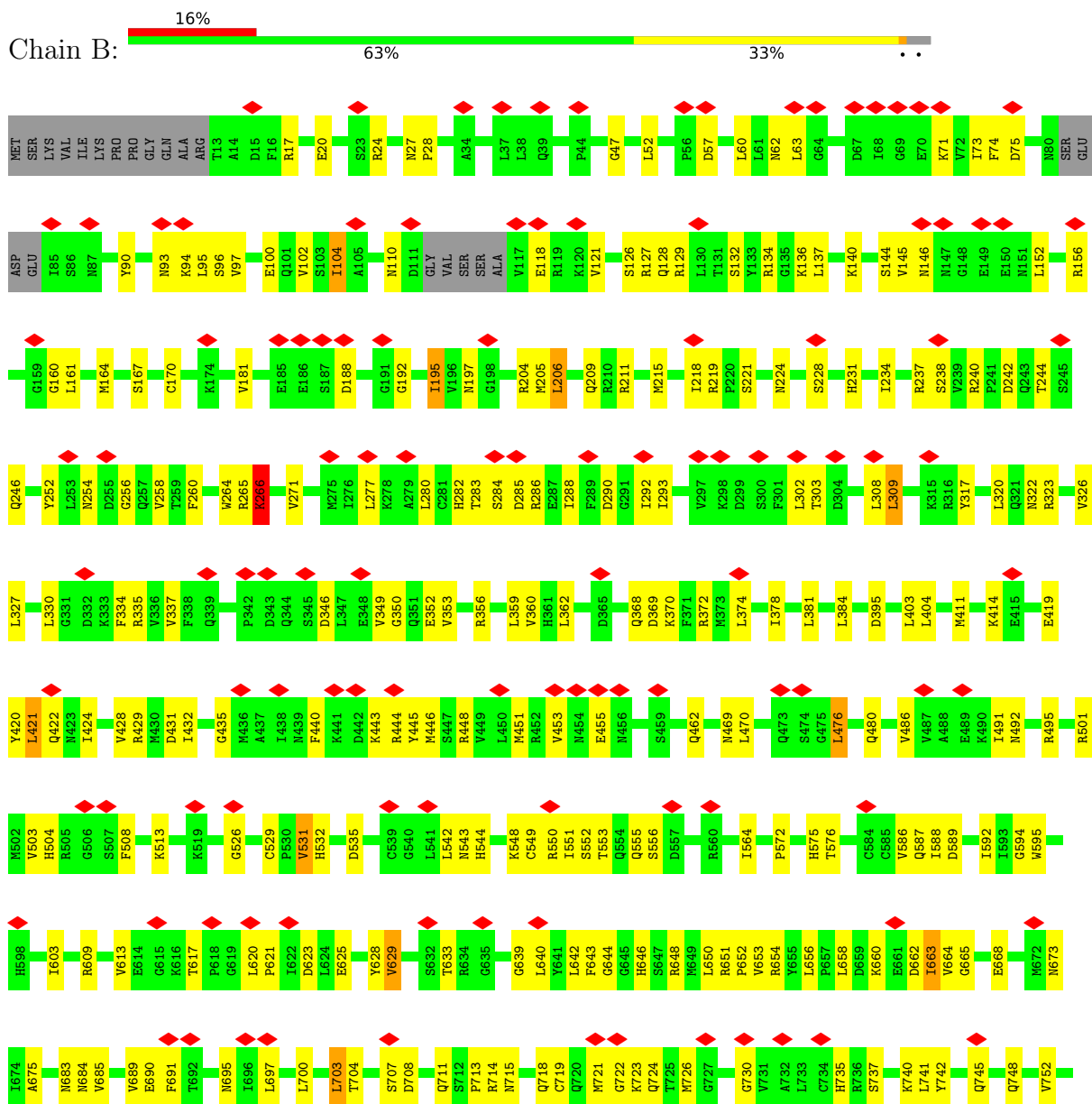
- Molecule 2: Nontemplate strand

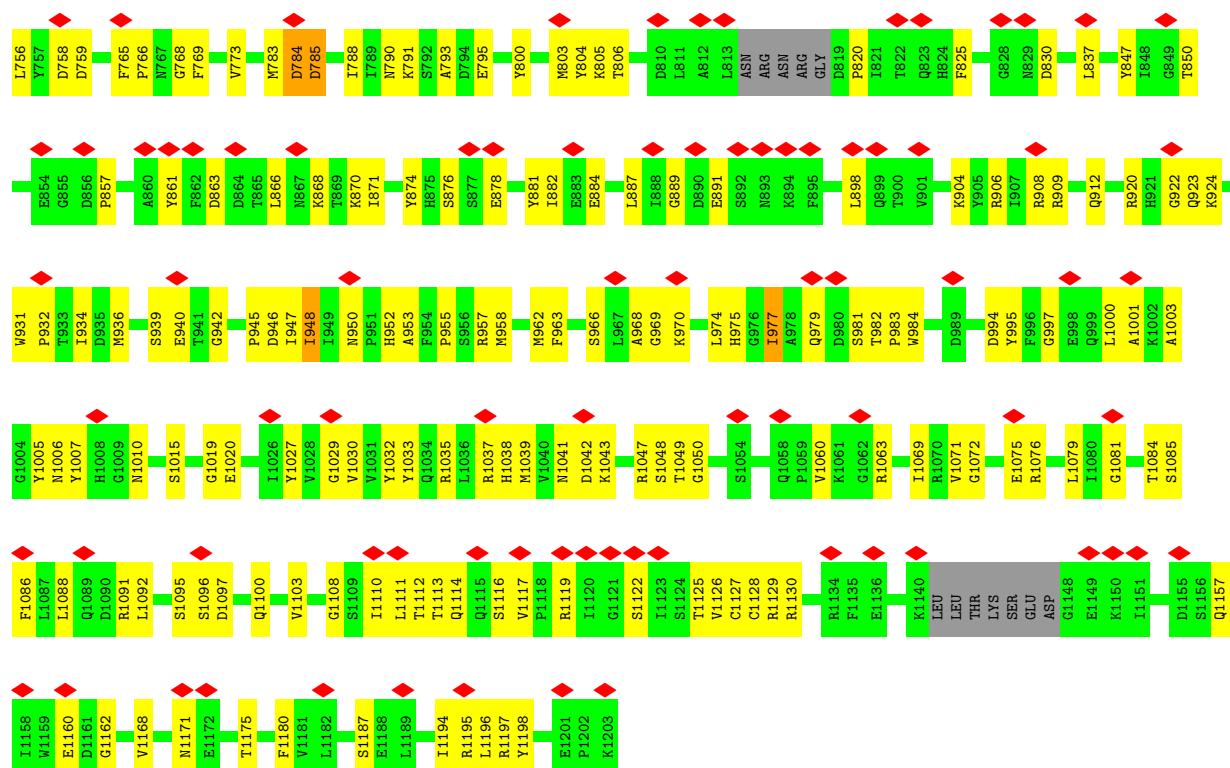


- Molecule 3: DNA-directed RNA polymerase I subunit RPA190

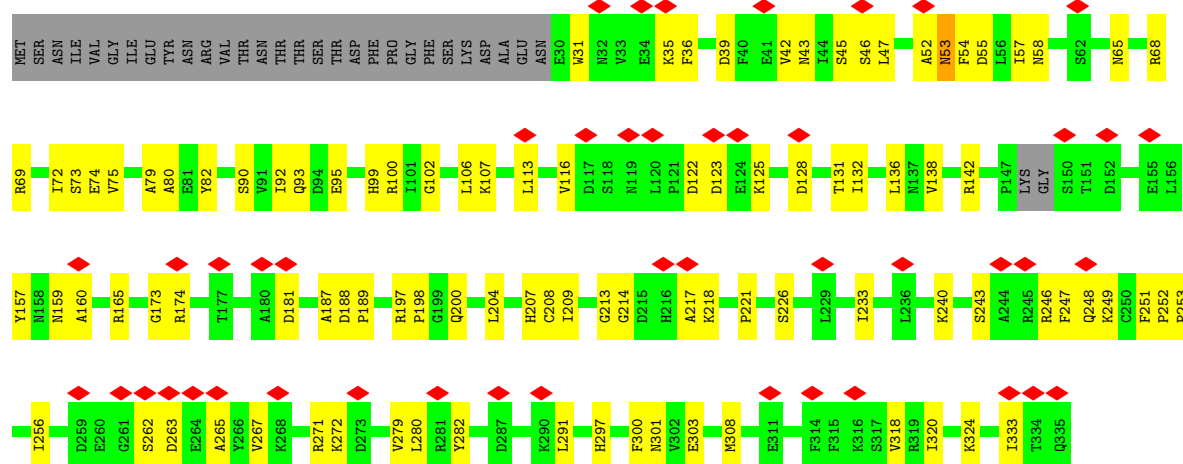




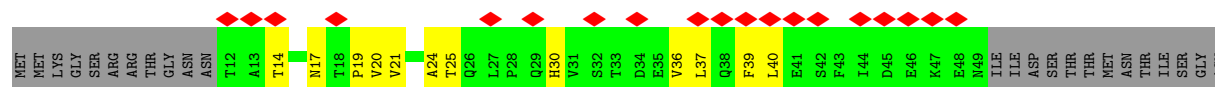


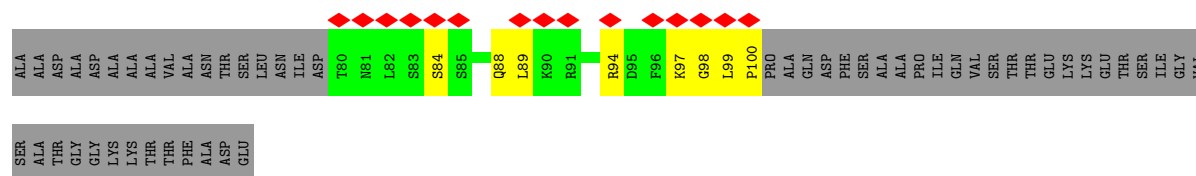


• Molecule 5: DNA-directed RNA polymerases I and III subunit RPAC1

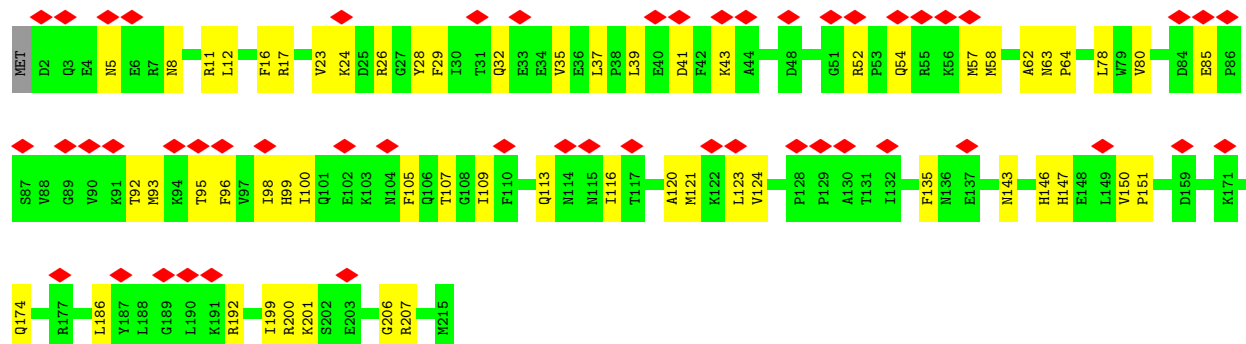


• Molecule 6: DNA-directed RNA polymerase I subunit RPA14

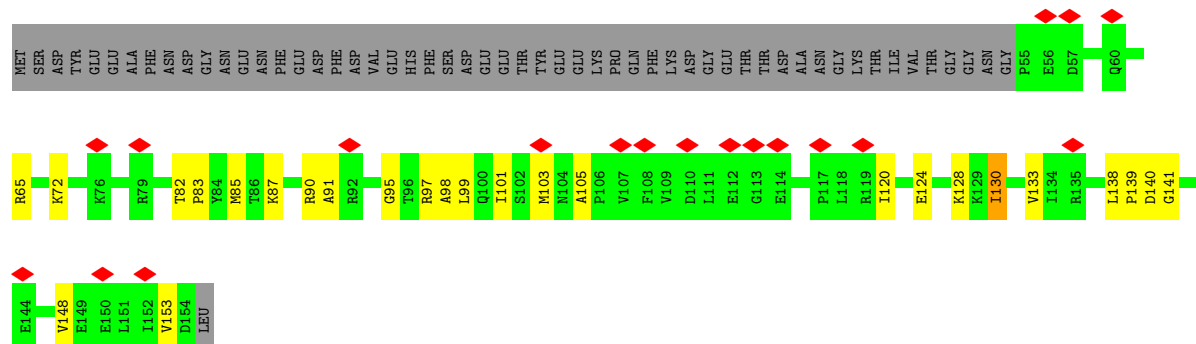




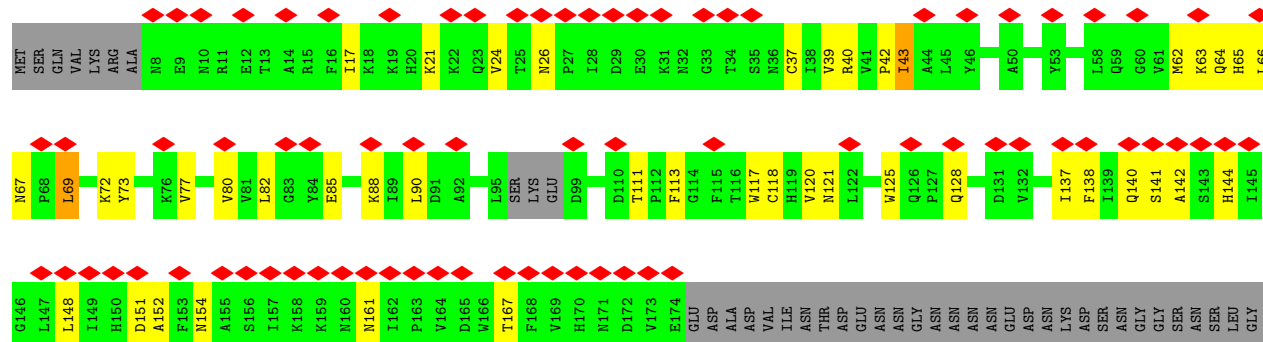
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



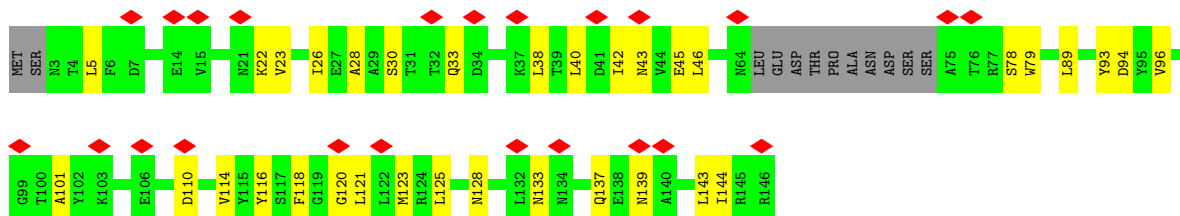
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



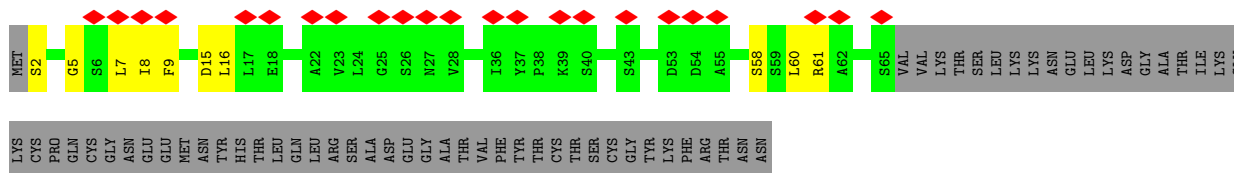
• Molecule 9: DNA-directed RNA polymerase I subunit RPA43



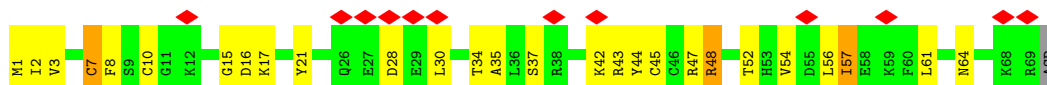
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3



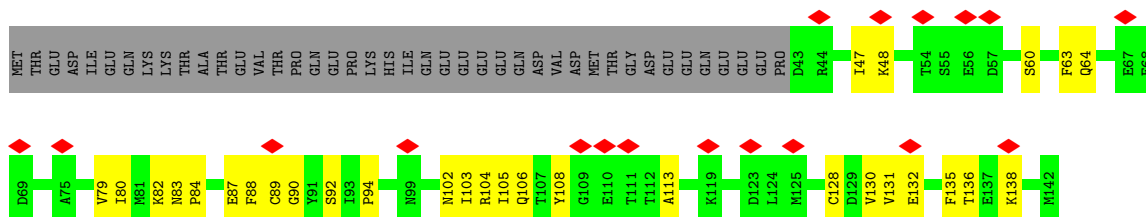
- Molecule 11: DNA-directed RNA polymerase I subunit RPA12



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5



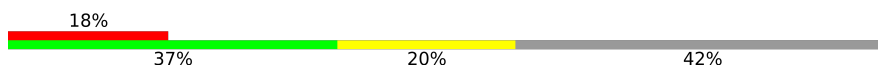
- Molecule 13: DNA-directed RNA polymerases I and III subunit RPAC2



- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC4



Response	Percentage
Good	66%
Not good	24%
Don't know	6%



Chain O:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9789	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 ($e^-/\text{\AA}^2$)	1.57175	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	0.286	Depositor
Minimum map value	-0.181	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	233.5168, 233.5168, 233.5168	wwPDB
Map dimensions	176, 176, 176	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3268, 1.3268, 1.3268	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	T	0.35	0/405	0.68	1/622 (0.2%)
2	U	0.33	0/330	0.58	1/508 (0.2%)
3	A	0.36	0/11782	0.72	4/15913 (0.0%)
4	B	0.38	1/9506 (0.0%)	0.73	5/12847 (0.0%)
5	C	0.34	0/2469	0.69	3/3347 (0.1%)
6	D	0.25	0/473	0.54	0/641
7	E	0.34	0/1787	0.66	0/2406
8	F	0.33	0/838	0.65	0/1129
9	G	0.28	0/1637	0.62	0/2226
10	H	0.32	0/1093	0.62	0/1480
11	I	0.29	0/478	0.68	0/647
12	J	0.44	0/578	0.85	2/775 (0.3%)
13	K	0.33	0/795	0.65	1/1072 (0.1%)
14	L	0.26	0/346	0.65	0/457
15	M	0.30	0/3150	0.71	5/4247 (0.1%)
16	N	0.31	0/1090	0.81	3/1466 (0.2%)
17	O	0.21	0/3897	0.59	3/5268 (0.1%)
All	All	0.34	1/40654 (0.0%)	0.70	28/55051 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	121	VAL	C-N	-5.33	1.22	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	O	163	ILE	CA-C-N	8.73	133.95	120.68
17	O	163	ILE	C-N-CA	8.73	133.95	120.68
16	N	169	GLU	CA-C-N	-7.96	111.78	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	N	169	GLU	C-N-CA	-7.96	111.78	123.00
5	C	53	ASN	N-CA-C	-7.87	98.82	110.23
17	O	325	ILE	N-CA-C	-7.83	105.85	113.53
3	A	813	LEU	N-CA-C	-6.67	104.09	111.36
13	K	131	VAL	N-CA-C	-6.36	106.25	111.91
3	A	530	TRP	CA-C-N	-6.29	113.28	119.76
3	A	530	TRP	C-N-CA	-6.29	113.28	119.76
15	M	265	LEU	N-CA-C	-6.10	104.64	111.28
12	J	7	CYS	CA-C-N	5.73	129.41	120.82
12	J	7	CYS	C-N-CA	5.73	129.41	120.82
15	M	268	LEU	N-CA-C	-5.61	105.06	111.07
1	T	12	DC	C2'-C3'-O3'	5.61	119.91	111.50
5	C	53	ASN	CA-C-N	-5.43	113.36	121.72
5	C	53	ASN	C-N-CA	-5.43	113.36	121.72
4	B	266	LYS	N-CA-C	-5.34	99.43	110.80
4	B	683	ASN	CA-C-N	5.25	131.56	121.54
4	B	683	ASN	C-N-CA	5.25	131.56	121.54
2	U	58	DA	C2'-C3'-O3'	5.23	119.34	111.50
3	A	503	VAL	N-CA-C	-5.21	108.77	113.71
15	M	148	ARG	CA-C-N	5.18	129.12	120.62
15	M	148	ARG	C-N-CA	5.18	129.12	120.62
4	B	266	LYS	CA-C-N	-5.18	113.68	121.86
4	B	266	LYS	C-N-CA	-5.18	113.68	121.86
16	N	169	GLU	N-CA-C	-5.13	103.01	110.24
15	M	193	ILE	N-CA-C	-5.12	108.29	113.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	364	0	206	17	0
2	U	293	0	158	15	0
3	A	11571	0	11653	387	0
4	B	9301	0	9194	358	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	2418	0	2401	74	0
6	D	467	0	468	16	0
7	E	1751	0	1776	40	0
8	F	823	0	841	17	0
9	G	1600	0	1600	38	0
10	H	1075	0	1046	25	0
11	I	472	0	474	7	0
12	J	569	0	587	23	0
13	K	785	0	782	23	0
14	L	344	0	365	8	0
15	M	3100	0	3210	107	0
16	N	1070	0	1085	62	0
17	O	3811	0	3804	54	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	39820	0	39650	1110	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 14.

