Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 01:44 PM EDT

PDB ID	:	3S1M
Title	:	RNA Polymerase II Initiation Complex with a 5-nt RNA (variant 1)
Authors	:	Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on	:	2011-05-15
Resolution	:	3.13 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

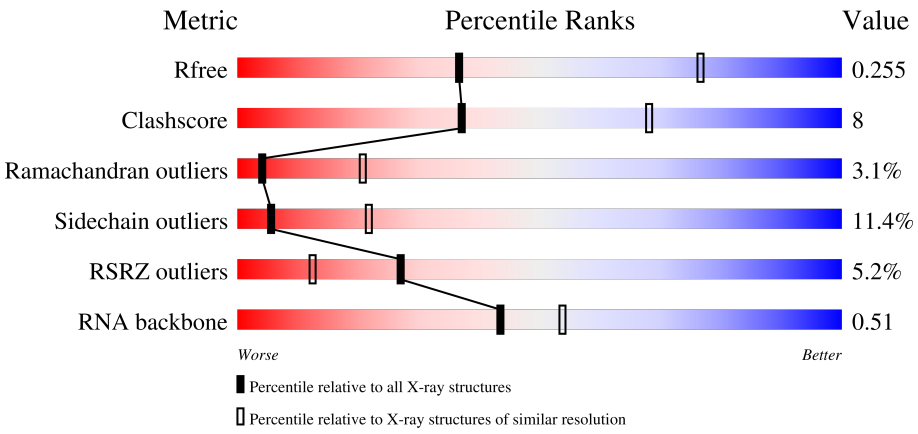
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.13 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)
RNA backbone	3102	1000 (3.46-2.82)

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	8% 58% 18% • 19%
2	B	1224	3% 65% 23% • 9%
3	C	318	60% 20% • 16%
4	E	215	% 81% 16% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	155	48% 7% 45%
6	H	146	3% 64% 21% 6% 9%
7	I	122	74% 21%
8	J	70	61% 24% 6% 7%
9	K	120	72% 18% 5%
10	L	70	3% 29% 30% 7% 34%
11	R	5	20% 80% 20%
12	T	29	10% 17% 72%

2 Entry composition (i)

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
			Total	C	N	O	S			
7	I	119	971	596	179	186	10	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
11	R	5	107	49	23	31	4	0	0	0

- 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*GP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
12	T	8	162	77	28	49	8	0	0	0

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

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

Continued on next page...

Continued from previous page...

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

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

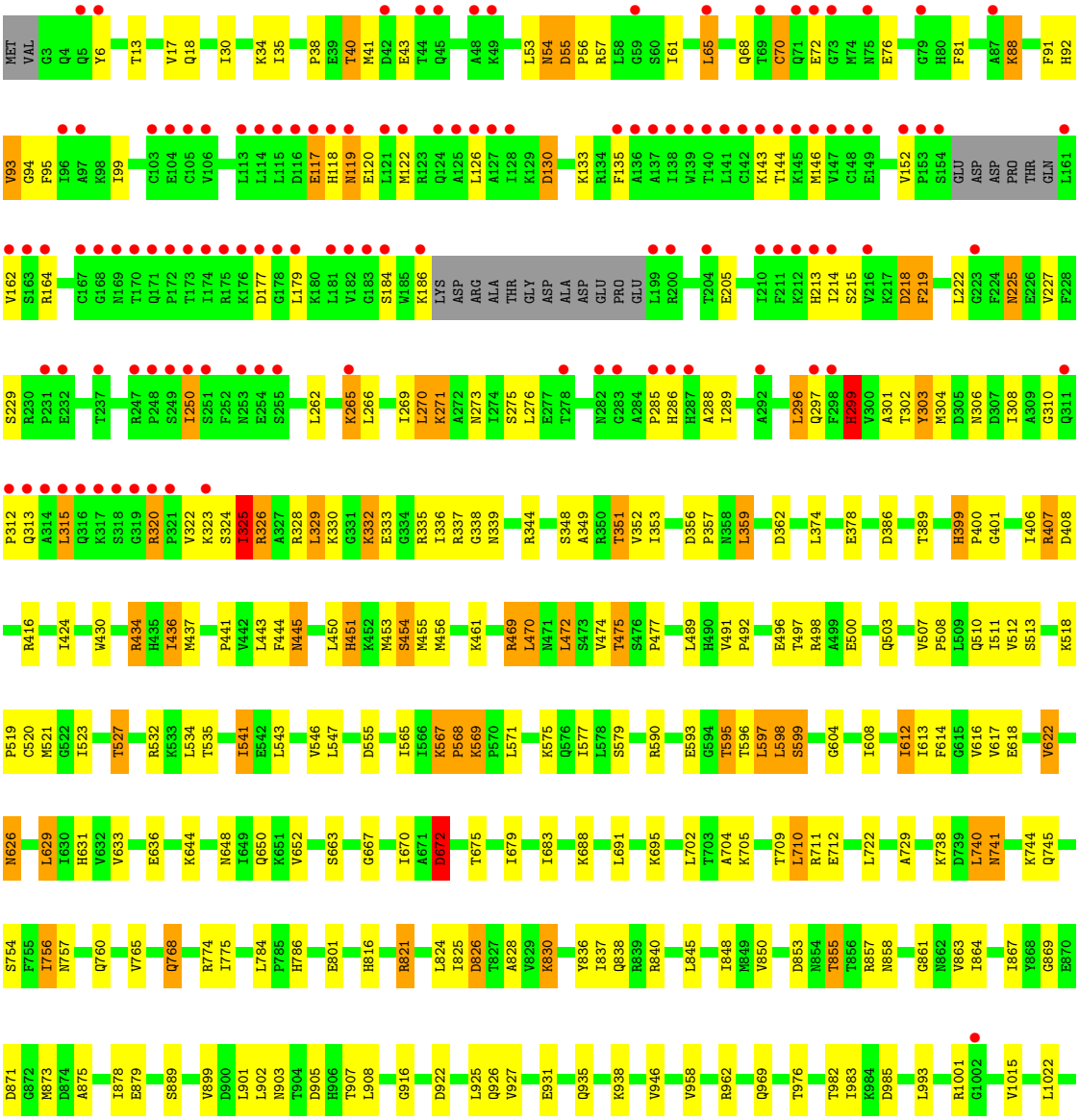
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
14	A	1	1	1	0	0

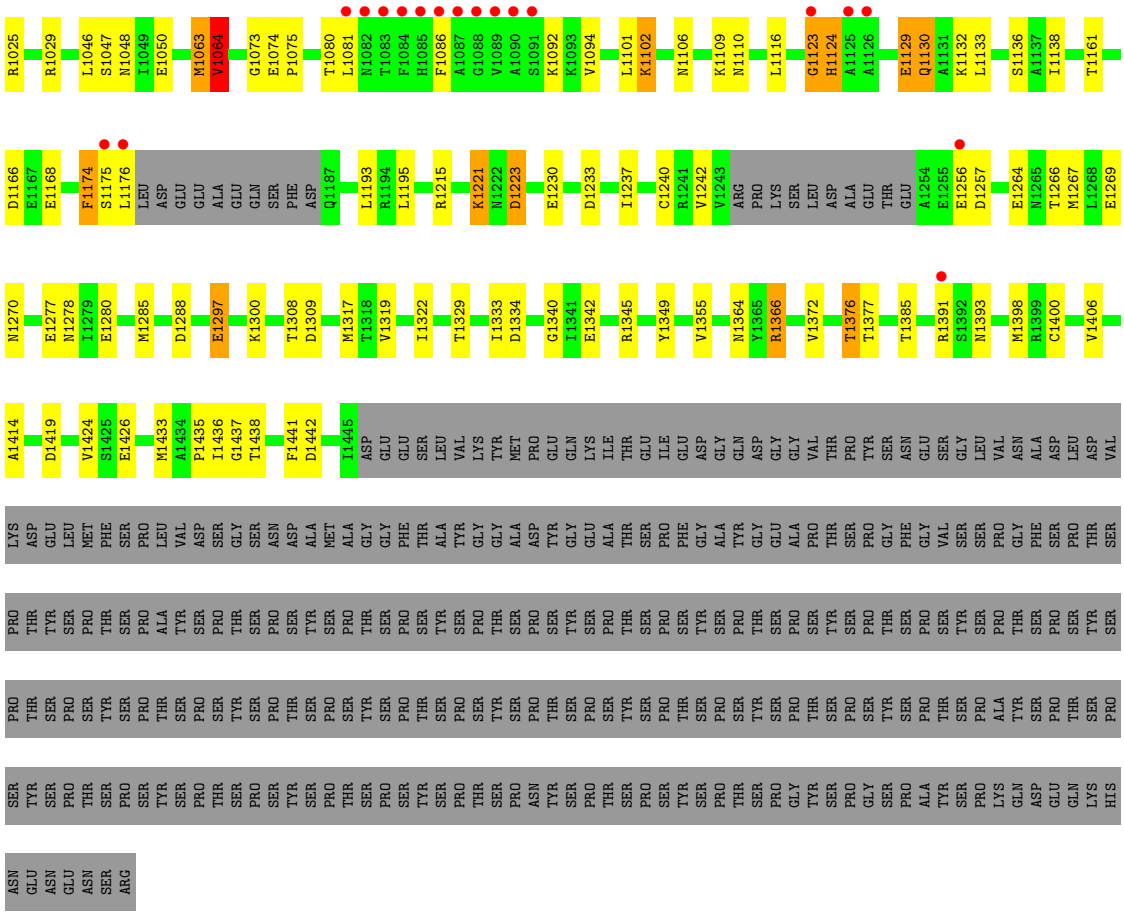
3 Residue-property plots (i)

