Full wwPDB X-ray Structure Validation Report (i)

May 18, 2016 – 02:18 PM EDT

PDB ID	:	3RZD
Title	:	RNA Polymerase II Initiation Complex with a 5-nt RNA
Authors	:	Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on	:	2011-05-11
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

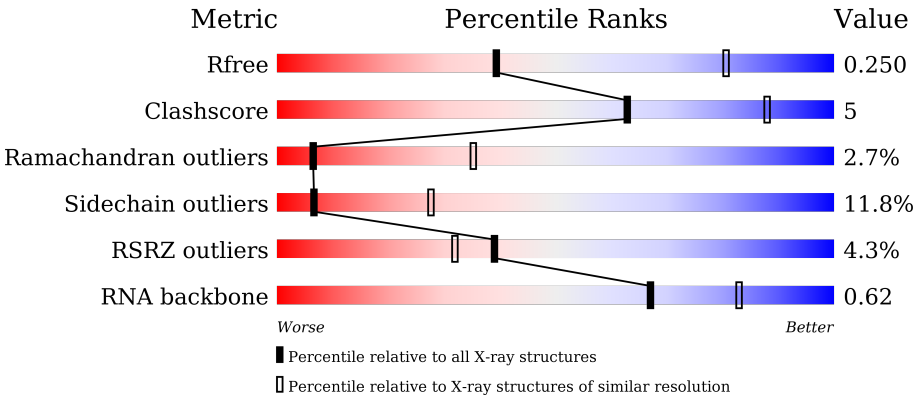
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	5% 62% 17% • 19%
2	B	1224	4% 68% 20% • 9%
3	C	318	% 62% 19% • 16%
4	E	215	2% 83% 16%

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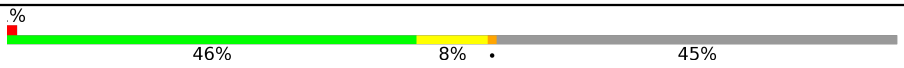
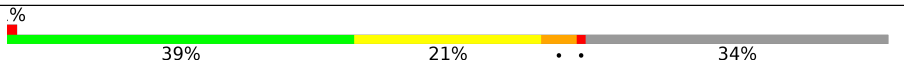
Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	5	
12	T	29	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28570 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1405	11043	6965	1936	2081	61	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1114	8861	5610	1549	1647	55	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	266	2095	1317	348	417	13	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	85	688	439	116	130	3	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	133	1068	673	180	211	4	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	5	Total	C	N	O	P	0	0	0
			110	50	25	31	4			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP *GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	8	Total	C	N	O	P	0	0	0
			159	76	26	49	8			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total Zn 1 1	0	0
13	I	2	Total Zn 2 2	0	0
13	C	1	Total Zn 1 1	0	0
13	A	2	Total Zn 2 2	0	0
13	L	1	Total Zn 1 1	0	0

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

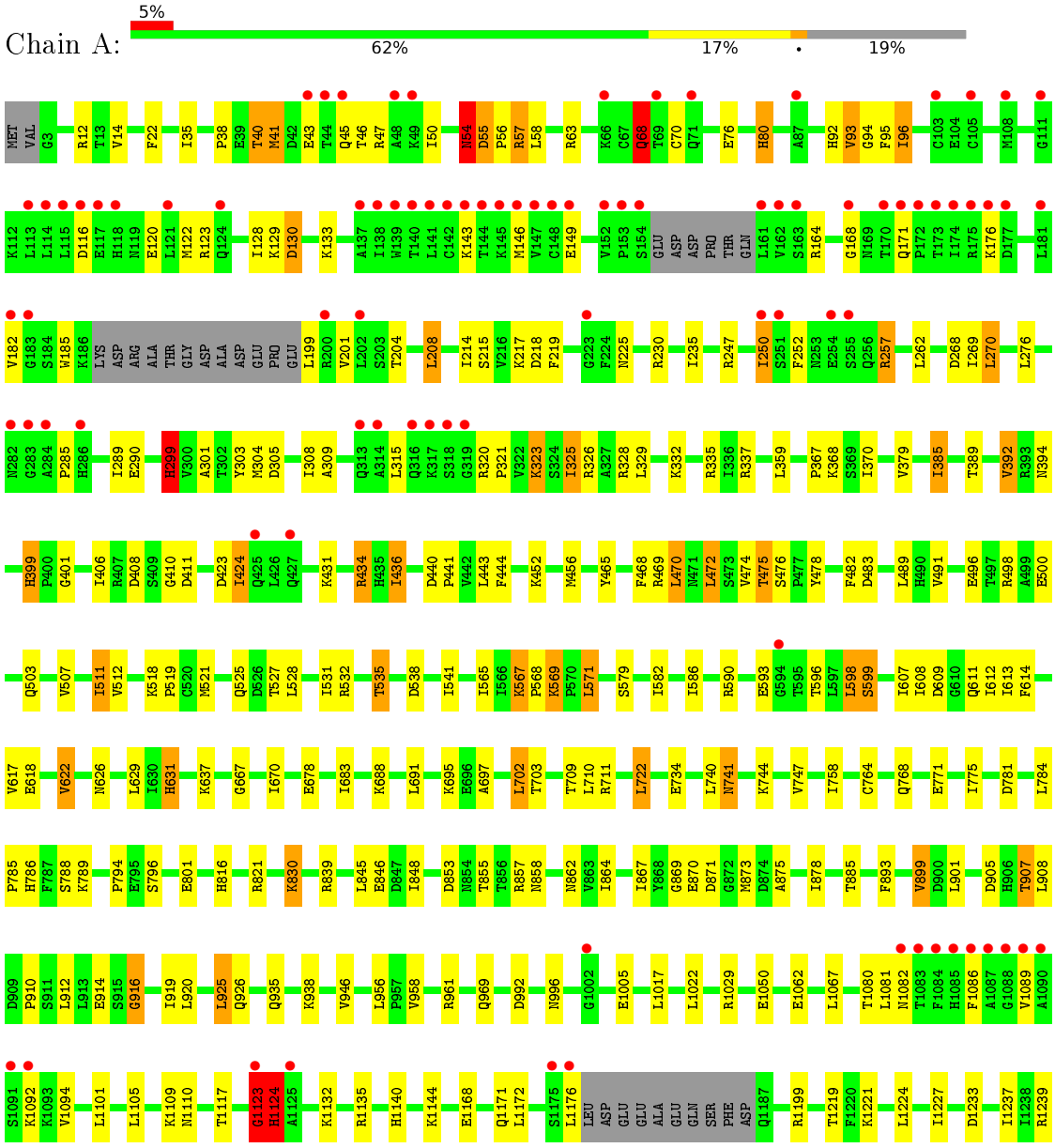
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total Mg 1 1	0	0