All (1110) 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)
3:A:912:VAL:HG22	3:A:913:PRO:CD	1.52	1.37
4:B:1005:TYR:HE1	16:N:171:PHE:CZ	1.54	1.26
3:A:41:LEU:HD12	3:A:43:HIS:ND1	1.53	1.21
4:B:1005:TYR:OH	16:N:169:GLU:HG3	1.39	1.21
4:B:1005:TYR:CE1	16:N:171:PHE:CZ	2.31	1.18
4:B:1005:TYR:HE1	16:N:171:PHE:CE2	1.63	1.14
4:B:1005:TYR:CE1	16:N:171:PHE:CE2	2.37	1.12
15:M:262:LEU:CG	15:M:265:LEU:HD12	1.78	1.11
3:A:32:ILE:HD11	3:A:54:LEU:HD12	1.30	1.10
3:A:912:VAL:CG2	3:A:913:PRO:HD2	1.82	1.08
4:B:470:LEU:HD11	4:B:476:LEU:HD11	1.27	1.08
3:A:466:LEU:HD22	3:A:470:HIS:ND1	1.68	1.07
3:A:985:ARG:HD3	3:A:986:PHE:N	1.68	1.07
3:A:669:LEU:HD13	3:A:813:LEU:HD12	1.36	1.07
15:M:262:LEU:HG	15:M:265:LEU:CD1	1.88	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:359:LEU:HD11	4:B:370:LYS:HG3	1.37	1.03
3:A:618:TYR:CD1	4:B:783:MET:CE	2.42	1.02
16:N:169:GLU:OE2	16:N:170:HIS:N	1.94	1.01
15:M:262:LEU:HG	15:M:265:LEU:HD12	1.03	0.99
3:A:912:VAL:CG2	3:A:913:PRO:CD	2.41	0.98
3:A:912:VAL:HG22	3:A:913:PRO:HD2	0.99	0.97
3:A:912:VAL:HG22	3:A:913:PRO:HD3	1.46	0.95
3:A:618:TYR:CD1	4:B:783:MET:HE1	2.02	0.94
3:A:985:ARG:NH2	3:A:986:PHE:HB2	1.83	0.94
15:M:262:LEU:HA	15:M:265:LEU:HG	1.47	0.94
4:B:1196:LEU:HD13	4:B:1197:ARG:N	1.84	0.93
15:M:262:LEU:HA	15:M:265:LEU:CG	2.00	0.92
5:C:45:SER:HB3	5:C:53:ASN:HB3	1.53	0.91
3:A:32:ILE:HD11	3:A:54:LEU:CD1	2.00	0.90
3:A:618:TYR:HA	4:B:783:MET:HE1	1.52	0.89
3:A:618:TYR:CD1	4:B:783:MET:HE3	2.04	0.89
3:A:942:GLN:O	3:A:985:ARG:CZ	2.21	0.88
3:A:466:LEU:CD2	3:A:470:HIS:ND1	2.35	0.88
4:B:470:LEU:CD1	4:B:476:LEU:HD11	2.04	0.86
4:B:359:LEU:CD1	4:B:370:LYS:HE3	2.06	0.85
3:A:1178:LEU:HD13	3:A:1179:ILE:N	1.92	0.84
4:B:703:LEU:O	4:B:703:LEU:HD22	1.77	0.84
4:B:703:LEU:HD13	4:B:704:THR:N	1.93	0.83
4:B:974:LEU:HD11	16:N:169:GLU:CG	2.09	0.83
4:B:974:LEU:HD21	16:N:169:GLU:HG2	1.60	0.83
4:B:327:LEU:HD23	4:B:330:LEU:HD12	1.61	0.82
3:A:669:LEU:HD13	3:A:813:LEU:CD1	2.11	0.80
15:M:250:LEU:HD23	15:M:250:LEU:H	1.46	0.80
3:A:943:ILE:HA	3:A:985:ARG:NH1	1.96	0.80
3:A:1306:TYR:O	3:A:1307:ASP:OD1	2.00	0.80
4:B:820:PRO:HD2	15:M:356:LYS:NZ	1.97	0.79
3:A:669:LEU:CD1	3:A:813:LEU:HD12	2.11	0.79
4:B:974:LEU:CD2	16:N:169:GLU:HG2	2.14	0.77
2:U:62:DG:H1'	2:U:63:DT:H5'	1.67	0.76
4:B:359:LEU:HD11	4:B:370:LYS:CG	2.15	0.76
3:A:943:ILE:HA	3:A:985:ARG:HH11	1.48	0.76
2:U:66:DA:H1'	2:U:67:DA:H5'	1.68	0.76
15:M:262:LEU:CB	15:M:265:LEU:HD12	2.16	0.75
4:B:359:LEU:HD12	4:B:359:LEU:O	1.87	0.74
3:A:41:LEU:HD13	3:A:41:LEU:O	1.86	0.74
3:A:618:TYR:CA	4:B:783:MET:HE1	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:875:LEU:C	3:A:875:LEU:HD13	2.13	0.74
7:E:186:LEU:O	7:E:186:LEU:HD23	1.88	0.74
4:B:1005:TYR:HE1	16:N:171:PHE:CE1	2.06	0.73
4:B:1005:TYR:CD1	16:N:171:PHE:CE2	2.76	0.73
3:A:54:LEU:O	3:A:54:LEU:HD23	1.87	0.73
3:A:1030:VAL:HG12	3:A:1040:ASP:HA	1.71	0.73
15:M:262:LEU:HA	15:M:265:LEU:CD1	2.18	0.73
3:A:461:GLU:HB3	3:A:464:GLU:HA	1.70	0.73
3:A:985:ARG:HH21	3:A:986:PHE:H	1.34	0.73
3:A:985:ARG:HD3	3:A:985:ARG:C	2.13	0.72
16:N:169:GLU:CD	16:N:170:HIS:N	2.47	0.72
4:B:714:ARG:HD2	4:B:957:ARG:HD2	1.72	0.72
1:T:13:DT:OP2	1:T:13:DT:H71	1.90	0.72
15:M:268:LEU:HG	15:M:331:TYR:CE2	2.24	0.72
7:E:135:PHE:CD1	7:E:186:LEU:HD21	2.25	0.71
5:C:165:ARG:HB3	5:C:189:PRO:HB3	1.71	0.71
10:H:116:TYR:HB3	10:H:123:MET:HB2	1.71	0.71
4:B:703:LEU:HD13	4:B:703:LEU:C	2.16	0.70
4:B:359:LEU:HD11	4:B:370:LYS:CE	2.21	0.70
4:B:820:PRO:HD2	15:M:356:LYS:HZ2	1.54	0.70
5:C:53:ASN:ND2	16:N:174:GLY:O	2.24	0.70
3:A:813:LEU:HD13	3:A:813:LEU:C	2.17	0.70
2:U:61:DA:H4'	3:A:1601:GLN:HE22	1.57	0.69
3:A:985:ARG:CD	3:A:987:TYR:H	2.04	0.69
3:A:930:LEU:HD13	3:A:930:LEU:O	1.92	0.69
4:B:1196:LEU:HD13	4:B:1196:LEU:C	2.16	0.69
3:A:875:LEU:O	3:A:875:LEU:HD22	1.93	0.69
4:B:359:LEU:CD1	4:B:370:LYS:CE	2.71	0.69
3:A:759:TYR:CE1	3:A:913:PRO:HG2	2.27	0.69
3:A:875:LEU:HD13	3:A:875:LEU:O	1.93	0.69
3:A:930:LEU:O	3:A:930:LEU:HD22	1.93	0.68
3:A:926:GLN:O	3:A:930:LEU:HB3	1.94	0.68
3:A:1178:LEU:HD13	3:A:1178:LEU:C	2.18	0.68
15:M:363:LEU:HD13	15:M:363:LEU:O	1.92	0.68
15:M:250:LEU:HD23	15:M:250:LEU:N	2.08	0.68
3:A:1256:LYS:CB	3:A:1307:ASP:OD2	2.43	0.67
4:B:703:LEU:HD22	4:B:703:LEU:C	2.19	0.67
3:A:943:ILE:HD12	3:A:985:ARG:NH1	2.10	0.67
9:G:148:LEU:HB3	9:G:151:ASP:HA	1.76	0.67
3:A:1443:GLN:NE2	3:A:1461:ASN:OD1	2.28	0.67
15:M:268:LEU:C	15:M:268:LEU:HD23	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:359:LEU:HD11	4:B:370:LYS:HE3	1.76	0.67
4:B:803:MET:SD	4:B:909:ARG:NH1	2.68	0.66
4:B:531:VAL:HG23	4:B:715:ASN:HB3	1.76	0.66
4:B:1005:TYR:OH	16:N:169:GLU:CG	2.31	0.66
1:T:13:DT:H3	2:U:56:DA:H2	1.44	0.66
15:M:363:LEU:O	15:M:363:LEU:HD22	1.95	0.66
4:B:96:SER:HB3	4:B:144:SER:HB3	1.76	0.66
3:A:1436:ASN:HB2	3:A:1461:ASN:HD21	1.60	0.66
4:B:362:LEU:HD12	4:B:369:ASP:HB3	1.77	0.66
4:B:110:ASN:HD21	4:B:118:GLU:HA	1.61	0.65
4:B:589:ASP:HB3	4:B:643:PHE:HA	1.78	0.65
3:A:126:GLN:HB2	3:A:343:PRO:HD3	1.79	0.65
5:C:197:ARG:HE	12:J:61:LEU:HB3	1.61	0.65
4:B:866:LEU:HD23	4:B:868:LYS:HD3	1.77	0.65
3:A:943:ILE:HD12	3:A:985:ARG:HH11	1.61	0.65
3:A:1634:LEU:HB2	3:A:1639:ALA:HB1	1.79	0.65
3:A:828:CYS:SG	3:A:829:GLY:N	2.70	0.65
3:A:618:TYR:CG	4:B:783:MET:HE1	2.32	0.65
4:B:1047:ARG:HE	4:B:1050:GLY:HA3	1.61	0.65
3:A:985:ARG:HD2	3:A:987:TYR:H	1.62	0.64
4:B:942:GLY:HA2	5:C:226:SER:HB3	1.80	0.64
4:B:1006:ASN:ND2	4:B:1010:ASN:OD1	2.29	0.64
3:A:40:ASN:O	3:A:41:LEU:HB3	1.97	0.64
4:B:1005:TYR:CE1	16:N:171:PHE:CE1	2.85	0.64
3:A:813:LEU:HD13	3:A:813:LEU:O	1.98	0.64
15:M:262:LEU:HA	15:M:265:LEU:HD12	1.78	0.64
4:B:244:THR:HA	4:B:411:MET:HE3	1.78	0.64
7:E:78:LEU:HD11	7:E:109:ILE:HG12	1.78	0.64
3:A:1085:LEU:HD11	3:A:1176:ARG:HH11	1.62	0.64
3:A:1138:GLU:HB3	7:E:206:GLY:HA3	1.80	0.64
3:A:1470:CYS:SG	3:A:1471:GLU:N	2.71	0.64
4:B:974:LEU:CD1	16:N:169:GLU:HG2	2.27	0.64
1:T:4:DT:O2	2:U:67:DA:H2	1.80	0.64
3:A:618:TYR:HD1	4:B:783:MET:HE1	1.58	0.64
4:B:429:ARG:HA	4:B:432:ILE:HG22	1.80	0.63
17:O:387:HIS:ND1	17:O:606:MET:SD	2.72	0.63
4:B:303:THR:HG21	11:I:5:GLY:HA3	1.79	0.63
4:B:1196:LEU:HD11	4:B:1198:TYR:CE1	2.34	0.63
4:B:134:ARG:HE	4:B:160:GLY:HA3	1.63	0.63
4:B:246:GLN:HE22	4:B:360:VAL:HG12	1.64	0.63
4:B:625:GLU:HB2	4:B:648:ARG:HH11	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:96:PHE:HA	7:E:99:HIS:HD2	1.64	0.63
17:O:432:LYS:HB3	17:O:609:TYR:HD1	1.63	0.63
17:O:62:ASP:HB3	17:O:67:ASP:HB3	1.80	0.63
3:A:15:ASP:O	4:B:1196:LEU:HD22	1.99	0.62
12:J:10:CYS:HB3	12:J:43:ARG:HH21	1.64	0.62
4:B:974:LEU:HD21	16:N:169:GLU:CG	2.30	0.62
5:C:80:ALA:HA	5:C:208:CYS:HA	1.80	0.62
3:A:41:LEU:HD11	15:M:323:GLN:HA	1.82	0.62
3:A:456:VAL:O	3:A:460:LEU:N	2.33	0.62
4:B:740:LYS:HE3	4:B:805:LYS:HG2	1.80	0.62
3:A:872:ASP:HB2	3:A:875:LEU:HB3	1.82	0.62
4:B:327:LEU:HD23	4:B:330:LEU:CD1	2.29	0.62
7:E:28:TYR:HA	7:E:64:PRO:HA	1.82	0.62
3:A:463:LYS:O	3:A:468:ARG:NH1	2.33	0.62
4:B:424:ILE:HG22	4:B:453:VAL:HG11	1.82	0.62
3:A:490:ILE:HG23	3:A:494:GLU:HB2	1.82	0.62
3:A:32:ILE:CD1	3:A:54:LEU:CD1	2.78	0.61
3:A:439:ASP:O	3:A:442:LYS:NZ	2.33	0.61
3:A:985:ARG:HD2	3:A:987:TYR:HB3	1.82	0.61
7:E:93:MET:HE2	7:E:120:ALA:HA	1.82	0.61
3:A:652:ASN:O	3:A:656:GLN:NE2	2.33	0.61
4:B:745:GLN:HE21	4:B:800:TYR:HB3	1.65	0.61
4:B:974:LEU:HD11	16:N:169:GLU:HG2	1.79	0.61
6:D:37:LEU:HD12	6:D:97:LYS:HE3	1.81	0.61
5:C:122:ASP:HA	5:C:125:LYS:HB3	1.82	0.61
8:F:85:MET:HB3	8:F:153:VAL:HA	1.83	0.61
13:K:105:ILE:HD11	13:K:113:ALA:HA	1.83	0.61
16:N:169:GLU:CD	16:N:170:HIS:H	2.07	0.61
3:A:618:TYR:CB	4:B:783:MET:HE1	2.30	0.61
5:C:246:ARG:HA	5:C:249:LYS:HE2	1.82	0.61
3:A:175:SER:HA	3:A:178:LEU:HD23	1.82	0.61
3:A:531:PRO:HB3	3:A:580:HIS:HB2	1.81	0.61
4:B:211:ARG:HH22	4:B:646:HIS:HB2	1.66	0.61
9:G:82:LEU:HD11	9:G:125:TRP:HB2	1.81	0.61
4:B:104:ILE:HG23	4:B:137:LEU:HD23	1.83	0.61
9:G:241:ARG:HG2	17:O:189:PHE:HB3	1.83	0.61
4:B:1003:ALA:HB1	4:B:1005:TYR:CD2	2.36	0.60
3:A:618:TYR:CG	4:B:783:MET:CE	2.83	0.60
4:B:285:ASP:HA	11:I:15:ASP:HB3	1.81	0.60
4:B:784:ASP:C	4:B:950:ASN:ND2	2.58	0.60
5:C:45:SER:HB3	5:C:53:ASN:CB	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:56:DA:N3	4:B:513:LYS:NZ	2.49	0.60
4:B:974:LEU:HD11	16:N:169:GLU:CB	2.31	0.60
17:O:116:ILE:HG23	17:O:143:LEU:HD21	1.83	0.60
3:A:912:VAL:O	3:A:914:ASP:N	2.33	0.60
4:B:63:LEU:O	4:B:63:LEU:HD23	2.01	0.60
17:O:213:SER:HB2	17:O:338:LEU:HD21	1.81	0.60
7:E:174:GLN:NE2	8:F:140:ASP:OD2	2.32	0.60
17:O:417:LYS:HD3	17:O:472:HIS:HB2	1.83	0.60
4:B:741:LEU:H	4:B:804:TYR:HB2	1.67	0.60
6:D:30:HIS:HA	9:G:39:VAL:HG23	1.84	0.60
3:A:1080:TYR:HB3	3:A:1172:LEU:HD22	1.84	0.59
15:M:262:LEU:CA	15:M:265:LEU:HD12	2.32	0.59
16:N:80:MET:HB2	16:N:87:TYR:HB2	1.83	0.59
17:O:118:SER:HA	17:O:121:ASN:HB2	1.82	0.59
3:A:985:ARG:CD	3:A:987:TYR:N	2.65	0.59
4:B:17:ARG:NH1	4:B:758:ASP:OD2	2.35	0.59
4:B:404:LEU:HD11	4:B:551:ILE:HG21	1.85	0.59
4:B:492:ASN:HB3	4:B:495:ARG:HG3	1.83	0.59
5:C:333:ILE:HG22	13:K:47:ILE:HG12	1.83	0.59
7:E:100:ILE:HG23	7:E:105:PHE:HB2	1.84	0.59
10:H:22:LYS:O	10:H:43:ASN:ND2	2.35	0.59
3:A:130:ILE:O	7:E:192:ARG:NH2	2.36	0.59
3:A:912:VAL:CG2	3:A:913:PRO:HD3	2.24	0.59
4:B:1039:MET:HG2	4:B:1042:ASP:H	1.65	0.59
3:A:85:CYS:SG	3:A:86:TYR:N	2.75	0.59
3:A:792:GLY:H	3:A:795:HIS:HB3	1.67	0.59
12:J:30:LEU:HB3	12:J:35:ALA:HB2	1.85	0.59
3:A:370:PRO:HB3	3:A:379:GLU:HA	1.85	0.59
15:M:268:LEU:HG	15:M:331:TYR:HE2	1.67	0.59
3:A:1459:LYS:HD3	3:A:1473:LYS:HE2	1.83	0.59
4:B:791:LYS:NZ	5:C:214:GLY:O	2.35	0.59
12:J:42:LYS:HG3	12:J:43:ARG:HG3	1.84	0.59
3:A:466:LEU:HD13	3:A:471:MET:SD	2.42	0.59
4:B:718:GLN:HB2	4:B:922:GLY:HA2	1.84	0.59
5:C:80:ALA:HB3	5:C:102:GLY:HA2	1.83	0.59
15:M:268:LEU:HG	15:M:331:TYR:CD2	2.37	0.59
3:A:332:GLN:HE22	3:A:350:VAL:HG22	1.68	0.59
3:A:465:GLY:HA2	3:A:468:ARG:HB3	1.84	0.59
3:A:588:LEU:HD21	3:A:600:MET:HG3	1.84	0.59
3:A:1306:TYR:C	3:A:1307:ASP:OD1	2.45	0.59
3:A:335:LEU:HA	3:A:338:VAL:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:100:GLU:HB3	4:B:140:LYS:HD2	1.85	0.59
6:D:24:ALA:HA	9:G:43:ILE:HG22	1.85	0.59
7:E:62:ALA:HB3	7:E:78:LEU:HB3	1.85	0.59
3:A:748:ASN:ND2	3:A:771:PHE:O	2.36	0.58
3:A:1600:ARG:HG3	3:A:1601:GLN:HG3	1.85	0.58
5:C:318:VAL:HG13	13:K:128:CYS:HB2	1.85	0.58
15:M:313:SER:O	17:O:117:GLN:NE2	2.36	0.58
3:A:1276:THR:OG1	3:A:1288:ARG:NH1	2.36	0.58
12:J:44:TYR:HA	12:J:47:ARG:HG2	1.84	0.58
3:A:892:LEU:HA	3:A:895:VAL:HG12	1.85	0.58
4:B:136:LYS:HA	4:B:160:GLY:HA2	1.83	0.58
3:A:1129:PRO:HB2	3:A:1178:LEU:HD23	1.84	0.58
5:C:248:GLN:HG3	5:C:256:ILE:HB	1.85	0.58
4:B:609:ARG:NH2	4:B:662:ASP:OD2	2.37	0.58
7:E:151:PRO:HA	7:E:201:LYS:HZ3	1.67	0.58
3:A:1180:ASN:HD22	8:F:87:LYS:HG2	1.69	0.58
15:M:42:LYS:HB2	16:N:30:LYS:HB2	1.86	0.58
3:A:41:LEU:HD13	15:M:322:PRO:O	2.03	0.58
3:A:79:ILE:HG22	3:A:360:LEU:H	1.67	0.58
4:B:277:LEU:HD23	4:B:374:LEU:HD12	1.84	0.58
15:M:187:PRO:HB3	15:M:327:LYS:HG2	1.85	0.58
17:O:144:CYS:HB3	17:O:151:TRP:HB2	1.85	0.58
17:O:431:ALA:O	17:O:487:ARG:NH2	2.36	0.58
3:A:496:GLY:HA3	3:A:608:LEU:HD13	1.84	0.58
3:A:936:SER:H	3:A:939:ASN:HB2	1.68	0.58
4:B:327:LEU:CD2	4:B:330:LEU:HD12	2.33	0.58
4:B:966:SER:HB3	4:B:1029:GLY:HA3	1.85	0.58
12:J:7:CYS:SG	12:J:8:PHE:N	2.77	0.58
4:B:205:MET:SD	4:B:206:LEU:N	2.77	0.58
5:C:157:TYR:HB2	5:C:160:ALA:HB2	1.86	0.58
17:O:532:ALA:HA	17:O:537:VAL:HB	1.85	0.58
3:A:28:SER:O	4:B:1129:ARG:NH1	2.37	0.57
3:A:671:GLN:O	4:B:952:HIS:NE2	2.37	0.57
3:A:1626:VAL:HG21	4:B:1194:ILE:HG12	1.86	0.57
5:C:142:ARG:HE	5:C:198:PRO:HG3	1.69	0.57
9:G:42:PRO:HA	9:G:121:ASN:HA	1.86	0.57
10:H:114:VAL:HG22	10:H:125:LEU:HB2	1.86	0.57
12:J:17:LYS:O	12:J:21:TYR:N	2.36	0.57
4:B:240:ARG:NH2	4:B:356:ARG:O	2.37	0.57
15:M:77:VAL:HG12	15:M:92:LYS:HA	1.86	0.57
4:B:372:ARG:NH1	4:B:592:ILE:O	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:116:TYR:OH	10:H:137:GLN:NE2	2.37	0.57
3:A:512:THR:HB	3:A:514:TYR:HB3	1.86	0.57
4:B:887:LEU:HD12	14:L:56:LEU:HB2	1.85	0.57
4:B:1003:ALA:O	4:B:1005:TYR:CD2	2.57	0.57
3:A:1028:GLU:OE2	3:A:1638:SER:N	2.36	0.57
3:A:1068:PHE:O	3:A:1072:ASN:ND2	2.37	0.57
3:A:618:TYR:HD1	4:B:783:MET:CE	2.12	0.57
10:H:110:ASP:OD2	10:H:128:ASN:ND2	2.37	0.57
15:M:80:LEU:HB3	16:N:51:GLN:HE21	1.69	0.57
1:T:13:DT:OP2	3:A:464:GLU:OE2	2.22	0.57
3:A:985:ARG:HD3	3:A:987:TYR:H	1.70	0.57
15:M:11:GLU:OE2	15:M:87:SER:OG	2.22	0.57
4:B:613:VAL:HB	4:B:660:LYS:HD2	1.86	0.57
4:B:1003:ALA:HB1	4:B:1005:TYR:HD2	1.70	0.57
4:B:1005:TYR:HE1	16:N:171:PHE:CD2	2.20	0.57
9:G:37:CYS:SG	9:G:125:TRP:NE1	2.78	0.57
4:B:675:ALA:HB3	4:B:689:VAL:HG12	1.86	0.56
4:B:791:LYS:HE3	4:B:932:PRO:HD3	1.87	0.56
4:B:352:GLU:HG3	4:B:356:ARG:HE	1.71	0.56
