Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 02:59 PM EDT

PDB ID	:	3S2H
Title	:	RNA Polymerase II Initiation Complex with a 6-nt RNA containing a 2[prime]-iodo ATP
Authors	:	Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on	:	2011-05-16
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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 (i)) were used in the production of this report:

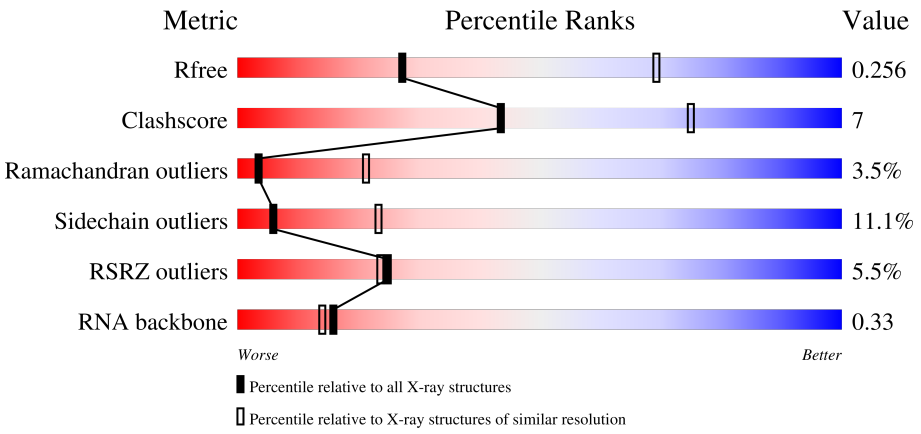
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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	7% 60% 18% • 19%
2	B	1224	3% 64% 24% • 9%
3	C	318	60% 22% • 16%
4	E	215	5% 80% 18% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	155	40% 14% •• 45%
6	H	146	12% 68% 23% • 9%
7	I	122	73% 21% • •
8	J	70	51% 34% 7% 7%
9	K	120	73% 19% • 5%
10	L	70	7% 46% 14% 6% 34%
11	R	6	33% 50% 17%
12	T	29	7% 14% 24% • 59%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 28674 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*GP*GP*(2IA))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	I	N	O	P			
11	R	6	132	60	1	30	36	5	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*CP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
12	T	12	241	115	41	73	12	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).

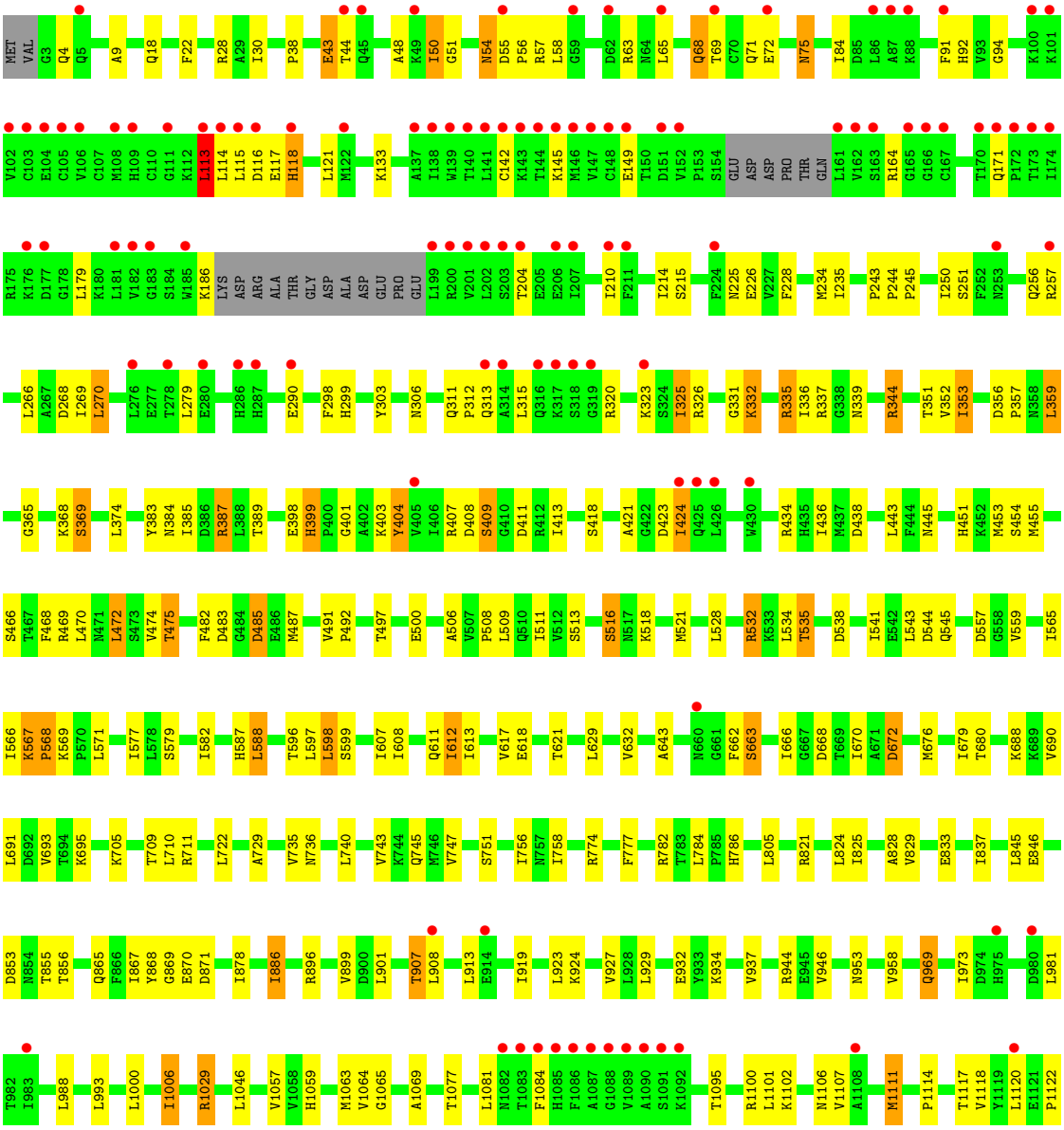
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
14	A	1	1	1	0	0

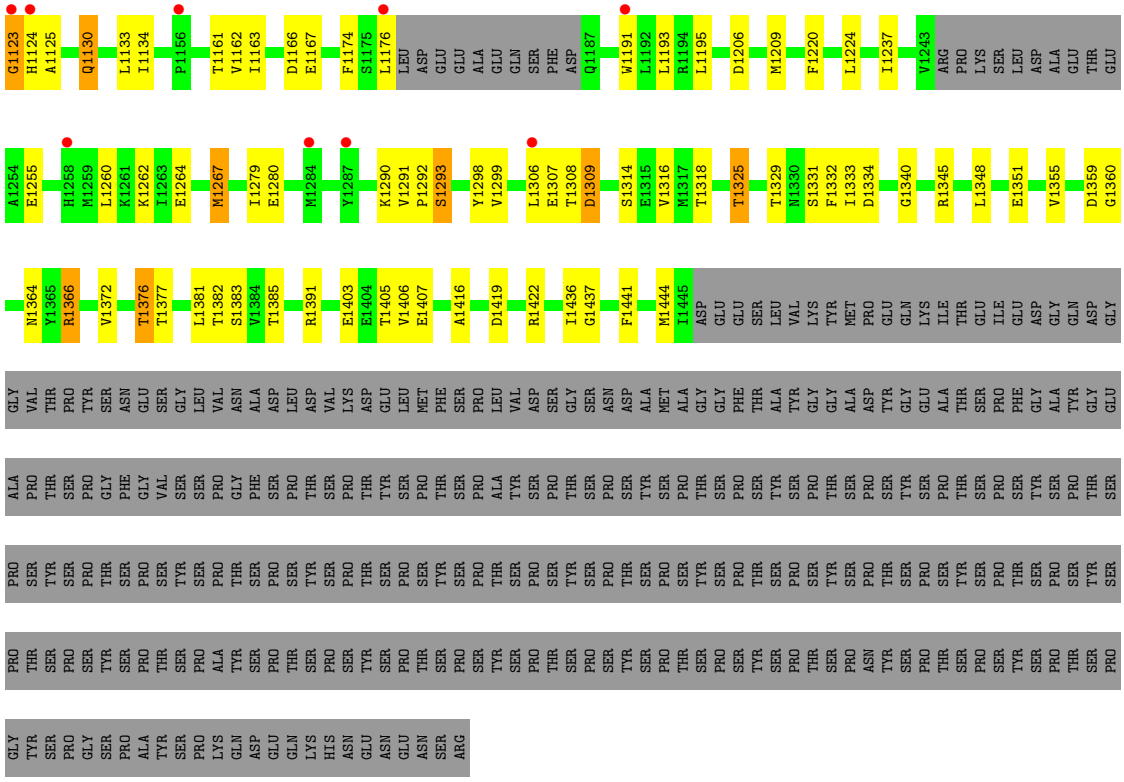
3 Residue-property plots (i)