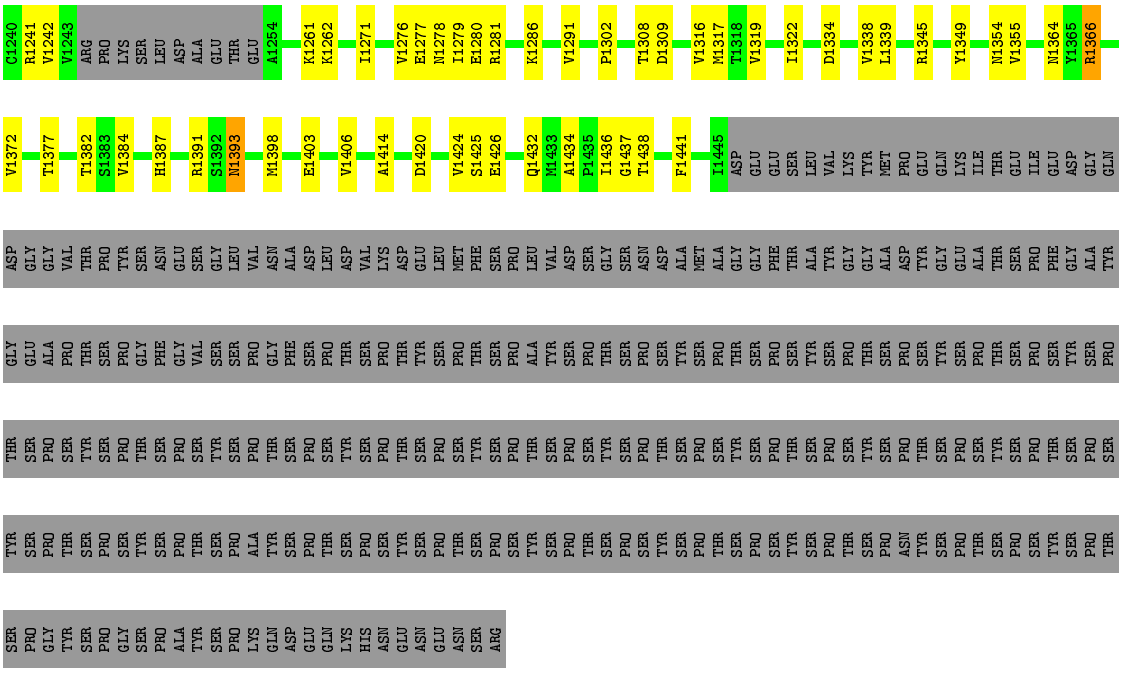
3 Residue-property plots (i)

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

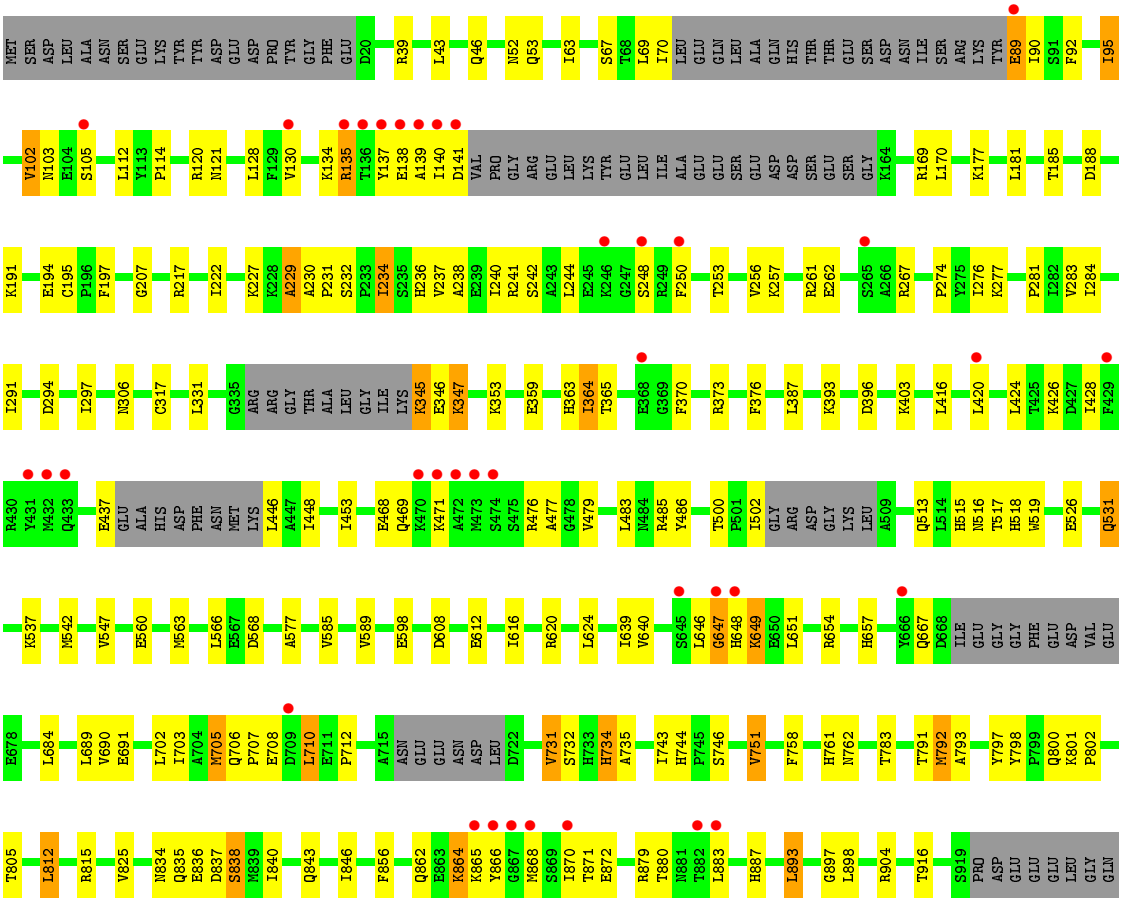
Chain A:

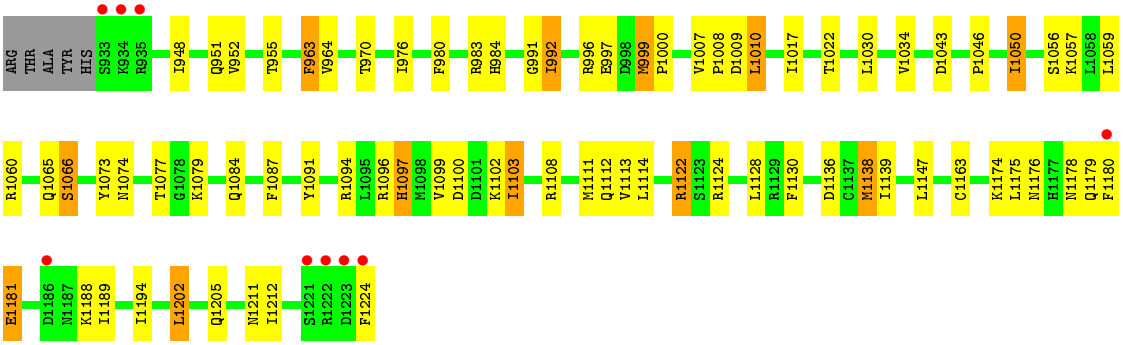


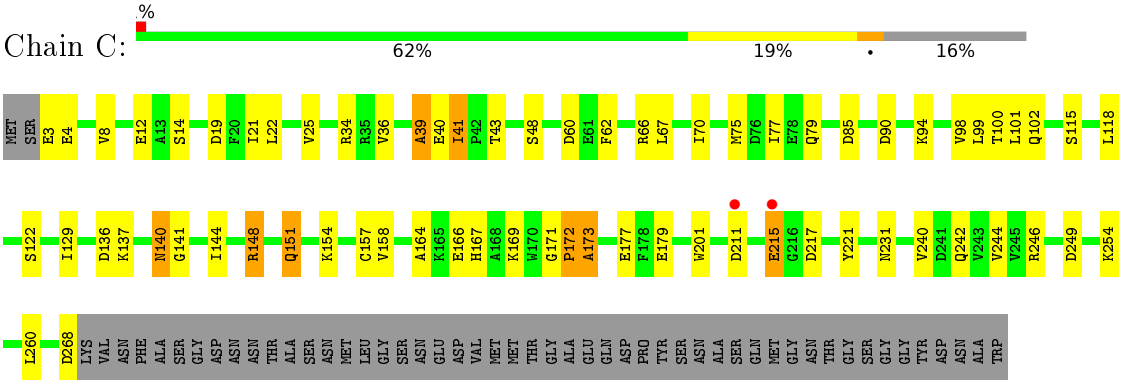


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

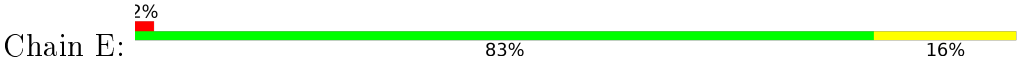


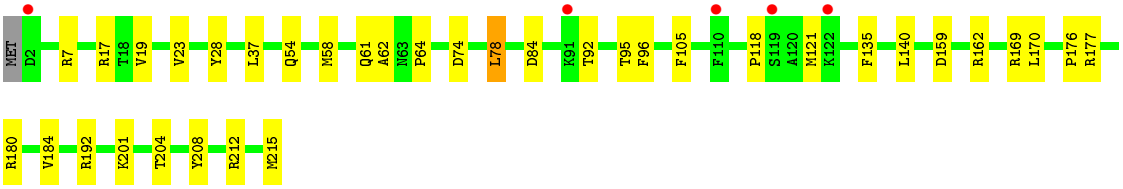




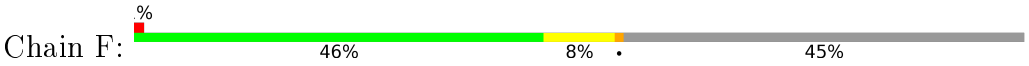
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

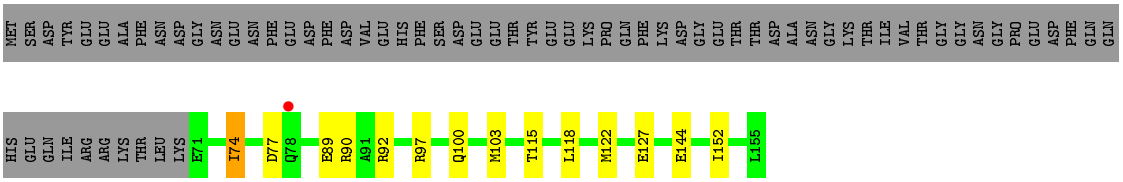
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



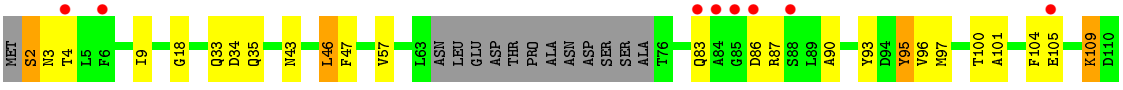


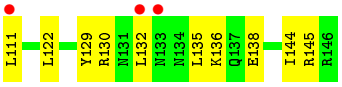
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2





• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3





• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

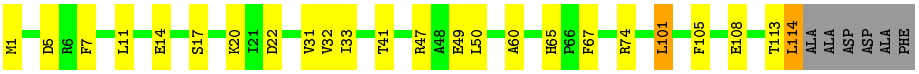
Chain I:

• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

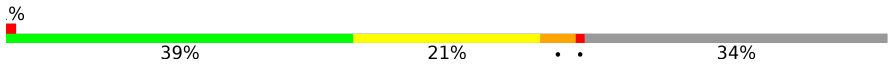
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

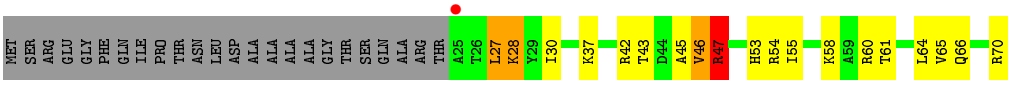
Chain K:



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:





• Molecule 11: RNA (5'-R(*AP*GP*AP*GP*G)-3')

Chain R:

• Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*C
P*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3')

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.54Å 221.27Å 192.18Å 90.00° 97.44° 90.00°	Depositor
Resolution (Å)	45.14 – 3.30 45.14 – 3.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.14-3.30) 98.8 (45.14-3.29)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.188 , 0.230 0.206 , 0.250	Depositor DCC
R_{free} test set	4842 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	69.4	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 68.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28570	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.41	0/11241	0.69	1/15199 (0.0%)
2	B	0.41	0/9033	0.70	1/12181 (0.0%)
3	C	0.38	0/2133	0.71	2/2891 (0.1%)
4	E	0.40	0/1788	0.63	0/2406
5	F	0.42	0/700	0.64	0/945
6	H	0.41	0/1086	0.72	1/1470 (0.1%)
7	I	0.38	0/989	0.71	0/1331
8	J	0.41	0/541	0.72	0/727
9	K	0.37	0/937	0.60	0/1265
10	L	0.47	0/365	0.84	0/485
11	R	0.79	0/124	1.28	0/193
12	T	1.15	0/176	1.91	6/268 (2.2%)
All	All	0.42	0/29113	0.71	11/39361 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	647	GLY	C-N-CA	7.64	140.81	121.70
12	T	22	DT	O4'-C1'-N1	6.51	112.56	108.00
3	C	172	PRO	C-N-CA	5.83	136.29	121.70
12	T	22	DT	N3-C2-O2	-5.78	118.83	122.30
12	T	22	DT	C4'-C3'-C2'	-5.57	98.08	103.10
1	A	1123	GLY	C-N-CA	5.53	135.52	121.70
12	T	20	DC	O4'-C1'-N1	5.49	111.84	108.00
12	T	22	DT	O4'-C4'-C3'	-5.44	102.33	104.50
12	T	16	DC	P-O3'-C3'	5.27	126.02	119.70
6	H	2	SER	C-N-CA	5.24	134.81	121.70
3	C	39	ALA	N-CA-C	5.06	124.67	111.00