4:B:788:ILE:HG22	4:B:948:ILE:HB	1.86	0.56
3:A:28:SER:OG	3:A:29:ALA:N	2.39	0.56
3:A:466:LEU:HD11	3:A:471:MET:HE1	1.87	0.56
3:A:650:LEU:HD23	4:B:1084:THR:HB	1.87	0.56
4:B:73:ILE:HD13	4:B:428:VAL:HB	1.86	0.56
4:B:994:ASP:OD1	4:B:1007:TYR:OH	2.24	0.56
9:G:88:LYS:H	9:G:120:VAL:HG12	1.70	0.56
16:N:54:TRP:HA	16:N:133:PHE:HE1	1.71	0.56
1:T:18:DC:N3	1:T:19:DA:N6	2.53	0.56
4:B:197:ASN:HD21	4:B:462:GLN:HE21	1.53	0.56
4:B:240:ARG:HD2	4:B:244:THR:HG23	1.88	0.56
5:C:240:LYS:HD3	5:C:265:ALA:H	1.70	0.56
9:G:154:ASN:HD22	17:O:148:PRO:HG3	1.71	0.56
10:H:30:SER:OG	10:H:33:GLN:O	2.24	0.56
3:A:466:LEU:CD2	3:A:470:HIS:CE1	2.88	0.56
4:B:359:LEU:HD12	4:B:370:LYS:NZ	2.21	0.56
13:K:89:CYS:SG	13:K:90:GLY:N	2.78	0.56
4:B:1157:GLN:HE22	4:B:1171:ASN:HB2	1.71	0.56
15:M:230:LYS:HD2	15:M:247:LEU:HD21	1.87	0.56
3:A:238:MET:SD	3:A:238:MET:N	2.78	0.56
4:B:492:ASN:ND2	4:B:722:GLY:O	2.39	0.56
3:A:629:ASP:O	4:B:924:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:135:PHE:CE1	7:E:186:LEU:CD2	2.89	0.56
15:M:336:ILE:HG21	15:M:349:LEU:HD11	1.88	0.56
2:U:61:DA:H4'	3:A:1601:GLN:NE2	2.20	0.56
3:A:673:HIS:HD2	3:A:817:PHE:HB2	1.71	0.56
4:B:623:ASP:HA	4:B:663:ILE:HD11	1.88	0.56
16:N:114:GLU:OE1	16:N:116:LYS:NZ	2.37	0.56
3:A:400:ASN:ND2	15:M:169:SER:OG	2.37	0.56
3:A:483:VAL:O	3:A:613:THR:OG1	2.23	0.56
3:A:818:THR:HA	3:A:821:ILE:HG22	1.88	0.56
3:A:325:ASP:OD1	3:A:329:ARG:NH2	2.39	0.55
3:A:1559:ARG:HH22	7:E:200:ARG:HG3	1.70	0.55
4:B:440:PHE:HA	4:B:445:TYR:HB3	1.88	0.55
4:B:1076:ARG:HH12	4:B:1088:LEU:HD22	1.70	0.55
5:C:100:ARG:HH12	12:J:2:ILE:HB	1.71	0.55
5:C:218:LYS:NZ	14:L:70:ARG:OXT	2.40	0.55
9:G:90:LEU:HD23	9:G:118:CYS:HA	1.88	0.55
3:A:41:LEU:HD13	3:A:41:LEU:C	2.31	0.55
3:A:942:GLN:O	3:A:985:ARG:NH1	2.38	0.55
5:C:90:SER:HA	5:C:200:GLN:HG2	1.88	0.55
3:A:1256:LYS:HB2	3:A:1307:ASP:OD2	2.05	0.55
4:B:703:LEU:HD13	4:B:704:THR:CA	2.36	0.55
3:A:729:LYS:HE2	10:H:120:GLY:HA3	1.87	0.55
4:B:652:PRO:HA	4:B:663:ILE:HA	1.88	0.55
15:M:262:LEU:O	15:M:265:LEU:HB2	2.05	0.55
3:A:1634:LEU:HD12	3:A:1634:LEU:O	2.06	0.55
9:G:161:ASN:HD22	9:G:248:THR:HG22	1.71	0.55
6:D:84:SER:O	6:D:88:GLN:NE2	2.40	0.55
14:L:31:CYS:SG	14:L:32:ALA:N	2.79	0.55
3:A:194:ALA:HA	3:A:197:LEU:HB2	1.88	0.55
4:B:97:VAL:HG21	4:B:424:ILE:HD11	1.88	0.55
9:G:218:VAL:HG13	9:G:222:GLY:HA2	1.89	0.55
3:A:250:LYS:HD2	3:A:316:LEU:HA	1.88	0.55
3:A:1450:ILE:O	3:A:1454:HIS:N	2.40	0.55
4:B:912:GLN:OE1	4:B:1041:ASN:ND2	2.39	0.55
5:C:116:VAL:HG21	5:C:209:ILE:HG13	1.87	0.55
9:G:140:GLN:HE21	9:G:215:GLY:H	1.52	0.55
3:A:532:GLY:H	3:A:580:HIS:CE1	2.25	0.55
4:B:1005:TYR:CE1	16:N:171:PHE:CD2	2.95	0.55
7:E:5:ASN:OD1	7:E:52:ARG:NH2	2.40	0.55
3:A:559:ASN:ND2	17:O:376:TYR:O	2.40	0.54
3:A:1053:ASP:OD1	3:A:1174:TYR:OH	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:444:ARG:HG3	4:B:448:ARG:HH11	1.72	0.54
4:B:673:ASN:ND2	4:B:685:VAL:O	2.40	0.54
4:B:766:PRO:HG3	12:J:54:VAL:HG21	1.89	0.54
4:B:1039:MET:HE2	4:B:1041:ASN:HA	1.89	0.54
4:B:997:GLY:O	4:B:1001:ALA:N	2.41	0.54
14:L:48:CYS:N	14:L:53:HIS:O	2.39	0.54
15:M:267:LEU:HG	15:M:270:GLY:HA3	1.88	0.54
3:A:15:ASP:HB3	4:B:1197:ARG:HB3	1.89	0.54
3:A:1047:GLN:HE21	3:A:1587:ASP:HB2	1.72	0.54
4:B:359:LEU:CD1	4:B:370:LYS:NZ	2.70	0.54
15:M:261:LEU:O	15:M:265:LEU:HG	2.07	0.54
15:M:268:LEU:HD23	15:M:268:LEU:O	2.06	0.54
3:A:438:ILE:HG22	3:A:457:LYS:HE2	1.89	0.54
3:A:1591:ARG:HE	3:A:1592:GLN:HE21	1.55	0.54
5:C:54:PHE:HB3	5:C:300:PHE:HB2	1.89	0.54
16:N:82:ILE:HG13	16:N:85:HIS:H	1.73	0.54
3:A:1256:LYS:O	3:A:1499:ARG:NH2	2.36	0.54
4:B:857:PRO:HB3	4:B:871:ILE:HG23	1.89	0.54
7:E:135:PHE:CE1	7:E:186:LEU:HD21	2.42	0.54
14:L:38:LEU:HD13	14:L:40:LEU:HD13	1.89	0.54
15:M:79:GLY:N	16:N:54:TRP:O	2.36	0.54
3:A:196:ALA:HB2	3:A:201:ARG:HH21	1.73	0.54
3:A:883:LEU:HD12	3:A:884:ARG:HE	1.73	0.54
4:B:974:LEU:HD11	16:N:169:GLU:HB3	1.89	0.54
5:C:128:ASP:OD2	5:C:174:ARG:N	2.40	0.54
17:O:382:GLN:NE2	17:O:593:PRO:O	2.40	0.54
3:A:516:ILE:HD11	17:O:588:LEU:HD11	1.89	0.54
3:A:592:GLN:NE2	3:A:634:ASN:OD1	2.35	0.54
3:A:1025:LYS:HZ2	3:A:1615:TYR:HB2	1.70	0.54
4:B:1000:LEU:HA	4:B:1003:ALA:HB3	1.90	0.54
9:G:26:ASN:OD1	9:G:128:GLN:NE2	2.40	0.54
1:T:13:DT:O4	2:U:56:DA:N1	2.40	0.54
4:B:280:LEU:HG	4:B:370:LYS:HB3	1.89	0.54
4:B:317:TYR:HD2	4:B:320:LEU:HB2	1.72	0.54
4:B:543:ASN:OD1	4:B:543:ASN:N	2.41	0.54
6:D:94:ARG:HA	6:D:98:GLY:H	1.73	0.54
11:I:2:SER:O	11:I:9:PHE:N	2.40	0.54
1:T:12:DC:H3'	1:T:12:DC:H6	1.72	0.54
4:B:555:GLN:OE1	4:B:646:HIS:ND1	2.40	0.54
4:B:588:ILE:HA	4:B:642:LEU:HB2	1.89	0.54
4:B:650:LEU:HD12	4:B:663:ILE:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:94:ARG:HD3	6:D:100:PRO:HD3	1.90	0.54
15:M:299:LEU:O	15:M:303:THR:OG1	2.26	0.54
3:A:499:PRO:HA	3:A:502:ALA:HB3	1.89	0.53
3:A:985:ARG:HD3	3:A:987:TYR:N	2.23	0.53
15:M:35:ASP:OD1	15:M:35:ASP:N	2.40	0.53
3:A:668:GLY:HA3	3:A:787:GLY:HA2	1.89	0.53
3:A:686:PHE:HB3	3:A:725:LEU:HD11	1.90	0.53
3:A:1055:ILE:O	3:A:1580:ARG:NH1	2.41	0.53
6:D:84:SER:OG	17:O:228:GLN:NE2	2.41	0.53
3:A:1046:VAL:HG22	3:A:1591:ARG:HD3	1.91	0.53
4:B:129:ARG:NH2	4:B:891:GLU:H	2.06	0.53
4:B:876:SER:OG	4:B:878:GLU:OE1	2.25	0.53
10:H:118:PHE:HB2	10:H:121:LEU:HB3	1.89	0.53
15:M:261:LEU:HD13	15:M:335:ILE:HG12	1.90	0.53
3:A:480:ALA:HB3	3:A:635:MET:HB3	1.91	0.53
4:B:265:ARG:O	4:B:266:LYS:HG2	2.09	0.53
5:C:303:GLU:OE2	12:J:43:ARG:NH1	2.41	0.53
3:A:832:ASP:OD1	3:A:923:ASN:ND2	2.41	0.53
3:A:1562:ILE:HD11	3:A:1586:ALA:HA	1.89	0.53
4:B:221:SER:HA	4:B:224:ASN:HB2	1.90	0.53
4:B:784:ASP:C	4:B:785:ASP:OD1	2.52	0.53
4:B:906:ARG:O	4:B:908:ARG:NH2	2.39	0.53
2:U:65:DG:O5'	2:U:65:DG:H8	1.92	0.53
3:A:1528:ALA:O	3:A:1532:GLN:NE2	2.41	0.53
4:B:690:GLU:OE2	4:B:695:ASN:ND2	2.42	0.53
5:C:39:ASP:O	5:C:58:ASN:ND2	2.39	0.53
9:G:24:VAL:O	9:G:128:GLN:NE2	2.42	0.53
11:I:58:SER:OG	11:I:61:ARG:N	2.40	0.53
3:A:815:ARG:O	3:A:819:ASN:ND2	2.41	0.53
13:K:60:SER:OG	13:K:104:ARG:NH2	2.42	0.53
3:A:1636:SER:O	3:A:1640:ARG:N	2.42	0.53
3:A:113:VAL:HG21	3:A:178:LEU:HD12	1.89	0.53
4:B:359:LEU:CD1	4:B:370:LYS:HG3	2.27	0.53
12:J:34:THR:HA	12:J:37:SER:HB2	1.91	0.53
4:B:908:ARG:NH1	5:C:93:GLN:OE1	2.41	0.52
10:H:28:ALA:HB3	10:H:38:LEU:HB3	1.91	0.52
13:K:79:VAL:HG23	13:K:82:LYS:HD2	1.91	0.52
15:M:360:VAL:HA	15:M:363:LEU:HB3	1.91	0.52
3:A:1439:MET:SD	3:A:1439:MET:N	2.82	0.52
4:B:95:LEU:HA	4:B:145:VAL:HA	1.90	0.52
4:B:748:GLN:HB2	4:B:769:PHE:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:85:GLU:O	7:E:113:GLN:NE2	2.42	0.52
1:T:19:DA:OP1	4:B:1063:ARG:NH1	2.42	0.52
3:A:830:MET:O	3:A:834:ARG:NH2	2.43	0.52
4:B:256:GLY:HA3	4:B:308:LEU:HD22	1.92	0.52
4:B:586:VAL:N	4:B:594:GLY:O	2.41	0.52
6:D:88:GLN:HG3	6:D:89:LEU:HD12	1.90	0.52
3:A:646:GLU:O	3:A:650:LEU:N	2.42	0.52
3:A:721:LYS:HE2	10:H:46:LEU:HD22	1.89	0.52
3:A:1097:TYR:OH	3:A:1121:ASP:OD1	2.27	0.52
4:B:127:ARG:HB3	4:B:195:ILE:HD13	1.91	0.52
3:A:41:LEU:HD12	3:A:43:HIS:CE1	2.38	0.52
4:B:167:SER:N	4:B:170:CYS:SG	2.76	0.52
4:B:244:THR:HG21	4:B:414:LYS:HD2	1.91	0.52
4:B:532:HIS:ND1	4:B:719:CYS:SG	2.70	0.52
4:B:1111:LEU:HD13	4:B:1187:SER:HB2	1.92	0.52
9:G:63:LYS:HD3	9:G:67:ASN:HD22	1.74	0.52
3:A:1038:ILE:HD11	3:A:1047:GLN:HB2	1.92	0.52
4:B:60:LEU:HD12	4:B:242:ASP:HA	1.92	0.52
8:F:101:ILE:HA	8:F:105:ALA:HB3	1.91	0.52
10:H:43:ASN:ND2	10:H:45:GLU:OE1	2.43	0.52
15:M:250:LEU:HG	15:M:250:LEU:O	2.10	0.52
17:O:480:LEU:HD12	17:O:483:ILE:HD12	1.92	0.52
3:A:985:ARG:HH21	3:A:986:PHE:N	2.04	0.52
4:B:219:ARG:HG2	4:B:221:SER:H	1.75	0.52
3:A:216:ARG:NH2	3:A:340:HIS:O	2.43	0.52
3:A:435:ASN:OD1	3:A:436:ALA:N	2.42	0.52
4:B:889:GLY:HA3	4:B:898:LEU:HD22	1.91	0.52
4:B:228:SER:O	4:B:254:ASN:ND2	2.42	0.52
3:A:99:ARG:O	3:A:109:ARG:NH2	2.38	0.51
3:A:252:PHE:HZ	15:M:144:LEU:HG	1.74	0.51
3:A:462:LYS:NZ	3:A:465:GLY:O	2.42	0.51
3:A:470:HIS:O	3:A:474:LYS:NZ	2.43	0.51
4:B:837:LEU:O	4:B:847:TYR:OH	2.26	0.51
5:C:301:ASN:HD21	16:N:174:GLY:HA2	1.75	0.51
9:G:73:TYR:HB2	9:G:80:VAL:HG22	1.92	0.51
17:O:163:ILE:HA	17:O:211:TYR:HB2	1.90	0.51
3:A:52:LEU:HD21	3:A:60:ASN:HD22	1.74	0.51
3:A:1333:ILE:HG12	3:A:1480:THR:HG21	1.92	0.51
4:B:784:ASP:C	4:B:950:ASN:HD22	2.18	0.51
4:B:784:ASP:OD1	4:B:785:ASP:N	2.43	0.51
10:H:40:LEU:HD21	10:H:42:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:363:LEU:HD13	15:M:363:LEU:C	2.35	0.51
17:O:428:ILE:HA	17:O:434:LEU:HD21	1.92	0.51
3:A:898:SER:O	3:A:902:ALA:N	2.43	0.51
4:B:576:THR:HB	4:B:595:TRP:HZ2	1.75	0.51
15:M:113:ILE:HG23	15:M:117:SER:HA	1.92	0.51
16:N:58:PHE:HB3	16:N:139:VAL:HB	1.91	0.51
3:A:908:VAL:HG23	3:A:941:SER:HB3	1.92	0.51
3:A:1042:ASP:OD1	3:A:1042:ASP:N	2.37	0.51
3:A:1588:MET:SD	3:A:1591:ARG:NH1	2.82	0.51
5:C:45:SER:CB	5:C:53:ASN:HB3	2.35	0.51
15:M:250:LEU:N	15:M:250:LEU:CD2	2.73	0.51
17:O:412:GLU:OE1	17:O:416:LYS:NZ	2.35	0.51
3:A:117:ARG:O	3:A:121:LYS:N	2.40	0.51
3:A:1072:ASN:HB3	3:A:1075:ALA:HB3	1.92	0.51
4:B:431:ASP:O	4:B:435:GLY:N	2.43	0.51
7:E:23:VAL:HG23	7:E:28:TYR:HD2	1.76	0.51
7:E:54:GLN:HE21	7:E:57:MET:HE3	1.75	0.51
13:K:88:PHE:O	13:K:106:GLN:N	2.41	0.51
3:A:813:LEU:CD1	3:A:813:LEU:C	2.83	0.51
3:A:1053:ASP:O	3:A:1174:TYR:OH	2.29	0.51
3:A:1484:LEU:O	3:A:1488:ILE:N	2.42	0.51
4:B:238:SER:OG	4:B:246:GLN:NE2	2.44	0.51
4:B:327:LEU:HD22	4:B:350:GLY:HA3	1.93	0.51
7:E:147:HIS:HB3	7:E:150:VAL:HG22	1.93	0.51
16:N:50:GLN:HE22	16:N:52:GLN:HB3	1.76	0.51
3:A:314:TYR:OH	15:M:146:ARG:O	2.26	0.51
3:A:463:LYS:HG3	3:A:468:ARG:HH12	1.75	0.51
3:A:1237:GLN:HE22	3:A:1520:VAL:HB	1.76	0.51
10:H:26:ILE:HB	10:H:40:LEU:HB3	1.92	0.51
3:A:214:ASP:O	3:A:218:LYS:N	2.42	0.51
4:B:346:ASP:HA	4:B:349:VAL:HG12	1.93	0.51
4:B:420:TYR:HE1	4:B:455:GLU:HG2	1.74	0.51
4:B:714:ARG:CD	4:B:957:ARG:HD2	2.38	0.51
3:A:613:THR:O	3:A:615:ARG:NH2	2.44	0.51
3:A:673:HIS:CD2	3:A:817:PHE:HB2	2.46	0.51
3:A:842:TRP:HA	3:A:845:ASP:HB2	1.93	0.51
4:B:205:MET:HE3	4:B:503:VAL:HA	1.93	0.51
4:B:863:ASP:OD1	4:B:870:LYS:NZ	2.36	0.51
5:C:320:ILE:O	5:C:324:LYS:N	2.44	0.51
3:A:912:VAL:CB	3:A:913:PRO:HD2	2.41	0.50
4:B:656:LEU:HD11	4:B:689:VAL:HG13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:711:GLN:HB3	4:B:713:PRO:HD2	1.93	0.50
8:F:97:ARG:O	8:F:101:ILE:N	2.35	0.50
9:G:17:ILE:O	9:G:21:LYS:N	2.43	0.50
17:O:139:PHE:HA	17:O:142:ILE:HG22	1.93	0.50
3:A:368:ARG:HH11	3:A:383:ASN:HD21	1.59	0.50
15:M:350:ALA:O	15:M:355:LEU:O	2.29	0.50
3:A:843:ARG:HH22	3:A:985:ARG:HB3	1.77	0.50
3:A:937:ASN:HA	3:A:940:VAL:HG22	1.93	0.50
3:A:1054:ALA:O	3:A:1178:LEU:HD22	2.11	0.50
3:A:1103:LYS:HA	3:A:1106:LYS:HG2	1.94	0.50
4:B:820:PRO:HD2	15:M:356:LYS:HZ1	1.74	0.50
17:O:67:ASP:OD2	17:O:69:THR:OG1	2.29	0.50
3:A:368:ARG:HD2	3:A:383:ASN:HD21	1.76	0.50
5:C:57:ILE:HG23	5:C:297:HIS:HA	1.92	0.50
13:K:63:PHE:N	13:K:103:ILE:O	2.44	0.50
3:A:481:ARG:HB2	4:B:1069:ILE:HD12	1.92	0.50
3:A:1610:PHE:HB2	3:A:1639:ALA:HB2	1.94	0.50
4:B:651:ARG:N	4:B:664:VAL:O	2.44	0.50
4:B:1112:THR:HG21	4:B:1130:ARG:HB2	1.94	0.50
5:C:100:ARG:NH2	12:J:3:VAL:O	2.45	0.50
15:M:42:LYS:HD2	16:N:32:CYS:HA	1.93	0.50
3:A:1091:VAL:HA	3:A:1133:LEU:HB2	1.92	0.50
3:A:1549:VAL:HG11	3:A:1561:THR:HG21	1.92	0.50
4:B:785:ASP:OD1	4:B:785:ASP:N	2.44	0.50
4:B:898:LEU:HD11	14:L:46:VAL:HG11	1.93	0.50
12:J:1:MET:HA	12:J:56:LEU:H	1.76	0.50
4:B:322:ASN:ND2	15:M:104:SER:O	2.45	0.50
4:B:806:THR:HA	4:B:904:LYS:HA	1.93	0.50
6:D:99:LEU:HD22	6:D:100:PRO:HD2	1.94	0.50
9:G:137:ILE:HB	9:G:227:GLY:HA2	1.94	0.50
16:N:169:GLU:OE2	16:N:170:HIS:C	2.54	0.50
3:A:836:THR:O	3:A:840:ASN:N	2.37	0.50
3:A:1270:VAL:HG11	3:A:1489:VAL:HG11	1.93	0.50
3:A:1634:LEU:HD13	3:A:1639:ALA:O	2.11	0.50
4:B:47:GLY:O	4:B:553:THR:OG1	2.27	0.50
7:E:8:ASN:HA	7:E:11:ARG:HG2	1.93	0.50
4:B:334:PHE:HA	4:B:337:VAL:HG12	1.93	0.50
13:K:83:ASN:HD22	13:K:84:PRO:HD2	1.77	0.50
3:A:237:GLY:O	3:A:263:ASN:ND2	2.44	0.49
3:A:732:ILE:O	3:A:736:LEU:HB2	2.12	0.49
3:A:843:ARG:NH2	3:A:985:ARG:HB3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:872:ASP:HB2	3:A:875:LEU:CB	2.42	0.49
3:A:1031:HIS:HB3	3:A:1649:VAL:HG13	1.94	0.49
3:A:1238:MET:HE3	3:A:1240:LEU:HD11	1.94	0.49
4:B:529:CYS:HB3	4:B:532:HIS:H	1.77	0.49
4:B:995:TYR:OH	16:N:161:PRO:O	2.26	0.49
5:C:233:ILE:HD12	5:C:291:LEU:HB3	1.94	0.49
16:N:73:ASP:HB2	16:N:77:SER:HB3	1.93	0.49
3:A:125:LEU:N	3:A:126:GLN:OE1	2.40	0.49
4:B:335:ARG:HH22	15:M:112:LYS:HD2	1.77	0.49
4:B:726:MET:SD	4:B:1035:ARG:NH1	2.85	0.49
5:C:197:ARG:HG2	12:J:61:LEU:HD22	1.94	0.49
17:O:438:GLN:HA	17:O:441:PHE:HB3	1.94	0.49
3:A:809:VAL:HA	3:A:812:VAL:HG22	1.95	0.49
3:A:947:LEU:HD11	3:A:950:GLN:HE21	1.77	0.49
3:A:1651:THR:HG22	4:B:1085:SER:H	1.78	0.49
4:B:1088:LEU:HA	4:B:1091:ARG:HB3	1.95	0.49
