



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 08:14 PM JST

PDB ID : 9K7F / pdb_00009k7f
EMDB ID : EMD-62148
Title : RNA polymerase II elongation complex apo structure.
Authors : Xu, J.; Zhao, W.; Zhu, L.
Deposited on : 2024-10-23
Resolution : 2.50 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	: FAILED
MolProbity	: 4-5-2 with Phenix2.0
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	: NOT EXECUTED
MapQ	: FAILED
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.49

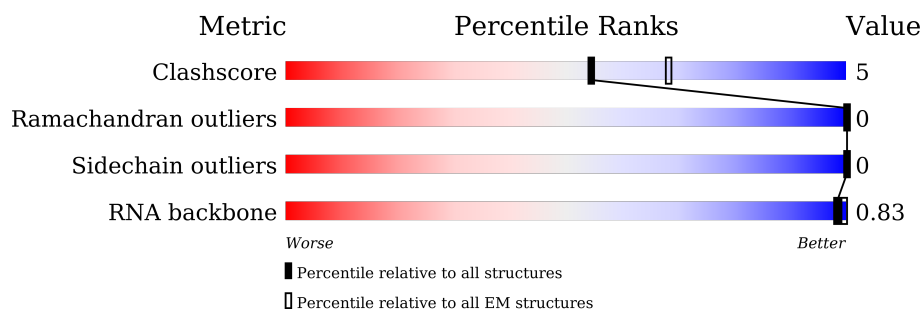
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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.



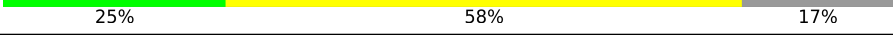
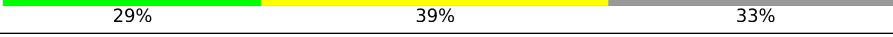
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1733	71% 10% 18%
2	B	1224	86% 10% .
3	C	318	71% 13% 17%
4	D	221	59% 16% 25%
5	E	215	89% 10%
6	F	155	50% 6% 44%
7	G	171	73% 27%
8	H	146	87% 9% .

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Mol	Chain	Length	Quality of chain
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	49	
14	P	12	
15	T	49	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 33011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1418	Total	C	N	O	S	0	0
			11153	7029	1947	2115	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1179	Total	C	N	O	S	0	0
			9400	5944	1642	1759	55		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	265	Total	C	N	O	S	0	0
			2086	1312	347	414	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	166	Total	C	N	O	S	0	0
			1332	823	238	269	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1339	861	222	248	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	704	188	224	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 13 is a DNA chain called NTS(non-template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	21	Total	C	N	O	P	0	0
			436	208	86	121	21		

- Molecule 14 is a RNA chain called RNA (5'-R(*CP*CP*CP*UP*AP*AP*GP*AP*GP*UP

*AP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	10	Total	C	N	O	P	0	0
			214	96	40	68	10		

- Molecule 15 is a DNA chain called TS(template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	33	Total	C	N	O	P	0	0
			669	324	105	207	33		

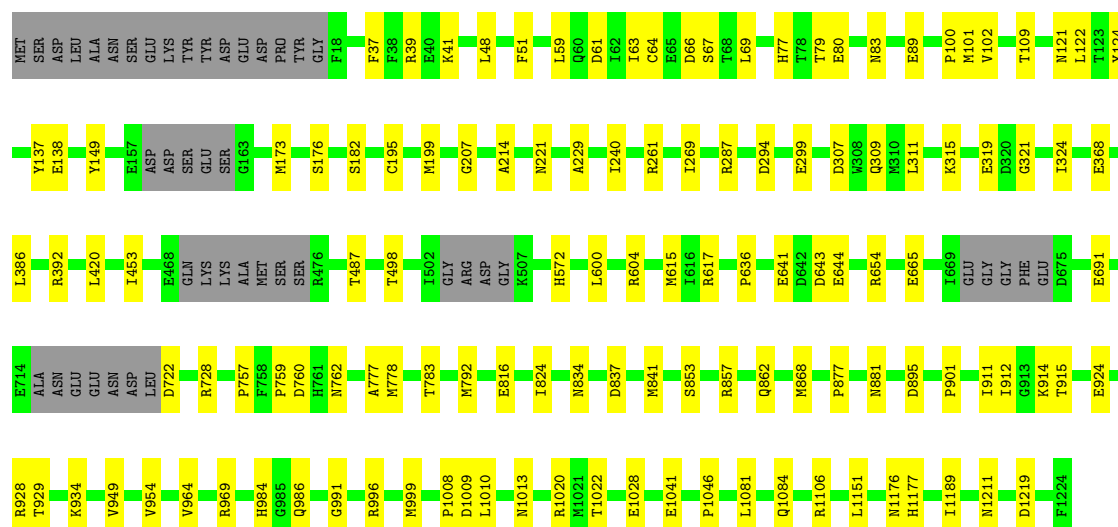
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