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

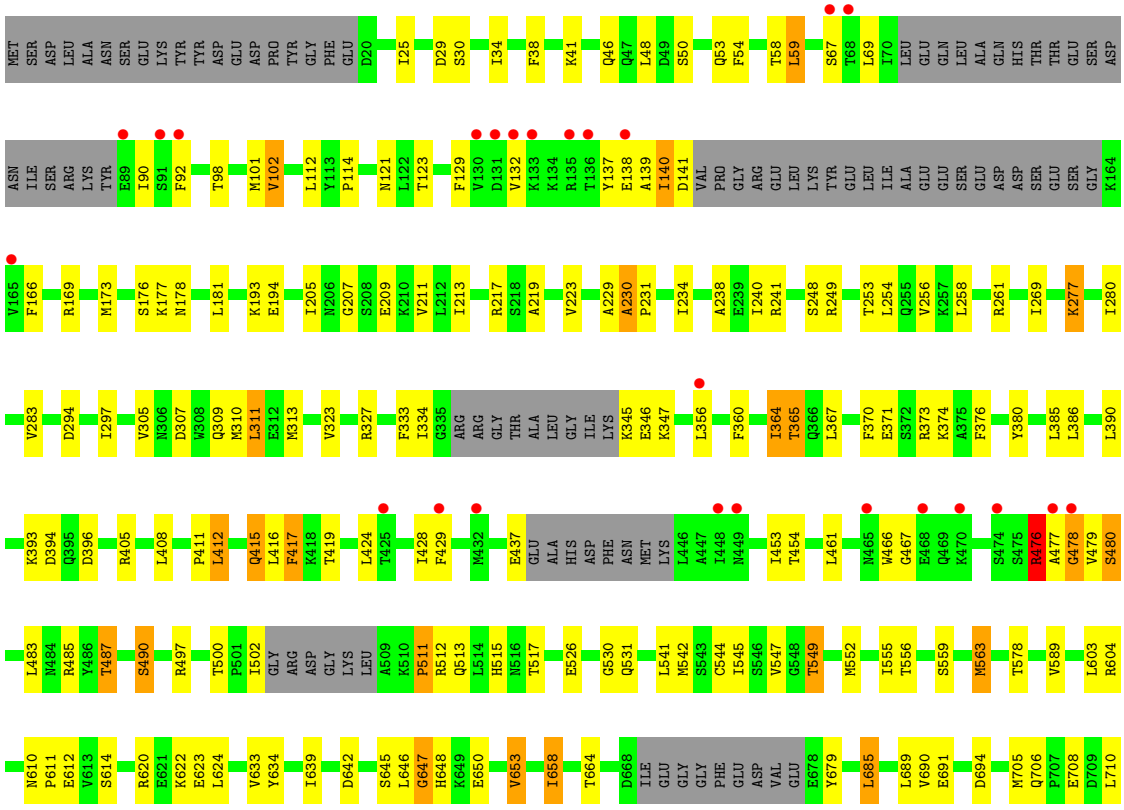
Chain A: 7% 60% 18% • 19%

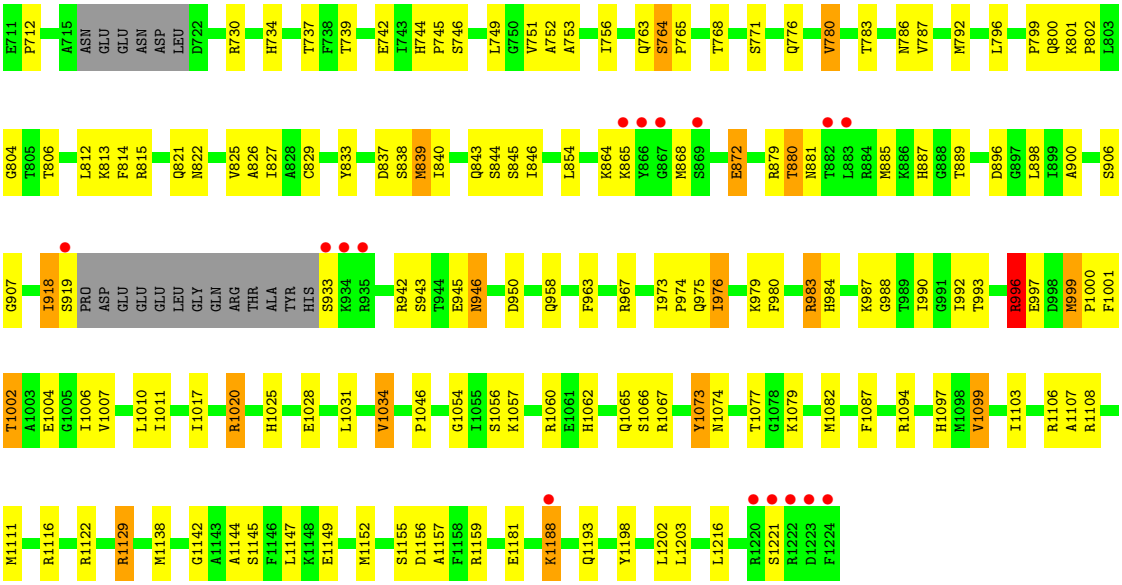




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

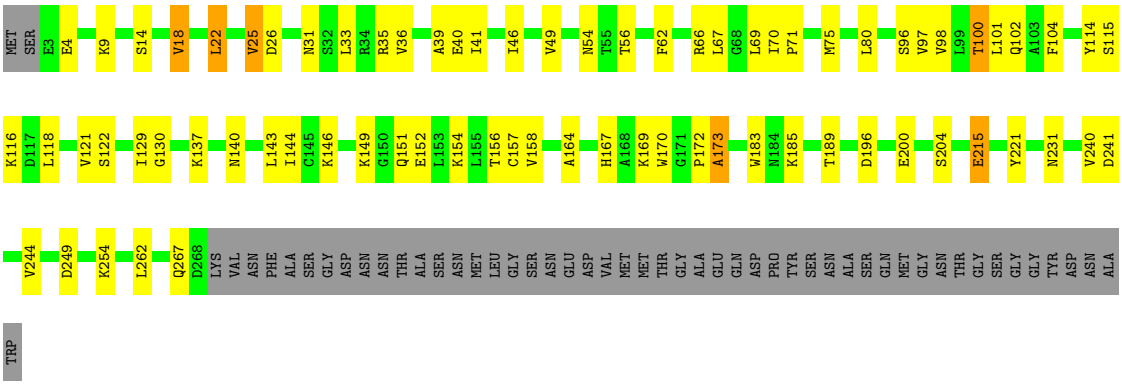
Chain B:





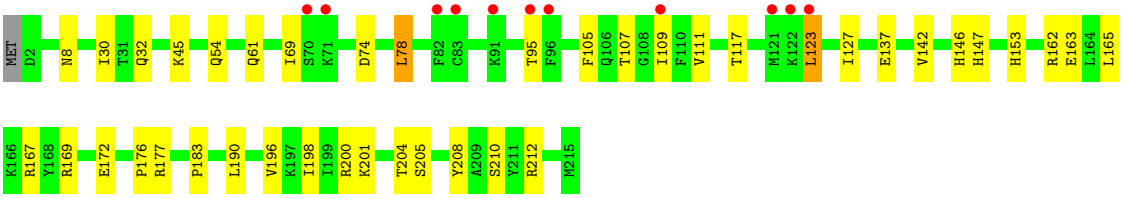
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



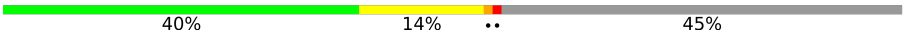
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

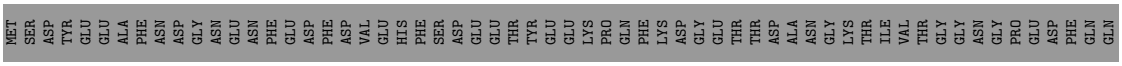
Chain E:



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

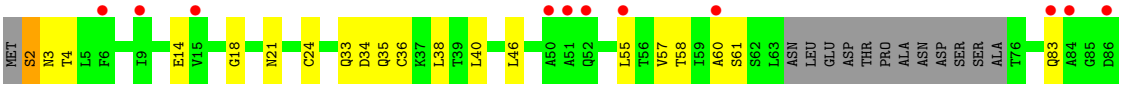
Chain F:

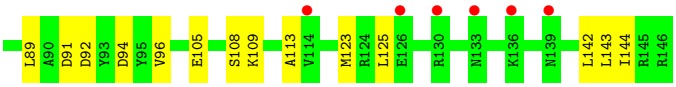




• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

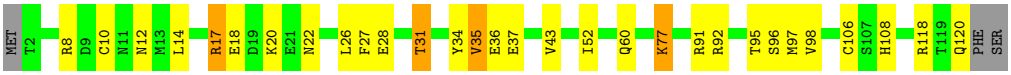
Chain H:





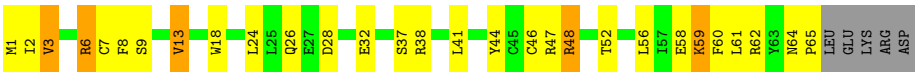
• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I:



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

Chain J:

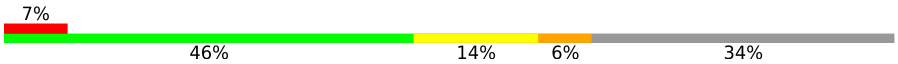


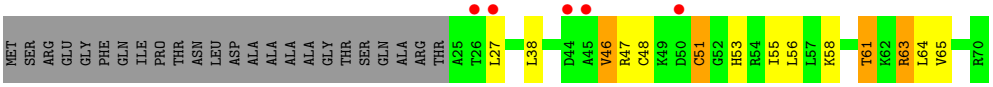
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:

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

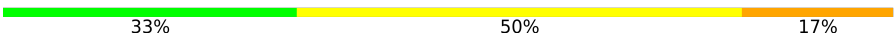
Chain L:





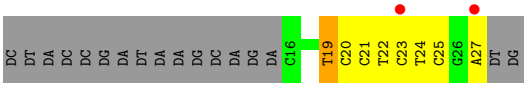
• Molecule 11: RNA (5'-R(*AP*GP*AP*GP*GP*(2IA))-3')

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

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	165.53Å 221.61Å 194.06Å 90.00° 99.67° 90.00°	Depositor
Resolution (Å)	49.81 – 3.30 49.81 – 3.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.81-3.30) 95.8 (49.81-3.29)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 3.33Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.191 , 0.240 0.209 , 0.256	Depositor DCC
R_{free} test set	4987 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	92.8	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 86.3	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	28674	wwPDB-VP
Average B, all atoms (Å^2)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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, 2IA

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	0.44	0/11241	0.72	0/15199
2	B	0.45	0/9033	0.74	1/12181 (0.0%)
3	C	0.40	0/2133	0.71	1/2891 (0.0%)
4	E	0.43	0/1788	0.67	0/2406
5	F	0.45	0/700	0.71	0/945
6	H	0.40	0/1086	0.68	0/1470
7	I	0.41	0/989	0.71	0/1331
8	J	0.47	0/541	0.80	0/727
9	K	0.38	0/937	0.66	0/1265
10	L	0.46	0/365	0.86	0/485
11	R	0.75	0/124	1.35	0/193
12	T	1.04	0/268	1.80	12/410 (2.9%)
All	All	0.45	0/29205	0.75	14/39503 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	23	DC	O4'-C1'-N1	6.90	112.83	108.00
12	T	21	DC	C4'-C3'-C2'	-6.53	97.22	103.10
12	T	25	DC	O4'-C1'-N1	6.45	112.51	108.00
3	C	172	PRO	C-N-CA	6.25	137.34	121.70
12	T	19	DT	O4'-C1'-N1	6.18	112.33	108.00
12	T	22	DT	O4'-C1'-N1	6.09	112.27	108.00
12	T	25	DC	C1'-O4'-C4'	-5.99	104.11	110.10
12	T	21	DC	O4'-C4'-C3'	-5.78	102.19	104.50
12	T	21	DC	O4'-C1'-N1	5.72	112.00	108.00
12	T	24	DT	P-O3'-C3'	5.64	126.47	119.70
12	T	19	DT	C4'-C3'-C2'	-5.53	98.12	103.10
12	T	27	DA	C1'-O4'-C4'	-5.14	104.96	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	140	ILE	C-N-CA	5.13	134.53	121.70
12	T	22	DT	O4'-C4'-C3'	-5.13	102.45	104.50

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	156	0
2	B	8861	0	8884	149	0
3	C	2095	0	2051	33	0
4	E	1752	0	1776	20	0
5	F	688	0	707	13	0
6	H	1068	0	1040	12	0
7	I	971	0	927	15	0
8	J	532	0	542	19	0
9	K	919	0	929	16	0
10	L	363	0	386	4	0
11	R	132	0	67	6	0
12	T	241	0	136	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	28674	0	28578	386	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 7.

