Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2024 – 09:55 am BST

PDB ID	:	4C3H
Title	:	Structure of 14-subunit RNA polymerase I at 3.27 A resolution, crystal form C2-93
Authors	:	Fernandez-Tornero, C.; Moreno-Morcillo, M.; Rashid, U.J.; Taylor, N.M.I.; Ruiz, F.M.; Gruene, T.; Legrand, P.; Steuerwald, U.; Muller, C.W.
Deposited on	:	2013-08-24
Resolution	:	3.27 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

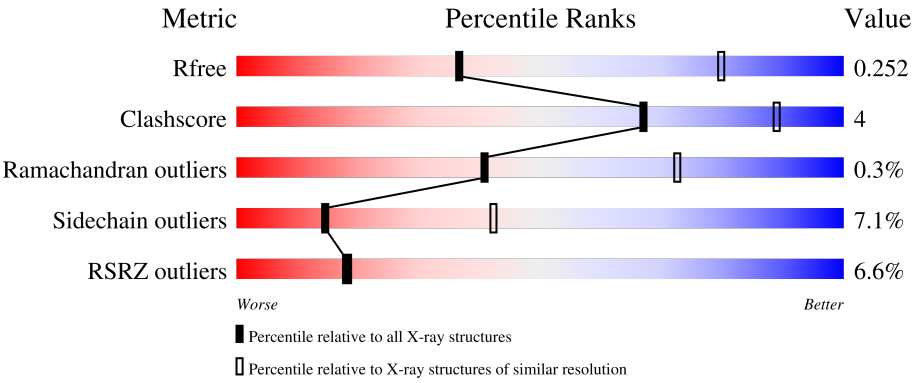
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.27 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	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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	1664	3% 77% 14% · 8%
2	B	1203	5% 80% 16% ··
3	C	335	5% 74% 17% 9%
4	D	137	4% 36% 7% 57%
5	E	215	6% 92% 8%

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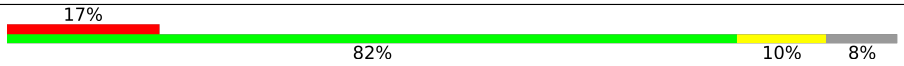
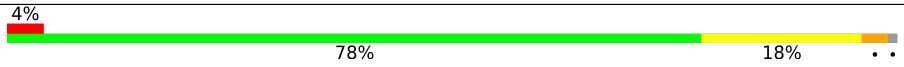
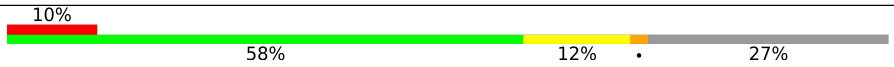
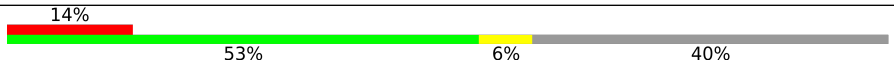
Mol	Chain	Length	Quality of chain
6	F	155	
7	G	326	
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 34552 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 I SUBUNIT RPA190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1523	Total	C	N	O	S	0	0	0
			12019	7577	2086	2292	64			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1176	Total	C	N	O	S	0	0	0
			9322	5898	1629	1745	50			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	304	Total	C	N	O	S	0	0	0
			2418	1536	414	460	8			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	59	Total	C	N	O	0	0	0
			466	292	80	94			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	12	SER	THR	conflict	UNP P50106

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	215	Total	C	N	O	S	0	0	0
			1759	1116	310	321	12			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			823	522	144	154	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	259	Total	C	N	O	S	0	0	0
			2052	1301	348	398	5			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1072	676	181	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	124	Total	C	N	O	S	0	0	0
			942	584	160	189	9			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	103	Total	C	N	O	S	0	0	0
			810	506	132	167	5			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

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

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	105	Total	C	N	O	0	0	0
			831	528	137	166			

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	139	Total	C	N	O	S	0	0	0
			1103	706	179	214	4			

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

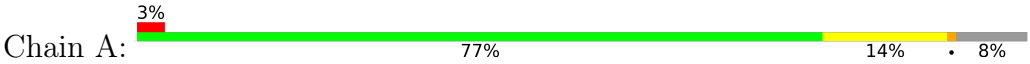
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Zn	0	0
			2	2		
15	B	1	Total	Zn	0	0
			1	1		
15	I	2	Total	Zn	0	0
			2	2		
15	J	1	Total	Zn	0	0
			1	1		
15	L	1	Total	Zn	0	0
			1	1		

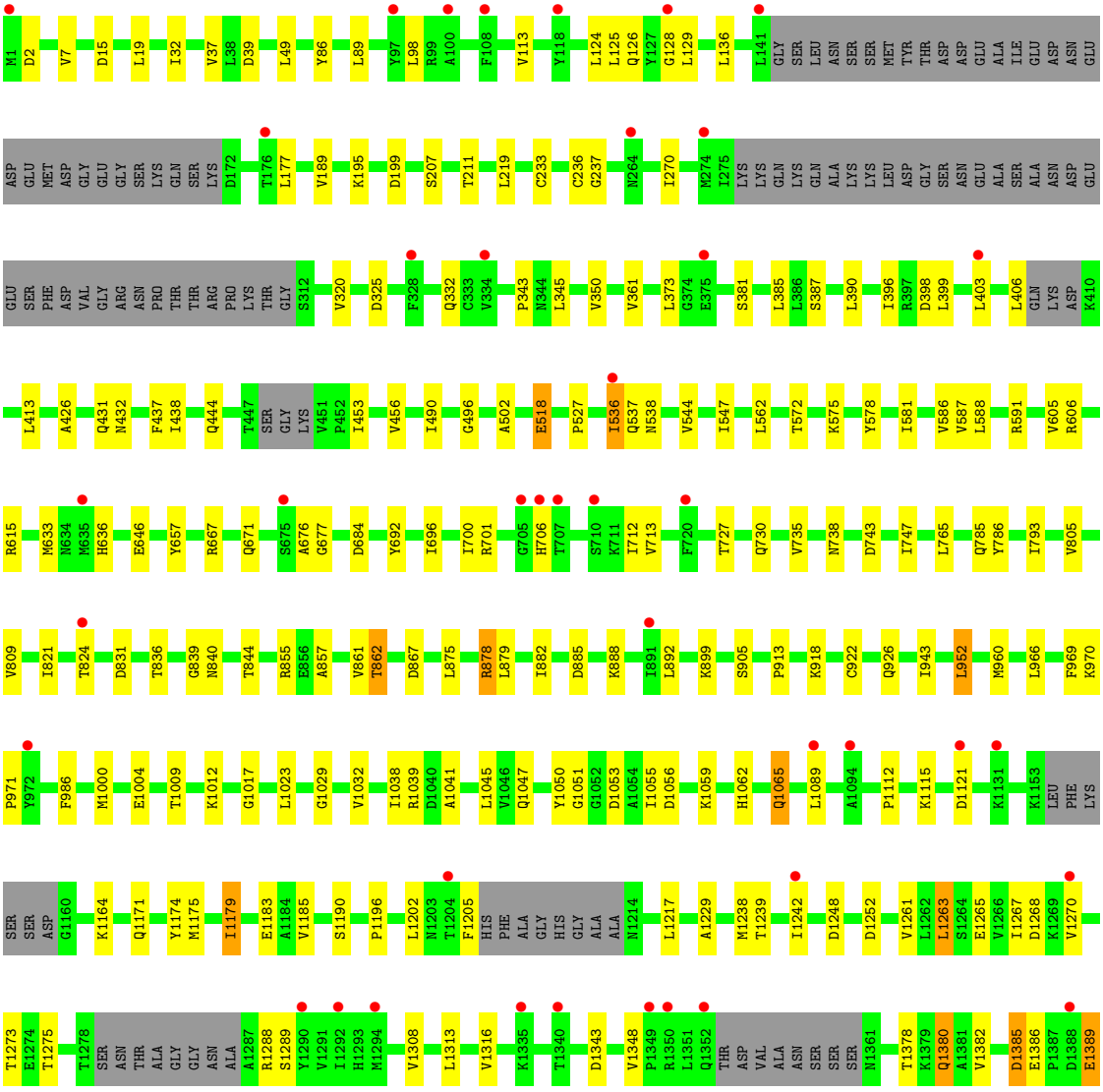
3 Residue-property plots (i)