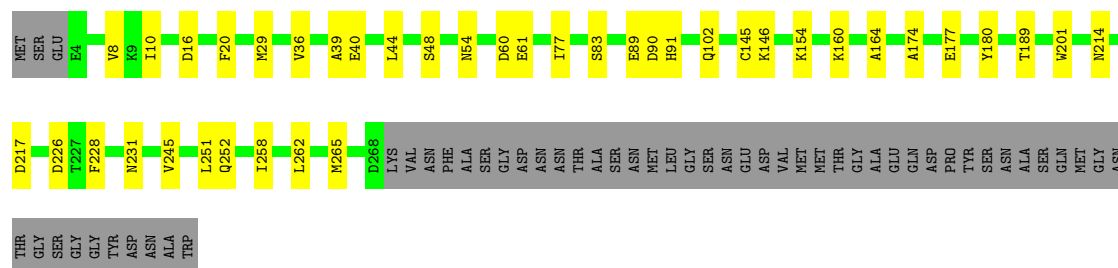
Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Mg	0
			1	1	

Chain B:  86% 10%



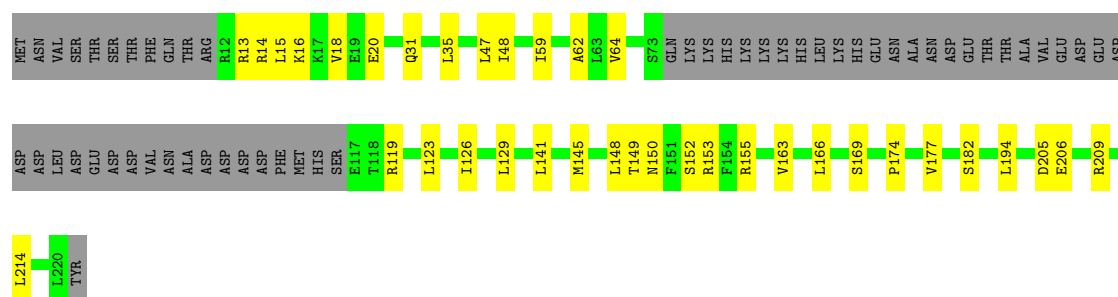
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:  71% 13% 17%



- Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:  59% 16% 25%



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

Chain E:  89% 10%



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

Chain F: 

MET SER GLU ASP TYR ILE ARG GLU ALA PHE ASN ASP GLY ASN GLU ASN PHE GLU PHE ASP PHE VAL GLU HIS PHE SER ASP GLU GLU THR TYR GLU LYS PRO GLN PHE PHE LYS ASP GLY THR THR ASP ALA ASN GLY LYS THR ILE VAL THR GLY GLY ASN GLY PRO GLU ASP PHE GLN

HIS GLU GLN F3 ILE ARG ARG LYS THR L69 E89 R97 Q100 M103 D116 R119 V133 R136 W146 S147 L156

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

Chain G: 

R1 F2 F3 I4 P15 F18 L30 L31 E32 E33 V34 E35 L45 L46 C47 V48 L49 R58 D65 Y74 R75 A76 W77 R83 G84 E85 V86 D87 D88 G89 R97 K112 M115 L119 A123 P128 S132 S133 E134 D135 T136 S141 R142

I143 R144 I147 E148 Q153 V154 S156 I163 Y167 L169 G169 A170 I171

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

Chain H: 

MET S2 V15 I26 T32 Q33 D34 S61 P69 ALA ASN ASP SER A75 P82 D86 R87 K103 S108 K109 R146

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

Chain I: 

MET T2 C7 L14 Y15 F16 R17 D19 N22 F23 R24 R30 R30 I52 D61 C78 V84 Q87 F101 L104 S105 C106 S112 K115 R116 R117 ARG THR GLN PHE SER

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

Chain J: 

R1 C7 L41 C46 R47 R48 N49 T52 L56 R69 ASP

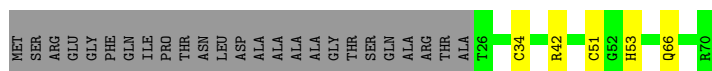
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K: 

R1 L42 L45 I46 R47 A48 E49 R54 T77 Y81 I94 I95 K102 F105 E106 T107 E108 Q112 T113 L114 A115 ALA ASP ASP ALA PHE

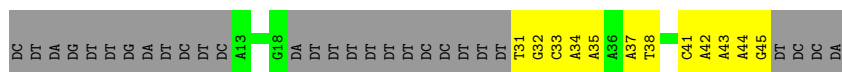
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  57% 7% 36%

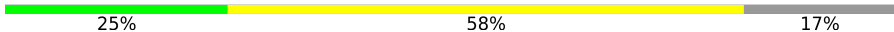


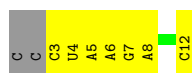
- Molecule 13: NTS(non-template strand)

Chain N:  18% 24% 57%

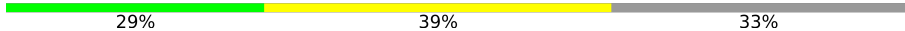


- Molecule 14: RNA (5'-R(*CP*CP*CP*UP*AP*AP*GP*AP*GP*UP*AP*C)-3')

