Full wwPDB EM Validation Report (i)

May 14, 2024 – 12:54 am BST

PDB ID	:	6RQL
EMDB ID	:	EMD-4984
Title	:	RNA Polymerase I Closed Conformation 2 (CC2)
Authors	:	Mueller, C.W.; Sadian, Y.; Tafur, L.
Deposited on	:	2019-05-16
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

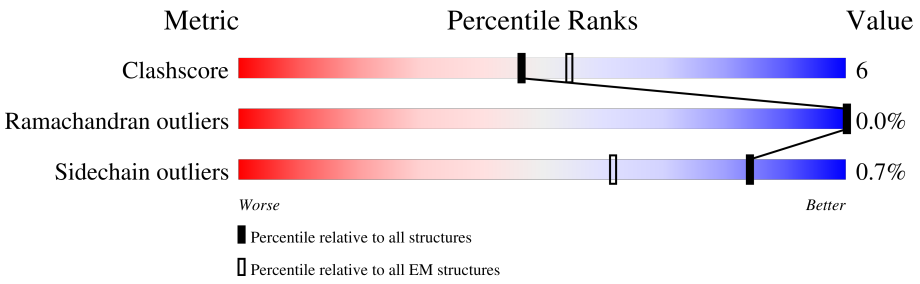
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	T	70	53% 7% 40%
2	U	70	56% • 40%
3	Q	514	75% 17% • 7%
4	S	894	53% 15% 32%
5	R	507	53% 12% 35%
6	M	415	21% 5% 74%
7	A	1664	80% 12% 7%
8	B	1203	82% 16% •
9	C	335	77% 13% 9%

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Mol	Chain	Length	Quality of chain
10	D	137	38% 13% 49%
11	E	215	90% 10%
12	F	155	57% 7% 35%
13	G	326	50% 11% 39%
14	H	146	83% 8% • 8%
15	I	125	79% 19% ••
16	J	70	86% 11% ••
17	K	142	60% 13% 27%
18	L	70	56% 9% 36%
19	N	233	50% 9% 40%
20	O	627	68% 12% 20%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 51626 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
			Total	C	N	O	P		
1	T	42	842	405	141	254	42	0	0

- Molecule 2 is a DNA chain called Nontemplate strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	U	42	877	417	171	248	41	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Q	476	3931	2526	674	711	20	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	A	1542	11953	7543	2086	2263	61	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

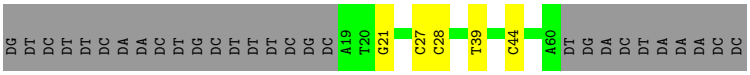
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	O	499	4086	2636	661	767	22	0	0

3 Residue-property plots (i)

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

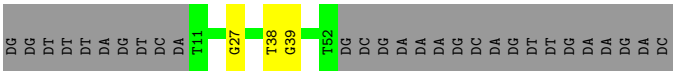
• Molecule 1: Template strand

Chain T: 53% 7% 40%



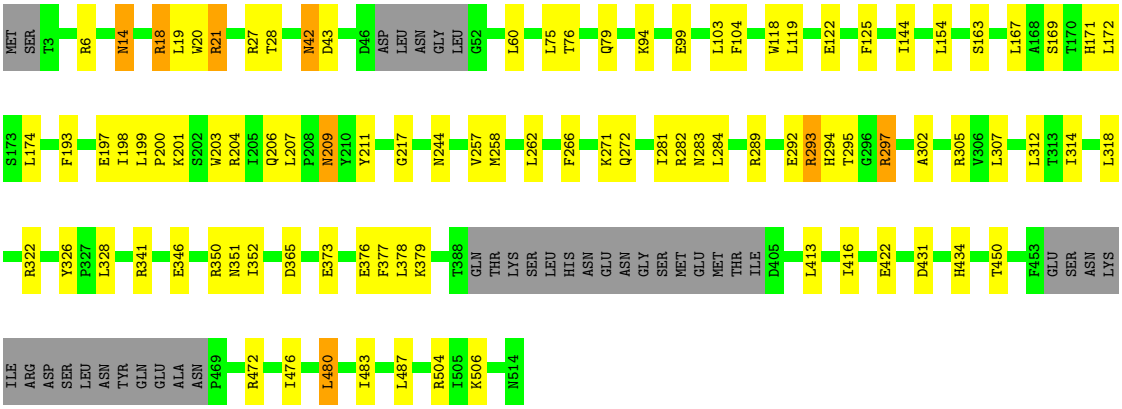
• Molecule 2: Nontemplate strand

Chain U: 56% • 40%



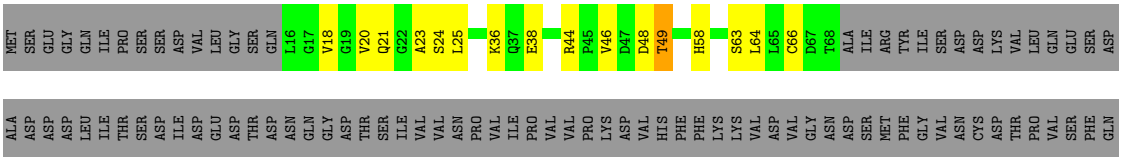
• Molecule 3: RNA polymerase I-specific transcription initiation factor RRN7

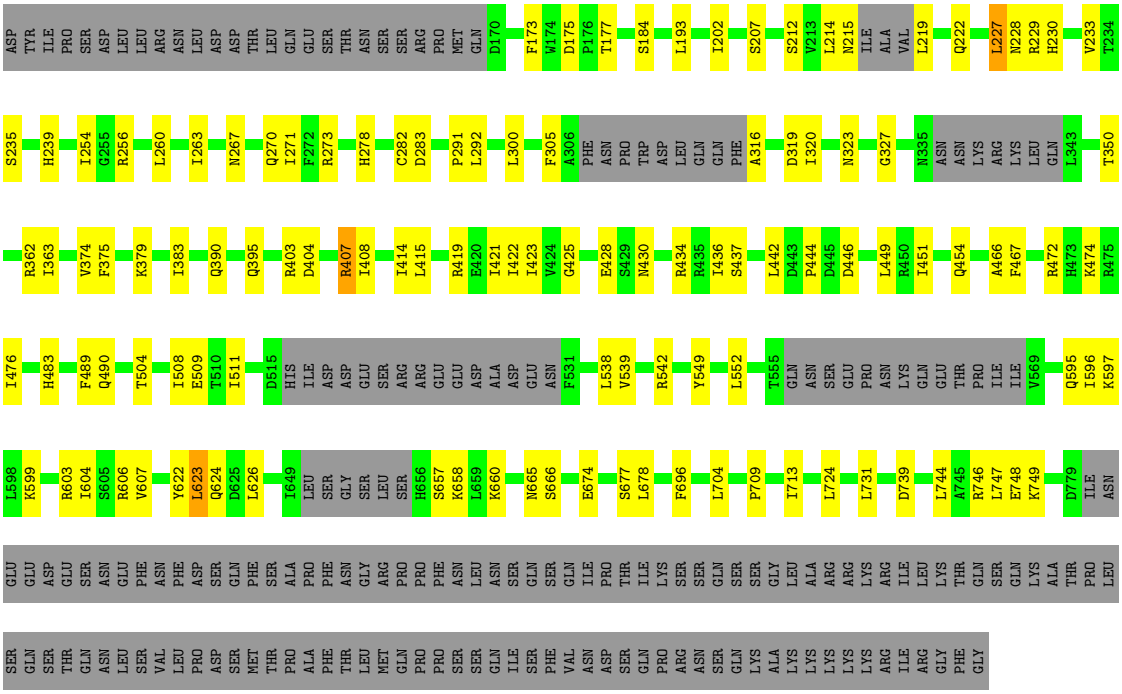
Chain Q: 75% 17% • 7%



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

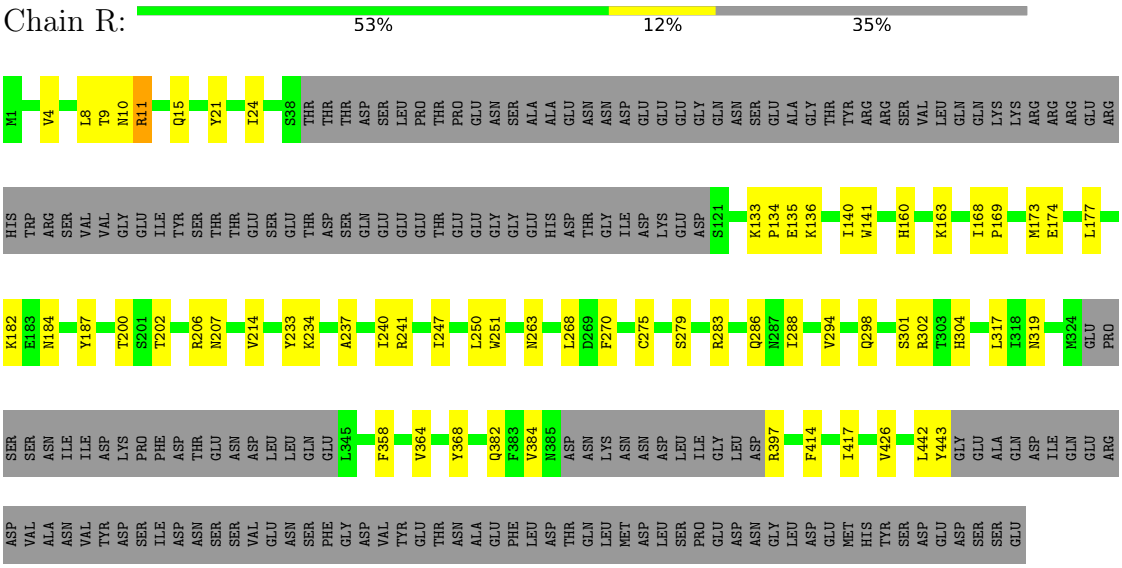
Chain S: 53% 15% 32%





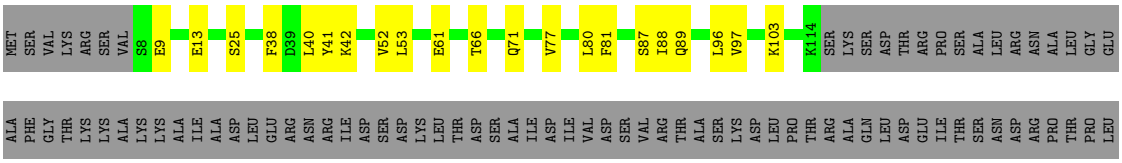
- Molecule 5: RNA polymerase I-specific transcription initiation factor RRN11