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	A	11043	0	11133	136	0
2	B	8861	0	8884	108	0
3	C	2095	0	2051	28	0
4	E	1752	0	1776	17	0
5	F	688	0	707	6	0
6	H	1068	0	1040	17	0
7	I	971	0	927	5	0
8	J	532	0	542	9	0
9	K	919	0	929	8	0
10	L	363	0	386	6	0
11	R	110	0	56	1	0
12	T	159	0	91	1	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	28570	0	28522	302	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 (302) 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:1123:GLY:HA3	1:A:1124:HIS:HB2	1.33	1.07
8:J:48:ARG:O	8:J:52:THR:HB	1.79	0.83
1:A:1123:GLY:CA	1:A:1124:HIS:HB2	2.10	0.80
7:I:63:GLY:HA3	7:I:104:LEU:HD11	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PRO:HD2	1:A:289:ILE:HD11	1.65	0.79
1:A:935:GLN:HE22	1:A:938:LYS:HD3	1.46	0.78
2:B:984:HIS:HB3	2:B:1022:THR:CG2	2.17	0.74
1:A:535:THR:HG21	1:A:617:VAL:H	1.51	0.74
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.70	0.72
2:B:654:ARG:H	2:B:657:HIS:HD2	1.37	0.71
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.39	0.70
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.74	0.70
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.72	0.70
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.23	0.69
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.40	0.68
1:A:567:LYS:HB3	6:H:96:VAL:H	1.57	0.68
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.75	0.67
3:C:167:HIS:HD2	3:C:169:LYS:H	1.40	0.67
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.77	0.67
5:F:74:ILE:HG21	5:F:144:GLU:HG2	1.76	0.66
9:K:65:HIS:HD2	9:K:67:PHE:H	1.41	0.66
2:B:984:HIS:HB3	2:B:1022:THR:HG21	1.75	0.66
2:B:1097:HIS:HB2	2:B:1102:LYS:HE3	1.78	0.66
1:A:14:VAL:HG12	1:A:1432:GLN:HE22	1.59	0.65
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.77	0.65
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.79	0.65
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	1.78	0.64
1:A:472:LEU:O	1:A:475:THR:HB	1.98	0.64
2:B:706:GLN:O	2:B:710:LEU:HB2	1.99	0.63
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.63	0.63
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.81	0.63
1:A:1276:VAL:HG21	1:A:1316:VAL:HG22	1.80	0.63
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.80	0.62
3:C:115:SER:HB3	3:C:141:GLY:HA3	1.81	0.62
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.81	0.62
1:A:215:SER:O	1:A:219:PHE:HB2	1.99	0.62
1:A:323:LYS:HE2	1:A:328:ARG:HE	1.65	0.61
2:B:234:ILE:HD11	2:B:237:VAL:HG23	1.82	0.61
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.80	0.61
10:L:27:LEU:HB3	10:L:37:LYS:HD2	1.81	0.61
3:C:41:ILE:HG12	3:C:172:PRO:HG3	1.83	0.61
6:H:2:SER:HB2	6:H:3:ASN:HB2	1.82	0.61
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.80	0.61
2:B:1074:ASN:HD22	2:B:1077:THR:H	1.49	0.60
2:B:798:TYR:HE2	3:C:66:ARG:HH21	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.37	0.58
2:B:1034:VAL:HG22	2:B:1059:LEU:HB2	1.84	0.58
1:A:1086:PHE:HB3	1:A:1092:LYS:HE2	1.86	0.58
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.49	0.58
1:A:95:PHE:HE2	1:A:1414:ALA:HB2	1.67	0.58
1:A:535:THR:HG21	1:A:617:VAL:N	2.19	0.58
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.85	0.58
2:B:744:HIS:HD2	2:B:746:SER:H	1.52	0.58
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.84	0.58
1:A:1089:VAL:HB	1:A:1092:LYS:HD3	1.85	0.57
1:A:579:SER:HB3	1:A:611:GLN:HA	1.86	0.57
2:B:234:ILE:HG13	2:B:257:LYS:HB3	1.86	0.57
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.40	0.57
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.86	0.57
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.86	0.57
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.69	0.56
1:A:535:THR:CG2	1:A:617:VAL:H	2.17	0.56
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.87	0.56
2:B:542:MET:HE1	2:B:743:ILE:HB	1.88	0.56
1:A:483:ASP:HB3	2:B:837:ASP:HB2	1.87	0.56
1:A:1239:ARG:HH12	1:A:1241:ARG:HH12	1.54	0.56
4:E:118:PRO:HA	4:E:121:MET:HB2	1.88	0.55
1:A:219:PHE:HZ	1:A:230:ARG:HG2	1.71	0.55
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.87	0.55
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.07	0.55
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.88	0.55
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.88	0.55
9:K:32:VAL:HG22	9:K:74:ARG:HG3	1.87	0.55
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.87	0.55
1:A:579:SER:HA	1:A:582:ILE:HD12	1.88	0.55
2:B:864:LYS:HG2	2:B:871:THR:HA	1.88	0.55
4:E:19:VAL:O	4:E:23:VAL:HG23	2.07	0.55
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.89	0.55
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.90	0.54
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.87	0.54
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.89	0.54
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.89	0.54
1:A:567:LYS:HB3	6:H:95:TYR:HA	1.89	0.54
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.88	0.54
1:A:1377:THR:HG22	4:E:176:PRO:HB3	1.89	0.54
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.89	0.54
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.72	0.54
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.44	0.53
2:B:89:GLU:HB3	2:B:135:ARG:HB3	1.91	0.53
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.90	0.53
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.91	0.53
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.90	0.53
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.91	0.53
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.38	0.53
11:R:8:A:H61	12:T:21:DC:H42	1.56	0.53
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.74	0.52
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.91	0.52
1:A:1281:ARG:HB2	1:A:1309:ASP:HB3	1.92	0.52
1:A:871:ASP:HB3	4:E:204:THR:HG22	1.92	0.52
1:A:567:LYS:NZ	6:H:46:LEU:HB2	2.23	0.52
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.91	0.52
1:A:304:MET:HG2	1:A:325:ILE:HD12	1.92	0.52
2:B:283:VAL:HG12	2:B:297:ILE:HG21	1.90	0.52
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.91	0.52
1:A:441:PRO:HG2	1:A:498:ARG:HB2	1.92	0.52
3:C:12:GLU:HB3	3:C:19:ASP:HB3	1.92	0.52
1:A:569:LYS:HG2	1:A:571:LEU:HD13	1.91	0.51
3:C:36:VAL:HG23	3:C:40:GLU:HB2	1.91	0.51
1:A:596:THR:C	1:A:598:LEU:H	2.14	0.51
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.76	0.51
1:A:456:MET:HE2	1:A:507:VAL:HA	1.91	0.51
2:B:486:TYR:OH	2:B:1096:ARG:HB3	2.10	0.51
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.93	0.51
3:C:171:GLY:C	3:C:173:ALA:H	2.14	0.51
1:A:392:VAL:HG13	1:A:424:ILE:HD12	1.93	0.51
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.93	0.50
1:A:55:ASP:O	1:A:57:ARG:N	2.43	0.50
1:A:626:ASN:O	1:A:631:HIS:HD2	1.94	0.50
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.11	0.50
1:A:1105:LEU:HB3	1:A:1384:VAL:HG22	1.93	0.50
2:B:1030:LEU:O	2:B:1034:VAL:HG23	2.11	0.50
1:A:469:ARG:NH2	2:B:991:GLY:O	2.44	0.50
1:A:709:THR:HG22	1:A:711:ARG:H	1.76	0.50
3:C:136:ASP:HB3	3:C:140:ASN:O	2.12	0.50
1:A:120:GLU:HA	1:A:123:ARG:HB2	1.94	0.50
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:109:LYS:HZ1	6:H:111:LEU:HD12	1.77	0.50
4:E:176:PRO:O	4:E:212:ARG:HA	2.12	0.49
1:A:586:ILE:HD11	1:A:637:LYS:HG3	1.93	0.49
7:I:47:GLU:HB3	7:I:50:THR:HG23	1.94	0.48
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.77	0.48
1:A:68:GLN:HG2	1:A:80:HIS:CE1	2.48	0.48
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.94	0.48
5:F:97:ARG:HH11	5:F:100:GLN:HG3	1.79	0.48
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.78	0.48
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.95	0.48
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.94	0.48
2:B:516:ASN:HD22	2:B:516:ASN:H	1.60	0.48
3:C:48:SER:HB3	3:C:158:VAL:HB	1.96	0.48
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.96	0.48
1:A:741:ASN:HD22	1:A:744:LYS:H	1.62	0.48
1:A:92:HIS:HD2	1:A:94:GLY:H	1.61	0.48
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.95	0.48
