Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 10:09 AM EDT

PDB ID	:	3S16
Title	:	RNA Polymerase II Initiation Complex with an 8-nt RNA
Authors	:	Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on	:	2011-05-14
Resolution	:	3.24 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
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:

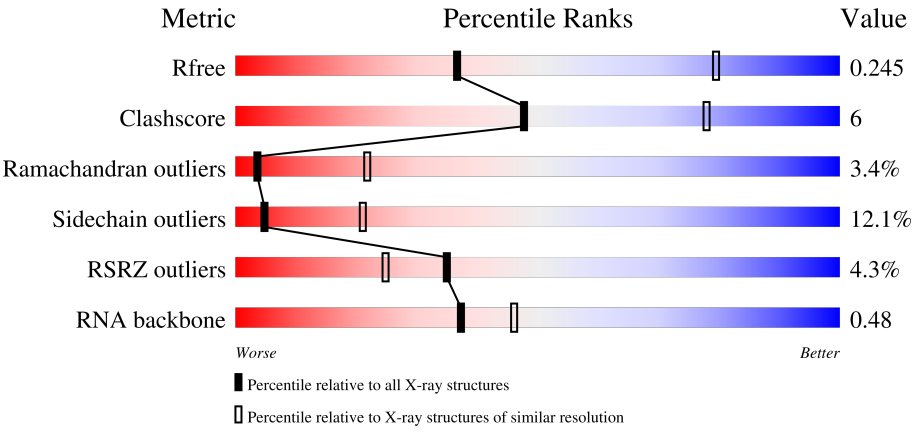
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.24 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}	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)
RNA backbone	3102	1034 (3.58-2.90)

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 of the lower 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% 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	4% 61% 17% · 19%
2	B	1224	4% 66% 22% · 9%
3	C	318	3% 58% 23% · 16%
4	E	215	3% 81% 18%

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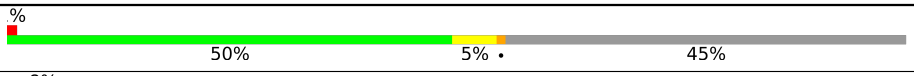
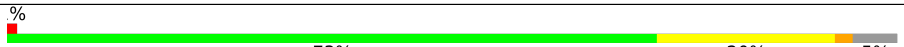
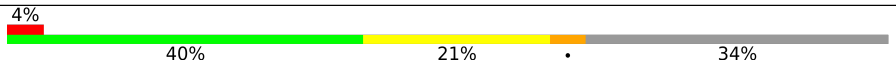
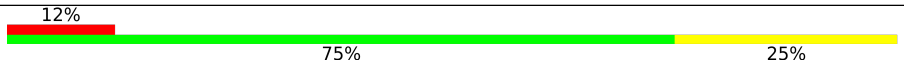
Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	8	
12	T	29	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28735 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(*UP*CP*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	8	Total	C	N	O	P	0	0	0
			173	78	35	53	7			

- 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	13	Total	C	N	O	P	0	0	0
			261	125	43	80	13			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		

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

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

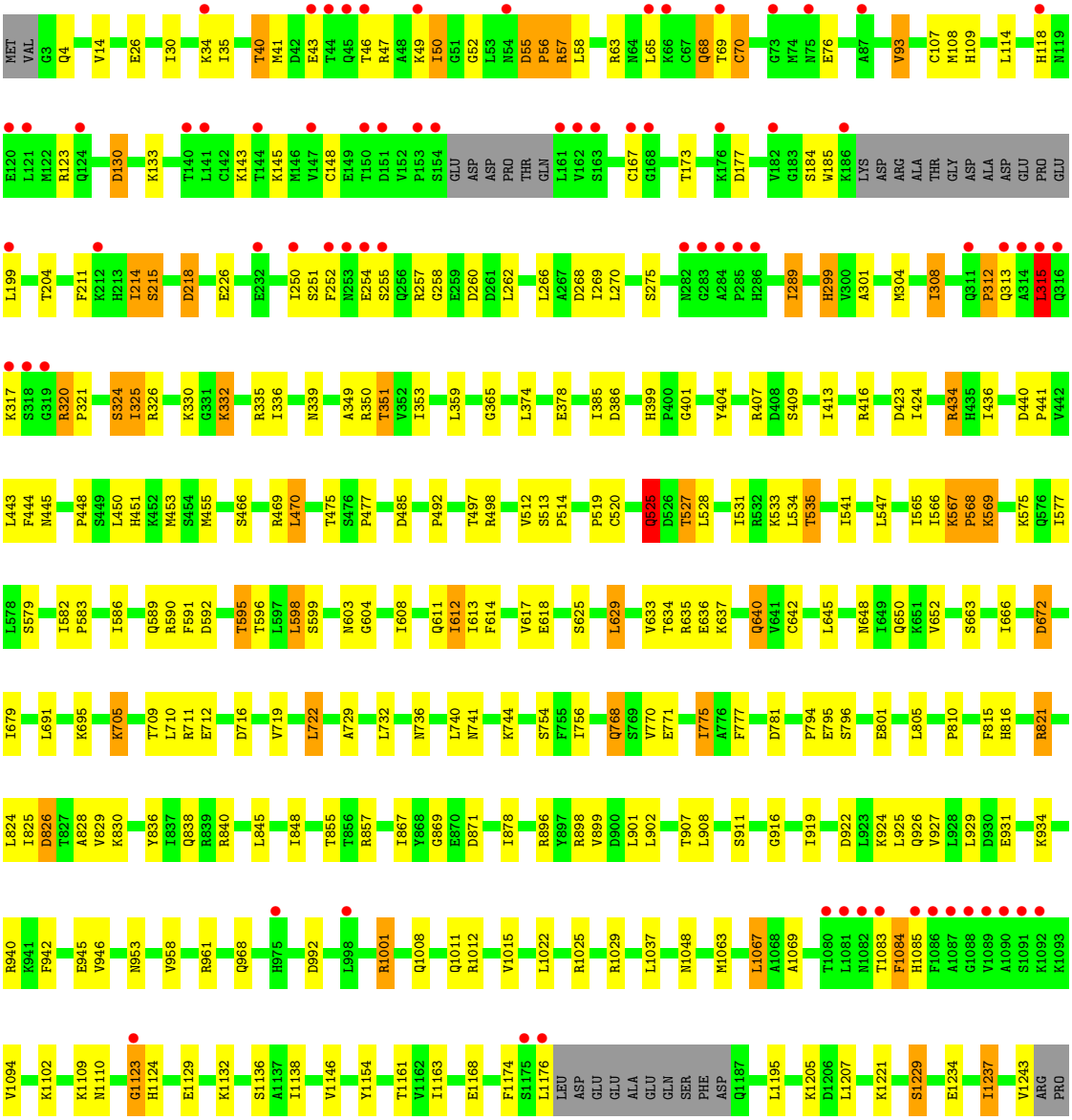
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total Mg 1 1	0	0

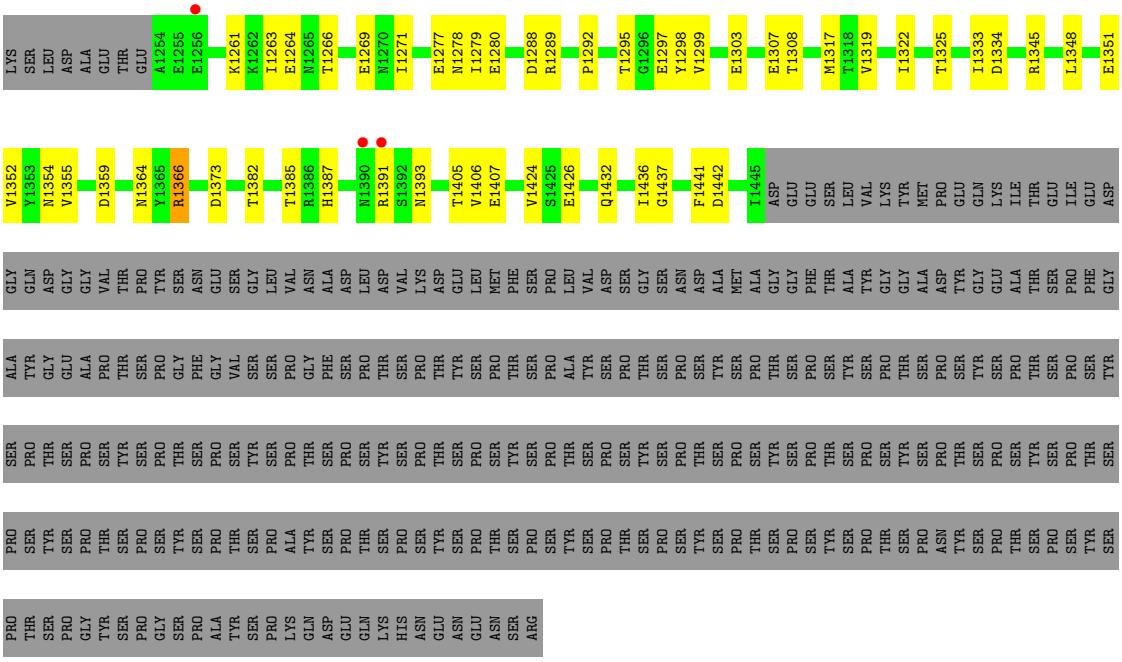
3 Residue-property plots (i)