All (386) 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)
2:B:664:THR:HG21	2:B:679:TYR:H	1.37	0.87
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.10	0.87
8:J:48:ARG:O	8:J:52:THR:HB	1.75	0.86
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.58	0.86
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.43	0.84
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.63	0.80
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.15	0.77
1:A:565:ILE:HG23	1:A:567:LYS:HD2	1.66	0.76
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.68	0.75
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.69	0.74
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	2.03	0.73
1:A:466:SER:HB3	2:B:1103:ILE:HD11	1.71	0.73
11:R:5:A:H2'	11:R:6:G:H8	1.52	0.73
1:A:1107:VAL:HG12	1:A:1383:SER:HB3	1.70	0.72
1:A:567:LYS:HB3	6:H:96:VAL:H	1.54	0.72
1:A:1118:VAL:HG13	1:A:1306:LEU:HB2	1.72	0.71
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.71	0.71
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.75	0.69
2:B:801:LYS:O	8:J:52:THR:HG23	1.93	0.68
3:C:167:HIS:HD2	3:C:169:LYS:H	1.39	0.68
1:A:1111:MET:HB3	1:A:1114:PRO:HG3	1.76	0.67
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.77	0.67
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.76	0.66
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.76	0.66
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.61	0.66
2:B:996:ARG:HH22	3:C:173:ALA:HB1	1.60	0.66
1:A:511:ILE:HA	1:A:521:MET:HE3	1.78	0.66
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.79	0.65
1:A:901:LEU:HA	1:A:907:THR:HG23	1.79	0.65
1:A:472:LEU:O	1:A:475:THR:HB	1.97	0.65
3:C:54:ASN:OD1	3:C:56:THR:HG22	1.97	0.64
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.78	0.64
1:A:336:ILE:HD11	2:B:1203:LEU:HD13	1.79	0.64
2:B:783:THR:HG21	8:J:59:LYS:HB3	1.79	0.64
3:C:104:PHE:HD1	3:C:152:GLU:HB3	1.63	0.64
1:A:1006:ILE:HD11	4:E:163:GLU:HG3	1.79	0.64
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.80	0.64
1:A:711:ARG:HH12	7:I:95:THR:HB	1.64	0.63
1:A:946:VAL:HG12	4:E:201:LYS:HB3	1.81	0.63
2:B:408:LEU:H	2:B:411:PRO:HG2	1.63	0.62
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.80	0.62
2:B:230:ALA:H	2:B:231:PRO:HD2	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:GLY:O	4:E:204:THR:HG21	2.01	0.61
2:B:327:ARG:HH22	2:B:371:GLU:HG2	1.66	0.61
1:A:399:HIS:O	1:A:401:GLY:N	2.32	0.60
1:A:899:VAL:HG23	1:A:1029:ARG:HG2	1.83	0.60
2:B:706:GLN:O	2:B:710:LEU:HB2	2.01	0.60
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.84	0.60
1:A:535:THR:HG21	1:A:617:VAL:H	1.66	0.60
1:A:924:LYS:O	1:A:927:VAL:HG12	2.02	0.60
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.84	0.59
2:B:1082:MET:HA	3:C:189:THR:HA	1.84	0.59
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.17	0.59
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.84	0.59
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.67	0.59
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.83	0.59
1:A:596:THR:C	1:A:598:LEU:H	2.06	0.59
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.03	0.59
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.66	0.59
1:A:332:LYS:H	1:A:337:ARG:HB2	1.68	0.58
2:B:511:PRO:O	2:B:513:GLN:N	2.36	0.58
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.69	0.58
3:C:196:ASP:O	3:C:200:GLU:HG2	2.04	0.58
1:A:485:ASP:HA	11:R:10:2IA:I	2.74	0.58
2:B:98:THR:O	2:B:178:ASN:ND2	2.36	0.57
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.85	0.57
2:B:345:LYS:HA	2:B:347:LYS:H	1.69	0.57
2:B:753:ALA:HA	2:B:756:ILE:HD12	1.86	0.57
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.51	0.57
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.86	0.57
2:B:744:HIS:CD2	2:B:746:SER:OG	2.57	0.57
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.84	0.57
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.87	0.57
2:B:578:THR:HG22	2:B:622:LYS:HA	1.87	0.57
6:H:89:LEU:C	6:H:91:ASP:H	2.06	0.57
2:B:976:ILE:O	2:B:990:ILE:HB	2.05	0.57
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.86	0.57
7:I:8:ARG:HB3	7:I:34:TYR:HE1	1.70	0.56
6:H:57:VAL:HG22	6:H:144:ILE:HG12	1.85	0.56
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.71	0.56
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.87	0.56
3:C:183:TRP:HB2	3:C:185:LYS:HG3	1.88	0.56
8:J:41:LEU:HD23	8:J:46:CYS:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:HG21	1:A:466:SER:O	2.05	0.56
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.71	0.56
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.71	0.56
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.88	0.55
8:J:1:MET:H1	8:J:56:LEU:H	1.54	0.55
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.71	0.55
1:A:1329:THR:HG22	1:A:1331:SER:H	1.72	0.55
2:B:54:PHE:HA	2:B:58:THR:HB	1.87	0.55
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.89	0.54
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.88	0.54
3:C:69:LEU:HD12	8:J:6:ARG:HD3	1.89	0.54
2:B:906:SER:HA	2:B:946:ASN:HB3	1.90	0.54
1:A:535:THR:CG2	1:A:617:VAL:H	2.21	0.54
2:B:744:HIS:HD2	2:B:746:SER:OG	1.91	0.54
9:K:92:ASN:HA	9:K:95:ILE:HD12	1.90	0.54
1:A:482:PHE:HB2	2:B:838:SER:OG	2.08	0.53
2:B:800:GLN:CB	8:J:52:THR:HG22	2.35	0.53
5:F:74:ILE:HG21	5:F:144:GLU:HG2	1.90	0.53
6:H:105:GLU:HB3	6:H:113:ALA:HB3	1.90	0.53
10:L:61:THR:HG21	10:L:63:ARG:HD3	1.90	0.53
2:B:69:LEU:HD12	2:B:90:ILE:HB	1.91	0.53
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.90	0.53
2:B:38:PHE:H	2:B:41:LYS:HB2	1.72	0.53
5:F:116:ASP:HB3	5:F:119:ARG:HB2	1.91	0.53
1:A:871:ASP:OD2	4:E:204:THR:HG23	2.09	0.53
1:A:43:GLU:HG3	1:A:50:ILE:HG12	1.91	0.52
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.91	0.52
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.39	0.52
1:A:1059:HIS:CE1	5:F:87:LYS:H	2.27	0.52
3:C:167:HIS:CD2	3:C:169:LYS:H	2.25	0.52
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.90	0.52
8:J:24:LEU:O	8:J:28:ASP:HB2	2.10	0.52
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.74	0.52
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.92	0.52
1:A:225:ASN:HD22	1:A:228:PHE:H	1.56	0.52
1:A:825:ILE:O	1:A:829:VAL:HG23	2.10	0.52
2:B:864:LYS:H	2:B:872:GLU:HB2	1.75	0.52
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.68	0.51
1:A:1318:THR:HG22	4:E:142:VAL:HG12	1.92	0.51
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.93	0.51
1:A:418:SER:HB3	1:A:421:ALA:HB2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.75	0.51
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.93	0.51
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.75	0.51
2:B:241:ARG:HA	2:B:253:THR:HG22	1.93	0.51
4:E:198:ILE:HD13	4:E:212:ARG:HG3	1.92	0.51
1:A:1308:THR:HG22	1:A:1309:ASP:H	1.75	0.51
5:F:134:ILE:HG22	5:F:136:ARG:HG3	1.93	0.51
1:A:351:THR:HG22	1:A:352:VAL:N	2.26	0.51
1:A:84:ILE:HD11	1:A:270:LEU:HG	1.92	0.50
1:A:1444:MET:HB2	5:F:133:VAL:HB	1.93	0.50
4:E:204:THR:HG22	4:E:205:SER:N	2.26	0.50
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.93	0.50
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.94	0.50
2:B:1054:GLY:HA2	2:B:1057:LYS:HE2	1.94	0.50
4:E:61:GLN:HG3	4:E:105:PHE:HE2	1.77	0.50
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.93	0.50
1:A:114:LEU:HB3	1:A:115:LEU:HD12	1.94	0.50
2:B:307:ASP:O	2:B:311:LEU:HD12	2.12	0.50
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.46	0.50
1:A:445:ASN:HB2	1:A:455:MET:HG3	1.94	0.49
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.94	0.49
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.93	0.49
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.93	0.49
2:B:563:MET:HA	2:B:589:VAL:O	2.11	0.49
2:B:843:GLN:HB2	2:B:993:THR:HB	1.93	0.49
5:F:72:LYS:HG2	5:F:142:SER:HA	1.94	0.49
3:C:18:VAL:O	3:C:231:ASN:HA	2.13	0.49
6:H:2:SER:HA	6:H:3:ASN:HB2	1.94	0.49
1:A:113:LEU:HD12	1:A:116:ASP:HB2	1.95	0.49
1:A:1308:THR:HG22	1:A:1309:ASP:N	2.28	0.49
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.78	0.49
1:A:1191:TRP:HZ3	7:I:43:VAL:HG21	1.79	0.48
9:K:12:LEU:HA	9:K:37:LYS:HE3	1.95	0.48
9:K:65:HIS:HD2	9:K:67:PHE:H	1.61	0.48
1:A:114:LEU:HD21	1:A:171:GLN:HE22	1.77	0.48
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.43	0.48
2:B:845:SER:HA	8:J:8:PHE:O	2.12	0.48
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.94	0.48
1:A:886:ILE:HG12	1:A:944:ARG:HG3	1.96	0.48
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.48	0.48
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.49	0.48
2:B:230:ALA:H	2:B:231:PRO:CD	2.26	0.48
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.77	0.48
3:C:46:ILE:HG23	3:C:157:CYS:HB2	1.95	0.48
1:A:68:GLN:HG3	1:A:69:THR:H	1.77	0.48
1:A:506:ALA:HB3	1:A:509:LEU:HD12	1.96	0.48
4:E:196:VAL:HG13	4:E:198:ILE:HD11	1.96	0.48
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.95	0.48
1:A:508:PRO:HB3	1:A:643:ALA:HB2	1.95	0.47
1:A:747:VAL:HG21	1:A:758:ILE:HD11	1.97	0.47
1:A:91:PHE:HA	1:A:235:ILE:HG22	1.96	0.47
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.95	0.47
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.96	0.47
1:A:670:ILE:HD12	2:B:1067:ARG:HD2	1.96	0.47
2:B:1020:ARG:H	2:B:1020:ARG:HG2	1.52	0.47
4:E:78:LEU:HD12	4:E:107:THR:HB	1.97	0.47
2:B:53:GLN:HG2	2:B:547:VAL:HB	1.95	0.47
2:B:639:ILE:HD11	2:B:691:GLU:HB3	1.96	0.47
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.44	0.47
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.96	0.47
11:R:6:G:H2'	11:R:7:A:C8	2.50	0.47
2:B:813:LYS:O	2:B:815:ARG:N	2.47	0.47
4:E:111:VAL:HG12	4:E:137:GLU:HG2	1.97	0.47
7:I:34:TYR:HE2	7:I:36:GLU:HB3	1.80	0.47
1:A:357:PRO:HD2	2:B:833:TYR:CE2	2.50	0.47
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.45	0.47