Chain P:  25% 58% 17%



- Molecule 15: TS(template strand)

Chain T:  29% 39% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128658	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.18	0/11352	0.32	0/15350
2	B	0.18	0/9585	0.33	0/12929
3	C	0.19	0/2124	0.31	0/2879
4	D	0.13	0/1340	0.33	0/1797
5	E	0.18	0/1788	0.33	0/2406
6	F	0.20	0/717	0.31	0/967
7	G	0.15	0/1367	0.35	0/1844
8	H	0.15	0/1139	0.28	0/1544
9	I	0.13	0/962	0.33	0/1295
10	J	0.20	0/578	0.30	0/775
11	K	0.16	0/942	0.29	0/1272
12	L	0.14	0/361	0.37	0/478
13	N	0.17	0/490	0.37	0/752
14	P	0.19	0/239	0.28	0/370
15	T	0.24	0/745	0.46	0/1147
All	All	0.18	0/33729	0.33	0/45805

There are no bond length outliers.

There are no bond angle outliers.

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	A	11153	0	11228	116	0
2	B	9400	0	9395	79	0
3	C	2086	0	2045	29	0
4	D	1332	0	1353	28	0
5	E	1752	0	1776	13	0
6	F	705	0	731	6	0
7	G	1339	0	1357	31	0
8	H	1120	0	1086	9	0
9	I	944	0	899	12	0
10	J	569	0	585	6	0
11	K	924	0	934	15	0
12	L	359	0	381	4	0
13	N	436	0	238	12	0
14	P	214	0	108	5	0
15	T	669	0	380	13	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	33011	0	32496	334	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 5.

