



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 07:02 PM UTC

PDB ID : 6RQH / pdb_00006rqh
EMDB ID : EMD-4982
Title : RNA Polymerase I Closed Conformation 1 (CC1)
Authors : Mueller, C.W.; Sadian, Y.; Tafur, L.
Deposited on : 2019-05-15
Resolution : 3.70 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

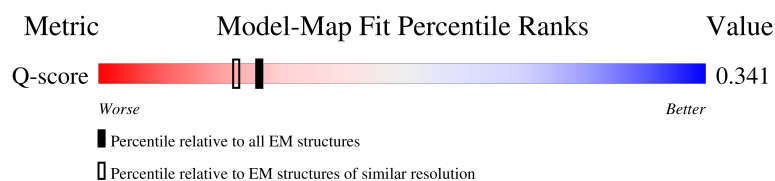
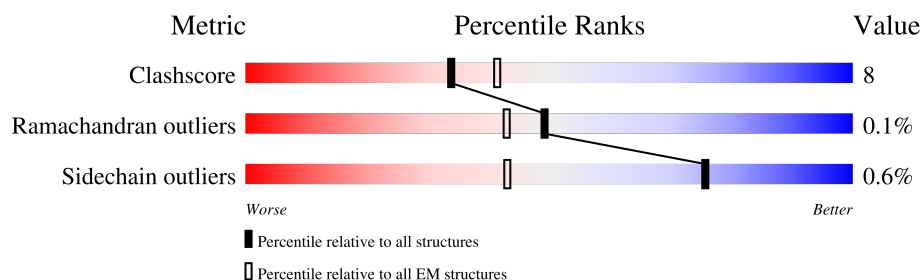
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	37% 47% 9% 44%
2	U	70	40% 46% 10% 44%
3	Q	514	63% 69% 17% 14%
4	S	894	49% 51% 16% 32%

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Mol	Chain	Length	Quality of chain
5	R	507	
6	M	415	
7	A	1664	
8	B	1203	
9	C	335	
10	D	137	
11	E	215	
12	F	155	
13	G	326	
14	H	146	
15	I	125	
16	J	70	
17	K	142	
18	L	70	
19	N	233	
20	O	627	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 50851 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	39	Total	C	N	O	P	0	0
			779	375	129	236	39		

- Molecule 2 is a DNA chain called Nontemplate strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	39	Total	C	N	O	P	0	0
			817	388	161	230	38		

- Molecule 3 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	442	Total	C	N	O	S	0	0
			3675	2373	624	658	20		

- Molecule 4 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	610	Total	C	N	O	S	0	0
			4963	3160	842	950	11		

- Molecule 5 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	330	Total	C	N	O	S	0	0
			2771	1791	489	480	11		

- Molecule 6 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	107	Total	C	N	O	0	0
			850	540	141	169		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1518	Total	C	N	O	S	0	0
			11836	7474	2062	2239	61		

- Molecule 8 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	1180	Total	C	N	O	S	0	0
			9371	5923	1644	1754	50		

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	70	Total	C	N	O	S	0	0
			551	340	100	109	2		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	199	Total	C	N	O	S	0	0
			1576	1012	273	286	5		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	134	Total	C	N	O	S	0	0
			1072	676	181	211	4		

- Molecule 15 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	124	Total	C	N	O	S	0	0
			942	584	160	189	9		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 17 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	103	Total	C	N	O	S	0	0
			810	506	132	167	5		

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

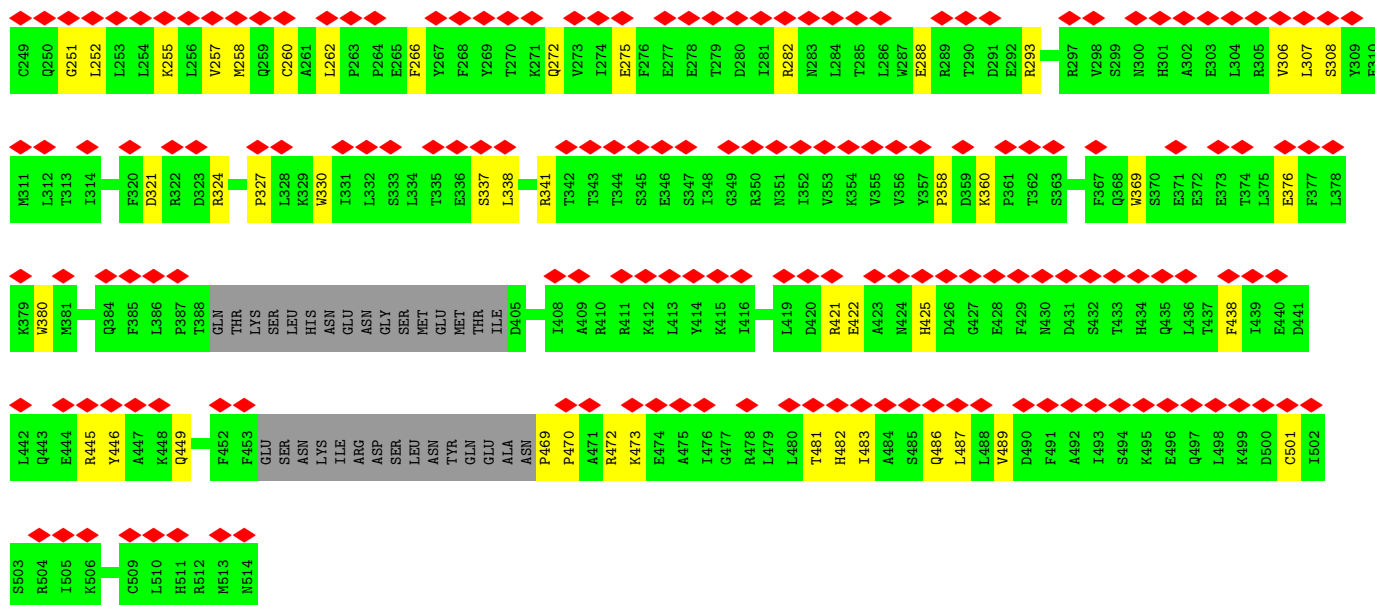
Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 19 is a protein called DNA-directed RNA polymerase I subunit RPA34.

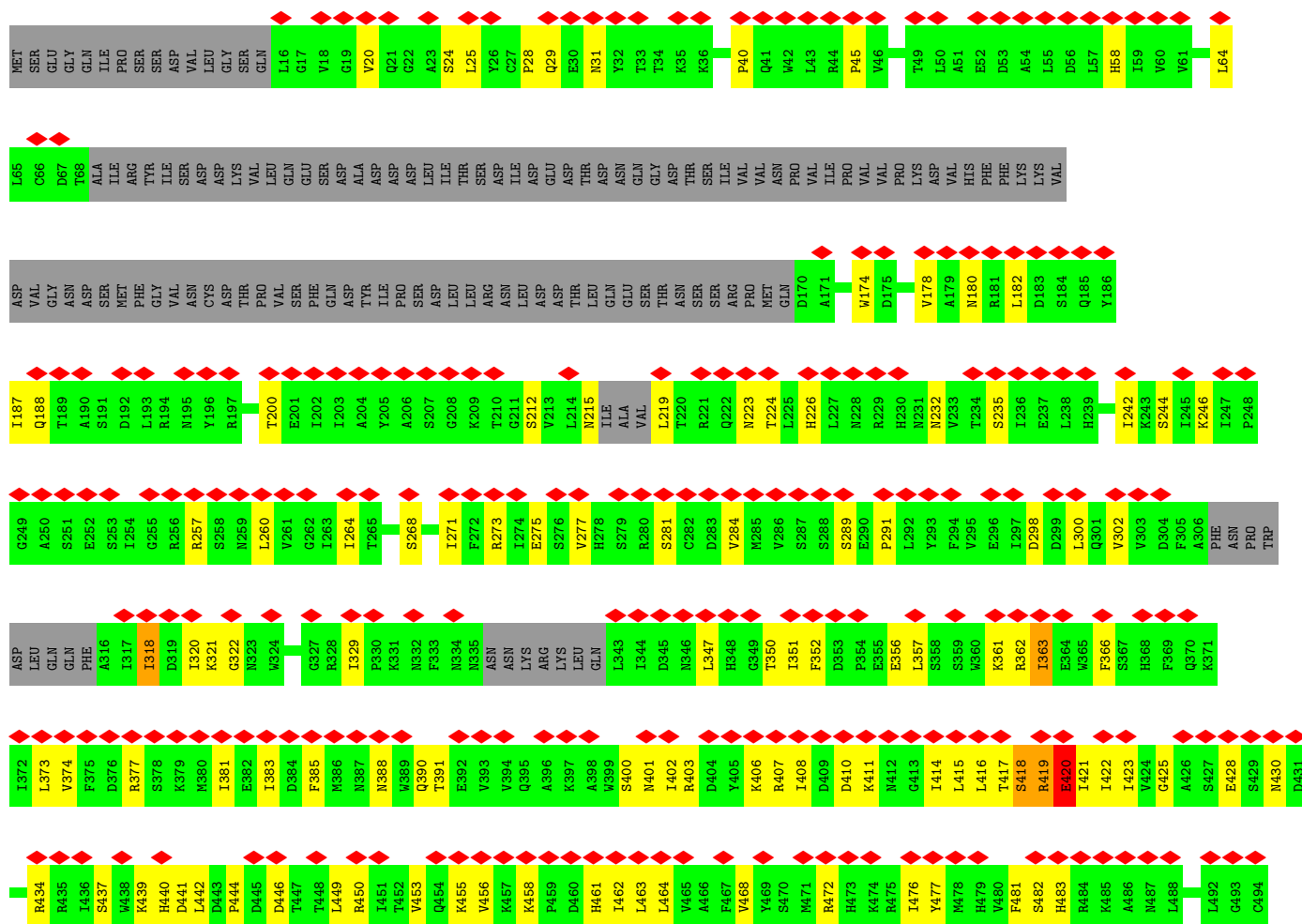
Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	139	Total	C	N	O	S	0	0
			1103	706	179	214	4		

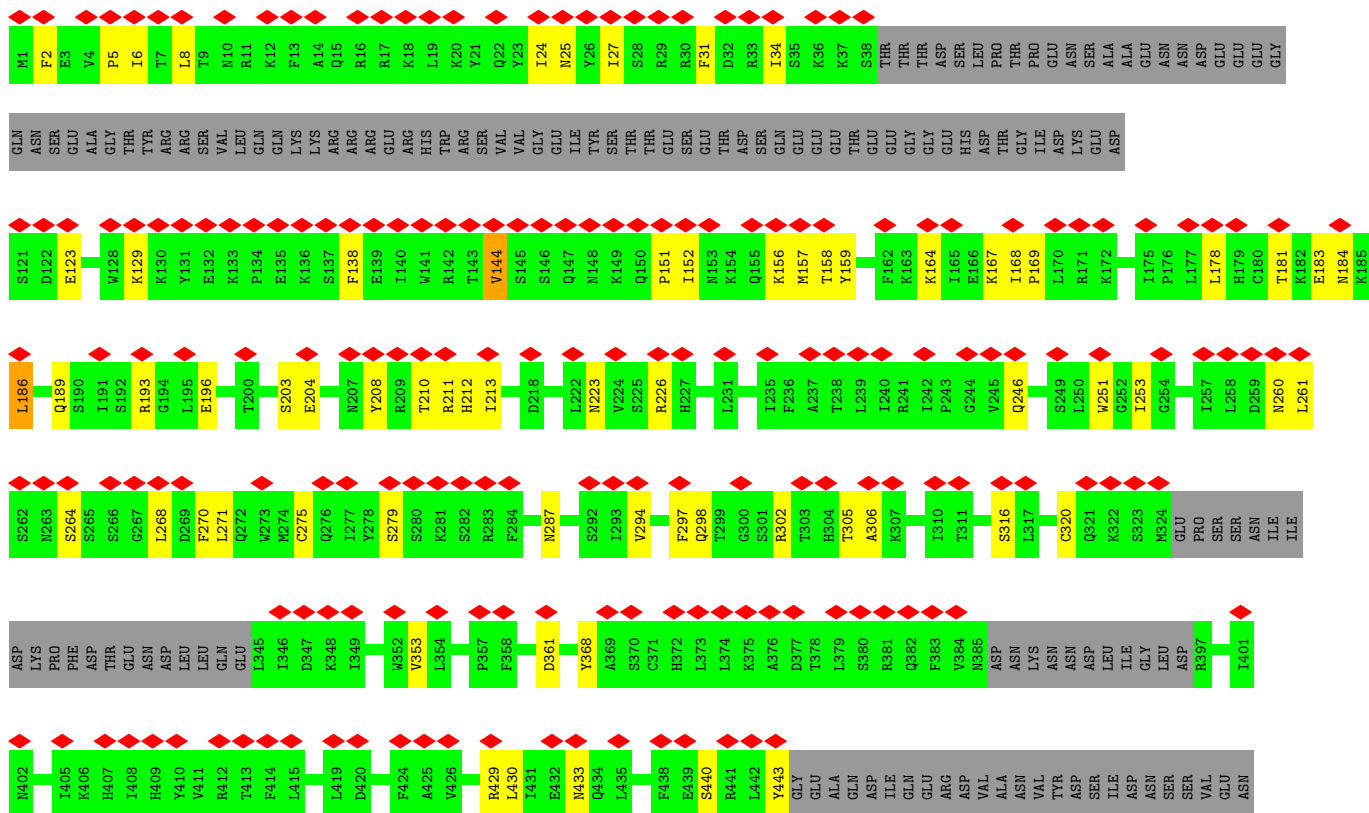
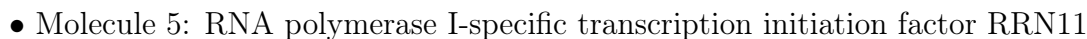
- Molecule 20 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	462	Total	C	N	O	S	0	0
			3807	2471	622	693	21		



• Molecule 4: RNA polymerase I-specific transcription initiation factor RRN6

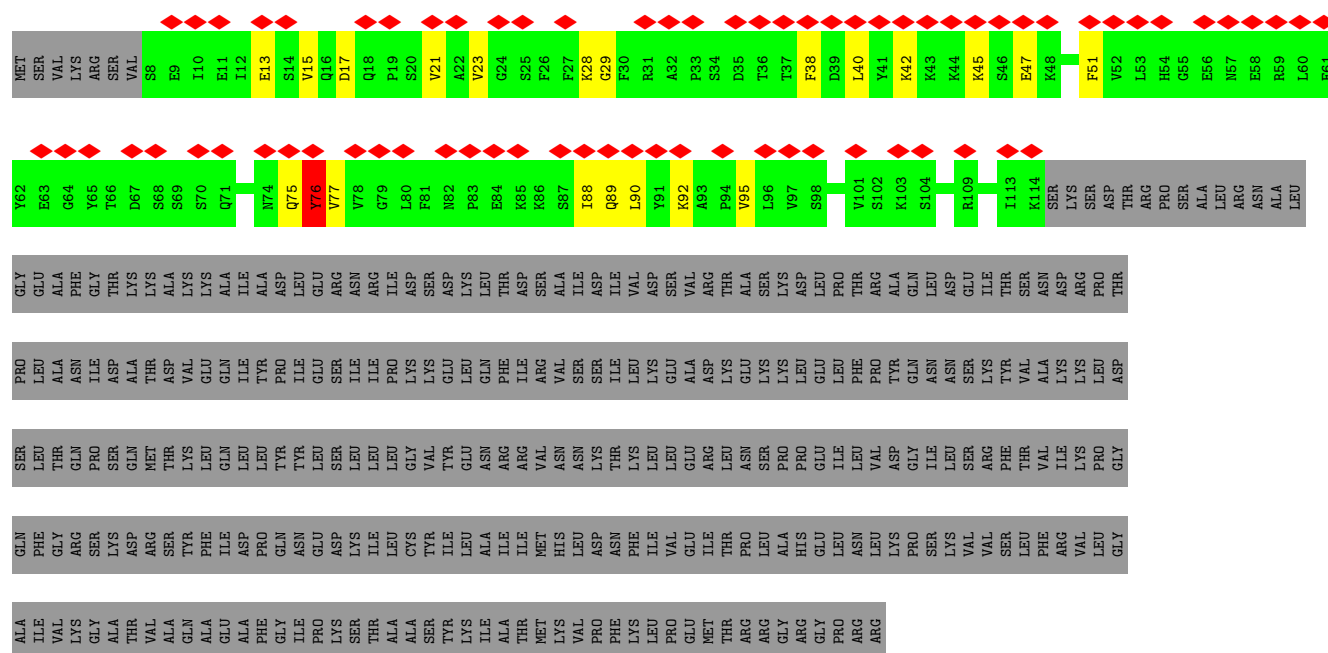




SER PHE GLY ASP VAL TYR GLU THR ASN ALA GLU PHE LEU ASP THR GLN LEU MET ASP LEU SER SER PRO GLU MET HIS TYR SER ASP GLU ASP SER SER GLU