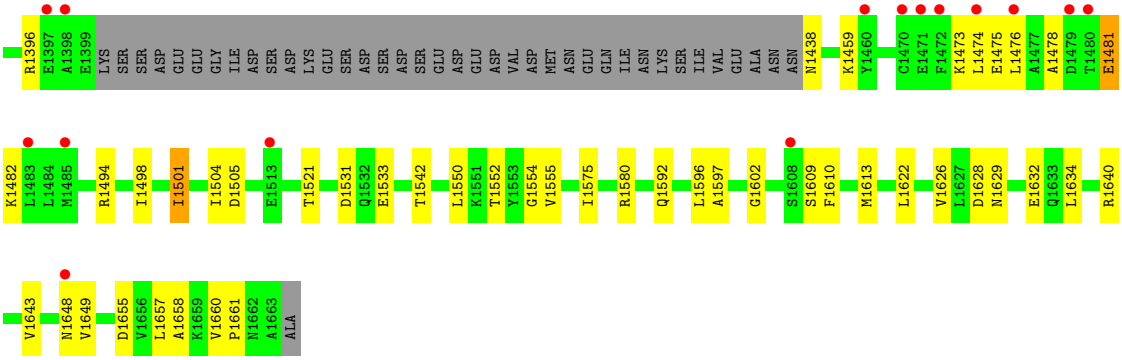
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 I SUBUNIT RPA190

Chain A:

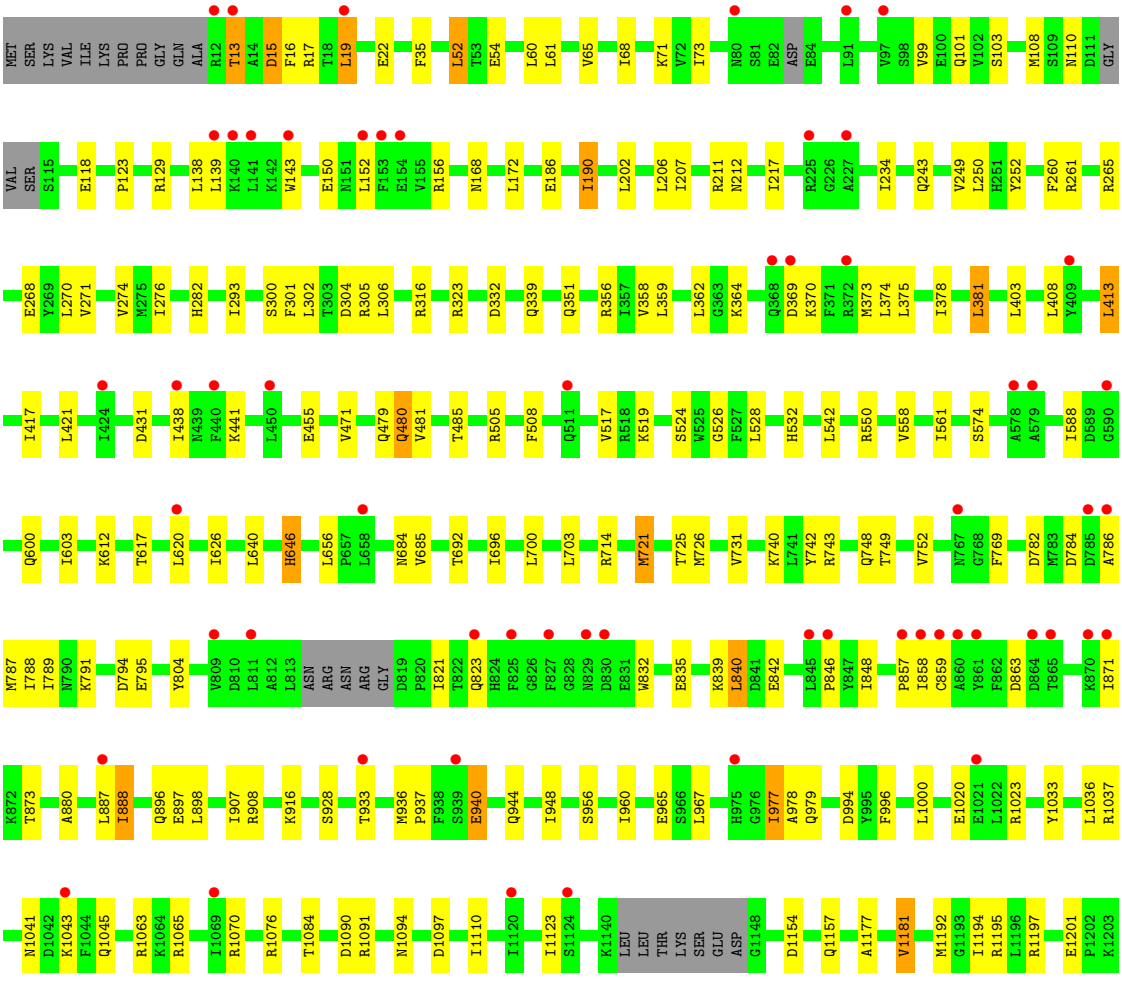






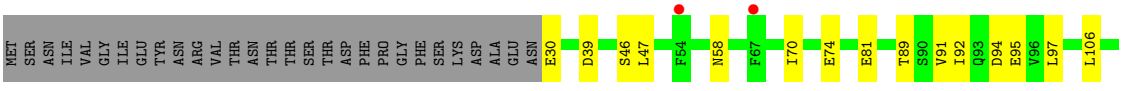
• Molecule 2: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135

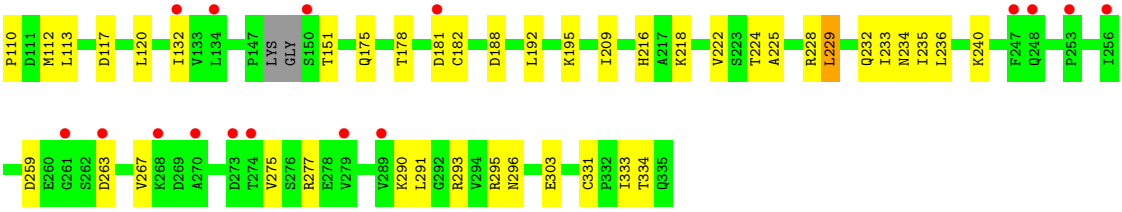
Chain B:



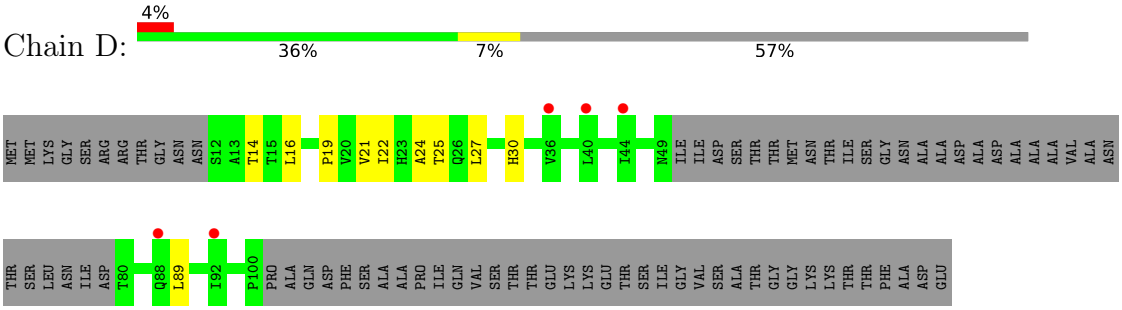
• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

Chain C:

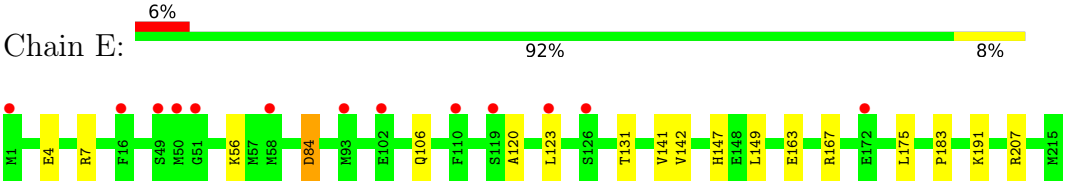




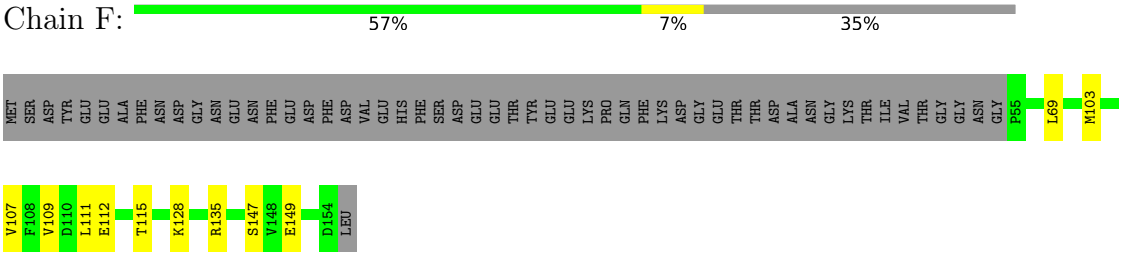
• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14



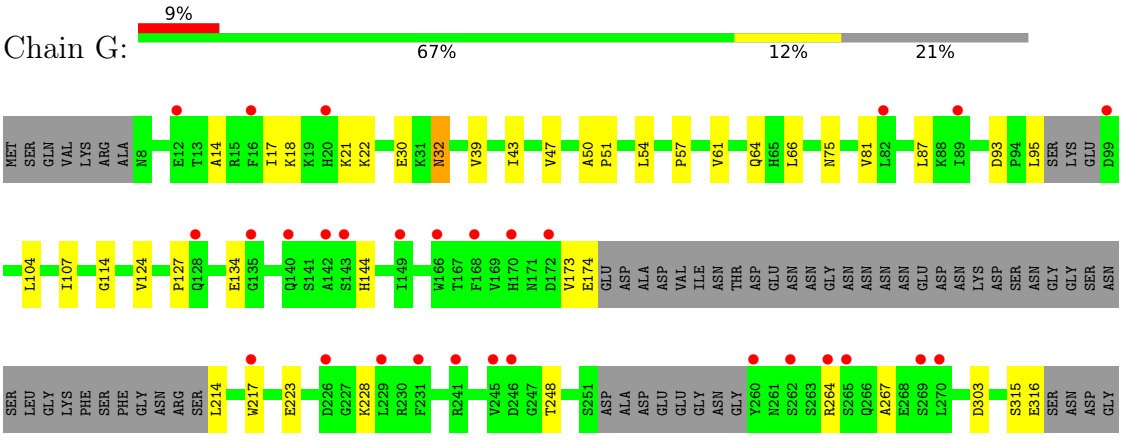
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

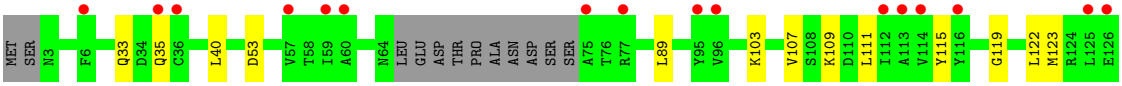


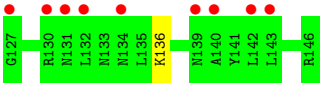
• Molecule 7: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43



• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:



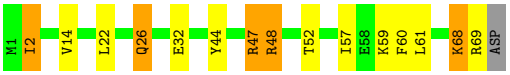


• Molecule 9: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12

Chain I:

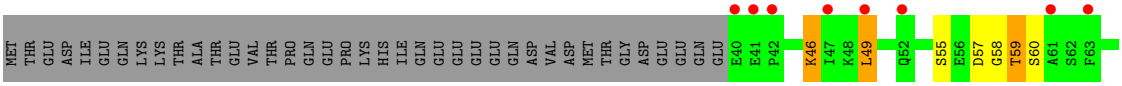
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

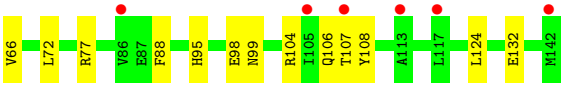
Chain J:



• Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2

Chain K:



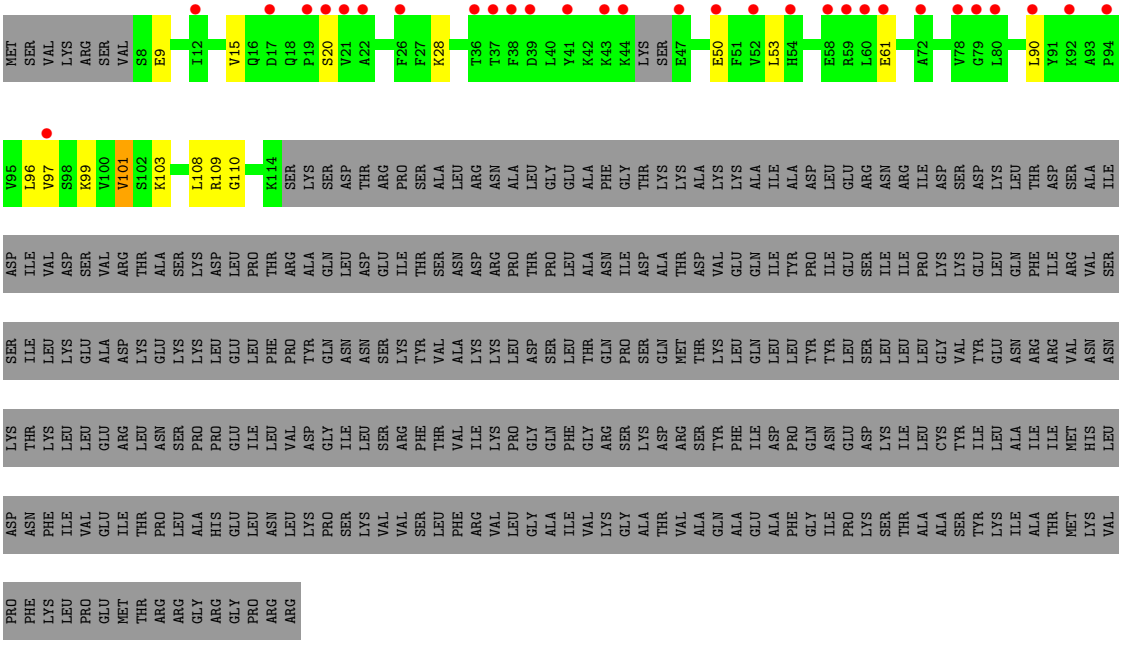


• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:

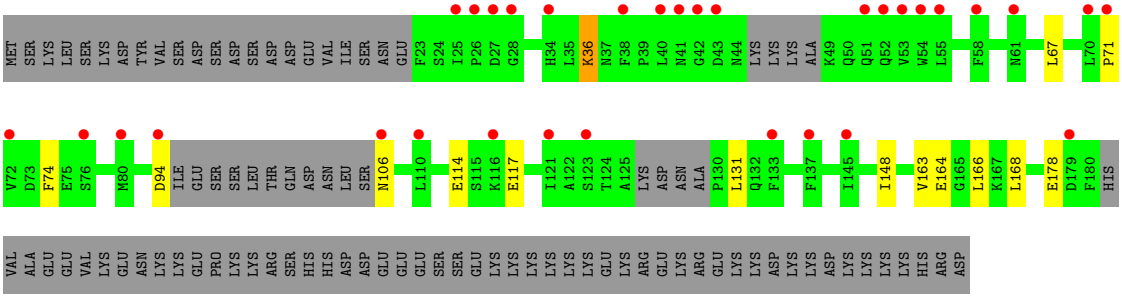
• Molecule 13: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49

Chain M:



• Molecule 14: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	425.24Å 140.62Å 139.72Å 90.00° 93.35° 90.00°	Depositor
Resolution (Å)	47.88 – 3.27 47.78 – 3.27	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.88-3.27) 97.7 (47.78-3.27)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.221 , 0.226 0.249 , 0.252	Depositor DCC
R_{free} test set	6209 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	135.5	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 101.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	34552	wwPDB-VP
Average B, all atoms (Å^2)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/12233	0.58	0/16523
2	B	0.41	0/9527	0.60	0/12879
3	C	0.40	0/2469	0.60	0/3347
4	D	0.39	0/472	0.52	0/639
5	E	0.41	0/1795	0.56	0/2416
6	F	0.40	0/838	0.54	0/1129
7	G	0.39	0/2094	0.58	0/2843
8	H	0.39	0/1090	0.57	0/1476
9	I	0.39	0/953	0.56	0/1282
10	J	0.41	0/578	0.62	0/775
11	K	0.39	0/821	0.59	0/1108
12	L	0.39	0/361	0.60	0/478
13	M	0.39	0/846	0.53	0/1136
14	N	0.39	0/1124	0.52	0/1512
All	All	0.40	0/35201	0.58	0/47543

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	12019	0	12051	127	0
2	B	9322	0	9187	92	0
3	C	2418	0	2401	21	0
4	D	466	0	466	3	0
5	E	1759	0	1788	8	0
6	F	823	0	841	6	0
7	G	2052	0	2016	15	0
8	H	1072	0	1042	6	0
9	I	942	0	928	14	0
10	J	569	0	585	12	0
11	K	810	0	801	12	0
12	L	359	0	381	1	0
13	M	831	0	820	10	0
14	N	1103	0	1106	6	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	34552	0	34413	272	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 4.