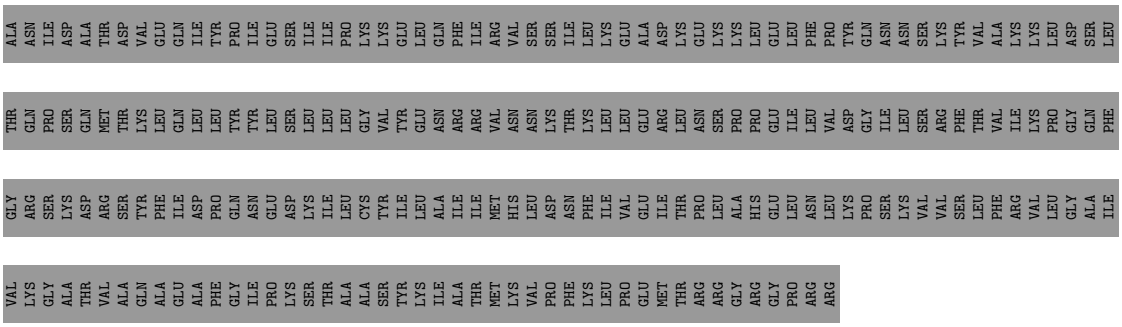
Chain R:



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

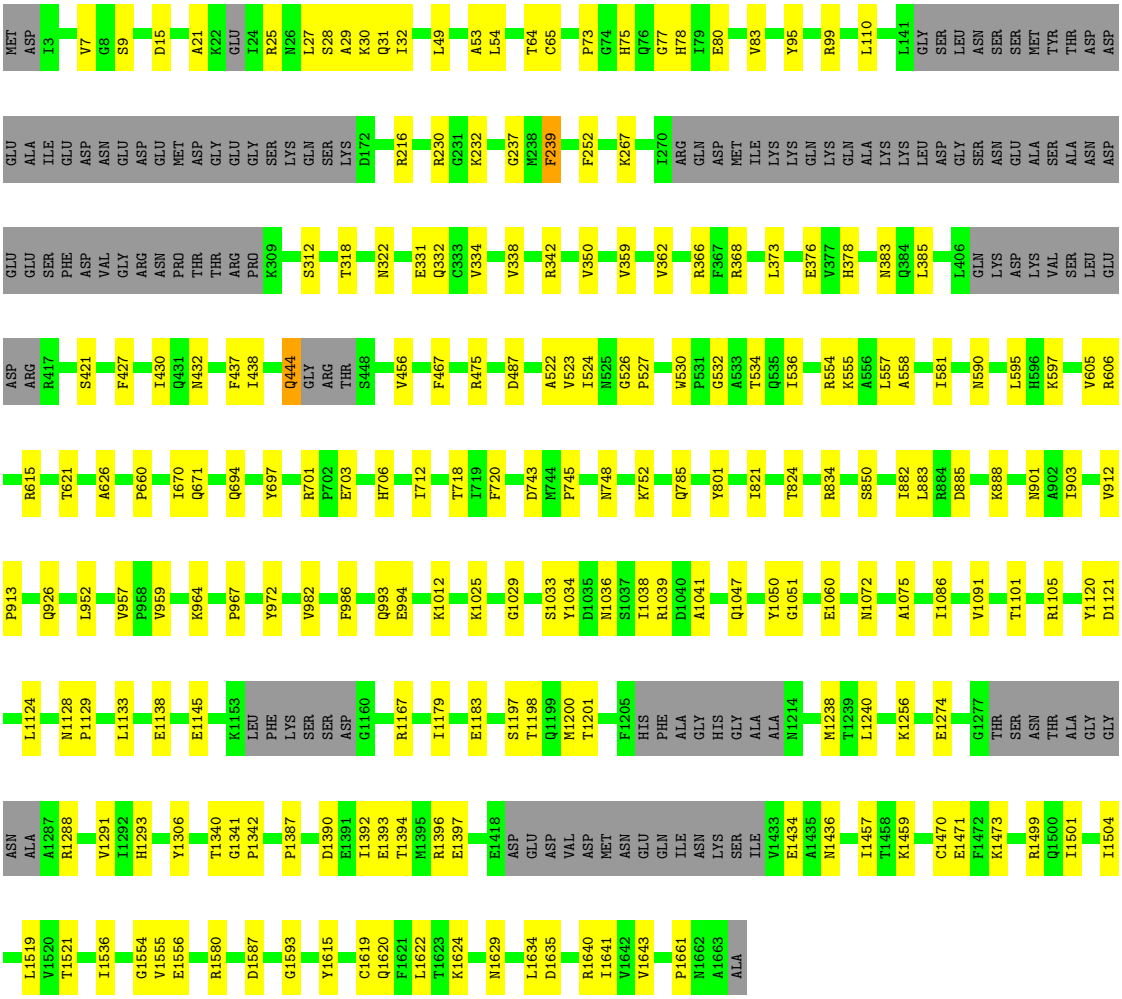
Chain M:





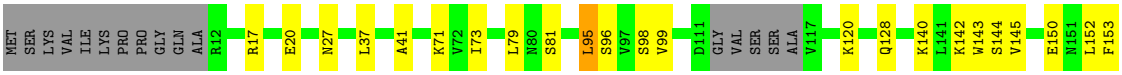
• Molecule 7: DNA-directed RNA polymerase I subunit RPA190

Chain A: 80% 12% 7%



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

Chain B: 82% 16% •



E154 V155 S167 N168 H171 L202 R210 R211 Q243 H251 Y252 V258 R261 V273 V274 M275 R286 F289 D290 G291 S300 R305 L306 R316 L330 E352 R356 L375 I378 N393 A396 L404 I417 D418 L421

I425 R429 I432 N433 R434 K441 I457 A488 E489 K490 R501 S524 L528 H532 I551 L568 I588 S597 H598 I604 E625 R634 L642 R648 M649 L650 R651 M672 N673 I674 Q679 E680 I681 Q682 H686 T692 P693 T694

S698 I699 D708 Q711 S712 P713 R714 C719 M726 V731 H735 K740 P750 K753 D759 N770 Y781 D782 M783 D784 D785 A786 M787 I788 K791 E795 M803 E807 K808 V809 R815 N816 R817 Q823 H824 E838 T850 I858

C859 A860 D863 I871 K872 T873 Y874 I882 E883 E884 L887 S892 E897 L898 Q899 Y905 R906 I913 K916 V926 C927 S928 R929 K930 W931 I934 D935 I948 R957 I960 F963 A971 L974 N987 L1000 N1006 Y1007 H1008 G1009 N1010

Y1014 S1015 G1016 R1023 A1024 D1025 I1026 Y1027 R1035 M1039 D1042 K1043 R1047 K1061 G1062 R1063 K1064 R1065 H1066 G1067 G1068 R1076 L1088 D1097 Y1098 T1099 C1107 G1108 S1109 Q1114 Q1115 R1119 I1123 S1124 C1128 R1129 R1130 K1140 LEU LEU THR LYS SER GLU

ASP G1148 D1155 S1156 Q1157 I1158 W1159 E1160 D1161 A1177 F1180 R1197 P1202 K1203

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

Chain C: 77% 13% 9%

MET SER ASN ILE VAL GLY ILE GLU TYR ASN ARG VAL THR ASN THR THR SER THR ASP PHE PRO GLY PHE SER LYS ASP ALA GLU ASN E30 W31 V42 R69 I70 E74 A80 Y84 V91 K107 W115 Y116 D117 L120 K125 P147 LYS GLY S150

Y157 A160 A164 A187 I191 L192 K195 L196 R197 C208 I212 H216 A217 K218 V222 A225 R228 I239 K240 Q248 I258 D259 E260 G261 S262 D263 E264 R271 R277 E278 R281 K288 R293 I320 K324 Q335

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

Chain D: 38% 13% 49%

M1 G4 S5 R6 N10 N11 T12 N17 T18 P19 T25 I44 N49 ILE ILE ASP SER THR THR MET ASN THR ILE SER GLY ASN ALA ALA ASP ALA ASP ALA ALA ALA VAL ALA ASN THR SER LEU ASN ILE ASP T80 I86 S87 Q88 L89 K90 Q93 R94

L99 P100 PRO ALA GLN ASP PHE SER ALA ALA PRO ILE GLN VAL SER THR THR GLU LYS LYS GLU THR SER ILE GLY VAL SER ALA THR GLY GLY LYS LYS THR THR PHE ALA ASP GLU

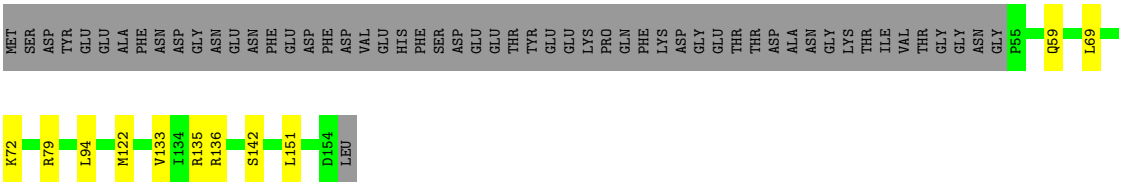
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 90% 10%

M1 R11 Y28 Q32 E36 P64 G76 S77 L78 V90 M93 V97 I100 Q106 T107 G108 I109 T117 P118 S119 A120 L123 I127 Y168 P183 R200 M215

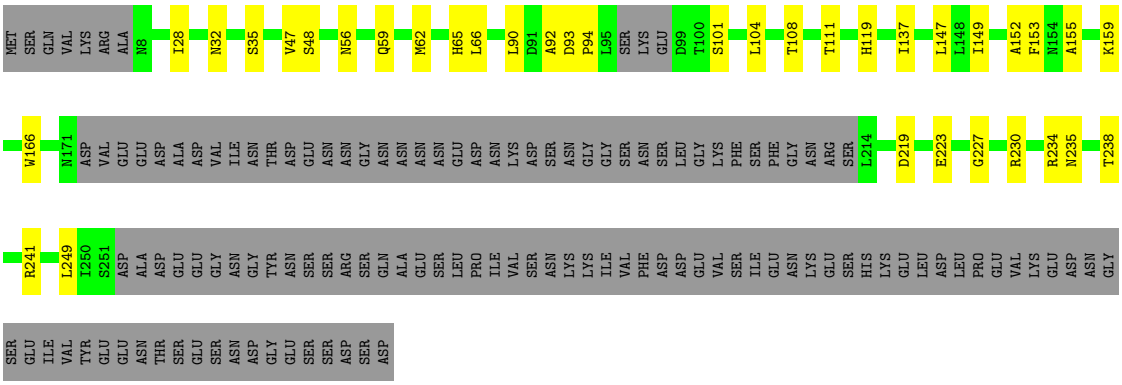
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 57% 7% 35%



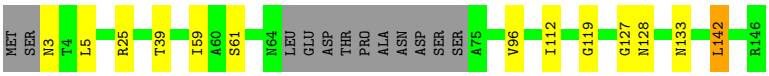
• Molecule 13: DNA-directed RNA polymerase I subunit RPA43