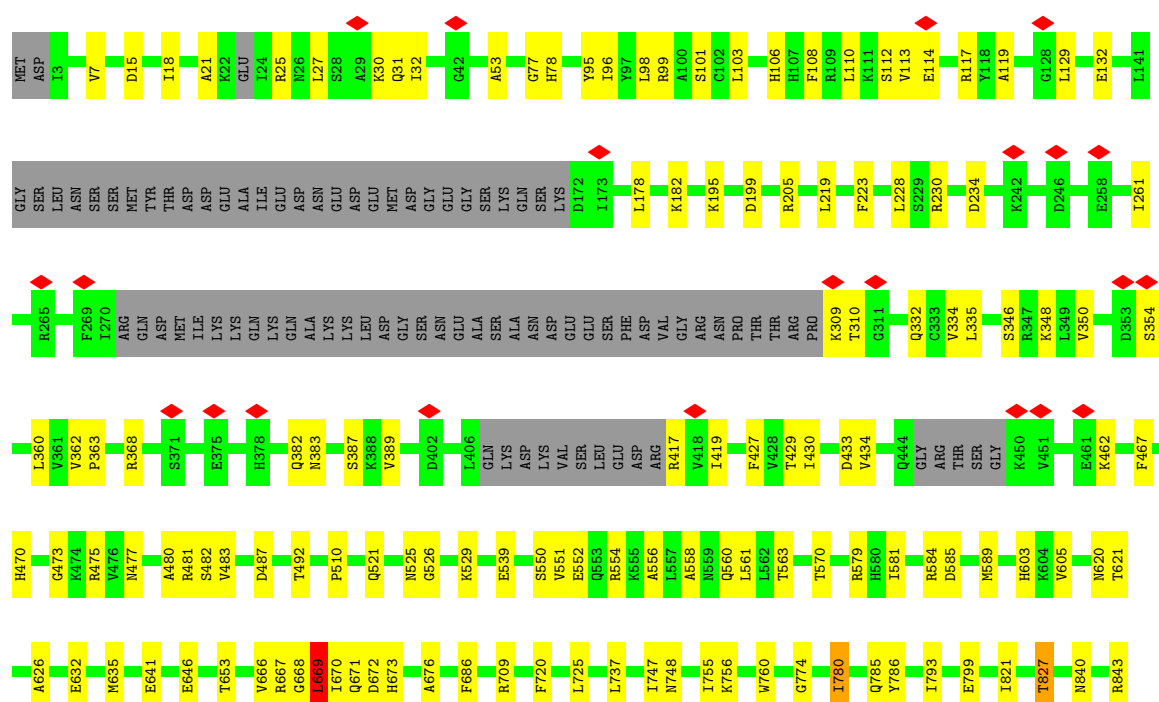
• Molecule 6: DNA-directed RNA polymerase I subunit RPA49

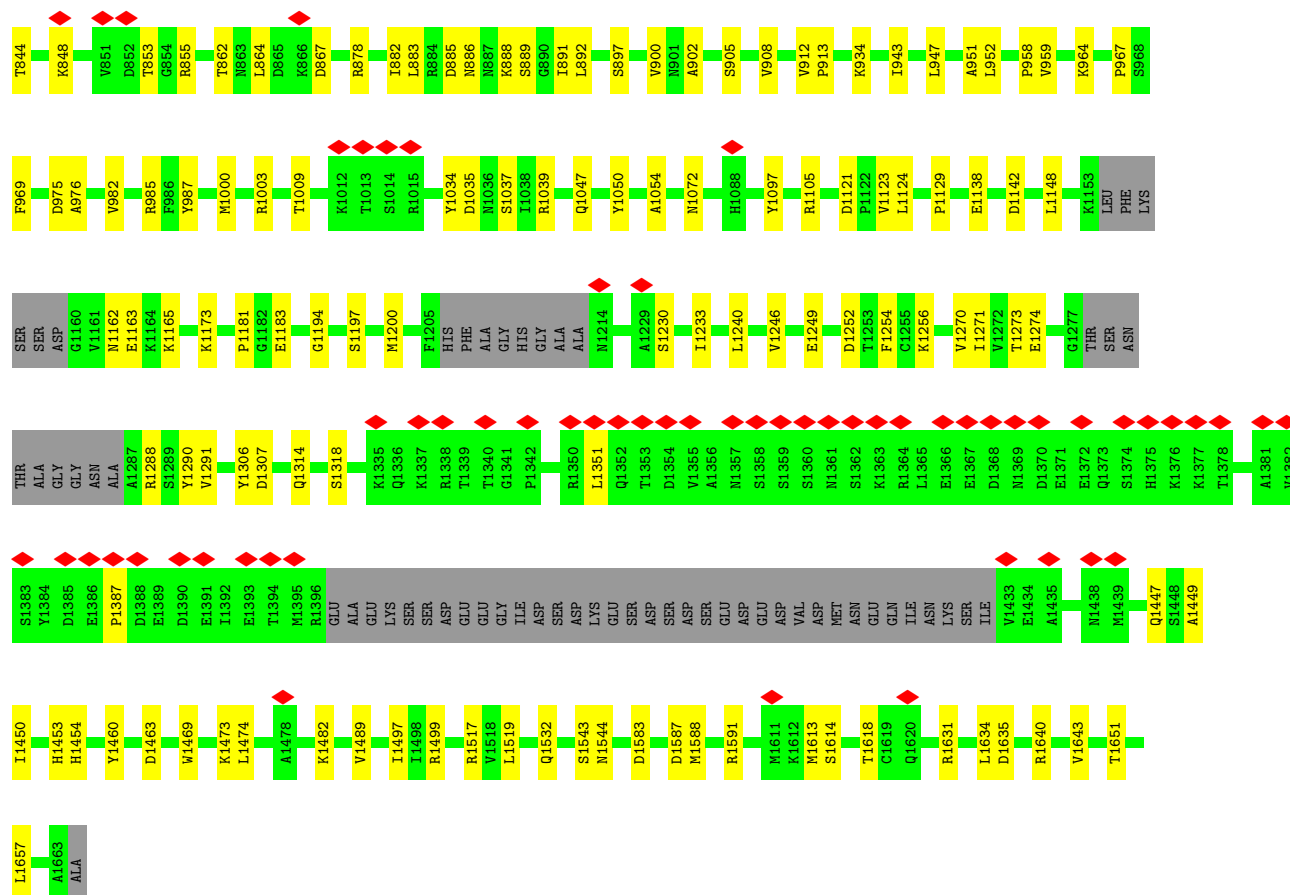
Chain M: 



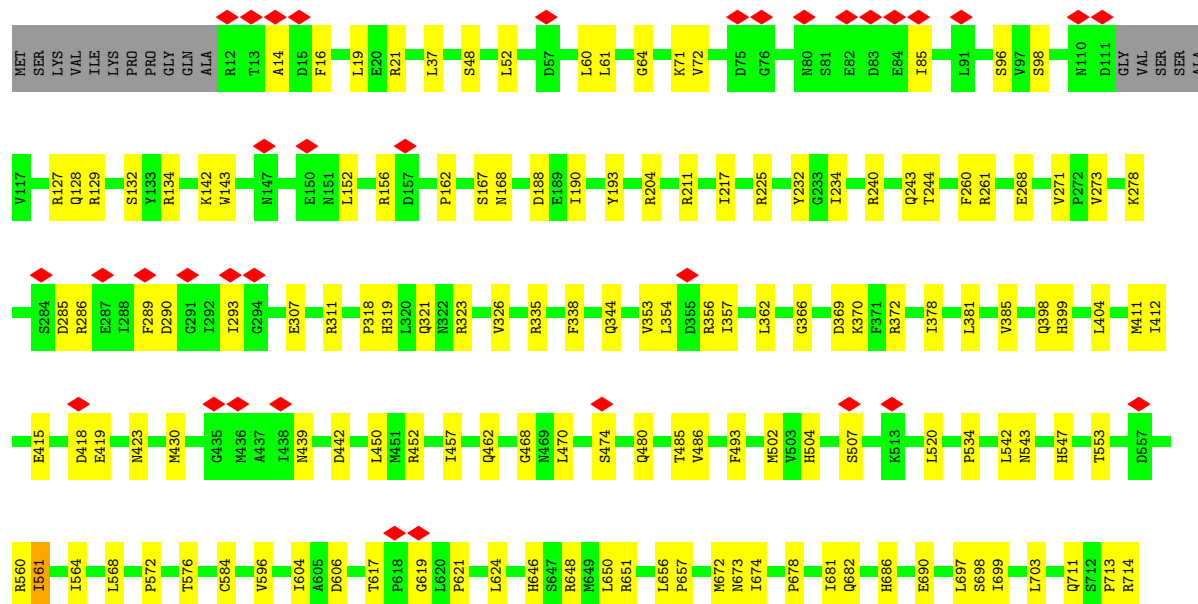
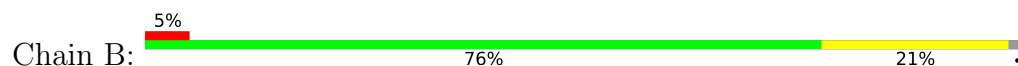
• Molecule 7: DNA-directed RNA polymerase I subunit RPA190

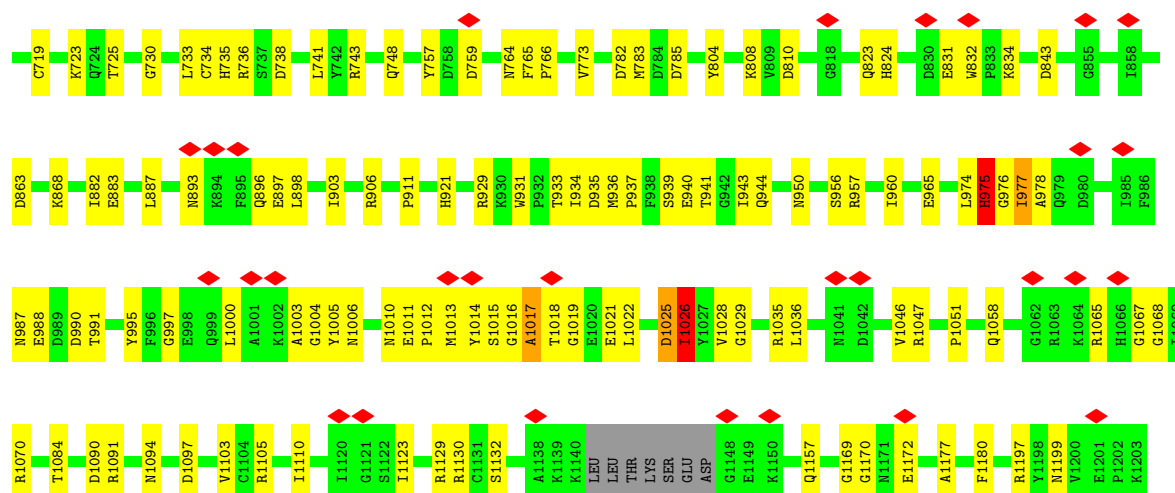
Chain A: 



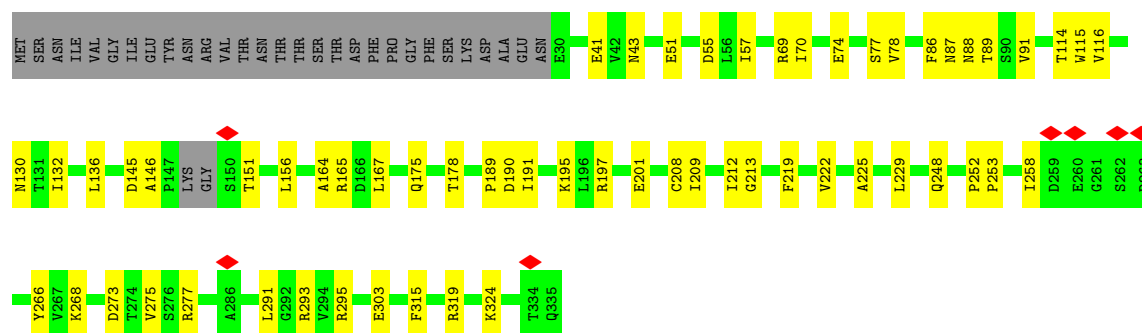


• Molecule 8: DNA-directed RNA polymerase I subunit RPA135

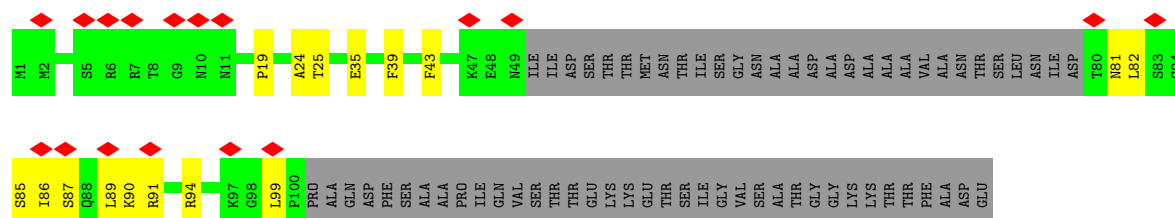
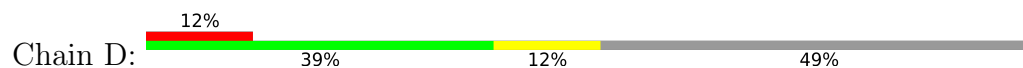




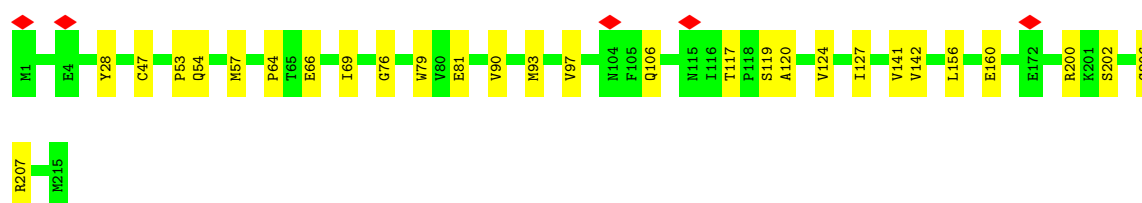
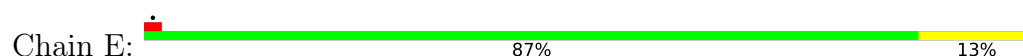
• Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC1



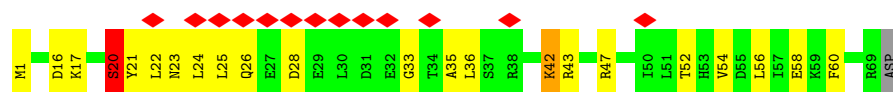
• Molecule 10: DNA-directed RNA polymerase I subunit RPA14



• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC1

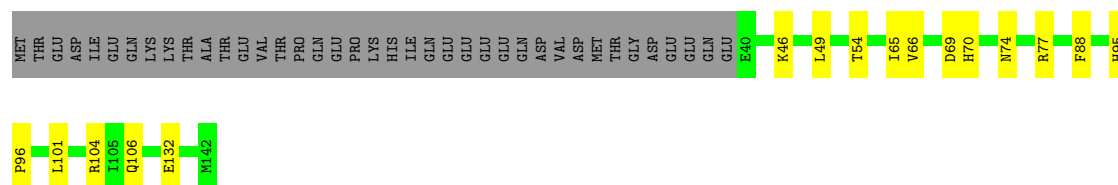


- Chain J: 19% 67% 29% ...



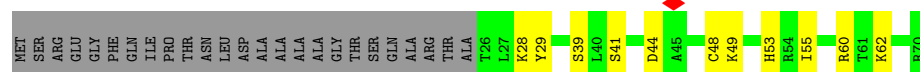
- Molecule 17: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K: 61% 11% 27%



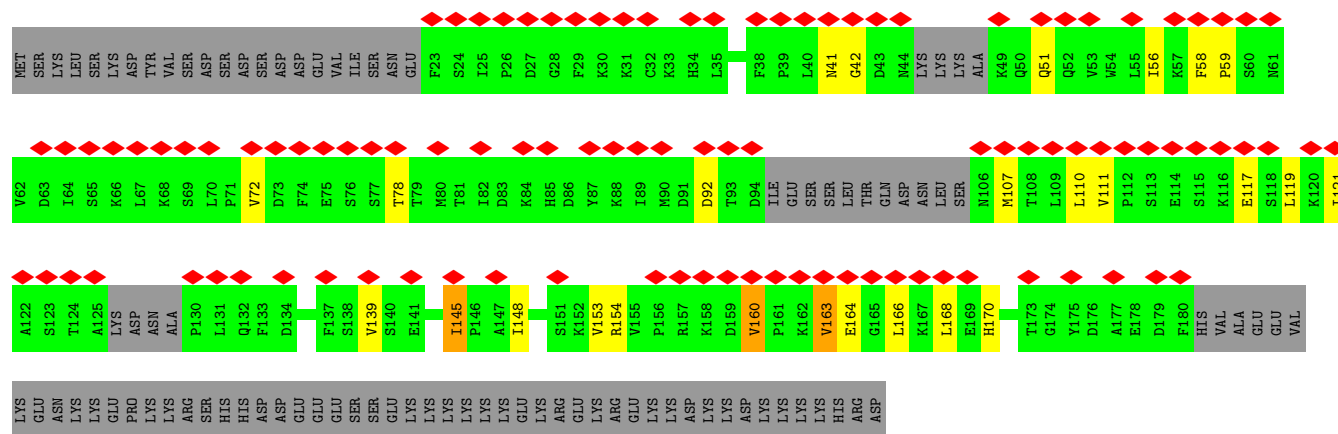
- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 49% 16% 36%



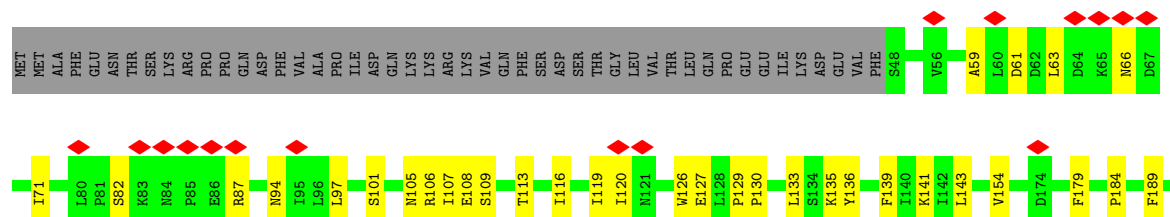
- Molecule 19: DNA-directed RNA polymerase I subunit RPA34