All (272) 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)
11:K:59:THR:HG22	11:K:107:THR:OG1	1.46	1.13
11:K:60:SER:OG	11:K:106:GLN:HG2	1.62	0.99
1:A:1382:VAL:HA	2:B:1070:ARG:NH1	1.78	0.97
2:B:99:VAL:HG21	2:B:417:ILE:HD11	1.58	0.85
3:C:222:VAL:HG21	3:C:225:ALA:HB2	1.68	0.75
2:B:16:PHE:HD2	2:B:978:ALA:HB2	1.53	0.73
1:A:86:TYR:H	1:A:431:GLN:HE22	1.36	0.73
1:A:432:ASN:HD21	1:A:444:GLN:H	1.38	0.71
1:A:824:THR:HG23	2:B:1023:ARG:HB2	1.72	0.71
1:A:712:ILE:H	11:K:106:GLN:HE22	1.39	0.70
1:A:1023:LEU:HB3	1:A:1190:SER:HB3	1.76	0.68
3:C:70:ILE:HG23	3:C:74:GLU:HB2	1.76	0.67
1:A:1265:GLU:HA	9:I:58:SER:HB3	1.78	0.66
2:B:524:SER:HB3	2:B:528:LEU:HB2	1.78	0.65
2:B:749:THR:O	10:J:52:THR:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:PRO:HB3	1:A:926:GLN:HE22	1.63	0.63
5:E:147:HIS:HD2	5:E:149:LEU:H	1.47	0.62
13:M:61:GLU:HB3	13:M:101:VAL:HG23	1.82	0.62
1:A:332:GLN:HE22	1:A:350:VAL:H	1.48	0.62
3:C:229:LEU:HB3	3:C:293:ARG:HG2	1.80	0.62
1:A:1382:VAL:HA	2:B:1070:ARG:HH11	1.61	0.61
2:B:558:VAL:HA	2:B:561:ILE:HD12	1.80	0.61
3:C:275:VAL:HG21	3:C:293:ARG:HH21	1.65	0.61
1:A:713:VAL:H	1:A:738:ASN:HD21	1.49	0.61
1:A:943:ILE:HG12	2:B:960:ILE:HD11	1.83	0.60
2:B:748:GLN:HB3	10:J:52:THR:HG22	1.83	0.60
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.84	0.60
2:B:1045:GLN:HB3	2:B:1063:ARG:HG3	1.83	0.59
1:A:581:ILE:HD11	1:A:605:VAL:HG21	1.84	0.59
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.84	0.59
2:B:211:ARG:HH22	2:B:243:GLN:HE22	1.51	0.58
1:A:701:ARG:H	1:A:706:HIS:HD2	1.49	0.58
1:A:1051:GLY:HA3	1:A:1580:ARG:HG2	1.85	0.58
1:A:1038:ILE:HB	1:A:1047:GLN:HB2	1.85	0.58
2:B:190:ILE:HD13	2:B:190:ILE:H	1.68	0.57
2:B:840:LEU:HD21	2:B:857:PRO:HB2	1.86	0.56
1:A:527:PRO:HG2	1:A:547:ILE:HA	1.86	0.56
2:B:839:LYS:HG3	2:B:857:PRO:HD2	1.86	0.56
10:J:48:ARG:O	10:J:52:THR:HB	2.05	0.56
1:A:952:LEU:HD21	1:A:1000:MET:HB3	1.88	0.56
1:A:15:ASP:HB2	2:B:1197:ARG:HB3	1.87	0.56
1:A:727:THR:HG22	1:A:730:GLN:HG3	1.87	0.56
1:A:438:ILE:HA	1:A:456:VAL:HG22	1.88	0.56
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.88	0.56
2:B:786:ALA:HB1	2:B:928:SER:HB2	1.87	0.56
1:A:1660:VAL:HB	7:G:57:PRO:HG3	1.87	0.55
2:B:857:PRO:HB3	2:B:871:ILE:HD13	1.89	0.55
3:C:232:GLN:HE21	3:C:234:ASN:HD21	1.55	0.55
1:A:1062:HIS:HA	1:A:1065:GLN:HB2	1.88	0.55
5:E:131:THR:HG21	5:E:191:LYS:HE2	1.89	0.54
2:B:323:ARG:HH22	2:B:351:GLN:HE22	1.56	0.54
1:A:1316:VAL:HG21	1:A:1498:ILE:HA	1.90	0.54
11:K:46:LYS:HA	11:K:66:VAL:HG22	1.89	0.54
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.89	0.54
1:A:701:ARG:H	1:A:706:HIS:CD2	2.25	0.54
3:C:91:VAL:HG11	10:J:60:PHE:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:ILE:HG12	10:J:2:ILE:HD11	1.89	0.54
1:A:438:ILE:HG23	2:B:1192:MET:HG2	1.89	0.53
2:B:52:LEU:HG	2:B:61:LEU:HD13	1.90	0.53
2:B:721:MET:HG3	2:B:1036:LEU:HD21	1.91	0.53
1:A:1382:VAL:HA	2:B:1070:ARG:HH12	1.71	0.53
1:A:1657:LEU:HD11	6:F:135:ARG:HB2	1.91	0.53
2:B:282:HIS:HD2	13:M:99:LYS:HD2	1.73	0.53
2:B:791:LYS:O	2:B:795:GLU:HG2	2.08	0.53
7:G:81:VAL:HA	7:G:124:VAL:HG12	1.91	0.53
13:M:9:GLU:HG2	14:N:71:PRO:HB3	1.89	0.53
1:A:970:LYS:HE2	2:B:685:VAL:HG21	1.90	0.52
13:M:28:LYS:HD2	14:N:106:ASN:HB2	1.91	0.52
1:A:381:SER:HB2	1:A:453:ILE:HG23	1.92	0.52
7:G:134:GLU:HB3	7:G:228:LYS:HE2	1.90	0.52
1:A:1056:ASP:HB3	1:A:1059:LYS:HD3	1.91	0.52
1:A:1239:THR:HB	1:A:1542:THR:HB	1.92	0.52
1:A:1501:ILE:HG23	1:A:1504:ILE:HB	1.91	0.52
2:B:748:GLN:HB2	2:B:769:PHE:HA	1.92	0.51
1:A:1378:THR:HB	2:B:1043:LYS:HG3	1.93	0.51
2:B:979:GLN:HG2	2:B:996:PHE:HE1	1.75	0.51
1:A:861:VAL:HG21	1:A:892:LEU:HA	1.92	0.51
1:A:1596:LEU:HD22	1:A:1602:GLY:HA2	1.91	0.51
2:B:293:ILE:HG12	2:B:302:LEU:HD23	1.92	0.51
2:B:574:SER:HB2	13:M:97:VAL:HG11	1.93	0.51
1:A:588:LEU:HB2	1:A:636:HIS:HB2	1.92	0.51
1:A:677:GLY:HA3	1:A:786:TYR:OH	2.10	0.51
10:J:2:ILE:HG23	10:J:57:ILE:HG21	1.92	0.51
7:G:51:PRO:HA	7:G:54:LEU:HD13	1.92	0.50
11:K:104:ARG:HD2	11:K:106:GLN:HG3	1.92	0.50
1:A:676:ALA:HB2	1:A:821:ILE:HD13	1.92	0.50
2:B:646:HIS:CD2	2:B:646:HIS:H	2.29	0.50
3:C:58:ASN:HA	3:C:296:ASN:HB3	1.92	0.50
9:I:112:TYR:HB2	9:I:121:PHE:HB3	1.92	0.50
1:A:1270:VAL:H	9:I:51:THR:HB	1.77	0.50
1:A:1478:ALA:HB1	9:I:21:ASN:HB3	1.92	0.50
3:C:333:ILE:HG22	11:K:49:LEU:HB2	1.93	0.50
7:G:50:ALA:H	7:G:64:GLN:HE22	1.58	0.50
1:A:518:GLU:HG3	6:F:115:THR:HG21	1.93	0.49
7:G:18:LYS:HA	7:G:21:LYS:HD2	1.93	0.49
1:A:19:LEU:HG	2:B:1195:ARG:HB2	1.94	0.49
10:J:68:LYS:HD3	10:J:69:ARG:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:LYS:HE2	1:A:922:CYS:HB3	1.94	0.49
1:A:986:PHE:HB2	2:B:960:ILE:HD12	1.94	0.49
1:A:37:VAL:HG12	1:A:49:LEU:HB2	1.95	0.49
1:A:1112:PRO:HD2	1:A:1115:LYS:HB2	1.95	0.49
2:B:731:VAL:HG21	10:J:59:LYS:HG2	1.94	0.49
13:M:53:LEU:HB2	13:M:96:LEU:HD22	1.93	0.49
2:B:252:TYR:HB2	2:B:381:LEU:HD21	1.95	0.49
7:G:14:ALA:HA	7:G:17:ILE:HD12	1.95	0.48
11:K:55:SER:HB2	11:K:60:SER:HB2	1.94	0.48
11:K:95:HIS:HB3	11:K:98:GLU:HG2	1.95	0.48
2:B:123:PRO:HG2	2:B:172:LEU:HD11	1.96	0.48
2:B:977:ILE:HD13	14:N:163:VAL:HG21	1.96	0.48
1:A:986:PHE:CB	2:B:960:ILE:HD12	2.44	0.48
2:B:700:LEU:HA	2:B:703:LEU:HD12	1.95	0.48
2:B:908:ARG:HD2	3:C:95:GLU:HG2	1.95	0.48
3:C:216:HIS:HD2	3:C:218:LYS:H	1.61	0.48
8:H:103:LYS:HB3	8:H:115:TYR:HB2	1.96	0.48
13:M:109:ARG:HG3	13:M:110:GLY:H	1.78	0.47
1:A:536:ILE:HD11	1:A:575:LYS:HD3	1.95	0.47
1:A:1038:ILE:HD12	1:A:1185:VAL:HG21	1.96	0.47
1:A:538:ASN:HA	1:A:575:LYS:HG2	1.97	0.47
1:A:1348:VAL:HG11	2:B:270:LEU:HD12	1.96	0.47
1:A:1263:LEU:HD22	1:A:1267:ILE:HD11	1.95	0.47
1:A:1382:VAL:CA	2:B:1070:ARG:NH1	2.66	0.47
2:B:375:LEU:HA	2:B:378:ILE:HD12	1.96	0.47
2:B:823:GLN:HG2	2:B:863:ASP:HB3	1.96	0.47
1:A:952:LEU:HD23	1:A:1004:GLU:HG3	1.96	0.47
2:B:19:LEU:HD11	10:J:26:GLN:HG2	1.96	0.47
1:A:862:THR:HA	9:I:67:VAL:HG12	1.97	0.47
1:A:1039:ARG:HD2	1:A:1045:LEU:HA	1.95	0.47
2:B:110:ASN:HB3	2:B:118:GLU:HG2	1.95	0.47
2:B:362:LEU:HD22	2:B:369:ASP:HB3	1.96	0.47
2:B:740:LYS:HA	2:B:804:TYR:O	2.15	0.47
1:A:836:THR:HG23	1:A:839:GLY:H	1.79	0.47
2:B:656:LEU:HB3	14:N:148:ILE:HG12	1.96	0.47
3:C:236:LEU:HD11	3:C:290:LYS:HG3	1.97	0.47
1:A:1610:PHE:CD2	1:A:1632:GLU:HG2	2.50	0.46
1:A:700:ILE:HD11	1:A:735:VAL:HA	1.97	0.46
2:B:916:LYS:HB3	2:B:1036:LEU:HD12	1.97	0.46
5:E:4:GLU:HG2	5:E:7:ARG:HH12	1.81	0.46
1:A:1288:ARG:HB2	1:A:1476:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ILE:HG21	1:A:49:LEU:HD13	1.97	0.46
1:A:124:LEU:HD21	1:A:189:VAL:HA	1.97	0.46
8:H:107:VAL:O	8:H:111:LEU:HB2	2.15	0.46
1:A:879:LEU:HA	1:A:882:ILE:HD12	1.97	0.46
6:F:128:LYS:HD2	6:F:149:GLU:HA	1.98	0.46
1:A:537:GLN:HB2	1:A:578:TYR:HE1	1.81	0.46
1:A:862:THR:OG1	1:A:878:ARG:HB3	2.15	0.46
2:B:103:SER:HB3	2:B:138:LEU:HB2	1.98	0.46
2:B:748:GLN:HB3	10:J:52:THR:CG2	2.46	0.46
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.98	0.45
1:A:1196:PRO:HB2	1:A:1575:ILE:HG21	1.97	0.45
1:A:862:THR:HG21	1:A:875:LEU:HD12	1.97	0.45
1:A:1032:VAL:HG21	1:A:1179:ILE:HG12	1.99	0.45
1:A:1275:THR:HG23	1:A:1289:SER:HB2	1.97	0.45
9:I:8:ILE:HG23	9:I:17:LEU:HB2	1.98	0.45
1:A:502:ALA:HA	1:A:581:ILE:CG2	2.46	0.45
1:A:1009:THR:HG21	9:I:102:ARG:HA	1.99	0.45
1:A:727:THR:H	1:A:730:GLN:HE21	1.63	0.45
1:A:1658:ALA:HB2	7:G:107:ILE:HD11	1.98	0.45
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.99	0.45
1:A:1634:LEU:HD13	1:A:1643:VAL:HG11	1.99	0.45
3:C:110:PRO:C	3:C:112:MET:H	2.20	0.45
7:G:30:GLU:HG2	7:G:32:ASN:HB2	1.99	0.45
1:A:1038:ILE:HD11	1:A:1050:TYR:HB2	1.99	0.44
2:B:561:ILE:HG12	2:B:620:LEU:HD12	1.99	0.44
5:E:56:LYS:HE2	5:E:84:ASP:H	1.81	0.44
5:E:120:ALA:HA	5:E:123:LEU:HD12	1.99	0.44
11:K:59:THR:CG2	11:K:108:TYR:O	2.65	0.44
1:A:671:GLN:HE22	2:B:784:ASP:HB2	1.82	0.44
1:A:1055:ILE:HD11	1:A:1174:TYR:CE2	2.52	0.44
3:C:192:LEU:HD21	3:C:195:LYS:HE3	1.97	0.44
1:A:456:VAL:HG21	2:B:1192:MET:HG3	2.00	0.44
1:A:1261:VAL:HG11	1:A:1308:VAL:HG21	2.00	0.44
2:B:721:MET:O	2:B:725:THR:HG23	2.18	0.44
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.98	0.44
6:F:107:VAL:HG12	6:F:109:VAL:H	1.83	0.44
1:A:126:GLN:HB3	1:A:343:PRO:HD3	1.98	0.44
1:A:1029:GLY:HA3	1:A:1041:ALA:HB2	1.99	0.44
1:A:1017:GLY:HA3	1:A:1385:ASP:HB2	2.00	0.44
2:B:65:VAL:HA	2:B:68:ILE:HG12	1.99	0.44
1:A:438:ILE:HD12	2:B:1192:MET:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:SER:HB3	9:I:81:THR:H	1.83	0.43
1:A:1626:VAL:HG21	2:B:1194:ILE:HG12	2.00	0.43
2:B:788:ILE:HB	2:B:948:ILE:HB	2.00	0.43
2:B:940:GLU:OE2	3:C:228:ARG:HB2	2.17	0.43
1:A:7:VAL:HG21	2:B:1177:ALA:HB2	2.01	0.43
1:A:692:TYR:O	1:A:696:ILE:HG12	2.19	0.43
2:B:129:ARG:HA	2:B:888:ILE:HG21	1.99	0.43
3:C:229:LEU:HD21	3:C:295:ARG:HA	2.00	0.43
9:I:72:LYS:HB2	9:I:75:GLU:HB2	2.01	0.43
1:A:1481:GLU:HB2	1:A:1482:LYS:H	1.72	0.43
1:A:1640:ARG:HH11	1:A:1648:ASN:HB3	1.83	0.43
2:B:300:SER:HB3	9:I:49:THR:HG22	2.00	0.43
3:C:113:LEU:HD11	3:C:132:ILE:HD12	1.99	0.43
2:B:301:PHE:O	2:B:305:ARG:HG2	2.18	0.43
1:A:1550:LEU:HD12	1:A:1555:VAL:HA	2.01	0.43
2:B:15:ASP:HA	2:B:978:ALA:HB3	2.01	0.43
1:A:387:SER:HA	1:A:390:LEU:HD12	2.01	0.43
2:B:612:LYS:HD3	2:B:626:ILE:HD11	2.01	0.43
2:B:1097:ASP:OD2	2:B:1181:VAL:HG22	2.19	0.43
1:A:1238:MET:HB2	1:A:1521:THR:HB	2.01	0.43
1:A:1613:MET:HE3	1:A:1622:LEU:HD13	2.00	0.43
2:B:13:THR:HG21	2:B:977:ILE:HB	2.00	0.43
2:B:480:GLN:HE21	2:B:508:PHE:H	1.65	0.43
2:B:526:GLY:HA2	2:B:696:ILE:HA	2.01	0.43
13:M:20:SER:HB3	14:N:36:LYS:HB2	2.01	0.43
1:A:646:GLU:HB3	2:B:1084:THR:OG1	2.19	0.42
7:G:264:ARG:H	7:G:267:ALA:HB3	1.84	0.42
9:I:52:ALA:C	9:I:54:ASP:H	2.22	0.42
2:B:249:VAL:HB	2:B:261:ARG:HB3	2.01	0.42
13:M:9:GLU:HA	14:N:71:PRO:HA	2.01	0.42
2:B:714:ARG:NH2	9:I:100:GLN:HE22	2.17	0.42
1:A:1494:ARG:H	1:A:1494:ARG:HG2	1.71	0.42
7:G:47:VAL:HG21	7:G:61:VAL:HG13	2.00	0.42
9:I:27:ASN:HA	9:I:38:PRO:HD3	2.00	0.42
1:A:128:GLY:H	1:A:207:SER:HB3	1.84	0.42
1:A:1655:ASP:HB2	6:F:135:ARG:HB3	2.01	0.42
3:C:195:LYS:HB3	10:J:61:LEU:HD11	2.01	0.42
1:A:490:ILE:HG22	1:A:606:ARG:HD3	2.01	0.42
1:A:591:ARG:HB2	1:A:633:MET:HG2	2.00	0.42
1:A:970:LYS:HG2	1:A:971:PRO:HD2	2.02	0.42
2:B:880:ALA:HB2	2:B:907:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:PRO:HG2	4:D:22:ILE:HD11	2.02	0.42
8:H:40:LEU:HB2	8:H:123:MET:HG3	2.02	0.42
11:K:59:THR:HG21	11:K:108:TYR:O	2.20	0.42
1:A:913:PRO:HD3	9:I:83:LYS:HE3	2.02	0.42
2:B:600:GLN:HA	2:B:603:ILE:HD12	2.02	0.42
7:G:66:LEU:HD11	7:G:87:LEU:HD13	2.02	0.42
1:A:855:ARG:HH21	1:A:867:ASP:HB3	1.85	0.42
1:A:1229:ALA:CB	1:A:1597:ALA:HB2	2.50	0.41
1:A:1459:LYS:HB2	1:A:1473:LYS:HB2	2.02	0.41
3:C:229:LEU:HD23	3:C:293:ARG:HB3	2.02	0.41
1:A:396:ILE:HG12	1:A:426:ALA:HB1	2.01	0.41
1:A:1121:ASP:HA	5:E:207:ARG:HH22	1.84	0.41
2:B:936:MET:HG3	2:B:937:PRO:HD2	2.01	0.41
1:A:536:ILE:HG23	1:A:544:VAL:HB	2.02	0.41
1:A:1554:GLY:HA2	5:E:183:PRO:HD2	2.02	0.41
2:B:61:LEU:HD21	2:B:413:LEU:HD13	2.01	0.41
2:B:403:LEU:HD21	2:B:408:LEU:HD13	2.02	0.41
5:E:141:VAL:HG12	5:E:142:VAL:HG23	2.02	0.41
1:A:765:LEU:HD12	8:H:122:LEU:HD13	2.03	0.41
1:A:885:ASP:HB3	1:A:888:LYS:HB2	2.02	0.41
1:A:233:CYS:HB3	1:A:236:CYS:O	2.20	0.41
2:B:358:VAL:HG13	2:B:370:LYS:HD3	2.02	0.41
11:K:57:ASP:HA	11:K:58:GLY:HA2	1.84	0.41
2:B:858:ILE:HD12	2:B:858:ILE:HA	1.99	0.41
4:D:30:HIS:HA	7:G:39:VAL:HG23	2.02	0.41
6:F:112:GLU:H	6:F:112:GLU:HG2	1.76	0.41
3:C:233:ILE:HB	3:C:267:VAL:HG11	2.03	0.41
1:A:385:LEU:HD13	1:A:437:PHE:HA	2.02	0.41
1:A:657:TYR:HA	1:A:667:ARG:HG3	2.01	0.41
1:A:805:VAL:O	1:A:809:VAL:HG23	2.20	0.41
2:B:71:LYS:HG3	2:B:421:LEU:HB3	2.03	0.41
2:B:840:LEU:HA	2:B:846:PRO:HA	2.03	0.41
2:B:1084:THR:O	2:B:1084:THR:HG23	2.21	0.41
7:G:107:ILE:HA	7:G:114:GLY:HA2	2.03	0.41
1:A:98:LEU:HD13	1:A:320:VAL:HG13	2.03	0.41
1:A:966:LEU:HB2	1:A:969:PHE:HD2	1.86	0.41
2:B:207:ILE:HB	2:B:505:ARG:HA	2.03	0.41
12:L:28:LYS:HB2	12:L:59:ALA:HB3	2.02	0.41
13:M:15:VAL:HG12	13:M:90:LEU:HB2	2.03	0.41
1:A:727:THR:HG21	8:H:119:GLY:O	2.21	0.40
2:B:260:PHE:HB3	2:B:271:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:HIS:HD2	2:B:1091:ARG:HH21	1.70	0.40
2:B:211:ARG:HH22	2:B:243:GLN:NE2	2.18	0.40
1:A:125:LEU:HD12	1:A:219:LEU:HD12	2.03	0.40
1:A:502:ALA:HA	1:A:581:ILE:HG22	2.04	0.40
1:A:857:ALA:HB2	1:A:899:LYS:HD2	2.04	0.40
1:A:1053:ASP:HB2	1:A:1174:TYR:OH	2.21	0.40
1:A:1380:GLN:H	1:A:1380:GLN:HG2	1.74	0.40
1:A:1660:VAL:HA	1:A:1661:PRO:HD3	1.96	0.40
3:C:175:GLN:HB3	3:C:178:THR:HG22	2.03	0.40
4:D:24:ALA:HA	7:G:43:ILE:HG22	2.03	0.40
8:H:35:GLN:HB3	8:H:111:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1503/1664 (90%)	1421 (94%)	78 (5%)	4 (0%)	41 72
2	B	1166/1203 (97%)	1095 (94%)	67 (6%)	4 (0%)	41 72
3	C	300/335 (90%)	283 (94%)	17 (6%)	0	100 100
4	D	55/137 (40%)	52 (94%)	3 (6%)	0	100 100
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100 100
6	F	98/155 (63%)	96 (98%)	2 (2%)	0	100 100
7	G	251/326 (77%)	232 (92%)	17 (7%)	2 (1%)	19 52
8	H	130/146 (89%)	119 (92%)	11 (8%)	0	100 100
9	I	118/125 (94%)	104 (88%)	12 (10%)	2 (2%)	9 37
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100 100
11	K	101/142 (71%)	95 (94%)	5 (5%)	1 (1%)	15 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	43/70 (61%)	40 (93%)	3 (7%)	0	100	100
13	M	101/415 (24%)	94 (93%)	7 (7%)	0	100	100
14	N	131/233 (56%)	122 (93%)	9 (7%)	0	100	100
All	All	4277/5236 (82%)	4017 (94%)	247 (6%)	13 (0%)	41	72