Chain G: 50% 11% 39%



• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 83% 8% • 8%

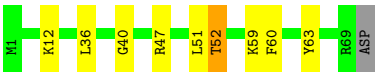


• Molecule 15: DNA-directed RNA polymerase I subunit RPA12

Chain I: 79% 19% ••

• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 86% 11% ••



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

Chain K: 60% 13% 27%

E98 N99 L100 R104 I105 Q106 A113 K138 M142

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

Chain L: 56% 9% 36%

MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN LEU ASP ALA ALA ALA ALA GLY THR SER GLN ALA ARG THR ALA T26 L27 K28 S39 V46 I55 R63 L64 R70

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

Chain N: 50% 9% 40%

MET SER LYS LEU SER LYS ASP TYR VAL SER ASP SER ASP SER ASP ASP GLU VAL ILE SER ASN GLU F23 K30 K31 C32 K33 N44 LYS LYS LYS ALA K49 Q52 V53 I56 K57 L70 P71 I89 D92 T93 D94 ILE GLU SER SER LEU THR GLN ASP ASN LEU

SER N106 L109 E117 S118 L119 A125 LYS ASP ASN ALA P130 F137 S138 V139 R154 V155 P156 R157 R158 D159 F180 HIS VAL ALA GLU GLU VAL LYS GLU ASN LYS LYS GLU PRO LYS LYS ARG SER HIS HIS ASP ASP GLU GLU GLU SER SER GLU LYS LYS LYS LYS LYS

LYS GLU LYS ARG GLU LYS ARG GLU LYS LYS ASP LYS ASP LYS LYS LYS LYS HIS ARG ASP

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

Chain O: 68% 12% 20%

MET MET ALA PHE GLU ASN THR SER LYS ARG PRO PRO GLN ASP PHE VAL ALA PRO ILE ASP GLN LYS LYS ARG LYS VAL GLN PHE SER ASP SER THR GLY LEU VAL THR LEU GLN PRO GLU GLU ILE LYS ASP GLU VAL PHE S48 A59 L60 D61 D62 L63 D64 K65 N66 Q70

Q77 I88 N94 L97 N105 R106 R111 P130 L133 S134 K135 S155 L158 L164 Q168 F179 M182 I183 P184 N200 K201 N202 R205 L208 S213 I240 L265 GLU ASP ASP ASP ASP LEU ASP ASP ASP SER GLY ASP ASP ASP

ASP GLU ASN CYS GLY ASN SER ASN GLU GLU LEU ARG SER GLY ALA ALA ASP GLY SER GLN SER ASP SER GLU ASP M305 T330 K331 L332 D333 L338 V339 S340 V343 V347 T348 P349 E350 S351 L352 L364 F368 R379 Q382 Y383 H387 L393 M396

Q422 Y423 R430 A431 I440 S444 S448 R452 Y453 V454 I455 R487 D503 L517 N521 V524 V537 C540 N547 E550 R551 LEU ARG GLY ILE ILE GLY LYS ALA ASP SER ASP LYS LYS GLU ASN SER ALA GLN ALA ASN THR THR SER SER SER