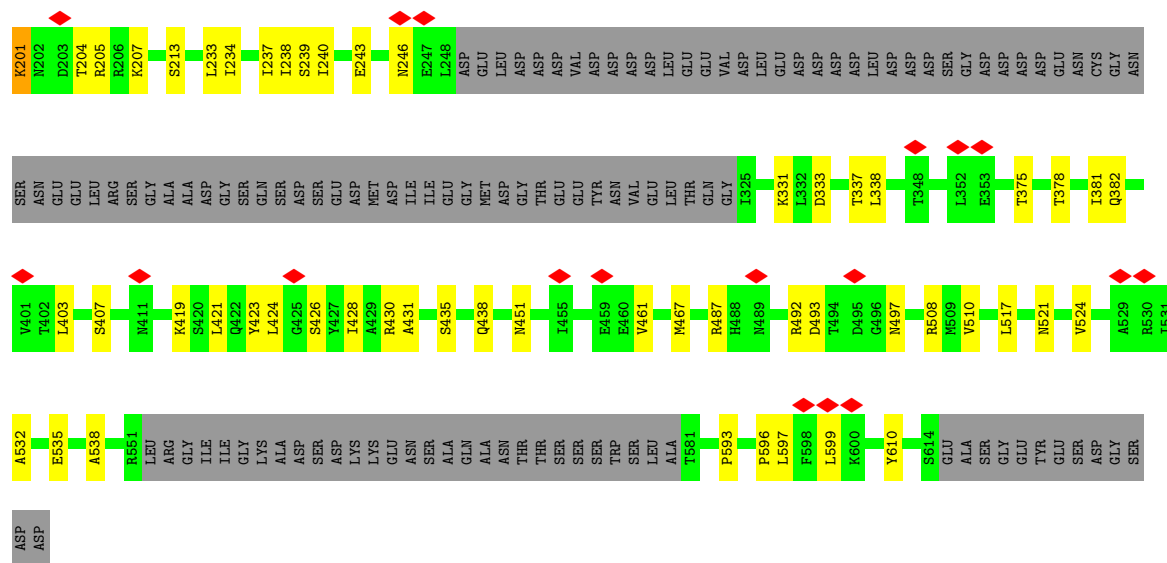
Chain N: 44% 48% 10% 40%



- Molecule 20: RNA polymerase I-specific transcription initiation factor RRN3

Chain O: 5% 60% 14% 26%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9483	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	0.171	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	395.58002, 395.58002, 395.58002	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.041, 1.041, 1.041	Depositor

5 Model quality

5.1 Standard geometry

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	0.28	0/868	0.54	0/1332
2	U	0.31	0/921	0.53	0/1425
3	Q	0.28	0/3766	0.66	0/5086
4	S	0.27	0/5065	0.63	0/6859
5	R	0.29	0/2836	0.68	2/3817 (0.1%)
6	M	0.30	0/866	0.65	2/1162 (0.2%)
7	A	0.39	0/12048	0.62	4/16288 (0.0%)
8	B	0.42	0/9578	0.66	5/12948 (0.0%)
9	C	0.40	0/2469	0.61	0/3347
10	D	0.33	0/557	0.65	0/750
11	E	0.37	1/1795 (0.1%)	0.58	0/2416
12	F	0.38	0/838	0.61	0/1129
13	G	0.35	0/1613	0.59	0/2193
14	H	0.37	0/1090	0.55	0/1476
15	I	0.30	0/955	0.67	2/1288 (0.2%)
16	J	0.41	0/578	0.84	3/775 (0.4%)
17	K	0.41	0/821	0.63	0/1108
18	L	0.40	0/361	0.64	0/478
19	N	0.33	0/1124	0.66	0/1512
20	O	0.32	0/3893	0.58	1/5263 (0.0%)
All	All	0.36	1/52042 (0.0%)	0.63	19/70652 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	124	VAL	C-N	5.23	1.37	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	O	107	ILE	N-CA-C	-8.52	105.62	113.71
8	B	560	ARG	CA-C-N	6.99	124.64	120.24
8	B	560	ARG	C-N-CA	6.99	124.64	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	20	SER	CA-C-N	-6.69	111.13	122.11
16	J	20	SER	C-N-CA	-6.69	111.13	122.11
8	B	457	ILE	N-CA-C	-6.56	106.12	112.29
15	I	18	GLU	CA-C-N	6.41	130.00	120.83
15	I	18	GLU	C-N-CA	6.41	130.00	120.83
6	M	17	ASP	CA-C-N	6.39	129.78	120.51
6	M	17	ASP	C-N-CA	6.39	129.78	120.51
7	A	1387	PRO	N-CA-CB	6.02	110.18	103.44
7	A	853	THR	N-CA-C	-6.00	105.99	113.55
16	J	42	LYS	N-CA-C	5.92	121.06	113.18
8	B	606	ASP	N-CA-C	-5.86	106.68	113.88
8	B	975	HIS	CB-CA-C	5.23	119.12	109.71
5	R	302	ARG	CA-C-N	5.09	131.26	121.54
5	R	302	ARG	C-N-CA	5.09	131.26	121.54
7	A	669	LEU	CA-C-N	-5.05	112.88	121.97
7	A	669	LEU	C-N-CA	-5.05	112.88	121.97

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	779	0	442	5	0
2	U	817	0	441	8	0
3	Q	3675	0	3660	59	0
4	S	4963	0	4890	112	0
5	R	2771	0	2844	49	0
6	M	850	0	850	25	0
7	A	11836	0	11794	185	0
8	B	9371	0	9243	220	0
9	C	2418	0	2401	45	0
10	D	551	0	558	14	0
11	E	1759	0	1788	15	0
12	F	823	0	841	11	0
13	G	1576	0	1581	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	H	1072	0	1042	12	0
15	I	942	0	935	28	0
16	J	569	0	587	20	0
17	K	810	0	801	11	0
18	L	359	0	385	9	0
19	N	1103	0	1106	27	0
20	O	3807	0	3801	54	0
All	All	50851	0	49990	813	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 8.