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

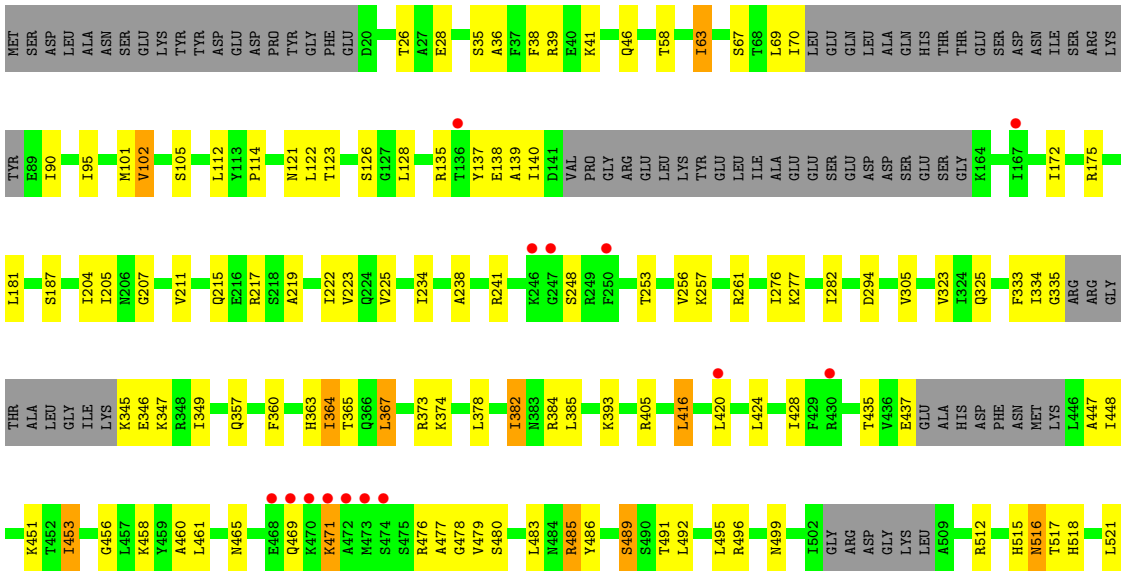
Chain A: 8% 58% 18% 19%

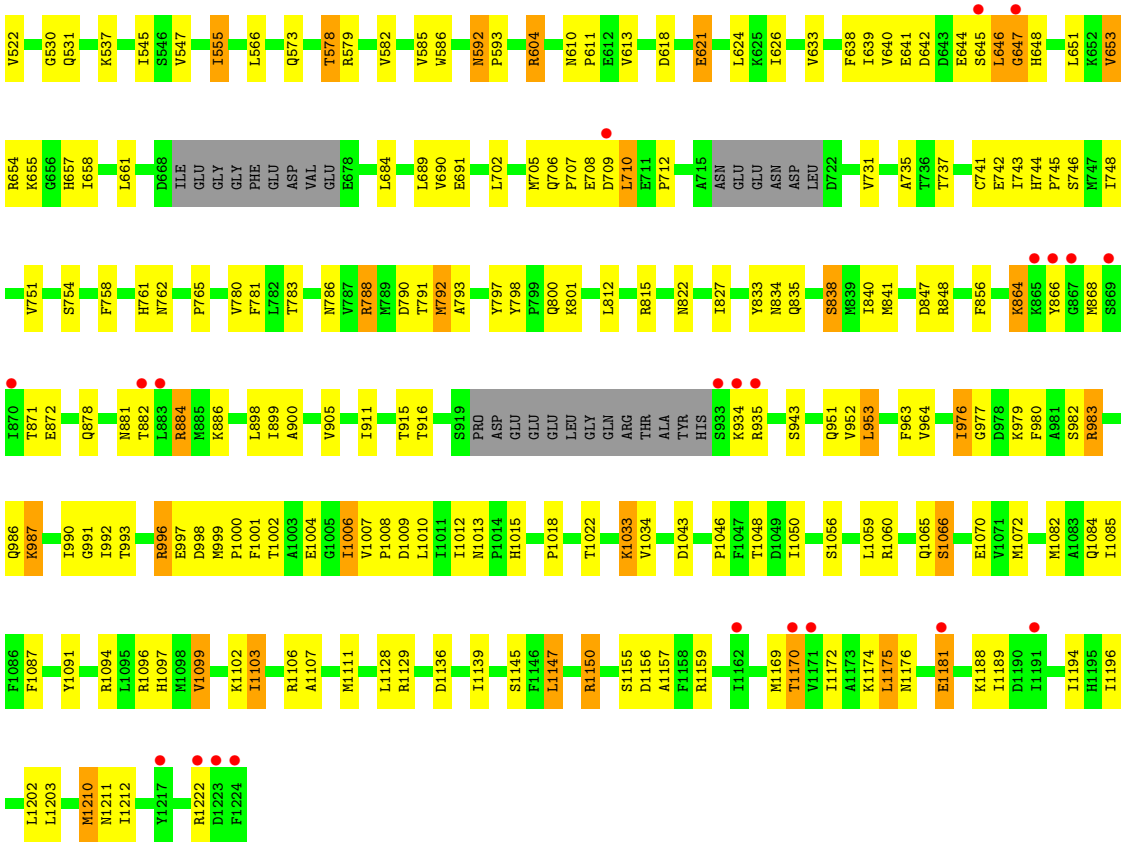




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

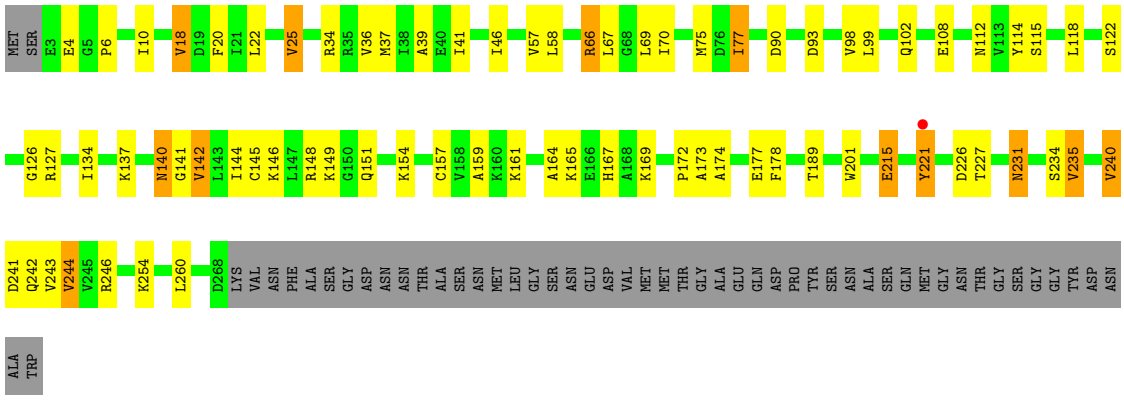
Chain B:





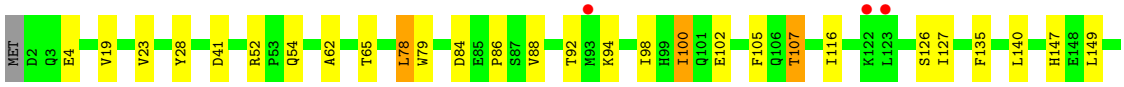
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

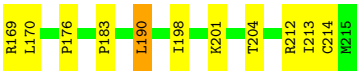
Chain C:



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

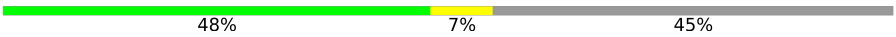
Chain E:

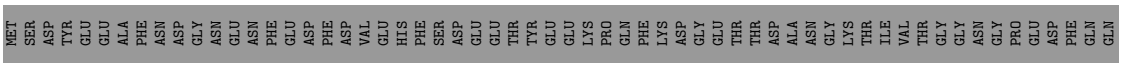


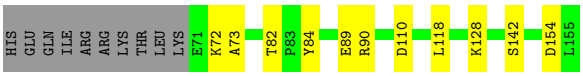


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:

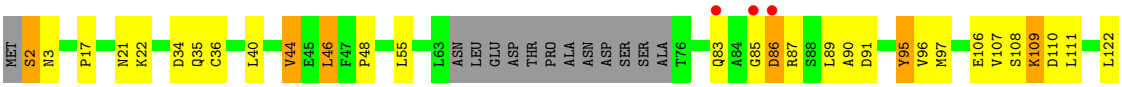


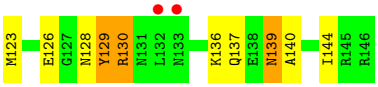




• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

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

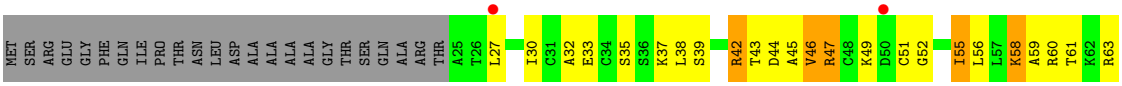
Chain J:

• 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:

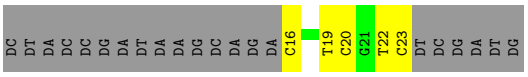


• Molecule 11: RNA (5'-R(*AP*GP*AP*CP*G)-3')

Chain R:

• Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*GP*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	156.92Å 220.71Å 191.77Å 90.00° 97.48° 90.00°	Depositor
Resolution (Å)	47.72 – 3.13 47.72 – 3.12	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.72-3.13) 98.7 (47.72-3.12)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 3.12Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.183 , 0.233 0.205 , 0.255	Depositor DCC
R_{free} test set	5668 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	79.3	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 84.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	28570	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: 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	0.47	0/11241	0.75	2/15199 (0.0%)
2	B	0.48	0/9033	0.76	1/12181 (0.0%)
3	C	0.44	0/2133	0.77	0/2891
4	E	0.43	0/1788	0.67	0/2406
5	F	0.44	0/700	0.68	0/945
6	H	0.44	0/1086	0.78	1/1470 (0.1%)
7	I	0.47	0/989	0.81	0/1331
8	J	0.49	0/541	0.83	0/727
9	K	0.43	0/937	0.68	0/1265
10	L	0.51	0/365	0.90	0/485
11	R	0.95	0/120	1.47	0/186
12	T	1.24	0/180	1.92	7/275 (2.5%)
All	All	0.48	0/29113	0.77	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})
12	T	22	DT	O4'-C1'-N1	7.68	113.38	108.00
1	A	218	ASP	C-N-CA	6.95	139.08	121.70
12	T	23	DC	O4'-C1'-N1	6.54	112.58	108.00
12	T	20	DC	O4'-C1'-N1	6.33	112.43	108.00
12	T	19	DT	O4'-C1'-N1	5.92	112.14	108.00
12	T	16	DC	O4'-C1'-N1	5.60	111.92	108.00
12	T	22	DT	N3-C2-O2	-5.50	119.00	122.30
2	B	140	ILE	C-N-CA	5.19	134.68	121.70
6	H	2	SER	C-N-CA	5.07	134.37	121.70
12	T	20	DC	C4'-C3'-C2'	-5.04	98.56	103.10
1	A	1063	MET	C-N-CA	5.02	134.25	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	196	0
2	B	8861	0	8884	152	0
3	C	2095	0	2051	46	0
4	E	1752	0	1776	23	0
5	F	688	0	707	6	0
6	H	1068	0	1040	19	0
7	I	971	0	927	14	0
8	J	532	0	542	22	0
9	K	919	0	929	20	0
10	L	363	0	386	11	0
11	R	107	0	56	0	0
12	T	162	0	91	0	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	447	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (447) 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:756:ILE:CG1	1:A:756:ILE:CD1	1.74	1.57
2:B:801:LYS:O	8:J:52:THR:HG23	1.74	0.87
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.58	0.86
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.41	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HB3	6:H:96:VAL:H	1.44	0.82
1:A:218:ASP:H	1:A:219:PHE:HB3	1.44	0.81
2:B:1002:THR:HG22	2:B:1004:GLU:H	1.45	0.81
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.62	0.80
2:B:345:LYS:HA	2:B:347:LYS:H	1.47	0.78
1:A:855:THR:HG21	1:A:857:ARG:HE	1.46	0.77
3:C:167:HIS:HD2	3:C:169:LYS:H	1.33	0.77
2:B:515:HIS:HD2	2:B:517:THR:H	1.29	0.77
2:B:864:LYS:HB3	2:B:872:GLU:H	1.48	0.77
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.68	0.76
2:B:706:GLN:O	2:B:710:LEU:HB2	1.86	0.75
2:B:1072:MET:HG3	2:B:1085:ILE:HB	1.67	0.75
2:B:1175:LEU:HD23	2:B:1176:ASN:H	1.52	0.75
9:K:65:HIS:HD2	9:K:67:PHE:H	1.33	0.75
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.70	0.74
1:A:869:GLY:O	4:E:204:THR:HG21	1.88	0.73
1:A:756:ILE:HD13	1:A:756:ILE:H	1.53	0.73
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.70	0.72
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.70	0.72
2:B:486:TYR:OH	2:B:1096:ARG:HB3	1.91	0.71
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.74	0.70
1:A:754:SER:H	1:A:757:ASN:HD22	1.40	0.70
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.73	0.69
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.76	0.69
2:B:744:HIS:HD2	2:B:746:SER:H	1.39	0.69
1:A:596:THR:O	1:A:598:LEU:N	2.27	0.68
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.75	0.68
1:A:567:LYS:O	1:A:569:LYS:N	2.24	0.68
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.58	0.67
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.77	0.67
1:A:567:LYS:HE3	6:H:46:LEU:HD12	1.76	0.66
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.78	0.65
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.28	0.65
2:B:486:TYR:CE2	2:B:1096:ARG:HD2	2.32	0.65
1:A:399:HIS:O	1:A:401:GLY:N	2.30	0.65
1:A:299:HIS:HA	1:A:302:THR:HG22	1.78	0.65
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.79	0.64
2:B:604:ARG:HD3	2:B:611:PRO:HA	1.78	0.64
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.80	0.64
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.79	0.64
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.13	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:654:ARG:H	2:B:657:HIS:HD2	1.44	0.64
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.78	0.64
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.44	0.64
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.80	0.64
1:A:472:LEU:O	1:A:475:THR:HB	1.98	0.64
2:B:241:ARG:HA	2:B:253:THR:HG22	1.80	0.63
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.80	0.63
3:C:98:VAL:H	3:C:122:SER:HB2	1.64	0.63
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.81	0.63
2:B:1034:VAL:HG22	2:B:1059:LEU:HB2	1.80	0.62
3:C:221:TYR:HB3	6:H:46:LEU:HD22	1.81	0.62
1:A:441:PRO:HG2	1:A:498:ARG:HB2	1.82	0.62
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.30	0.61
1:A:901:LEU:HA	1:A:907:THR:HG23	1.83	0.61
1:A:907:THR:HG22	1:A:908:LEU:H	1.66	0.61
2:B:835:GLN:O	2:B:838:SER:HB2	2.00	0.61
1:A:503:GLN:NE2	5:F:90:ARG:HH22	1.99	0.60
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.84	0.60
2:B:651:LEU:HD21	2:B:741:CYS:HB3	1.82	0.60
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.84	0.60
3:C:235:VAL:HG22	8:J:13:VAL:HG23	1.84	0.59
1:A:863:VAL:HG23	4:E:170:LEU:HD21	1.83	0.59
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.82	0.59
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.83	0.59
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.84	0.58
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.85	0.58
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.31	0.58
2:B:363:HIS:O	2:B:364:ILE:HB	2.03	0.58
1:A:91:PHE:HE1	1:A:99:ILE:HG21	1.67	0.58
9:K:32:VAL:HG22	9:K:74:ARG:HG3	1.85	0.58
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.86	0.58
7:I:111:THR:HG23	7:I:113:ASP:H	1.68	0.58
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	1.86	0.57
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.34	0.57
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.86	0.57
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.86	0.57
2:B:705:MET:H	2:B:710:LEU:HG	1.69	0.57
3:C:46:ILE:HA	3:C:159:ALA:HA	1.87	0.57
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.86	0.57
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.04	0.57
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.86	0.57
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.87	0.57
1:A:1377:THR:HG22	4:E:176:PRO:HB3	1.87	0.57
9:K:7:PHE:O	9:K:11:LEU:HB2	2.05	0.57
6:H:2:SER:HB3	6:H:3:ASN:HB2	1.87	0.56
1:A:667:GLY:HA2	1:A:670:ILE:HG12	1.86	0.56
1:A:511:ILE:HA	1:A:521:MET:HE3	1.87	0.56
10:L:27:LEU:HD23	10:L:37:LYS:HD3	1.86	0.56
1:A:513:SER:HB3	1:A:520:CYS:HB3	1.88	0.56
1:A:1086:PHE:HB3	1:A:1092:LYS:HB3	1.86	0.56
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.88	0.56
2:B:223:VAL:HG13	2:B:384:ARG:HH21	1.71	0.56
1:A:527:THR:HG21	1:A:650:GLN:HA	1.88	0.56
1:A:456:MET:HE2	1:A:507:VAL:HA	1.87	0.56
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.88	0.56
6:H:44:VAL:HG12	6:H:48:PRO:HA	1.87	0.56
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.39	0.56
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.88	0.55
1:A:848:ILE:HD12	1:A:864:ILE:HG13	1.87	0.55
1:A:541:ILE:HD11	1:A:577:ILE:HG12	1.88	0.55
3:C:165:LYS:O	9:K:6:ARG:NH1	2.39	0.55
1:A:741:ASN:HB3	1:A:744:LYS:HB2	1.88	0.55
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.89	0.55
2:B:277:LYS:NZ	2:B:335:GLY:H	2.04	0.55
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.70	0.55
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.89	0.55