TRP SER LEU ALA T581 Q589 S590 Y591 F592 P593 L599 Y610 S614 GLU ALA SER GLY GLU TYR GLU SER ASP GLY SER ASP ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24482	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 ($e^-/Å^2$)	1.1075	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.75	0/939	1.05	0/1442
2	U	0.64	0/988	0.92	0/1528
3	Q	0.36	0/4023	0.64	1/5434 (0.0%)
4	S	0.35	0/5065	0.63	0/6859
5	R	0.41	0/2836	0.65	0/3817
6	M	0.35	0/866	0.61	0/1162
7	A	0.47	0/12165	0.60	1/16450 (0.0%)
8	B	0.53	0/9578	0.65	0/12948
9	C	0.48	0/2469	0.61	0/3347
10	D	0.35	0/557	0.59	0/750
11	E	0.41	0/1795	0.54	0/2416
12	F	0.52	0/838	0.60	0/1129
13	G	0.40	0/1613	0.59	0/2193
14	H	0.49	0/1090	0.61	0/1476
15	I	0.37	0/955	0.61	0/1288
16	J	0.58	0/578	0.71	0/775
17	K	0.48	0/821	0.61	0/1108
18	L	0.49	0/361	0.77	0/478
19	N	0.32	0/1124	0.58	0/1512
20	O	0.36	0/4173	0.57	0/5645
All	All	0.46	0/52834	0.64	2/71757 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	60	LEU	CA-CB-CG	5.55	128.07	115.30
7	A	1387	PRO	N-CA-CB	5.17	109.50	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	842	0	476	9	0
2	U	877	0	475	2	0
3	Q	3931	0	3918	67	0
4	S	4963	0	4890	99	0
5	R	2771	0	2844	42	0
6	M	850	0	850	15	0
7	A	11953	0	11848	152	0
8	B	9371	0	9243	141	0
9	C	2418	0	2401	41	0
10	D	551	0	558	14	0
11	E	1759	0	1788	13	0
12	F	823	0	841	7	0
13	G	1576	0	1581	24	0
14	H	1072	0	1042	8	0
15	I	942	0	937	17	0
16	J	569	0	589	8	0
17	K	810	0	801	15	0
18	L	359	0	385	5	0
19	N	1103	0	1106	18	0
20	O	4086	0	4024	43	0
All	All	51626	0	50597	644	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (644) 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:232:LYS:HG2	7:A:239:PHE:CD1	1.59	1.36
4:S:442:LEU:HD21	4:S:444:PRO:CG	1.63	1.27
4:S:623:LEU:HD12	4:S:624:GLN:N	1.56	1.19
7:A:30:LYS:HD2	7:A:53:ALA:HB1	1.29	1.15
4:S:442:LEU:HD23	4:S:444:PRO:HD2	1.32	1.11
4:S:442:LEU:CD2	4:S:444:PRO:HG2	1.78	1.10
8:B:73:ILE:CD1	8:B:95:LEU:HD11	1.83	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:30:LYS:HD2	7:A:53:ALA:CB	1.89	1.03
7:A:232:LYS:CG	7:A:239:PHE:HD1	1.72	1.03
4:S:442:LEU:HD23	4:S:444:PRO:CD	1.90	1.01
9:C:120:LEU:HD11	9:C:125:LYS:HA	1.41	1.01
4:S:442:LEU:CD2	4:S:444:PRO:CD	2.39	1.00
7:A:432:ASN:ND2	7:A:444:GLN:OE1	1.99	0.96
4:S:442:LEU:CD2	4:S:444:PRO:CG	2.42	0.95
4:S:442:LEU:CD2	4:S:444:PRO:HD2	1.95	0.94
7:A:30:LYS:CD	7:A:53:ALA:HB1	1.98	0.92
7:A:232:LYS:HG2	7:A:239:PHE:HD1	0.79	0.91
1:T:39:DT:C7	5:R:11:ARG:NH2	2.34	0.91
4:S:623:LEU:HD12	4:S:624:GLN:H	1.36	0.89
9:C:120:LEU:HD11	9:C:125:LYS:CA	2.02	0.88
4:S:442:LEU:HD21	4:S:444:PRO:HG2	0.88	0.88
8:B:740:LYS:HE2	8:B:803:MET:SD	2.13	0.87
10:D:11:ASN:O	10:D:12:THR:HG22	1.74	0.87
7:A:373:LEU:CD2	7:A:378:HIS:NE2	2.42	0.83
8:B:934:ILE:HD12	9:C:69:ARG:HD2	1.60	0.82
8:B:807:GLU:OE1	8:B:905:TYR:OH	1.98	0.82
9:C:117:ASP:HB3	9:C:120:LEU:HD23	1.62	0.82
7:A:373:LEU:HD23	7:A:378:HIS:NE2	1.96	0.81
4:S:193:LEU:HD11	4:S:256:ARG:HH21	1.49	0.77
7:A:748:ASN:H	7:A:1072:ASN:HD21	1.32	0.77
8:B:73:ILE:HD11	8:B:95:LEU:HD11	1.67	0.76
9:C:120:LEU:O	9:C:120:LEU:HD12	1.85	0.76
10:D:12:THR:HG23	10:D:12:THR:O	1.85	0.76
1:T:39:DT:C5	5:R:11:ARG:NH2	2.55	0.75
8:B:73:ILE:CG1	8:B:95:LEU:HD11	2.17	0.75
3:Q:262:LEU:HD13	3:Q:266:PHE:HB2	1.70	0.73
8:B:73:ILE:HD12	8:B:95:LEU:HD11	1.66	0.73
9:C:117:ASP:HB3	9:C:120:LEU:CD2	2.19	0.72
8:B:898:LEU:HB3	18:L:46:VAL:HG21	1.70	0.72
7:A:373:LEU:HD23	7:A:378:HIS:CD2	2.24	0.72
7:A:232:LYS:CG	7:A:239:PHE:CD1	2.55	0.71
13:G:108:THR:HG1	13:G:111:THR:HG1	1.38	0.71
3:Q:266:PHE:CE1	3:Q:314:ILE:HD12	2.27	0.70
8:B:73:ILE:CD1	8:B:95:LEU:CD1	2.68	0.70
1:T:39:DT:H73	5:R:11:ARG:NH2	2.07	0.70
9:C:120:LEU:HD12	9:C:120:LEU:C	2.13	0.69
9:C:120:LEU:HD11	9:C:125:LYS:CB	2.23	0.69
4:S:46:VAL:HG22	4:S:48:ASP:H	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:15:ASP:HB2	8:B:1197:ARG:HB3	1.76	0.68
8:B:73:ILE:HG13	8:B:95:LEU:HD11	1.75	0.68
4:S:66:CYS:HB3	4:S:227:LEU:HD13	1.78	0.66
7:A:373:LEU:HD21	7:A:378:HIS:NE2	2.09	0.66
7:A:701:ARG:H	7:A:706:HIS:HD2	1.44	0.66
7:A:670:ILE:HG12	7:A:671:GLN:HG3	1.78	0.66
7:A:606:ARG:NH2	17:K:98:GLU:OE2	2.29	0.66
4:S:623:LEU:HB2	4:S:678:LEU:HD12	1.78	0.65
4:S:442:LEU:HD21	4:S:444:PRO:CD	2.11	0.65
8:B:714:ARG:HH12	15:I:105:ASP:HA	1.62	0.65
7:A:232:LYS:HG2	7:A:239:PHE:CE1	2.29	0.65
6:M:53:LEU:HB2	6:M:96:LEU:HD13	1.80	0.64
6:M:80:LEU:HD23	6:M:89:GLN:HE21	1.63	0.64
8:B:785:ASP:OD2	8:B:957:ARG:NH2	2.31	0.64
15:I:113:THR:HG23	15:I:120:LYS:HE2	1.79	0.64
8:B:73:ILE:HD12	8:B:95:LEU:CD1	2.27	0.63
20:O:431:ALA:O	20:O:487:ARG:NH2	2.31	0.63
8:B:95:LEU:HD12	8:B:95:LEU:H	1.64	0.63
7:A:964:LYS:NZ	8:B:672:MET:O	2.24	0.63
7:A:65:CYS:SG	7:A:75:HIS:NE2	2.62	0.63
8:B:79:LEU:HD22	8:B:81:SER:HB3	1.80	0.62
8:B:143:TRP:HB3	8:B:152:LEU:HB2	1.81	0.62
3:Q:292:GLU:HG3	3:Q:294:HIS:CD2	2.34	0.62
7:A:526:GLY:HA3	7:A:554:ARG:HH11	1.64	0.62
8:B:931:TRP:NE1	8:B:935:ASP:O	2.30	0.62
5:R:358:PHE:HB2	5:R:364:VAL:HG11	1.82	0.62
20:O:547:ASN:HA	20:O:550:GLU:HB3	1.82	0.62
4:S:362:ARG:HB3	4:S:375:PHE:HB2	1.81	0.62
3:Q:289:ARG:HH22	3:Q:295:THR:HG22	1.64	0.61
7:A:1459:LYS:HD3	7:A:1473:LYS:HD3	1.82	0.61
4:S:623:LEU:HD12	4:S:623:LEU:C	2.19	0.61
11:E:97:VAL:HG13	11:E:127:ILE:HD11	1.83	0.61
14:H:3:ASN:HB3	14:H:61:SER:HB3	1.83	0.61
9:C:120:LEU:CD1	9:C:125:LYS:HA	2.23	0.61
4:S:442:LEU:HD23	4:S:442:LEU:C	2.20	0.61
9:C:70:ILE:HG23	9:C:74:GLU:HB2	1.82	0.61
7:A:1179:ILE:HD11	7:A:1183:GLU:HG2	1.83	0.60
8:B:417:ILE:HG22	8:B:457:ILE:HD13	1.83	0.60
4:S:454:GLN:NE2	4:S:511:ILE:O	2.34	0.60
8:B:211:ARG:HH12	8:B:243:GLN:HE22	1.47	0.60
6:M:38:PHE:HB2	19:N:119:LEU:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:104:ARG:HE	17:K:106:GLN:HE21	1.48	0.60
3:Q:292:GLU:HG3	3:Q:294:HIS:CG	2.37	0.60
15:I:78:ASP:O	15:I:95:ASN:ND2	2.35	0.60
8:B:1014:TYR:OH	9:C:293:ARG:NH1	2.34	0.59
7:A:850:SER:HB3	7:A:903:ILE:HG21	1.82	0.59
15:I:114:CYS:SG	15:I:115:THR:N	2.75	0.59
7:A:1101:THR:HG22	7:A:1120:TYR:HB3	1.84	0.59
3:Q:289:ARG:NH1	3:Q:294:HIS:O	2.36	0.59
8:B:17:ARG:HB3	8:B:20:GLU:HB3	1.84	0.59
5:R:15:GLN:OE1	5:R:184:ASN:ND2	2.36	0.59
8:B:300:SER:HB3	15:I:49:THR:HG22	1.85	0.59
14:H:5:LEU:O	14:H:133:ASN:ND2	2.36	0.59
3:Q:272:GLN:HG3	4:S:596:ILE:HD13	1.85	0.58
9:C:278:GLU:OE2	9:C:281:ARG:NH1	2.36	0.58
7:A:536:ILE:HG12	7:A:557:LEU:HD21	1.86	0.58
20:O:340:SER:HA	20:O:343:VAL:HG12	1.85	0.58
3:Q:14:ASN:ND2	20:O:200:ASN:OD1	2.37	0.58
7:A:475:ARG:NH1	8:B:1068:GLY:O	2.35	0.58
20:O:66:ASN:HA	20:O:111:ARG:HH12	1.69	0.58
8:B:41:ALA:HA	8:B:501:ARG:HH21	1.69	0.57
9:C:248:GLN:HE21	9:C:258:ILE:HG23	1.69	0.57
20:O:179:PHE:HA	20:O:182:MET:HB3	1.86	0.57
3:Q:193:PHE:HA	3:Q:217:GLY:HA3	1.86	0.57
7:A:30:LYS:HD2	7:A:53:ALA:HB3	1.82	0.57
7:A:21:ALA:O	7:A:25:ARG:NH1	2.37	0.57
7:A:982:VAL:HG22	7:A:994:GLU:HB2	1.85	0.57
3:Q:171:HIS:ND1	3:Q:244:ASN:OD1	2.37	0.57
3:Q:271:LYS:NZ	4:S:739:ASP:OD2	2.37	0.57
8:B:568:LEU:HD23	8:B:604:ILE:HG12	1.86	0.57
13:G:149:ILE:HB	13:G:153:PHE:HB2	1.87	0.57
20:O:97:LEU:HD22	20:O:135:LYS:HG2	1.86	0.57
16:J:36:LEU:HB2	16:J:47:ARG:HH21	1.68	0.57
8:B:974:LEU:O	16:J:47:ARG:NH1	2.37	0.57
4:S:511:ILE:HD11	4:S:538:LEU:HD23	1.87	0.56
8:B:1016:GLY:O	9:C:69:ARG:NH2	2.38	0.56
8:B:1047:ARG:HH11	8:B:1067:GLY:HA3	1.70	0.56
3:Q:293:ARG:O	3:Q:293:ARG:HG3	2.05	0.56
4:S:222:GLN:HE21	4:S:229:ARG:HH22	1.51	0.56
8:B:251:HIS:HE1	8:B:261:ARG:HD3	1.71	0.56
4:S:603:ARG:HE	4:S:606:ARG:HH21	1.54	0.56
4:S:623:LEU:CD1	4:S:624:GLN:N	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:32:ASN:O	13:G:230:ARG:NH2	2.38	0.56
7:A:30:LYS:HE3	7:A:53:ALA:O	2.05	0.56
13:G:219:ASP:OD1	13:G:223:GLU:N	2.36	0.56
7:A:1274:GLU:OE2	7:A:1288:ARG:NH2	2.35	0.56
4:S:508:ILE:HG12	4:S:539:VAL:HG12	1.88	0.55
7:A:27:LEU:HB3	8:B:1130:ARG:HB3	1.88	0.55
7:A:1256:LYS:O	7:A:1499:ARG:NH2	2.38	0.55
8:B:681:ILE:O	19:N:154:ARG:NH1	2.39	0.55
8:B:817:ARG:HH12	8:B:892:SER:HB2	1.70	0.55
7:A:1556:GLU:OE1	11:E:200:ARG:NH1	2.39	0.55
17:K:98:GLU:HG3	17:K:100:LEU:HD12	1.88	0.55
17:K:74:ASN:OD1	17:K:77:ARG:NH2	2.40	0.55
5:R:160:HIS:HA	5:R:163:LYS:HE3	1.88	0.55
20:O:66:ASN:HD22	20:O:111:ARG:HH22	1.54	0.55
8:B:291:GLY:HA3	8:B:375:LEU:HD13	1.88	0.55
8:B:1119:ARG:NH2	8:B:1160:GLU:OE2	2.40	0.55
3:Q:203:TRP:HD1	3:Q:206:GLN:HE21	1.55	0.55
8:B:95:LEU:HD12	8:B:95:LEU:N	2.20	0.55
8:B:934:ILE:HD12	9:C:69:ARG:CD	2.35	0.55
9:C:42:VAL:O	17:K:138:LYS:NZ	2.38	0.55
5:R:8:LEU:HD21	5:R:202:THR:HG22	1.88	0.54
7:A:7:VAL:HG21	8:B:1177:ALA:HB2	1.88	0.54
7:A:368:ARG:HH11	7:A:383:ASN:HD21	1.55	0.54
5:R:442:LEU:O	5:R:443:TYR:CD2	2.60	0.54
20:O:503:ASP:HA	20:O:537:VAL:HG13	1.89	0.54
3:Q:118:TRP:NE1	3:Q:122:GLU:OE1	2.37	0.54
7:A:1036:ASN:ND2	7:A:1128:ASN:OD1	2.40	0.54
4:S:442:LEU:HD23	4:S:444:PRO:N	2.21	0.54
8:B:1097:ASP:N	8:B:1097:ASP:OD1	2.40	0.54
15:I:95:ASN:HB2	15:I:113:THR:HB	1.90	0.54
1:T:39:DT:H71	5:R:11:ARG:NH2	2.22	0.54
10:D:12:THR:O	10:D:17:ASN:ND2	2.38	0.54
3:Q:328:LEU:HD13	3:Q:472:ARG:HG3	1.89	0.54
4:S:278:HIS:HB2	4:S:283:ASP:H	1.73	0.54
8:B:1076:ARG:HG3	8:B:1088:LEU:HD11	1.90	0.54
9:C:157:TYR:HB2	9:C:160:ALA:HB2	1.90	0.54
13:G:152:ALA:HA	20:O:184:PRO:HG2	1.90	0.54
4:S:300:LEU:HA	4:S:320:ILE:HA	1.89	0.54
5:R:136:LYS:HD2	5:R:304:HIS:HD2	1.73	0.54
4:S:451:ILE:HD11	4:S:466:ALA:HB1	1.89	0.54
7:A:237:GLY:HA3	7:A:267:LYS:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1042:ASP:OD1	8:B:1043:LYS:NZ	2.41	0.53
3:Q:94:LYS:NZ	3:Q:207:LEU:O	2.34	0.53
3:Q:341:ARG:NH2	3:Q:373:GLU:OE2	2.40	0.53
4:S:407:ARG:HA	4:S:414:ILE:HG23	1.89	0.53
4:S:423:ILE:HD13	5:R:141:TRP:HZ2	1.73	0.53
7:A:32:ILE:HD11	7:A:54:LEU:HD11	1.91	0.53
9:C:196:LEU:O	9:C:197:ARG:NH1	2.41	0.53
13:G:147:LEU:HB2	13:G:155:ALA:HB3	1.90	0.53
3:Q:341:ARG:NH2	3:Q:351:ASN:OD1	2.42	0.53
7:A:1340:THR:HG23	8:B:316:ARG:HD3	1.90	0.53
7:A:1434:GLU:OE1	7:A:1436:ASN:ND2	2.42	0.53
9:C:120:LEU:CD1	9:C:125:LYS:CA	2.83	0.53
20:O:422:GLN:NE2	20:O:591:TYR:O	2.40	0.53
1:T:44:DC:H42	2:U:27:DG:H1	1.57	0.53
8:B:27:ASN:OD1	9:C:150:SER:N	2.41	0.53
4:S:623:LEU:O	4:S:626:LEU:N	2.41	0.53
8:B:1042:ASP:O	8:B:1063:ARG:NH1	2.42	0.53
8:B:883:GLU:HG3	8:B:884:GLU:HG3	1.91	0.53
8:B:731:VAL:HG21	16:J:59:LYS:HG2	1.91	0.53
12:F:136:ARG:HH12	12:F:151:LEU:HD21	1.73	0.53
3:Q:169:SER:HA	3:Q:174:LEU:HD12	1.91	0.53
4:S:63:SER:HB3	4:S:549:TYR:HB3	1.90	0.53
5:R:294:VAL:H	5:R:298:GLN:HE21	1.56	0.53
8:B:71:LYS:NZ	8:B:418:ASP:OD1	2.41	0.53
3:Q:14:ASN:O	20:O:200:ASN:ND2	2.42	0.52
3:Q:104:PHE:HE1	3:Q:211:TYR:O	1.92	0.52
4:S:18:VAL:HG23	5:R:426:VAL:HA	1.91	0.52
8:B:1039:MET:O	8:B:1043:LYS:NZ	2.42	0.52
20:O:521:ASN:HB3	20:O:524:VAL:HG12	1.92	0.52
11:E:28:TYR:HA	11:E:64:PRO:HA	1.92	0.52
9:C:91:VAL:HG11	16:J:60:PHE:HB3	1.91	0.52
3:Q:422:GLU:HG3	5:R:263:ASN:HD22	1.74	0.52
5:R:382:GLN:HE22	5:R:442:LEU:HA	1.74	0.52