All (813) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:669:LEU:HD22	7:A:786:TYR:CD2	1.85	1.10
4:S:401:ASN:H	4:S:419:ARG:CB	1.65	1.09
4:S:401:ASN:H	4:S:419:ARG:HB2	0.94	1.06
8:B:1014:TYR:CE1	8:B:1021:GLU:HB2	1.90	1.05
7:A:30:LYS:CE	7:A:53:ALA:HB1	1.89	1.03
7:A:669:LEU:CD2	7:A:786:TYR:CE2	2.42	1.02
7:A:669:LEU:HD22	7:A:786:TYR:CE2	1.94	1.01
8:B:14:ALA:HB3	8:B:977:ILE:CD1	1.89	1.01
4:S:401:ASN:N	4:S:419:ARG:HB2	1.76	1.01
7:A:30:LYS:HE2	7:A:53:ALA:HB1	1.44	0.99
8:B:14:ALA:HB3	8:B:977:ILE:HD12	1.47	0.95
8:B:16:PHE:HD1	8:B:976:GLY:O	1.50	0.93
16:J:20:SER:O	16:J:24:LEU:HG	1.73	0.89
8:B:940:GLU:HB2	8:B:1012:PRO:HG2	1.57	0.87
7:A:669:LEU:HD23	7:A:786:TYR:HE2	1.40	0.85
8:B:1013:MET:HG2	8:B:1026:ILE:HG21	1.60	0.83
8:B:1013:MET:CG	8:B:1026:ILE:HG21	2.08	0.82
8:B:16:PHE:CD1	8:B:976:GLY:O	2.33	0.82
8:B:1014:TYR:CD1	8:B:1021:GLU:HA	2.14	0.82
8:B:937:PRO:HB3	8:B:1015:SER:HA	1.62	0.82
10:D:82:LEU:O	10:D:86:ILE:HG13	1.80	0.81
5:R:6:ILE:HG21	5:R:8:LEU:HD23	1.66	0.77
8:B:211:ARG:HH22	8:B:243:GLN:HE22	1.32	0.77
4:S:401:ASN:HB2	4:S:419:ARG:HG3	1.65	0.76
3:Q:246:GLU:O	3:Q:247:ILE:C	2.28	0.76
8:B:1013:MET:O	8:B:1026:ILE:HG12	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:668:GLY:O	7:A:669:LEU:O	2.04	0.76
5:R:138:PHE:CZ	5:R:297:PHE:HE2	2.03	0.76
4:S:420:GLU:HA	4:S:442:LEU:HB3	1.67	0.75
7:A:669:LEU:HD23	7:A:786:TYR:CE2	2.18	0.75
16:J:20:SER:O	16:J:24:LEU:CG	2.35	0.75
8:B:974:LEU:HB2	8:B:975:HIS:CD2	2.23	0.74
7:A:669:LEU:HG	7:A:673:HIS:CB	2.19	0.73
4:S:444:PRO:HA	5:R:2:PHE:HA	1.71	0.72
7:A:30:LYS:CE	7:A:53:ALA:CB	2.68	0.71
4:S:418:SER:OG	4:S:421:ILE:HG22	1.91	0.70
8:B:204:ARG:HH21	8:B:486:VAL:HG11	1.57	0.69
4:S:400:SER:HA	4:S:419:ARG:HD3	1.75	0.69
8:B:1014:TYR:CD1	8:B:1021:GLU:HB2	2.27	0.69
20:O:61:ASP:HA	20:O:106:ARG:HH22	1.57	0.69
7:A:672:ASP:HB3	8:B:783:MET:HE3	1.75	0.68
7:A:27:LEU:HB3	8:B:1130:ARG:HB3	1.76	0.68
3:Q:275:GLU:OE2	3:Q:282:ARG:NH1	2.26	0.68
16:J:20:SER:O	16:J:24:LEU:CD1	2.42	0.68
8:B:1014:TYR:HD1	8:B:1022:LEU:H	1.42	0.68
7:A:669:LEU:HG	7:A:673:HIS:HB3	1.76	0.67
8:B:991:THR:O	8:B:995:TYR:N	2.27	0.67
8:B:14:ALA:N	8:B:977:ILE:HD13	2.09	0.67
4:S:391:THR:HG21	5:R:144:VAL:HG23	1.76	0.67
8:B:1014:TYR:CD1	8:B:1021:GLU:CA	2.78	0.66
7:A:332:GLN:HE22	7:A:350:VAL:H	1.42	0.66
4:S:298:ASP:HB3	4:S:321:LYS:HB2	1.76	0.66
5:R:6:ILE:CG2	5:R:8:LEU:HD23	2.24	0.66
6:M:77:VAL:HG22	6:M:92:LYS:HG2	1.77	0.66
7:A:113:VAL:HG11	7:A:178:LEU:HD22	1.78	0.65
6:M:75:GLN:O	6:M:76:TYR:O	2.15	0.65
11:E:54:GLN:HE21	11:E:57:MET:HE3	1.61	0.65
3:Q:235:GLY:HA2	3:Q:288:GLU:HB2	1.78	0.65
8:B:743:ARG:NH2	16:J:1:MET:SD	2.70	0.65
8:B:1014:TYR:CG	8:B:1021:GLU:HA	2.32	0.65
4:S:260:LEU:HD12	4:S:260:LEU:C	2.21	0.64
19:N:41:ASN:HB2	19:N:51:GLN:HG3	1.78	0.64
18:L:28:LYS:HG2	18:L:39:SER:HB2	1.80	0.64
7:A:1124:LEU:HD22	7:A:1129:PRO:HG3	1.79	0.64
3:Q:154:LEU:O	3:Q:154:LEU:HG	1.97	0.64
4:S:300:LEU:HA	4:S:320:ILE:HA	1.80	0.63
7:A:668:GLY:C	7:A:669:LEU:O	2.39	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:81:ASN:O	10:D:82:LEU:HB3	1.97	0.63
8:B:1025:ASP:OD2	9:C:277:ARG:NH1	2.32	0.63
9:C:70:ILE:HG23	9:C:74:GLU:HB2	1.81	0.63
13:G:159:LYS:HB3	20:O:105:ASN:HD21	1.63	0.63
8:B:1016:GLY:O	8:B:1018:THR:N	2.31	0.63
9:C:43:ASN:HB2	9:C:55:ASP:HB2	1.81	0.63
7:A:30:LYS:HD2	7:A:53:ALA:CB	2.29	0.63
8:B:1014:TYR:HE2	9:C:293:ARG:HH22	1.43	0.63
13:G:234:ARG:H	13:G:247:GLY:HA2	1.64	0.63
5:R:8:LEU:HD12	5:R:8:LEU:O	1.98	0.63
20:O:510:VAL:HG13	20:O:517:LEU:HD11	1.81	0.62
4:S:401:ASN:N	4:S:419:ARG:CB	2.50	0.62
6:M:76:TYR:CD2	19:N:107:MET:HE1	2.34	0.62
7:A:481:ARG:NH2	7:A:632:GLU:OE1	2.32	0.62
16:J:20:SER:O	16:J:24:LEU:HD12	2.00	0.62
4:S:407:ARG:HH11	4:S:411:LYS:HG2	1.64	0.62
9:C:69:ARG:HH12	17:K:70:HIS:HB2	1.63	0.62
8:B:1047:ARG:NH2	8:B:1051:PRO:O	2.33	0.62
15:I:3:VAL:HG22	15:I:8:ILE:HA	1.81	0.62
4:S:416:LEU:HD23	4:S:423:ILE:HD12	1.82	0.62
4:S:180:ASN:HD22	4:S:246:LYS:HE2	1.63	0.62
8:B:1105:ARG:NH2	8:B:1172:GLU:OE1	2.32	0.62
8:B:156:ARG:HH11	8:B:450:LEU:HD22	1.65	0.62
8:B:240:ARG:NH2	8:B:356:ARG:O	2.33	0.62
9:C:87:ASN:ND2	9:C:201:GLU:OE2	2.33	0.62
10:D:94:ARG:NH2	10:D:99:LEU:O	2.32	0.62
4:S:401:ASN:H	4:S:419:ARG:CG	2.12	0.62
6:M:76:TYR:O	6:M:77:VAL:CG2	2.48	0.62
6:M:76:TYR:C	6:M:77:VAL:HG23	2.25	0.62
4:S:232:ASN:ND2	4:S:281:SER:O	2.33	0.61
6:M:28:LYS:O	8:B:286:ARG:NH2	2.33	0.61
4:S:390:GLN:HB2	5:R:152:ILE:HG13	1.83	0.61
17:K:104:ARG:HE	17:K:106:GLN:HE21	1.48	0.61
4:S:606:ARG:NH1	4:S:667:ASP:O	2.33	0.61
7:A:7:VAL:HG21	8:B:1177:ALA:HB2	1.80	0.61
7:A:670:ILE:HG12	7:A:671:GLN:HG3	1.80	0.61
8:B:617:THR:HG22	8:B:619:GLY:H	1.63	0.61
6:M:38:PHE:HB2	19:N:119:LEU:HB2	1.82	0.61
6:M:76:TYR:O	6:M:77:VAL:HG23	2.00	0.61
7:A:389:VAL:HG22	7:A:433:ASP:HB3	1.82	0.61
5:R:440:SER:O	5:R:443:TYR:CE2	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:110:LEU:HD12	7:A:114:GLU:HG2	1.83	0.61
4:S:363:ILE:HG22	4:S:374:VAL:HA	1.81	0.61
4:S:425:GLY:HA3	4:S:434:ARG:HH11	1.66	0.61
7:A:669:LEU:HD22	7:A:786:TYR:HD2	1.61	0.61
3:Q:337:SER:O	3:Q:445:ARG:NH1	2.35	0.60
3:Q:307:LEU:HD22	3:Q:487:LEU:HD11	1.82	0.60
5:R:5:PRO:HB2	5:R:246:GLN:H	1.66	0.60
8:B:278:LYS:NZ	8:B:285:ASP:OD1	2.34	0.60
14:H:28:ALA:HB3	14:H:38:LEU:HB3	1.82	0.60
4:S:476:ILE:HG22	4:S:497:VAL:H	1.65	0.60
4:S:464:LEU:HB2	4:S:481:PHE:HB2	1.83	0.60
7:A:1274:GLU:OE2	7:A:1288:ARG:NH2	2.33	0.60
8:B:974:LEU:HB2	8:B:975:HIS:HD2	1.67	0.60
7:A:1273:THR:HG22	15:I:48:VAL:HG23	1.84	0.60
7:A:799:GLU:OE2	7:A:1173:LYS:NZ	2.34	0.60
8:B:977:ILE:HD12	8:B:978:ALA:N	2.16	0.60
11:E:97:VAL:HG13	11:E:127:ILE:HD11	1.84	0.60
7:A:908:VAL:O	15:I:83:LYS:NZ	2.34	0.59
8:B:1047:ARG:HD2	8:B:1067:GLY:HA2	1.84	0.59
3:Q:246:GLU:O	3:Q:248:SER:N	2.35	0.59
9:C:248:GLN:HE21	9:C:258:ILE:HG23	1.66	0.59
9:C:293:ARG:HB2	9:C:295:ARG:HE	1.68	0.59
3:Q:258:MET:HE1	4:S:704:LEU:HD23	1.84	0.59
7:A:1138:GLU:OE2	11:E:207:ARG:NH1	2.35	0.59
15:I:40:SER:HB3	15:I:43:SER:HB3	1.83	0.59
4:S:597:LYS:HD2	4:S:601:ARG:HE	1.66	0.59
15:I:30:CYS:SG	15:I:31:SER:N	2.75	0.59
8:B:1026:ILE:HG22	8:B:1028:VAL:HG23	1.83	0.59
20:O:492:ARG:NH2	20:O:535:GLU:OE1	2.36	0.59
8:B:711:GLN:HG2	8:B:713:PRO:HD2	1.83	0.59
15:I:33:CYS:SG	15:I:34:LYS:N	2.76	0.59
9:C:165:ARG:NH1	9:C:190:ASP:OD1	2.36	0.59
13:G:149:ILE:HB	13:G:153:PHE:HB2	1.85	0.58
13:G:32:ASN:O	13:G:230:ARG:NH2	2.36	0.58
5:R:138:PHE:CZ	5:R:297:PHE:CE2	2.89	0.58
8:B:741:LEU:HB2	8:B:804:TYR:HB2	1.85	0.58
20:O:451:ASN:OD1	20:O:508:ARG:NH2	2.36	0.58
2:U:43:DG:H1	8:B:452:ARG:HA	1.68	0.58
4:S:402:ILE:HG12	4:S:418:SER:HB3	1.85	0.58
8:B:167:SER:OG	8:B:168:ASN:N	2.35	0.58
8:B:188:ASP:OD2	8:B:764:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:782:ASP:O	8:B:950:ASN:ND2	2.37	0.58
4:S:383:ILE:HG12	5:R:152:ILE:HG12	1.86	0.57
8:B:353:VAL:HG13	8:B:357:ILE:HD12	1.86	0.57
10:D:87:SER:HA	10:D:90:LYS:HB2	1.85	0.57
4:S:541:LEU:HB2	4:S:544:SER:HB3	1.85	0.57
8:B:975:HIS:CD2	8:B:975:HIS:N	2.71	0.57
8:B:1014:TYR:CE1	8:B:1021:GLU:CB	2.78	0.57
16:J:42:LYS:HE2	16:J:43:ARG:HG3	1.86	0.57
4:S:351:ILE:HG21	4:S:374:VAL:HG11	1.85	0.57
7:A:477:ASN:OD1	8:B:1047:ARG:NH1	2.28	0.57
8:B:823:GLN:HA	8:B:863:ASP:HA	1.86	0.57
8:B:1003:ALA:HA	19:N:168:LEU:HG	1.85	0.57
4:S:401:ASN:OD1	4:S:419:ARG:HD2	2.04	0.57
7:A:709:ARG:NH1	7:A:737:LEU:O	2.37	0.57
8:B:232:TYR:HD2	8:B:385:VAL:HG12	1.68	0.57
8:B:1026:ILE:HG22	8:B:1028:VAL:CG2	2.34	0.57
20:O:423:TYR:HA	20:O:593:PRO:HG2	1.87	0.57
3:Q:240:LYS:O	3:Q:241:GLU:HG3	2.04	0.57
13:G:158:LYS:NZ	20:O:108:GLU:OE1	2.37	0.57
4:S:417:THR:HG22	4:S:417:THR:O	2.03	0.57
5:R:275:CYS:O	5:R:279:SER:OG	2.23	0.57
7:A:952:LEU:HD11	7:A:1000:MET:HB3	1.87	0.57
8:B:785:ASP:OD2	8:B:957:ARG:NH2	2.33	0.57
1:T:32:DC:N4	2:U:39:DG:O6	2.38	0.56
4:S:446:ASP:HA	4:S:472:ARG:HH12	1.70	0.56
7:A:1651:THR:O	12:F:92:ARG:NH1	2.37	0.56
9:C:116:VAL:HB	9:C:209:ILE:HD11	1.86	0.56
2:U:38:DT:OP1	5:R:287:ASN:ND2	2.38	0.56
7:A:30:LYS:HD2	7:A:53:ALA:HB3	1.86	0.56
7:A:492:THR:O	7:A:620:ASN:ND2	2.38	0.56
6:M:76:TYR:CE2	19:N:107:MET:HE1	2.40	0.56
7:A:429:THR:O	7:A:433:ASP:N	2.38	0.56
7:A:1249:GLU:HA	7:A:1252:ASP:HB2	1.86	0.56
8:B:14:ALA:CB	8:B:977:ILE:CD1	2.77	0.56
8:B:1014:TYR:CD1	8:B:1021:GLU:CB	2.87	0.56
16:J:43:ARG:O	16:J:47:ARG:N	2.38	0.56
4:S:407:ARG:HA	4:S:414:ILE:HG23	1.87	0.56
15:I:23:VAL:HG11	15:I:28:VAL:HG12	1.87	0.56
3:Q:177:TYR:OH	3:Q:248:SER:O	2.24	0.56
7:A:1447:GLN:HG3	7:A:1460:TYR:HB3	1.87	0.56
3:Q:102:LEU:HD11	4:S:773:SER:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:234:ILE:HD13	20:O:237:ILE:HD12	1.87	0.56
4:S:449:LEU:HD22	4:S:468:VAL:HB	1.87	0.56
7:A:1105:ARG:NH2	7:A:1142:ASP:OD1	2.38	0.56
7:A:1291:VAL:HG22	7:A:1473:LYS:HG2	1.88	0.56
8:B:60:LEU:O	8:B:64:GLY:N	2.39	0.56
17:K:65:ILE:HB	17:K:101:LEU:HB3	1.87	0.56
20:O:94:ASN:HD22	20:O:135:LYS:HD2	1.70	0.55
7:A:1009:THR:HG21	15:I:103:SER:HB2	1.88	0.55
20:O:430:ARG:NH1	20:O:610:TYR:OH	2.39	0.55
7:A:27:LEU:O	8:B:1129:ARG:NE	2.32	0.55
7:A:195:LYS:NZ	7:A:199:ASP:OD2	2.38	0.55
7:A:840:ASN:OD1	7:A:844:THR:OG1	2.23	0.55
8:B:748:GLN:HB3	16:J:52:THR:HG22	1.88	0.55
13:G:63:LYS:HA	13:G:67:ASN:HD22	1.72	0.55
16:J:21:TYR:HA	16:J:24:LEU:HB2	1.87	0.55
8:B:1016:GLY:C	8:B:1018:THR:N	2.63	0.55
6:M:90:LEU:HD13	6:M:92:LYS:HD2	1.88	0.55
8:B:204:ARG:HD3	8:B:504:HIS:HB2	1.88	0.55
8:B:651:ARG:NH2	8:B:690:GLU:OE2	2.39	0.55
20:O:431:ALA:O	20:O:487:ARG:NH2	2.40	0.55
4:S:219:LEU:N	4:S:226:HIS:O	2.40	0.55
4:S:402:ILE:HG12	4:S:418:SER:CB	2.37	0.55
7:A:219:LEU:O	7:A:223:PHE:N	2.36	0.55
8:B:273:VAL:HG11	8:B:378:ILE:HD11	1.89	0.55
3:Q:111:ILE:HD11	3:Q:200:PRO:HG3	1.89	0.55
7:A:32:ILE:HD12	7:A:362:VAL:HG21	1.87	0.55
7:A:114:GLU:OE2	7:A:117:ARG:NH2	2.40	0.55
8:B:719:CYS:O	8:B:723:LYS:NZ	2.39	0.55
16:J:33:GLY:HA2	16:J:36:LEU:HB2	1.88	0.55
7:A:346:SER:OG	7:A:348:LYS:NZ	2.36	0.54
7:A:560:GLN:HE22	20:O:239:SER:HA	1.72	0.54
4:S:178:VAL:O	4:S:450:ARG:NH2	2.40	0.54
8:B:204:ARG:NH1	8:B:502:MET:SD	2.74	0.54
5:R:189:GLN:HB3	5:R:193:ARG:HH12	1.72	0.54
7:A:30:LYS:CD	7:A:53:ALA:HB1	2.35	0.54
7:A:309:LYS:HG3	7:A:310:THR:HG23	1.88	0.54
7:A:666:VAL:HG23	7:A:667:ARG:HG3	1.88	0.54
7:A:785:GLN:HB3	7:A:793:ILE:HG22	1.89	0.54
7:A:985:ARG:HG2	7:A:987:TYR:H	1.71	0.54
7:A:1037:SER:OG	7:A:1039:ARG:NE	2.41	0.54
8:B:1016:GLY:O	8:B:1017:ALA:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1097:ASP:OD2	8:B:1180:PHE:N	2.39	0.54
7:A:129:LEU:HD13	7:A:132:GLU:HB2	1.90	0.54
8:B:1021:GLU:OE2	9:C:295:ARG:NH2	2.41	0.54
8:B:1090:ASP:HA	8:B:1094:ASN:HB2	1.89	0.54
15:I:91:ASN:ND2	15:I:115:THR:OG1	2.40	0.54
15:I:119:TYR:HE2	15:I:121:PHE:HD1	1.56	0.54
6:M:23:VAL:HG12	19:N:107:MET:HE2	1.89	0.54
7:A:964:LYS:NZ	8:B:672:MET:O	2.30	0.54
8:B:1090:ASP:O	8:B:1091:ARG:NE	2.40	0.54
20:O:97:LEU:HD22	20:O:135:LYS:HG2	1.89	0.54
7:A:891:ILE:HD12	15:I:71:LEU:HG	1.90	0.54
7:A:951:ALA:O	15:I:98:THR:OG1	2.24	0.54
8:B:16:PHE:HD1	8:B:976:GLY:C	2.15	0.54
8:B:714:ARG:NH1	15:I:104:ALA:O	2.39	0.54
5:R:203:SER:O	5:R:211:ARG:NH1	2.38	0.54
7:A:1254:PHE:HZ	7:A:1532:GLN:HB3	1.73	0.54
8:B:14:ALA:HB3	8:B:977:ILE:HD13	1.85	0.54
8:B:1006:ASN:ND2	8:B:1010:ASN:O	2.41	0.54
9:C:175:GLN:HA	9:C:178:THR:HG22	1.90	0.54
20:O:521:ASN:HB3	20:O:524:VAL:HG12	1.90	0.54
8:B:621:PRO:HG2	8:B:624:LEU:HB2	1.90	0.53
15:I:74:ASN:O	15:I:77:LYS:NZ	2.40	0.53
7:A:934:LYS:HD2	8:B:956:SER:HB3	1.90	0.53
7:A:18:ILE:HG21	7:A:354:SER:HA	1.91	0.53
15:I:112:TYR:HB2	15:I:121:PHE:HB3	1.90	0.53
8:B:1014:TYR:OH	9:C:293:ARG:NH2	2.41	0.53
7:A:862:THR:HG23	7:A:864:LEU:H	1.74	0.53
7:A:1588:MET:O	7:A:1591:ARG:NH1	2.37	0.53
3:Q:24:ASP:HB3	8:B:1065:ARG:HG3	1.90	0.53
4:S:423:ILE:HG22	4:S:425:GLY:H	1.73	0.53
9:C:114:THR:OG1	9:C:130:ASN:ND2	2.41	0.53
7:A:1256:LYS:O	7:A:1499:ARG:NH2	2.41	0.53
8:B:1013:MET:HB3	8:B:1026:ILE:CG2	2.38	0.53
9:C:164:ALA:HB2	9:C:191:ILE:HB	1.91	0.53
9:C:165:ARG:HB3	9:C:189:PRO:HB2	1.90	0.53
18:L:48:CYS:SG	18:L:49:LYS:N	2.82	0.53
3:Q:152:LEU:HD23	3:Q:152:LEU:H	1.74	0.53
8:B:736:ARG:NH2	8:B:738:ASP:OD2	2.42	0.53
8:B:1004:GLY:O	19:N:170:HIS:ND1	2.42	0.53
20:O:233:LEU:O	20:O:237:ILE:N	2.42	0.53
7:A:882:ILE:HG22	7:A:888:LYS:HB3	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:63:LEU:O	20:O:66:ASN:ND2	2.42	0.52
7:A:521:GLN:O	7:A:525:ASN:ND2	2.42	0.52
7:A:912:VAL:HG23	7:A:913:PRO:HD3	1.91	0.52
7:A:480:ALA:HB2	8:B:1046:VAL:HG23	1.91	0.52
7:A:1449:ALA:O	7:A:1453:HIS:ND1	2.43	0.52
8:B:37:LEU:HD12	8:B:759:ASP:HB3	1.91	0.52
7:A:1306:TYR:O	7:A:1499:ARG:NH2	2.43	0.52
8:B:286:ARG:HA	8:B:289:PHE:HB3	1.92	0.52
8:B:883:GLU:OE1	8:B:906:ARG:NH1	2.42	0.52
8:B:939:SER:OG	8:B:940:GLU:N	2.41	0.52
3:Q:252:LEU:HD22	3:Q:306:VAL:HG12	1.91	0.52
4:S:601:ARG:HA	4:S:604:ILE:HB	1.90	0.52
7:A:30:LYS:CD	7:A:53:ALA:CB	2.87	0.52
7:A:1450:ILE:O	7:A:1454:HIS:ND1	2.34	0.52
8:B:71:LYS:NZ	8:B:418:ASP:OD1	2.42	0.52
13:G:147:LEU:O	13:G:154:ASN:ND2	2.39	0.52
7:A:556:ALA:HB1	20:O:243:GLU:HG2	1.92	0.52
8:B:190:ILE:HD11	8:B:493:PHE:HE1	1.75	0.52
8:B:808:LYS:HE2	8:B:810:ASP:HB2	1.91	0.52
12:F:106:PRO:HG3	13:G:55:GLU:HB2	1.91	0.52
3:Q:169:SER:HA	3:Q:174:LEU:HD12	1.92	0.52
8:B:568:LEU:HD23	8:B:604:ILE:HG12	1.92	0.52
7:A:526:GLY:HA3	7:A:554:ARG:HH11	1.75	0.52
8:B:933:THR:OG1	8:B:944:GLN:OE1	2.26	0.52
16:J:22:LEU:O	16:J:26:GLN:N	2.43	0.52
20:O:213:SER:HB2	20:O:338:LEU:HD21	1.92	0.52
8:B:311:ARG:HE	15:I:16:LEU:HD11	1.74	0.52
9:C:319:ARG:NH1	17:K:132:GLU:OE2	2.42	0.52
19:N:42:GLY:H	19:N:51:GLN:HB2	1.74	0.52
8:B:843:ASP:OD2	18:L:29:TYR:OH	2.27	0.52
7:A:943:ILE:HG12	8:B:960:ILE:HD11	1.92	0.51
8:B:584:CYS:HB3	8:B:596:VAL:HG23	1.92	0.51
8:B:997:GLY:HA2	8:B:1000:LEU:HD13	1.92	0.51
1:T:30:DC:H2''	1:T:31:DC:H5'	1.91	0.51
6:M:29:GLY:HA3	8:B:286:ARG:HH21	1.75	0.51
8:B:940:GLU:HB2	8:B:1012:PRO:CG	2.35	0.51
20:O:201:LYS:HG3	20:O:240:ILE:HG13	1.92	0.51
4:S:456:VAL:HB	4:S:463:LEU:HB2	1.91	0.51
7:A:1047:GLN:HE22	7:A:1583:ASP:HB3	1.74	0.51
4:S:462:ILE:HB	4:S:483:HIS:HB3	1.92	0.51
8:B:127:ARG:NH2	8:B:193:TYR:OH	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:19:PRO:HB3	13:G:47:VAL:HG12	1.92	0.51
3:Q:229:LYS:HA	3:Q:232:LEU:HD23	1.93	0.51
4:S:28:PRO:HG2	4:S:31:ASN:HD21	1.74	0.51
4:S:587:GLU:O	4:S:591:ALA:N	2.44	0.51
8:B:16:PHE:CD1	8:B:976:GLY:C	2.87	0.51
7:A:1613:MET:HB3	7:A:1618:THR:HG23	1.92	0.51
8:B:323:ARG:HA	8:B:326:VAL:HG12	1.92	0.51
4:S:58:HIS:HB3	4:S:552:LEU:HD22	1.92	0.51
4:S:377:ARG:HA	4:S:402:ILE:HB	1.91	0.51
6:M:88:ILE:HB	19:N:56:ILE:HD13	1.93	0.51
8:B:129:ARG:HB2	18:L:55:ILE:HD11	1.92	0.51
4:S:422:ILE:HB	4:S:440:HIS:HB3	1.92	0.51
7:A:96:ILE:HG23	7:A:228:LEU:HD13	1.92	0.51
7:A:1034:TYR:HA	7:A:1181:PRO:HB3	1.93	0.51
7:A:1274:GLU:HB3	15:I:47:VAL:HG23	1.91	0.51
8:B:1015:SER:HB3	8:B:1022:LEU:HD11	1.93	0.51
11:E:202:SER:N	11:E:206:GLY:O	2.42	0.51
16:J:24:LEU:HA	16:J:28:ASP:HB2	1.91	0.51
18:L:41:SER:OG	18:L:44:ASP:OD2	2.25	0.51
20:O:119:ILE:O	20:O:136:TYR:OH	2.28	0.51
3:Q:262:LEU:HD13	3:Q:266:PHE:HB2	1.93	0.51
7:A:473:GLY:O	8:B:1070:ARG:NH1	2.44	0.51
8:B:733:LEU:HD22	8:B:741:LEU:HD13	1.93	0.51
3:Q:154:LEU:HD23	3:Q:154:LEU:H	1.76	0.50
8:B:261:ARG:NH2	8:B:268:GLU:OE2	2.45	0.50
5:R:168:ILE:HG23	5:R:169:PRO:HD3	1.93	0.50
5:R:361:ASP:OD1	5:R:361:ASP:N	2.42	0.50
7:A:21:ALA:O	7:A:25:ARG:NH1	2.45	0.50
7:A:646:GLU:OE1	8:B:1084:THR:OG1	2.27	0.50
7:A:827:THR:HG21	8:B:1026:ILE:HA	1.92	0.50
7:A:1288:ARG:HH22	7:A:1482:LYS:HA	1.76	0.50
8:B:52:LEU:HD23	8:B:61:LEU:HD11	1.92	0.50
15:I:39:LYS:HD2	15:I:41:GLN:HB2	1.94	0.50
3:Q:251:GLY:O	3:Q:255:LYS:N	2.42	0.50
3:Q:96:ILE:HB	3:Q:100:ALA:HB2	1.93	0.50
4:S:635:ASN:OD1	4:S:686:TYR:OH	2.30	0.50
7:A:368:ARG:HG2	7:A:382:GLN:HG3	1.93	0.50
10:D:25:THR:OG1	12:F:59:GLN:OE1	2.29	0.50
7:A:669:LEU:CD2	7:A:786:TYR:HE2	1.93	0.50
8:B:831:GLU:OE1	8:B:868:LYS:NZ	2.38	0.50
19:N:72:VAL:HA	19:N:78:THR:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:439:ASN:HB3	8:B:442:ASP:HB2	1.94	0.50
3:Q:240:LYS:C	3:Q:241:GLU:HG3	2.36	0.50
7:A:363:PRO:O	7:A:368:ARG:NH2	2.42	0.50
14:H:112:ILE:HD12	14:H:131:ASN:HD22	1.77	0.50
6:M:42:LYS:HG3	6:M:51:PHE:HE1	1.76	0.49
15:I:80:ALA:HB3	15:I:95:ASN:HD22	1.77	0.49
2:U:24:DT:O4	3:Q:293:ARG:NH1	2.46	0.49
3:Q:115:GLN:HE22	3:Q:161:THR:HG21	1.77	0.49
3:Q:171:HIS:ND1	3:Q:244:ASN:OD1	2.44	0.49
7:A:15:ASP:HB2	8:B:1197:ARG:HB3	1.93	0.49
7:A:108:PHE:HZ	7:A:335:LEU:HD11	1.76	0.49
8:B:14:ALA:H	8:B:977:ILE:HD13	1.76	0.49
8:B:1015:SER:H	8:B:1022:LEU:HD13	1.76	0.49
4:S:374:VAL:HB	4:S:381:ILE:HB	1.94	0.49
5:R:429:ARG:O	5:R:433:ASN:ND2	2.46	0.49
14:H:93:TYR:HE1	14:H:145:ARG:HH11	1.59	0.49
20:O:130:PRO:HA	20:O:133:LEU:HB3	1.93	0.49
4:S:322:GLY:O	4:S:350:THR:OG1	2.25	0.49
8:B:419:GLU:O	8:B:423:ASN:ND2	2.44	0.49
8:B:534:PRO:HG3	8:B:542:LEU:HD23	1.94	0.49
8:B:1018:THR:OG1	8:B:1019:GLY:N	2.45	0.49
10:D:35:GLU:O	10:D:39:PHE:N	2.43	0.49
12:F:86:THR:N	12:F:89:GLU:OE1	2.45	0.49
4:S:420:GLU:HB2	4:S:442:LEU:O	2.12	0.49
8:B:318:PRO:O	8:B:321:GLN:NE2	2.45	0.49
11:E:93:MET:O	11:E:97:VAL:N	2.34	0.49
20:O:403:LEU:HD22	20:O:424:LEU:HD13	1.95	0.49
8:B:415:GLU:OE1	8:B:474:SER:OG	2.28	0.49
20:O:141:LYS:HA	20:O:179:PHE:HZ	1.77	0.49
7:A:1307:ASP:O	7:A:1499:ARG:NH1	2.46	0.49
8:B:1014:TYR:HD1	8:B:1022:LEU:N	2.09	0.49
14:H:106:GLU:HA	14:H:112:ILE:HA	1.94	0.49
17:K:69:ASP:N	17:K:69:ASP:OD1	2.43	0.49
3:Q:111:ILE:HG21	3:Q:195:ALA:HB1	1.95	0.49
3:Q:116:ILE:HA	3:Q:119:LEU:HD12	1.95	0.49
19:N:110:LEU:HD23	19:N:121:ILE:HG13	1.94	0.49
20:O:419:LYS:O	20:O:423:TYR:N	2.43	0.49
4:S:388:ASN:HB3	5:R:151:PRO:HB3	1.94	0.48
4:S:402:ILE:HA	4:S:418:SER:HB2	1.94	0.48
7:A:383:ASN:O	7:A:387:SER:N	2.44	0.48
7:A:1288:ARG:NH2	7:A:1290:TYR:OH	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:272:GLN:NE2	3:Q:275:GLU:OE1	2.46	0.48
4:S:273:ARG:HG2	4:S:275:GLU:HG3	1.95	0.48
7:A:843:ARG:NH2	8:B:988:GLU:OE2	2.46	0.48
4:S:408:ILE:HD11	4:S:415:LEU:HB2	1.94	0.48
16:J:24:LEU:HB3	16:J:35:ALA:HB1	1.95	0.48
7:A:747:ILE:HG22	7:A:774:GLY:HA2	1.96	0.48
7:A:1543:SER:OG	7:A:1544:ASN:N	2.46	0.48
19:N:163:VAL:HB	19:N:166:LEU:HD11	1.94	0.48
3:Q:321:ASP:OD2	3:Q:324:ARG:N	2.47	0.48
5:R:129:LYS:HE2	5:R:287:ASN:HD21	1.78	0.48
7:A:77:GLY:O	7:A:362:VAL:N	2.46	0.48
7:A:1270:VAL:HG11	7:A:1489:VAL:HG11	1.95	0.48
7:A:1634:LEU:HD13	7:A:1643:VAL:HG11	1.95	0.48
8:B:1011:GLU:O	8:B:1026:ILE:O	2.32	0.48
9:C:195:LYS:NZ	16:J:58:GLU:OE2	2.35	0.48
4:S:187:ILE:O	4:S:200:THR:OG1	2.26	0.48
8:B:698:SER:OG	8:B:699:ILE:N	2.44	0.48
8:B:782:ASP:N	8:B:782:ASP:OD1	2.47	0.48
8:B:931:TRP:HD1	8:B:936:MET:HE3	1.78	0.48
8:B:1103:VAL:HG22	8:B:1110:ILE:HG12	1.96	0.48
9:C:91:VAL:HG11	16:J:60:PHE:HB3	1.95	0.48
5:R:8:LEU:HD12	5:R:8:LEU:C	2.39	0.48
6:M:76:TYR:HD2	19:N:107:MET:HE1	1.79	0.48