All (334) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ARG:NH2	2:B:991:GLY:O	2.15	0.80
1:A:597:LEU:HD21	8:H:103:LYS:HG2	1.65	0.78
2:B:837:ASP:OD1	2:B:1020:ARG:NH2	2.17	0.78
2:B:287:ARG:NH1	2:B:321:GLY:O	2.20	0.74
1:A:1166:ASP:HB2	1:A:1169:ILE:HD12	1.68	0.74
1:A:120:GLU:OE1	1:A:123:ARG:NH2	2.23	0.72
1:A:119:ASN:O	1:A:123:ARG:NH1	2.24	0.71
1:A:1446:ASP:OD1	7:G:58:ARG:NH1	2.24	0.71
5:E:106:GLN:HG2	5:E:107:THR:HG23	1.72	0.70
7:G:84:GLY:N	7:G:147:ILE:O	2.25	0.69
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.25	0.69
2:B:307:ASP:OD2	2:B:392:ARG:NH1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:901:PRO:HA	2:B:949:VAL:HG13	1.73	0.68
1:A:548:ASN:ND2	11:K:47:ARG:HH12	1.92	0.68
8:H:2:SER:N	8:H:61:SER:HG	1.92	0.68
1:A:767:GLN:NE2	1:A:768:GLN:O	2.27	0.67
1:A:1166:ASP:OD2	1:A:1239:ARG:NH1	2.27	0.67
2:B:487:THR:OG1	2:B:777:ALA:O	2.13	0.67
2:B:1219:ASP:O	4:D:13:ARG:NH2	2.27	0.67
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.77	0.67
1:A:700:ASN:O	9:I:115:LYS:NZ	2.28	0.66
2:B:928:ARG:NH1	2:B:929:THR:O	2.28	0.66
4:D:126:ILE:HD12	4:D:145:MET:HG3	1.78	0.66
1:A:157:ASP:OD1	1:A:160:GLN:NE2	2.30	0.65
2:B:617:ARG:NH2	9:I:61:ASP:OD2	2.30	0.64
1:A:346:ASP:OD1	2:B:1106:ARG:NE	2.29	0.64
15:T:7:DT:H2'	15:T:8:DT:H71	1.79	0.64
15:T:8:DT:H2''	15:T:9:DG:C8	2.33	0.64
1:A:840:ARG:NH1	1:A:1106:ASN:OD1	2.30	0.64
13:N:31:DT:H1'	13:N:32:DG:C8	2.33	0.64
1:A:355:GLY:O	1:A:469:ARG:NH1	2.31	0.63
1:A:1378:GLN:OE1	5:E:177:ARG:NH1	2.31	0.63
7:G:34:VAL:HG22	7:G:45:ILE:HG21	1.80	0.63
13:N:33:DC:H2'	13:N:34:DA:C8	2.33	0.62
7:G:88:ASP:OD1	7:G:89:GLY:N	2.33	0.62
2:B:895:ASP:O	12:L:42:ARG:NH2	2.33	0.61
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.81	0.61
1:A:1187:GLN:O	1:A:1244:ARG:N	2.29	0.61
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.74	0.61
8:H:86:ASP:O	8:H:87:ARG:NH1	2.34	0.60
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.33	0.60
1:A:922:ASP:OD1	1:A:923:LEU:N	2.35	0.60
13:N:43:DA:H2''	13:N:44:DA:H5''	1.83	0.60
2:B:643:ASP:OD2	2:B:654:ARG:NH2	2.34	0.60
7:G:133:SER:OG	7:G:134:GLU:OE1	2.20	0.59
1:A:147:VAL:HG13	1:A:149:GLU:HG2	1.84	0.59
2:B:604:ARG:NH2	2:B:691:GLU:OE2	2.35	0.59
1:A:473:SER:OG	1:A:650:GLN:NE2	2.36	0.59
2:B:792:MET:SD	2:B:857:ARG:NH2	2.76	0.59
2:B:319:GLU:OE1	9:I:30:ARG:NH1	2.36	0.58
2:B:1041:GLU:N	2:B:1041:GLU:OE1	2.34	0.58
1:A:63:ARG:NE	1:A:63:ARG:O	2.37	0.58
8:H:82:PRO:O	11:K:54:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:O	1:A:471:ASN:ND2	2.36	0.58
14:P:5:A:H2'	14:P:6:A:C8	2.39	0.58
1:A:402:ALA:HA	1:A:434:ARG:HA	1.86	0.58
1:A:1279:ILE:HD12	1:A:1308:THR:HG21	1.86	0.58
4:D:48:ILE:HD11	7:G:4:ILE:HD11	1.86	0.57
6:F:133:VAL:HG12	6:F:147:SER:HA	1.87	0.57
1:A:881:GLN:NE2	1:A:958:VAL:O	2.35	0.57
2:B:229:ALA:O	2:B:261:ARG:NH1	2.35	0.57
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.87	0.57
1:A:1244:ARG:NH2	1:A:1249:ASP:OD2	2.38	0.56
9:I:19:ASP:OD2	9:I:24:ARG:NH1	2.38	0.56
2:B:80:GLU:OE1	2:B:83:ASN:ND2	2.37	0.56
2:B:728:ARG:NH1	2:B:760:ASP:OD2	2.31	0.56
1:A:918:GLU:N	1:A:918:GLU:OE1	2.38	0.56
2:B:911:ILE:HG13	2:B:912:ILE:HG13	1.88	0.56
2:B:996:ARG:NH1	3:C:174:ALA:O	2.37	0.56
7:G:132:SER:OG	7:G:135:ASP:OD1	2.23	0.56
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.88	0.56
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.20	0.56
1:A:443:LEU:HD13	1:A:501:LEU:HD11	1.87	0.55