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.07	0.55
2:B:1082:MET:HA	3:C:189:THR:HA	1.88	0.55
1:A:535:THR:HG21	1:A:617:VAL:H	1.70	0.55
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.41	0.55
1:A:315:LEU:HA	1:A:320:ARG:HB3	1.89	0.55
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.42	0.55
1:A:273:ASN:HA	1:A:296:LEU:HD11	1.88	0.55
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.22	0.54
2:B:38:PHE:H	2:B:41:LYS:HB2	1.72	0.54
2:B:346:GLU:HA	2:B:349:ILE:HD12	1.89	0.54
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.89	0.54
2:B:492:LEU:O	2:B:496:ARG:HG3	2.08	0.54
2:B:916:THR:HG23	2:B:935:ARG:HB3	1.88	0.54
2:B:979:LYS:HE3	2:B:987:LYS:HB2	1.88	0.54
10:L:47:ARG:HG3	10:L:52:GLY:HA2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:ILE:CD1	1:A:756:ILE:H	2.21	0.54
2:B:983:ARG:HH11	2:B:983:ARG:HB2	1.73	0.54
1:A:225:ASN:HD22	1:A:227:VAL:H	1.56	0.54
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.42	0.54
3:C:37:MET:HE2	3:C:244:VAL:HA	1.90	0.54
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.90	0.53
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.90	0.53
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.90	0.53
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.91	0.53
9:K:57:LEU:HB2	9:K:76:GLN:HG2	1.90	0.53
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.43	0.53
2:B:515:HIS:CD2	2:B:517:THR:H	2.19	0.53
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.73	0.53
2:B:864:LYS:H	2:B:872:GLU:HB2	1.73	0.53
3:C:142:VAL:H	8:J:16:ASP:HB3	1.74	0.53
1:A:6:TYR:O	2:B:1175:LEU:HD21	2.08	0.53
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.72	0.53
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.91	0.53
3:C:37:MET:HG2	3:C:243:VAL:HG12	1.91	0.53
1:A:629:LEU:O	1:A:633:VAL:HG23	2.09	0.52
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.90	0.52
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.89	0.52
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.90	0.52
3:C:148:ARG:HB3	3:C:151:GLN:HG3	1.91	0.52
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.92	0.52
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.43	0.52
1:A:982:THR:HB	1:A:985:ASP:H	1.74	0.52
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.74	0.52
2:B:516:ASN:H	2:B:516:ASN:HD22	1.57	0.52
4:E:190:LEU:HD23	4:E:214:CYS:HB2	1.91	0.52
1:A:265:LYS:HD3	1:A:322:VAL:HG21	1.92	0.52
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.75	0.52
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.56	0.52
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.92	0.52
2:B:1048:THR:OG1	2:B:1050:ILE:HD12	2.10	0.52
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.91	0.52
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.91	0.52
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.50	0.52
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.92	0.52
2:B:578:THR:HB	2:B:593:PRO:HG3	1.91	0.52
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:GLU:HG3	4:E:198:ILE:HG21	1.92	0.51
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.40	0.51
8:J:1:MET:H2	8:J:57:ILE:HG22	1.74	0.51
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.91	0.51
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.92	0.51
2:B:915:THR:HG21	2:B:934:LYS:HD2	1.93	0.51
7:I:50:THR:HG22	7:I:52:ILE:H	1.76	0.51
10:L:61:THR:HB	10:L:63:ARG:H	1.74	0.51
2:B:834:ASN:HA	2:B:838:SER:HB3	1.92	0.51
6:H:2:SER:CB	6:H:3:ASN:HB2	2.41	0.51
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.92	0.51
1:A:925:LEU:HD23	1:A:983:ILE:HB	1.92	0.51
1:A:648:ASN:O	1:A:652:VAL:HG23	2.11	0.51
2:B:882:THR:HB	2:B:934:LYS:O	2.10	0.51
9:K:58:PHE:HE2	9:K:74:ARG:HB3	1.76	0.51
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.91	0.51
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.93	0.51
2:B:424:LEU:O	2:B:428:ILE:HG12	2.10	0.50
1:A:469:ARG:NH2	2:B:991:GLY:O	2.37	0.50
1:A:571:LEU:HD22	6:H:46:LEU:HD11	1.94	0.50
2:B:36:ALA:HB2	2:B:661:LEU:HD22	1.92	0.50
1:A:709:THR:HB	1:A:712:GLU:HB2	1.94	0.50
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.93	0.50
3:C:66:ARG:NH2	8:J:3:VAL:O	2.35	0.50
4:E:78:LEU:HD12	4:E:107:THR:HB	1.93	0.50
1:A:541:ILE:HG12	1:A:546:VAL:HG22	1.93	0.50
2:B:953:LEU:O	2:B:964:VAL:HG23	2.12	0.50
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.93	0.50
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.93	0.50
6:H:40:LEU:HD13	6:H:123:MET:HG3	1.94	0.50
1:A:324:SER:O	1:A:326:ARG:N	2.45	0.50
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.93	0.50
7:I:75:CYS:O	7:I:78:CYS:O	2.30	0.50
1:A:626:ASN:O	1:A:631:HIS:CD2	2.65	0.50
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.92	0.50
2:B:489:SER:HA	2:B:492:LEU:HD12	1.94	0.50
10:L:42:ARG:NH1	10:L:43:THR:OG1	2.44	0.50
2:B:35:SER:O	2:B:39:ARG:HB2	2.12	0.49
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.93	0.49
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.44	0.49
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.44	0.49
2:B:345:LYS:HA	2:B:347:LYS:N	2.22	0.49
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.95	0.49
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.45	0.49
1:A:218:ASP:N	1:A:219:PHE:HB3	2.21	0.49
1:A:451:HIS:HB3	1:A:454:SER:H	1.76	0.49
6:H:137:GLN:HB3	6:H:139:ASN:HB2	1.94	0.49
8:J:48:ARG:O	8:J:52:THR:HB	2.13	0.49
1:A:95:PHE:HE2	1:A:1414:ALA:HB2	1.78	0.49
1:A:374:LEU:HA	2:B:1107:ALA:HB2	1.94	0.49
1:A:30:ILE:HG13	2:B:1170:THR:HG23	1.95	0.48
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.94	0.48
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.43	0.48
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.95	0.48
2:B:976:ILE:O	2:B:990:ILE:O	2.31	0.48
2:B:1172:ILE:HG22	2:B:1174:LYS:HG3	1.95	0.48
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.59	0.48
2:B:234:ILE:HD13	2:B:257:LYS:HD2	1.95	0.48
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.28	0.48
2:B:797:TYR:O	8:J:1:MET:HG2	2.12	0.48
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.48	0.48
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.95	0.48
4:E:147:HIS:CD2	4:E:149:LEU:HB2	2.49	0.48
7:I:102:VAL:HG22	7:I:109:ILE:HG12	1.95	0.48
1:A:285:PRO:HD2	1:A:289:ILE:HB	1.96	0.48
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.96	0.48
1:A:709:THR:HG22	1:A:711:ARG:H	1.78	0.48
2:B:977:GLY:HA3	2:B:1099:VAL:HG13	1.95	0.47
3:C:10:ILE:HD13	3:C:20:PHE:HB3	1.96	0.47
1:A:503:GLN:HE21	5:F:90:ARG:NH1	2.12	0.47
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.95	0.47
1:A:857:ARG:HD3	1:A:861:GLY:O	2.13	0.47
1:A:512:VAL:HA	1:A:519:PRO:HA	1.96	0.47
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.96	0.47
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.95	0.47
10:L:55:ILE:H	10:L:55:ILE:HG12	1.55	0.47
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.96	0.47
3:C:108:GLU:HA	3:C:149:LYS:HD3	1.97	0.47
1:A:135:PHE:HD1	1:A:222:LEU:HB2	1.80	0.47
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.29	0.47
1:A:119:ASN:HB3	1:A:122:MET:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.96	0.47
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.97	0.47
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.50	0.47
1:A:378:GLU:OE2	1:A:434:ARG:HD3	2.15	0.46
6:H:95:TYR:HB3	6:H:144:ILE:HB	1.96	0.46
1:A:276:LEU:HD13	1:A:296:LEU:HD12	1.97	0.46
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.80	0.46
1:A:535:THR:HG22	1:A:616:VAL:HA	1.97	0.46
1:A:596:THR:O	1:A:599:SER:N	2.49	0.46
2:B:745:PRO:O	2:B:748:ILE:HG12	2.16	0.46
4:E:79:TRP:HB3	4:E:100:ILE:HD11	1.96	0.46
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.96	0.46
3:C:134:ILE:HG23	3:C:141:GLY:H	1.81	0.46
4:E:147:HIS:CD2	4:E:149:LEU:H	2.33	0.46
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.48	0.46
2:B:126:SER:HB2	2:B:172:ILE:HD11	1.98	0.46
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.96	0.46
3:C:20:PHE:HE1	3:C:22:LEU:HD13	1.80	0.46
7:I:101:PHE:O	7:I:109:ILE:HA	2.16	0.46
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.39	0.46
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.96	0.46
3:C:241:ASP:HB3	9:K:109:TRP:CD2	2.50	0.46
1:A:1080:THR:HG22	1:A:1081:LEU:HD12	1.97	0.46
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.49	0.46
2:B:982:SER:OG	2:B:986:GLN:HB2	2.16	0.46
1:A:225:ASN:HB3	1:A:229:SER:H	1.80	0.46
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.97	0.46