7:A:15:ASP:OD2	8:B:1199:ASN:ND2	2.42	0.48
7:A:525:ASN:HB3	7:A:529:LYS:HB3	1.96	0.48
3:Q:227:TYR:HA	3:Q:230:ILE:HD12	1.96	0.48
6:M:45:LYS:HE2	6:M:47:GLU:HG2	1.96	0.48
7:A:584:ARG:NH1	12:F:116:ASP:OD1	2.47	0.48
10:D:91:ARG:HD3	20:O:184:PRO:HB3	1.96	0.48
3:Q:224:GLY:HA2	3:Q:227:TYR:HD2	1.79	0.48
3:Q:260:CYS:HB2	3:Q:338:LEU:HD21	1.95	0.48
3:Q:341:ARG:HH22	3:Q:369:TRP:HE1	1.62	0.48
4:S:402:ILE:HA	4:S:418:SER:CB	2.44	0.48
4:S:29:GLN:NE2	4:S:477:TYR:OH	2.32	0.47
5:R:223:ASN:HA	5:R:226:ARG:HB2	1.96	0.47
7:A:1162:ASN:HB2	7:A:1165:LYS:HG2	1.95	0.47
19:N:56:ILE:HD12	19:N:58:PHE:HE2	1.79	0.47
3:Q:446:TYR:HA	3:Q:449:GLN:HG2	1.96	0.47
8:B:19:LEU:HD12	16:J:25:LEU:HD12	1.96	0.47
8:B:882:ILE:HG12	8:B:903:ILE:HD11	1.95	0.47
4:S:357:LEU:HD11	5:R:24:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:597:LYS:HA	4:S:600:GLU:HB3	1.96	0.47
5:R:25:ASN:ND2	5:R:123:GLU:O	2.47	0.47
1:T:26:DA:N6	2:U:44:DG:O6	2.47	0.47
4:S:174:TRP:O	5:R:196:GLU:N	2.47	0.47
4:S:318:ILE:HD13	4:S:320:ILE:HG13	1.96	0.47
7:A:952:LEU:HD12	7:A:958:PRO:HD3	1.95	0.47
8:B:730:GLY:HA2	8:B:765:PHE:HE1	1.79	0.47
19:N:110:LEU:HD13	19:N:119:LEU:HD13	1.96	0.47
4:S:401:ASN:N	4:S:419:ARG:CG	2.77	0.47
4:S:215:ASN:HB3	4:S:235:SER:HA	1.97	0.47
4:S:461:HIS:HB2	4:S:482:SER:HB2	1.95	0.47
6:M:15:VAL:HA	6:M:90:LEU:HD12	1.97	0.47
10:D:24:ALA:HA	13:G:43:ILE:HG22	1.97	0.47
11:E:141:VAL:HG12	11:E:142:VAL:HG23	1.97	0.47
7:A:844:THR:O	7:A:848:LYS:N	2.38	0.47
7:A:1240:LEU:HB2	7:A:1519:LEU:HB2	1.97	0.47
8:B:468:GLY:HA2	8:B:485:THR:HG22	1.96	0.47
3:Q:422:GLU:OE2	5:R:260:ASN:ND2	2.48	0.47
4:S:64:LEU:HA	4:S:548:TYR:HA	1.97	0.47
8:B:824:HIS:ND1	8:B:897:GLU:OE1	2.45	0.47
15:I:8:ILE:O	15:I:17:LEU:N	2.44	0.47
4:S:704:LEU:HB3	4:S:706:GLU:HG2	1.97	0.47
5:R:138:PHE:CE2	5:R:297:PHE:HE2	2.33	0.47
7:A:885:ASP:OD1	7:A:886:ASN:N	2.48	0.47
7:A:1314:GLN:HE21	7:A:1318:SER:HB3	1.80	0.47
11:E:28:TYR:HA	11:E:64:PRO:HA	1.96	0.47
20:O:120:ILE:HG12	20:O:154:VAL:HG22	1.97	0.47
10:D:86:ILE:O	10:D:90:LYS:N	2.45	0.46
10:D:87:SER:O	10:D:91:ARG:N	2.48	0.46
3:Q:240:LYS:C	3:Q:241:GLU:CG	2.86	0.46
4:S:418:SER:OG	4:S:421:ILE:CG2	2.60	0.46
8:B:362:LEU:HD13	8:B:366:GLY:HA3	1.97	0.46
8:B:1015:SER:HG	8:B:1018:THR:HG23	1.80	0.46
4:S:505:PRO:HA	4:S:541:LEU:HA	1.97	0.46
6:M:76:TYR:C	6:M:77:VAL:CG2	2.88	0.46
10:D:81:ASN:O	10:D:82:LEU:CB	2.61	0.46
7:A:1162:ASN:HB2	7:A:1165:LYS:HE3	1.97	0.46
8:B:937:PRO:HB2	8:B:1014:TYR:O	2.15	0.46
8:B:48:SER:HB2	8:B:404:LEU:HD13	1.96	0.46
11:E:156:LEU:HD22	11:E:160:GLU:HG3	1.97	0.46
13:G:219:ASP:OD1	13:G:222:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:64:ASN:H	14:H:89:LEU:HB2	1.81	0.46
14:H:88:SER:OG	14:H:89:LEU:N	2.47	0.46
4:S:277:VAL:HG12	4:S:284:VAL:HA	1.96	0.46
7:A:1003:ARG:HD3	8:B:520:LEU:HB2	1.97	0.46
20:O:430:ARG:HH12	20:O:596:PRO:HD3	1.80	0.46
7:A:967:PRO:O	8:B:674:ILE:N	2.48	0.46
19:N:92:ASP:OD1	19:N:92:ASP:N	2.47	0.46
1:T:44:DC:O2	2:U:28:DG:N2	2.48	0.46
7:A:1148:LEU:HD22	7:A:1163:GLU:HG2	1.98	0.46
8:B:14:ALA:O	8:B:977:ILE:HB	2.16	0.46
8:B:21:ARG:HH12	16:J:54:VAL:HA	1.80	0.46
8:B:260:PHE:HB3	8:B:271:VAL:HG23	1.98	0.46
8:B:911:PRO:HA	8:B:1035:ARG:HH21	1.80	0.46
8:B:1015:SER:OG	8:B:1018:THR:HG23	2.15	0.46
9:C:51:GLU:HA	9:C:303:GLU:HA	1.98	0.46
9:C:213:GLY:HA2	9:C:219:PHE:HB2	1.98	0.46
14:H:125:LEU:HD13	14:H:130:ARG:HH12	1.80	0.46
17:K:46:LYS:HA	17:K:66:VAL:HG22	1.98	0.46
4:S:591:ALA:O	4:S:595:GLN:N	2.49	0.46
7:A:427:PHE:HA	7:A:430:ILE:HG22	1.98	0.46
7:A:579:ARG:NH1	7:A:585:ASP:OD2	2.44	0.46
8:B:656:LEU:HD22	19:N:153:VAL:HG11	1.98	0.46
8:B:773:VAL:N	8:B:1029:GLY:O	2.47	0.46
3:Q:308:SER:HB2	3:Q:501:CYS:SG	2.55	0.46
5:R:261:LEU:H	5:R:264:SER:HB2	1.80	0.46
7:A:480:ALA:O	7:A:635:MET:N	2.41	0.46
7:A:1003:ARG:HD3	8:B:520:LEU:HD22	1.98	0.46
7:A:1047:GLN:NE2	7:A:1587:ASP:OD2	2.42	0.46
7:A:1194:GLY:O	7:A:1197:SER:OG	2.26	0.46
7:A:1351:LEU:HA	8:B:225:ARG:HH22	1.80	0.46
8:B:553:THR:O	8:B:646:HIS:ND1	2.27	0.46
13:G:38:ILE:HG13	13:G:125:TRP:HD1	1.80	0.46
13:G:134:GLU:HG2	13:G:230:ARG:HA	1.97	0.46
17:K:49:LEU:HD21	17:K:54:THR:HG21	1.97	0.46
5:R:440:SER:O	5:R:443:TYR:CD2	2.69	0.45
6:M:75:GLN:C	6:M:76:TYR:O	2.58	0.45
7:A:669:LEU:HG	7:A:673:HIS:HB2	1.97	0.45
8:B:128:GLN:HB2	18:L:55:ILE:HD13	1.98	0.45
8:B:290:ASP:HA	8:B:293:ILE:HB	1.98	0.45
8:B:354:LEU:O	8:B:370:LYS:NZ	2.46	0.45
8:B:398:GLN:HG3	8:B:399:HIS:ND1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:76:TYR:HE2	19:N:107:MET:SD	2.39	0.45
7:A:103:LEU:O	7:A:106:HIS:NE2	2.50	0.45
8:B:72:VAL:HG12	8:B:96:SER:HA	1.98	0.45
8:B:98:SER:HB3	8:B:142:LYS:HB3	1.98	0.45
8:B:893:ASN:HD21	8:B:896:GLN:HG3	1.80	0.45
8:B:934:ILE:HD12	9:C:69:ARG:HD2	1.99	0.45
20:O:428:ILE:HG22	20:O:487:ARG:HD2	1.99	0.45
3:Q:482:HIS:O	3:Q:486:GLN:N	2.48	0.45
7:A:947:LEU:HD22	7:A:982:VAL:HG11	1.97	0.45
8:B:1026:ILE:N	8:B:1026:ILE:CD1	2.79	0.45
4:S:188:GLN:HB2	4:S:257:ARG:HD2	1.98	0.45
5:R:353:VAL:HG11	5:R:368:TYR:HB2	1.98	0.45
6:M:21:VAL:HG22	19:N:111:VAL:HA	1.97	0.45
7:A:550:SER:OG	7:A:551:VAL:N	2.48	0.45
7:A:686:PHE:HB3	7:A:725:LEU:HD13	1.98	0.45
15:I:101:LEU:HD23	15:I:102:ARG:HH12	1.82	0.45
20:O:238:ILE:HD12	20:O:378:THR:HG21	1.98	0.45
3:Q:120:ILE:HD11	3:Q:130:GLU:HB2	1.98	0.45
3:Q:161:THR:HA	3:Q:164:ILE:HG12	1.97	0.45
3:Q:481:THR:OG1	4:S:570:ASP:OD1	2.28	0.45
7:A:30:LYS:HE3	7:A:53:ALA:CB	2.44	0.45
8:B:682:GLN:H	8:B:686:HIS:HD2	1.64	0.45
3:Q:25:GLY:HA3	8:B:1051:PRO:HB3	1.99	0.45
8:B:941:THR:HB	8:B:943:ILE:HG13	1.98	0.45
8:B:1157:GLN:HB3	8:B:1169:GLY:H	1.81	0.45
9:C:151:THR:HB	9:C:156:LEU:HD22	1.97	0.45
5:R:294:VAL:H	5:R:298:GLN:HE21	1.65	0.45
6:M:13:GLU:HG3	6:M:89:GLN:HB3	1.99	0.45
7:A:878:ARG:NH1	15:I:66:VAL:O	2.50	0.45
7:A:1183:GLU:OE1	12:F:88:TYR:OH	2.32	0.45
8:B:480:GLN:HG3	8:B:507:SER:HB3	1.99	0.45
8:B:887:LEU:HD23	8:B:898:LEU:HD22	1.98	0.45
15:I:10:CYS:SG	15:I:11:LEU:N	2.90	0.45
4:S:271:ILE:HD12	4:S:329:ILE:HD11	1.98	0.45
4:S:302:VAL:HG11	4:S:362:ARG:HD2	1.99	0.45
4:S:350:THR:HB	5:R:156:LYS:HA	1.98	0.45
7:A:1635:ASP:OD1	7:A:1635:ASP:N	2.48	0.45
8:B:369:ASP:OD1	8:B:372:ARG:NH1	2.49	0.45
13:G:234:ARG:HG2	13:G:235:ASN:H	1.82	0.45
14:H:113:ALA:HA	14:H:126:GLU:HA	1.98	0.45
7:A:470:HIS:O	8:B:1058:GLN:NE2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:902:ALA:O	7:A:905:SER:OG	2.25	0.45
8:B:319:HIS:HA	8:B:321:GLN:HE22	1.82	0.45
11:E:47:CYS:HA	11:E:53:PRO:HA	1.99	0.45
7:A:1463:ASP:HB2	7:A:1469:TRP:CE2	2.52	0.45
8:B:1013:MET:SD	8:B:1026:ILE:HG21	2.56	0.45
8:B:1016:GLY:C	8:B:1018:THR:H	2.25	0.45
9:C:89:THR:HB	9:C:201:GLU:H	1.81	0.45
14:H:35:GLN:OE1	14:H:128:ASN:ND2	2.50	0.45
14:H:127:GLY:HA3	14:H:130:ARG:HE	1.81	0.45
20:O:493:ASP:OD1	20:O:497:ASN:N	2.50	0.45
20:O:532:ALA:HB1	20:O:538:ALA:H	1.82	0.45
5:R:268:LEU:HD11	5:R:316:SER:HB3	1.99	0.44
20:O:205:ARG:HG2	20:O:331:LYS:HG2	1.98	0.44
13:G:143:SER:OG	20:O:101:SER:O	2.35	0.44
20:O:426:SER:HB3	20:O:593:PRO:HD2	1.98	0.44
3:Q:421:ARG:HB3	3:Q:425:HIS:HB3	1.99	0.44
5:R:430:LEU:HA	5:R:433:ASN:HD22	1.83	0.44
6:M:76:TYR:CE2	19:N:107:MET:SD	3.11	0.44
8:B:132:SER:OG	8:B:462:GLN:NE2	2.51	0.44
8:B:921:HIS:NE2	8:B:965:GLU:OE1	2.43	0.44
11:E:117:THR:HG22	11:E:119:SER:H	1.81	0.44
8:B:14:ALA:HB1	8:B:978:ALA:HB3	1.99	0.44
9:C:151:THR:HG21	9:C:156:LEU:HD13	1.99	0.44
13:G:59:GLN:HE21	13:G:63:LYS:NZ	2.15	0.44
4:S:244:SER:HB3	4:S:264:ILE:HB	2.00	0.44
8:B:52:LEU:HA	8:B:60:LEU:HB2	2.00	0.44
9:C:86:PHE:HB3	18:L:62:LYS:HG3	2.00	0.44
17:K:74:ASN:OD1	17:K:77:ARG:NH2	2.51	0.44
19:N:59:PRO:HD2	19:N:139:VAL:HB	1.98	0.44
19:N:145:ILE:H	19:N:145:ILE:HG13	1.65	0.44
7:A:563:THR:HG22	20:O:375:THR:HG22	1.99	0.44
9:C:51:GLU:HB3	9:C:303:GLU:HG2	2.00	0.44
20:O:382:GLN:NE2	20:O:593:PRO:O	2.37	0.44
3:Q:445:ARG:O	3:Q:449:GLN:N	2.39	0.44
4:S:410:ASP:HB2	4:S:455:LYS:NZ	2.33	0.44
8:B:14:ALA:CA	8:B:977:ILE:HD13	2.47	0.44
8:B:956:SER:OG	8:B:957:ARG:NH1	2.50	0.44
9:C:136:LEU:HB2	9:C:167:LEU:HD23	2.00	0.44
3:Q:376:GLU:O	3:Q:380:TRP:N	2.51	0.44
4:S:440:HIS:ND1	4:S:441:ASP:O	2.36	0.44
5:R:181:THR:H	5:R:184:ASN:HD22	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:467:PHE:HE2	7:A:1614:SER:HB3	1.82	0.44
7:A:603:HIS:CE1	7:A:653:THR:HG21	2.53	0.44
8:B:234:ILE:HG12	8:B:381:LEU:HD13	1.99	0.44
14:H:59:ILE:HG12	14:H:142:LEU:HD12	1.99	0.44
20:O:461:VAL:HG13	20:O:467:MET:HE1	2.00	0.44
3:Q:258:MET:HE2	3:Q:438:PHE:HE2	1.83	0.44
4:S:733:THR:HA	4:S:736:ILE:HD12	1.99	0.44
7:A:1635:ASP:HA	7:A:1640:ARG:HE	1.83	0.44
7:A:554:ARG:O	7:A:558:ALA:N	2.41	0.43
8:B:657:PRO:HG3	19:N:148:ILE:HG23	1.99	0.43
8:B:1000:LEU:HA	8:B:1005:TYR:HD2	1.82	0.43
9:C:252:PRO:HG2	9:C:273:ASP:HA	1.99	0.43
5:R:316:SER:O	5:R:320:CYS:N	2.51	0.43
6:M:76:TYR:CD2	6:M:95:VAL:CG2	3.01	0.43
8:B:19:LEU:HD23	8:B:19:LEU:HA	1.87	0.43
4:S:352:PHE:HB3	5:R:157:MET:HG3	2.00	0.43
7:A:985:ARG:HH11	7:A:987:TYR:HD2	1.66	0.43
8:B:939:SER:HA	8:B:1013:MET:HA	2.00	0.43
8:B:1014:TYR:CE2	9:C:293:ARG:NH2	2.80	0.43
8:B:766:PRO:HD2	16:J:56:LEU:HD11	2.01	0.43
9:C:88:ASN:O	18:L:60:ARG:NH1	2.51	0.43
3:Q:469:PRO:HB2	3:Q:472:ARG:HB3	2.00	0.43
4:S:535:VAL:HG12	4:S:552:LEU:HB2	2.00	0.43
4:S:537:PHE:HE1	4:S:552:LEU:HG	1.83	0.43
4:S:662:LEU:HD11	4:S:666:SER:HB3	2.00	0.43
8:B:16:PHE:CE1	8:B:976:GLY:HA3	2.53	0.43
12:F:93:ILE:HG23	12:F:132:LEU:HD12	2.00	0.43
7:A:539:GLU:HB3	7:A:570:THR:HB	2.01	0.43
7:A:1230:SER:HB3	7:A:1233:ILE:HG13	2.01	0.43
8:B:725:THR:HA	8:B:1036:LEU:HA	2.00	0.43
11:E:76:GLY:N	11:E:106:GLN:OE1	2.40	0.43
11:E:90:VAL:HG23	11:E:120:ALA:HA	2.01	0.43
20:O:82:SER:HA	20:O:87:ARG:HH11	1.84	0.43
3:Q:195:ALA:HA	3:Q:199:LEU:HD23	2.00	0.43
4:S:40:PRO:HA	4:S:45:PRO:HB3	2.00	0.43
8:B:143:TRP:HB3	8:B:152:LEU:HB2	2.01	0.43
8:B:285:ASP:HB2	15:I:15:ASP:HA	2.00	0.43
8:B:1097:ASP:OD1	8:B:1097:ASP:N	2.52	0.43
9:C:266:TYR:OH	9:C:268:LYS:NZ	2.46	0.43
10:D:43:PHE:HE2	10:D:89:LEU:HD22	1.83	0.43
4:S:630:LEU:HD11	4:S:662:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:208:TYR:O	5:R:212:HIS:ND1	2.47	0.43
7:A:119:ALA:HB2	7:A:334:VAL:HG23	2.01	0.43
8:B:734:CYS:SG	8:B:735:HIS:ND1	2.81	0.43
9:C:197:ARG:HA	9:C:197:ARG:HD3	1.81	0.43
4:S:425:GLY:HA2	4:S:437:SER:HB2	1.99	0.43
4:S:536:ASP:OD1	4:S:536:ASP:N	2.51	0.43
7:A:368:ARG:HH11	7:A:383:ASN:HD21	1.66	0.43
7:A:882:ILE:O	7:A:889:SER:OG	2.32	0.43
8:B:1123:ILE:HD11	13:G:241:ARG:HH11	1.83	0.43
8:B:1132:SER:HB3	8:B:1170:GLY:HA3	2.01	0.43
11:E:66:GLU:HG2	11:E:69:ILE:HD12	2.01	0.43
13:G:237:HIS:HB2	13:G:244:SER:HB3	2.01	0.43
15:I:13:CYS:HB3	15:I:33:CYS:H	1.84	0.43
4:S:20:VAL:HG12	4:S:25:LEU:HD13	2.00	0.43
4:S:400:SER:HA	4:S:419:ARG:HB3	2.00	0.43
7:A:581:ILE:HD11	7:A:605:VAL:HG21	2.01	0.43
7:A:882:ILE:HD12	7:A:892:LEU:HD22	2.00	0.43
9:C:41:GLU:HB2	9:C:57:ILE:HD13	2.00	0.43
17:K:88:PHE:HB3	17:K:106:GLN:HB2	1.99	0.43
20:O:59:ALA:HB1	20:O:71:ILE:HD13	2.00	0.43
7:A:510:PRO:HG2	12:F:102:SER:HB2	2.01	0.42
7:A:552:GLU:O	20:O:246:ASN:ND2	2.49	0.42
8:B:995:TYR:CZ	19:N:160:VAL:HG23	2.54	0.42
8:B:1013:MET:CB	8:B:1026:ILE:HG21	2.48	0.42
9:C:252:PRO:HA	9:C:253:PRO:HD3	1.86	0.42
13:G:159:LYS:HA	13:G:162:ILE:HD12	2.00	0.42
4:S:366:PHE:HD1	4:S:373:LEU:HD11	1.84	0.42
4:S:686:TYR:HB2	4:S:693:PHE:HE2	1.83	0.42
7:A:205:ARG:HD2	7:A:1631:ARG:HH12	1.84	0.42
7:A:230:ARG:NH2	7:A:234:ASP:OD2	2.53	0.42
8:B:412:ILE:HD12	8:B:470:LEU:HD12	2.01	0.42
12:F:55:PRO:HB2	12:F:56:GLU:H	1.68	0.42
4:S:212:SER:HA	4:S:242:ILE:HG12	2.01	0.42
7:A:969:PHE:O	8:B:673:ASN:ND2	2.52	0.42
7:A:1003:ARG:HH22	8:B:543:ASN:HB3	1.84	0.42
9:C:275:VAL:HG21	9:C:293:ARG:HH21	1.84	0.42
13:G:137:ILE:H	13:G:227:GLY:HA2	1.83	0.42
20:O:109:SER:O	20:O:113:THR:OG1	2.31	0.42
20:O:126:TRP:CD1	20:O:127:GLU:HG3	2.54	0.42
7:A:368:ARG:NH1	7:A:383:ASN:HD21	2.18	0.42
7:A:475:ARG:NH1	8:B:1068:GLY:O	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:23:ASN:O	16:J:28:ASP:N	2.50	0.42
8:B:307:GLU:HG2	15:I:7:LEU:HD11	2.02	0.42
9:C:145:ASP:OD1	9:C:146:ALA:N	2.51	0.42
11:E:79:TRP:NE1	11:E:81:GLU:OE1	2.28	0.42
15:I:13:CYS:HB2	15:I:32:GLN:HB2	2.00	0.42
3:Q:135:ILE:HA	3:Q:138:LEU:HB2	2.01	0.42
3:Q:470:PRO:HA	3:Q:473:LYS:HG2	2.01	0.42
5:R:24:ILE:HA	5:R:27:ILE:HG22	2.02	0.42
5:R:183:GLU:HA	5:R:186:LEU:HB2	2.01	0.42
7:A:334:VAL:HG13	7:A:335:LEU:HG	2.01	0.42
7:A:883:LEU:HD11	7:A:959:VAL:HG11	2.00	0.42
8:B:929:ARG:HH21	17:K:96:PRO:HB2	1.85	0.42
8:B:931:TRP:NE1	8:B:935:ASP:O	2.50	0.42
11:E:64:PRO:HB2	11:E:69:ILE:HD11	2.01	0.42
4:S:420:GLU:CA	4:S:442:LEU:HB3	2.45	0.42
8:B:572:PRO:O	8:B:576:THR:OG1	2.35	0.42
5:R:164:LYS:HB2	5:R:167:LYS:HE3	2.02	0.42
6:M:40:LEU:HB3	19:N:117:GLU:HG3	2.02	0.42
7:A:975:ASP:OD1	7:A:976:ALA:N	2.53	0.42
7:A:1121:ASP:OD1	7:A:1121:ASP:N	2.52	0.42
8:B:987:ASN:H	8:B:990:ASP:HB3	1.84	0.42
4:S:174:TRP:N	5:R:196:GLU:O	2.46	0.42
4:S:271:ILE:HB	4:S:289:SER:HB3	2.01	0.42
7:A:1197:SER:HA	7:A:1200:MET:HE3	2.02	0.42
9:C:115:TRP:O	9:C:130:ASN:ND2	2.53	0.42
9:C:115:TRP:HH2	9:C:212:ILE:HG23	1.84	0.42
3:Q:172:LEU:HB3	3:Q:174:LEU:HG	2.00	0.42
3:Q:257:VAL:HG22	3:Q:262:LEU:HD11	2.01	0.42
7:A:621:THR:OG1	7:A:626:ALA:O	2.35	0.42
7:A:720:PHE:HE2	14:H:141:TYR:HE1	1.67	0.42
20:O:407:SER:HB2	20:O:421:LEU:HG	2.02	0.42
2:U:42:DA:H2'	2:U:43:DG:C8	2.55	0.41
7:A:417:ARG:HG3	7:A:419:ILE:H	1.84	0.41
7:A:897:SER:HA	7:A:900:VAL:HG22	2.02	0.41
8:B:14:ALA:CB	8:B:977:ILE:HD13	2.47	0.41
8:B:338:PHE:HZ	8:B:357:ILE:HD11	1.85	0.41
8:B:937:PRO:CB	8:B:1014:TYR:O	2.67	0.41
13:G:241:ARG:HE	20:O:189:PHE:HB3	1.85	0.41
20:O:116:ILE:HG23	20:O:143:LEU:HD21	2.01	0.41
4:S:347:LEU:HD11	4:S:385:PHE:HD2	1.85	0.41
7:A:31:GLN:HB3	7:A:78:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:95:TYR:CZ	7:A:99:ARG:HD2	2.55	0.41
8:B:561:ILE:HA	8:B:564:ILE:HD12	2.01	0.41
20:O:382:GLN:HB2	20:O:423:TYR:OH	2.20	0.41
20:O:435:SER:HB3	20:O:438:GLN:HG3	2.01	0.41
4:S:406:LYS:HE2	4:S:453:VAL:H	1.85	0.41
7:A:589:MET:HE2	7:A:589:MET:HB2	1.93	0.41
7:A:676:ALA:HB2	7:A:821:ILE:HD11	2.02	0.41
8:B:134:ARG:HA	8:B:162:PRO:HA	2.01	0.41
8:B:547:HIS:N	8:B:697:LEU:O	2.53	0.41
15:I:61:ARG:HA	15:I:64:LYS:HB2	2.02	0.41
7:A:98:LEU:O	7:A:101:SER:OG	2.32	0.41
8:B:682:GLN:H	8:B:686:HIS:CD2	2.38	0.41
8:B:703:LEU:HD22	8:B:757:TYR:HD1	1.86	0.41
20:O:238:ILE:HD11	20:O:381:ILE:HG12	2.02	0.41
20:O:333:ASP:O	20:O:337:THR:OG1	2.34	0.41
20:O:597:LEU:HD11	20:O:599:LEU:HB2	2.02	0.41
3:Q:198:ILE:HG13	3:Q:199:LEU:HD22	2.03	0.41
5:R:31:PHE:HA	5:R:34:ILE:HB	2.01	0.41
5:R:158:THR:OG1	5:R:159:TYR:N	2.52	0.41
5:R:210:THR:HA	5:R:213:ILE:HD12	2.03	0.41
5:R:270:PHE:HD2	5:R:271:LEU:HD12	1.85	0.41
7:A:482:SER:OG	7:A:483:VAL:N	2.52	0.41
7:A:487:ASP:OD2	17:K:95:HIS:NE2	2.38	0.41
8:B:714:ARG:HA	8:B:714:ARG:HD3	1.85	0.41
9:C:132:ILE:HB	9:C:208:CYS:HB2	2.03	0.41
9:C:277:ARG:HG2	9:C:291:LEU:HD22	2.01	0.41
10:D:82:LEU:HD12	10:D:85:SER:HB2	2.02	0.41
1:T:27:DC:H42	8:B:430:MET:HE2	1.86	0.41
3:Q:483:ILE:HD12	3:Q:486:GLN:HB3	2.02	0.41
4:S:223:ASN:OD1	4:S:224:THR:N	2.54	0.41
7:A:1035:ASP:N	7:A:1035:ASP:OD1	2.52	0.41
7:A:1097:TYR:HD2	7:A:1123:VAL:HG23	1.85	0.41
7:A:1290:TYR:O	7:A:1474:LEU:N	2.54	0.41
8:B:678:PRO:HA	8:B:681:ILE:HG13	2.02	0.41
8:B:832:TRP:CD1	8:B:834:LYS:HA	2.56	0.41
8:B:1025:ASP:O	8:B:1026:ILE:HB	2.20	0.41
4:S:182:LEU:HD21	4:S:507:GLY:HA3	2.01	0.41
7:A:561:LEU:HD23	7:A:561:LEU:HA	1.94	0.41
7:A:748:ASN:N	7:A:1072:ASN:HD21	2.18	0.41
9:C:77:SER:OG	9:C:78:VAL:N	2.53	0.41
3:Q:42:ASN:HD21	8:B:1065:ARG:NH2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:356:GLU:OE1	4:S:361:LYS:NZ	2.54	0.41
4:S:638:LEU:HD21	4:S:691:VAL:HB	2.03	0.41
4:S:757:GLN:HA	4:S:760:ILE:HG12	2.02	0.41
5:R:251:TRP:HZ2	5:R:297:PHE:HB3	1.86	0.41
7:A:1246:VAL:O	7:A:1517:ARG:NH1	2.47	0.41
8:B:648:ARG:HH12	8:B:650:LEU:HD21	1.86	0.41
13:G:241:ARG:HH21	20:O:189:PHE:HB2	1.86	0.41
19:N:110:LEU:HB3	19:N:119:LEU:HB3	2.01	0.41
20:O:129:PRO:HA	20:O:130:PRO:HD3	1.91	0.41
4:S:268:SER:HB2	4:S:291:PRO:HB2	2.02	0.41
4:S:401:ASN:CB	4:S:419:ARG:HG3	2.43	0.41
8:B:906:ARG:HH11	8:B:906:ARG:HD3	1.77	0.41
8:B:1026:ILE:N	8:B:1026:ILE:HD12	2.36	0.41
9:C:315:PHE:HB3	9:C:319:ARG:HH22	1.85	0.41
18:L:48:CYS:HB3	18:L:53:HIS:H	1.86	0.41
3:Q:327:PRO:HG2	3:Q:330:TRP:HB2	2.03	0.40
8:B:335:ARG:NH2	8:B:344:GLN:O	2.38	0.40
9:C:222:VAL:HG21	9:C:225:ALA:HB2	2.03	0.40
5:R:305:THR:OG1	5:R:306:ALA:N	2.54	0.40
7:A:855:ARG:NH2	7:A:867:ASP:HB3	2.37	0.40
2:U:38:DT:H6	2:U:38:DT:H2'	1.73	0.40
3:Q:358:PRO:HG3	5:R:204:GLU:HA	2.03	0.40
4:S:24:SER:HB2	4:S:439:LYS:HE3	2.04	0.40
4:S:403:ARG:HD3	4:S:403:ARG:HA	1.83	0.40
7:A:360:LEU:HD11	7:A:434:VAL:HG23	2.04	0.40
7:A:641:GLU:HB2	12:F:99:LEU:HD13	2.02	0.40
7:A:1657:LEU:HG	13:G:106:LYS:HA	2.02	0.40
7:A:1657:LEU:HD11	13:G:106:LYS:HE2	2.03	0.40
13:G:90:LEU:HD11	13:G:119:HIS:CE1	2.57	0.40
13:G:142:ALA:O	13:G:159:LYS:NZ	2.42	0.40
19:N:110:LEU:HD22	19:N:119:LEU:HB3	2.02	0.40
20:O:97:LEU:HD21	20:O:139:PHE:HB2	2.03	0.40
3:Q:43:ASP:OD1	3:Q:43:ASP:N	2.55	0.40
3:Q:360:LYS:HE2	3:Q:489:VAL:HA	2.04	0.40
4:S:410:ASP:HB2	4:S:455:LYS:HZ2	1.86	0.40
4:S:456:VAL:HG12	4:S:458:LYS:HG3	2.02	0.40
4:S:536:ASP:HA	4:S:551:ALA:HA	2.02	0.40
7:A:112:SER:O	7:A:182:LYS:NZ	2.43	0.40
7:A:755:ILE:HG21	7:A:760:TRP:HE1	1.86	0.40
7:A:780:ILE:H	7:A:780:ILE:HG13	1.49	0.40
8:B:244:THR:HA	8:B:411:MET:HE3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:974:LEU:CB	8:B:975:HIS:CD2	3.00	0.40
9:C:229:LEU:HD12	9:C:229:LEU:HA	1.87	0.40
16:J:16:ASP:OD1	16:J:17:LYS:N	2.54	0.40
20:O:204:THR:HG23	20:O:207:LYS:H	1.86	0.40
4:S:428:GLU:HG2	4:S:430:ASN:H	1.87	0.40
7:A:230:ARG:HA	7:A:230:ARG:HD2	1.82	0.40
7:A:1050:TYR:HB3	7:A:1054:ALA:HA	2.02	0.40
12:F:76:LYS:HD3	12:F:79:ARG:HD3	2.02	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	
3	Q	434/514 (84%)	375 (86%)	58 (13%)	1 (0%)	43	72
4	S	594/894 (66%)	509 (86%)	83 (14%)	2 (0%)	36	65
5	R	322/507 (64%)	274 (85%)	48 (15%)	0	100	100
6	M	105/415 (25%)	84 (80%)	20 (19%)	1 (1%)	12	43
7	A	1500/1664 (90%)	1372 (92%)	127 (8%)	1 (0%)	48	78
8	B	1174/1203 (98%)	1046 (89%)	126 (11%)	2 (0%)	43	72
9	C	300/335 (90%)	279 (93%)	21 (7%)	0	100	100
10	D	66/137 (48%)	61 (92%)	5 (8%)	0	100	100
11	E	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
12	F	98/155 (63%)	92 (94%)	6 (6%)	0	100	100
13	G	193/326 (59%)	170 (88%)	23 (12%)	0	100	100
14	H	130/146 (89%)	120 (92%)	10 (8%)	0	100	100
15	I	122/125 (98%)	103 (84%)	19 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	J	67/70 (96%)	51 (76%)	16 (24%)	0	100	100
17	K	101/142 (71%)	98 (97%)	3 (3%)	0	100	100
18	L	43/70 (61%)	38 (88%)	5 (12%)	0	100	100
19	N	131/233 (56%)	105 (80%)	24 (18%)	2 (2%)	8	36
20	O	456/627 (73%)	424 (93%)	32 (7%)	0	100	100
All	All	6049/7778 (78%)	5403 (89%)	637 (10%)	9 (0%)	49	78