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.88	0.55
15:T:10:DT:H2''	15:T:11:DC:C6	2.42	0.55
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.88	0.55
1:A:997:LEU:O	1:A:1011:GLN:NE2	2.40	0.55
1:A:1215:ARG:NH2	1:A:1272:THR:O	2.40	0.55
4:D:62:ALA:HB2	7:G:49:LEU:HD13	1.89	0.55
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.89	0.54
7:G:115:MET:HG2	7:G:119:LEU:HD23	1.89	0.54
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.72	0.54
1:A:804:TYR:OH	1:A:816:HIS:NE2	2.40	0.54
4:D:152:SER:OG	4:D:155:ARG:NH2	2.41	0.54
2:B:287:ARG:NH1	2:B:324:ILE:O	2.41	0.54
12:L:51:CYS:SG	12:L:53:HIS:HB2	2.48	0.54
1:A:1030:ARG:NH2	1:A:1035:TYR:OH	2.35	0.54
1:A:1140:HIS:NE2	1:A:1277:GLU:OE2	2.41	0.54
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.90	0.54
1:A:528:LEU:O	1:A:531:ILE:HG22	2.08	0.53
1:A:1329:THR:HG22	1:A:1331:SER:H	1.73	0.53
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.42	0.53
2:B:881:ASN:O	2:B:934:LYS:NZ	2.41	0.53
1:A:1116:LEU:HD21	1:A:1327:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:64:VAL:HG12	4:D:129:LEU:HD11	1.91	0.53
9:I:78:CYS:SG	9:I:106:CYS:HB3	2.48	0.53
11:K:102:LYS:NZ	11:K:106:GLU:OE2	2.37	0.53
3:C:36:VAL:HG13	3:C:40:GLU:HB2	1.90	0.52
7:G:15:PRO:HA	7:G:18:PHE:CD2	2.44	0.52
2:B:644:GLU:N	2:B:644:GLU:OE1	2.37	0.52
13:N:44:DA:H2''	13:N:45:DG:C8	2.44	0.52
7:G:15:PRO:HA	7:G:18:PHE:CE2	2.45	0.52
1:A:119:ASN:OD1	1:A:120:GLU:N	2.43	0.52
4:D:166:LEU:O	4:D:169:SER:OG	2.24	0.52
1:A:596:THR:OG1	1:A:598:LEU:O	2.23	0.51
3:C:102:GLN:HG2	3:C:154:LYS:HG2	1.92	0.51
13:N:41:DC:H2''	13:N:42:DA:N7	2.25	0.51
2:B:641:GLU:OE1	2:B:641:GLU:N	2.43	0.51
1:A:1168:GLU:O	1:A:1171:GLN:HG3	2.10	0.51
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.92	0.51
7:G:83:LYS:NZ	7:G:148:GLU:O	2.35	0.51
1:A:1454:MET:SD	1:A:1454:MET:N	2.84	0.51
2:B:722:ASP:OD1	2:B:722:ASP:N	2.43	0.51
2:B:868:MET:N	2:B:868:MET:SD	2.83	0.51
2:B:102:VAL:HG21	2:B:122:LEU:HD13	1.92	0.51
3:C:145:CYS:SG	3:C:146:LYS:N	2.84	0.51
4:D:174:PRO:HA	4:D:177:VAL:HG22	1.92	0.51
15:T:26:DC:H2'	15:T:27:DT:H71	1.92	0.51
1:A:121:LEU:HB3	1:A:141:LEU:HD21	1.92	0.50
1:A:1115:SER:HA	1:A:1308:THR:O	2.12	0.50
4:D:126:ILE:HD13	4:D:149:THR:HG21	1.93	0.50
3:C:258:ILE:HG13	11:K:42:LEU:HD21	1.92	0.50
4:D:15:LEU:O	4:D:16:LYS:HG2	2.11	0.50
4:D:20:GLU:OE1	4:D:20:GLU:N	2.42	0.50
3:C:83:SER:HB3	3:C:160:LYS:HG2	1.93	0.50
1:A:844:ALA:HB2	1:A:1384:VAL:HG13	1.94	0.49
15:T:5:DC:H2'	15:T:6:DT:C6	2.47	0.49
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.48	0.49
1:A:1172:LEU:O	1:A:1175:SER:OG	2.20	0.49
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.77	0.49
1:A:528:LEU:HD23	1:A:751:SER:HA	1.94	0.49
7:G:97:HIS:O	7:G:112:LYS:N	2.44	0.49
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.94	0.49
1:A:451:HIS:ND1	1:A:453:MET:HE2	2.28	0.49
1:A:896:ARG:HD2	1:A:1030:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.95	0.49
1:A:339:ASN:O	1:A:343:LYS:HE2	2.12	0.49
7:G:84:GLY:CA	7:G:147:ILE:O	2.60	0.49
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.48	0.49
1:A:852:TYR:OH	6:F:89:GLU:OE2	2.18	0.48
13:N:42:DA:H8	13:N:42:DA:H5''	1.77	0.48
1:A:446:ARG:HB2	1:A:487:MET:HE3	1.94	0.48
2:B:51:PHE:HB2	2:B:173:MET:HE3	1.94	0.48
2:B:862:GLN:O	2:B:914:LYS:NZ	2.41	0.48
8:H:108:SER:OG	8:H:109:LYS:N	2.46	0.48
9:I:84:VAL:HG13	9:I:104:LEU:HD21	1.95	0.48
2:B:1081:LEU:O	3:C:189:THR:HG22	2.14	0.48