9:G:64:GLN:HG3	9:G:65:HIS:CD2	2.48	0.49
3:A:506:THR:O	3:A:639:GLN:NE2	2.33	0.49
3:A:1032:VAL:O	3:A:1182:GLY:N	2.40	0.49
7:E:80:VAL:HG22	7:E:109:ILE:HB	1.95	0.49
12:J:16:ASP:OD1	12:J:16:ASP:N	2.42	0.49
15:M:58:GLU:OE2	15:M:59:ARG:NH1	2.46	0.49
3:A:1178:LEU:C	3:A:1178:LEU:CD1	2.86	0.49
3:A:1437:ASN:HD22	3:A:1438:ASN:H	1.60	0.49
7:E:95:THR:HA	7:E:98:ILE:HD12	1.94	0.49
12:J:45:CYS:O	12:J:48:ARG:NE	2.39	0.49
3:A:715:LEU:HD22	3:A:730:GLN:HE22	1.77	0.49
3:A:975:ASP:N	3:A:975:ASP:OD1	2.44	0.49
3:A:1256:LYS:HB3	3:A:1307:ASP:OD2	2.12	0.49
4:B:1196:LEU:C	4:B:1196:LEU:CD1	2.86	0.49
4:B:286:ARG:O	4:B:290:ASP:N	2.35	0.49
4:B:572:PRO:HB2	4:B:575:HIS:HD2	1.77	0.49
5:C:65:ASN:HD22	5:C:68:ARG:HE	1.61	0.49
15:M:268:LEU:C	15:M:268:LEU:CD2	2.86	0.49
15:M:321:ASP:OD1	15:M:324:ASN:ND2	2.46	0.49
3:A:466:LEU:HD23	3:A:470:HIS:CE1	2.48	0.49
3:A:972:TYR:OH	4:B:633:THR:OG1	2.29	0.49
8:F:65:ARG:HH12	9:G:117:TRP:HE3	1.61	0.49
17:O:348:THR:OG1	17:O:350:GLU:OE1	2.31	0.49
3:A:24:ILE:HA	3:A:27:LEU:HD22	1.95	0.49
3:A:720:PHE:HB2	10:H:96:VAL:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1634:LEU:CD1	3:A:1639:ALA:O	2.61	0.49
4:B:947:ILE:HG21	4:B:1033:TYR:HE2	1.77	0.49
11:I:58:SER:HB2	11:I:60:LEU:HD23	1.95	0.49
13:K:92:SER:OG	13:K:102:ASN:O	2.31	0.49
16:N:57:LYS:HB3	16:N:138:SER:HA	1.93	0.49
17:O:81:PRO:HB2	17:O:83:LYS:HG2	1.94	0.49
4:B:974:LEU:CD1	16:N:169:GLU:CG	2.84	0.48
17:O:241:ASP:OD2	17:O:380:SER:N	2.46	0.48
17:O:445:TYR:O	17:O:449:TRP:N	2.46	0.48
3:A:1648:ASN:OD1	3:A:1648:ASN:N	2.46	0.48
4:B:152:LEU:HD23	4:B:443:LYS:HG3	1.95	0.48
4:B:653:VAL:N	4:B:662:ASP:O	2.40	0.48
17:O:198:PHE:HB2	17:O:232:LEU:HD21	1.95	0.48
4:B:556:SER:HB2	4:B:621:PRO:HG3	1.95	0.48
4:B:1015:SER:HG	4:B:1020:GLU:H	1.60	0.48
4:B:1116:SER:OG	4:B:1160:GLU:O	2.31	0.48
8:F:72:LYS:HE3	8:F:141:GLY:HA2	1.94	0.48
3:A:110:LEU:HA	3:A:227:LEU:HD13	1.95	0.48
4:B:218:ILE:HD12	4:B:231:HIS:HD2	1.78	0.48
4:B:756:LEU:HD13	4:B:759:ASP:HB3	1.95	0.48
7:E:143:ASN:HD22	7:E:146:HIS:CE1	2.31	0.48
3:A:862:THR:HG23	3:A:864:LEU:H	1.78	0.48
4:B:27:ASN:OD1	4:B:27:ASN:N	2.47	0.48
4:B:969:GLY:HA3	4:B:1030:VAL:HG23	1.94	0.48
3:A:912:VAL:C	3:A:914:ASP:H	2.20	0.48
4:B:204:ARG:HD2	4:B:486:VAL:HG13	1.95	0.48
4:B:283:THR:OG1	4:B:323:ARG:NH2	2.47	0.48
5:C:200:GLN:NE2	12:J:64:ASN:OD1	2.42	0.48
17:O:101:SER:HA	17:O:104:ILE:HD13	1.95	0.48
3:A:224:HIS:HA	3:A:228:LEU:HD22	1.94	0.48
3:A:399:LEU:HD23	3:A:422:ARG:HD3	1.95	0.48
4:B:742:TYR:HE2	4:B:1037:ARG:HG3	1.79	0.48
6:D:19:PRO:HD3	9:G:65:HIS:HB3	1.96	0.48
3:A:381:SER:HB2	3:A:453:ILE:HD11	1.94	0.48
3:A:1550:LEU:HA	3:A:1554:GLY:H	1.79	0.48
3:A:1578:SER:OG	3:A:1579:PHE:N	2.46	0.48
15:M:22:ALA:HB3	16:N:110:LEU:HD21	1.95	0.48
3:A:912:VAL:CB	3:A:913:PRO:CD	2.92	0.48
4:B:126:SER:OG	4:B:132:SER:O	2.31	0.48
4:B:931:TRP:CD2	4:B:932:PRO:HD2	2.49	0.48
3:A:911:CYS:O	3:A:911:CYS:SG	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1032:VAL:HB	3:A:1181:PRO:HA	1.95	0.48
4:B:564:ILE:HD11	4:B:620:LEU:HD21	1.96	0.48
7:E:12:LEU:O	7:E:16:PHE:N	2.41	0.48
8:F:87:LYS:O	8:F:91:ALA:N	2.45	0.48
3:A:736:LEU:HD22	3:A:736:LEU:HA	1.60	0.47
3:A:1657:LEU:HB2	8:F:133:VAL:HB	1.96	0.47
3:A:52:LEU:HD11	3:A:60:ASN:HB2	1.95	0.47
3:A:885:ASP:N	3:A:885:ASP:OD1	2.42	0.47
3:A:1019:LEU:HD23	3:A:1227:MET:HE2	1.96	0.47
15:M:78:VAL:HA	16:N:55:LEU:HA	1.96	0.47
4:B:1097:ASP:OD1	4:B:1180:PHE:N	2.43	0.47
4:B:1100:GLN:HB3	4:B:1175:THR:HB	1.96	0.47
4:B:1116:SER:O	4:B:1125:THR:OG1	2.30	0.47
8:F:130:ILE:HG23	8:F:148:VAL:HG11	1.95	0.47
3:A:33:THR:HG22	3:A:394:LEU:HD11	1.96	0.47
3:A:41:LEU:CD1	15:M:323:GLN:HA	2.43	0.47
3:A:41:LEU:CD1	15:M:322:PRO:O	2.62	0.47
3:A:96:ILE:HG21	3:A:224:HIS:HD2	1.78	0.47
3:A:726:TRP:HE3	3:A:730:GLN:HG2	1.80	0.47
3:A:781:LEU:HD21	3:A:786:TYR:HE1	1.80	0.47
3:A:1027:LEU:HD13	3:A:1186:GLY:HA2	1.97	0.47
3:A:1531:ASP:OD1	3:A:1532:GLN:NE2	2.47	0.47
4:B:830:ASP:N	4:B:830:ASP:OD1	2.43	0.47
10:H:28:ALA:O	10:H:38:LEU:N	2.48	0.47
17:O:478:GLN:O	17:O:482:TYR:N	2.47	0.47
3:A:400:ASN:HD22	15:M:167:THR:HG23	1.78	0.47
3:A:672:ASP:OD1	3:A:673:HIS:ND1	2.48	0.47
3:A:1044:THR:HA	7:E:174:GLN:HE21	1.79	0.47
4:B:52:LEU:HA	4:B:60:LEU:HD23	1.96	0.47
5:C:73:SER:OG	5:C:74:GLU:OE1	2.28	0.47
17:O:344:GLU:HG3	17:O:388:VAL:HG23	1.96	0.47
3:A:14:VAL:O	3:A:1631:ARG:NH1	2.48	0.47
4:B:104:ILE:HG21	4:B:161:LEU:HB3	1.97	0.47
6:D:39:PHE:HD2	9:G:40:ARG:HH22	1.60	0.47
15:M:153:LYS:HB2	15:M:156:ASP:HB2	1.96	0.47
15:M:305:ILE:HG21	15:M:316:ARG:HH21	1.80	0.47
3:A:1178:LEU:CD1	3:A:1179:ILE:O	2.63	0.47
3:A:1256:LYS:C	3:A:1307:ASP:OD2	2.57	0.47
4:B:359:LEU:CG	4:B:370:LYS:HE3	2.44	0.47
4:B:623:ASP:OD1	4:B:623:ASP:N	2.35	0.47
4:B:707:SER:H	4:B:983:PRO:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:975:HIS:CE1	16:N:166:LEU:HB3	2.50	0.47
5:C:107:LYS:HE3	5:C:187:ALA:HA	1.96	0.47
3:A:23:GLU:OE1	4:B:1130:ARG:NH1	2.47	0.47
3:A:985:ARG:HD2	3:A:987:TYR:N	2.26	0.47
3:A:1057:ILE:HG13	3:A:1581:HIS:HE1	1.80	0.47
4:B:825:PHE:HA	4:B:861:TYR:HB2	1.97	0.47
5:C:93:GLN:HE22	5:C:95:GLU:HB3	1.79	0.47
7:E:151:PRO:HB3	7:E:200:ARG:HA	1.95	0.47
10:H:137:GLN:OE1	10:H:139:ASN:N	2.48	0.47
15:M:8:SER:OG	15:M:9:GLU:N	2.46	0.47
17:O:238:ILE:HG23	17:O:378:THR:HG21	1.97	0.47
3:A:43:HIS:HA	15:M:322:PRO:HG2	1.97	0.47
3:A:64:THR:HA	4:B:1162:GLY:HA3	1.96	0.47
3:A:759:TYR:CD1	3:A:913:PRO:HG2	2.50	0.47
4:B:589:ASP:OD1	4:B:589:ASP:N	2.42	0.47
6:D:36:VAL:HG22	6:D:40:LEU:HG	1.96	0.47
14:L:32:ALA:HB3	14:L:53:HIS:HE1	1.80	0.47
15:M:306:LYS:HG3	15:M:319:PHE:HB2	1.96	0.47
16:N:169:GLU:CD	16:N:169:GLU:C	2.82	0.47
3:A:836:THR:OG1	3:A:839:GLY:N	2.46	0.47
4:B:395:ASP:OD1	4:B:395:ASP:N	2.39	0.47
4:B:724:GLN:HE21	4:B:1037:ARG:HB3	1.80	0.47
4:B:790:ASN:HB3	4:B:793:ALA:HB3	1.96	0.47
5:C:272:LYS:HG2	16:N:175:TYR:CZ	2.50	0.47
3:A:942:GLN:HG2	3:A:947:LEU:HB2	1.96	0.46
5:C:42:VAL:HB	13:K:138:LYS:HG3	1.98	0.46
9:G:80:VAL:N	9:G:125:TRP:O	2.48	0.46
4:B:20:GLU:O	4:B:24:ARG:NE	2.47	0.46
4:B:939:SER:O	5:C:226:SER:OG	2.33	0.46
10:H:101:ALA:HB3	10:H:137:GLN:H	1.79	0.46
12:J:48:ARG:O	12:J:52:THR:N	2.47	0.46
17:O:420:SER:HA	17:O:423:TYR:HD2	1.79	0.46
3:A:561:LEU:HA	3:A:575:LYS:HD2	1.96	0.46
4:B:1113:THR:OG1	4:B:1127:CYS:O	2.28	0.46
3:A:949:GLN:HG2	3:A:981:TYR:HA	1.97	0.46
4:B:258:VAL:HG11	4:B:378:ILE:HD11	1.98	0.46
4:B:480:GLN:OE1	4:B:508:PHE:N	2.46	0.46
4:B:963:PHE:O	4:B:1027:TYR:OH	2.24	0.46
5:C:181:ASP:OD1	5:C:181:ASP:N	2.46	0.46
7:E:39:LEU:O	7:E:43:LYS:N	2.34	0.46
15:M:42:LYS:HA	15:M:51:PHE:HD1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:140:SER:OG	16:N:141:GLU:N	2.48	0.46
17:O:440:ILE:O	17:O:444:SER:OG	2.29	0.46
3:A:61:LEU:HG	15:M:306:LYS:HG2	1.97	0.46
3:A:1613:MET:HE3	3:A:1622:LEU:HD11	1.97	0.46
4:B:1047:ARG:HH12	4:B:1060:VAL:H	1.63	0.46
7:E:93:MET:HG3	7:E:120:ALA:HB1	1.96	0.46
9:G:138:PHE:HE2	17:O:183:ILE:HG12	1.81	0.46
16:N:39:PRO:HB2	16:N:51:GLN:HE22	1.81	0.46
3:A:127:TYR:HB2	3:A:129:LEU:HD23	1.98	0.46
3:A:985:ARG:C	3:A:985:ARG:CD	2.86	0.46
3:A:1114:TYR:HB2	7:E:146:HIS:HD2	1.81	0.46
5:C:36:PHE:HE2	13:K:130:VAL:HG11	1.81	0.46
15:M:231:LEU:HD11	15:M:244:ALA:HB2	1.96	0.46
15:M:388:THR:OG1	15:M:391:SER:OG	2.33	0.46
3:A:267:LYS:HB2	3:A:270:ILE:HD11	1.96	0.46
3:A:514:TYR:CZ	8:F:120:ILE:HD11	2.50	0.46
3:A:759:TYR:CZ	3:A:913:PRO:HG2	2.51	0.46
3:A:1256:LYS:HB3	3:A:1307:ASP:CG	2.41	0.46
4:B:629:VAL:HG13	4:B:639:GLY:H	1.81	0.46
4:B:730:GLY:HA2	4:B:765:PHE:HE1	1.80	0.46
16:N:33:LYS:O	16:N:115:SER:OG	2.33	0.46
4:B:850:THR:H	4:B:882:ILE:HG13	1.81	0.46
4:B:881:TYR:HB2	4:B:908:ARG:NH2	2.31	0.46
10:H:5:LEU:HD12	10:H:133:ASN:HB2	1.96	0.46
15:M:9:GLU:HA	16:N:71:PRO:HA	1.97	0.46
3:A:489:ASN:ND2	13:K:94:PRO:O	2.49	0.46
3:A:1337:LYS:HZ1	3:A:1480:THR:HA	1.81	0.46
4:B:71:LYS:HZ3	4:B:421:LEU:HD12	1.79	0.46
4:B:96:SER:OG	4:B:97:VAL:N	2.49	0.46
4:B:532:HIS:HE1	4:B:723:LYS:HD3	1.81	0.46
4:B:586:VAL:HG22	4:B:640:LEU:HB3	1.97	0.46
4:B:1015:SER:OG	4:B:1020:GLU:N	2.49	0.46
4:B:1103:VAL:HG22	4:B:1110:ILE:HG13	1.97	0.46
17:O:401:VAL:HA	17:O:404:ILE:HD12	1.97	0.46
2:U:65:DG:H2'	2:U:66:DA:C8	2.50	0.46
3:A:14:VAL:HG12	3:A:1632:GLU:HB2	1.97	0.46
3:A:1167:ARG:HA	3:A:1170:MET:HE2	1.97	0.46
3:A:252:PHE:HB2	3:A:314:TYR:HA	1.98	0.45
3:A:883:LEU:HA	3:A:889:SER:HB2	1.97	0.45
3:A:1178:LEU:HD13	3:A:1179:ILE:O	2.16	0.45
4:B:977:ILE:H	4:B:977:ILE:HG13	1.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:12:LEU:HD11	7:E:58:MET:HE1	1.98	0.45
13:K:88:PHE:HB3	13:K:106:GLN:HB2	1.98	0.45
3:A:484:ILE:HG21	3:A:633:MET:HE3	1.98	0.45
3:A:1085:LEU:HD12	3:A:1172:LEU:HD11	1.98	0.45
4:B:1003:ALA:CB	4:B:1005:TYR:HD2	2.29	0.45
5:C:252:PRO:HA	5:C:253:PRO:HD3	1.84	0.45
15:M:82:ASN:HB2	15:M:85:LYS:HB3	1.99	0.45
3:A:56:ALA:HB2	3:A:62:CYS:HB2	1.97	0.45
3:A:602:GLY:N	3:A:651:ALA:O	2.49	0.45
4:B:359:LEU:HG	4:B:370:LYS:HE3	1.99	0.45
4:B:974:LEU:HD23	12:J:44:TYR:HB3	1.99	0.45
5:C:53:ASN:HD21	5:C:271:ARG:NH1	2.15	0.45
1:T:7:DA:H2"	1:T:8:DA:C8	2.51	0.45
3:A:61:LEU:HD23	15:M:306:LYS:HZ1	1.81	0.45
4:B:1039:MET:HG3	4:B:1043:LYS:HG2	1.98	0.45
4:B:1119:ARG:H	4:B:1122:SER:HB2	1.81	0.45
15:M:235:PRO:HG2	15:M:263:TYR:HE1	1.81	0.45
3:A:538:ASN:HA	3:A:575:LYS:HG2	1.98	0.45
4:B:644:GLY:HA2	4:B:648:ARG:HG3	1.99	0.45
4:B:711:GLN:HE21	4:B:958:MET:HE2	1.81	0.45
9:G:228:LYS:HE2	9:G:230:ARG:HH12	1.82	0.45
10:H:38:LEU:HD12	10:H:125:LEU:HD21	1.97	0.45
13:K:102:ASN:N	13:K:102:ASN:OD1	2.48	0.45
3:A:1197:SER:HA	3:A:1200:MET:HG2	1.99	0.45
9:G:62:MET:HG3	9:G:66:LEU:HD23	1.99	0.45
17:O:540:CYS:HA	17:O:543:ILE:HD12	1.98	0.45
3:A:397:ARG:HD3	15:M:172:LEU:HB2	1.99	0.45
3:A:757:ASN:HD21	3:A:767:ASN:H	1.63	0.45
3:A:1221:ARG:NH2	3:A:1544:ASN:OD1	2.49	0.45
4:B:350:GLY:HA2	4:B:353:VAL:HG22	1.99	0.45
4:B:419:GLU:HA	4:B:422:GLN:HB2	1.97	0.45
4:B:773:VAL:N	4:B:1029:GLY:O	2.50	0.45
4:B:939:SER:OG	4:B:940:GLU:N	2.50	0.45
4:B:1072:GLY:H	4:B:1075:GLU:HB3	1.81	0.45
6:D:14:THR:H	6:D:17:ASN:HB2	1.81	0.45
15:M:41:TYR:HB3	15:M:52:VAL:HG13	1.99	0.45
3:A:536:ILE:HD12	3:A:577:VAL:HG22	1.98	0.45
4:B:535:ASP:OD1	4:B:535:ASP:N	2.44	0.45
5:C:69:ARG:HA	5:C:72:ILE:HG22	1.99	0.45
15:M:246:LYS:O	15:M:250:LEU:CD2	2.64	0.45
3:A:1193:VAL:HG22	3:A:1222:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1502:PRO:HD2	3:A:1525:ASN:HD21	1.81	0.45
4:B:654:ARG:NE	4:B:691:PHE:HB3	2.31	0.45
7:E:116:ILE:HG21	7:E:121:MET:HE3	1.99	0.45
10:H:40:LEU:HD12	10:H:123:MET:HE1	1.98	0.45
4:B:790:ASN:HB2	4:B:946:ASP:HA	1.99	0.44
4:B:884:GLU:HB2	4:B:904:LYS:HB3	1.99	0.44
5:C:46:SER:OG	5:C:53:ASN:HB2	2.17	0.44
5:C:240:LYS:HD3	5:C:265:ALA:N	2.32	0.44
11:I:9:PHE:HA	11:I:16:LEU:HA	1.98	0.44
2:U:65:DG:O5'	2:U:65:DG:C8	2.71	0.44
3:A:687:PHE:O	3:A:726:TRP:N	2.46	0.44
3:A:827:THR:OG1	3:A:828:CYS:N	2.50	0.44
3:A:894:ALA:HA	3:A:897:SER:HB3	1.98	0.44
4:B:280:LEU:HD11	4:B:370:LYS:HD2	1.99	0.44
4:B:282:HIS:CE1	15:M:101:VAL:HA	2.52	0.44
1:T:12:DC:C5	1:T:12:DC:OP2	2.70	0.44
2:U:58:DA:H2''	2:U:59:DG:H5''	1.98	0.44
3:A:1236:PRO:HG2	3:A:1523:GLY:HA2	1.99	0.44
3:A:1298:ASP:OD1	3:A:1298:ASP:N	2.50	0.44
4:B:359:LEU:HD12	4:B:370:LYS:CE	2.48	0.44
4:B:526:GLY:HA3	4:B:651:ARG:HH22	1.82	0.44
4:B:768:GLY:N	4:B:1032:TYR:OH	2.50	0.44
5:C:136:LEU:HB3	5:C:204:LEU:HG	1.99	0.44
16:N:39:PRO:O	16:N:51:GLN:NE2	2.50	0.44
3:A:467:PHE:HA	3:A:471:MET:HB2	2.00	0.44
3:A:882:ILE:HA	3:A:888:LYS:HB3	1.99	0.44
4:B:334:PHE:HB3	4:B:353:VAL:HG11	2.00	0.44
4:B:658:LEU:HD22	4:B:660:LYS:HE2	2.00	0.44
4:B:1113:THR:HA	4:B:1128:CYS:HA	1.98	0.44
4:B:1128:CYS:SG	4:B:1129:ARG:N	2.90	0.44
16:N:55:LEU:HG	16:N:136:VAL:HG23	2.00	0.44
3:A:404:SER:HB3	15:M:170:LYS:HE3	2.00	0.44
4:B:75:ASP:HA	4:B:432:ILE:HG12	1.99	0.44
6:D:94:ARG:NH1	9:G:151:ASP:OD2	2.51	0.44
15:M:22:ALA:H	16:N:110:LEU:HD11	1.83	0.44
3:A:397:ARG:NH2	15:M:172:LEU:H	2.16	0.44
3:A:928:MET:HE3	4:B:952:HIS:CD2	2.53	0.44
4:B:1071:VAL:HG23	4:B:1091:ARG:HH21	1.82	0.44
5:C:128:ASP:HB2	5:C:173:GLY:HA3	1.99	0.44
8:F:82:THR:HA	8:F:83:PRO:HD3	1.77	0.44
13:K:104:ARG:HE	13:K:106:GLN:HE22	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:107:HIS:CE1	3:A:330:LYS:HD3	2.53	0.44
3:A:316:LEU:HG	3:A:318:THR:H	1.81	0.44
3:A:1333:ILE:HD11	3:A:1476:LEU:HD21	2.00	0.44
4:B:936:MET:HB3	4:B:945:PRO:HD2	2.00	0.44
5:C:188:ASP:OD1	5:C:188:ASP:N	2.43	0.44
10:H:93:TYR:HD2	10:H:143:LEU:HD23	1.82	0.44
12:J:57:ILE:O	12:J:61:LEU:N	2.48	0.44
3:A:264:ASN:HA	3:A:267:LYS:HG2	2.00	0.44
3:A:399:LEU:HD22	3:A:402:ASP:HB3	1.99	0.44
3:A:790:LYS:HE3	3:A:791:TYR:CZ	2.53	0.44
3:A:985:ARG:HD3	3:A:986:PHE:H	1.72	0.44
4:B:282:HIS:CG	15:M:101:VAL:HG12	2.53	0.44