2:B:884:ARG:HE	2:B:935:ARG:HH21	1.64	0.46
3:C:18:VAL:HG22	3:C:240:VAL:HB	1.98	0.46
1:A:55:ASP:O	1:A:57:ARG:N	2.49	0.45
1:A:219:PHE:H	1:A:222:LEU:HG	1.81	0.45
1:A:855:THR:CG2	1:A:857:ARG:HE	2.22	0.45
2:B:1034:VAL:CG2	2:B:1059:LEU:HB2	2.46	0.45
3:C:70:ILE:HG21	3:C:115:SER:HB2	1.98	0.45
1:A:53:LEU:HG	1:A:54:ASN:HD22	1.81	0.45
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.46	0.45
1:A:456:MET:HG2	1:A:510:GLN:HG3	1.98	0.45
1:A:738:LYS:HD2	1:A:740:LEU:HD21	1.99	0.45
8:J:1:MET:N	8:J:57:ILE:H	2.14	0.45
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.98	0.45
2:B:219:ALA:HB3	2:B:222:ILE:HD11	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:THR:HG23	1:A:54:ASN:HD21	1.82	0.45
2:B:1139:ILE:HG13	2:B:1147:LEU:HD11	1.99	0.45
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.52	0.45
3:C:164:ALA:HA	3:C:167:HIS:O	2.17	0.45
3:C:235:VAL:HG11	8:J:6:ARG:NH2	2.32	0.45
7:I:10:CYS:SG	7:I:31:THR:HB	2.58	0.45
7:I:62:ILE:HG12	7:I:84:VAL:HG11	1.98	0.45
1:A:306:ASN:HD21	1:A:313:GLN:HB2	1.82	0.44
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.99	0.44
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.17	0.44
4:E:19:VAL:O	4:E:23:VAL:HG23	2.17	0.44
1:A:899:VAL:HG22	1:A:1029:ARG:HH11	1.82	0.44
2:B:225:VAL:HG11	2:B:385:LEU:HA	1.97	0.44
3:C:148:ARG:H	3:C:151:GLN:HG3	1.82	0.44
1:A:1129:GLU:HA	1:A:1132:LYS:HE3	1.98	0.44
3:C:93:ASP:O	3:C:127:ARG:NH2	2.48	0.44
10:L:61:THR:HB	10:L:63:ARG:HB2	1.98	0.44
1:A:663:SER:HB2	2:B:1085:ILE:HG13	1.97	0.44
2:B:654:ARG:H	2:B:657:HIS:CD2	2.31	0.44
6:H:36:CYS:HB2	6:H:129:TYR:OH	2.18	0.44
1:A:271:LYS:O	1:A:275:SER:HB2	2.18	0.44
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.51	0.44
3:C:57:VAL:HG12	3:C:58:LEU:HD23	1.99	0.44
3:C:234:SER:HB2	3:C:240:VAL:HG13	2.00	0.44
7:I:63:GLY:O	7:I:70:ARG:NH2	2.50	0.44
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.99	0.44
2:B:1097:HIS:HB3	2:B:1102:LYS:HE3	2.00	0.44
3:C:70:ILE:CD1	3:C:144:ILE:HD12	2.48	0.44
9:K:65:HIS:CD2	9:K:67:PHE:H	2.23	0.44
1:A:567:LYS:HD2	1:A:568:PRO:HD2	2.00	0.44
8:J:48:ARG:HD2	8:J:49:MET:HE2	2.00	0.44
8:J:52:THR:HG22	8:J:52:THR:O	2.18	0.44
1:A:304:MET:HG2	1:A:325:ILE:HD12	1.99	0.43
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.52	0.43
1:A:982:THR:H	1:A:985:ASP:HB2	1.83	0.43
2:B:63:ILE:O	2:B:67:SER:HB3	2.18	0.43
2:B:102:VAL:HG11	2:B:122:LEU:HD13	2.00	0.43
1:A:595:THR:HG21	1:A:604:GLY:HA3	2.00	0.43
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.48	0.43
2:B:420:LEU:HB3	2:B:453:ILE:HG13	2.00	0.43
6:H:89:LEU:C	6:H:91:ASP:H	2.22	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.99	0.43
1:A:828:ALA:HB2	2:B:530:GLY:HA2	2.00	0.43
1:A:837:ILE:HD11	1:A:1102:LYS:HG3	2.00	0.43
1:A:848:ILE:HD13	1:A:858:ASN:HB3	2.00	0.43
2:B:123:THR:HA	2:B:204:ILE:O	2.18	0.43
4:E:88:VAL:HB	4:E:116:ILE:HD13	2.00	0.43
6:H:83:GLN:C	6:H:85:GLY:H	2.22	0.43
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.53	0.43
1:A:492:PRO:HB3	1:A:497:THR:HG22	2.00	0.43
1:A:826:ASP:HB2	1:A:830:LYS:HZ3	1.83	0.43
1:A:901:LEU:H	1:A:926:GLN:NE2	2.17	0.43
2:B:211:VAL:HG13	2:B:495:LEU:HD23	2.00	0.43
2:B:592:ASN:H	2:B:593:PRO:HD3	1.84	0.43
7:I:45:ARG:HE	7:I:47:GLU:HG3	1.84	0.43
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	2.00	0.43
1:A:362:ASP:HB3	1:A:508:PRO:HD3	2.00	0.43
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	2.00	0.43
2:B:647:GLY:HA2	2:B:648:HIS:C	2.39	0.43
2:B:898:LEU:HD21	2:B:964:VAL:HG11	2.00	0.43
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.54	0.43
1:A:614:PHE:HB3	6:H:122:LEU:HD21	2.01	0.43
2:B:485:ARG:HG3	2:B:781:PHE:CD1	2.54	0.43
2:B:1013:ASN:OD1	2:B:1015:HIS:HD2	1.99	0.43
2:B:1056:SER:HB3	2:B:1066:SER:HB2	2.00	0.43
3:C:177:GLU:HB2	3:C:231:ASN:HB3	2.01	0.43
1:A:348:SER:HA	1:A:489:LEU:O	2.19	0.43
6:H:109:LYS:HG3	6:H:110:ASP:H	1.83	0.43
9:K:23:PRO:HA	9:K:31:VAL:HG23	2.01	0.43
1:A:672:ASP:HB3	1:A:675:THR:H	1.83	0.43
1:A:993:LEU:HD22	1:A:1046:LEU:HG	2.01	0.43
10:L:32:ALA:HB3	10:L:55:ILE:HG13	2.01	0.43
3:C:18:VAL:O	3:C:231:ASN:HA	2.19	0.42
5:F:72:LYS:HE2	5:F:142:SER:HB3	2.01	0.42
7:I:47:GLU:OE1	7:I:50:THR:HG23	2.19	0.42
1:A:38:PRO:HA	1:A:270:LEU:HD13	2.00	0.42
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.00	0.42
1:A:266:LEU:HA	1:A:269:ILE:HG12	2.01	0.42
1:A:356:ASP:OD2	9:K:65:HIS:HE1	2.02	0.42
1:A:935:GLN:HE22	1:A:938:LYS:HD2	1.84	0.42
2:B:792:MET:HA	2:B:856:PHE:O	2.19	0.42
4:E:100:ILE:HG13	4:E:105:PHE:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.85	0.42
2:B:360:PHE:HE2	2:B:374:LYS:HB3	1.83	0.42
2:B:841:MET:O	2:B:993:THR:HA	2.19	0.42
8:J:1:MET:H2	8:J:57:ILE:H	1.66	0.42
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	2.00	0.42
8:J:14:VAL:HA	8:J:17:LYS:HD2	2.00	0.42
1:A:88:LYS:HE2	1:A:205:GLU:HB2	2.00	0.42
1:A:1116:LEU:HB3	1:A:1308:THR:HB	2.02	0.42
2:B:1006:ILE:CD1	8:J:43:ARG:HB2	2.49	0.42
4:E:94:LYS:O	4:E:98:ILE:HG12	2.19	0.42
1:A:760:GLN:HG2	1:A:765:VAL:HA	2.01	0.42
2:B:378:LEU:HG	2:B:382:ILE:HD11	2.02	0.42
2:B:1210:MET:HB3	2:B:1212:ILE:HD12	2.02	0.42
4:E:135:PHE:HB3	4:E:140:LEU:HD11	2.01	0.42
1:A:1266:THR:HG23	1:A:1270:ASN:HD22	1.84	0.42
4:E:147:HIS:HD2	4:E:149:LEU:HB2	1.85	0.42
10:L:38:LEU:HD21	10:L:49:LYS:H	1.85	0.42
1:A:92:HIS:HD2	1:A:94:GLY:H	1.67	0.42
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.68	0.42
2:B:516:ASN:H	2:B:516:ASN:ND2	2.16	0.42
2:B:800:GLN:CB	8:J:52:THR:HG22	2.45	0.42
1:A:325:ILE:O	1:A:328:ARG:HB2	2.20	0.42
1:A:445:ASN:HB2	1:A:455:MET:HG3	2.02	0.42
2:B:515:HIS:H	2:B:518:HIS:CD2	2.38	0.42
8:J:14:VAL:HB	8:J:50:ILE:HD11	2.01	0.42
1:A:565:ILE:HG22	1:A:569:LYS:O	2.20	0.41
3:C:114:TYR:CG	3:C:140:ASN:HB2	2.55	0.41
5:F:82:THR:HG22	5:F:84:TYR:H	1.85	0.41
1:A:152:VAL:HG23	1:A:162:VAL:HB	2.02	0.41
1:A:117:GLU:N	1:A:118:HIS:HB2	2.36	0.41
2:B:95:ILE:HD11	2:B:128:LEU:HB3	2.02	0.41
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.84	0.41
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.52	0.41
6:H:126:GLU:C	6:H:130:ARG:HH22	2.24	0.41
1:A:265:LYS:HG2	1:A:303:TYR:HB2	2.03	0.41
1:A:333:GLU:HA	1:A:338:GLY:HA3	2.02	0.41
1:A:903:ASN:O	1:A:907:THR:OG1	2.39	0.41
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	2.21	0.41
2:B:545:ILE:HG12	2:B:633:VAL:HG22	2.03	0.41
1:A:265:LYS:HE3	1:A:299:HIS:HB3	2.03	0.41
2:B:282:ILE:HG21	2:B:382:ILE:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.34	0.41
2:B:1099:VAL:O	2:B:1103:ILE:HG13	2.20	0.41
3:C:98:VAL:H	3:C:122:SER:CB	2.32	0.41
1:A:541:ILE:CD1	1:A:577:ILE:HG12	2.50	0.41
1:A:1174:PHE:HD1	1:A:1175:SER:H	1.69	0.41
2:B:277:LYS:HZ2	2:B:335:GLY:H	1.68	0.41
2:B:618:ASP:OD2	2:B:621:GLU:HB2	2.20	0.41
7:I:55:THR:HG23	7:I:58:VAL:HG21	2.02	0.41
1:A:70:CYS:HA	2:B:1174:LYS:HG2	2.03	0.41
1:A:523:ILE:HG23	1:A:527:THR:HB	2.03	0.41
1:A:597:LEU:HD12	1:A:597:LEU:H	1.86	0.41
2:B:69:LEU:HD12	2:B:90:ILE:HB	2.01	0.41
2:B:219:ALA:HB2	2:B:405:ARG:HG2	2.02	0.41
2:B:333:PHE:O	2:B:334:ILE:HG13	2.21	0.41
2:B:420:LEU:HD21	2:B:456:GLY:HA3	2.03	0.41
2:B:610:ASN:HB3	2:B:613:VAL:HG23	2.03	0.41
1:A:351:THR:HG22	1:A:352:VAL:H	1.85	0.41
10:L:46:VAL:HG23	10:L:47:ARG:H	1.86	0.41
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.86	0.40
1:A:568:PRO:O	1:A:569:LYS:HB2	2.21	0.40
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	2.03	0.40
2:B:555:ILE:H	2:B:555:ILE:HG12	1.58	0.40
1:A:567:LYS:HB3	6:H:95:TYR:HA	2.02	0.40
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.57	0.40
1:A:946:VAL:HG13	4:E:201:LYS:HB3	2.04	0.40
7:I:84:VAL:HB	7:I:104:LEU:HD21	2.04	0.40
1:A:741:ASN:HD22	1:A:744:LYS:H	1.69	0.40
1:A:889:SER:HB3	1:A:1297:GLU:HG3	2.04	0.40
2:B:798:TYR:HE2	3:C:66:ARG:HH21	1.69	0.40
3:C:22:LEU:HG	3:C:25:VAL:HG21	2.02	0.40
7:I:58:VAL:HG11	7:I:109:ILE:HD11	2.04	0.40
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.03	0.40
2:B:900:ALA:HB3	10:L:61:THR:HG23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	1242 (89%)	110 (8%)	43 (3%)	4 21
2	B	1096/1224 (90%)	949 (87%)	112 (10%)	35 (3%)	4 20
3	C	264/318 (83%)	239 (90%)	18 (7%)	7 (3%)	5 23
4	E	212/215 (99%)	202 (95%)	8 (4%)	2 (1%)	17 50
5	F	83/155 (54%)	74 (89%)	6 (7%)	3 (4%)	3 18
6	H	129/146 (88%)	107 (83%)	14 (11%)	8 (6%)	1 8
7	I	117/122 (96%)	101 (86%)	15 (13%)	1 (1%)	17 50
8	J	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4 20
9	K	112/120 (93%)	105 (94%)	6 (5%)	1 (1%)	17 50
10	L	44/70 (63%)	26 (59%)	10 (23%)	8 (18%)	0 0
All	All	3515/4173 (84%)	3102 (88%)	303 (9%)	110 (3%)	4 21