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	76	TYR
7	A	669	LEU
4	S	418	SER
8	B	1017	ALA
19	N	163	VAL
19	N	164	GLU
3	Q	247	ILE
4	S	420	GLU
8	B	1026	ILE

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	Q	407/476 (86%)	407 (100%)	0	100	100
4	S	563/828 (68%)	558 (99%)	5 (1%)	70	75
5	R	313/474 (66%)	309 (99%)	4 (1%)	61	71
6	M	97/371 (26%)	96 (99%)	1 (1%)	68	74
7	A	1297/1465 (88%)	1289 (99%)	8 (1%)	78	79
8	B	1030/1053 (98%)	1023 (99%)	7 (1%)	76	77
9	C	269/296 (91%)	268 (100%)	1 (0%)	84	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	D	65/116 (56%)	65 (100%)	0	100	100
11	E	197/197 (100%)	196 (100%)	1 (0%)	81	80
12	F	90/137 (66%)	90 (100%)	0	100	100
13	G	177/291 (61%)	177 (100%)	0	100	100
14	H	116/128 (91%)	116 (100%)	0	100	100
15	I	109/110 (99%)	109 (100%)	0	100	100
16	J	64/65 (98%)	63 (98%)	1 (2%)	55	68
17	K	93/130 (72%)	93 (100%)	0	100	100
18	L	40/57 (70%)	40 (100%)	0	100	100
19	N	128/220 (58%)	125 (98%)	3 (2%)	44	62
20	O	427/576 (74%)	426 (100%)	1 (0%)	87	86
All	All	5482/6990 (78%)	5450 (99%)	32 (1%)	76	79