4:B:1116:SER:N	4:B:1125:THR:O	2.50	0.44
4:B:1195:ARG:HH12	4:B:1197:ARG:NE	2.16	0.44
17:O:117:GLN:HE21	17:O:150:TRP:HH2	1.64	0.44
17:O:482:TYR:HD1	17:O:524:VAL:HG11	1.83	0.44
3:A:910:LYS:C	3:A:912:VAL:H	2.26	0.44
3:A:124:LEU:HD12	3:A:189:VAL:HG13	2.00	0.43
3:A:520:ARG:HH22	17:O:377:TYR:HB3	1.82	0.43
3:A:551:VAL:HA	3:A:554:ARG:HB2	2.00	0.43
3:A:1131:LYS:HG3	3:A:1132:TYR:CD2	2.53	0.43
3:A:1558:ALA:HA	3:A:1561:THR:HG22	1.99	0.43
5:C:113:LEU:HD21	5:C:132:ILE:HD11	2.00	0.43
6:D:20:VAL:HG22	6:D:21:VAL:HG23	2.00	0.43
15:M:235:PRO:HB3	15:M:287:LEU:HB3	2.00	0.43
2:U:55:DT:H72	2:U:56:DA:H61	1.82	0.43
3:A:41:LEU:CD1	3:A:43:HIS:ND1	2.49	0.43
3:A:537:GLN:HE21	3:A:576:LYS:H	1.66	0.43
3:A:683:LYS:HB3	10:H:23:VAL:HG21	2.00	0.43
3:A:1012:LYS:HB3	3:A:1198:THR:HG23	1.99	0.43
5:C:221:PRO:HB2	5:C:308:MET:HG3	2.00	0.43
7:E:17:ARG:NH2	7:E:35:VAL:O	2.51	0.43
1:T:12:DC:C3'	1:T:12:DC:C6	3.01	0.43
3:A:1069:CYS:HB2	3:A:1076:LEU:HD21	1.99	0.43
3:A:1090:ASP:HB3	3:A:1132:TYR:HD1	1.83	0.43
4:B:252:TYR:HB2	4:B:381:LEU:HD11	1.99	0.43
15:M:252:GLN:HG3	15:M:254:SER:H	1.83	0.43
15:M:384:ILE:HG12	15:M:392:TYR:CE1	2.54	0.43
17:O:60:LEU:HD11	17:O:100:LEU:HA	2.00	0.43
17:O:475:ALA:O	17:O:479:ALA:N	2.48	0.43
1:T:7:DA:H2''	1:T:8:DA:N7	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1040:ASP:HB3	3:A:1044:THR:HG23	2.01	0.43
4:B:1015:SER:HG	4:B:1020:GLU:N	2.17	0.43
16:N:157:ARG:NH1	16:N:159:ASP:OD1	2.51	0.43
4:B:654:ARG:HE	4:B:691:PHE:HB3	1.84	0.43
4:B:663:ILE:H	4:B:663:ILE:HG13	1.62	0.43
4:B:1038:HIS:HB3	4:B:1039:MET:H	1.65	0.43
5:C:243:SER:O	5:C:247:PHE:N	2.48	0.43
9:G:141:SER:HB2	9:G:144:HIS:HB3	2.01	0.43
12:J:3:VAL:HG11	12:J:15:GLY:HA2	2.00	0.43
3:A:102:CYS:HB2	3:A:109:ARG:HG2	2.00	0.43
3:A:600:MET:HE3	4:B:1079:LEU:HB2	2.00	0.43
3:A:1020:GLN:O	3:A:1024:THR:OG1	2.30	0.43
3:A:1128:ASN:OD1	3:A:1131:LYS:N	2.43	0.43
4:B:658:LEU:CD2	4:B:660:LYS:HE2	2.49	0.43
4:B:953:ALA:O	4:B:957:ARG:N	2.43	0.43
5:C:57:ILE:HD12	5:C:297:HIS:CG	2.53	0.43
13:K:132:GLU:O	13:K:136:THR:OG1	2.28	0.43
15:M:264:TYR:O	15:M:268:LEU:N	2.51	0.43
16:N:80:MET:H	16:N:87:TYR:H	1.67	0.43
17:O:141:LYS:O	17:O:145:SER:OG	2.36	0.43
3:A:749:LEU:H	3:A:771:PHE:HB2	1.84	0.43
4:B:445:TYR:HA	4:B:448:ARG:HE	1.83	0.43
7:E:24:LYS:NZ	7:E:32:GLN:OE1	2.51	0.43
15:M:361:VAL:HA	15:M:364:PHE:HD2	1.83	0.43
3:A:1559:ARG:HG2	3:A:1586:ALA:HB1	2.01	0.43
4:B:795:GLU:HG3	5:C:217:ALA:H	1.83	0.43
4:B:234:ILE:HG23	4:B:381:LEU:HD23	2.01	0.43
4:B:292:ILE:HG22	4:B:293:ILE:N	2.34	0.43
4:B:742:TYR:CE2	4:B:1037:ARG:HG3	2.54	0.43
7:E:37:LEU:HG	7:E:41:ASP:HB3	2.01	0.43
9:G:111:THR:HG23	9:G:113:PHE:H	1.84	0.43
1:T:12:DC:H2'	1:T:13:DT:C7	2.49	0.43
3:A:495:ILE:HB	3:A:605:VAL:HG12	2.01	0.43
3:A:745:PRO:HD2	3:A:1075:ALA:HA	2.01	0.43
4:B:703:LEU:HD21	4:B:920:ARG:HH22	1.83	0.43
4:B:1196:LEU:HD13	4:B:1197:ARG:CA	2.48	0.43
7:E:100:ILE:HA	7:E:105:PHE:HD2	1.84	0.43
8:F:95:GLY:HA2	8:F:98:ALA:HB3	2.00	0.43
13:K:104:ARG:HE	13:K:106:GLN:NE2	2.17	0.43
3:A:681:THR:HA	3:A:728:GLY:HA3	2.01	0.42
3:A:875:LEU:C	3:A:875:LEU:CD1	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1094:ALA:O	3:A:1098:SER:N	2.51	0.42
3:A:1260:LYS:N	3:A:1505:ASP:O	2.40	0.42
3:A:1525:ASN:HD21	3:A:1528:ALA:HB3	1.84	0.42
4:B:617:THR:HB	4:B:620:LEU:HB2	2.01	0.42
8:F:124:GLU:O	8:F:128:LYS:N	2.44	0.42
17:O:62:ASP:O	17:O:67:ASP:N	2.46	0.42
3:A:68:ASP:OD1	3:A:68:ASP:N	2.51	0.42
3:A:771:PHE:HB3	3:A:774:GLY:HA2	2.01	0.42
3:A:1004:GLU:HA	3:A:1007:ILE:HB	2.01	0.42
4:B:700:LEU:O	4:B:703:LEU:HD12	2.19	0.42
4:B:752:VAL:HG22	4:B:981:SER:HB3	2.00	0.42
4:B:785:ASP:OD2	4:B:957:ARG:NH2	2.53	0.42
4:B:847:TYR:HD2	4:B:850:THR:HG21	1.84	0.42
5:C:279:VAL:HG23	5:C:280:LEU:HD12	2.01	0.42
15:M:12:ILE:HD12	16:N:68:LYS:HA	2.02	0.42
4:B:820:PRO:CD	15:M:356:LYS:HZ2	2.28	0.42
5:C:82:TYR:O	5:C:207:HIS:N	2.50	0.42
7:E:29:PHE:N	7:E:63:ASN:O	2.49	0.42
11:I:7:LEU:HD22	11:I:8:ILE:H	1.83	0.42
4:B:215:MET:HE2	4:B:215:MET:HB3	1.84	0.42
4:B:264:TRP:CD1	4:B:265:ARG:HD3	2.54	0.42
4:B:284:SER:HA	4:B:288:ILE:HD11	2.02	0.42
5:C:79:ALA:HA	5:C:106:LEU:HD12	2.00	0.42
5:C:262:SER:OG	5:C:263:ASP:N	2.53	0.42
15:M:39:ASP:HA	16:N:118:SER:HB2	2.02	0.42
3:A:369:LEU:HD22	3:A:370:PRO:HD2	2.01	0.42
3:A:530:TRP:O	3:A:531:PRO:C	2.63	0.42
4:B:258:VAL:HG12	4:B:309:LEU:HG	2.01	0.42
4:B:491:ILE:HD11	4:B:742:TYR:CG	2.55	0.42
4:B:552:SER:HB3	4:B:648:ARG:HB3	2.01	0.42
4:B:708:ASP:OD2	4:B:984:TRP:N	2.51	0.42
4:B:721:MET:HE2	4:B:924:LYS:HG2	2.01	0.42
4:B:874:TYR:CZ	4:B:876:SER:HB3	2.55	0.42
5:C:42:VAL:HG11	13:K:135:PHE:HD1	1.84	0.42
7:E:92:THR:HA	7:E:95:THR:HG22	2.00	0.42
9:G:167:THR:HG23	9:G:218:VAL:HB	2.02	0.42
10:H:78:SER:OG	10:H:79:TRP:N	2.51	0.42
12:J:28:ASP:HB3	12:J:30:LEU:HD23	2.01	0.42
15:M:71:GLN:NE2	15:M:95:VAL:O	2.52	0.42
3:A:985:ARG:HH21	3:A:986:PHE:HB2	1.79	0.42
4:B:164:MET:HG3	4:B:192:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:41:ASN:HD21	16:N:51:GLN:H	1.68	0.42
3:A:516:ILE:HG21	17:O:376:TYR:HE2	1.85	0.42
3:A:964:LYS:HZ1	4:B:673:ASN:HB3	1.85	0.42
4:B:368:GLN:HE22	15:M:99:LYS:NZ	2.17	0.42
5:C:131:THR:HG23	5:C:208:CYS:H	1.85	0.42
5:C:279:VAL:HA	5:C:282:TYR:HD2	1.85	0.42
15:M:360:VAL:O	15:M:364:PHE:N	2.52	0.42
1:T:13:DT:H6	1:T:13:DT:O5'	2.03	0.42
3:A:489:ASN:OD1	3:A:701:ARG:NH2	2.44	0.42
3:A:642:ASN:HB3	4:B:1086:PHE:CE2	2.54	0.42
3:A:1637:PRO:HA	3:A:1640:ARG:HB3	2.00	0.42
4:B:156:ARG:HH12	4:B:451:MET:HB3	1.84	0.42
4:B:504:HIS:ND1	4:B:542:LEU:HB3	2.35	0.42
5:C:138:VAL:HG13	5:C:159:ASN:HB3	2.01	0.42
2:U:64:DT:H4'	2:U:64:DT:OP1	2.19	0.42
3:A:912:VAL:C	3:A:914:ASP:N	2.78	0.42
4:B:470:LEU:HD11	4:B:476:LEU:CD1	2.19	0.42
4:B:981:SER:OG	4:B:982:THR:N	2.52	0.42
7:E:26:ARG:HH12	7:E:107:THR:HG21	1.83	0.42
9:G:219:ASP:OD1	9:G:219:ASP:N	2.46	0.42
3:A:614:LEU:HD13	3:A:614:LEU:HA	1.92	0.42
3:A:985:ARG:HD3	3:A:986:PHE:CA	2.46	0.42
3:A:1294:MET:HB3	3:A:1470:CYS:HB3	2.02	0.42
4:B:57:ASP:O	4:B:62:ASN:ND2	2.53	0.42
4:B:90:TYR:OH	4:B:146:ASN:OD1	2.38	0.42
15:M:332:ILE:HG23	15:M:336:ILE:HB	2.01	0.42
15:M:342:PHE:O	15:M:396:THR:OG1	2.27	0.42
3:A:771:PHE:HE2	3:A:793:ILE:HD13	1.84	0.41
3:A:1224:GLU:O	3:A:1228:THR:OG1	2.29	0.41
4:B:469:ASN:OD1	4:B:469:ASN:N	2.52	0.41
4:B:947:ILE:HG21	4:B:1033:TYR:CE2	2.54	0.41
15:M:77:VAL:HG22	16:N:58:PHE:HE1	1.84	0.41
16:N:113:SER:N	16:N:117:GLU:OE2	2.51	0.41
3:A:649:ASN:OD1	8:F:90:ARG:NH1	2.53	0.41
3:A:990:ILE:HD11	3:A:995:TYR:HB2	2.02	0.41
4:B:28:PRO:HG2	4:B:181:VAL:HG21	2.03	0.41
4:B:206:LEU:HD12	4:B:403:LEU:HD12	2.02	0.41
4:B:501:ARG:HH12	4:B:550:ARG:HH12	1.66	0.41
3:A:75:HIS:HE1	4:B:1114:GLN:HG2	1.85	0.41
4:B:327:LEU:O	4:B:330:LEU:HG	2.20	0.41
4:B:923:GLN:HG2	4:B:962:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1015:SER:OG	4:B:1019:GLY:N	2.53	0.41
5:C:43:ASN:HB2	5:C:55:ASP:HB2	2.01	0.41
5:C:92:ILE:HD12	12:J:2:ILE:HD11	2.02	0.41
15:M:247:LEU:HA	15:M:250:LEU:HD21	2.01	0.41
15:M:332:ILE:HD13	15:M:353:LEU:HD21	2.01	0.41
3:A:597:LYS:NZ	4:B:1081:GLY:O	2.53	0.41
3:A:792:GLY:O	3:A:796:SER:OG	2.36	0.41
3:A:1105:ARG:HH21	7:E:207:ARG:NH1	2.19	0.41
4:B:260:PHE:HB2	4:B:271:VAL:HG12	2.02	0.41
4:B:446:MET:HE2	4:B:446:MET:HB2	1.85	0.41
4:B:549:CYS:O	4:B:550:ARG:NE	2.49	0.41
5:C:65:ASN:HA	5:C:68:ARG:HB3	2.02	0.41
5:C:99:HIS:HB3	14:L:69:ALA:HA	2.02	0.41
15:M:21:VAL:HB	15:M:91:TYR:HE2	1.84	0.41
15:M:305:ILE:HA	15:M:318:TYR:HA	2.01	0.41
1:T:14:DT:H4'	3:A:1014:SER:HA	2.02	0.41
3:A:51:ASP:OD1	3:A:52:LEU:N	2.54	0.41
3:A:263:ASN:HA	3:A:266:VAL:HG12	2.02	0.41
3:A:1121:ASP:OD1	3:A:1121:ASP:N	2.48	0.41
3:A:1563:VAL:HG23	3:A:1582:LEU:HB3	2.02	0.41
4:B:934:ILE:HD12	5:C:69:ARG:HG3	2.02	0.41
15:M:361:VAL:HA	15:M:364:PHE:CD2	2.55	0.41
16:N:82:ILE:HG13	16:N:84:LYS:H	1.86	0.41
3:A:54:LEU:HD22	3:A:368:ARG:NH2	2.35	0.41
3:A:107:HIS:ND1	3:A:331:GLU:OE2	2.38	0.41
4:B:93:ASN:OD1	4:B:93:ASN:N	2.53	0.41
4:B:970:LYS:HZ3	4:B:1005:TYR:HD1	1.54	0.41
5:C:122:ASP:HA	5:C:125:LYS:HE3	2.03	0.41
3:A:462:LYS:HG3	3:A:463:LYS:H	1.84	0.41
3:A:1612:LYS:HE3	3:A:1612:LYS:HB2	1.89	0.41
4:B:968:ALA:C	4:B:979:GLN:HE22	2.28	0.41
5:C:73:SER:O	5:C:213:GLY:N	2.54	0.41
9:G:142:ALA:N	17:O:142:ILE:O	2.54	0.41
13:K:80:ILE:HD13	13:K:80:ILE:HA	1.94	0.41
15:M:112:LYS:HE2	15:M:112:LYS:HB2	1.85	0.41
16:N:86:ASP:OD1	16:N:86:ASP:N	2.53	0.41
17:O:234:ILE:HG13	17:O:367:LEU:HD21	2.01	0.41
3:A:57:PHE:HE1	3:A:370:PRO:HD2	1.86	0.41
4:B:320:LEU:HG	4:B:326:VAL:HG22	2.02	0.41
4:B:501:ARG:HG3	4:B:544:HIS:HB2	2.01	0.41
4:B:703:LEU:HD13	4:B:704:THR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:714:ARG:CZ	4:B:957:ARG:HD2	2.51	0.41
8:F:138:LEU:HA	8:F:139:PRO:HD3	1.80	0.41
17:O:428:ILE:HD12	17:O:439:ILE:HD12	2.02	0.41
3:A:481:ARG:NH2	3:A:592:GLN:HE22	2.19	0.41
3:A:934:LYS:HG2	4:B:955:PRO:HB2	2.03	0.41
3:A:1137:SER:OG	3:A:1138:GLU:N	2.53	0.41
4:B:73:ILE:HD11	4:B:429:ARG:HB3	2.02	0.41
4:B:74:PHE:HE1	4:B:94:LYS:HA	1.86	0.41
4:B:128:GLN:HE22	4:B:735:HIS:C	2.28	0.41
4:B:188:ASP:OD1	4:B:188:ASP:N	2.52	0.41
4:B:359:LEU:HD12	4:B:370:LYS:HE3	1.95	0.41
4:B:480:GLN:HB3	4:B:508:PHE:HB2	2.02	0.41
4:B:564:ILE:H	4:B:564:ILE:HG13	1.75	0.41
5:C:123:ASP:OD1	5:C:123:ASP:N	2.53	0.41
13:K:87:GLU:HB3	13:K:108:TYR:CE2	2.56	0.41
15:M:10:ILE:HD12	15:M:10:ILE:HA	1.83	0.41
15:M:320:ILE:HG23	15:M:324:ASN:HB2	2.03	0.41
3:A:185:ARG:HA	3:A:188:TYR:HB3	2.03	0.41
3:A:721:LYS:NZ	10:H:94:ASP:HB2	2.36	0.41
4:B:529:CYS:SG	4:B:532:HIS:HB3	2.60	0.41
4:B:1048:SER:OG	4:B:1049:THR:N	2.54	0.41
5:C:31:TRP:CD2	13:K:82:LYS:HD3	2.56	0.41
13:K:48:LYS:HB3	13:K:64:GLN:HB3	2.02	0.41
15:M:268:LEU:CG	15:M:331:TYR:HE2	2.33	0.41
17:O:426:SER:HB3	17:O:594:TYR:HB2	2.03	0.41
3:A:208:PHE:CZ	3:A:213:ASN:HB3	2.56	0.40
3:A:529:LYS:C	3:A:530:TRP:O	2.64	0.40
3:A:749:LEU:HA	3:A:749:LEU:HD13	1.89	0.40
3:A:1050:TYR:HB3	3:A:1054:ALA:HA	2.02	0.40
4:B:628:TYR:HD1	4:B:640:LEU:HD23	1.85	0.40
4:B:665:GLY:N	4:B:668:GLU:OE1	2.39	0.40
6:D:25:THR:HB	9:G:42:PRO:HG2	2.02	0.40
16:N:57:LYS:N	16:N:137:PHE:O	2.49	0.40
16:N:133:PHE:HE2	16:N:136:VAL:HB	1.86	0.40
1:T:12:DC:H3'	1:T:12:DC:C6	2.55	0.40
1:T:13:DT:O5'	1:T:13:DT:C6	2.74	0.40
3:A:3:ILE:HD13	8:F:103:MET:HE3	2.02	0.40
3:A:529:LYS:O	3:A:530:TRP:C	2.64	0.40
3:A:585:ASP:OD1	3:A:585:ASP:N	2.54	0.40
3:A:1019:LEU:HD11	3:A:1193:VAL:HG13	2.04	0.40
4:B:587:GLN:HA	4:B:592:ILE:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:69:LEU:HA	9:G:72:LYS:HE3	2.03	0.40
15:M:262:LEU:CG	15:M:265:LEU:CD1	2.69	0.40
15:M:298:ILE:HA	15:M:302:PHE:HD2	1.85	0.40
17:O:94:ASN:HD21	17:O:132:THR:HA	1.85	0.40
3:A:757:ASN:HD22	3:A:765:LEU:HD13	1.84	0.40
3:A:942:GLN:HA	3:A:947:LEU:HA	2.04	0.40
4:B:359:LEU:CD1	4:B:370:LYS:HZ2	2.34	0.40
4:B:737:SER:HA	4:B:904:LYS:NZ	2.36	0.40
4:B:1108:GLY:HA3	4:B:1198:TYR:H	1.86	0.40
5:C:47:LEU:HA	5:C:52:ALA:HA	2.03	0.40
15:M:312:ARG:NH1	15:M:317:SER:H	2.19	0.40
17:O:530:ARG:HH22	17:O:613:TRP:HE1	1.68	0.40
3:A:586:VAL:HG21	3:A:648:LEU:HB2	2.02	0.40
3:A:995:TYR:HE2	4:B:697:LEU:HD11	1.87	0.40
9:G:85:GLU:OE2	9:G:121:ASN:ND2	2.54	0.40
9:G:152:ALA:O	17:O:185:SER:OG	2.38	0.40
10:H:26:ILE:N	10:H:40:LEU:O	2.42	0.40
15:M:203:PRO:O	15:M:206:SER:OG	2.32	0.40
17:O:205:ARG:HG3	17:O:331:LYS:HE2	2.04	0.40
2:U:63:DT:H2"	2:U:64:DT:C6	2.57	0.40
3:A:537:GLN:NE2	3:A:576:LYS:HG2	2.36	0.40
3:A:709:ARG:HG2	3:A:710:SER:H	1.86	0.40
3:A:1550:LEU:HD11	3:A:1594:THR:HA	2.03	0.40
4:B:209:GLN:HE22	4:B:237:ARG:HB2	1.85	0.40
4:B:240:ARG:HG2	4:B:360:VAL:HG11	2.02	0.40
4:B:292:ILE:HG22	4:B:302:LEU:HD11	2.03	0.40
4:B:1095:SER:OG	4:B:1096:SER:N	2.54	0.40
9:G:137:ILE:N	9:G:227:GLY:O	2.42	0.40
15:M:242:TYR:CE1	15:M:352:GLU:HB2	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	
3	A	1450/1664 (87%)	1234 (85%)	212 (15%)	4 (0%)	36	70
4	B	1160/1203 (96%)	980 (84%)	177 (15%)	3 (0%)	36	70
5	C	300/335 (90%)	269 (90%)	31 (10%)	0	100	100
6	D	55/137 (40%)	50 (91%)	5 (9%)	0	100	100
7	E	212/215 (99%)	192 (91%)	20 (9%)	0	100	100
8	F	98/155 (63%)	87 (89%)	11 (11%)	0	100	100
9	G	196/326 (60%)	168 (86%)	28 (14%)	0	100	100
10	H	130/146 (89%)	112 (86%)	18 (14%)	0	100	100
11	I	62/125 (50%)	49 (79%)	13 (21%)	0	100	100
12	J	67/70 (96%)	59 (88%)	8 (12%)	0	100	100
13	K	98/142 (69%)	87 (89%)	11 (11%)	0	100	100
14	L	41/70 (59%)	36 (88%)	5 (12%)	0	100	100
15	M	386/415 (93%)	303 (78%)	83 (22%)	0	100	100
16	N	127/233 (54%)	96 (76%)	31 (24%)	0	100	100
17	O	457/627 (73%)	392 (86%)	65 (14%)	0	100	100
All	All	4839/5863 (82%)	4114 (85%)	718 (15%)	7 (0%)	49	81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	913	PRO
3	A	757	ASN
4	B	784	ASP
4	B	684	ASN
3	A	530	TRP
4	B	266	LYS
3	A	35	PRO