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

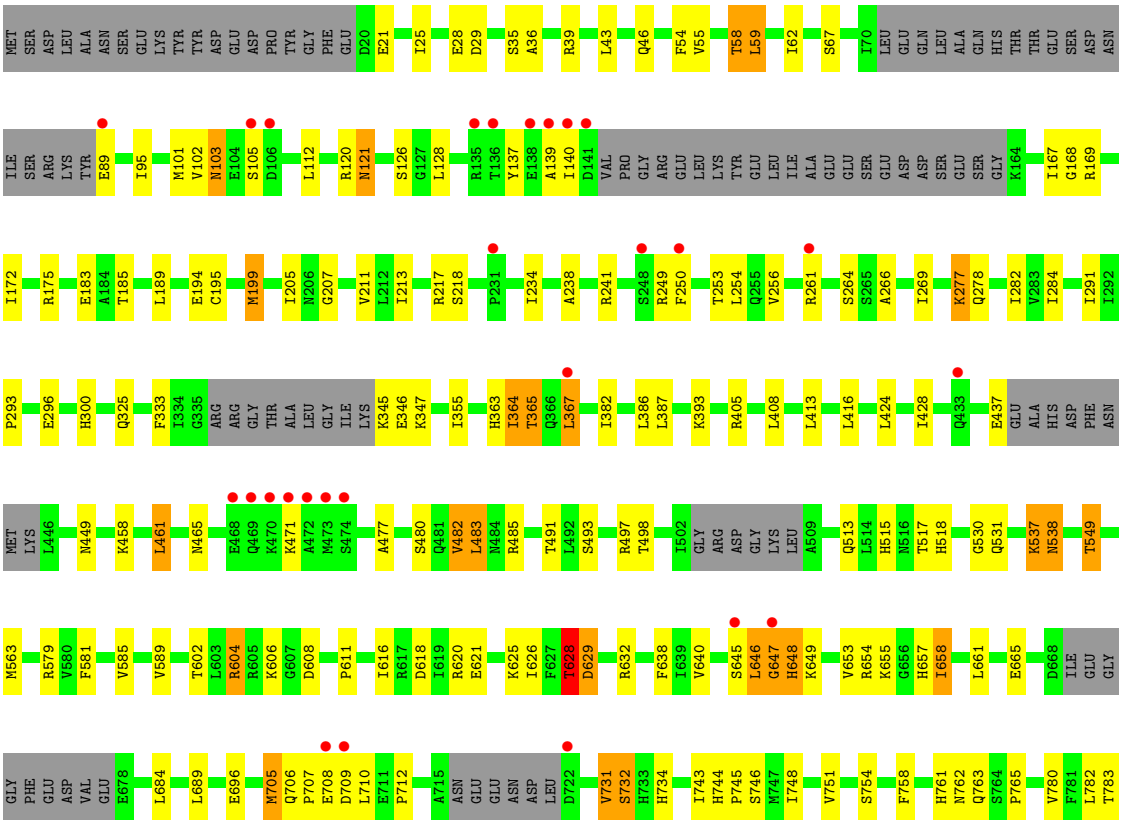
Chain A:

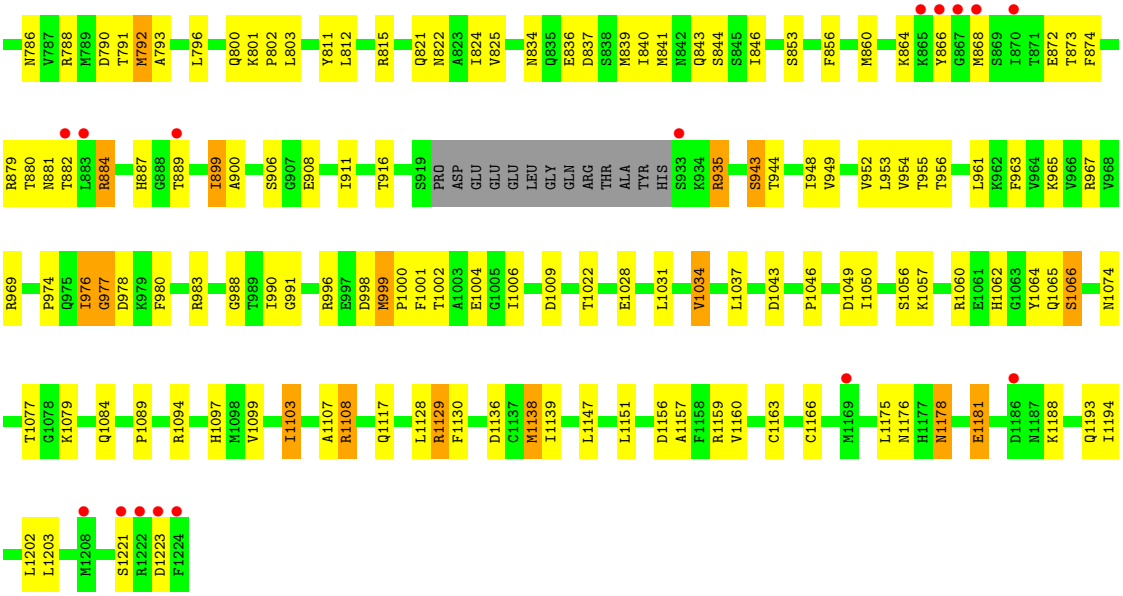




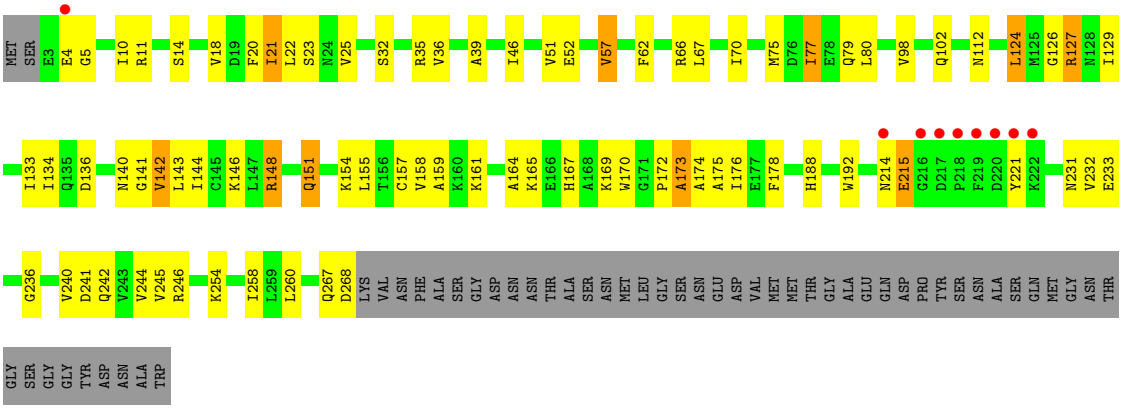
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