2:B:768:THR:O	2:B:771:SER:HB2	2.15	0.47
3:C:14:SER:HA	9:K:114:LEU:HD22	1.96	0.47
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.97	0.46
1:A:777:PHE:CD1	1:A:782:ARG:HA	2.49	0.46
1:A:1436:ILE:HB	2:B:1144:ALA:HB2	1.97	0.46
2:B:950:ASP:HB3	2:B:967:ARG:HG2	1.97	0.46
12:T:19:DT:H2'	12:T:20:DC:O4'	2.15	0.46
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.98	0.46
8:J:58:GLU:HA	8:J:61:LEU:HD12	1.96	0.46
1:A:58:LEU:HD23	1:A:244:PRO:HD3	1.98	0.46
1:A:663:SER:OG	2:B:827:ILE:O	2.27	0.46
3:C:31:ASN:O	3:C:35:ARG:HG3	2.16	0.46
5:F:110:ASP:O	5:F:123:LYS:HE2	2.15	0.46
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.97	0.46
1:A:374:LEU:HA	2:B:1107:ALA:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.81	0.46
1:A:369:SER:HB3	9:K:2:ASN:HD21	1.81	0.46
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.98	0.46
9:K:32:VAL:HG22	9:K:74:ARG:HG3	1.97	0.46
9:K:58:PHE:HE2	9:K:74:ARG:HB3	1.81	0.46
2:B:896:ASP:OD2	10:L:58:LYS:HE2	2.15	0.46
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.98	0.46
1:A:1220:PHE:CD1	1:A:1224:LEU:HD22	2.51	0.46
1:A:690:VAL:HA	1:A:693:VAL:HG12	1.98	0.45
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.98	0.45
1:A:1006:ILE:HD12	4:E:167:ARG:HB2	1.98	0.45
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.98	0.45
2:B:424:LEU:O	2:B:428:ILE:HG12	2.16	0.45
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.51	0.45
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.98	0.45
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.98	0.45
7:I:17:ARG:HE	7:I:28:GLU:HG2	1.82	0.45
1:A:587:HIS:HE1	1:A:969:GLN:HE21	1.64	0.45
2:B:1156:ASP:HB2	2:B:1198:TYR:H	1.81	0.45
3:C:33:LEU:HA	3:C:36:VAL:HG12	1.98	0.45
1:A:670:ILE:HG12	1:A:805:LEU:HD11	1.97	0.45
1:A:9:ALA:HB3	2:B:1193:GLN:HE21	1.80	0.45
1:A:408:ASP:O	1:A:409:SER:HB2	2.15	0.45
1:A:344:ARG:O	2:B:1155:SER:OG	2.35	0.45
1:A:404:TYR:HA	1:A:413:ILE:O	2.17	0.45
1:A:907:THR:HG22	1:A:908:LEU:H	1.82	0.45
2:B:223:VAL:HG11	2:B:380:TYR:HE2	1.82	0.45
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.99	0.45
1:A:786:HIS:HE1	2:B:742:GLU:OE1	2.00	0.45
2:B:283:VAL:HG12	2:B:297:ILE:HG21	1.98	0.45
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.98	0.45
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.52	0.45
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.51	0.45
3:C:49:VAL:HG22	3:C:157:CYS:HB3	1.98	0.45
3:C:101:LEU:HD13	3:C:118:LEU:HG	1.99	0.45
2:B:48:LEU:HD23	2:B:173:MET:SD	2.57	0.44
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.32	0.44
2:B:476:ARG:O	2:B:478:GLY:N	2.50	0.44
2:B:864:LYS:N	2:B:872:GLU:HB2	2.32	0.44
3:C:262:LEU:HD11	9:K:87:LEU:HD12	1.98	0.44
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:HD2	2:B:517:THR:OG1	2.00	0.44
3:C:100:THR:HB	3:C:121:VAL:HG21	1.99	0.44
1:A:557:ASP:OD2	1:A:559:VAL:HB	2.17	0.44
2:B:1031:LEU:O	2:B:1034:VAL:HG12	2.17	0.44
1:A:913:LEU:HD11	1:A:981:LEU:O	2.17	0.44
3:C:18:VAL:CG1	9:K:109:TRP:HZ3	2.30	0.44
4:E:153:HIS:HB3	4:E:196:VAL:HG21	2.00	0.44
1:A:528:LEU:HD23	1:A:751:SER:HA	2.00	0.44
2:B:211:VAL:HG21	2:B:483:LEU:HD13	2.00	0.44
2:B:360:PHE:HE2	2:B:374:LYS:HB3	1.82	0.44
6:H:4:THR:HA	6:H:60:ALA:HA	2.00	0.44
7:I:26:LEU:HD23	7:I:37:GLU:HA	2.00	0.44
8:J:64:ASN:N	8:J:65:PRO:HD2	2.33	0.44
1:A:567:LYS:HE3	6:H:96:VAL:O	2.17	0.44
7:I:34:TYR:CD2	7:I:35:VAL:N	2.86	0.44
1:A:516:SER:HB3	1:A:518:LYS:HG2	2.00	0.44
1:A:1325:THR:HA	4:E:147:HIS:HA	2.00	0.44
2:B:975:GLN:O	2:B:990:ILE:HD12	2.17	0.44
7:I:92:ARG:HB3	7:I:95:THR:OG1	2.18	0.44
11:R:5:A:H2'	11:R:6:G:C8	2.43	0.44
1:A:1107:VAL:HG23	1:A:1332:PHE:HE1	1.83	0.44
1:A:1117:THR:HG22	1:A:1307:GLU:HG2	2.00	0.44
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.66	0.44
2:B:59:LEU:HD13	2:B:417:PHE:HE1	1.83	0.44
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.99	0.44
7:I:10:CYS:SG	7:I:31:THR:HB	2.58	0.44
2:B:487:THR:HG22	2:B:490:SER:H	1.83	0.44
2:B:763:GLN:NE2	2:B:765:PRO:HD2	2.33	0.44
2:B:764:SER:HB3	2:B:765:PRO:HD3	1.99	0.44
2:B:826:ALA:HB2	2:B:1087:PHE:CD1	2.52	0.44
2:B:310:MET:HE2	2:B:386:LEU:HD12	1.99	0.43
2:B:749:LEU:HB3	2:B:753:ALA:HB3	2.00	0.43
11:R:6:G:H2'	11:R:7:A:H8	1.81	0.43
1:A:298:PHE:HZ	1:A:311:GLN:H	1.66	0.43
6:H:123:MET:HE2	6:H:142:LEU:HD22	2.00	0.43
1:A:856:THR:HB	1:A:865:GLN:HB2	1.99	0.43
2:B:919:SER:HG	2:B:933:SER:N	2.16	0.43
8:J:32:GLU:CD	8:J:32:GLU:H	2.22	0.43
4:E:198:ILE:HB	4:E:210:SER:HB3	2.00	0.43
1:A:269:ILE:HG22	1:A:299:HIS:HB3	2.01	0.43
1:A:1101:LEU:HB2	1:A:1355:VAL:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:783:THR:CG2	8:J:59:LYS:HB3	2.46	0.43
2:B:840:ILE:HG12	2:B:992:ILE:HG22	2.01	0.43
2:B:942:ARG:HB3	2:B:945:GLU:HB2	2.01	0.43
2:B:1152:MET:O	2:B:1157:ALA:HB2	2.18	0.43
1:A:92:HIS:HD2	1:A:94:GLY:H	1.65	0.43
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.66	0.43
1:A:579:SER:HA	1:A:582:ILE:HD12	1.99	0.43
1:A:1195:LEU:HD11	1:A:1267:MET:SD	2.59	0.43
6:H:33:GLN:HB2	6:H:36:CYS:HB3	2.01	0.43
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.00	0.43
1:A:588:LEU:HD12	1:A:632:VAL:HG21	2.01	0.43
1:A:837:ILE:HD11	1:A:1102:LYS:HG3	2.01	0.43
1:A:353:ILE:HG21	1:A:487:MET:HB2	2.01	0.43
3:C:36:VAL:HG23	3:C:40:GLU:HB2	2.00	0.43
7:I:106:CYS:SG	7:I:108:HIS:HB3	2.59	0.43
1:A:934:LYS:HA	1:A:937:VAL:HG22	2.01	0.42
2:B:67:SER:HB2	2:B:92:PHE:H	1.84	0.42
2:B:552:MET:HA	2:B:555:ILE:HD12	2.01	0.42
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.01	0.42
2:B:211:VAL:HG23	2:B:483:LEU:HB2	2.00	0.42
2:B:280:ILE:HD13	2:B:334:ILE:HG12	2.00	0.42
2:B:327:ARG:NH2	2:B:371:GLU:HG2	2.32	0.42
1:A:993:LEU:HD22	1:A:1046:LEU:HG	2.01	0.42
1:A:1107:VAL:HG21	1:A:1381:LEU:HB3	2.01	0.42
2:B:140:ILE:HB	2:B:141:ASP:HB2	2.02	0.42
2:B:364:ILE:HG22	2:B:365:THR:HG22	2.01	0.42
2:B:839:MET:HG2	2:B:990:ILE:HA	2.01	0.42
3:C:71:PRO:HG3	8:J:13:VAL:HG11	2.00	0.42
1:A:51:GLY:HA2	1:A:56:PRO:HB3	2.01	0.42
1:A:116:ASP:HA	1:A:117:GLU:HA	1.85	0.42
4:E:78:LEU:HD11	4:E:109:ILE:HD13	2.00	0.42
7:I:18:GLU:HG2	7:I:20:LYS:H	1.84	0.42
7:I:96:SER:HB2	7:I:98:VAL:HG23	2.02	0.42
1:A:1122:PRO:HA	1:A:1125:ALA:HB2	2.02	0.42
1:A:4:GLN:HE22	2:B:1159:ARG:H	1.66	0.42
1:A:492:PRO:HB3	1:A:497:THR:HG22	2.02	0.42
1:A:899:VAL:HG23	1:A:1029:ARG:CG	2.48	0.42
2:B:30:SER:O	2:B:34:ILE:HG12	2.19	0.42
2:B:412:LEU:HA	2:B:415:GLN:HB2	2.00	0.42
2:B:541:LEU:HD21	2:B:812:LEU:HD21	2.02	0.42
2:B:804:GLY:O	2:B:983:ARG:NH2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ASP:HB3	2:B:837:ASP:HB3	2.00	0.42
1:A:571:LEU:HD22	6:H:46:LEU:HD11	2.01	0.42
2:B:653:VAL:HG22	2:B:689:LEU:HB3	2.02	0.42
2:B:706:GLN:H	2:B:710:LEU:HD23	1.85	0.42
2:B:900:ALA:HA	10:L:58:LYS:HD3	2.01	0.42
3:C:115:SER:HA	3:C:144:ILE:HD11	2.02	0.42
9:K:65:HIS:HD2	9:K:67:PHE:HB2	1.85	0.42
1:A:901:LEU:HD22	1:A:919:ILE:HG22	2.01	0.41
2:B:50:SER:OG	2:B:411:PRO:HD2	2.20	0.41
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.85	0.41
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.54	0.41
1:A:325:ILE:H	1:A:325:ILE:HG13	1.75	0.41
1:A:1107:VAL:HG23	1:A:1332:PHE:CE1	2.56	0.41
2:B:25:ILE:HG23	2:B:29:ASP:HB2	2.01	0.41
3:C:18:VAL:HG11	9:K:109:TRP:HZ3	1.85	0.41
11:R:10:2IA:C2	12:T:19:DT:H3	2.33	0.41
1:A:709:THR:HG22	1:A:711:ARG:H	1.86	0.41
2:B:313:MET:HE1	2:B:390:LEU:HG	2.01	0.41
9:K:7:PHE:HA	9:K:10:PHE:CE2	2.56	0.41
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.55	0.41
3:C:62:PHE:O	3:C:66:ARG:HG3	2.20	0.41
1:A:1290:LYS:HE2	1:A:1298:TYR:HB3	2.01	0.41
2:B:705:MET:HG3	2:B:745:PRO:HG3	2.02	0.41
1:A:1293:SER:HB3	1:A:1299:VAL:HG23	2.01	0.41
1:A:1436:ILE:HG22	2:B:1142:GLY:HA2	2.03	0.41
8:J:44:TYR:HA	8:J:47:ARG:HB2	2.03	0.41
10:L:48:CYS:SG	10:L:51:CYS:HB3	2.60	0.41
1:A:306:ASN:HD21	1:A:313:GLN:HB2	1.85	0.41
2:B:846:ILE:HG23	2:B:974:PRO:HD2	2.03	0.41
5:F:72:LYS:HE2	5:F:142:SER:HB3	2.02	0.41
5:F:87:LYS:HE2	5:F:88:TYR:CZ	2.55	0.41
2:B:123:THR:H	2:B:958:GLN:HE22	1.67	0.41
6:H:58:THR:HG23	6:H:143:LEU:HB2	2.03	0.41
1:A:579:SER:HB3	1:A:611:GLN:HA	2.02	0.41
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.56	0.41
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.54	0.41
2:B:114:PRO:HG2	2:B:181:LEU:HD11	2.03	0.41
3:C:241:ASP:HB3	9:K:109:TRP:CD2	2.56	0.41
4:E:176:PRO:O	4:E:212:ARG:HA	2.21	0.41
5:F:90:ARG:HD3	5:F:155:LEU:HD11	2.02	0.41
1:A:384:ASN:HB2	1:A:387:ARG:HH21	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:424:LEU:HD22	2:B:453:ILE:HD11	2.03	0.41
2:B:1074:ASN:HD22	2:B:1077:THR:H	1.69	0.41
1:A:608:ILE:HD12	1:A:613:ILE:HG13	2.02	0.40
2:B:408:LEU:HD11	2:B:545:ILE:HD13	2.02	0.40
7:I:34:TYR:HD2	7:I:35:VAL:N	2.18	0.40
1:A:55:ASP:N	1:A:56:PRO:HD3	2.37	0.40
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.04	0.40
1:A:71:GLN:HB3	1:A:72:GLU:H	1.77	0.40
2:B:647:GLY:HA2	2:B:648:HIS:C	2.41	0.40
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	2.03	0.40
2:B:345:LYS:HA	2:B:347:LYS:N	2.34	0.40
2:B:515:HIS:CD2	2:B:517:THR:H	2.40	0.40
2:B:549:THR:HG21	2:B:610:ASN:HD22	1.86	0.40
2:B:999:MET:HE2	2:B:1011:ILE:HD11	2.04	0.40
4:E:167:ARG:HA	4:E:167:ARG:HD3	1.93	0.40
5:F:112:GLU:H	5:F:112:GLU:HG3	1.69	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%)	1181 (85%)	165 (12%)	49 (4%)	3 21
2	B	1096/1224 (90%)	936 (85%)	112 (10%)	48 (4%)	2 16
3	C	264/318 (83%)	242 (92%)	18 (7%)	4 (2%)	10 38
4	E	212/215 (99%)	194 (92%)	15 (7%)	3 (1%)	11 38
5	F	83/155 (54%)	68 (82%)	13 (16%)	2 (2%)	6 28
6	H	129/146 (88%)	99 (77%)	26 (20%)	4 (3%)	4 23
7	I	117/122 (96%)	100 (86%)	15 (13%)	2 (2%)	9 35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	J	63/70 (90%)	56 (89%)	4 (6%)	3 (5%)	2 14
9	K	112/120 (93%)	107 (96%)	5 (4%)	0	100 100
10	L	44/70 (63%)	30 (68%)	7 (16%)	7 (16%)	0 1
All	All	3515/4173 (84%)	3013 (86%)	380 (11%)	122 (4%)	3 21