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1385	ASP
1	A	237	GLY
1	A	1389	GLU
2	B	1154	ASP
9	I	78	ASP
11	K	46	LYS
2	B	532	HIS
1	A	1386	GLU
2	B	359	LEU
9	I	102	ARG
2	B	339	GLN
7	G	173	VAL
7	G	127	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	1343/1465 (92%)	1271 (95%)	72 (5%)	22	53
2	B	1024/1053 (97%)	927 (90%)	97 (10%)	8	29
3	C	269/296 (91%)	242 (90%)	27 (10%)	7	28
4	D	56/116 (48%)	50 (89%)	6 (11%)	6	25
5	E	197/197 (100%)	192 (98%)	5 (2%)	47	72
6	F	90/137 (66%)	86 (96%)	4 (4%)	28	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	G	234/291 (80%)	219 (94%)	15 (6%)	17 47
8	H	116/128 (91%)	111 (96%)	5 (4%)	29 59
9	I	109/110 (99%)	99 (91%)	10 (9%)	9 31
10	J	64/65 (98%)	56 (88%)	8 (12%)	4 19
11	K	93/130 (72%)	86 (92%)	7 (8%)	13 39
12	L	40/57 (70%)	37 (92%)	3 (8%)	13 39
13	M	94/371 (25%)	90 (96%)	4 (4%)	29 59
14	N	128/220 (58%)	117 (91%)	11 (9%)	10 34
All	All	3857/4636 (83%)	3583 (93%)	274 (7%)	14 42