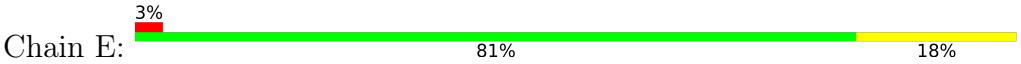


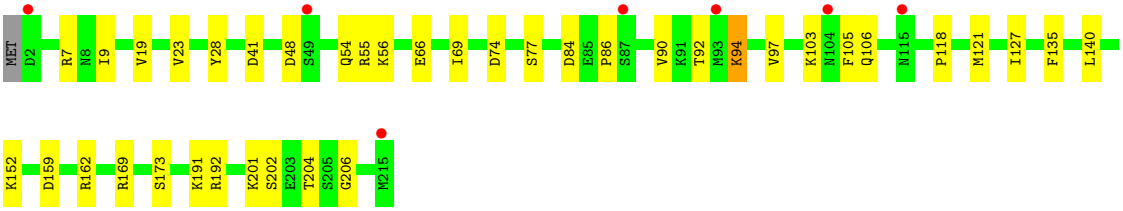


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

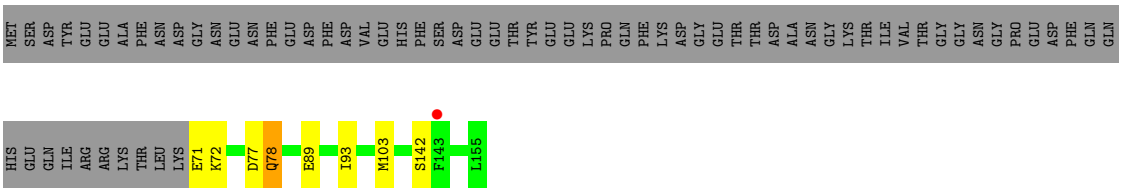


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



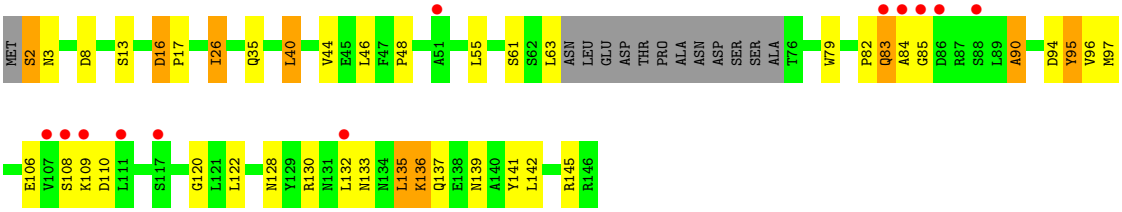


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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

Chain H:

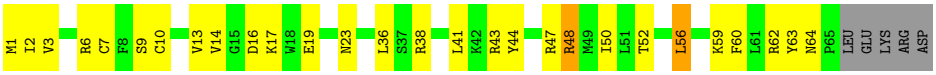


• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I:

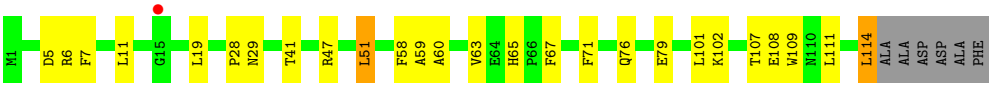
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



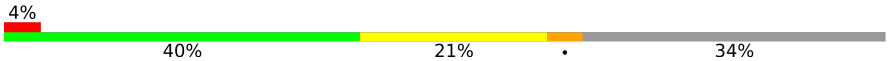
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

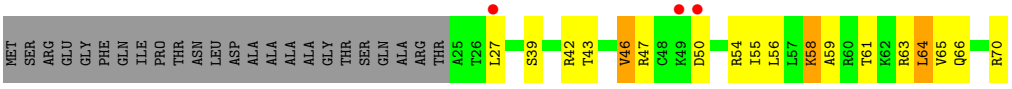
Chain K:



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

Chain L:

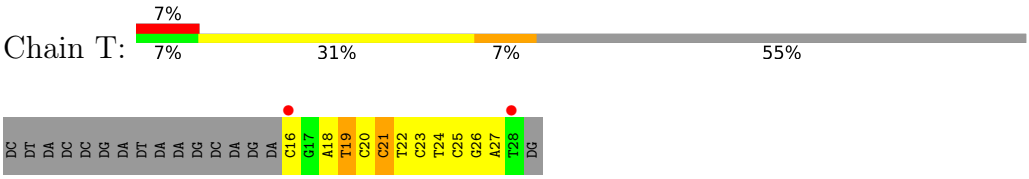




• Molecule 11: RNA (5'-R(*UP*CP*GP*AP*GP*AP*GP*G)-3')

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')



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.84Å 221.12Å 192.75Å 90.00° 97.61° 90.00°	Depositor
Resolution (Å)	29.86 – 3.24 29.87 – 3.24	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.86-3.24) 99.5 (29.87-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 3.24Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.183 , 0.227 0.201 , 0.245	Depositor DCC
R_{free} test set	5152 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	84.1	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 104.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	28735	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.43	0/11241	0.72	0/15199
2	B	0.45	0/9033	0.73	3/12181 (0.0%)
3	C	0.41	0/2133	0.73	1/2891 (0.0%)
4	E	0.40	0/1788	0.64	0/2406
5	F	0.43	0/700	0.67	0/945
6	H	0.40	0/1086	0.72	1/1470 (0.1%)
7	I	0.42	0/989	0.72	0/1331
8	J	0.44	0/541	0.78	0/727
9	K	0.39	0/937	0.68	0/1265
10	L	0.46	0/365	0.85	0/485
11	R	0.91	0/194	1.34	1/302 (0.3%)
12	T	1.07	0/290	2.00	15/444 (3.4%)
All	All	0.45	0/29297	0.75	21/39646 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	26	DG	P-O3'-C3'	9.90	131.58	119.70
12	T	16	DC	P-O3'-C3'	9.83	131.49	119.70
12	T	24	DT	O4'-C1'-N1	9.37	114.56	108.00
12	T	21	DC	O4'-C4'-C3'	-7.87	101.28	106.00
12	T	23	DC	O4'-C1'-N1	7.68	113.38	108.00
12	T	22	DT	C4'-C3'-C2'	-7.23	96.59	103.10
2	B	647	GLY	C-N-CA	7.20	139.69	121.70
12	T	19	DT	O4'-C1'-N1	7.07	112.95	108.00
12	T	25	DC	O4'-C1'-N1	6.53	112.57	108.00
11	R	4	C	O4'-C1'-N1	6.43	113.34	108.20
12	T	27	DA	P-O3'-C3'	6.05	126.96	119.70
12	T	21	DC	C4'-C3'-C2'	-5.93	97.76	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	20	DC	O4'-C1'-N1	5.86	112.10	108.00
12	T	22	DT	O4'-C4'-C3'	-5.66	102.23	104.50
3	C	172	PRO	C-N-CA	5.48	135.40	121.70
12	T	16	DC	O4'-C1'-N1	5.37	111.76	108.00
12	T	20	DC	P-O3'-C3'	5.33	126.10	119.70
2	B	140	ILE	C-N-CA	5.22	134.75	121.70
12	T	19	DT	P-O3'-C3'	5.16	125.89	119.70
2	B	628	THR	C-N-CA	5.06	134.34	121.70
6	H	2	SER	C-N-CA	5.01	134.22	121.70