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ARG
1	A	853	ASP
1	A	1437	GLY
2	B	137	TYR
2	B	229	ALA
2	B	230	ALA
2	B	249	ARG
2	B	477	ALA
2	B	512	ARG
2	B	531	GLN
2	B	646	LEU
2	B	712	PRO
2	B	734	HIS
2	B	751	VAL
2	B	814	PHE
2	B	880	THR
2	B	889	THR
2	B	976	ILE
2	B	1221	SER
3	C	4	GLU
3	C	173	ALA
8	J	2	ILE
10	L	64	LEU
1	A	54	ASN
1	A	57	ARG
1	A	68	GLN
1	A	113	LEU
1	A	121	LEU
1	A	214	ILE
1	A	251	SER
1	A	331	GLY
1	A	385	ILE
1	A	423	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	424	ILE
1	A	662	PHE
1	A	672	ASP
1	A	846	GLU
1	A	923	LEU
1	A	1081	LEU
1	A	1123	GLY
1	A	1405	THR
2	B	138	GLU
2	B	176	SER
2	B	277	LYS
2	B	480	SER
2	B	511	PRO
2	B	647	GLY
2	B	792	MET
2	B	943	SER
2	B	1046	PRO
2	B	1099	VAL
6	H	83	GLN
7	I	77	LYS
8	J	6	ARG
8	J	13	VAL
10	L	56	LEU
10	L	63	ARG
1	A	118	HIS
1	A	145	LYS
1	A	907	THR
1	A	1167	GLU
1	A	1377	THR
1	A	1416	ALA
2	B	248	SER
2	B	526	GLU
2	B	881	ASN
2	B	1017	ILE
2	B	1097	HIS
3	C	215	GLU
3	C	267	GLN
4	E	123	LEU
5	F	112	GLU
10	L	51	CYS
1	A	48	ALA
1	A	215	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	399	HIS
1	A	404	TYR
1	A	569	LYS
1	A	597	LEU
1	A	599	SER
1	A	736	ASN
1	A	1255	GLU
2	B	139	ALA
2	B	476	ARG
2	B	478	GLY
2	B	563	MET
2	B	764	SER
2	B	907	GLY
2	B	918	ILE
2	B	1108	ARG
4	E	45	LYS
4	E	172	GLU
6	H	109	LYS
7	I	60	GLN
1	A	63	ARG
1	A	149	GLU
1	A	226	GLU
1	A	250	ILE
1	A	332	LYS
1	A	958	VAL
1	A	1166	ASP
2	B	177	LYS
2	B	752	ALA
2	B	996	ARG
2	B	1181	GLU
5	F	114	GLU
6	H	108	SER
10	L	47	ARG
1	A	312	PRO
1	A	409	SER
2	B	346	GLU
2	B	467	GLY
2	B	1188	LYS
1	A	568	PRO
1	A	735	VAL
1	A	1360	GLY
2	B	364	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	18	GLY
10	L	46	VAL
2	B	780	VAL
10	L	55	ILE
1	A	210	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	1085 (89%)	140 (11%)	5	22
2	B	967/1061 (91%)	856 (88%)	111 (12%)	5	22
3	C	234/274 (85%)	209 (89%)	25 (11%)	6	25
4	E	196/197 (100%)	178 (91%)	18 (9%)	9	31
5	F	75/137 (55%)	69 (92%)	6 (8%)	12	37
6	H	117/128 (91%)	106 (91%)	11 (9%)	8	30
7	I	113/116 (97%)	103 (91%)	10 (9%)	10	33
8	J	60/65 (92%)	51 (85%)	9 (15%)	3	13
9	K	99/102 (97%)	88 (89%)	11 (11%)	6	23
10	L	40/57 (70%)	34 (85%)	6 (15%)	3	13
All	All	3126/3657 (86%)	2779 (89%)	347 (11%)	6	23