7:G:115:MET:HG3	7:G:163:ILE:HD11	1.96	0.48
4:D:141:LEU:HA	7:G:46:LEU:HD12	1.96	0.48
13:N:37:DA:H1'	13:N:38:DT:H5'	1.94	0.48
3:C:245:VAL:HG13	11:K:102:LYS:HE2	1.94	0.48
1:A:548:ASN:HD21	11:K:47:ARG:HH12	1.62	0.48
2:B:199:MET:SD	2:B:199:MET:N	2.73	0.48
11:K:114:LEU:H	11:K:114:LEU:HD23	1.78	0.48
2:B:214:ALA:HB3	2:B:498:THR:HG22	1.95	0.47
3:C:89:GLU:HG2	3:C:90:ASP:H	1.79	0.47
4:D:59:ILE:HD11	7:G:77:VAL:HG11	1.96	0.47
2:B:48:LEU:HD23	2:B:173:MET:SD	2.55	0.47
14:P:4:U:H2'	14:P:5:A:C8	2.49	0.47
1:A:515:GLN:NE2	1:A:1363:VAL:HG22	2.30	0.47
2:B:100:PRO:HG2	2:B:124:TYR:CZ	2.50	0.47
3:C:214:ASN:ND2	3:C:217:ASP:OD2	2.42	0.47
5:E:74:ASP:N	5:E:74:ASP:OD1	2.46	0.47
1:A:1143:LEU:HD12	1:A:1267:MET:O	2.15	0.47
7:G:31:LEU:HD22	7:G:35:GLU:HG3	1.96	0.47
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.96	0.47
1:A:404:TYR:HB2	1:A:433:GLU:HB3	1.97	0.47
2:B:69:LEU:O	2:B:89:GLU:HA	2.14	0.47
5:E:126:SER:OG	5:E:127:ILE:N	2.47	0.47
7:G:153:GLN:HB2	7:G:156:SER:O	2.13	0.47
4:D:119:ARG:NH1	4:D:150:ASN:O	2.46	0.47
11:K:49:GLU:HG2	11:K:94:ILE:HG12	1.97	0.47
1:A:350:ARG:NH1	1:A:488:ASN:OD1	2.48	0.47
10:J:1:MET:HA	10:J:56:LEU:HB2	1.96	0.47
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.54	0.46
1:A:1428:VAL:HG13	2:B:1151:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:LEU:O	4:D:47:LEU:N	2.41	0.46
1:A:562:THR:O	1:A:576:GLN:NE2	2.48	0.46
1:A:512:VAL:HA	1:A:519:PRO:HA	1.98	0.46
2:B:924:GLU:O	2:B:928:ARG:HB3	2.15	0.46
8:H:32:THR:OG1	8:H:33:GLN:OE1	2.34	0.46
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.51	0.46
1:A:557:ASP:OD1	1:A:557:ASP:N	2.49	0.46
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.47	0.46
1:A:1397:LEU:HB2	1:A:1426:GLU:HG3	1.97	0.46
2:B:999:MET:HE3	2:B:1008:PRO:HG2	1.98	0.46
13:N:34:DA:H1'	13:N:35:DA:C8	2.50	0.46
2:B:420:LEU:HG	2:B:453:ILE:HD13	1.97	0.46
4:D:31:GLN:OE1	4:D:31:GLN:N	2.48	0.46
2:B:39:ARG:NH2	2:B:665:GLU:HB2	2.31	0.46
4:D:206:GLU:OE2	4:D:209:ARG:NH1	2.49	0.46
5:E:190:LEU:HD11	5:E:196:VAL:HG13	1.98	0.46
6:F:97:ARG:NH1	6:F:100:GLN:OE1	2.49	0.46
1:A:485:ASP:OD1	14:P:12:C:O2'	2.17	0.46
1:A:122:MET:HE2	1:A:141:LEU:HD23	1.98	0.45
3:C:8:VAL:HG11	11:K:105:PHE:HA	1.98	0.45
10:J:48:ARG:NH1	10:J:49:MET:SD	2.89	0.45
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.17	0.45
1:A:451:HIS:CE1	1:A:453:MET:HB2	2.51	0.45
1:A:1115:SER:OG	1:A:1330:ASN:OD1	2.25	0.45
1:A:1196:GLU:N	1:A:1196:GLU:OE1	2.49	0.45
3:C:16:ASP:OD1	3:C:16:ASP:N	2.50	0.45
6:F:116:ASP:HB3	6:F:119:ARG:HG2	1.97	0.45
10:J:7:CYS:HA	10:J:49:MET:HG3	1.98	0.45
1:A:548:ASN:CG	11:K:47:ARG:HH12	2.25	0.45
1:A:848:ILE:HB	1:A:1065:GLY:HA3	1.97	0.45
2:B:311:LEU:O	2:B:315:LYS:HG2	2.16	0.45
4:D:148:LEU:HD21	7:G:2:PHE:HE2	1.81	0.45
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.98	0.45
5:E:76:GLY:C	5:E:106:GLN:HE22	2.25	0.45
1:A:1017:LEU:HB2	5:E:206:GLY:N	2.31	0.45
6:F:103:MET:HE1	7:G:65:ASP:O	2.17	0.45
11:K:77:THR:OG1	11:K:81:TYR:O	2.31	0.45
2:B:368:GLU:N	2:B:368:GLU:OE1	2.50	0.45
10:J:7:CYS:HA	10:J:49:MET:HE2	1.99	0.45
15:T:14:DT:H2'	15:T:15:DT:H71	1.98	0.45
1:A:351:THR:OG1	1:A:352:VAL:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:GLU:N	2:B:138:GLU:OE1	2.50	0.44
3:C:48:SER:OG	12:L:66:GLN:OE1	2.35	0.44
5:E:43:LYS:O	5:E:47:CYS:HB3	2.17	0.44
5:E:85:GLU:OE2	5:E:92:THR:HG21	2.18	0.44
7:G:144:ARG:NE	7:G:167:TYR:O	2.40	0.44
15:T:35:DT:H2''	15:T:36:DA:C8	2.52	0.44