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	11043	0	11133	142	0
2	B	8861	0	8884	134	0
3	C	2095	0	2051	47	0
4	E	1752	0	1776	11	0
5	F	688	0	707	4	0
6	H	1068	0	1040	19	0
7	I	971	0	927	8	0
8	J	532	0	542	17	0
9	K	919	0	929	14	0
10	L	363	0	386	7	0
11	R	173	0	88	0	0
12	T	261	0	148	2	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	28735	0	28611	348	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 (348) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.38	1.01
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.23	1.00
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.85	0.92
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.61	0.82
2:B:996:ARG:HH22	3:C:173:ALA:HB1	1.46	0.79
3:C:167:HIS:HD2	3:C:169:LYS:H	1.31	0.78
6:H:40:LEU:HD21	6:H:142:LEU:HD21	1.65	0.78
2:B:345:LYS:HA	2:B:347:LYS:H	1.48	0.76
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.52	0.75
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.70	0.73
2:B:54:PHE:HA	2:B:58:THR:HB	1.69	0.72
1:A:351:THR:HG21	1:A:466:SER:O	1.90	0.72
2:B:801:LYS:O	8:J:52:THR:HG23	1.90	0.72
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.72	0.71
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.72	0.71
1:A:441:PRO:HG2	1:A:498:ARG:HB2	1.72	0.71
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.76	0.69
1:A:469:ARG:NH2	2:B:991:GLY:O	2.27	0.67
1:A:869:GLY:O	4:E:204:THR:HG21	1.94	0.67
1:A:567:LYS:HE2	6:H:46:LEU:CB	2.25	0.67
2:B:604:ARG:HD3	2:B:611:PRO:HA	1.77	0.67
2:B:345:LYS:HA	2:B:347:LYS:N	2.11	0.66
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.78	0.66
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.77	0.65
1:A:567:LYS:HE2	6:H:46:LEU:HB2	1.77	0.65
1:A:55:ASP:H	1:A:56:PRO:HD2	1.61	0.65
2:B:955:THR:HG22	2:B:956:THR:H	1.62	0.65
2:B:1163:CYS:HB3	2:B:1166:CYS:HB2	1.77	0.65
1:A:535:THR:HG21	1:A:617:VAL:H	1.62	0.64
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.64	0.63
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.81	0.63
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.63	0.63
2:B:365:THR:HG23	2:B:367:LEU:H	1.64	0.63
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.81	0.62
3:C:11:ARG:HD2	3:C:21:ILE:HD11	1.82	0.61
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.48	0.61
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:THR:HG22	2:B:1004:GLU:H	1.66	0.60
2:B:1181:GLU:HG2	2:B:1188:LYS:HG2	1.84	0.60
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.83	0.60
1:A:57:ARG:HB3	1:A:68:GLN:HB3	1.82	0.60
1:A:711:ARG:HA	7:I:97:MET:HE1	1.84	0.60
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.83	0.59
3:C:242:GLN:HA	3:C:245:VAL:HG22	1.83	0.59
1:A:596:THR:C	1:A:598:LEU:H	2.05	0.59
1:A:741:ASN:HD22	1:A:744:LYS:H	1.49	0.59
1:A:567:LYS:HB3	6:H:96:VAL:H	1.66	0.59
1:A:855:THR:HG21	1:A:857:ARG:HE	1.68	0.58
1:A:709:THR:HB	1:A:712:GLU:HB2	1.85	0.58
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.39	0.58
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.85	0.58
3:C:66:ARG:NH2	8:J:3:VAL:O	2.37	0.58
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.84	0.58
3:C:62:PHE:O	3:C:66:ARG:HG3	2.03	0.58
2:B:976:ILE:O	2:B:990:ILE:HB	2.03	0.58
1:A:512:VAL:HA	1:A:519:PRO:HA	1.86	0.57
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.85	0.57
1:A:899:VAL:HG22	1:A:1029:ARG:HD3	1.85	0.57
1:A:592:ASP:HB2	1:A:603:ASN:HD22	1.70	0.57
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.86	0.56
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.86	0.56
3:C:167:HIS:CD2	3:C:169:LYS:H	2.18	0.56
1:A:4:GLN:HE22	2:B:1159:ARG:H	1.54	0.56
1:A:535:THR:HG21	1:A:617:VAL:N	2.21	0.56
2:B:549:THR:HB	2:B:628:THR:HG22	1.88	0.56
2:B:640:VAL:HG12	2:B:649:LYS:HB3	1.88	0.55
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.87	0.55
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.87	0.55
1:A:795:GLU:HG3	2:B:731:VAL:HG11	1.89	0.55
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.70	0.55
2:B:864:LYS:H	2:B:872:GLU:HB2	1.72	0.55
1:A:49:LYS:HB3	1:A:55:ASP:HB3	1.88	0.55
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.53	0.55
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.89	0.55
1:A:531:ILE:O	1:A:535:THR:HB	2.07	0.55
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.05	0.55
8:J:36:LEU:HD13	8:J:47:ARG:HG2	1.89	0.55
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:ASP:HB3	4:E:204:THR:HG22	1.89	0.55
2:B:497:ARG:HE	2:B:538:ASN:HD21	1.55	0.54
2:B:745:PRO:O	2:B:748:ILE:HG12	2.08	0.54
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.72	0.54
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.89	0.54
8:J:1:MET:H1	8:J:56:LEU:HB2	1.72	0.54
1:A:513:SER:HB3	1:A:520:CYS:HB3	1.88	0.54
2:B:1107:ALA:O	2:B:1108:ARG:HB2	2.07	0.53
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.90	0.53
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.42	0.53
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.73	0.53
2:B:1074:ASN:HD22	2:B:1077:THR:H	1.56	0.53
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.90	0.53
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.44	0.53
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.91	0.53
2:B:976:ILE:HG23	2:B:977:GLY:H	1.74	0.53
9:K:65:HIS:CD2	9:K:67:PHE:H	2.27	0.53
1:A:705:LYS:HE3	1:A:705:LYS:H	1.73	0.52
1:A:55:ASP:O	1:A:57:ARG:N	2.42	0.52
3:C:164:ALA:HA	3:C:167:HIS:O	2.10	0.52
2:B:955:THR:HG22	2:B:956:THR:N	2.23	0.52
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.92	0.52
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.92	0.52
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.90	0.52
2:B:996:ARG:NH2	3:C:174:ALA:O	2.43	0.52
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.40	0.52
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.91	0.52
2:B:980:PHE:CE2	2:B:1094:ARG:HD2	2.45	0.52
1:A:1292:PRO:HA	1:A:1298:TYR:HA	1.92	0.52
2:B:1129:ARG:HB3	12:T:21:DC:H5"	1.92	0.52
1:A:315:LEU:HG	1:A:320:ARG:HH21	1.76	0.51
1:A:399:HIS:O	1:A:401:GLY:N	2.37	0.51
2:B:95:ILE:HD11	2:B:128:LEU:HB3	1.92	0.51
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.43	0.51
2:B:935:ARG:CZ	2:B:935:ARG:HA	2.40	0.51
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.93	0.51
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.91	0.51
2:B:803:LEU:H	2:B:822:ASN:HD21	1.55	0.51
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.93	0.51
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.75	0.51
2:B:908:GLU:HG2	2:B:943:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.93	0.51
2:B:126:SER:HB2	2:B:172:ILE:HD11	1.93	0.51
2:B:860:MET:HG3	2:B:965:LYS:HG2	1.93	0.51
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.92	0.51
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.60	0.51
1:A:466:SER:HB3	2:B:1103:ILE:CD1	2.41	0.50
1:A:1279:ILE:HD12	1:A:1308:THR:HG21	1.94	0.50
2:B:39:ARG:HH12	2:B:665:GLU:HG3	1.75	0.50
1:A:629:LEU:O	1:A:633:VAL:HG23	2.11	0.50
2:B:515:HIS:CD2	2:B:517:THR:H	2.30	0.50
2:B:55:VAL:HA	2:B:59:LEU:HD23	1.93	0.50
1:A:640:GLN:CD	1:A:640:GLN:H	2.15	0.49
1:A:899:VAL:HB	1:A:929:LEU:HD22	1.94	0.49
1:A:916:GLY:O	1:A:919:ILE:HG22	2.12	0.49
1:A:185:TRP:HB2	1:A:199:LEU:HD12	1.94	0.49
5:F:77:ASP:O	5:F:78:GLN:HB2	2.13	0.49
2:B:846:ILE:HG23	2:B:974:PRO:HD2	1.93	0.49
3:C:20:PHE:HE1	3:C:22:LEU:HD13	1.78	0.49
1:A:595:THR:HG21	1:A:604:GLY:HA3	1.95	0.49
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.95	0.49
2:B:654:ARG:H	2:B:657:HIS:HD2	1.61	0.49
3:C:170:TRP:HH2	10:L:70:ARG:HH21	1.60	0.49
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.95	0.49
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.93	0.49
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.95	0.49
1:A:434:ARG:NH2	1:A:440:ASP:OD1	2.45	0.48
8:J:1:MET:N	8:J:56:LEU:H	2.10	0.48
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.94	0.48
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.78	0.48
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.96	0.48
2:B:43:LEU:HD11	2:B:811:TYR:O	2.13	0.48
3:C:14:SER:HA	9:K:114:LEU:HD22	1.94	0.48
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.46	0.48
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.96	0.48
6:H:2:SER:HB3	6:H:3:ASN:HB2	1.95	0.48
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.93	0.48
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.94	0.48
7:I:111:THR:HG23	7:I:113:ASP:H	1.79	0.48
2:B:706:GLN:H	2:B:710:LEU:HG	1.78	0.48
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.95	0.48
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HA	3:C:159:ALA:HA	1.94	0.48
1:A:567:LYS:HE2	6:H:46:LEU:HB3	1.95	0.48
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.96	0.48
2:B:955:THR:HG23	10:L:54:ARG:O	2.13	0.48
3:C:10:ILE:HD12	9:K:108:GLU:HB3	1.96	0.48
3:C:124:LEU:O	3:C:127:ARG:HG2	2.13	0.48
1:A:924:LYS:O	1:A:927:VAL:HG12	2.14	0.47
3:C:165:LYS:O	9:K:6:ARG:NH1	2.47	0.47
1:A:68:GLN:HE21	1:A:70:CYS:HB3	1.79	0.47
2:B:640:VAL:CG1	2:B:649:LYS:HB3	2.43	0.47