All (347) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	22	PHE
1	A	28	ARG
1	A	30	ILE
1	A	43	GLU
1	A	44	THR
1	A	50	ILE
1	A	54	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	65	LEU
1	A	75	ASN
1	A	113	LEU
1	A	118	HIS
1	A	133	LYS
1	A	142	CYS
1	A	164	ARG
1	A	179	LEU
1	A	186	LYS
1	A	204	THR
1	A	234	MET
1	A	256	GLN
1	A	266	LEU
1	A	268	ASP
1	A	270	LEU
1	A	279	LEU
1	A	290	GLU
1	A	303	TYR
1	A	315	LEU
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	335	ARG
1	A	344	ARG
1	A	353	ILE
1	A	359	LEU
1	A	368	LYS
1	A	369	SER
1	A	383	TYR
1	A	387	ARG
1	A	389	THR
1	A	398	GLU
1	A	403	LYS
1	A	411	ASP
1	A	424	ILE
1	A	434	ARG
1	A	438	ASP
1	A	443	LEU
1	A	451	HIS
1	A	453	MET
1	A	454	SER
1	A	468	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	485	ASP
1	A	500	GLU
1	A	513	SER
1	A	516	SER
1	A	532	ARG
1	A	534	LEU
1	A	535	THR
1	A	538	ASP
1	A	541	ILE
1	A	543	LEU
1	A	544	ASP
1	A	545	GLN
1	A	566	ILE
1	A	567	LYS
1	A	577	ILE
1	A	588	LEU
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	621	THR
1	A	629	LEU
1	A	663	SER
1	A	666	ILE
1	A	672	ASP
1	A	676	MET
1	A	680	THR
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	705	LYS
1	A	710	LEU
1	A	722	LEU
1	A	740	LEU
1	A	756	ILE
1	A	774	ARG
1	A	821	ARG
1	A	833	GLU
1	A	855	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	867	ILE
1	A	878	ILE
1	A	886	ILE
1	A	896	ARG
1	A	929	LEU
1	A	932	GLU
1	A	953	ASN
1	A	969	GLN
1	A	973	ILE
1	A	988	LEU
1	A	1000	LEU
1	A	1006	ILE
1	A	1029	ARG
1	A	1057	VAL
1	A	1077	THR
1	A	1084	PHE
1	A	1095	THR
1	A	1111	MET
1	A	1120	LEU
1	A	1130	GLN
1	A	1134	ILE
1	A	1162	VAL
1	A	1174	PHE
1	A	1176	LEU
1	A	1206	ASP
1	A	1209	MET
1	A	1237	ILE
1	A	1262	LYS
1	A	1264	GLU
1	A	1267	MET
1	A	1280	GLU
1	A	1293	SER
1	A	1309	ASP
1	A	1314	SER
1	A	1316	VAL
1	A	1325	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1359	ASP
1	A	1366	ARG
1	A	1376	THR
1	A	1382	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1385	THR
1	A	1391	ARG
1	A	1403	GLU
1	A	1407	GLU
1	A	1419	ASP
1	A	1422	ARG
2	B	46	GLN
2	B	59	LEU
2	B	101	MET
2	B	102	VAL
2	B	132	VAL
2	B	194	GLU
2	B	209	GLU
2	B	217	ARG
2	B	234	ILE
2	B	240	ILE
2	B	254	LEU
2	B	261	ARG
2	B	277	LYS
2	B	305	VAL
2	B	309	GLN
2	B	311	LEU
2	B	323	VAL
2	B	333	PHE
2	B	365	THR
2	B	367	LEU
2	B	376	PHE
2	B	393	LYS
2	B	394	ASP
2	B	396	ASP
2	B	412	LEU
2	B	415	GLN
2	B	416	LEU
2	B	417	PHE
2	B	419	THR
2	B	429	PHE
2	B	437	GLU
2	B	466	TRP
2	B	476	ARG
2	B	479	VAL
2	B	480	SER
2	B	485	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	487	THR
2	B	490	SER
2	B	500	THR
2	B	502	ILE
2	B	542	MET
2	B	549	THR
2	B	556	THR
2	B	559	SER
2	B	603	LEU
2	B	604	ARG
2	B	612	GLU
2	B	614	SER
2	B	620	ARG
2	B	623	GLU
2	B	624	LEU
2	B	633	VAL
2	B	642	ASP
2	B	645	SER
2	B	650	GLU
2	B	653	VAL
2	B	658	ILE
2	B	685	LEU
2	B	690	VAL
2	B	694	ASP
2	B	708	GLU
2	B	730	ARG
2	B	737	THR
2	B	739	THR
2	B	776	GLN
2	B	780	VAL
2	B	786	ASN
2	B	806	THR
2	B	825	VAL
2	B	829	CYS
2	B	839	MET
2	B	844	SER
2	B	854	LEU
2	B	865	LYS
2	B	868	MET
2	B	872	GLU
2	B	879	ARG
2	B	880	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	885	MET
2	B	887	HIS
2	B	898	LEU
2	B	918	ILE
2	B	946	ASN
2	B	963	PHE
2	B	973	ILE
2	B	979	LYS
2	B	983	ARG
2	B	987	LYS
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1020	ARG
2	B	1028	GLU
2	B	1034	VAL
2	B	1060	ARG
2	B	1062	HIS
2	B	1065	GLN
2	B	1073	TYR
2	B	1099	VAL
2	B	1106	ARG
2	B	1111	MET
2	B	1129	ARG
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1149	GLU
2	B	1188	LYS
2	B	1202	LEU
2	B	1216	LEU
3	C	9	LYS
3	C	18	VAL
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	41	ILE
3	C	75	MET
3	C	80	LEU
3	C	96	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	100	THR
3	C	116	LYS
3	C	122	SER
3	C	129	ILE
3	C	137	LYS
3	C	149	LYS
3	C	151	GLN
3	C	156	THR
3	C	170	TRP
3	C	204	SER
3	C	215	GLU
3	C	221	TYR
3	C	240	VAL
3	C	244	VAL
3	C	249	ASP
3	C	254	LYS
4	E	8	ASN
4	E	30	ILE
4	E	32	GLN
4	E	54	GLN
4	E	69	ILE
4	E	74	ASP
4	E	78	LEU
4	E	95	THR
4	E	117	THR
4	E	123	LEU
4	E	127	ILE
4	E	146	HIS
4	E	162	ARG
4	E	165	LEU
4	E	169	ARG
4	E	177	ARG
4	E	190	LEU
4	E	200	ARG
5	F	74	ILE
5	F	82	THR
5	F	111	LEU
5	F	112	GLU
5	F	138	LEU
5	F	152	ILE
6	H	2	SER
6	H	14	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	21	ASN
6	H	24	CYS
6	H	34	ASP
6	H	35	GLN
6	H	40	LEU
6	H	55	LEU
6	H	61	SER
6	H	92	ASP
6	H	94	ASP
7	I	17	ARG
7	I	22	ASN
7	I	31	THR
7	I	35	VAL
7	I	52	ILE
7	I	77	LYS
7	I	91	ARG
7	I	97	MET
7	I	118	ARG
7	I	120	GLN
8	J	3	VAL
8	J	7	CYS
8	J	9	SER
8	J	26	GLN
8	J	37	SER
8	J	38	ARG
8	J	48	ARG
8	J	59	LYS
8	J	62	ARG
9	K	18	LYS
9	K	20	LYS
9	K	21	ILE
9	K	29	ASN
9	K	71	PHE
9	K	74	ARG
9	K	78	THR
9	K	92	ASN
9	K	103	THR
9	K	111	LEU
9	K	114	LEU
10	L	27	LEU
10	L	38	LEU
10	L	46	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	L	53	HIS
10	L	61	THR
10	L	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	83	HIS
1	A	92	HIS
1	A	118	HIS
1	A	171	GLN
1	A	225	ASN
1	A	339	ASN
1	A	358	ASN
1	A	439	ASN
1	A	451	HIS
1	A	471	ASN
1	A	517	ASN
1	A	654	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	935	GLN
1	A	965	GLN
1	A	969	GLN
1	A	1106	ASN
1	A	1278	ASN
1	A	1364	ASN
2	B	121	ASN
2	B	178	ASN
2	B	255	GLN
2	B	300	HIS
2	B	325	GLN
2	B	357	GLN
2	B	383	ASN
2	B	415	GLN
2	B	484	ASN
2	B	515	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	516	ASN
2	B	686	ASN
2	B	744	HIS
2	B	762	ASN
2	B	763	GLN
2	B	776	GLN
2	B	822	ASN
2	B	958	GLN
2	B	984	HIS
2	B	1013	ASN
2	B	1025	HIS
2	B	1074	ASN
2	B	1117	GLN
2	B	1193	GLN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	167	HIS
4	E	106	GLN
5	F	100	GLN
7	I	12	ASN
7	I	60	GLN
7	I	83	ASN
9	K	52	ASN
9	K	65	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	4/6 (66%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	2IA	R	10	11,14	17,24,25	0.86	1 (5%)	15,35,38	1.73	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	2IA	R	10	11,14	-	1/3/25/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	10	2IA	C2-N3	2.00	1.35	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	R	10	2IA	N3-C2-N1	-5.03	120.82	128.68
11	R	10	2IA	C4-C5-N7	-2.10	107.21	109.40
11	R	10	2IA	C1'-N9-C4	-2.04	123.06	126.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	R	10	2IA	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	R	10	2IA	2	0