8:B:698:SER:OG	8:B:699:ILE:N	2.42	0.52
8:B:786:ALA:HB1	8:B:928:SER:HB2	1.92	0.52
3:Q:266:PHE:CD1	3:Q:314:ILE:HD12	2.44	0.52
8:B:963:PHE:O	8:B:1027:TYR:OH	2.28	0.52
4:S:657:SER:HA	4:S:748:GLU:HB2	1.91	0.52
8:B:883:GLU:OE1	8:B:906:ARG:NH1	2.38	0.52
14:H:25:ARG:HE	14:H:39:THR:HG23	1.75	0.52
4:S:595:GLN:OE1	4:S:599:LYS:NZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:73:PRO:O	7:A:366:ARG:NH2	2.43	0.52
7:A:1291:VAL:HG22	7:A:1473:LYS:HG2	1.92	0.52
10:D:11:ASN:O	10:D:12:THR:CG2	2.54	0.52
1:T:39:DT:C7	5:R:11:ARG:HH22	2.15	0.51
3:Q:302:ALA:HA	3:Q:305:ARG:HE	1.75	0.51
7:A:1619:CYS:HA	7:A:1622:LEU:HB3	1.91	0.51
7:A:1635:ASP:HA	7:A:1640:ARG:HE	1.75	0.51
4:S:316:ALA:HB3	4:S:327:GLY:HA3	1.90	0.51
5:R:4:VAL:HG11	5:R:214:VAL:HG22	1.91	0.51
6:M:13:GLU:OE2	6:M:87:SER:OG	2.27	0.51
9:C:69:ARG:HH12	17:K:70:HIS:HB2	1.75	0.51
7:A:883:LEU:HD11	7:A:959:VAL:HG11	1.92	0.51
6:M:25:SER:HB3	6:M:97:VAL:HA	1.92	0.51
8:B:858:ILE:HD13	8:B:874:TYR:HB2	1.93	0.51
4:S:260:LEU:HA	4:S:273:ARG:HA	1.93	0.51
4:S:604:ILE:HD12	4:S:731:LEU:HD11	1.90	0.51
5:R:133:LYS:H	5:R:286:GLN:HE21	1.57	0.51
7:A:239:PHE:HD2	7:A:239:PHE:O	1.93	0.51
8:B:286:ARG:HH22	15:I:4:VAL:HG21	1.76	0.51
9:C:80:ALA:HA	9:C:208:CYS:HA	1.92	0.51
9:C:228:ARG:NH2	9:C:271:ARG:O	2.40	0.51
7:A:1051:GLY:HA3	7:A:1580:ARG:HG2	1.92	0.51
7:A:1306:TYR:O	7:A:1499:ARG:NH2	2.44	0.51
20:O:213:SER:HB2	20:O:338:LEU:HD21	1.91	0.51
3:Q:352:ILE:CD1	3:Q:377:PHE:CE1	2.93	0.51
7:A:888:LYS:HE2	15:I:69:THR:HG22	1.93	0.51
7:A:1039:ARG:NH2	11:E:168:TYR:O	2.44	0.51
8:B:142:LYS:HG3	8:B:153:PHE:HE1	1.75	0.51
5:R:136:LYS:HD2	5:R:304:HIS:CD2	2.46	0.51
7:A:252:PHE:HB3	7:A:312:SER:HB2	1.92	0.51
15:I:26:SER:OG	15:I:38:PRO:O	2.29	0.51
20:O:423:TYR:HA	20:O:593:PRO:HG2	1.92	0.51
7:A:487:ASP:HB2	7:A:615:ARG:HG2	1.93	0.51
3:Q:284:LEU:HB3	3:Q:302:ALA:HB1	1.93	0.51
3:Q:431:ASP:OD2	3:Q:434:HIS:ND1	2.41	0.51
7:A:993:GLN:NE2	8:B:680:GLU:OE1	2.44	0.51
3:Q:378:LEU:HD13	5:R:234:LYS:HB3	1.91	0.50
4:S:607:VAL:HB	4:S:731:LEU:HD13	1.93	0.50
7:A:712:ILE:H	17:K:106:GLN:HE22	1.59	0.50
8:B:916:LYS:HG2	8:B:926:VAL:HG12	1.92	0.50
9:C:239:ILE:HG22	9:C:288:LYS:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:200:ASN:ND2	20:O:202:ASN:OD1	2.44	0.50
7:A:885:ASP:HB3	7:A:888:LYS:HB2	1.92	0.50
16:J:12:LYS:NZ	16:J:40:GLY:O	2.44	0.50
20:O:94:ASN:HD22	20:O:135:LYS:HD2	1.76	0.50
4:S:408:ILE:HD11	4:S:415:LEU:HB2	1.93	0.50
8:B:987:ASN:HD22	19:N:157:ARG:HE	1.60	0.50
8:B:1061:LYS:O	8:B:1065:ARG:NH1	2.40	0.50
3:Q:119:LEU:HB3	3:Q:125:PHE:HD2	1.76	0.50
8:B:99:VAL:HG23	8:B:421:LEU:HD21	1.94	0.50
4:S:709:PRO:HD2	4:S:713:ILE:HD11	1.93	0.50
7:A:216:ARG:NH2	7:A:338:VAL:O	2.44	0.50
7:A:1145:GLU:OE2	7:A:1167:ARG:NH1	2.43	0.50
8:B:1156:SER:HB3	13:G:238:THR:HG21	1.93	0.50
15:I:52:ALA:HB3	15:I:55:ALA:HB2	1.94	0.50
20:O:348:THR:HG23	20:O:350:GLU:HG2	1.94	0.50
4:S:404:ASP:OD2	4:S:451:ILE:N	2.44	0.50
7:A:824:THR:HG23	8:B:1023:ARG:HB2	1.94	0.50
7:A:964:LYS:HZ1	7:A:967:PRO:HA	1.76	0.50
8:B:252:TYR:OH	8:B:305:ARG:NE	2.40	0.50
3:Q:198:ILE:HG13	3:Q:199:LEU:HD22	1.94	0.50
4:S:214:LEU:HD22	4:S:263:ILE:HD13	1.94	0.50
4:S:415:LEU:HD21	4:S:422:ILE:HG23	1.94	0.50
7:A:912:VAL:O	7:A:926:GLN:NE2	2.45	0.50
7:A:1341:GLY:HA3	8:B:316:ARG:HE	1.77	0.50
8:B:37:LEU:HD12	8:B:759:ASP:HB3	1.93	0.50
3:Q:200:PRO:HB3	3:Q:203:TRP:HB2	1.94	0.49
8:B:393:ASN:HB3	8:B:396:ALA:HB2	1.94	0.49
8:B:809:VAL:HG13	8:B:872:LYS:HE2	1.94	0.49
20:O:60:LEU:O	20:O:106:ARG:NH1	2.39	0.49
8:B:404:LEU:HD21	8:B:551:ILE:HG21	1.94	0.49
9:C:222:VAL:HG21	9:C:225:ALA:HB2	1.95	0.49
13:G:149:ILE:HD11	13:G:155:ALA:HB2	1.94	0.49
7:A:444:GLN:NE2	7:A:444:GLN:N	2.60	0.49
8:B:1014:TYR:HH	9:C:293:ARG:HH12	1.61	0.49
11:E:90:VAL:HA	11:E:120:ALA:HB2	1.93	0.49
4:S:173:PHE:HZ	5:R:187:TYR:HA	1.77	0.49
4:S:383:ILE:HG12	4:S:390:GLN:HG3	1.93	0.49
3:Q:346:GLU:OE2	3:Q:350:ARG:NH1	2.45	0.49
7:A:1293:HIS:ND1	7:A:1471:GLU:OE1	2.46	0.49
3:Q:322:ARG:HB3	4:S:597:LYS:HZ3	1.78	0.49
7:A:697:TYR:OH	7:A:703:GLU:OE2	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:834:ARG:HH12	8:B:1008:HIS:CD2	2.31	0.49
8:B:167:SER:OG	8:B:168:ASN:N	2.46	0.49
8:B:726:MET:SD	8:B:1035:ARG:NH1	2.85	0.49
10:D:25:THR:OG1	12:F:59:GLN:OE1	2.30	0.49
7:A:80:GLU:HA	7:A:359:VAL:HG12	1.95	0.49
8:B:95:LEU:HA	8:B:145:VAL:HA	1.94	0.49
8:B:1114:GLN:HE22	8:B:1161:ASP:HB3	1.78	0.49
4:S:21:GLN:OE1	4:S:24:SER:OG	2.26	0.49
4:S:49:THR:HG22	4:S:490:GLN:HA	1.94	0.49
8:B:1025:ASP:OD2	9:C:277:ARG:NH1	2.46	0.49
20:O:347:VAL:HG23	20:O:352:LEU:HD11	1.95	0.49
4:S:260:LEU:HB3	4:S:273:ARG:HG3	1.93	0.48
7:A:373:LEU:O	7:A:373:LEU:HG	2.13	0.48
7:A:752:LYS:O	7:A:785:GLN:NE2	2.47	0.48
7:A:1038:ILE:HD11	7:A:1050:TYR:HB2	1.95	0.48
8:B:823:GLN:HB3	8:B:863:ASP:HB3	1.95	0.48
13:G:28:ILE:HA	13:G:35:SER:HA	1.95	0.48
20:O:440:ILE:O	20:O:444:SER:N	2.44	0.48
4:S:25:LEU:HD23	4:S:437:SER:HA	1.94	0.48
7:A:332:GLN:HE22	7:A:350:VAL:H	1.61	0.48
8:B:971:ALA:HB2	8:B:1000:LEU:HD12	1.95	0.48
11:E:117:THR:HG22	11:E:119:SER:H	1.77	0.48
5:R:135:GLU:OE2	5:R:301:SER:OG	2.32	0.48
8:B:1107:CYS:SG	8:B:1109:SER:OG	2.60	0.48
10:D:19:PRO:HB3	13:G:47:VAL:HG12	1.95	0.48
4:S:483:HIS:HA	4:S:489:PHE:HB3	1.95	0.48
8:B:682:GLN:H	8:B:686:HIS:HD2	1.61	0.48
17:K:62:SER:OG	17:K:104:ARG:NH1	2.41	0.48
3:Q:6:ARG:HE	3:Q:18:ARG:HB3	1.78	0.48
4:S:425:GLY:HA3	4:S:434:ARG:HH11	1.78	0.48
8:B:95:LEU:HD13	8:B:95:LEU:C	2.34	0.48
18:L:28:LYS:HG2	18:L:39:SER:HB2	1.94	0.48
14:H:59:ILE:HG12	14:H:142:LEU:HD12	1.96	0.48
3:Q:307:LEU:HD22	3:Q:487:LEU:HD21	1.95	0.48
5:R:9:THR:O	5:R:10:ASN:OD1	2.30	0.48
10:D:44:ILE:HD11	10:D:89:LEU:HB3	1.96	0.48
13:G:90:LEU:HD11	13:G:119:HIS:CE1	2.48	0.48
20:O:430:ARG:NH1	20:O:610:TYR:OH	2.46	0.48
4:S:395:GLN:HB3	5:R:140:ILE:HG23	1.96	0.48
7:A:1238:MET:HB3	7:A:1521:THR:HB	1.96	0.48
8:B:202:LEU:HD23	8:B:488:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:289:PHE:HD1	8:B:306:LEU:HD22	1.77	0.48
5:R:21:TYR:HA	5:R:24:ILE:HB	1.94	0.48
8:B:913:ILE:HG13	8:B:930:LYS:HE2	1.95	0.48
8:B:1006:ASN:HD22	8:B:1010:ASN:HB2	1.78	0.48
14:H:112:ILE:N	14:H:127:GLY:O	2.46	0.48
20:O:448:SER:O	20:O:452:ARG:N	2.47	0.48
4:S:421:ILE:HA	4:S:442:LEU:H	1.79	0.47
7:A:720:PHE:HB2	14:H:96:VAL:HB	1.96	0.47
8:B:672:MET:HE1	8:B:674:ILE:HD11	1.94	0.47
12:F:94:LEU:HD13	12:F:122:MET:HG2	1.96	0.47
6:M:40:LEU:HD22	19:N:119:LEU:HD11	1.97	0.47
8:B:750:PRO:HG2	8:B:753:LYS:HB3	1.96	0.47
20:O:330:THR:HA	20:O:333:ASP:HB2	1.96	0.47
4:S:215:ASN:HB2	4:S:233:VAL:HB	1.96	0.47
8:B:95:LEU:HD13	8:B:95:LEU:O	2.14	0.47
8:B:588:ILE:HG22	8:B:642:LEU:HB2	1.96	0.47
8:B:860:ALA:HA	8:B:871:ILE:HG22	1.96	0.47
5:R:442:LEU:O	5:R:443:TYR:CG	2.67	0.47
7:A:1124:LEU:HD22	7:A:1129:PRO:HG3	1.96	0.47
4:S:270:GLN:HG2	4:S:291:PRO:HB3	1.97	0.47
7:A:882:ILE:HG22	7:A:888:LYS:HB3	1.97	0.47
7:A:1555:VAL:HG21	7:A:1593:GLY:HA2	1.96	0.47
4:S:428:GLU:HG2	4:S:430:ASN:H	1.80	0.47
5:R:247:ILE:HA	5:R:250:LEU:HD12	1.96	0.47
6:M:41:TYR:HB2	6:M:52:VAL:HB	1.95	0.47
7:A:1047:GLN:NE2	7:A:1587:ASP:OD2	2.45	0.47
17:K:46:LYS:HA	17:K:66:VAL:HG22	1.96	0.47
3:Q:312:LEU:HD21	3:Q:506:LYS:HB2	1.96	0.47
4:S:184:SER:N	4:S:509:GLU:OE2	2.45	0.47
7:A:1197:SER:HA	7:A:1200:MET:HG2	1.97	0.47
19:N:89:ILE:HG13	19:N:139:VAL:HG22	1.96	0.47
20:O:383:TYR:O	20:O:387:HIS:N	2.45	0.47
4:S:472:ARG:NH2	5:R:200:THR:OG1	2.48	0.46
7:A:883:LEU:HD22	7:A:972:TYR:HE1	1.81	0.46
8:B:708:ASP:OD1	8:B:708:ASP:N	2.46	0.46
3:Q:21:ARG:HA	3:Q:27:ARG:HA	1.96	0.46
4:S:20:VAL:HG12	4:S:25:LEU:HD13	1.96	0.46
7:A:1091:VAL:HG13	7:A:1133:LEU:HD23	1.98	0.46
8:B:98:SER:HB3	8:B:142:LYS:HB3	1.96	0.46
15:I:86:CYS:HB3	15:I:91:ASN:HB3	1.96	0.46
4:S:230:HIS:ND1	4:S:282:CYS:SG	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:133:VAL:HG21	13:G:104:LEU:HD22	1.97	0.46
20:O:521:ASN:HB2	20:O:589:GLN:HB3	1.97	0.46
3:Q:297:ARG:O	3:Q:504:ARG:NH2	2.49	0.46
4:S:622:TYR:O	4:S:626:LEU:N	2.48	0.46
7:A:1641:ILE:HD11	8:B:1088:LEU:HD21	1.97	0.46
6:M:88:ILE:HD11	19:N:70:LEU:HD13	1.97	0.46
7:A:49:LEU:HD23	7:A:383:ASN:HD22	1.81	0.46
7:A:524:ILE:HG12	7:A:555:LYS:HG2	1.97	0.46
9:C:84:TYR:HB3	18:L:64:LEU:HD11	1.97	0.46
9:C:107:LYS:HE3	9:C:187:ALA:HA	1.98	0.46
10:D:86:ILE:HG22	10:D:90:LYS:HE3	1.98	0.46
11:E:97:VAL:HG21	11:E:123:LEU:HB3	1.97	0.46
1:T:28:DC:OP1	8:B:434:ARG:NH1	2.49	0.46
19:N:117:GLU:HG2	19:N:118:SER:H	1.81	0.46
5:R:237:ALA:O	5:R:241:ARG:NH2	2.41	0.46
7:A:318:THR:O	7:A:322:ASN:ND2	2.49	0.46
7:A:694:GLN:NE2	17:K:91:TYR:O	2.43	0.46
8:B:634:ARG:NH1	15:I:54:ASP:OD2	2.49	0.46
1:T:21:DG:OP1	7:A:421:SER:OG	2.34	0.46
8:B:824:HIS:ND1	8:B:897:GLU:OE1	2.40	0.46
15:I:30:CYS:SG	15:I:31:SER:N	2.89	0.46
4:S:175:ASP:OD2	4:S:177:THR:OG1	2.26	0.45
7:A:342:ARG:NH1	7:A:1629:ASN:O	2.48	0.45
13:G:93:ASP:HB2	13:G:104:LEU:HD11	1.98	0.45
20:O:379:ARG:HA	20:O:382:GLN:HE22	1.81	0.45
5:R:169:PRO:O	5:R:173:MET:N	2.49	0.45
11:E:93:MET:HG3	11:E:120:ALA:HB1	1.98	0.45
4:S:58:HIS:HB3	4:S:552:LEU:HD22	1.99	0.45
7:A:718:THR:HG21	14:H:119:GLY:HA3	1.98	0.45
13:G:159:LYS:HB3	20:O:105:ASN:HD21	1.82	0.45
4:S:442:LEU:CD2	4:S:444:PRO:N	2.80	0.45
6:M:13:GLU:HB2	6:M:89:GLN:HB3	1.98	0.45
7:A:239:PHE:O	7:A:239:PHE:CD2	2.70	0.45
7:A:581:ILE:HD11	7:A:605:VAL:HG21	1.99	0.45
8:B:887:LEU:HD23	8:B:898:LEU:HD22	1.98	0.45
8:B:935:ASP:N	8:B:935:ASP:OD1	2.38	0.45
3:Q:450:THR:HB	4:S:724:LEU:HD21	1.98	0.45
4:S:504:THR:O	4:S:542:ARG:N	2.39	0.45
4:S:746:ARG:HH22	4:S:749:LYS:HD2	1.82	0.45
7:A:77:GLY:O	7:A:362:VAL:N	2.46	0.45
8:B:711:GLN:HG2	8:B:713:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:239:HIS:O	4:S:267:ASN:ND2	2.50	0.45
7:A:32:ILE:HD12	7:A:362:VAL:HG21	1.98	0.45
13:G:166:TRP:HZ3	13:G:249:LEU:HD13	1.81	0.45
14:H:128:ASN:N	14:H:128:ASN:OD1	2.48	0.45
3:Q:172:LEU:HD23	3:Q:174:LEU:HD11	1.99	0.45
3:Q:413:LEU:HD21	5:R:240:ILE:HD12	1.99	0.45
7:A:1240:LEU:HB2	7:A:1519:LEU:HB2	1.98	0.45
8:B:128:GLN:HB2	18:L:55:ILE:HD13	1.98	0.45
8:B:735:HIS:HE1	16:J:63:TYR:HB3	1.82	0.45
8:B:770:ASN:HD22	16:J:52:THR:HG21	1.81	0.45
19:N:92:ASP:OD1	19:N:92:ASP:N	2.50	0.45
3:Q:99:GLU:O	3:Q:103:LEU:N	2.47	0.45
4:S:202:ILE:HA	4:S:219:LEU:HD13	1.98	0.45
5:R:302:ARG:NH2	8:B:155:VAL:O	2.49	0.45
7:A:331:GLU:HB3	7:A:334:VAL:HG12	1.97	0.45
12:F:135:ARG:NH2	13:G:92:ALA:O	2.42	0.45
3:Q:289:ARG:HH12	3:Q:294:HIS:C	2.20	0.44
4:S:215:ASN:HB3	4:S:235:SER:HA	1.98	0.44
5:R:268:LEU:HD22	5:R:319:ASN:HD22	1.82	0.44
7:A:373:LEU:HD11	7:A:376:GLU:OE1	2.17	0.44
7:A:438:ILE:HA	7:A:456:VAL:HG22	1.98	0.44
8:B:838:GLU:O	18:L:63:ARG:NH2	2.50	0.44
9:C:192:LEU:HD21	9:C:195:LYS:HE3	1.99	0.44
9:C:216:HIS:HD2	9:C:218:LYS:H	1.65	0.44
4:S:674:GLU:O	4:S:677:SER:OG	2.30	0.44
7:A:1038:ILE:HB	7:A:1047:GLN:HB2	1.99	0.44
9:C:259:ASP:HB3	9:C:263:ASP:HB3	1.99	0.44
7:A:427:PHE:HA	7:A:430:ILE:HG22	2.00	0.44