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.49	0.47
1:A:777:PHE:HD1	1:A:781:ASP:C	2.18	0.47
3:C:174:ALA:HB3	3:C:233:GLU:O	2.14	0.47
1:A:826:ASP:HA	1:A:829:VAL:HB	1.96	0.47
2:B:36:ALA:HB2	2:B:661:LEU:HD22	1.96	0.47
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.61	0.47
1:A:336:ILE:HD11	2:B:1203:LEU:HD13	1.97	0.47
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.79	0.47
6:H:63:LEU:HB2	6:H:90:ALA:HB2	1.95	0.47
9:K:65:HIS:HD2	9:K:67:PHE:H	1.62	0.47
1:A:579:SER:HB3	1:A:611:GLN:HA	1.96	0.47
1:A:919:ILE:HD11	1:A:925:LEU:HG	1.97	0.47
2:B:35:SER:O	2:B:39:ARG:HB2	2.15	0.46
2:B:241:ARG:HA	2:B:253:THR:HG22	1.96	0.46
2:B:916:THR:HG23	2:B:935:ARG:HB3	1.96	0.46
2:B:705:MET:H	2:B:710:LEU:HD12	1.80	0.46
1:A:107:CYS:HB3	1:A:114:LEU:HD21	1.97	0.46
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.96	0.46
1:A:50:ILE:HG23	1:A:52:GLY:H	1.80	0.46
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.97	0.46
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.97	0.46
2:B:731:VAL:O	2:B:732:SER:HB2	2.16	0.46
1:A:648:ASN:O	1:A:652:VAL:HG23	2.15	0.46
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.89	0.46
1:A:315:LEU:HD23	1:A:317:LYS:H	1.81	0.46
1:A:770:VAL:HG12	1:A:771:GLU:HG2	1.97	0.46
2:B:58:THR:O	2:B:62:ILE:HG12	2.15	0.46
2:B:199:MET:SD	2:B:199:MET:N	2.88	0.46
2:B:837:ASP:O	2:B:988:GLY:HA2	2.16	0.46
4:E:118:PRO:HA	4:E:121:MET:HB2	1.97	0.46
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:PHE:HB3	6:H:122:LEU:HD21	1.98	0.46
1:A:1129:GLU:HA	1:A:1132:LYS:HE3	1.98	0.46
1:A:374:LEU:HD23	2:B:1107:ALA:HB2	1.98	0.45
1:A:525:GLN:NE2	2:B:836:GLU:H	2.14	0.45
1:A:709:THR:HB	1:A:712:GLU:H	1.81	0.45
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.97	0.45
9:K:7:PHE:O	9:K:11:LEU:HB2	2.17	0.45
7:I:92:ARG:HD2	7:I:94:ASP:OD2	2.16	0.45
1:A:26:GLU:HG2	1:A:30:ILE:HD13	1.97	0.45
1:A:514:PRO:HG2	1:A:1067:LEU:HD21	1.97	0.45
1:A:810:PRO:HG2	2:B:705:MET:HG2	1.98	0.45
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.82	0.45
2:B:291:ILE:HG12	2:B:300:HIS:NE2	2.32	0.45
2:B:618:ASP:OD2	2:B:621:GLU:HB2	2.15	0.45
4:E:19:VAL:O	4:E:23:VAL:HG23	2.16	0.45
1:A:535:THR:CG2	1:A:617:VAL:H	2.28	0.45
1:A:1229:SER:HB3	1:A:1237:ILE:H	1.82	0.45
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.99	0.45
2:B:872:GLU:HG2	2:B:916:THR:HB	1.98	0.45
3:C:11:ARG:HD2	3:C:21:ILE:CD1	2.47	0.45
3:C:148:ARG:H	3:C:151:GLN:HG3	1.80	0.45
1:A:4:GLN:HE22	2:B:1159:ARG:N	2.15	0.45
1:A:901:LEU:HD23	1:A:907:THR:HG23	1.99	0.45
2:B:579:ARG:HA	2:B:589:VAL:HG12	1.99	0.45
6:H:136:LYS:H	6:H:136:LYS:HD3	1.81	0.45
12:T:18:DA:H5"	12:T:19:DT:H5'	1.98	0.45
1:A:378:GLU:OE2	1:A:434:ARG:HD3	2.17	0.45
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.99	0.44
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.41	0.44
1:A:591:PHE:HD2	1:A:595:THR:HB	1.82	0.44
2:B:498:THR:HB	2:B:537:LYS:HB2	2.00	0.44
8:J:14:VAL:HA	8:J:17:LYS:HD2	1.99	0.44
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.99	0.44
1:A:586:ILE:HD11	1:A:637:LYS:HG3	1.99	0.44
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.99	0.44
3:C:66:ARG:NH1	3:C:144:ILE:O	2.51	0.44
1:A:575:LYS:HD2	6:H:120:GLY:HA3	1.99	0.44
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	1.99	0.44
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.98	0.44
3:C:258:ILE:HD12	9:K:19:LEU:HD21	1.99	0.44
2:B:102:VAL:HG23	2:B:112:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.32	0.44
1:A:211:PHE:HA	1:A:214:ILE:HD11	1.98	0.44
1:A:567:LYS:HD3	6:H:95:TYR:CG	2.52	0.44
2:B:647:GLY:HA3	2:B:648:HIS:HB2	1.99	0.44
2:B:1031:LEU:O	2:B:1034:VAL:HG12	2.18	0.44
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	2.00	0.44
3:C:133:ILE:HG21	3:C:236:GLY:HA3	1.99	0.44
2:B:744:HIS:CD2	2:B:746:SER:OG	2.70	0.44
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.82	0.44
2:B:424:LEU:O	2:B:428:ILE:HG12	2.18	0.43
2:B:1037:LEU:HD13	2:B:1062:HIS:HB3	2.00	0.43
2:B:882:THR:HA	2:B:935:ARG:HH12	1.83	0.43
4:E:77:SER:HB2	4:E:105:PHE:HA	1.99	0.43
2:B:128:LEU:HB2	2:B:167:ILE:HB	2.00	0.43
4:E:202:SER:HB3	4:E:206:GLY:H	1.82	0.43
1:A:642:CYS:O	1:A:645:LEU:HB3	2.19	0.43
1:A:824:LEU:HD21	2:B:765:PRO:HB3	2.01	0.43
2:B:293:PRO:HG2	2:B:296:GLU:HB2	2.00	0.43
6:H:135:LEU:C	6:H:137:GLN:H	2.22	0.43
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.00	0.43
2:B:956:THR:HB	10:L:46:VAL:HG21	1.99	0.43
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.19	0.43
3:C:175:ALA:HB2	8:J:10:CYS:HB2	2.01	0.43
5:F:72:LYS:HG2	5:F:142:SER:HA	2.00	0.43
1:A:527:THR:HG21	1:A:650:GLN:HG2	2.01	0.43
1:A:567:LYS:O	1:A:569:LYS:N	2.52	0.43
1:A:251:SER:HB3	1:A:258:GLY:HA3	2.01	0.43
1:A:596:THR:C	1:A:598:LEU:N	2.72	0.43
1:A:528:LEU:O	1:A:531:ILE:HG22	2.19	0.42
1:A:946:VAL:HG22	4:E:201:LYS:HD2	2.01	0.42
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.19	0.42
3:C:70:ILE:HD11	3:C:144:ILE:HD12	2.02	0.42
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.55	0.42
3:C:142:VAL:H	8:J:16:ASP:HB3	1.84	0.42
8:J:14:VAL:HB	8:J:50:ILE:HD11	2.02	0.42
1:A:148:CYS:HB3	1:A:167:CYS:O	2.19	0.42
2:B:1060:ARG:HA	2:B:1064:TYR:O	2.20	0.42
1:A:173:THR:HB	1:A:184:SER:HB3	2.01	0.42
1:A:304:MET:HG2	1:A:325:ILE:HD12	2.01	0.42
1:A:729:ALA:HA	1:A:732:LEU:HD12	2.01	0.42
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:SER:HA	1:A:582:ILE:HD12	2.01	0.42
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.01	0.42
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.60	0.42
1:A:1352:VAL:O	1:A:1355:VAL:HG12	2.19	0.42
1:A:324:SER:O	1:A:326:ARG:N	2.53	0.42
2:B:900:ALA:HB3	10:L:61:THR:HG23	2.02	0.42
3:C:18:VAL:O	3:C:231:ASN:HA	2.20	0.42
1:A:775:ILE:HG21	1:A:815:PHE:CE2	2.55	0.42
2:B:515:HIS:H	2:B:518:HIS:CD2	2.38	0.42
3:C:143:LEU:HD21	3:C:146:LYS:HE3	2.01	0.42
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.55	0.42
1:A:466:SER:HB3	2:B:1103:ILE:HD11	2.01	0.42
3:C:46:ILE:HG23	3:C:157:CYS:HB2	2.02	0.42
2:B:824:ILE:HD13	2:B:1089:PRO:HB3	2.01	0.41
2:B:1079:LYS:HE2	3:C:188:HIS:CE1	2.54	0.41
1:A:289:ILE:H	1:A:289:ILE:HG13	1.59	0.41
1:A:756:ILE:H	1:A:756:ILE:HG13	1.55	0.41
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.20	0.41
8:J:1:MET:H1	8:J:56:LEU:H	1.68	0.41
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.55	0.41
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.03	0.41
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.02	0.41
3:C:241:ASP:HB3	9:K:109:TRP:CD2	2.56	0.41
6:H:79:TRP:CZ2	6:H:82:PRO:HD3	2.55	0.41
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.03	0.41
2:B:976:ILE:O	2:B:978:ASP:N	2.45	0.41
4:E:94:LYS:HA	4:E:97:VAL:HB	2.01	0.41
1:A:1154:TYR:CD2	7:I:25:LEU:HB2	2.55	0.41
2:B:899:ILE:HD12	2:B:949:VAL:HG21	2.03	0.41
3:C:52:GLU:HA	10:L:64:LEU:HD22	2.03	0.41
6:H:83:GLN:HE21	6:H:85:GLY:H	1.68	0.41
7:I:26:LEU:HD23	7:I:37:GLU:HA	2.01	0.41
1:A:312:PRO:HB2	1:A:313:GLN:H	1.76	0.41
6:H:26:ILE:HG22	6:H:40:LEU:HB3	2.03	0.41
10:L:61:THR:HB	10:L:63:ARG:H	1.86	0.41
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.21	0.41
2:B:581:PHE:HB2	2:B:625:LYS:HG2	2.02	0.41
5:F:89:GLU:O	5:F:93:ILE:HG12	2.21	0.41
1:A:453:MET:HB3	1:A:477:PRO:HB2	2.03	0.41
1:A:942:PHE:O	1:A:945:GLU:HG2	2.21	0.41
3:C:134:ILE:HG12	3:C:141:GLY:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:66:GLU:HA	4:E:69:ILE:HD12	2.02	0.41
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.52	0.41
2:B:277:LYS:H	2:B:277:LYS:HG3	1.65	0.41
1:A:466:SER:HB3	2:B:1103:ILE:HD12	2.02	0.40
2:B:282:ILE:HD13	2:B:382:ILE:HD13	2.03	0.40
3:C:51:VAL:HG12	3:C:155:LEU:HB3	2.03	0.40
6:H:61:SER:HA	6:H:141:TYR:HD1	1.86	0.40
1:A:547:LEU:HD22	9:K:58:PHE:HD1	1.87	0.40
8:J:17:LYS:HD3	8:J:41:LEU:HD21	2.03	0.40
1:A:586:ILE:HD11	1:A:637:LYS:CG	2.52	0.40
1:A:775:ILE:HG21	1:A:815:PHE:CD2	2.56	0.40
1:A:1205:LYS:HB2	1:A:1207:LEU:HD12	2.03	0.40
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.22	0.40
2:B:803:LEU:N	2:B:822:ASN:HD21	2.18	0.40
7:I:65:ASP:HB3	7:I:68:LEU:HD12	2.04	0.40
1:A:589:GLN:HB3	1:A:961:ARG:HH22	1.86	0.40
1:A:591:PHE:HA	1:A:595:THR:HG21	2.03	0.40
2:B:213:ILE:HD12	2:B:497:ARG:HB3	2.03	0.40
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.57	0.40
3:C:176:ILE:HG12	3:C:232:VAL:HG12	2.03	0.40
7:I:84:VAL:HG23	7:I:104:LEU:HD11	2.04	0.40
1:A:492:PRO:HB3	1:A:497:THR:HG22	2.04	0.40
1:A:821:ARG:HG3	1:A:825:ILE:HD11	2.03	0.40
9:K:7:PHE:HB2	9:K:11:LEU:HD22	2.04	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%)	1212 (87%)	137 (10%)	46 (3%)	4 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	1096/1224 (90%)	960 (88%)	91 (8%)	45 (4%)	3 18
3	C	264/318 (83%)	234 (89%)	24 (9%)	6 (2%)	6 31
4	E	212/215 (99%)	191 (90%)	18 (8%)	3 (1%)	11 43
5	F	83/155 (54%)	73 (88%)	9 (11%)	1 (1%)	13 46
6	H	129/146 (88%)	100 (78%)	23 (18%)	6 (5%)	2 15
7	I	117/122 (96%)	100 (86%)	14 (12%)	3 (3%)	5 28
8	J	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4 23
9	K	112/120 (93%)	102 (91%)	8 (7%)	2 (2%)	8 38
10	L	44/70 (63%)	27 (61%)	11 (25%)	6 (14%)	0 1
All	All	3515/4173 (84%)	3056 (87%)	339 (10%)	120 (3%)	3 22