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%)	0.39	121 (8%)	10	10	72, 120, 213, 242	0
2	B	1114/1224 (91%)	0.16	41 (3%)	41	38	67, 110, 181, 232	0
3	C	266/318 (83%)	-0.12	0	100	100	83, 111, 153, 201	0
4	E	214/215 (99%)	0.21	11 (5%)	28	26	85, 153, 214, 225	0
5	F	85/155 (54%)	-0.19	0	100	100	88, 126, 166, 188	0
6	H	133/146 (91%)	0.68	17 (12%)	3	3	128, 170, 186, 196	0
7	I	119/122 (97%)	-0.15	0	100	100	89, 129, 162, 181	0
8	J	65/70 (92%)	-0.16	0	100	100	67, 101, 131, 145	0
9	K	114/120 (95%)	0.00	0	100	100	84, 121, 148, 155	0
10	L	46/70 (65%)	0.17	5 (10%)	5	5	98, 139, 169, 173	0
11	R	5/6 (83%)	-0.37	0	100	100	152, 160, 171, 177	0
12	T	12/29 (41%)	1.10	2 (16%)	1	1	184, 198, 229, 229	0
All	All	3578/4208 (85%)	0.22	197 (5%)	25	23	67, 119, 201, 242	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	CYS	8.5
1	A	105	CYS	8.1
1	A	1176	LEU	8.0
1	A	44	THR	6.6
2	B	1224	PHE	6.3
1	A	141	LEU	6.0
2	B	1222	ARG	5.7
1	A	317	LYS	5.7
1	A	182	VAL	5.6
1	A	1082	ASN	5.4
1	A	202	LEU	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	199	LEU	5.3
1	A	106	VAL	5.2
1	A	142	CYS	5.2
1	A	49	LYS	5.1
1	A	174	ILE	4.8
4	E	83	CYS	4.7
1	A	114	LEU	4.7
1	A	1091	SER	4.7
1	A	1085	HIS	4.7
1	A	163	SER	4.6
1	A	145	LYS	4.6
4	E	122	LYS	4.5
6	H	86	ASP	4.5
1	A	108	MET	4.5
1	A	69	THR	4.5
1	A	181	LEU	4.5
1	A	1124	HIS	4.5
1	A	144	THR	4.4
2	B	1223	ASP	4.3
1	A	116	ASP	4.2
4	E	123	LEU	4.2
1	A	72	GLU	4.2
1	A	1089	VAL	4.1
1	A	138	ILE	4.1
1	A	45	GLN	4.1
6	H	84	ALA	4.1
1	A	314	ALA	4.1
1	A	286	HIS	4.1
4	E	95	THR	4.0
1	A	149	GLU	4.0
1	A	183	GLY	4.0
6	H	83	GLN	3.9
4	E	82	PHE	3.9
2	B	89	GLU	3.8
1	A	257	ARG	3.8
1	A	253	ASN	3.8
2	B	136	THR	3.8
1	A	210	ILE	3.7
1	A	55	ASP	3.7
1	A	143	LYS	3.7
1	A	318	SER	3.7
1	A	200	ARG	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	206	GLU	3.6
1	A	109	HIS	3.6
2	B	883	LEU	3.6
2	B	866	TYR	3.6
1	A	201	VAL	3.6
1	A	171	GLN	3.6
1	A	172	PRO	3.5
2	B	468	GLU	3.5
2	B	448	ILE	3.5
1	A	176	LYS	3.5
1	A	1087	ALA	3.5
1	A	152	VAL	3.5
1	A	319	GLY	3.5
2	B	1188	LYS	3.4
1	A	161	LEU	3.4
1	A	91	PHE	3.4
1	A	1083	THR	3.4
2	B	92	PHE	3.4
2	B	882	THR	3.4
6	H	9	ILE	3.3
2	B	477	ALA	3.3
1	A	287	HIS	3.3
1	A	1306	LEU	3.3
1	A	151	ASP	3.3
1	A	146	MET	3.3
1	A	100	LYS	3.3
1	A	177	ASP	3.3
1	A	1088	GLY	3.3
1	A	167	CYS	3.2
1	A	111	GLY	3.2
2	B	356	LEU	3.2
2	B	1221	SER	3.2
1	A	316	GLN	3.2
1	A	173	THR	3.2
2	B	165	VAL	3.1
1	A	276	LEU	3.1
1	A	113	LEU	3.1
1	A	914	GLU	3.1
2	B	432	MET	3.1
10	L	27	LEU	3.1
2	B	934	LYS	3.1
1	A	148	CYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	104	GLU	3.1
1	A	86	LEU	3.0
1	A	140	THR	3.0
1	A	147	VAL	3.0
4	E	91	LYS	3.0
12	T	27	DA	3.0
1	A	165	GLY	2.9
1	A	166	GLY	2.9
1	A	162	VAL	2.9
6	H	52	GLN	2.9
1	A	65	LEU	2.9
1	A	118	HIS	2.8
2	B	865	LYS	2.8
6	H	51	ALA	2.8
1	A	207	ILE	2.8
1	A	101	LYS	2.8
4	E	121	MET	2.8
10	L	26	THR	2.8
10	L	50	ASP	2.8
1	A	426	LEU	2.7
1	A	1092	LYS	2.7
2	B	135	ARG	2.7
1	A	115	LEU	2.7
1	A	975	HIS	2.7
1	A	1123	GLY	2.7
1	A	1084	PHE	2.7
1	A	1156	PRO	2.7
6	H	55	LEU	2.6
1	A	139	TRP	2.6
1	A	211	PHE	2.6
2	B	133	LYS	2.6
2	B	919	SER	2.6
1	A	87	ALA	2.5
1	A	280	GLU	2.5
1	A	122	MET	2.5
2	B	132	VAL	2.5
1	A	980	ASP	2.5
1	A	405	VAL	2.5
1	A	1108	ALA	2.5
1	A	290	GLU	2.5
1	A	313	GLN	2.5
1	A	1258	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	660	ASN	2.5
2	B	138	GLU	2.4
1	A	323	LYS	2.4
2	B	933	SER	2.4
1	A	424	ILE	2.4
1	A	102	VAL	2.4
2	B	130	VAL	2.4
1	A	1284	MET	2.3
1	A	908	LEU	2.3
6	H	15	VAL	2.3
1	A	170	THR	2.3
2	B	470	LYS	2.3
1	A	5	GLN	2.3
1	A	278	THR	2.3
1	A	224	PHE	2.3
1	A	1090	ALA	2.3
2	B	131	ASP	2.3
1	A	1120	LEU	2.3
2	B	429	PHE	2.3
2	B	1220	ARG	2.3
6	H	130	ARG	2.3
6	H	50	ALA	2.2
1	A	185	TRP	2.2
2	B	465	ASN	2.2
2	B	67	SER	2.2
2	B	935	ARG	2.2
1	A	430	TRP	2.2
6	H	139	ASN	2.2
1	A	88	LYS	2.2
2	B	474	SER	2.2
2	B	869	SER	2.2
10	L	45	ALA	2.2
12	T	23	DC	2.2
1	A	1086	PHE	2.2
6	H	136	LYS	2.2
1	A	983	ILE	2.1
1	A	1287	TYR	2.1
1	A	1191	TRP	2.1
1	A	137	ALA	2.1
1	A	425	GLN	2.1
2	B	449	ASN	2.1
6	H	133	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	478	GLY	2.1
2	B	867	GLY	2.1
1	A	204	THR	2.1
6	H	6	PHE	2.1
4	E	70	SER	2.1
1	A	59	GLY	2.1
2	B	68	THR	2.1
4	E	96	PHE	2.1
6	H	114	VAL	2.0
4	E	109	ILE	2.0
2	B	91	SER	2.0
6	H	60	ALA	2.0
2	B	425	THR	2.0
1	A	62	ASP	2.0
1	A	203	SER	2.0
4	E	71	LYS	2.0
6	H	126	GLU	2.0
10	L	44	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
11	2IA	R	10	22/23	0.88	0.18	147,150,152,152	1

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	0.56	0.25	300,300,300,300	0
13	ZN	A	1735	1/1	0.71	0.11	198,198,198,198	0
13	ZN	B	1307	1/1	0.95	0.05	226,226,226,226	0
13	ZN	L	105	1/1	0.97	0.09	169,169,169,169	0
14	MG	A	2001	1/1	0.97	0.21	47,47,47,47	0
13	ZN	I	203	1/1	0.98	0.12	129,129,129,129	0
13	ZN	J	101	1/1	0.99	0.20	112,112,112,112	0
13	ZN	C	319	1/1	0.99	0.11	126,126,126,126	0
13	ZN	I	204	1/1	0.99	0.12	118,118,118,118	0

6.5 Other polymers (i)

There are no such residues in this entry.