2:B:345:LYS:HA	2:B:347:LYS:H	1.78	0.48
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.78	0.48
2:B:516:ASN:ND2	2:B:516:ASN:H	2.12	0.48
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.79	0.48
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.94	0.48
1:A:869:GLY:O	4:E:204:THR:HG21	2.13	0.48
3:C:98:VAL:H	3:C:122:SER:HB2	1.77	0.48
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.96	0.48
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.96	0.47
1:A:858:ASN:HD22	1:A:864:ILE:HD11	1.79	0.47
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.78	0.47
1:A:250:ILE:HD13	2:B:1113:VAL:HG11	1.95	0.47
2:B:53:GLN:HG2	2:B:547:VAL:HB	1.96	0.47
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.80	0.47
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.96	0.47
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.95	0.47
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.96	0.47
1:A:399:HIS:O	1:A:401:GLY:N	2.47	0.46
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.97	0.46
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.48	0.46
2:B:801:LYS:O	8:J:52:THR:HG23	2.15	0.46
2:B:825:VAL:HG23	2:B:1010:LEU:HB3	1.97	0.46
1:A:711:ARG:HH12	7:I:95:THR:HG22	1.79	0.46
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1144:LYS:HG3	7:I:48:LEU:HD22	1.97	0.46
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.97	0.46
2:B:980:PHE:CE2	2:B:1094:ARG:HD2	2.50	0.46
2:B:893:LEU:HD13	2:B:897:GLY:HA2	1.98	0.46
4:E:159:ASP:HA	4:E:162:ARG:HD3	1.98	0.46
1:A:567:LYS:HZ1	6:H:43:ASN:HB3	1.80	0.46
2:B:862:GLN:HG2	2:B:963:PHE:HB2	1.98	0.46
3:C:3:GLU:HG3	3:C:4:GLU:HG2	1.98	0.46
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.98	0.45
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.51	0.45
9:K:7:PHE:O	9:K:11:LEU:HB2	2.17	0.45
2:B:486:TYR:CZ	2:B:1096:ARG:HB3	2.51	0.45
1:A:899:VAL:HG13	1:A:1029:ARG:HD3	1.98	0.45
6:H:101:ALA:HB1	6:H:104:PHE:HE1	1.80	0.45
1:A:830:LYS:HE3	1:A:1082:ASN:HB3	1.97	0.45
1:A:367:PRO:HB3	1:A:465:TYR:O	2.16	0.45
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.81	0.45
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.99	0.45
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.82	0.45
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.52	0.45
2:B:835:GLN:O	2:B:838:SER:HB2	2.17	0.45
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.99	0.45
1:A:919:ILE:HD11	1:A:925:LEU:HG	1.97	0.45
2:B:428:ILE:HD11	2:B:448:ILE:HG23	1.98	0.45
1:A:456:MET:HB2	1:A:478:TYR:OH	2.17	0.44
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.97	0.44
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.50	0.44
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.98	0.44
2:B:232:SER:HB3	2:B:261:ARG:HH22	1.83	0.44
1:A:406:ILE:HB	1:A:431:LYS:HB2	2.00	0.44
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.47	0.44
4:E:61:GLN:HG3	4:E:105:PHE:HE2	1.82	0.44
9:K:7:PHE:HB2	9:K:11:LEU:HD22	2.00	0.44
2:B:291:ILE:HG22	2:B:297:ILE:HG13	2.00	0.44
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	2.16	0.44
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	1.99	0.44
6:H:100:THR:HG23	6:H:138:GLU:HA	1.98	0.44
3:C:22:LEU:HD11	9:K:101:LEU:HD21	2.00	0.44
1:A:910:PRO:HA	1:A:916:GLY:HA3	2.00	0.44
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.50	0.44
2:B:1100:ASP:HA	2:B:1103:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.98	0.44
3:C:166:GLU:HG2	10:L:70:ARG:HH21	1.83	0.44
1:A:1199:ARG:NH2	1:A:1233:ASP:O	2.50	0.43
1:A:567:LYS:NZ	6:H:43:ASN:HB3	2.33	0.43
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.18	0.43
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	2.01	0.43
2:B:1181:GLU:HA	2:B:1188:LYS:HA	2.01	0.43
1:A:528:LEU:O	1:A:531:ILE:HG22	2.18	0.43
3:C:101:LEU:HB2	3:C:118:LEU:HD23	2.00	0.43
4:E:28:TYR:HA	4:E:64:PRO:HA	2.01	0.43
1:A:614:PHE:HB3	6:H:122:LEU:HD21	2.00	0.43
1:A:781:ASP:HB2	1:A:789:LYS:HG2	2.00	0.43
2:B:1056:SER:HB3	2:B:1066:SER:HB2	2.00	0.43
2:B:515:HIS:HD2	2:B:517:THR:OG1	2.01	0.43
2:B:834:ASN:HA	2:B:838:SER:HB3	2.01	0.43
2:B:744:HIS:CD2	2:B:746:SER:OG	2.72	0.43
1:A:845:LEU:HA	1:A:848:ILE:HD12	2.01	0.42
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.53	0.42
4:E:177:ARG:HB3	4:E:215:MET:HG3	2.00	0.42
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	2.00	0.42
1:A:208:LEU:HD23	1:A:235:ILE:HD11	2.01	0.42
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.52	0.42
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.99	0.42
2:B:684:LEU:HA	2:B:689:LEU:HD12	2.01	0.42
6:H:93:TYR:HA	6:H:145:ARG:HB3	2.00	0.42
1:A:182:VAL:HG12	1:A:201:VAL:HA	2.01	0.42
1:A:512:VAL:HA	1:A:519:PRO:HA	2.01	0.42
1:A:567:LYS:HD2	1:A:568:PRO:HD2	2.00	0.42
2:B:1174:LYS:HB2	2:B:1179:GLN:O	2.19	0.42
2:B:955:THR:HG23	10:L:54:ARG:O	2.18	0.42
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.20	0.42
2:B:515:HIS:H	2:B:518:HIS:HD2	1.68	0.42
2:B:751:VAL:HA	2:B:812:LEU:HD21	2.01	0.42
1:A:185:TRP:HB2	1:A:199:LEU:HD12	2.01	0.42
1:A:747:VAL:HG21	1:A:758:ILE:HD11	2.00	0.42
1:A:875:ALA:HA	1:A:878:ILE:HD12	2.02	0.42
2:B:95:ILE:HD12	2:B:130:VAL:HB	2.00	0.42
3:C:167:HIS:CD2	3:C:169:LYS:H	2.29	0.42
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.55	0.42
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.20	0.42
2:B:188:ASP:HA	2:B:191:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:ILE:HG13	1:A:1308:THR:HG21	2.02	0.42
1:A:567:LYS:CB	1:A:568:PRO:CD	2.96	0.42
1:A:697:ALA:HA	1:A:702:LEU:HB2	2.02	0.42
2:B:229:ALA:HB1	2:B:231:PRO:HD2	2.01	0.41
10:L:27:LEU:HB2	10:L:28:LYS:H	1.73	0.41
3:C:14:SER:HA	9:K:114:LEU:HB3	2.02	0.41
1:A:1109:LYS:H	1:A:1109:LYS:HE2	1.85	0.41
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.56	0.41
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	2.02	0.41
4:E:61:GLN:HG3	4:E:105:PHE:CE2	2.55	0.41
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.24	0.41
1:A:503:GLN:HE21	5:F:90:ARG:NH1	2.11	0.41
2:B:52:ASN:OD1	2:B:177:LYS:HB2	2.20	0.41
2:B:241:ARG:HA	2:B:253:THR:HG22	2.02	0.41
2:B:420:LEU:HB3	2:B:453:ILE:HD13	2.02	0.41
1:A:40:THR:HG22	1:A:41:MET:HG3	2.03	0.41
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.86	0.41
1:A:1338:VAL:HG12	1:A:1339:LEU:HG	2.03	0.41
1:A:96:ILE:HD12	1:A:176:LYS:HE3	2.03	0.41
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.86	0.41
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.21	0.41
9:K:47:ARG:HD2	9:K:60:ALA:HA	2.02	0.41
1:A:531:ILE:HG21	1:A:622:VAL:HG11	2.03	0.41
2:B:128:LEU:HD11	2:B:170:LEU:HB2	2.02	0.41
2:B:373:ARG:HA	2:B:566:LEU:HD23	2.03	0.41
6:H:57:VAL:HG22	6:H:144:ILE:HG12	2.03	0.41
10:L:47:ARG:HD2	10:L:54:ARG:HG3	2.03	0.41
1:A:1438:THR:HG23	5:F:92:ARG:HD3	2.02	0.41
1:A:855:THR:HG23	1:A:857:ARG:HG3	2.01	0.41
2:B:999:MET:HG2	2:B:1007:VAL:HG13	2.02	0.41
3:C:62:PHE:O	3:C:66:ARG:HG2	2.21	0.41
1:A:901:LEU:HA	1:A:907:THR:HG23	2.01	0.41
1:A:511:ILE:HA	1:A:521:MET:HE3	2.02	0.40
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.49	0.40
2:B:577:ALA:HB1	2:B:589:VAL:HB	2.02	0.40
3:C:148:ARG:HB3	3:C:151:GLN:HG3	2.02	0.40
2:B:363:HIS:O	2:B:364:ILE:HB	2.21	0.40
2:B:802:PRO:HG2	2:B:805:THR:HG22	2.03	0.40
2:B:904:ARG:HG2	2:B:948:ILE:HG12	2.04	0.40
1:A:567:LYS:HE3	6:H:46:LEU:HD13	2.02	0.40
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:LEU:HB3	1:A:1384:VAL:CG2	2.50	0.40
1:A:1286:LYS:HE2	1:A:1302:PRO:HB2	2.02	0.40
1:A:367:PRO:HG2	1:A:370:ILE:HD12	2.03	0.40
1:A:858:ASN:HD21	1:A:862:ASN:HB2	1.86	0.40
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.56	0.40
2:B:244:LEU:HD12	2:B:250:PHE:HB2	2.04	0.40
2:B:640:VAL:HG12	2:B:649:LYS:HB3	2.04	0.40
1:A:571:LEU:HD12	1:A:571:LEU:HA	1.93	0.40
2:B:1122:ARG:C	2:B:1124:ARG:H	2.25	0.40
2:B:69:LEU:HD12	2:B:90:ILE:HB	2.04	0.40
2:B:898:LEU:HD21	2:B:964:VAL:HG11	2.03	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 X-ray entries followed by that with respect to entries of similar resolution.