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	50	ILE
1	A	56	PRO
1	A	257	ARG
1	A	315	LEU
1	A	324	SER
1	A	325	ILE
1	A	404	TYR
1	A	409	SER
1	A	1001	ARG
2	B	67	SER
2	B	168	GLY
2	B	250	PHE
2	B	264	SER
2	B	266	ALA
2	B	477	ALA
2	B	482	VAL
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	944	THR

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Mol	Chain	Res	Type
2	B	1046	PRO
2	B	1097	HIS
2	B	1156	ASP
3	C	173	ALA
6	H	109	LYS
8	J	2	ILE
9	K	28	PRO
1	A	55	ASP
1	A	76	GLU
1	A	214	ILE
1	A	332	LYS
1	A	385	ILE
1	A	423	ASP
1	A	1083	THR
1	A	1084	PHE
1	A	1123	GLY
1	A	1437	GLY
2	B	137	TYR
2	B	139	ALA
2	B	465	ASN
2	B	629	ASP
2	B	646	LEU
2	B	792	MET
2	B	884	ARG
2	B	943	SER
2	B	1066	SER
2	B	1108	ARG
2	B	1178	ASN
2	B	1223	ASP
3	C	5	GLY
3	C	142	VAL
3	C	215	GLU
4	E	90	VAL
5	F	78	GLN
6	H	136	LYS
8	J	6	ARG
10	L	55	ILE
1	A	65	LEU
1	A	109	HIS
1	A	130	ASP
1	A	312	PRO
1	A	330	LYS

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Mol	Chain	Res	Type
1	A	775	ILE
1	A	911	SER
2	B	105	SER
2	B	563	MET
2	B	707	PRO
2	B	881	ASN
2	B	976	ILE
2	B	1221	SER
3	C	267	GLN
4	E	86	PRO
6	H	128	ASN
7	I	3	THR
7	I	20	LYS
9	K	71	PHE
10	L	39	SER
1	A	215	SER
1	A	250	ILE
1	A	275	SER
1	A	525	GLN
1	A	567	LYS
1	A	569	LYS
1	A	583	PRO
1	A	958	VAL
1	A	1221	LYS
2	B	483	LEU
2	B	734	HIS
2	B	1157	ALA
2	B	1181	GLU
6	H	84	ALA
6	H	108	SER
1	A	308	ILE
1	A	424	ILE
1	A	568	PRO
1	A	599	SER
1	A	672	ASP
1	A	922	ASP
1	A	1278	ASN
2	B	346	GLU
2	B	367	LEU
2	B	887	HIS
2	B	977	GLY
4	E	103	LYS

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Mol	Chain	Res	Type
6	H	90	ALA
7	I	77	LYS
10	L	46	VAL
10	L	59	ALA
10	L	64	LEU
1	A	35	ILE
1	A	1405	THR
10	L	56	LEU
1	A	321	PRO
2	B	364	ILE
3	C	126	GLY

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%)	1069 (87%)	156 (13%)	4 19
2	B	967/1061 (91%)	853 (88%)	114 (12%)	5 22
3	C	234/274 (85%)	208 (89%)	26 (11%)	6 24
4	E	196/197 (100%)	176 (90%)	20 (10%)	7 28
5	F	75/137 (55%)	73 (97%)	2 (3%)	44 73
6	H	117/128 (91%)	99 (85%)	18 (15%)	2 12
7	I	113/116 (97%)	103 (91%)	10 (9%)	10 34
8	J	60/65 (92%)	48 (80%)	12 (20%)	1 5
9	K	99/102 (97%)	88 (89%)	11 (11%)	6 24
10	L	40/57 (70%)	32 (80%)	8 (20%)	1 5
All	All	3126/3657 (86%)	2749 (88%)	377 (12%)	5 21