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	S	318	ILE
4	S	363	ILE
4	S	419	ARG
4	S	420	GLU
4	S	744	LEU
5	R	144	VAL
5	R	178	LEU
5	R	186	LEU
5	R	253	ILE
6	M	76	TYR
7	A	261	ILE
7	A	462	LYS
7	A	669	LEU
7	A	756	LYS
7	A	780	ILE
7	A	827	THR
7	A	1271	ILE
7	A	1497	ILE
8	B	85	ILE
8	B	217	ILE
8	B	561	ILE
8	B	975	HIS

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Mol	Chain	Res	Type
8	B	977	ILE
8	B	1025	ASP
8	B	1026	ILE
9	C	324	LYS
11	E	200	ARG
16	J	20	SER
19	N	145	ILE
19	N	154	ARG
19	N	160	VAL
20	O	201	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
3	Q	14	ASN
3	Q	42	ASN
3	Q	149	GLN
3	Q	228	ASN
3	Q	514	ASN
4	S	37	GLN
4	S	180	ASN
4	S	230	HIS
4	S	461	HIS
4	S	479	HIS
4	S	483	HIS
4	S	554	ASN
4	S	579	ASN
4	S	580	ASN
4	S	613	HIS
4	S	642	GLN
4	S	665	ASN
4	S	684	GLN
5	R	25	ASN
5	R	179	HIS
5	R	184	ASN
5	R	207	ASN
5	R	223	ASN
5	R	260	ASN
5	R	287	ASN
5	R	304	HIS
5	R	433	ASN
6	M	54	HIS

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Mol	Chain	Res	Type
6	M	71	GLN
7	A	93	GLN
7	A	179	ASN
7	A	332	GLN
7	A	431	GLN
7	A	432	ASN
7	A	470	HIS
7	A	489	ASN
7	A	537	GLN
7	A	592	GLN
7	A	596	HIS
7	A	636	HIS
7	A	656	GLN
7	A	671	GLN
7	A	694	GLN
7	A	706	HIS
7	A	748	ASN
7	A	753	ASN
7	A	785	GLN
7	A	819	ASN
7	A	880	GLN
7	A	1062	HIS
7	A	1072	ASN
7	A	1108	HIS
7	A	1250	GLN
7	A	1314	GLN
7	A	1447	GLN
8	B	62	ASN
8	B	128	GLN
8	B	168	ASN
8	B	212	ASN
8	B	213	HIS
8	B	351	GLN
8	B	422	GLN
8	B	423	ASN
8	B	439	ASN
8	B	462	GLN
8	B	532	HIS
8	B	575	HIS
8	B	598	HIS
8	B	673	ASN
8	B	702	ASN

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Mol	Chain	Res	Type
8	B	710	ASN
8	B	715	ASN
8	B	764	ASN
8	B	912	GLN
8	B	923	GLN
8	B	1045	GLN
8	B	1066	HIS
8	B	1094	ASN
9	C	99	HIS
9	C	130	ASN
9	C	216	HIS
9	C	248	GLN
9	C	323	ASN
10	D	93	GLN
11	E	54	GLN
11	E	61	GLN
11	E	99	HIS
11	E	147	HIS
13	G	26	ASN
13	G	56	ASN
13	G	59	GLN
13	G	67	ASN
13	G	75	ASN
13	G	119	HIS
13	G	150	HIS
13	G	216	HIS
15	I	32	GLN
15	I	41	GLN
15	I	91	ASN
15	I	95	ASN
16	J	23	ASN
16	J	53	HIS
17	K	64	GLN
17	K	106	GLN
20	O	66	ASN
20	O	94	ASN
20	O	103	ASN
20	O	168	GLN
20	O	362	ASN
20	O	390	GLN
20	O	438	GLN
20	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

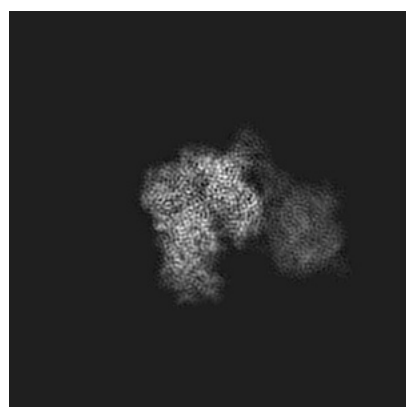
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4982. These allow visual inspection of the internal detail of the map and identification of artifacts.

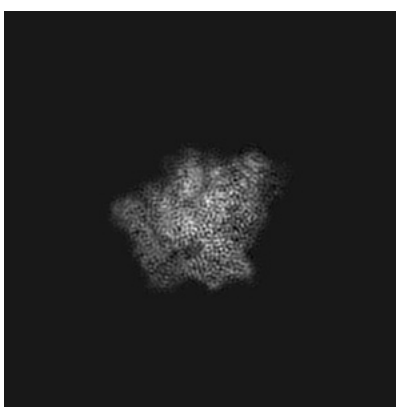
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

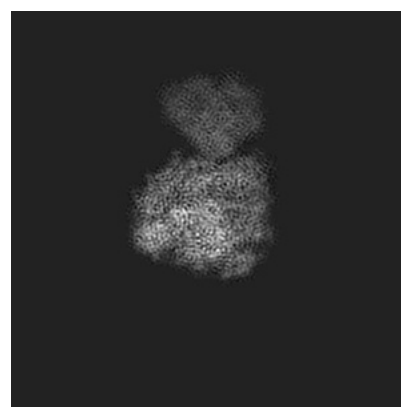
6.1.1 Primary map



X



Y

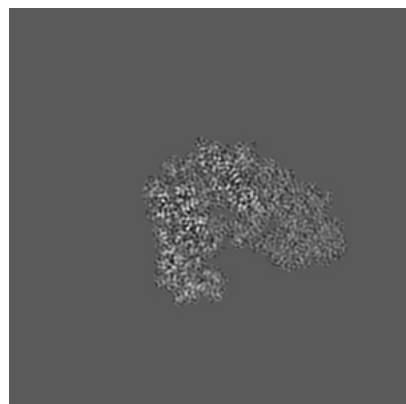


Z

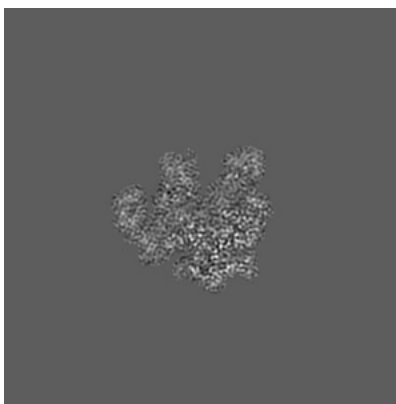
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

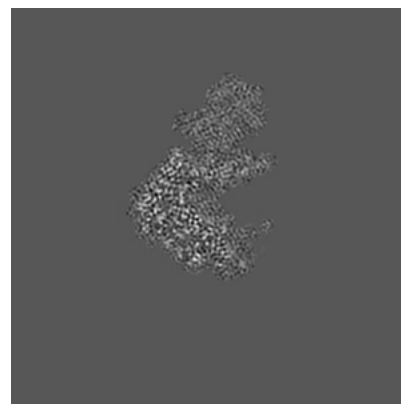
6.2.1 Primary map



X Index: 190



Y Index: 190

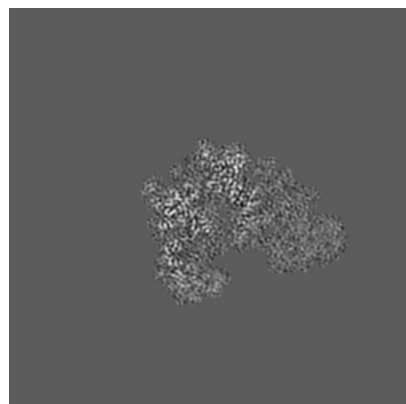


Z Index: 190

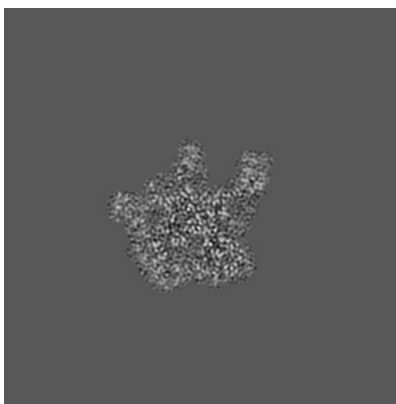
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 183



Y Index: 168

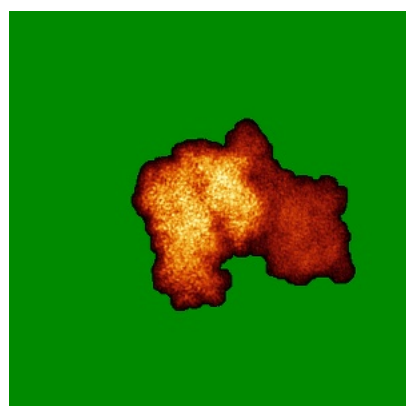


Z Index: 202

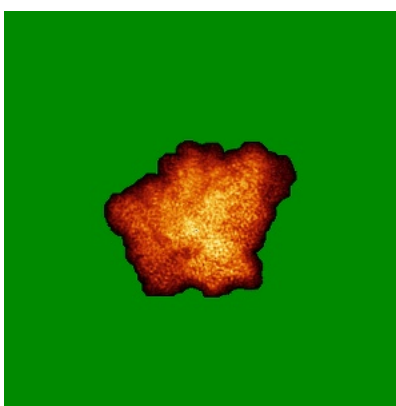
The images above show the largest variance slices of the map in three orthogonal directions.

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

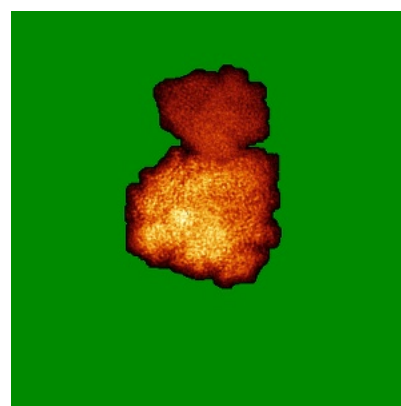
6.4.1 Primary map



X



Y

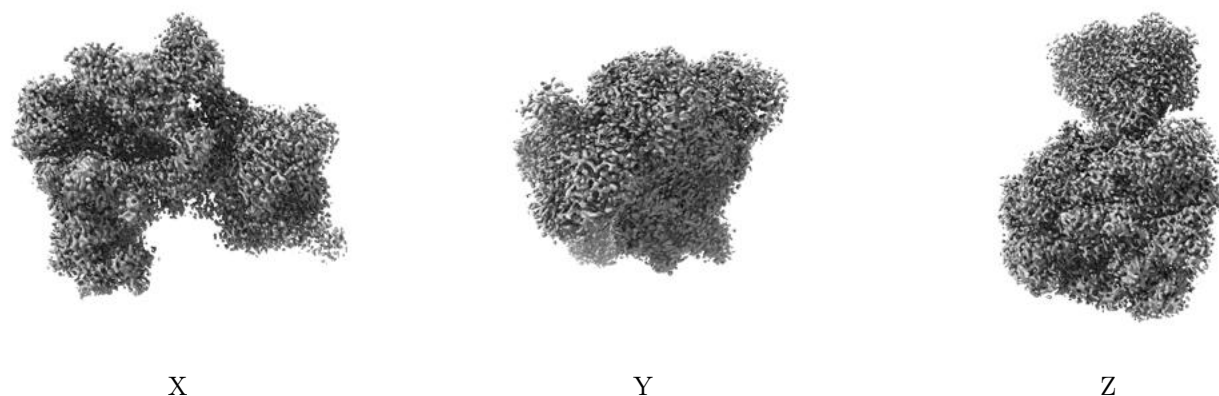


Z

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

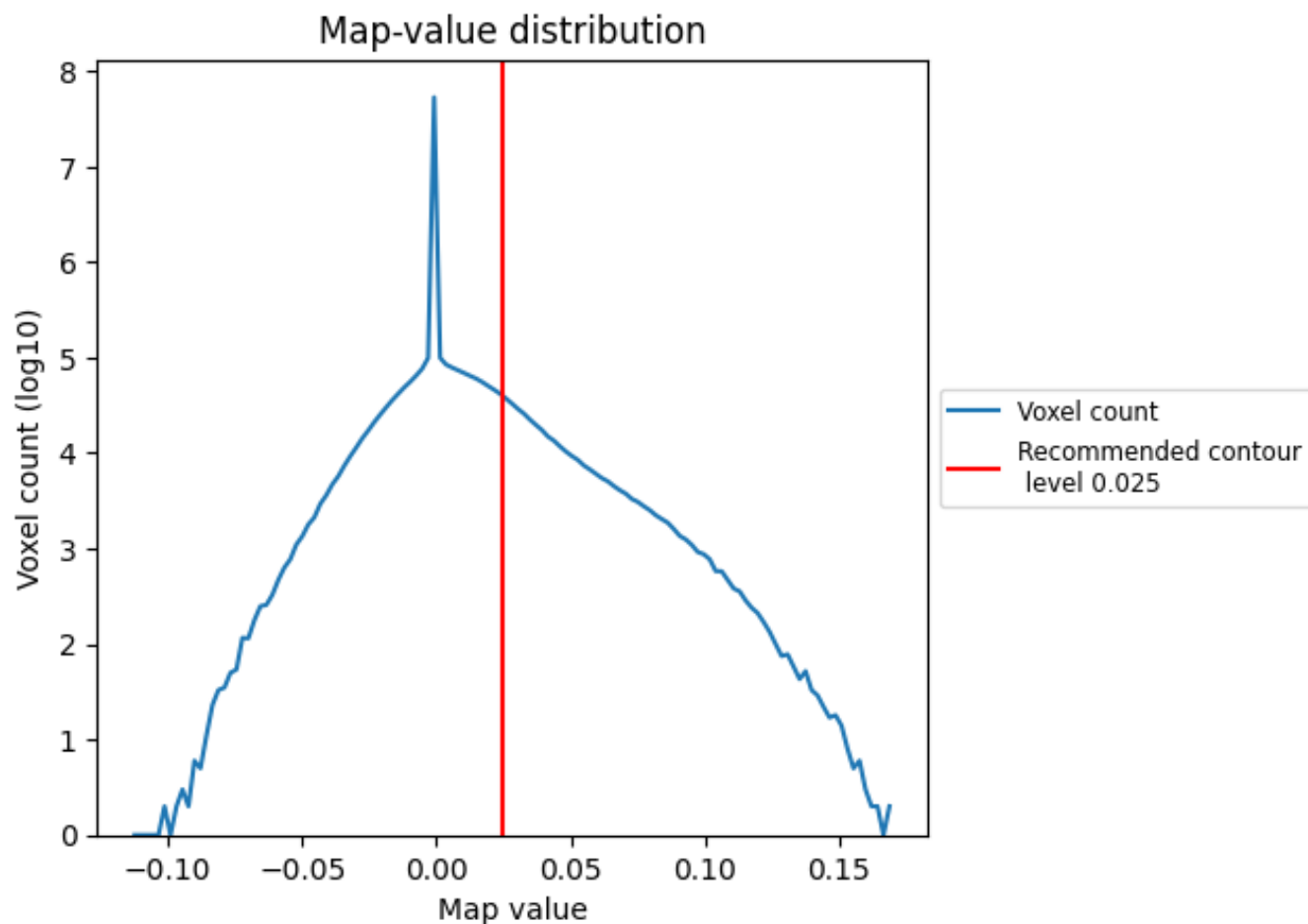
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