1:A:711:ARG:NH2	9:I:87:GLN:OE1	2.50	0.44
2:B:101:MET:HE2	2:B:109:THR:HG22	1.99	0.44
2:B:600:LEU:HB3	2:B:615:MET:SD	2.57	0.44
7:G:30:LEU:O	7:G:34:VAL:HG12	2.17	0.44
10:J:41:LEU:HD22	10:J:46:CYS:HB3	1.99	0.44
1:A:317:LYS:NZ	15:T:31:DT:OP1	2.34	0.44
3:C:10:ILE:HA	3:C:20:PHE:HA	1.99	0.44
14:P:7:G:H2'	14:P:8:A:C8	2.53	0.44
8:H:2:SER:N	8:H:61:SER:OG	2.50	0.44
15:T:31:DT:H2''	15:T:32:DC:C5	2.52	0.44
1:A:16:GLU:OE1	4:D:13:ARG:NH1	2.47	0.44
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.53	0.44
2:B:137:TYR:HB3	2:B:149:TYR:HB3	1.99	0.44
2:B:816:GLU:N	2:B:816:GLU:OE1	2.51	0.44
1:A:187:LYS:HE2	1:A:197:PRO:N	2.33	0.44
1:A:527:THR:HG23	1:A:653:VAL:HB	2.00	0.44
1:A:531:ILE:HD11	1:A:578:LEU:HD21	2.00	0.44
2:B:66:ASP:CG	2:B:67:SER:H	2.25	0.44
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	2.00	0.43
4:D:163:VAL:HG13	4:D:214:LEU:HD11	2.00	0.43
1:A:106:VAL:HG11	1:A:214:ILE:HG12	2.00	0.43
13:N:43:DA:H2''	13:N:44:DA:H8	1.84	0.43
7:G:74:TYR:CE2	7:G:76:ALA:HB2	2.52	0.43
3:C:180:TYR:HB3	3:C:228:PHE:CD2	2.53	0.43
1:A:43:GLU:OE1	1:A:43:GLU:N	2.47	0.43
1:A:325:ILE:HA	1:A:328:ARG:HD3	2.00	0.43
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.50	0.43
2:B:61:ASP:HA	2:B:64:CYS:SG	2.58	0.43
2:B:760:ASP:OD1	2:B:760:ASP:N	2.51	0.43
2:B:762:ASN:HD21	2:B:984:HIS:HB3	1.83	0.43
4:D:206:GLU:HA	4:D:209:ARG:HG2	1.98	0.43
7:G:47:CYS:SG	7:G:48:VAL:N	2.92	0.43
5:E:12:LEU:HG	5:E:58:MET:HE1	2.00	0.43
1:A:120:GLU:HA	1:A:123:ARG:NH2	2.33	0.43
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:THR:OG1	1:A:160:GLN:OE1	2.35	0.42
1:A:227:VAL:HG21	4:D:14:ARG:HD3	2.01	0.42
1:A:387:ARG:HH21	1:A:437:MET:HE1	1.83	0.42
2:B:121:ASN:HA	2:B:207:GLY:HA3	2.01	0.42
3:C:10:ILE:HG23	11:K:108:GLU:HG2	2.01	0.42
7:G:123:ALA:HA	7:G:128:PRO:HB3	2.00	0.42
7:G:138:THR:O	7:G:141:SER:OG	2.30	0.42
9:I:7:CYS:HB2	9:I:14:LEU:HD21	2.00	0.42
1:A:534:LEU:O	1:A:574:GLY:HA3	2.19	0.42
1:A:1127:ASP:OD2	1:A:1130:GLN:HB2	2.20	0.42
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.19	0.42
5:E:94:LYS:HA	5:E:97:VAL:HG12	2.01	0.42
13:N:33:DC:H2''	13:N:34:DA:O4'	2.19	0.42
15:T:29:DA:H2''	15:T:30:DT:H5''	2.02	0.42
2:B:195:CYS:SG	2:B:783:THR:OG1	2.55	0.42
5:E:121:MET:HE1	5:E:134:THR:HG21	2.01	0.42
2:B:59:LEU:O	2:B:63:ILE:HG12	2.20	0.42
3:C:10:ILE:HD11	11:K:112:GLN:CG	2.50	0.42
3:C:29:MET:HA	11:K:45:LEU:HD13	2.02	0.42
3:C:252:GLN:HE21	11:K:95:ILE:HG23	1.85	0.42
1:A:690:VAL:HG11	1:A:794:PRO:HG3	2.01	0.42
2:B:636:PRO:HA	2:B:691:GLU:O	2.20	0.42
3:C:177:GLU:HB2	3:C:231:ASN:HB3	2.02	0.42
1:A:130:ASP:OD1	1:A:130:ASP:N	2.53	0.42
1:A:583:PRO:HG2	1:A:586:ILE:HG13	2.02	0.42
1:A:1281:ARG:NH2	1:A:1309:ASP:OD2	2.52	0.42
1:A:1288:ASP:OD2	1:A:1300:LYS:HB3	2.20	0.42
4:D:123:LEU:HA	4:D:126:ILE:HG12	2.02	0.42
7:G:143:ILE:HG13	7:G:169:GLY:C	2.45	0.42
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.85	0.42
15:T:11:DC:H2''	15:T:12:DA:C8	2.55	0.42
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.02	0.42
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	2.02	0.42
2:B:221:ASN:HA	2:B:240:ILE:HD11	2.02	0.42
4:D:16:LYS:NZ	4:D:18:VAL:HG13	2.34	0.42
13:N:41:DC:H2''	13:N:42:DA:C8	2.55	0.42
2:B:778:MET:SD	2:B:853:SER:OG	2.66	0.41
2:B:824:ILE:O	2:B:1009:ASP:N	2.52	0.41
12:L:34:CYS:SG	12:L:51:CYS:HB3	2.59	0.41
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.20	0.41