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	39	ASP
1	A	89	LEU
1	A	113	VAL
1	A	129	LEU
1	A	136	LEU
1	A	177	LEU
1	A	195	LYS
1	A	199	ASP
1	A	211	THR
1	A	270	ILE
1	A	325	ASP
1	A	345	LEU
1	A	361	VAL
1	A	373	LEU
1	A	398	ASP
1	A	399	LEU
1	A	403	LEU
1	A	406	LEU
1	A	413	LEU
1	A	518	GLU
1	A	536	ILE
1	A	562	LEU
1	A	572	THR
1	A	586	VAL
1	A	587	VAL

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Mol	Chain	Res	Type
1	A	684	ASP
1	A	743	ASP
1	A	747	ILE
1	A	831	ASP
1	A	840	ASN
1	A	844	THR
1	A	862	THR
1	A	878	ARG
1	A	952	LEU
1	A	960	MET
1	A	1012	LYS
1	A	1065	GLN
1	A	1089	LEU
1	A	1164	LYS
1	A	1171	GLN
1	A	1175	MET
1	A	1179	ILE
1	A	1183	GLU
1	A	1202	LEU
1	A	1205	PHE
1	A	1217	LEU
1	A	1242	ILE
1	A	1248	ASP
1	A	1252	ASP
1	A	1263	LEU
1	A	1268	ASP
1	A	1273	THR
1	A	1313	LEU
1	A	1343	ASP
1	A	1380	GLN
1	A	1389	GLU
1	A	1396	ARG
1	A	1438	ASN
1	A	1474	LEU
1	A	1475	GLU
1	A	1481	GLU
1	A	1501	ILE
1	A	1505	ASP
1	A	1531	ASP
1	A	1533	GLU
1	A	1552	THR
1	A	1592	GLN

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Mol	Chain	Res	Type
1	A	1609	SER
1	A	1628	ASP
1	A	1629	ASN
1	A	1649	VAL
2	B	13	THR
2	B	15	ASP
2	B	17	ARG
2	B	19	LEU
2	B	22	GLU
2	B	35	PHE
2	B	52	LEU
2	B	54	GLU
2	B	60	LEU
2	B	73	ILE
2	B	101	GLN
2	B	108	MET
2	B	139	LEU
2	B	150	GLU
2	B	156	ARG
2	B	168	ASN
2	B	186	GLU
2	B	190	ILE
2	B	202	LEU
2	B	206	LEU
2	B	212	ASN
2	B	217	ILE
2	B	234	ILE
2	B	250	LEU
2	B	265	ARG
2	B	268	GLU
2	B	274	VAL
2	B	276	ILE
2	B	304	ASP
2	B	306	LEU
2	B	316	ARG
2	B	332	ASP
2	B	356	ARG
2	B	364	LYS
2	B	373	MET
2	B	374	LEU
2	B	381	LEU
2	B	413	LEU

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Mol	Chain	Res	Type
2	B	431	ASP
2	B	438	ILE
2	B	441	LYS
2	B	455	GLU
2	B	471	VAL
2	B	479	GLN
2	B	480	GLN
2	B	481	VAL
2	B	485	THR
2	B	517	VAL
2	B	519	LYS
2	B	542	LEU
2	B	550	ARG
2	B	588	ILE
2	B	617	THR
2	B	640	LEU
2	B	646	HIS
2	B	684	ASN
2	B	692	THR
2	B	721	MET
2	B	743	ARG
2	B	752	VAL
2	B	782	ASP
2	B	787	MET
2	B	789	ILE
2	B	794	ASP
2	B	821	ILE
2	B	832	TRP
2	B	835	GLU
2	B	840	LEU
2	B	842	GLU
2	B	848	ILE
2	B	859	CYS
2	B	873	THR
2	B	887	LEU
2	B	888	ILE
2	B	896	GLN
2	B	897	GLU
2	B	898	LEU
2	B	933	THR
2	B	940	GLU
2	B	944	GLN

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Mol	Chain	Res	Type
2	B	956	SER
2	B	965	GLU
2	B	967	LEU
2	B	977	ILE
2	B	994	ASP
2	B	1000	LEU
2	B	1020	GLU
2	B	1033	TYR
2	B	1037	ARG
2	B	1041	ASN
2	B	1065	ARG
2	B	1076	ARG
2	B	1110	ILE
2	B	1123	ILE
2	B	1157	GLN
2	B	1181	VAL
2	B	1201	GLU
3	C	30	GLU
3	C	39	ASP
3	C	46	SER
3	C	47	LEU
3	C	81	GLU
3	C	89	THR
3	C	94	ASP
3	C	97	LEU
3	C	106	LEU
3	C	117	ASP
3	C	120	LEU
3	C	151	THR
3	C	181	ASP
3	C	182	CYS
3	C	188	ASP
3	C	209	ILE
3	C	224	THR
3	C	229	LEU
3	C	235	ILE
3	C	240	LYS
3	C	259	ASP
3	C	263	ASP
3	C	277	ARG
3	C	291	LEU
3	C	303	GLU