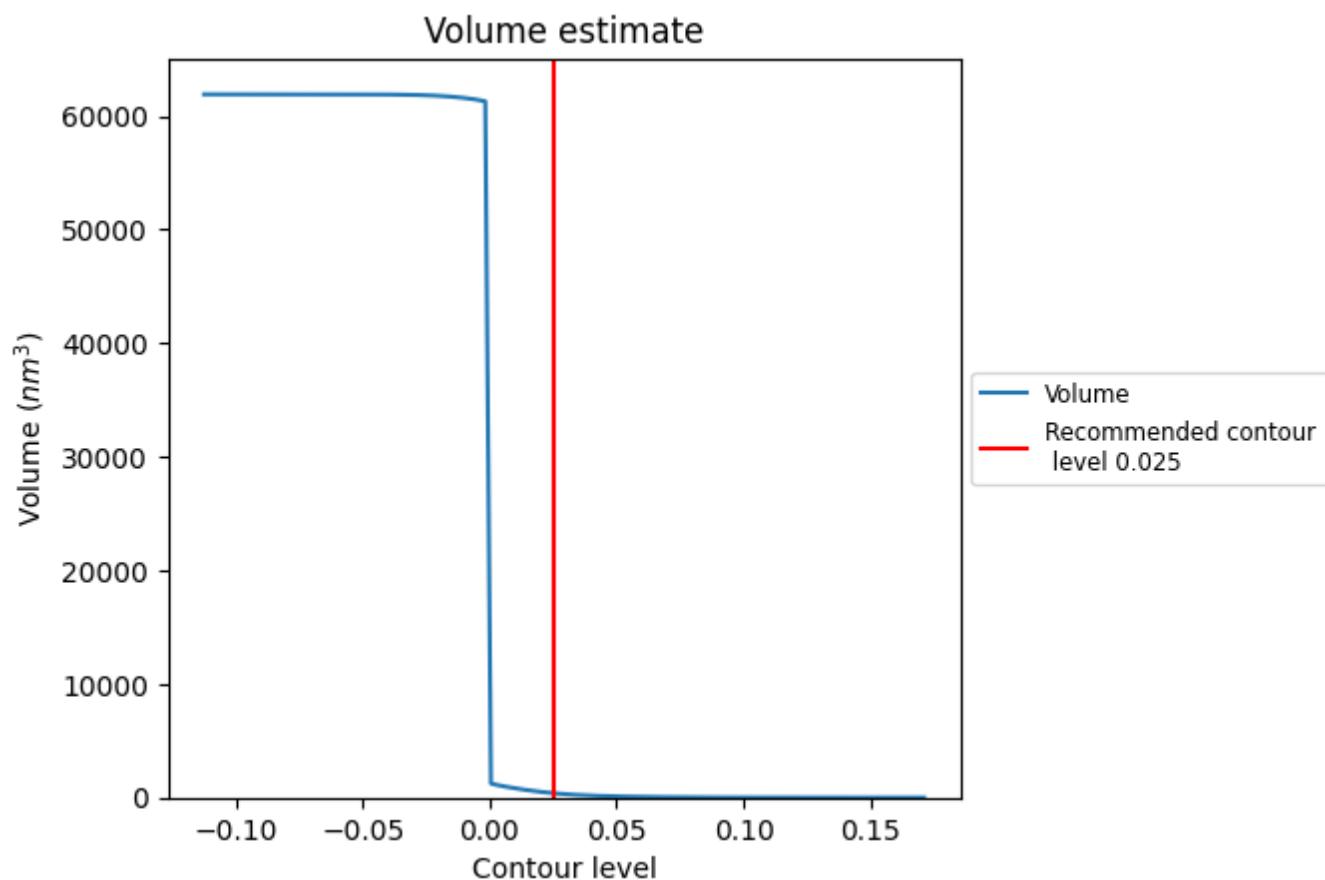
This section contains the results of statistical analysis of the map.

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.

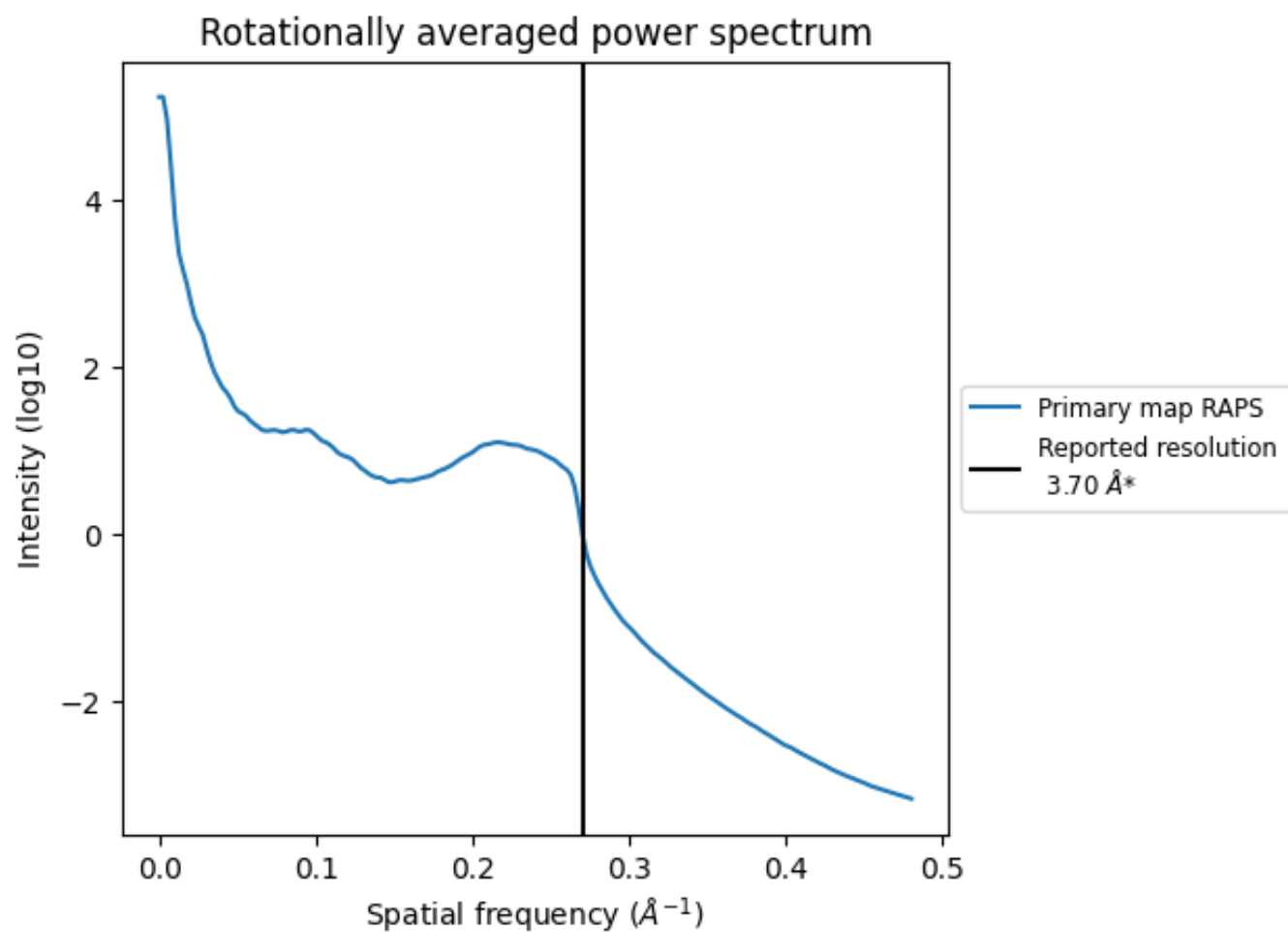
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 387 nm³; this corresponds to an approximate mass of 350 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 0.270 Å⁻¹

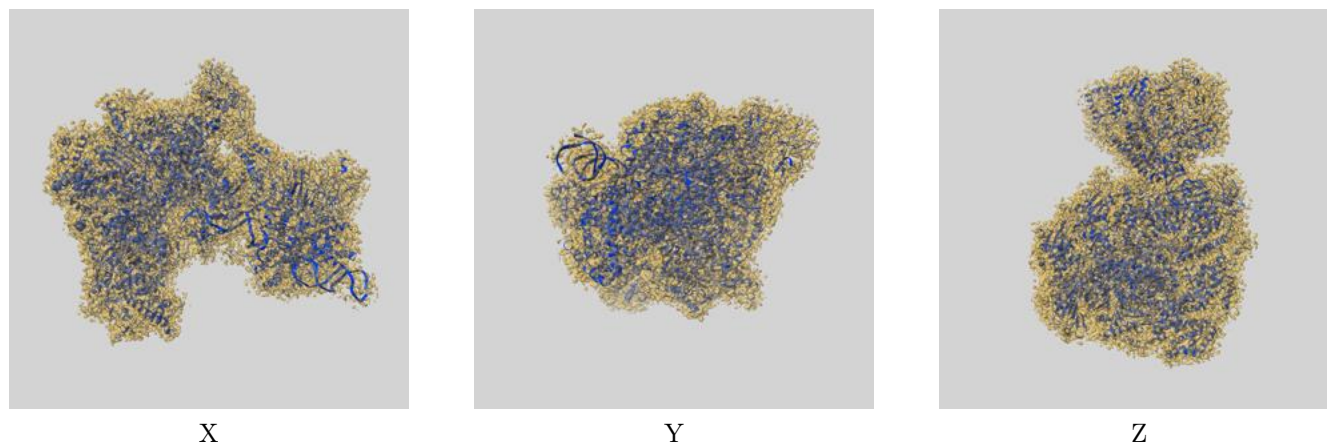
8 Fourier-Shell correlation ⓘ

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-4982 and PDB model 6RQH. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



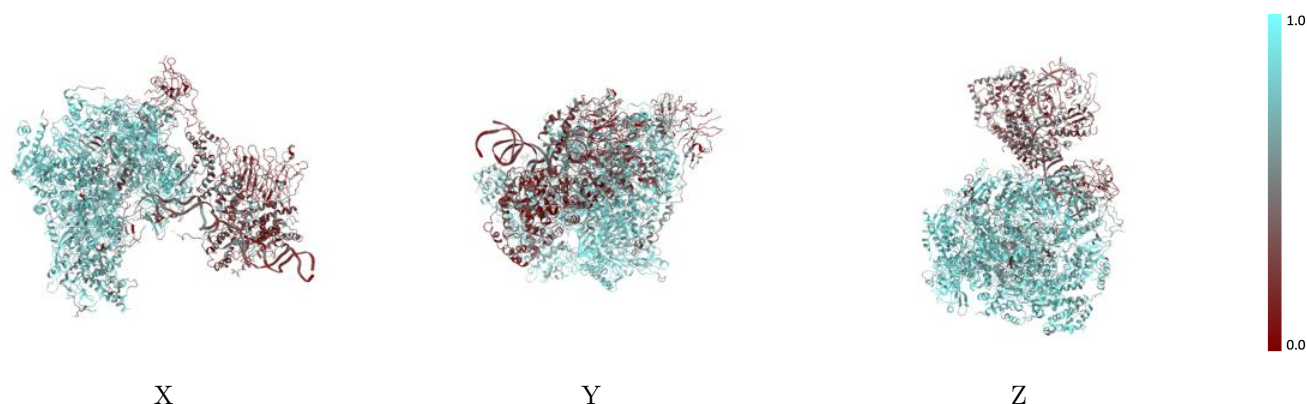
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



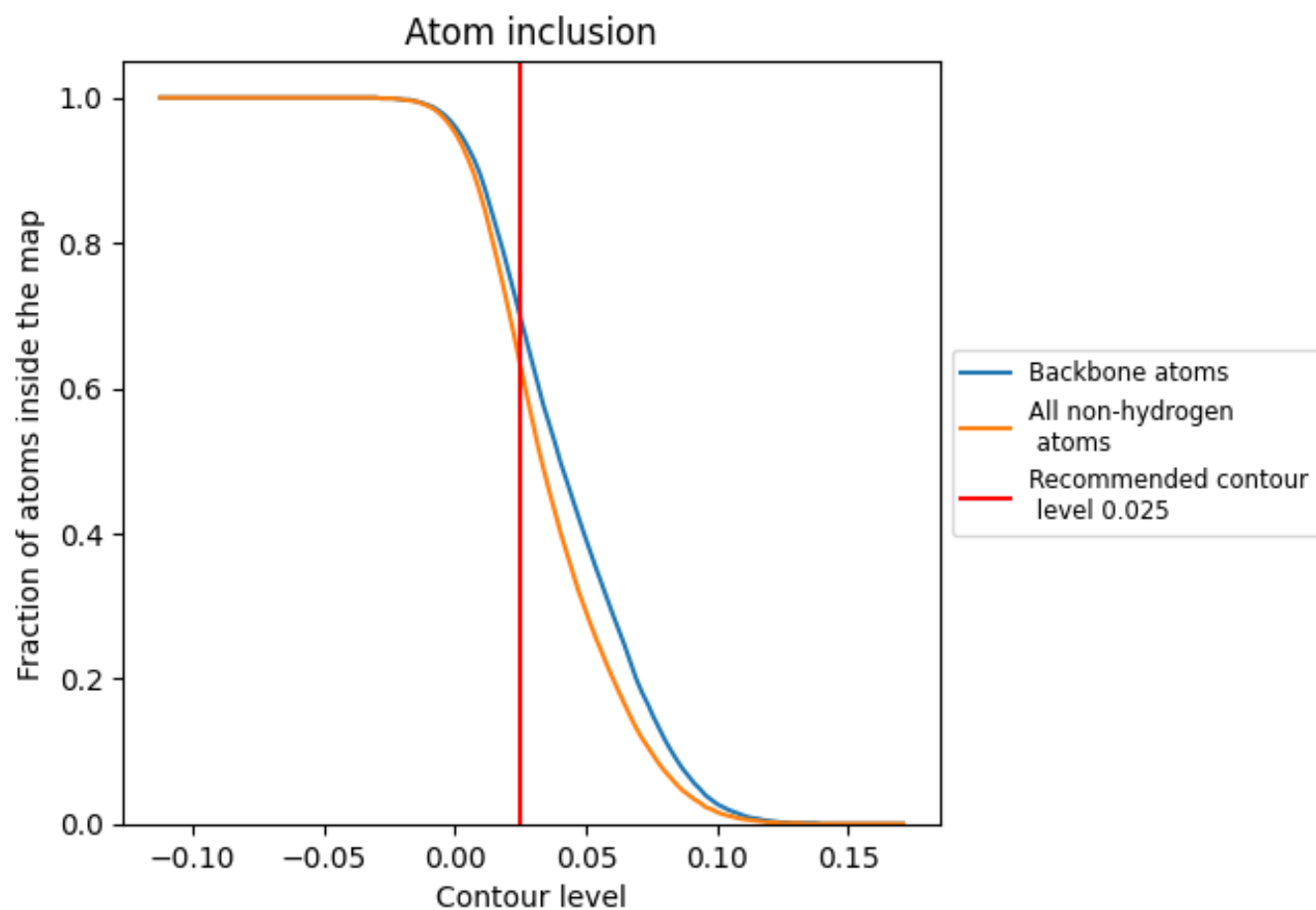
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 63% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6310	 0.3410
A	 0.7810	 0.4180
B	 0.7710	 0.4130
C	 0.8110	 0.4300
D	 0.5970	 0.3000
E	 0.7870	 0.4130
F	 0.8250	 0.4500
G	 0.7640	 0.3900
H	 0.8060	 0.4130
I	 0.5150	 0.2270
J	 0.7110	 0.3230
K	 0.8000	 0.4450
L	 0.7600	 0.4060
M	 0.3140	 0.1830
N	 0.2930	 0.1810
O	 0.7220	 0.3430
Q	 0.2900	 0.1830
R	 0.3610	 0.2190
S	 0.2950	 0.1960
T	 0.3310	 0.2070
U	 0.3200	 0.2140