All (110) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	ASP
1	A	325	ILE
1	A	399	HIS
1	A	543	LEU
1	A	567	LYS
1	A	597	LEU
1	A	1123	GLY
2	B	139	ALA
2	B	248	SER
2	B	364	ILE
2	B	469	GLN
2	B	477	ALA
2	B	531	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	646	LEU
2	B	712	PRO
2	B	731	VAL
2	B	1046	PRO
2	B	1156	ASP
2	B	1181	GLU
3	C	173	ALA
3	C	174	ALA
3	C	215	GLU
4	E	126	SER
6	H	109	LYS
6	H	140	ALA
8	J	6	ARG
10	L	46	VAL
10	L	60	ARG
10	L	64	LEU
1	A	219	PHE
1	A	672	ASP
1	A	775	ILE
1	A	1064	VAL
1	A	1221	LYS
1	A	1393	ASN
1	A	1437	GLY
2	B	137	TYR
2	B	465	ASN
2	B	592	ASN
2	B	647	GLY
2	B	709	ASP
2	B	886	LYS
2	B	1066	SER
3	C	142	VAL
3	C	227	THR
6	H	90	ALA
6	H	128	ASN
7	I	91	ARG
8	J	2	ILE
9	K	14	GLU
10	L	39	SER
10	L	45	ALA
10	L	51	CYS
10	L	56	LEU
1	A	40	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	56	PRO
1	A	65	LEU
1	A	117	GLU
1	A	286	HIS
1	A	299	HIS
1	A	312	PRO
1	A	568	PRO
1	A	569	LYS
1	A	916	GLY
1	A	1223	ASP
1	A	1278	ASN
2	B	105	SER
2	B	367	LEU
2	B	471	LYS
2	B	478	GLY
2	B	792	MET
2	B	1155	SER
2	B	1157	ALA
6	H	86	ASP
1	A	130	ASP
1	A	214	ILE
1	A	250	ILE
1	A	310	GLY
1	A	332	LYS
2	B	138	GLU
2	B	447	ALA
2	B	881	ASN
4	E	86	PRO
5	F	154	ASP
6	H	34	ASP
6	H	108	SER
1	A	72	GLU
1	A	76	GLU
1	A	400	PRO
1	A	593	GLU
1	A	599	SER
1	A	922	ASP
1	A	958	VAL
1	A	1124	HIS
2	B	448	ILE
2	B	707	PRO
2	B	751	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	943	SER
2	B	1169	MET
3	C	90	ASP
5	F	128	LYS
10	L	59	ALA
1	A	213	HIS
3	C	126	GLY
5	F	73	ALA
1	A	35	ILE
6	H	17	PRO
1	A	424	ILE
2	B	1018	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%)	1067 (87%)	158 (13%)	4	17
2	B	967/1061 (91%)	863 (89%)	104 (11%)	6	24
3	C	234/274 (85%)	213 (91%)	21 (9%)	9	32
4	E	196/197 (100%)	181 (92%)	15 (8%)	13	39
5	F	75/137 (55%)	73 (97%)	2 (3%)	44	72
6	H	117/128 (91%)	101 (86%)	16 (14%)	3	15
7	I	113/116 (97%)	103 (91%)	10 (9%)	10	33
8	J	60/65 (92%)	48 (80%)	12 (20%)	1	5
9	K	99/102 (97%)	90 (91%)	9 (9%)	9	31
10	L	40/57 (70%)	31 (78%)	9 (22%)	1	3
All	All	3126/3657 (86%)	2770 (89%)	356 (11%)	5	22