7:A:1105:ARG:NH1	7:A:1138:GLU:HB3	2.33	0.44
19:N:57:LYS:HB2	19:N:138:SER:HA	1.98	0.44
19:N:157:ARG:HH12	19:N:159:ASP:HA	1.82	0.44
20:O:454:VAL:HG13	20:O:455:ILE:HG13	1.99	0.44
19:N:53:VAL:HG11	19:N:109:LEU:HD22	2.00	0.44
3:Q:163:SER:O	3:Q:167:LEU:N	2.42	0.44
3:Q:209:ASN:OD1	3:Q:209:ASN:N	2.37	0.44
3:Q:257:VAL:HG22	3:Q:262:LEU:HD11	1.99	0.44
7:A:31:GLN:HB3	7:A:78:HIS:CE1	2.52	0.44
7:A:1390:ASP:O	7:A:1394:THR:N	2.43	0.44
9:C:120:LEU:C	9:C:120:LEU:CD1	2.85	0.44
12:F:72:LYS:HB3	12:F:142:SER:HA	2.00	0.44
5:R:251:TRP:HA	5:R:270:PHE:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:745:PRO:HG2	7:A:1075:ALA:HB2	2.00	0.44
8:B:1123:ILE:HD11	13:G:241:ARG:HH11	1.82	0.44
8:B:1128:CYS:SG	8:B:1129:ARG:N	2.91	0.44
10:D:1:MET:HG3	10:D:4:GLY:H	1.82	0.44
7:A:701:ARG:H	7:A:706:HIS:CD2	2.29	0.44
7:A:901:ASN:HB3	15:I:80:ALA:N	2.33	0.44
7:A:1029:GLY:HA3	7:A:1041:ALA:HB2	2.00	0.44
7:A:1501:ILE:HG23	7:A:1504:ILE:HB	2.00	0.44
7:A:1634:LEU:HD13	7:A:1643:VAL:HG11	2.00	0.44
10:D:94:ARG:HH12	10:D:100:PRO:HA	1.83	0.44
20:O:130:PRO:HA	20:O:133:LEU:HB3	1.99	0.44
4:S:623:LEU:C	4:S:623:LEU:CD1	2.85	0.44
7:A:1086:ILE:H	7:A:1086:ILE:HG13	1.57	0.44
8:B:352:GLU:OE2	8:B:356:ARG:NH2	2.51	0.44
8:B:429:ARG:HA	8:B:432:ILE:HG12	1.99	0.44
8:B:1115:GLN:NE2	8:B:1124:SER:OG	2.49	0.44
4:S:442:LEU:CD2	4:S:442:LEU:C	2.86	0.43
5:R:233:TYR:CD2	5:R:233:TYR:C	2.91	0.43
3:Q:144:ILE:HD12	3:Q:154:LEU:HB2	2.00	0.43
8:B:95:LEU:CD1	8:B:95:LEU:C	2.86	0.43
8:B:1155:ASP:HA	8:B:1158:ILE:HD12	1.99	0.43
6:M:9:GLU:HA	19:N:71:PRO:HA	2.00	0.43
9:C:31:TRP:HB3	17:K:82:LYS:HB3	1.99	0.43
4:S:23:ALA:HA	4:S:436:ILE:HD13	2.01	0.43
8:B:532:HIS:ND1	8:B:719:CYS:HB3	2.34	0.43
8:B:781:TYR:HE2	17:K:96:PRO:HG2	1.84	0.43
20:O:63:LEU:O	20:O:66:ASN:ND2	2.52	0.43
20:O:201:LYS:HG3	20:O:240:ILE:HG13	1.99	0.43
4:S:323:ASN:HA	4:S:350:THR:HA	2.01	0.43
6:M:77:VAL:HB	19:N:56:ILE:HG13	2.01	0.43
13:G:234:ARG:HG2	13:G:235:ASN:H	1.83	0.43
20:O:62:ASP:HA	20:O:65:LYS:HB2	2.00	0.43
4:S:44:ARG:O	4:S:46:VAL:N	2.51	0.43
7:A:1012:LYS:HG3	7:A:1201:THR:HG21	1.98	0.43
10:D:88:GLN:NE2	20:O:184:PRO:O	2.51	0.43
3:Q:42:ASN:HD22	3:Q:43:ASP:N	2.17	0.43
3:Q:198:ILE:O	3:Q:201:LYS:NZ	2.51	0.43
4:S:363:ILE:HG22	4:S:374:VAL:HG22	2.00	0.43
5:R:133:LYS:HA	5:R:134:PRO:HD3	1.90	0.43
5:R:275:CYS:O	5:R:279:SER:OG	2.32	0.43
6:M:66:THR:HB	6:M:71:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1470:CYS:SG	7:A:1471:GLU:N	2.92	0.43
8:B:850:THR:HB	8:B:882:ILE:HD13	2.01	0.43
16:J:36:LEU:HD11	16:J:51:LEU:HD12	2.00	0.43
20:O:517:LEU:HD11	20:O:540:CYS:HB2	2.01	0.43
3:Q:42:ASN:HD22	3:Q:43:ASP:H	1.66	0.43
3:Q:352:ILE:HD13	3:Q:377:PHE:CE1	2.54	0.43
7:A:83:VAL:HG11	7:A:427:PHE:HE1	1.83	0.43
7:A:1393:GLU:O	7:A:1397:GLU:N	2.49	0.43
4:S:228:ASN:HD22	4:S:282:CYS:HB3	1.83	0.43
7:A:64:THR:O	8:B:1114:GLN:NE2	2.52	0.43
7:A:1274:GLU:HB3	15:I:47:VAL:HG23	2.01	0.43
3:Q:20:TRP:N	3:Q:28:THR:O	2.52	0.43
7:A:595:LEU:HD13	7:A:1198:THR:HG21	2.01	0.43
7:A:1060:GLU:OE2	7:A:1580:ARG:NH1	2.44	0.43
7:A:1240:LEU:HB3	7:A:1536:ILE:HD12	2.01	0.43
8:B:651:ARG:HH11	8:B:651:ARG:HD3	1.72	0.43
13:G:48:SER:H	13:G:65:HIS:CE1	2.37	0.43
13:G:56:ASN:ND2	13:G:59:GLN:OE1	2.52	0.43
20:O:205:ARG:HA	20:O:208:LEU:HB2	2.01	0.43
3:Q:351:ASN:ND2	3:Q:373:GLU:OE2	2.49	0.42
4:S:474:LYS:HE3	4:S:474:LYS:HB2	1.87	0.42
7:A:432:ASN:CG	7:A:444:GLN:OE1	2.55	0.42
7:A:444:GLN:NE2	7:A:444:GLN:CA	2.81	0.42
7:A:1457:ILE:HD13	7:A:1457:ILE:HA	1.84	0.42
20:O:77:GLN:HG2	20:O:88:ILE:HB	1.99	0.42
11:E:76:GLY:N	11:E:106:GLN:OE1	2.39	0.42
12:F:69:LEU:HD23	13:G:94:PRO:HG3	2.01	0.42
19:N:31:LYS:HG3	19:N:33:LYS:HE3	2.01	0.42
4:S:254:ILE:HG23	4:S:256:ARG:H	1.84	0.42
7:A:373:LEU:HG	7:A:376:GLU:HB2	2.01	0.42
7:A:1025:LYS:HG3	7:A:1615:TYR:HD1	1.84	0.42
7:A:1554:GLY:HA2	11:E:183:PRO:HD2	2.01	0.42
7:A:1620:GLN:HE21	7:A:1624:LYS:NZ	2.17	0.42
8:B:140:LYS:HB3	8:B:155:VAL:HG22	2.00	0.42
8:B:692:THR:HG22	8:B:694:THR:H	1.84	0.42
13:G:137:ILE:HB	13:G:227:GLY:HA2	2.00	0.42
8:B:815:ARG:NH2	8:B:899:GLN:OE1	2.52	0.42
17:K:67:GLU:HA	17:K:99:ASN:HB3	2.02	0.42
4:S:696:PHE:HZ	4:S:747:LEU:HD11	1.85	0.42
7:A:444:GLN:N	7:A:444:GLN:CD	2.73	0.42
4:S:36:LYS:HG2	4:S:38:GLU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:33:CYS:SG	15:I:34:LYS:N	2.92	0.42
3:Q:413:LEU:HA	3:Q:416:ILE:HG22	2.02	0.42
5:R:174:GLU:HA	5:R:177:LEU:HD12	2.00	0.42
7:A:110:LEU:HD13	7:A:230:ARG:HH11	1.84	0.42
7:A:530:TRP:O	7:A:532:GLY:N	2.53	0.42
8:B:150:GLU:HG2	8:B:441:LYS:HG2	2.01	0.42
8:B:524:SER:HB3	8:B:528:LEU:HB2	2.02	0.42
10:D:89:LEU:O	10:D:93:GLN:N	2.44	0.42
15:I:8:ILE:HG23	15:I:17:LEU:HB2	2.01	0.42
4:S:36:LYS:HG3	4:S:46:VAL:HG23	2.02	0.42
5:R:414:PHE:HA	5:R:417:ILE:HG22	2.02	0.42
7:A:28:SER:O	7:A:78:HIS:ND1	2.51	0.42
7:A:743:ASP:N	7:A:743:ASP:OD1	2.49	0.42
8:B:258:VAL:HG12	8:B:273:VAL:HG21	2.00	0.42
7:A:95:TYR:CZ	7:A:99:ARG:HD2	2.55	0.42
7:A:1121:ASP:OD1	7:A:1121:ASP:N	2.50	0.42
8:B:96:SER:N	8:B:144:SER:O	2.48	0.42
20:O:332:LEU:HD23	20:O:599:LEU:HD11	2.02	0.42
7:A:9:SER:HA	8:B:1202:PRO:HG2	2.01	0.42
7:A:621:THR:OG1	7:A:626:ALA:O	2.37	0.42
7:A:745:PRO:O	7:A:801:TYR:OH	2.34	0.42
3:Q:341:ARG:NH1	3:Q:365:ASP:OD2	2.54	0.41
3:Q:480:LEU:HA	3:Q:483:ILE:HG22	2.01	0.41
6:M:81:PHE:HB3	19:N:52:GLN:HB2	2.02	0.41
8:B:273:VAL:HG11	8:B:378:ILE:HD11	2.02	0.41
3:Q:197:GLU:HA	3:Q:204:ARG:HH22	1.85	0.41
4:S:63:SER:OG	4:S:64:LEU:N	2.53	0.41
4:S:271:ILE:HD12	4:S:305:PHE:HZ	1.85	0.41
7:A:239:PHE:CD2	7:A:239:PHE:C	2.94	0.41
8:B:210:ARG:NH1	8:B:625:GLU:OE2	2.53	0.41
8:B:714:ARG:HD3	8:B:714:ARG:HA	1.75	0.41
9:C:115:TRP:HH2	9:C:212:ILE:HG23	1.86	0.41
10:D:99:LEU:HD12	10:D:100:PRO:HD2	2.02	0.41
3:Q:326:TYR:O	3:Q:472:ARG:NH2	2.37	0.41
5:R:442:LEU:C	5:R:443:TYR:CD2	2.93	0.41
7:A:986:PHE:HB3	8:B:960:ILE:HD12	2.02	0.41
13:G:62:MET:HA	13:G:66:LEU:HD12	2.02	0.41
20:O:59:ALA:HB2	20:O:70:GLN:HB2	2.01	0.41
3:Q:376:GLU:HA	3:Q:379:LYS:HB2	2.02	0.41
7:A:952:LEU:HD12	7:A:957:VAL:HA	2.03	0.41
8:B:71:LYS:HB3	8:B:425:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1014:TYR:HE2	9:C:228:ARG:HA	1.85	0.41
4:S:467:PHE:HB3	4:S:476:ILE:HD11	2.01	0.41
4:S:626:LEU:HD11	4:S:666:SER:HA	2.01	0.41
4:S:658:LYS:HG3	4:S:660:LYS:H	1.86	0.41
5:R:384:VAL:HG22	5:R:397:ARG:HD3	2.03	0.41
7:A:597:LYS:HE3	7:A:660:PRO:HG2	2.02	0.41
7:A:821:ILE:HD13	7:A:821:ILE:HA	1.89	0.41
8:B:788:ILE:HB	8:B:948:ILE:HB	2.02	0.41
8:B:823:GLN:HA	8:B:863:ASP:HA	2.02	0.41
9:C:320:ILE:O	9:C:324:LYS:N	2.51	0.41
6:M:42:LYS:N	19:N:30:LYS:O	2.53	0.41
7:A:239:PHE:HD2	7:A:239:PHE:C	2.23	0.41
7:A:1661:PRO:O	13:G:101:SER:OG	2.33	0.41
20:O:364:LEU:O	20:O:368:PHE:N	2.53	0.41
4:S:446:ASP:HB3	4:S:449:LEU:HG	2.03	0.41
7:A:522:ALA:HA	7:A:532:GLY:HA2	2.02	0.41
11:E:32:GLN:HE21	11:E:36:GLU:HG3	1.86	0.41
7:A:385:LEU:HD13	7:A:437:PHE:HA	2.03	0.41
9:C:264:GLU:H	9:C:264:GLU:HG2	1.66	0.41
20:O:393:LEU:HA	20:O:396:MET:HE3	2.03	0.41
3:Q:258:MET:HE3	4:S:704:LEU:HD23	2.02	0.41
3:Q:284:LEU:HA	3:Q:284:LEU:HD23	1.88	0.41
4:S:207:SER:O	4:S:212:SER:N	2.54	0.41
4:S:319:ASP:HB2	4:S:363:ILE:HG12	2.03	0.41
7:A:912:VAL:HG23	7:A:913:PRO:HD3	2.02	0.41
7:A:1392:ILE:O	7:A:1396:ARG:N	2.52	0.41
8:B:597:SER:OG	8:B:598:HIS:N	2.54	0.41
8:B:679:GLN:NE2	19:N:155:VAL:O	2.52	0.41
17:K:104:ARG:HE	17:K:106:GLN:NE2	2.18	0.41
20:O:155:SER:HA	20:O:158:LEU:HB2	2.03	0.41
4:S:472:ARG:HH21	4:S:472:ARG:HD3	1.74	0.41
11:E:78:LEU:HD11	11:E:109:ILE:HG13	2.02	0.41
11:E:100:ILE:HD11	11:E:108:GLY:HA3	2.02	0.41
19:N:56:ILE:HG22	19:N:137:PHE:HB2	2.02	0.41
2:U:38:DT:H2'	2:U:39:DG:C8	2.56	0.40
3:Q:19:LEU:HD13	3:Q:27:ARG:HE	1.85	0.40
4:S:230:HIS:CE1	4:S:282:CYS:HG	2.39	0.40
7:A:1341:GLY:HA2	7:A:1342:PRO:HD3	1.93	0.40
8:B:791:LYS:O	8:B:795:GLU:HG2	2.21	0.40
9:C:164:ALA:HB2	9:C:191:ILE:HB	2.03	0.40
20:O:164:LEU:HB3	20:O:168:GLN:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:75:LEU:HD13	3:Q:76:THR:HG23	2.03	0.40
4:S:403:ARG:HH21	4:S:419:ARG:HD2	1.86	0.40
5:R:168:ILE:HG23	5:R:169:PRO:HD3	2.04	0.40
7:A:373:LEU:O	7:A:373:LEU:CG	2.69	0.40
7:A:1033:SER:OG	7:A:1034:TYR:N	2.54	0.40
9:C:240:LYS:HB2	9:C:261:GLY:HA2	2.03	0.40
3:Q:318:LEU:HB3	3:Q:476:ILE:HD12	2.03	0.40
3:Q:352:ILE:CD1	3:Q:377:PHE:CD1	3.04	0.40
7:A:523:VAL:HB	7:A:558:ALA:HB2	2.03	0.40
8:B:648:ARG:NH1	8:B:650:LEU:HD21	2.36	0.40
10:D:6:ARG:O	10:D:10:ASN:N	2.54	0.40
17:K:105:ILE:HB	17:K:113:ALA:HB1	2.02	0.40
7:A:29:ALA:HA	7:A:78:HIS:HE1	1.86	0.40
1:T:27:DC:H5'	8:B:434:ARG:HD2	2.04	0.40
3:Q:103:LEU:HD21	3:Q:206:GLN:HG3	2.02	0.40
3:Q:282:ARG:HG3	3:Q:283:ASN:H	1.86	0.40
6:M:61:GLU:HB2	6:M:103:LYS:HD2	2.03	0.40
7:A:527:PRO:HB3	7:A:534:THR:HG22	2.02	0.40
8:B:120:LYS:HG3	8:B:171:HIS:CE1	2.57	0.40
8:B:275:MET:HG2	8:B:330:LEU:HD12	2.04	0.40
8:B:490:LYS:HD2	8:B:490:LYS:HA	1.90	0.40
8:B:1099:THR:HG21	8:B:1180:PHE:HD1	1.86	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	468/514 (91%)	409 (87%)	58 (12%)	1 (0%)	47 78
4	S	594/894 (66%)	509 (86%)	85 (14%)	0	100 100
5	R	322/507 (64%)	292 (91%)	30 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	M	105/415 (25%)	98 (93%)	7 (7%)	0	100	100
7	A	1524/1664 (92%)	1416 (93%)	108 (7%)	0	100	100
8	B	1174/1203 (98%)	1095 (93%)	79 (7%)	0	100	100
9	C	300/335 (90%)	283 (94%)	17 (6%)	0	100	100
10	D	66/137 (48%)	62 (94%)	4 (6%)	0	100	100
11	E	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
12	F	98/155 (63%)	93 (95%)	5 (5%)	0	100	100
13	G	193/326 (59%)	178 (92%)	15 (8%)	0	100	100
14	H	130/146 (89%)	118 (91%)	12 (9%)	0	100	100
15	I	122/125 (98%)	104 (85%)	18 (15%)	0	100	100
16	J	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
17	K	101/142 (71%)	95 (94%)	6 (6%)	0	100	100
18	L	43/70 (61%)	41 (95%)	2 (5%)	0	100	100
19	N	131/233 (56%)	115 (88%)	16 (12%)	0	100	100
20	O	493/627 (79%)	453 (92%)	40 (8%)	0	100	100
All	All	6144/7778 (79%)	5633 (92%)	510 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Q	281	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	436/476 (92%)	427 (98%)	9 (2%)	53	81
4	S	563/828 (68%)	555 (99%)	8 (1%)	67	89
5	R	313/474 (66%)	305 (97%)	8 (3%)	46	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	M	97/371 (26%)	97 (100%)	0	100	100
7	A	1297/1465 (88%)	1293 (100%)	4 (0%)	92	98
8	B	1030/1053 (98%)	1026 (100%)	4 (0%)	91	97
9	C	269/296 (91%)	268 (100%)	1 (0%)	91	97
10	D	65/116 (56%)	65 (100%)	0	100	100
11	E	197/197 (100%)	195 (99%)	2 (1%)	76	92
12	F	90/137 (66%)	89 (99%)	1 (1%)	73	92
13	G	177/291 (61%)	177 (100%)	0	100	100
14	H	116/128 (91%)	115 (99%)	1 (1%)	78	93
15	I	109/110 (99%)	108 (99%)	1 (1%)	78	93
16	J	64/65 (98%)	63 (98%)	1 (2%)	62	86
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%)	128 (100%)	0	100	100
20	O	457/576 (79%)	457 (100%)	0	100	100
All	All	5541/6990 (79%)	5501 (99%)	40 (1%)	84	95