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	
3	A	1293/1465 (88%)	1277 (99%)	16 (1%)	63	73
4	B	1025/1053 (97%)	1004 (98%)	21 (2%)	48	66
5	C	269/296 (91%)	265 (98%)	4 (2%)	57	70
6	D	56/116 (48%)	56 (100%)	0	100	100
7	E	196/197 (100%)	193 (98%)	3 (2%)	57	70
8	F	90/137 (66%)	88 (98%)	2 (2%)	45	65
9	G	180/291 (62%)	177 (98%)	3 (2%)	53	68
10	H	117/128 (91%)	115 (98%)	2 (2%)	53	68
11	I	56/110 (51%)	56 (100%)	0	100	100
12	J	64/65 (98%)	62 (97%)	2 (3%)	35	56
13	K	90/130 (69%)	90 (100%)	0	100	100
14	L	38/57 (67%)	38 (100%)	0	100	100
15	M	350/371 (94%)	349 (100%)	1 (0%)	86	85
16	N	125/220 (57%)	121 (97%)	4 (3%)	34	56
17	O	427/576 (74%)	426 (100%)	1 (0%)	87	87
All	All	4376/5212 (84%)	4317 (99%)	59 (1%)	59	72

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	27	LEU
3	A	59	ARG
3	A	466	LEU
3	A	605	VAL
3	A	712	ILE
3	A	736	LEU
3	A	777	LEU
3	A	781	LEU
3	A	813	LEU
3	A	875	LEU
3	A	919	LYS
3	A	930	LEU
3	A	946	LEU
3	A	1027	LEU
3	A	1055	ILE
3	A	1634	LEU
4	B	102	VAL
4	B	104	ILE