1:A:905:ASP:OD1	1:A:905:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:GLU:N	1:A:979:SER:O	2.50	0.41
1:A:506:ALA:O	1:A:510:GLN:HG2	2.20	0.41
7:G:31:LEU:C	7:G:33:GLU:H	2.27	0.41
1:A:667:GLY:HA2	1:A:670:ILE:HD12	2.03	0.41
1:A:1198:ASP:OD1	1:A:1200:ALA:N	2.53	0.41
2:B:299:GLU:OE2	2:B:572:HIS:ND1	2.53	0.41
5:E:31:THR:OG1	5:E:33:GLU:OE1	2.36	0.41
2:B:877:PRO:HG3	2:B:915:THR:HG23	2.01	0.41
14:P:3:C:H2'	14:P:4:U:C6	2.56	0.41
2:B:77:HIS:HB2	2:B:79:THR:O	2.20	0.41
3:C:90:ASP:OD1	3:C:91:HIS:N	2.47	0.41
2:B:37:PHE:CE2	2:B:41:LYS:HG3	2.56	0.41
4:D:205:ASP:OD1	4:D:206:GLU:N	2.52	0.41
3:C:36:VAL:HG21	3:C:251:LEU:HD13	2.03	0.41
15:T:29:DA:H2''	15:T:30:DT:O4'	2.20	0.41
2:B:309:GLN:NE2	9:I:52:ILE:HD11	2.36	0.41
2:B:757:PRO:CG	2:B:1028:GLU:HG3	2.51	0.41
2:B:954:VAL:HG12	2:B:964:VAL:HG12	2.02	0.41
13:N:31:DT:H1'	13:N:32:DG:N7	2.36	0.41
1:A:1420:ASP:OD1	1:A:1420:ASP:N	2.47	0.40
2:B:1176:ASN:OD1	2:B:1177:HIS:N	2.53	0.40
2:B:1189:ILE:HG21	7:G:154:VAL:HG21	2.03	0.40
15:T:25:DT:H2'	15:T:26:DC:C6	2.55	0.40
2:B:176:SER:O	2:B:182:SER:HB3	2.21	0.40
3:C:226:ASP:HA	3:C:228:PHE:CE1	2.56	0.40
4:D:148:LEU:HD23	4:D:148:LEU:HA	1.92	0.40
4:D:153:ARG:NE	4:D:182:SER:O	2.54	0.40
3:C:262:LEU:HD12	3:C:265:MET:HE2	2.02	0.40
8:H:34:ASP:OD1	8:H:34:ASP:N	2.54	0.40
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	2.04	0.40
2:B:63:ILE:O	2:B:67:SER:OG	2.26	0.40
9:I:15:TYR:OH	9:I:17:ARG:NH2	2.54	0.40
2:B:841:MET:HE3	2:B:1010:LEU:HD21	2.04	0.40
9:I:22:ASN:HB2	9:I:24:ARG:HH11	1.86	0.40
10:J:48:ARG:O	10:J:52:THR:OG1	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1408/1733 (81%)	1375 (98%)	33 (2%)	0	100	100
2	B	1167/1224 (95%)	1124 (96%)	43 (4%)	0	100	100
3	C	263/318 (83%)	254 (97%)	9 (3%)	0	100	100
4	D	162/221 (73%)	156 (96%)	6 (4%)	0	100	100
5	E	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
6	F	85/155 (55%)	84 (99%)	1 (1%)	0	100	100
7	G	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
8	H	136/146 (93%)	131 (96%)	5 (4%)	0	100	100
9	I	114/122 (93%)	109 (96%)	5 (4%)	0	100	100
10	J	67/70 (96%)	67 (100%)	0	0	100	100
11	K	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
12	L	43/70 (61%)	41 (95%)	2 (5%)	0	100	100
All	All	3939/4565 (86%)	3822 (97%)	117 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1240/1520 (82%)	1240 (100%)	0	100	100
2	B	1024/1061 (96%)	1024 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	233/274 (85%)	233 (100%)	0	100	100
4	D	148/200 (74%)	148 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	77/137 (56%)	77 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	123/128 (96%)	123 (100%)	0	100	100
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	64/65 (98%)	64 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
All	All	3506/4009 (88%)	3506 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	92	HIS
1	A	339	ASN
1	A	548	ASN
1	A	767	GLN
1	A	877	HIS
1	A	975	HIS
1	A	1078	GLN
1	A	1387	HIS
1	A	1390	ASN
2	B	110	HIS
2	B	115	GLN
2	B	357	GLN
2	B	366	GLN
2	B	383	ASN
2	B	1104	HIS
2	B	1205	GLN
3	C	73	GLN
3	C	206	ASN
3	C	252	GLN
4	D	28	GLN

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Mol	Chain	Res	Type
5	E	114	ASN
6	F	104	ASN
7	G	24	GLN
7	G	57	GLN
7	G	122	ASN
8	H	11	GLN
8	H	139	ASN
9	I	90	GLN
9	I	108	HIS
11	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/12 (75%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.