All (356) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	18	GLN
1	A	34	LYS
1	A	41	MET
1	A	43	GLU
1	A	61	ILE
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS
1	A	81	PHE
1	A	88	LYS
1	A	93	VAL
1	A	119	ASN
1	A	120	GLU
1	A	126	LEU
1	A	143	LYS
1	A	144	THR
1	A	146	MET
1	A	164	ARG
1	A	177	ASP
1	A	179	LEU
1	A	184	SER
1	A	186	LYS
1	A	225	ASN
1	A	250	ILE
1	A	262	LEU
1	A	265	LYS
1	A	270	LEU
1	A	271	LYS
1	A	296	LEU
1	A	299	HIS
1	A	303	TYR
1	A	308	ILE
1	A	315	LEU
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	326	ARG
1	A	329	LEU
1	A	330	LYS
1	A	332	LYS
1	A	336	ILE
1	A	337	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	344	ARG
1	A	351	THR
1	A	353	ILE
1	A	359	LEU
1	A	386	ASP
1	A	389	THR
1	A	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	416	ARG
1	A	434	ARG
1	A	436	ILE
1	A	437	MET
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	461	LYS
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	496	GLU
1	A	518	LYS
1	A	527	THR
1	A	541	ILE
1	A	555	ASP
1	A	579	SER
1	A	590	ARG
1	A	595	THR
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	626	ASN
1	A	629	LEU
1	A	636	GLU
1	A	644	LYS
1	A	672	ASP
1	A	688	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	691	LEU
1	A	695	LYS
1	A	702	LEU
1	A	705	LYS
1	A	710	LEU
1	A	722	LEU
1	A	740	LEU
1	A	741	ASN
1	A	756	ILE
1	A	768	GLN
1	A	774	ARG
1	A	821	ARG
1	A	826	ASP
1	A	830	LYS
1	A	845	LEU
1	A	855	THR
1	A	867	ILE
1	A	905	ASP
1	A	927	VAL
1	A	931	GLU
1	A	969	GLN
1	A	976	THR
1	A	1001	ARG
1	A	1015	VAL
1	A	1022	LEU
1	A	1025	ARG
1	A	1047	SER
1	A	1048	ASN
1	A	1050	GLU
1	A	1064	VAL
1	A	1094	VAL
1	A	1102	LYS
1	A	1109	LYS
1	A	1110	ASN
1	A	1129	GLU
1	A	1130	GLN
1	A	1136	SER
1	A	1168	GLU
1	A	1174	PHE
1	A	1176	LEU
1	A	1195	LEU
1	A	1215	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1221	LYS
1	A	1223	ASP
1	A	1230	GLU
1	A	1233	ASP
1	A	1237	ILE
1	A	1242	VAL
1	A	1256	GLU
1	A	1257	ASP
1	A	1264	GLU
1	A	1267	MET
1	A	1269	GLU
1	A	1277	GLU
1	A	1280	GLU
1	A	1285	MET
1	A	1288	ASP
1	A	1297	GLU
1	A	1300	LYS
1	A	1309	ASP
1	A	1329	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1366	ARG
1	A	1376	THR
1	A	1385	THR
1	A	1391	ARG
1	A	1398	MET
1	A	1400	CYS
1	A	1426	GLU
1	A	1433	MET
1	A	1435	PRO
1	A	1442	ASP
2	B	26	THR
2	B	28	GLU
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	70	ILE
2	B	101	MET
2	B	102	VAL
2	B	135	ARG
2	B	175	ARG
2	B	187	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	217	ARG
2	B	261	ARG
2	B	276	ILE
2	B	305	VAL
2	B	323	VAL
2	B	325	GLN
2	B	357	GLN
2	B	365	THR
2	B	367	LEU
2	B	382	ILE
2	B	393	LYS
2	B	416	LEU
2	B	435	THR
2	B	437	GLU
2	B	451	LYS
2	B	453	ILE
2	B	458	LYS
2	B	471	LYS
2	B	476	ARG
2	B	479	VAL
2	B	480	SER
2	B	485	ARG
2	B	489	SER
2	B	516	ASN
2	B	522	VAL
2	B	537	LYS
2	B	547	VAL
2	B	555	ILE
2	B	573	GLN
2	B	578	THR
2	B	604	ARG
2	B	621	GLU
2	B	624	LEU
2	B	641	GLU
2	B	642	ASP
2	B	644	GLU
2	B	645	SER
2	B	646	LEU
2	B	653	VAL
2	B	655	LYS
2	B	658	ILE
2	B	690	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	708	GLU
2	B	710	LEU
2	B	737	THR
2	B	780	VAL
2	B	786	ASN
2	B	788	ARG
2	B	791	THR
2	B	815	ARG
2	B	838	SER
2	B	864	LYS
2	B	866	TYR
2	B	868	MET
2	B	878	GLN
2	B	884	ARG
2	B	905	VAL
2	B	951	GLN
2	B	953	LEU
2	B	963	PHE
2	B	976	ILE
2	B	983	ARG
2	B	987	LYS
2	B	996	ARG
2	B	997	GLU
2	B	998	ASP
2	B	1006	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1033	LYS
2	B	1060	ARG
2	B	1065	GLN
2	B	1099	VAL
2	B	1103	ILE
2	B	1106	ARG
2	B	1111	MET
2	B	1128	LEU
2	B	1129	ARG
2	B	1145	SER
2	B	1147	LEU
2	B	1150	ARG
2	B	1159	ARG
2	B	1170	THR
2	B	1175	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1181	GLU
2	B	1188	LYS
2	B	1189	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1210	MET
2	B	1211	ASN
2	B	1222	ARG
3	C	4	GLU
3	C	18	VAL
3	C	25	VAL
3	C	34	ARG
3	C	36	VAL
3	C	66	ARG
3	C	69	LEU
3	C	75	MET
3	C	77	ILE
3	C	137	LYS
3	C	140	ASN
3	C	145	CYS
3	C	215	GLU
3	C	221	TYR
3	C	226	ASP
3	C	231	ASN
3	C	235	VAL
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	260	LEU
4	E	4	GLU
4	E	41	ASP
4	E	52	ARG
4	E	54	GLN
4	E	65	THR
4	E	78	LEU
4	E	84	ASP
4	E	92	THR
4	E	100	ILE
4	E	102	GLU
4	E	107	THR
4	E	127	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	169	ARG
4	E	190	LEU
4	E	213	ILE
5	F	110	ASP
5	F	118	LEU
6	H	21	ASN
6	H	22	LYS
6	H	35	GLN
6	H	44	VAL
6	H	46	LEU
6	H	55	LEU
6	H	86	ASP
6	H	87	ARG
6	H	95	TYR
6	H	106	GLU
6	H	107	VAL
6	H	111	LEU
6	H	129	TYR
6	H	130	ARG
6	H	136	LYS
6	H	139	ASN
7	I	24	ARG
7	I	37	GLU
7	I	51	ASN
7	I	55	THR
7	I	60	GLN
7	I	77	LYS
7	I	84	VAL
7	I	87	GLN
7	I	97	MET
7	I	111	THR
8	J	3	VAL
8	J	6	ARG
8	J	7	CYS
8	J	22	LEU
8	J	26	GLN
8	J	31	ASP
8	J	37	SER
8	J	43	ARG
8	J	48	ARG
8	J	57	ILE
8	J	59	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	J	62	ARG
9	K	6	ARG
9	K	12	LEU
9	K	20	LYS
9	K	22	ASP
9	K	31	VAL
9	K	47	ARG
9	K	51	LEU
9	K	63	VAL
9	K	101	LEU
10	L	30	ILE
10	L	33	GLU
10	L	35	SER
10	L	42	ARG
10	L	44	ASP
10	L	47	ARG
10	L	55	ILE
10	L	58	LYS
10	L	65	VAL