All (377) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	40	THR

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Mol	Chain	Res	Type
1	A	41	MET
1	A	43	GLU
1	A	46	THR
1	A	47	ARG
1	A	57	ARG
1	A	58	LEU
1	A	63	ARG
1	A	68	GLN
1	A	69	THR
1	A	70	CYS
1	A	93	VAL
1	A	108	MET
1	A	118	HIS
1	A	123	ARG
1	A	143	LYS
1	A	145	LYS
1	A	177	ASP
1	A	204	THR
1	A	218	ASP
1	A	226	GLU
1	A	252	PHE
1	A	254	GLU
1	A	255	SER
1	A	260	ASP
1	A	262	LEU
1	A	266	LEU
1	A	270	LEU
1	A	289	ILE
1	A	299	HIS
1	A	308	ILE
1	A	315	LEU
1	A	320	ARG
1	A	332	LYS
1	A	335	ARG
1	A	351	THR
1	A	353	ILE
1	A	359	LEU
1	A	386	ASP
1	A	416	ARG
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU

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Mol	Chain	Res	Type
1	A	445	ASN
1	A	448	PRO
1	A	450	LEU
1	A	451	HIS
1	A	455	MET
1	A	470	LEU
1	A	475	THR
1	A	485	ASP
1	A	525	GLN
1	A	527	THR
1	A	533	LYS
1	A	535	THR
1	A	541	ILE
1	A	566	ILE
1	A	590	ARG
1	A	595	THR
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	625	SER
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	636	GLU
1	A	640	GLN
1	A	663	SER
1	A	666	ILE
1	A	691	LEU
1	A	695	LYS
1	A	705	LYS
1	A	710	LEU
1	A	716	ASP
1	A	719	VAL
1	A	722	LEU
1	A	740	LEU
1	A	754	SER
1	A	768	GLN
1	A	796	SER
1	A	801	GLU
1	A	805	LEU
1	A	821	ARG
1	A	826	ASP

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Mol	Chain	Res	Type
1	A	830	LYS
1	A	838	GLN
1	A	848	ILE
1	A	867	ILE
1	A	878	ILE
1	A	896	ARG
1	A	898	ARG
1	A	908	LEU
1	A	931	GLU
1	A	934	LYS
1	A	940	ARG
1	A	953	ASN
1	A	968	GLN
1	A	992	ASP
1	A	1001	ARG
1	A	1008	GLN
1	A	1011	GLN
1	A	1012	ARG
1	A	1015	VAL
1	A	1022	LEU
1	A	1025	ARG
1	A	1037	LEU
1	A	1048	ASN
1	A	1067	LEU
1	A	1084	PHE
1	A	1085	HIS
1	A	1094	VAL
1	A	1102	LYS
1	A	1109	LYS
1	A	1110	ASN
1	A	1136	SER
1	A	1146	VAL
1	A	1168	GLU
1	A	1174	PHE
1	A	1176	LEU
1	A	1195	LEU
1	A	1229	SER
1	A	1234	GLU
1	A	1237	ILE
1	A	1243	VAL
1	A	1261	LYS
1	A	1263	ILE

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Mol	Chain	Res	Type
1	A	1264	GLU
1	A	1266	THR
1	A	1269	GLU
1	A	1271	ILE
1	A	1277	GLU
1	A	1280	GLU
1	A	1288	ASP
1	A	1289	ARG
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1303	GLU
1	A	1307	GLU
1	A	1325	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1351	GLU
1	A	1354	ASN
1	A	1359	ASP
1	A	1366	ARG
1	A	1382	THR
1	A	1385	THR
1	A	1387	HIS
1	A	1391	ARG
1	A	1393	ASN
1	A	1407	GLU
1	A	1426	GLU
1	A	1442	ASP
2	B	21	GLU
2	B	25	ILE
2	B	28	GLU
2	B	46	GLN
2	B	58	THR
2	B	59	LEU
2	B	89	GLU
2	B	101	MET
2	B	103	ASN
2	B	121	ASN
2	B	175	ARG
2	B	183	GLU
2	B	185	THR
2	B	189	LEU

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Mol	Chain	Res	Type
2	B	194	GLU
2	B	199	MET
2	B	217	ARG
2	B	218	SER
2	B	234	ILE
2	B	249	ARG
2	B	254	LEU
2	B	261	ARG
2	B	277	LYS
2	B	278	GLN
2	B	325	GLN
2	B	355	ILE
2	B	364	ILE
2	B	365	THR
2	B	387	LEU
2	B	393	LYS
2	B	405	ARG
2	B	408	LEU
2	B	413	LEU
2	B	416	LEU
2	B	437	GLU
2	B	449	ASN
2	B	458	LYS
2	B	461	LEU
2	B	471	LYS
2	B	480	SER
2	B	482	VAL
2	B	485	ARG
2	B	493	SER
2	B	513	GLN
2	B	537	LYS
2	B	538	ASN
2	B	549	THR
2	B	602	THR
2	B	604	ARG
2	B	616	ILE
2	B	620	ARG
2	B	626	ILE
2	B	628	THR
2	B	645	SER
2	B	646	LEU
2	B	653	VAL

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Mol	Chain	Res	Type
2	B	655	LYS
2	B	658	ILE
2	B	696	GLU
2	B	705	MET
2	B	708	GLU
2	B	709	ASP
2	B	762	ASN
2	B	780	VAL
2	B	786	ASN
2	B	791	THR
2	B	792	MET
2	B	796	LEU
2	B	815	ARG
2	B	825	VAL
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	853	SER
2	B	866	TYR
2	B	868	MET
2	B	873	THR
2	B	874	PHE
2	B	879	ARG
2	B	884	ARG
2	B	889	THR
2	B	899	ILE
2	B	906	SER
2	B	911	ILE
2	B	935	ARG
2	B	948	ILE
2	B	953	LEU
2	B	954	VAL
2	B	961	LEU
2	B	963	PHE
2	B	967	ARG
2	B	969	ARG
2	B	983	ARG
2	B	998	ASP
2	B	999	MET
2	B	1006	ILE
2	B	1022	THR
2	B	1028	GLU

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Mol	Chain	Res	Type
2	B	1034	VAL
2	B	1049	ASP
2	B	1057	LYS
2	B	1065	GLN
2	B	1099	VAL
2	B	1103	ILE
2	B	1129	ARG
2	B	1138	MET
2	B	1147	LEU
2	B	1151	LEU
2	B	1160	VAL
2	B	1175	LEU
2	B	1176	ASN
2	B	1178	ASN
2	B	1194	ILE
2	B	1202	LEU
3	C	4	GLU
3	C	21	ILE
3	C	23	SER
3	C	32	SER
3	C	35	ARG
3	C	36	VAL
3	C	57	VAL
3	C	75	MET
3	C	77	ILE
3	C	79	GLN
3	C	80	LEU
3	C	124	LEU
3	C	127	ARG
3	C	129	ILE
3	C	136	ASP
3	C	140	ASN
3	C	148	ARG
3	C	151	GLN
3	C	214	ASN
3	C	215	GLU
3	C	221	TYR
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	260	LEU
3	C	268	ASP

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Mol	Chain	Res	Type
4	E	7	ARG
4	E	9	ILE
4	E	41	ASP
4	E	48	ASP
4	E	54	GLN
4	E	55	ARG
4	E	56	LYS
4	E	74	ASP
4	E	84	ASP
4	E	92	THR
4	E	94	LYS
4	E	106	GLN
4	E	127	ILE
4	E	152	LYS
4	E	159	ASP
4	E	162	ARG
4	E	169	ARG
4	E	173	SER
4	E	191	LYS
4	E	192	ARG
5	F	71	GLU
5	F	103	MET
6	H	8	ASP
6	H	13	SER
6	H	16	ASP
6	H	26	ILE
6	H	35	GLN
6	H	40	LEU
6	H	55	LEU
6	H	83	GLN
6	H	94	ASP
6	H	95	TYR
6	H	106	GLU
6	H	110	ASP
6	H	130	ARG
6	H	132	LEU
6	H	133	ASN
6	H	135	LEU
6	H	139	ASN
6	H	145	ARG
7	I	4	PHE
7	I	29	CYS