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	14	ASN
3	Q	18	ARG
3	Q	21	ARG
3	Q	42	ASN
3	Q	79	GLN
3	Q	209	ASN
3	Q	293	ARG
3	Q	297	ARG
3	Q	480	LEU
4	S	49	THR
4	S	227	LEU
4	S	292	LEU
4	S	379	LYS
4	S	407	ARG
4	S	623	LEU
4	S	665	ASN
4	S	744	LEU

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Mol	Chain	Res	Type
5	R	11	ARG
5	R	182	LYS
5	R	206	ARG
5	R	207	ASN
5	R	283	ARG
5	R	288	ILE
5	R	317	LEU
5	R	368	TYR
7	A	239	PHE
7	A	444	GLN
7	A	467	PHE
7	A	590	ASN
8	B	95	LEU
8	B	306	LEU
8	B	651	ARG
8	B	783	MET
9	C	281	ARG
11	E	11	ARG
11	E	200	ARG
12	F	79	ARG
14	H	142	LEU
15	I	47	VAL
16	J	52	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
3	Q	14	ASN
3	Q	42	ASN
3	Q	149	GLN
3	Q	206	GLN
3	Q	228	ASN
3	Q	294	HIS
3	Q	482	HIS
4	S	222	GLN
4	S	267	ASN
4	S	440	HIS
4	S	461	HIS
4	S	483	HIS
4	S	487	ASN
5	R	207	ASN
5	R	263	ASN