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	1395/1733 (80%)	1252 (90%)	103 (7%)	40 (3%)	6 34
2	B	1096/1224 (90%)	969 (88%)	88 (8%)	39 (4%)	4 28
3	C	264/318 (83%)	241 (91%)	19 (7%)	4 (2%)	13 49
4	E	212/215 (99%)	201 (95%)	11 (5%)	0	100 100
5	F	83/155 (54%)	73 (88%)	10 (12%)	0	100 100
6	H	129/146 (88%)	105 (81%)	20 (16%)	4 (3%)	5 32
7	I	117/122 (96%)	103 (88%)	13 (11%)	1 (1%)	21 60
8	J	63/70 (90%)	59 (94%)	1 (2%)	3 (5%)	3 20
9	K	112/120 (93%)	108 (96%)	4 (4%)	0	100 100
10	L	44/70 (63%)	30 (68%)	9 (20%)	5 (11%)	0 3
All	All	3515/4173 (84%)	3141 (89%)	278 (8%)	96 (3%)	6 35

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	ASP
1	A	56	PRO
1	A	257	ARG
1	A	423	ASP
1	A	424	ILE
1	A	567	LYS
1	A	1221	LYS
2	B	137	TYR
2	B	469	GLN
2	B	477	ALA
2	B	531	GLN
2	B	648	HIS
2	B	712	PRO
2	B	731	VAL
2	B	732	SER
2	B	751	VAL
2	B	880	THR
2	B	883	LEU
2	B	1046	PRO
2	B	1180	PHE
3	C	173	ALA
3	C	215	GLU
8	J	2	ILE
8	J	6	ARG
10	L	28	LYS
1	A	40	THR
1	A	50	ILE
1	A	214	ILE
1	A	299	HIS
1	A	410	GLY
1	A	846	GLU
1	A	1123	GLY
1	A	1124	HIS
1	A	1437	GLY
2	B	364	ILE
2	B	646	LEU
2	B	887	HIS
6	H	18	GLY
6	H	90	ALA
6	H	136	LYS
10	L	64	LEU

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Mol	Chain	Res	Type
1	A	68	GLN
1	A	130	ASP
1	A	958	VAL
1	A	1393	ASN
2	B	105	SER
2	B	138	GLU
2	B	139	ALA
2	B	229	ALA
2	B	248	SER
2	B	346	GLU
2	B	468	GLU
2	B	483	LEU
2	B	563	MET
2	B	707	PRO
2	B	734	HIS
2	B	1066	SER
2	B	1097	HIS
3	C	148	ARG
6	H	135	LEU
7	I	77	LYS
10	L	45	ALA
10	L	46	VAL
1	A	46	THR
1	A	76	GLU
1	A	168	GLY
1	A	309	ALA
1	A	332	LYS
1	A	775	ILE
1	A	907	THR
1	A	1278	ASN
2	B	306	ASN
2	B	526	GLU
2	B	792	MET
2	B	1017	ILE
2	B	1108	ARG
3	C	90	ASP
1	A	45	GLN
1	A	399	HIS
2	B	1103	ILE
2	B	1181	GLU
8	J	13	VAL
10	L	47	ARG

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Mol	Chain	Res	Type
1	A	149	GLU
1	A	250	ILE
1	A	511	ILE
1	A	599	SER
2	B	865	LYS
1	A	35	ILE
1	A	385	ILE
1	A	569	LYS
2	B	647	GLY
1	A	916	GLY
2	B	230	ALA
1	A	321	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1225/1520 (81%)	1074 (88%)	151 (12%)	6 25
2	B	967/1061 (91%)	859 (89%)	108 (11%)	7 30
3	C	234/274 (85%)	208 (89%)	26 (11%)	8 31
4	E	196/197 (100%)	181 (92%)	15 (8%)	16 51
5	F	75/137 (55%)	67 (89%)	8 (11%)	8 32
6	H	117/128 (91%)	102 (87%)	15 (13%)	5 23
7	I	113/116 (97%)	100 (88%)	13 (12%)	7 29
8	J	60/65 (92%)	53 (88%)	7 (12%)	7 28
9	K	99/102 (97%)	84 (85%)	15 (15%)	3 16
10	L	40/57 (70%)	28 (70%)	12 (30%)	0 1
All	All	3126/3657 (86%)	2756 (88%)	370 (12%)	6 27

All (370) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG

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Mol	Chain	Res	Type
1	A	22	PHE
1	A	41	MET
1	A	43	GLU
1	A	47	ARG
1	A	54	ASN
1	A	57	ARG
1	A	58	LEU
1	A	63	ARG
1	A	68	GLN
1	A	70	CYS
1	A	80	HIS
1	A	93	VAL
1	A	96	ILE
1	A	116	ASP
1	A	122	MET
1	A	128	ILE
1	A	129	LYS
1	A	143	LYS
1	A	146	MET
1	A	164	ARG
1	A	171	GLN
1	A	204	THR
1	A	208	LEU
1	A	217	LYS
1	A	225	ASN
1	A	252	PHE
1	A	257	ARG
1	A	262	LEU
1	A	268	ASP
1	A	270	LEU
1	A	276	LEU
1	A	290	GLU
1	A	299	HIS
1	A	303	TYR
1	A	305	ASP
1	A	308	ILE
1	A	315	LEU
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	329	LEU
1	A	335	ARG

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Mol	Chain	Res	Type
1	A	337	ARG
1	A	359	LEU
1	A	368	LYS
1	A	385	ILE
1	A	389	THR
1	A	392	VAL
1	A	394	ASN
1	A	408	ASP
1	A	411	ASP
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	452	LYS
1	A	468	PHE
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	496	GLU
1	A	518	LYS
1	A	525	GLN
1	A	527	THR
1	A	532	ARG
1	A	535	THR
1	A	538	ASP
1	A	541	ILE
1	A	571	LEU
1	A	590	ARG
1	A	593	GLU
1	A	598	LEU
1	A	599	SER
1	A	609	ASP
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	631	HIS
1	A	678	GLU
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS

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Mol	Chain	Res	Type
1	A	702	LEU
1	A	703	THR
1	A	710	LEU
1	A	722	LEU
1	A	734	GLU
1	A	740	LEU
1	A	741	ASN
1	A	764	CYS
1	A	771	GLU
1	A	788	SER
1	A	796	SER
1	A	821	ARG
1	A	830	LYS
1	A	839	ARG
1	A	867	ILE
1	A	899	VAL
1	A	905	ASP
1	A	908	LEU
1	A	912	LEU
1	A	914	GLU
1	A	920	LEU
1	A	925	LEU
1	A	926	GLN
1	A	961	ARG
1	A	969	GLN
1	A	992	ASP
1	A	996	ASN
1	A	1005	GLU
1	A	1022	LEU
1	A	1050	GLU
1	A	1062	GLU
1	A	1067	LEU
1	A	1080	THR
1	A	1081	LEU
1	A	1094	VAL
1	A	1110	ASN
1	A	1117	THR
1	A	1124	HIS
1	A	1132	LYS
1	A	1135	ARG
1	A	1168	GLU
1	A	1171	GLN

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Mol	Chain	Res	Type
1	A	1172	LEU
1	A	1176	LEU
1	A	1224	LEU
1	A	1227	ILE
1	A	1237	ILE
1	A	1242	VAL
1	A	1261	LYS
1	A	1262	LYS
1	A	1277	GLU
1	A	1280	GLU
1	A	1291	VAL
1	A	1319	VAL
1	A	1334	ASP
1	A	1354	ASN
1	A	1366	ARG
1	A	1382	THR
1	A	1387	HIS
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1403	GLU
1	A	1420	ASP
1	A	1425	SER
1	A	1426	GLU
2	B	39	ARG
2	B	43	LEU
2	B	46	GLN
2	B	63	ILE
2	B	70	ILE
2	B	89	GLU
2	B	95	ILE
2	B	102	VAL
2	B	134	LYS
2	B	135	ARG
2	B	140	ILE
2	B	141	ASP
2	B	185	THR
2	B	194	GLU
2	B	217	ARG
2	B	222	ILE
2	B	234	ILE
2	B	240	ILE

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Mol	Chain	Res	Type
2	B	242	SER
2	B	262	GLU
2	B	267	ARG
2	B	276	ILE
2	B	277	LYS
2	B	317	CYS
2	B	331	LEU
2	B	345	LYS
2	B	347	LYS
2	B	353	LYS
2	B	376	PHE
2	B	387	LEU
2	B	393	LYS
2	B	396	ASP
2	B	403	LYS
2	B	416	LEU
2	B	424	LEU
2	B	426	LYS
2	B	437	GLU
2	B	446	LEU
2	B	471	LYS
2	B	476	ARG
2	B	479	VAL
2	B	485	ARG
2	B	500	THR
2	B	502	ILE
2	B	513	GLN
2	B	531	GLN
2	B	537	LYS
2	B	560	GLU
2	B	568	ASP
2	B	598	GLU
2	B	608	ASP
2	B	612	GLU
2	B	616	ILE
2	B	620	ARG
2	B	624	LEU
2	B	649	LYS
2	B	667	GLN
2	B	690	VAL
2	B	705	MET
2	B	708	GLU

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Mol	Chain	Res	Type
2	B	710	LEU
2	B	731	VAL
2	B	734	HIS
2	B	762	ASN
2	B	791	THR
2	B	792	MET
2	B	797	TYR
2	B	812	LEU
2	B	815	ARG
2	B	838	SER
2	B	864	LYS
2	B	866	TYR
2	B	868	MET
2	B	870	ILE
2	B	879	ARG
2	B	893	LEU
2	B	951	GLN
2	B	963	PHE
2	B	970	THR
2	B	976	ILE
2	B	992	ILE
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1010	LEU
2	B	1050	ILE
2	B	1057	LYS
2	B	1060	ARG
2	B	1065	GLN
2	B	1079	LYS
2	B	1099	VAL
2	B	1111	MET
2	B	1112	GLN
2	B	1122	ARG
2	B	1128	LEU
2	B	1138	MET
2	B	1147	LEU
2	B	1163	CYS
2	B	1175	LEU
2	B	1176	ASN
2	B	1178	ASN
2	B	1189	ILE

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Mol	Chain	Res	Type
2	B	1194	ILE
2	B	1202	LEU
2	B	1205	GLN
2	B	1211	ASN
2	B	1212	ILE
2	B	1224	PHE
3	C	21	ILE
3	C	25	VAL
3	C	34	ARG
3	C	41	ILE
3	C	43	THR
3	C	60	ASP
3	C	75	MET
3	C	77	ILE
3	C	79	GLN
3	C	85	ASP
3	C	94	LYS
3	C	100	THR
3	C	129	ILE
3	C	137	LYS
3	C	140	ASN
3	C	151	GLN
3	C	211	ASP
3	C	215	GLU
3	C	217	ASP
3	C	221	TYR
3	C	240	VAL
3	C	244	VAL
3	C	249	ASP
3	C	254	LYS
3	C	260	LEU
3	C	268	ASP
4	E	7	ARG
4	E	17	ARG
4	E	37	LEU
4	E	54	GLN
4	E	58	MET
4	E	74	ASP
4	E	78	LEU
4	E	84	ASP
4	E	92	THR
4	E	95	THR

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Mol	Chain	Res	Type
4	E	96	PHE
4	E	169	ARG
4	E	170	LEU
4	E	184	VAL
4	E	192	ARG
5	F	74	ILE
5	F	77	ASP
5	F	103	MET
5	F	115	THR
5	F	118	LEU
5	F	122	MET
5	F	127	GLU
5	F	152	ILE
6	H	4	THR
6	H	9	ILE
6	H	33	GLN
6	H	34	ASP
6	H	35	GLN
6	H	46	LEU
6	H	83	GLN
6	H	86	ASP
6	H	87	ARG
6	H	95	TYR
6	H	105	GLU
6	H	109	LYS
6	H	129	TYR
6	H	130	ARG
6	H	132	LEU
7	I	28	GLU
7	I	50	THR
7	I	60	GLN
7	I	70	ARG
7	I	77	LYS
7	I	90	GLN
7	I	94	ASP
7	I	95	THR
7	I	97	MET
7	I	104	LEU
7	I	107	SER
7	I	111	THR
7	I	120	GLN
8	J	3	VAL

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Mol	Chain	Res	Type
8	J	13	VAL
8	J	20	SER
8	J	30	LEU
8	J	31	ASP
8	J	48	ARG
8	J	62	ARG
9	K	1	MET
9	K	5	ASP
9	K	14	GLU
9	K	17	SER
9	K	20	LYS
9	K	22	ASP
9	K	31	VAL
9	K	33	ILE
9	K	41	THR
9	K	49	GLU
9	K	50	LEU
9	K	101	LEU
9	K	108	GLU
9	K	113	THR
9	K	114	LEU
10	L	27	LEU
10	L	30	ILE
10	L	42	ARG
10	L	43	THR
10	L	46	VAL
10	L	47	ARG
10	L	53	HIS
10	L	55	ILE
10	L	60	ARG
10	L	61	THR
10	L	65	VAL
10	L	66	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	80	HIS
1	A	83	HIS
1	A	92	HIS
1	A	171	GLN

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Mol	Chain	Res	Type
1	A	306	ASN
1	A	339	ASN
1	A	503	GLN
1	A	517	ASN
1	A	525	GLN
1	A	545	GLN
1	A	631	HIS
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	935	GLN
1	A	1085	HIS
1	A	1265	ASN
1	A	1312	ASN
1	A	1364	ASN
1	A	1387	HIS
1	A	1432	GLN
2	B	46	GLN
2	B	47	GLN
2	B	121	ASN
2	B	357	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	744	HIS
2	B	762	ASN
2	B	822	ASN
2	B	984	HIS
2	B	1025	HIS
2	B	1074	ASN
2	B	1161	HIS
2	B	1195	HIS
2	B	1211	ASN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	167	HIS
3	C	195	GLN
3	C	242	GLN
4	E	54	GLN