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Mol	Chain	Res	Type
4	B	195	ILE
4	B	206	LEU
4	B	309	LEU
4	B	384	LEU
4	B	421	LEU
4	B	476	LEU
4	B	531	VAL
4	B	548	LYS
4	B	603	ILE
4	B	629	VAL
4	B	663	ILE
4	B	703	LEU
4	B	785	ASP
4	B	948	ILE
4	B	977	ILE
4	B	1092	LEU
4	B	1117	VAL
4	B	1126	VAL
4	B	1168	VAL
5	C	35	LYS
5	C	75	VAL
5	C	251	PHE
5	C	267	VAL
7	E	123	LEU
7	E	124	VAL
7	E	199	ILE
8	F	99	LEU
8	F	130	ILE
9	G	43	ILE
9	G	69	LEU
9	G	77	VAL
10	H	89	LEU
10	H	144	ILE
12	J	48	ARG
12	J	57	ILE
15	M	267	LEU
16	N	89	ILE
16	N	111	VAL
16	N	120	LYS
16	N	169	GLU
17	O	490	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105)

such sidechains are listed below:

Mol	Chain	Res	Type
3	A	26	ASN
3	A	60	ASN
3	A	92	ASN
3	A	93	GLN
3	A	116	HIS
3	A	179	ASN
3	A	224	HIS
3	A	263	ASN
3	A	332	GLN
3	A	344	ASN
3	A	400	ASN
3	A	515	ASN
3	A	525	ASN
3	A	537	GLN
3	A	560	GLN
3	A	592	GLN
3	A	634	ASN
3	A	640	ASN
3	A	730	GLN
3	A	753	ASN
3	A	795	HIS
3	A	798	HIS
3	A	906	GLN
3	A	923	ASN
3	A	937	ASN
3	A	939	ASN
3	A	950	GLN
3	A	1047	GLN
3	A	1072	ASN
3	A	1088	HIS
3	A	1113	HIS
3	A	1139	ASN
3	A	1237	GLN
3	A	1319	ASN
3	A	1436	ASN
3	A	1437	ASN
3	A	1532	GLN
3	A	1592	GLN
4	B	45	HIS
4	B	87	ASN
4	B	110	ASN
4	B	128	GLN

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Mol	Chain	Res	Type
4	B	151	ASN
4	B	168	ASN
4	B	197	ASN
4	B	224	ASN
4	B	246	GLN
4	B	267	ASN
4	B	368	GLN
4	B	422	GLN
4	B	547	HIS
4	B	575	HIS
4	B	711	GLN
4	B	715	ASN
4	B	724	GLN
4	B	745	GLN
4	B	790	ASN
4	B	944	GLN
4	B	975	HIS
4	B	979	GLN
4	B	1058	GLN
4	B	1115	GLN
4	B	1157	GLN
4	B	1171	ASN
5	C	53	ASN
5	C	65	ASN
5	C	161	HIS
5	C	232	GLN
5	C	301	ASN
5	C	323	ASN
6	D	29	GLN
7	E	99	HIS
7	E	146	HIS
7	E	147	HIS
7	E	179	GLN
8	F	60	GLN
8	F	61	HIS
8	F	104	ASN
9	G	8	ASN
9	G	65	HIS
9	G	67	ASN
9	G	75	ASN
9	G	154	ASN
9	G	160	ASN

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Mol	Chain	Res	Type
10	H	43	ASN
10	H	128	ASN
10	H	134	ASN
11	I	19	ASN
12	J	53	HIS
13	K	83	ASN
14	L	53	HIS
15	M	57	ASN
15	M	75	GLN
15	M	126	ASN
15	M	274	ASN
15	M	278	ASN
15	M	351	HIS
16	N	37	ASN
16	N	50	GLN
16	N	51	GLN
16	N	52	GLN
16	N	85	HIS
17	O	92	ASN
17	O	228	GLN
17	O	549	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

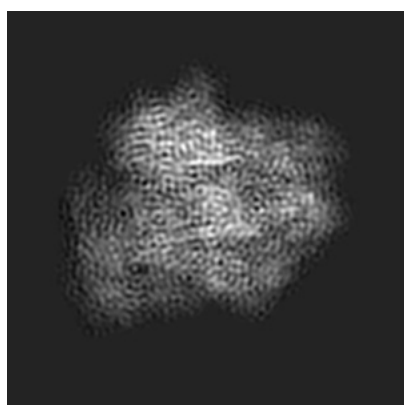
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4985. These allow visual inspection of the internal detail of the map and identification of artifacts.

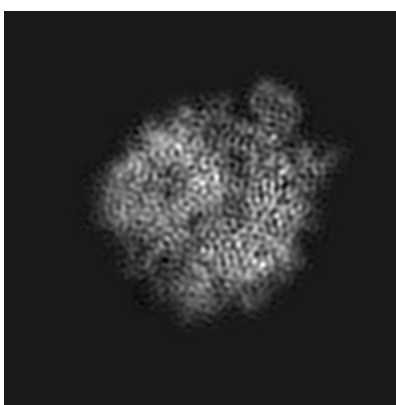
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

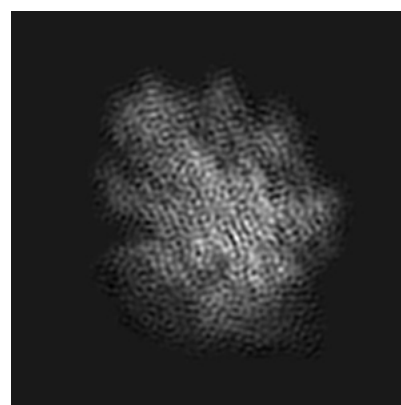
6.1.1 Primary map



X



Y

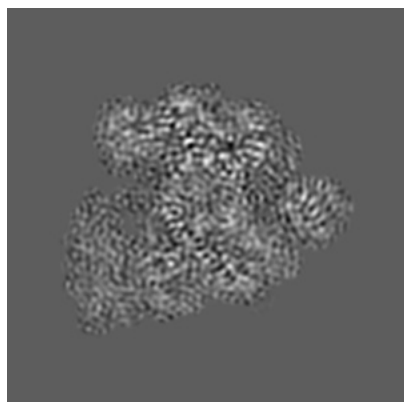


Z

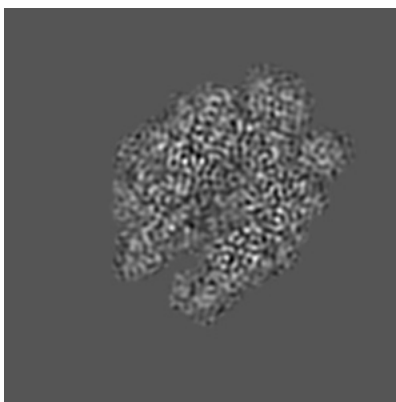
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

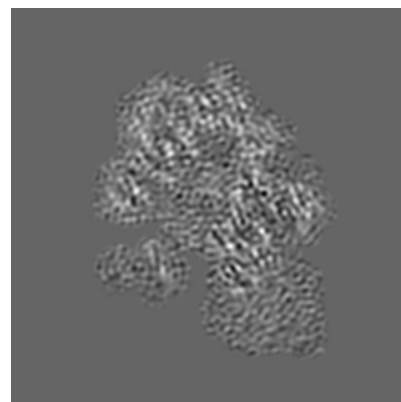
6.2.1 Primary map



X Index: 88



Y Index: 88

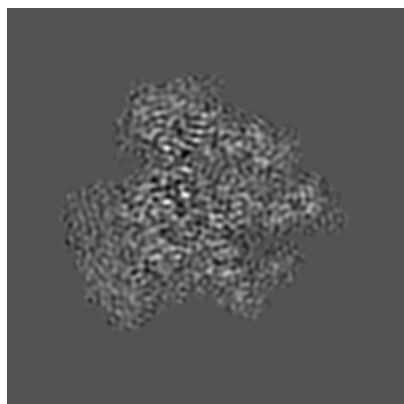


Z Index: 88

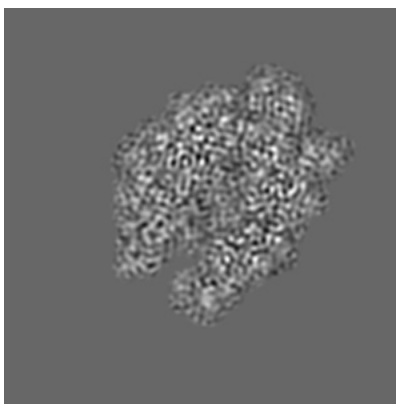
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

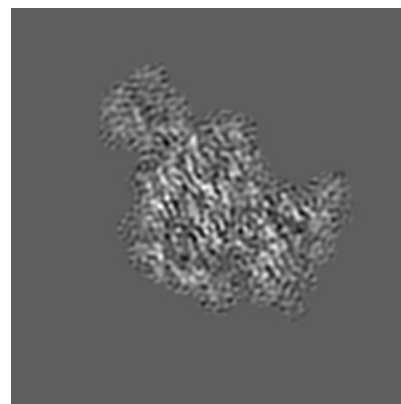
6.3.1 Primary map



X Index: 101



Y Index: 89

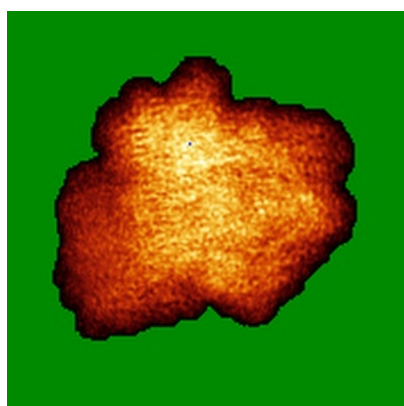


Z Index: 110

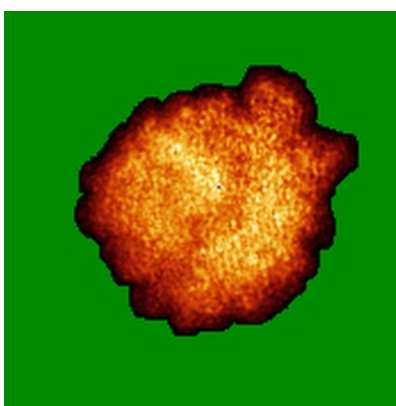
The images above show the largest variance slices of the map in three orthogonal directions.

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

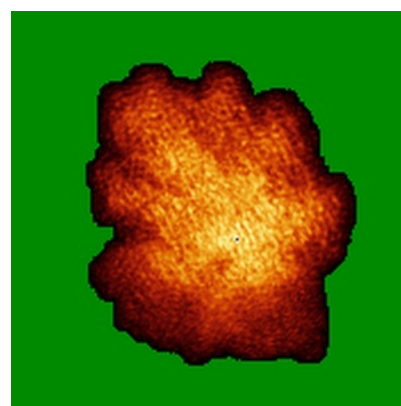
6.4.1 Primary map



X



Y

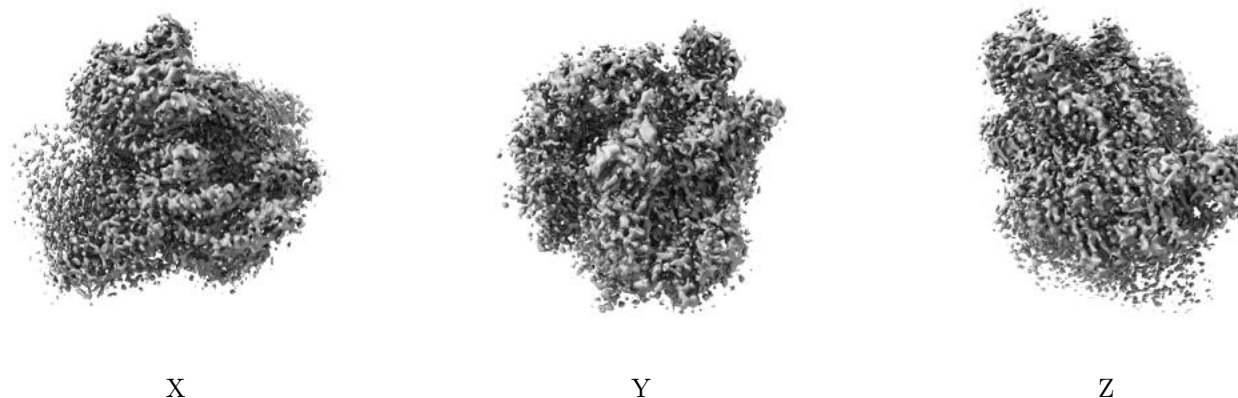


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

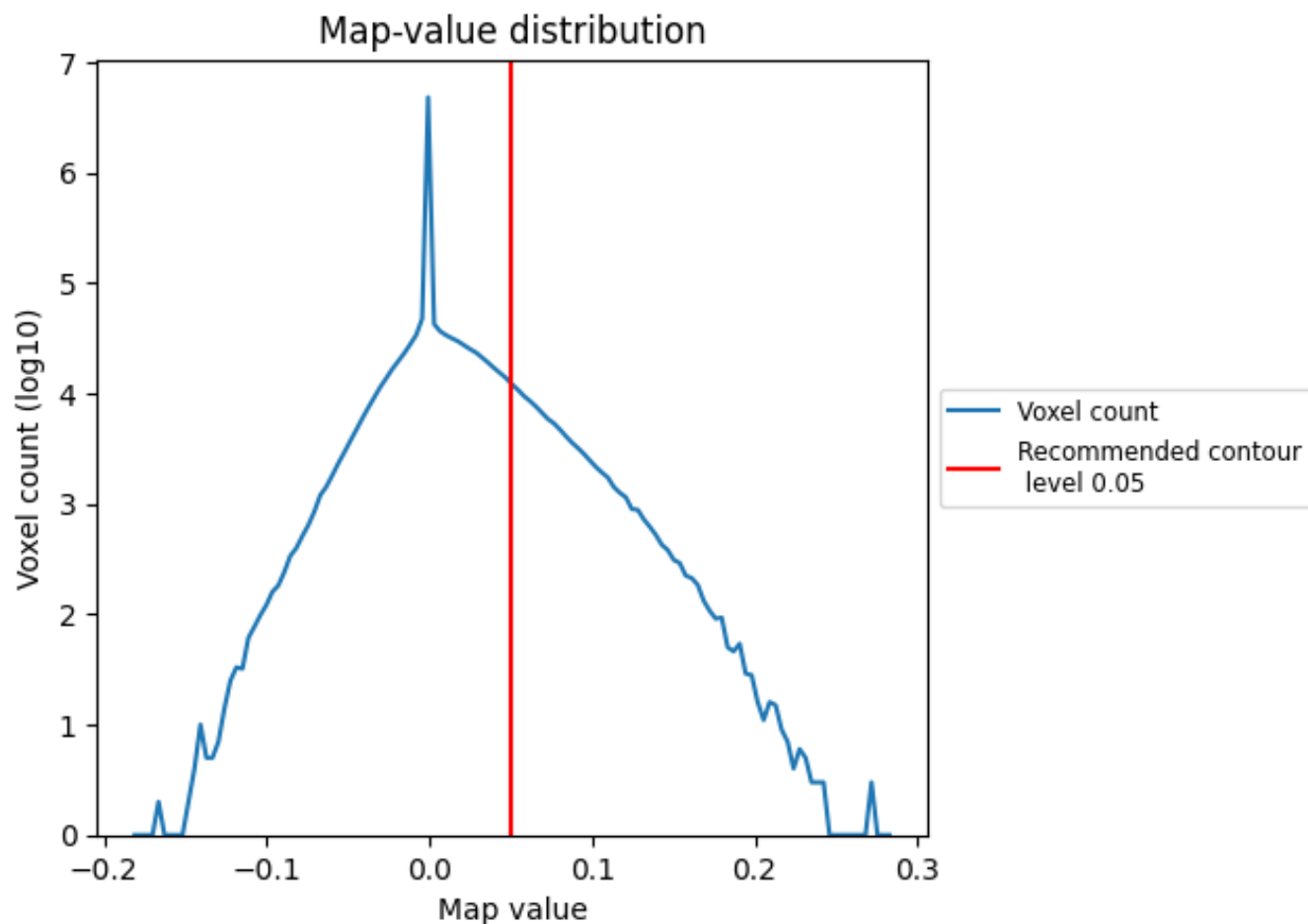
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