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Mol	Chain	Res	Type
5	R	286	GLN
5	R	304	HIS
5	R	319	ASN
5	R	382	GLN
6	M	89	GLN
7	A	322	ASN
7	A	332	GLN
7	A	383	ASN
7	A	431	GLN
7	A	592	GLN
7	A	636	HIS
7	A	706	HIS
7	A	748	ASN
7	A	785	GLN
7	A	880	GLN
7	A	926	GLN
7	A	1062	HIS
7	A	1072	ASN
7	A	1436	ASN
7	A	1487	ASN
7	A	1620	GLN
7	A	1629	ASN
8	B	62	ASN
8	B	212	ASN
8	B	231	HIS
8	B	243	GLN
8	B	248	ASN
8	B	251	HIS
8	B	361	HIS
8	B	427	GLN
8	B	456	ASN
8	B	686	HIS
8	B	735	HIS
8	B	770	ASN
8	B	1008	HIS
8	B	1041	ASN
8	B	1115	GLN
9	C	248	GLN
9	C	297	HIS
11	E	32	GLN
11	E	147	HIS
13	G	65	HIS

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Mol	Chain	Res	Type
15	I	95	ASN
17	K	106	GLN
20	O	66	ASN
20	O	94	ASN
20	O	105	ASN
20	O	200	ASN
20	O	318	ASN
20	O	547	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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-4984. 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)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

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)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit (i)

This section was not generated.