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Mol	Chain	Res	Type
4	E	114	ASN
6	H	3	ASN
7	I	60	GLN
9	K	65	HIS
9	K	110	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	4/5 (80%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	7	G

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 carbohydrates 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1405/1733 (81%)	0.14	88 (6%) 23 19	40, 85, 170, 224	0
2	B	1114/1224 (91%)	0.03	46 (4%) 41 34	42, 82, 148, 194	0
3	C	266/318 (83%)	-0.14	2 (0%) 87 84	52, 79, 120, 144	0
4	E	214/215 (99%)	0.10	5 (2%) 64 57	63, 117, 165, 185	0
5	F	85/155 (54%)	-0.10	1 (1%) 81 76	65, 96, 135, 155	0
6	H	133/146 (91%)	0.52	11 (8%) 14 11	83, 126, 152, 165	0
7	I	119/122 (97%)	-0.11	0 100 100	57, 89, 122, 131	0
8	J	65/70 (92%)	-0.28	0 100 100	51, 74, 110, 122	0
9	K	114/120 (95%)	-0.12	0 100 100	45, 79, 110, 132	0
10	L	46/70 (65%)	0.10	1 (2%) 65 59	66, 114, 132, 143	0
11	R	5/5 (100%)	-0.09	0 100 100	133, 136, 153, 156	0
12	T	8/29 (27%)	0.40	0 100 100	125, 134, 149, 156	0
All	All	3574/4207 (84%)	0.07	154 (4%) 39 32	40, 86, 160, 224	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	6.8
6	H	86	ASP	6.7
1	A	1082	ASN	6.4
1	A	44	THR	6.0
2	B	883	LEU	6.0
1	A	1085	HIS	5.2
2	B	138	GLU	5.2
1	A	69	THR	5.1
1	A	182	VAL	5.0
1	A	1091	SER	4.9
1	A	174	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	173	THR	4.7
2	B	865	LYS	4.7
1	A	1083	THR	4.7
1	A	1087	ALA	4.6
1	A	176	LYS	4.4
1	A	1002	GLY	4.4
1	A	183	GLY	4.3
1	A	103	CYS	4.2
1	A	141	LEU	4.2
2	B	1224	PHE	4.2
2	B	645	SER	4.2
1	A	105	CYS	4.1
1	A	144	THR	4.1
1	A	318	SER	4.1
6	H	85	GLY	4.1
1	A	168	GLY	4.0
2	B	1223	ASP	4.0
1	A	161	LEU	3.9
2	B	433	GLN	3.9
2	B	136	THR	3.9
1	A	142	CYS	3.8
2	B	474	SER	3.8
1	A	138	ILE	3.8
1	A	115	LEU	3.7
1	A	116	ASP	3.6
1	A	250	ILE	3.6
1	A	314	ALA	3.6
1	A	254	GLU	3.5
1	A	1123	GLY	3.5
2	B	866	TYR	3.5
1	A	49	LYS	3.4
1	A	1086	PHE	3.4
1	A	1089	VAL	3.4
2	B	139	ALA	3.4
1	A	170	THR	3.4
1	A	319	GLY	3.4
1	A	171	GLN	3.4
1	A	87	ALA	3.3
1	A	111	GLY	3.3
1	A	154	SER	3.3
2	B	471	LYS	3.2
2	B	431	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	282	ASN	3.2
1	A	283	GLY	3.2
2	B	1222	ARG	3.2
2	B	473	MET	3.2
2	B	709	ASP	3.2
1	A	181	LEU	3.1
1	A	177	ASP	3.1
1	A	1090	ALA	3.1
1	A	147	VAL	3.1
1	A	66	LYS	3.1
1	A	1088	GLY	3.1
1	A	163	SER	3.1
1	A	153	PRO	3.1
4	E	2	ASP	3.1
2	B	472	ALA	3.1
1	A	1084	PHE	3.1
2	B	368	GLU	3.1
1	A	1175	SER	3.0
1	A	118	HIS	3.0
2	B	248	SER	2.9
1	A	200	ARG	2.9
3	C	215	GLU	2.9
1	A	255	SER	2.9
1	A	139	TRP	2.8
1	A	108	MET	2.8
2	B	432	MET	2.8
6	H	132	LEU	2.8
1	A	146	MET	2.8
6	H	133	ASN	2.8
1	A	114	LEU	2.8
1	A	145	LYS	2.7
1	A	1125	ALA	2.7
2	B	89	GLU	2.7
2	B	135	ARG	2.6
1	A	427	GLN	2.6
2	B	647	GLY	2.6
2	B	250	PHE	2.6
1	A	113	LEU	2.6
1	A	137	ALA	2.6
2	B	935	ARG	2.5
4	E	122	LYS	2.5
1	A	48	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	175	ARG	2.5
6	H	83	GLN	2.5
1	A	223	GLY	2.5
1	A	316	GLN	2.4
2	B	933	SER	2.4
1	A	121	LEU	2.4
1	A	149	GLU	2.4
2	B	870	ILE	2.4
5	F	78	GLN	2.4
1	A	43	GLU	2.4
2	B	470	LYS	2.4
1	A	1092	LYS	2.4
2	B	130	VAL	2.4
2	B	882	THR	2.4
1	A	124	GLN	2.3
2	B	1186	ASP	2.3
2	B	140	ILE	2.3
2	B	420	LEU	2.3
1	A	317	LYS	2.3
1	A	594	GLY	2.3
6	H	4	THR	2.3
4	E	110	PHE	2.3
1	A	313	GLN	2.3
1	A	140	THR	2.3
1	A	284	ALA	2.3
1	A	251	SER	2.3
1	A	45	GLN	2.3
2	B	648	HIS	2.3
4	E	119	SER	2.2
6	H	105	GLU	2.2
1	A	172	PRO	2.2
2	B	141	ASP	2.2
3	C	211	ASP	2.2
2	B	265	SER	2.2
6	H	111	LEU	2.2
2	B	429	PHE	2.2
2	B	867	GLY	2.2
10	L	25	ALA	2.2
2	B	934	LYS	2.2
2	B	1221	SER	2.2
2	B	1180	PHE	2.2
1	A	152	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	LYS	2.1
6	H	88	SER	2.1
6	H	6	PHE	2.1
1	A	162	VAL	2.1
1	A	202	LEU	2.1
2	B	137	TYR	2.1
1	A	117	GLU	2.1
2	B	246	LYS	2.1
6	H	84	ALA	2.1
1	A	148	CYS	2.1
4	E	91	LYS	2.1
1	A	71	GLN	2.0
1	A	425	GLN	2.0
1	A	286	HIS	2.0
2	B	868	MET	2.0
2	B	105	SER	2.0
2	B	666	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	ZN	I	203	1/1	0.95	0.10	-1.21	94,94,94,94	0
13	ZN	C	319	1/1	0.99	0.09	-1.24	64,64,64,64	0
13	ZN	L	105	1/1	0.98	0.07	-1.33	96,96,96,96	0
13	ZN	I	204	1/1	0.99	0.09	-1.45	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	ZN	B	1307	1/1	0.91	0.09	-1.51	146,146,146,146	0
13	ZN	A	1735	1/1	0.92	0.09	-2.00	116,116,116,116	0
13	ZN	A	1734	1/1	0.75	0.09	-2.45	274,274,274,274	0
13	ZN	J	101	1/1	0.99	0.17	-2.47	63,63,63,63	0
14	MG	A	2001	1/1	0.97	0.14	-	38,38,38,38	0

6.5 Other polymers

There are no such residues in this entry.