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Mol	Chain	Res	Type
7	I	52	ILE
7	I	62	ILE
7	I	70	ARG
7	I	73	ARG
7	I	105	SER
7	I	107	SER
7	I	111	THR
7	I	116	ASN
8	J	7	CYS
8	J	9	SER
8	J	13	VAL
8	J	19	GLU
8	J	23	ASN
8	J	38	ARG
8	J	43	ARG
8	J	48	ARG
8	J	56	LEU
8	J	59	LYS
8	J	62	ARG
8	J	64	ASN
9	K	5	ASP
9	K	29	ASN
9	K	41	THR
9	K	51	LEU
9	K	63	VAL
9	K	79	GLU
9	K	101	LEU
9	K	102	LYS
9	K	107	THR
9	K	111	LEU
9	K	114	LEU
10	L	27	LEU
10	L	42	ARG
10	L	43	THR
10	L	47	ARG
10	L	50	ASP
10	L	58	LYS
10	L	65	VAL
10	L	66	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	68	GLN
1	A	299	HIS
1	A	313	GLN
1	A	503	GLN
1	A	517	ASN
1	A	525	GLN
1	A	584	ASN
1	A	603	ASN
1	A	626	ASN
1	A	631	HIS
1	A	741	ASN
1	A	757	ASN
1	A	926	GLN
1	A	1140	HIS
1	A	1171	GLN
1	A	1203	ASN
1	A	1218	GLN
1	A	1354	ASN
1	A	1364	ASN
1	A	1432	GLN
2	B	215	GLN
2	B	363	HIS
2	B	383	ASN
2	B	449	ASN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	587	HIS
2	B	734	HIS
2	B	744	HIS
2	B	762	ASN
2	B	822	ASN
2	B	1013	ASN
2	B	1015	HIS
2	B	1074	ASN
2	B	1084	GLN
2	B	1117	GLN
2	B	1141	HIS
2	B	1161	HIS
3	C	73	GLN

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Mol	Chain	Res	Type
3	C	91	HIS
3	C	112	ASN
3	C	167	HIS
3	C	242	GLN
4	E	61	GLN
4	E	63	ASN
6	H	3	ASN
6	H	83	GLN
7	I	60	GLN
7	I	83	ASN
9	K	65	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	7/8 (87%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	10	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 monosaccharides 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.

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%)	-0.05	74 (5%) 26 17	46, 104, 194, 237	0
2	B	1114/1224 (91%)	-0.18	43 (3%) 39 28	45, 98, 166, 201	0
3	C	266/318 (83%)	-0.19	9 (3%) 45 33	67, 96, 146, 180	0
4	E	214/215 (99%)	-0.04	7 (3%) 46 34	74, 135, 177, 193	0
5	F	85/155 (54%)	-0.31	1 (1%) 79 70	77, 114, 151, 168	0
6	H	133/146 (91%)	0.23	12 (9%) 9 7	98, 141, 173, 183	0
7	I	119/122 (97%)	-0.17	0 100 100	72, 113, 145, 163	0
8	J	65/70 (92%)	-0.19	0 100 100	60, 88, 127, 138	0
9	K	114/120 (95%)	-0.24	1 (0%) 84 78	64, 96, 127, 141	0
10	L	46/70 (65%)	0.20	3 (6%) 18 12	84, 137, 162, 175	0
11	R	8/8 (100%)	0.40	1 (12%) 3 3	100, 128, 162, 169	0
12	T	13/29 (44%)	0.98	2 (15%) 2 1	109, 134, 191, 198	0
All	All	3582/4210 (85%)	-0.10	153 (4%) 35 25	45, 105, 180, 237	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	11.7
1	A	317	LYS	11.0
1	A	69	THR	6.3
1	A	318	SER	6.3
1	A	163	SER	6.0
1	A	154	SER	5.2
2	B	883	LEU	5.1
2	B	1222	ARG	4.8
2	B	1224	PHE	4.8
1	A	1087	ALA	4.6
6	H	86	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
3	C	218	PRO	4.5
2	B	106	ASP	4.4
1	A	118	HIS	4.4
1	A	1088	GLY	4.3
1	A	319	GLY	4.3
1	A	1175	SER	4.3
1	A	254	GLU	4.3
6	H	85	GLY	4.2
2	B	474	SER	4.1
2	B	865	LYS	4.0
1	A	49	LYS	3.9
1	A	161	LEU	3.8
2	B	1223	ASP	3.8
1	A	1080	THR	3.8
6	H	83	GLN	3.8
1	A	44	THR	3.8
1	A	975	HIS	3.8
1	A	212	LYS	3.7
1	A	255	SER	3.7
1	A	1085	HIS	3.6
3	C	219	PHE	3.5
2	B	136	THR	3.5
1	A	316	GLN	3.5
2	B	882	THR	3.5
1	A	153	PRO	3.4
1	A	285	PRO	3.4
1	A	124	GLN	3.4
12	T	28	DT	3.4
12	T	16	DC	3.3
1	A	1092	LYS	3.3
6	H	84	ALA	3.3
1	A	140	THR	3.3
1	A	252	PHE	3.3
2	B	889	THR	3.3
1	A	168	GLY	3.2
1	A	182	VAL	3.2
2	B	1186	ASP	3.2
6	H	108	SER	3.2
2	B	1221	SER	3.1
1	A	65	LEU	3.1
3	C	220	ASP	3.1
2	B	250	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	722	ASP	3.1
1	A	1091	SER	3.1
2	B	647	GLY	3.1
2	B	105	SER	3.1
1	A	284	ALA	3.1
1	A	1082	ASN	3.1
2	B	141	ASP	3.0
2	B	870	ILE	3.0
1	A	34	LYS	3.0
10	L	49	LYS	3.0
1	A	46	THR	3.0
2	B	471	LYS	3.0
6	H	107	VAL	2.9
1	A	1090	ALA	2.9
1	A	250	ILE	2.9
1	A	144	THR	2.9
2	B	866	TYR	2.9
4	E	115	ASN	2.9
2	B	867	GLY	2.9
1	A	998	LEU	2.8
1	A	314	ALA	2.8
1	A	147	VAL	2.8
1	A	162	VAL	2.8
2	B	140	ILE	2.8
1	A	121	LEU	2.8
2	B	472	ALA	2.8
3	C	216	GLY	2.8
1	A	1123	GLY	2.8
1	A	286	HIS	2.7
11	R	3	U	2.7
1	A	283	GLY	2.7
10	L	50	ASP	2.6
1	A	1256	GLU	2.6
6	H	109	LYS	2.6
1	A	1086	PHE	2.6
2	B	473	MET	2.6
4	E	215	MET	2.6
2	B	1169	MET	2.6
2	B	708	GLU	2.6
2	B	469	GLN	2.6
1	A	1089	VAL	2.6
1	A	141	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	66	LYS	2.5
4	E	2	ASP	2.5
2	B	868	MET	2.5
3	C	4	GLU	2.5
6	H	51	ALA	2.5
1	A	150	THR	2.5
3	C	221	TYR	2.4
6	H	88	SER	2.4
1	A	232	GLU	2.4
2	B	709	ASP	2.4
1	A	282	ASN	2.4
2	B	89	GLU	2.4
1	A	87	ALA	2.4
1	A	1391	ARG	2.3
2	B	1208	MET	2.3
1	A	1390	ASN	2.3
2	B	231	PRO	2.3
1	A	75	ASN	2.3
1	A	176	LYS	2.3
3	C	217	ASP	2.2
1	A	54	ASN	2.2
4	E	93	MET	2.2
6	H	132	LEU	2.2
1	A	315	LEU	2.2
1	A	120	GLU	2.2
2	B	933	SER	2.2
4	E	49	SER	2.2
2	B	433	GLN	2.2
1	A	1083	THR	2.2
1	A	199	LEU	2.2
2	B	135	ARG	2.2
2	B	470	LYS	2.2
1	A	45	GLN	2.2
1	A	167	CYS	2.2
1	A	253	ASN	2.2
6	H	111	LEU	2.2
6	H	117	SER	2.2
1	A	151	ASP	2.1
4	E	104	ASN	2.1
2	B	248	SER	2.1
5	F	143	PHE	2.1
2	B	367	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
9	K	15	GLY	2.1
1	A	311	GLN	2.1
1	A	73	GLY	2.1
1	A	313	GLN	2.1
2	B	139	ALA	2.1
1	A	43	GLU	2.1
1	A	186	LYS	2.1
2	B	645	SER	2.1
1	A	1081	LEU	2.0
10	L	27	LEU	2.0
3	C	214	ASN	2.0
2	B	468	GLU	2.0
4	E	87	SER	2.0
2	B	138	GLU	2.0
2	B	261	ARG	2.0
3	C	222	LYS	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
13	ZN	A	1734	1/1	0.51	0.11	300,300,300,300	0
13	ZN	B	1307	1/1	0.92	0.11	174,174,174,174	0
13	ZN	A	1735	1/1	0.96	0.14	133,133,133,133	0
14	MG	A	2001	1/1	0.96	0.12	41,41,41,41	0
13	ZN	I	204	1/1	0.98	0.07	79,79,79,79	0
13	ZN	C	319	1/1	0.99	0.08	91,91,91,91	0
13	ZN	I	203	1/1	0.99	0.06	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	ZN	L	105	1/1	1.00	0.04	139,139,139,139	0
13	ZN	J	101	1/1	1.00	0.13	71,71,71,71	0

6.5 Other polymers (i)

There are no such residues in this entry.