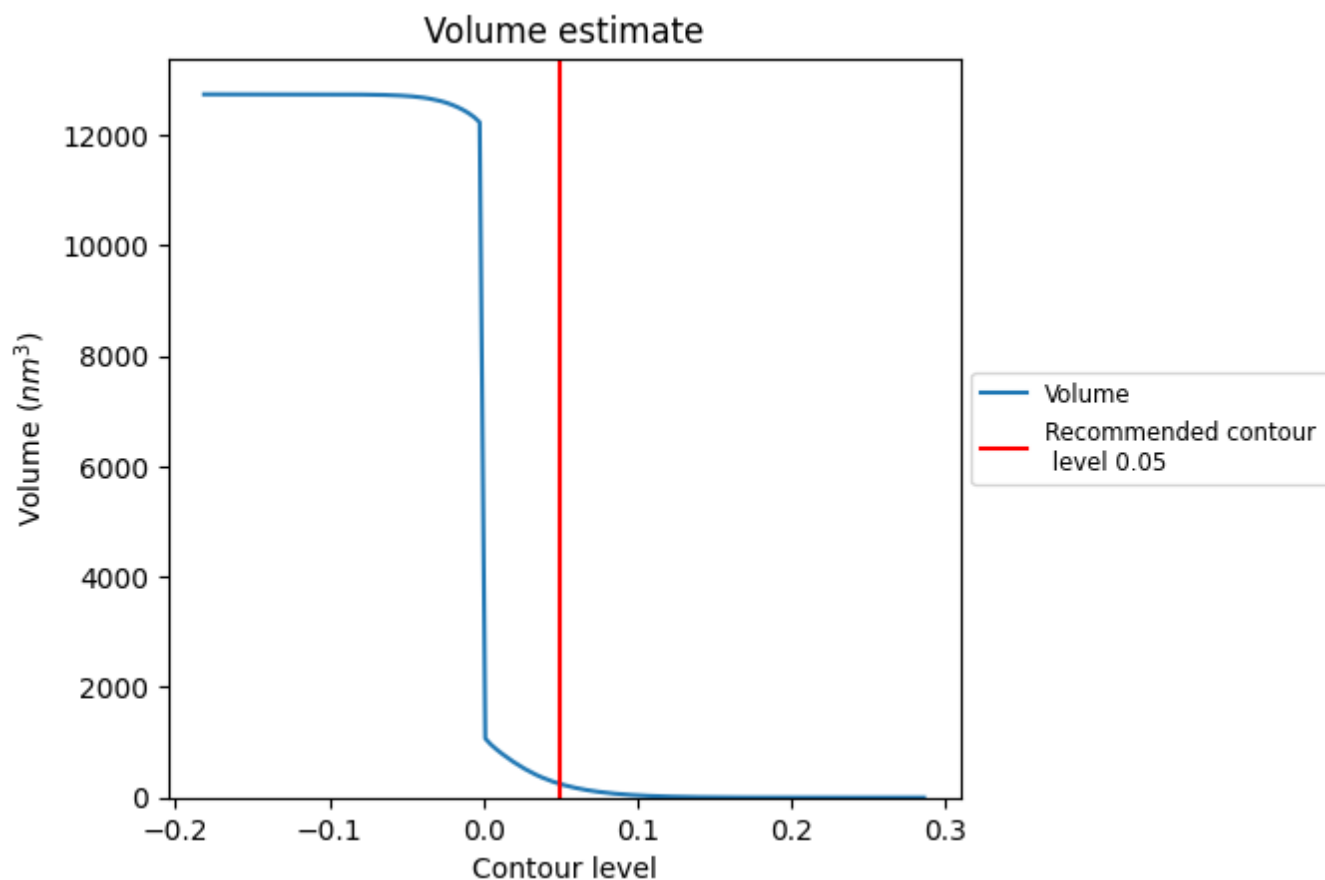
This section contains the results of statistical analysis of the map.

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.

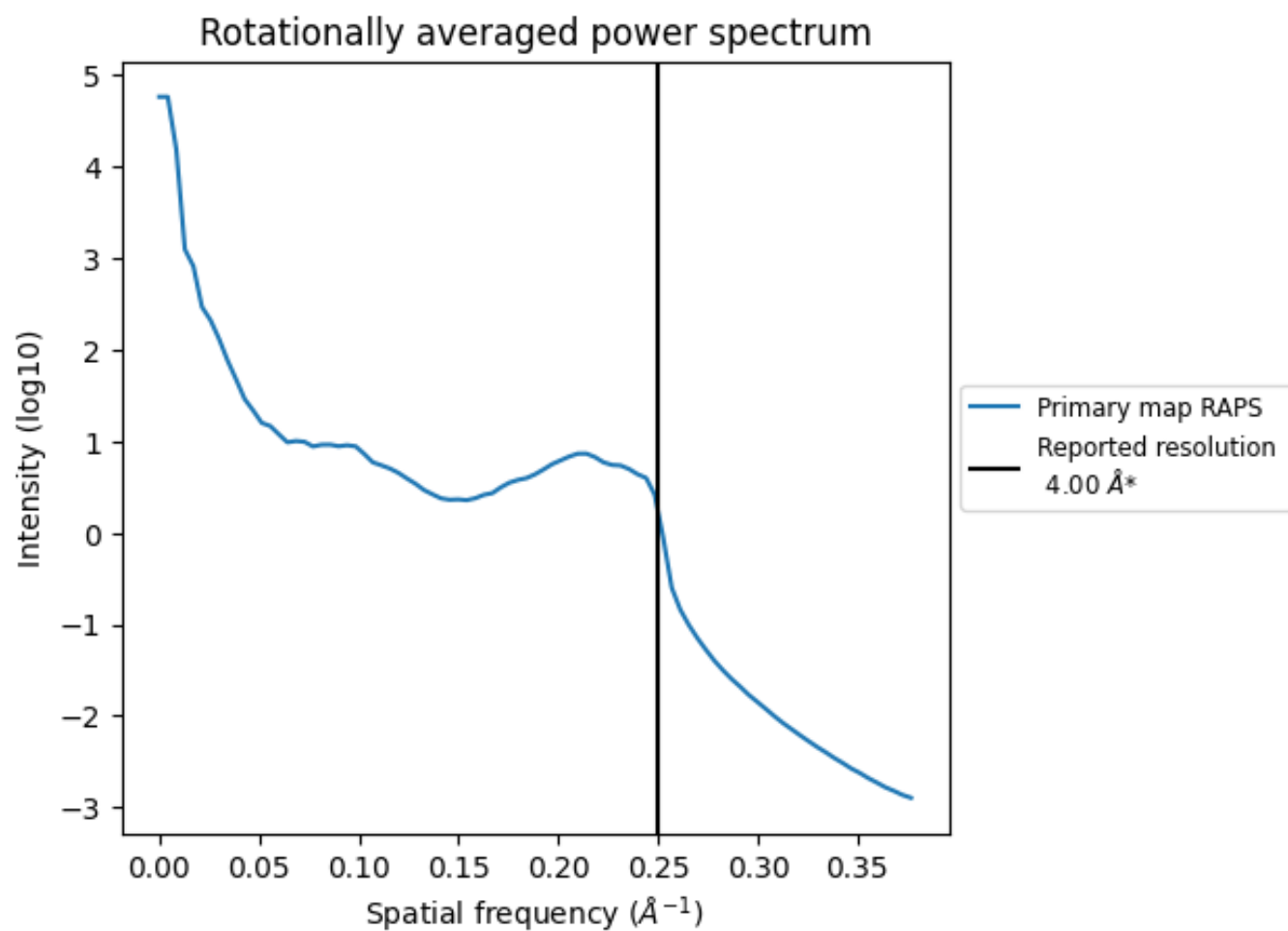
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm^3 ; this corresponds to an approximate mass of 223 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

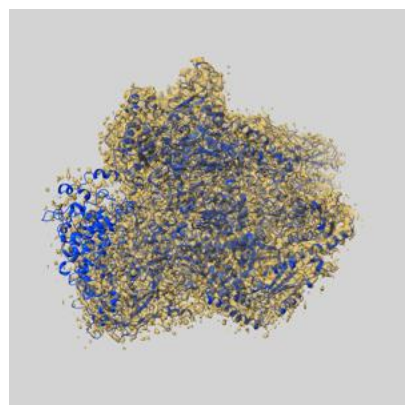
8 Fourier-Shell correlation

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

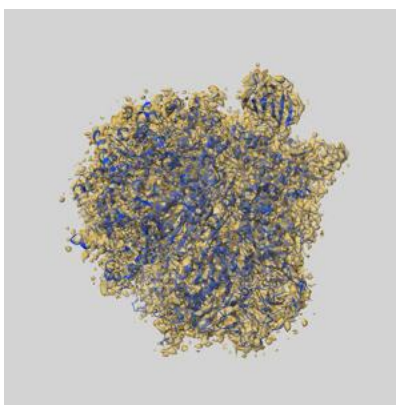
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4985 and PDB model 6RQT. Per-residue inclusion information can be found in section [3](#) on page [7](#).

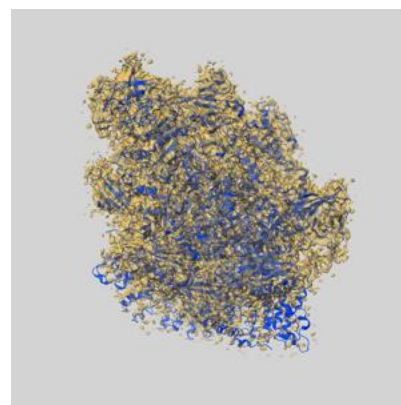
9.1 Map-model overlay [i](#)



X



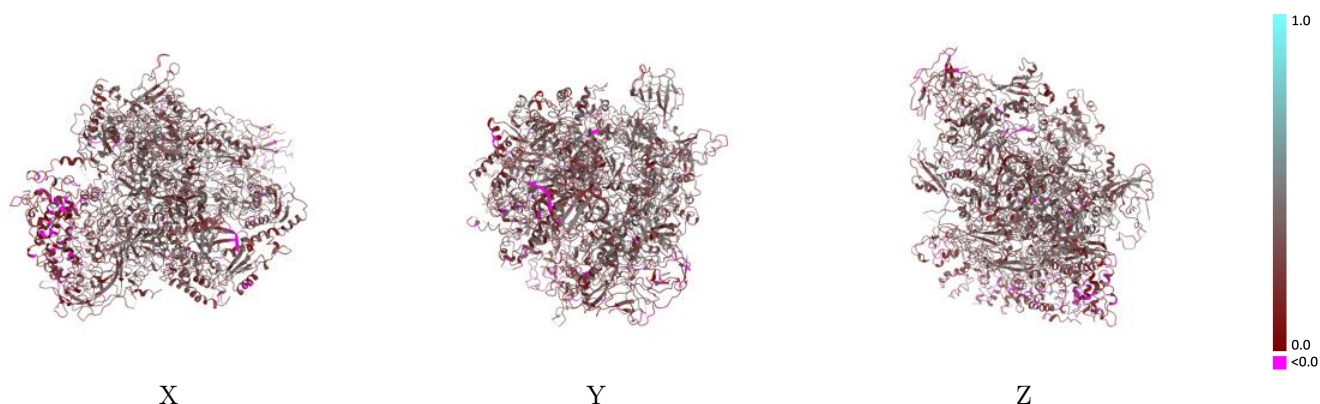
Y



Z

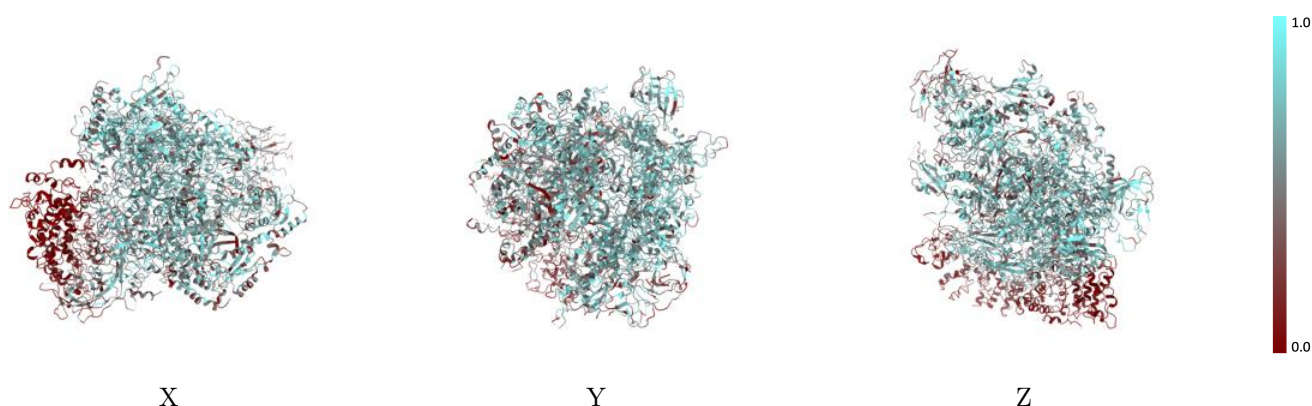
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



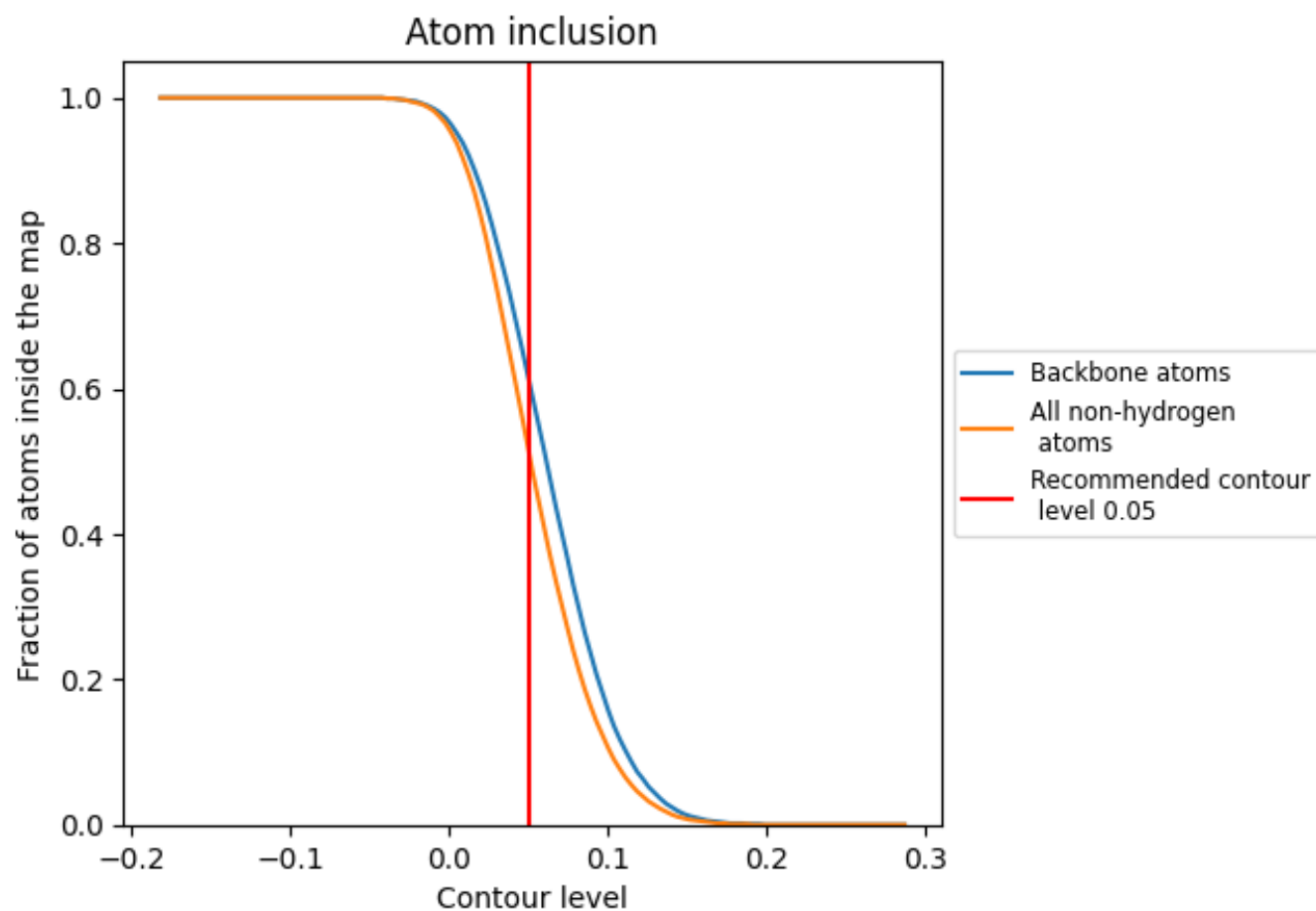
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 52% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5160	 0.2950
A	 0.6030	 0.3270
B	 0.6300	 0.3340
C	 0.6380	 0.3400
D	 0.4040	 0.2660
E	 0.5860	 0.3040
F	 0.6120	 0.3580
G	 0.4050	 0.2720
H	 0.6290	 0.3260
I	 0.5130	 0.3020
J	 0.6740	 0.3220
K	 0.6130	 0.3220
L	 0.5270	 0.2890
M	 0.2760	 0.2050
N	 0.4870	 0.2550
O	 0.0590	 0.1670
T	 0.3820	 0.1360
U	 0.3480	 0.1270