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

Mol	Chain	Res	Type
1	A	4	GLN
1	A	54	ASN
1	A	68	GLN
1	A	171	GLN
1	A	225	ASN
1	A	306	ASN
1	A	313	GLN
1	A	339	ASN
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	626	ASN
1	A	631	HIS
1	A	659	HIS
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	786	HIS
1	A	851	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	926	GLN
1	A	1082	ASN
1	A	1140	HIS
1	A	1258	HIS
1	A	1270	ASN
2	B	46	GLN
2	B	121	ASN
2	B	215	GLN
2	B	363	HIS
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	657	HIS
2	B	744	HIS
2	B	762	ASN
2	B	957	ASN
2	B	958	GLN
2	B	984	HIS
2	B	1015	HIS
2	B	1025	HIS
2	B	1076	HIS
2	B	1084	GLN
2	B	1141	HIS
2	B	1161	HIS
2	B	1211	ASN
3	C	73	GLN
3	C	112	ASN
3	C	167	HIS
3	C	242	GLN
4	E	147	HIS
6	H	133	ASN
9	K	65	HIS

5.3.3 RNA (i)

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 (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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%)	0.25	138 (9%) 7 3	62, 106, 212, 241	0
2	B	1114/1224 (91%)	0.02	36 (3%) 47 26	60, 101, 178, 207	0
3	C	266/318 (83%)	-0.25	1 (0%) 92 86	72, 98, 138, 170	0
4	E	214/215 (99%)	-0.07	3 (1%) 75 59	79, 137, 185, 197	0
5	F	85/155 (54%)	-0.31	0 100 100	87, 119, 155, 169	0
6	H	133/146 (91%)	0.30	5 (3%) 40 21	100, 141, 173, 184	0
7	I	119/122 (97%)	-0.27	0 100 100	77, 107, 146, 158	0
8	J	65/70 (92%)	-0.17	0 100 100	64, 94, 131, 144	0
9	K	114/120 (95%)	-0.17	0 100 100	64, 101, 127, 143	0
10	L	46/70 (65%)	-0.03	2 (4%) 35 17	79, 135, 168, 176	0
11	R	5/5 (100%)	0.84	1 (20%) 1 0	211, 213, 220, 220	0
12	T	8/29 (27%)	0.42	0 100 100	193, 198, 203, 205	0
All	All	3574/4207 (84%)	0.07	186 (5%) 27 12	60, 107, 200, 241	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1087	ALA	9.2
1	A	1088	GLY	8.7
1	A	317	LYS	7.3
1	A	44	THR	7.2
1	A	1176	LEU	6.5
1	A	49	LYS	6.5
1	A	141	LEU	6.3
1	A	255	SER	6.1
1	A	173	THR	5.7
6	H	86	ASP	5.6
1	A	144	THR	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	318	SER	5.4
2	B	883	LEU	5.2
1	A	314	ALA	5.2
1	A	124	GLN	5.0
2	B	1224	PHE	4.9
1	A	115	LEU	4.8
1	A	174	ILE	4.8
1	A	154	SER	4.8
1	A	319	GLY	4.8
2	B	865	LYS	4.8
1	A	114	LEU	4.6
1	A	282	ASN	4.6
1	A	121	LEU	4.5
1	A	177	ASP	4.5
1	A	147	VAL	4.4
1	A	176	LYS	4.4
1	A	69	THR	4.4
1	A	138	ILE	4.4
1	A	287	HIS	4.3
1	A	1256	GLU	4.3
1	A	73	GLY	4.3
1	A	183	GLY	4.3
1	A	313	GLN	4.2
1	A	142	CYS	4.2
6	H	85	GLY	4.1
1	A	316	GLN	4.1
1	A	1175	SER	4.1
2	B	474	SER	4.1
1	A	139	TRP	4.1
1	A	45	GLN	4.0
1	A	320	ARG	4.0
1	A	137	ALA	3.9
1	A	175	ARG	3.9
1	A	1085	HIS	3.9
1	A	140	THR	3.8
1	A	143	LYS	3.8
1	A	146	MET	3.8
2	B	468	GLU	3.8
1	A	171	GLN	3.7
2	B	420	LEU	3.6
1	A	5	GLN	3.6
1	A	122	MET	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	253	ASN	3.5
10	L	27	LEU	3.5
2	B	469	GLN	3.5
1	A	211	PHE	3.5
1	A	1086	PHE	3.5
1	A	105	CYS	3.4
10	L	50	ASP	3.4
1	A	182	VAL	3.4
1	A	79	GLY	3.4
2	B	1223	ASP	3.4
1	A	96	ILE	3.3
6	H	132	LEU	3.3
2	B	866	TYR	3.3
1	A	117	GLU	3.2
1	A	75	ASN	3.2
1	A	283	GLY	3.1
1	A	297	GLN	3.1
1	A	323	LYS	3.1
1	A	125	ALA	3.1
1	A	87	ALA	3.1
1	A	210	ILE	3.1
1	A	1082	ASN	3.1
1	A	292	ALA	3.1
1	A	232	GLU	3.0
1	A	181	LEU	3.0
2	B	471	LYS	3.0
4	E	122	LYS	3.0
2	B	647	GLY	2.9
1	A	59	GLY	2.9
1	A	148	CYS	2.9
1	A	1002	GLY	2.9
2	B	870	ILE	2.9
1	A	178	GLY	2.9
2	B	882	THR	2.9
1	A	135	PHE	2.9
1	A	1089	VAL	2.9
2	B	1191	ILE	2.8
2	B	1181	GLU	2.8
1	A	286	HIS	2.8
2	B	1170	THR	2.8
1	A	116	ASP	2.8
2	B	247	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	254	GLU	2.8
1	A	1084	PHE	2.8
1	A	214	ILE	2.8
2	B	470	LYS	2.7
1	A	97	ALA	2.7
1	A	212	LYS	2.7
1	A	1090	ALA	2.7
2	B	935	ARG	2.7
1	A	216	VAL	2.7
1	A	145	LYS	2.6
1	A	106	VAL	2.6
1	A	1091	SER	2.6
2	B	709	ASP	2.6
1	A	321	PRO	2.6
1	A	169	ASN	2.6
1	A	118	HIS	2.6
1	A	179	LEU	2.6
1	A	248	PRO	2.6
2	B	136	THR	2.6
1	A	71	GLN	2.6
1	A	152	VAL	2.6
1	A	213	HIS	2.6
2	B	1222	ARG	2.5
1	A	298	PHE	2.5
2	B	1171	VAL	2.5
1	A	1391	ARG	2.5
1	A	127	ALA	2.5
1	A	199	LEU	2.5
1	A	285	PRO	2.5
1	A	168	GLY	2.5
1	A	153	PRO	2.5
2	B	1162	ILE	2.5
1	A	312	PRO	2.5
2	B	933	SER	2.5
2	B	1217	TYR	2.4
1	A	250	ILE	2.4
2	B	472	ALA	2.4
1	A	170	THR	2.4
1	A	1125	ALA	2.4
6	H	133	ASN	2.4
1	A	48	ALA	2.4
1	A	251	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	430	ARG	2.4
1	A	1123	GLY	2.4
1	A	126	LEU	2.4
1	A	6	TYR	2.4
1	A	231	PRO	2.4
1	A	1083	THR	2.4
1	A	161	LEU	2.4
1	A	163	SER	2.4
1	A	1081	LEU	2.4
1	A	72	GLU	2.3
1	A	172	PRO	2.3
1	A	167	CYS	2.3
1	A	184	SER	2.3
1	A	113	LEU	2.3
1	A	315	LEU	2.3
1	A	223	GLY	2.3
1	A	249	SER	2.3
2	B	473	MET	2.3
4	E	93	MET	2.3
1	A	149	GLU	2.3
1	A	65	LEU	2.3
6	H	83	GLN	2.3
1	A	103	CYS	2.3
1	A	237	THR	2.2
1	A	200	ARG	2.2
1	A	204	THR	2.2
1	A	1126	ALA	2.2
1	A	119	ASN	2.2
1	A	164	ARG	2.2
4	E	123	LEU	2.2
1	A	186	LYS	2.2
1	A	42	ASP	2.2
1	A	104	GLU	2.2
1	A	265	LYS	2.1
2	B	246	LYS	2.1
1	A	247	ARG	2.1
1	A	128	ILE	2.1
1	A	136	ALA	2.1
1	A	162	VAL	2.1
2	B	867	GLY	2.1
2	B	645	SER	2.1
1	A	278	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	250	PHE	2.1
2	B	869	SER	2.1
2	B	167	ILE	2.0
2	B	934	LYS	2.0
1	A	311	GLN	2.0
11	R	6	A	2.0
3	C	221	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 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, 95th 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	0.50	0.27	300,300,300,300	0
13	ZN	B	1307	1/1	0.81	0.06	202,202,202,202	0
13	ZN	A	1735	1/1	0.85	0.06	190,190,190,190	0
13	ZN	I	203	1/1	0.97	0.12	108,108,108,108	0
13	ZN	C	319	1/1	0.98	0.12	92,92,92,92	0
14	MG	A	2001	1/1	0.98	0.14	60,60,60,60	0
13	ZN	J	101	1/1	0.99	0.21	85,85,85,85	0
13	ZN	L	105	1/1	0.99	0.12	129,129,129,129	0
13	ZN	I	204	1/1	0.99	0.13	83,83,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.