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Mol	Chain	Res	Type
3	C	331	CYS
3	C	334	THR
4	D	14	THR
4	D	16	LEU
4	D	21	VAL
4	D	25	THR
4	D	27	LEU
4	D	89	LEU
5	E	84	ASP
5	E	106	GLN
5	E	163	GLU
5	E	167	ARG
5	E	175	LEU
6	F	69	LEU
6	F	103	MET
6	F	111	LEU
6	F	147	SER
7	G	22	LYS
7	G	32	ASN
7	G	75	ASN
7	G	93	ASP
7	G	95	LEU
7	G	104	LEU
7	G	144	HIS
7	G	174	GLU
7	G	214	LEU
7	G	217	TRP
7	G	223	GLU
7	G	248	THR
7	G	303	ASP
7	G	315	SER
7	G	316	GLU
8	H	33	GLN
8	H	53	ASP
8	H	89	LEU
8	H	109	LYS
8	H	136	LYS
9	I	24	LEU
9	I	47	VAL
9	I	51	THR
9	I	53	ASP
9	I	60	LEU

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Mol	Chain	Res	Type
9	I	66	VAL
9	I	71	LEU
9	I	73	LYS
9	I	81	THR
9	I	83	LYS
10	J	2	ILE
10	J	14	VAL
10	J	22	LEU
10	J	26	GLN
10	J	32	GLU
10	J	47	ARG
10	J	48	ARG
10	J	68	LYS
11	K	49	LEU
11	K	59	THR
11	K	72	LEU
11	K	77	ARG
11	K	99	ASN
11	K	124	LEU
11	K	132	GLU
12	L	27	LEU
12	L	38	LEU
12	L	62	LYS
13	M	50	GLU
13	M	101	VAL
13	M	103	LYS
13	M	108	LEU
14	N	36	LYS
14	N	67	LEU
14	N	74	PHE
14	N	94	ASP
14	N	114	GLU
14	N	117	GLU
14	N	131	LEU
14	N	164	GLU
14	N	166	LEU
14	N	168	LEU
14	N	178	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	332	GLN
1	A	431	GLN
1	A	432	ASN
1	A	580	HIS
1	A	590	ASN
1	A	592	GLN
1	A	636	HIS
1	A	671	GLN
1	A	693	GLN
1	A	706	HIS
1	A	730	GLN
1	A	738	ASN
1	A	926	GLN
1	A	937	ASN
1	A	1026	GLN
1	A	1036	ASN
1	A	1113	HIS
1	A	1128	ASN
1	A	1380	GLN
1	A	1599	ASN
1	A	1620	GLN
2	B	146	ASN
2	B	151	ASN
2	B	212	ASN
2	B	243	GLN
2	B	251	HIS
2	B	351	GLN
2	B	361	HIS
2	B	400	GLN
2	B	480	GLN
2	B	646	HIS
2	B	686	HIS
2	B	695	ASN
2	B	755	ASN
2	B	896	GLN
2	B	975	HIS
2	B	987	ASN
2	B	999	GLN
2	B	1041	ASN
2	B	1053	ASN
2	B	1114	GLN
3	C	130	ASN

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Mol	Chain	Res	Type
3	C	232	GLN
4	D	30	HIS
5	E	147	HIS
5	E	179	GLN
7	G	20	HIS
7	G	26	ASN
7	G	32	ASN
7	G	64	GLN
7	G	65	HIS
7	G	128	GLN
7	G	140	GLN
7	G	150	HIS
8	H	35	GLN
9	I	91	ASN
9	I	100	GLN
10	J	64	ASN
11	K	106	GLN
13	M	16	GLN
14	N	132	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	65:SER	C	66:VAL	N	3.24
1	I	51:THR	C	52:ALA	N	2.96

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1523/1664 (91%)	0.28	56 (3%) 41 39	110, 151, 210, 241	0
2	B	1176/1203 (97%)	0.46	59 (5%) 28 27	111, 155, 215, 239	0
3	C	304/335 (90%)	0.38	18 (5%) 22 22	147, 180, 216, 228	0
4	D	59/137 (43%)	0.11	5 (8%) 10 11	154, 230, 241, 253	0
5	E	215/215 (100%)	0.26	13 (6%) 21 21	131, 191, 235, 241	0
6	F	100/155 (64%)	0.00	0 100 100	121, 155, 195, 205	0
7	G	259/326 (79%)	0.56	29 (11%) 5 5	135, 213, 249, 261	0
8	H	134/146 (91%)	0.81	25 (18%) 1 1	153, 190, 223, 233	0
9	I	124/125 (99%)	0.18	5 (4%) 38 36	130, 171, 227, 234	0
10	J	69/70 (98%)	0.17	0 100 100	144, 160, 191, 218	0
11	K	103/142 (72%)	0.50	14 (13%) 3 3	133, 180, 208, 231	0
12	L	45/70 (64%)	-0.12	0 100 100	157, 192, 219, 224	0
13	M	105/415 (25%)	1.30	30 (28%) 0 0	214, 235, 251, 258	0
14	N	139/233 (59%)	1.13	32 (23%) 0 1	152, 236, 266, 275	0
All	All	4355/5236 (83%)	0.41	286 (6%) 18 18	110, 165, 235, 275	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	N	27	ASP	7.7
1	A	706	HIS	7.6
13	M	22	ALA	6.5
14	N	121	ILE	6.2
13	M	17	ASP	6.2
2	B	440	PHE	5.8
14	N	54	TRP	5.7
8	H	125	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
2	B	830	ASP	5.3
14	N	28	GLY	5.2
1	A	1340	THR	5.1
2	B	152	LEU	5.1
14	N	72	VAL	5.1
14	N	43	ASP	5.0
7	G	172	ASP	5.0
3	C	256	ILE	5.0
1	A	1479	ASP	4.9
7	G	260	TYR	4.9
2	B	97	VAL	4.9
13	M	39	ASP	4.9
1	A	1480	THR	4.8
7	G	246	ASP	4.7
1	A	707	THR	4.7
2	B	141	LEU	4.6
1	A	1242	ILE	4.6
7	G	99	ASP	4.6
1	A	274	MET	4.5
1	A	1352	GLN	4.5
14	N	70	LEU	4.4
8	H	59	ILE	4.4
14	N	61	ASN	4.4
13	M	47	GLU	4.4
8	H	131	ASN	4.4
7	G	229	LEU	4.3
13	M	50	GLU	4.2
8	H	60	ALA	4.2
8	H	113	ALA	4.2
3	C	150	SER	4.1
2	B	578	ALA	4.1
14	N	26	PRO	4.1
13	M	44	LYS	4.0
2	B	12	ARG	4.0
1	A	1388	ASP	4.0
13	M	79	GLY	4.0
8	H	139	ASN	4.0
14	N	53	VAL	4.0
1	A	1204	THR	3.9
1	A	1350	ARG	3.9
11	K	63	PHE	3.9
1	A	1460	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
4	D	44	ILE	3.9
8	H	77	ARG	3.8
1	A	264	ASN	3.8
2	B	859	CYS	3.8
13	M	61	GLU	3.8
7	G	20	HIS	3.8
7	G	12	GLU	3.7
11	K	113	ALA	3.7
11	K	142	MET	3.7
2	B	227	ALA	3.7
3	C	248	GLN	3.7
5	E	93	MET	3.7
14	N	42	GLY	3.6
13	M	94	PRO	3.6
1	A	1335	LYS	3.6
14	N	41	ASN	3.5
7	G	217	TRP	3.5
3	C	181	ASP	3.5
1	A	1290	TYR	3.5
3	C	273	ASP	3.5
2	B	846	PRO	3.4
14	N	110	LEU	3.4
5	E	1	MET	3.4
14	N	25	ILE	3.4
2	B	785	ASP	3.4
1	A	1121	ASP	3.4
13	M	38	PHE	3.3
7	G	16	PHE	3.3
2	B	1120	ILE	3.3
11	K	105	ILE	3.3
7	G	135	GLY	3.3
13	M	37	THR	3.3
14	N	80	MET	3.3
14	N	133	PHE	3.3
7	G	140	GLN	3.2
5	E	49	SER	3.2
2	B	372	ARG	3.2
13	M	78	VAL	3.2
2	B	825	PHE	3.2
5	E	102	GLU	3.2
9	I	74	ASN	3.2
2	B	857	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1483	LEU	3.2
1	A	1470	CYS	3.1
2	B	658	LEU	3.1
13	M	59	ARG	3.1
1	A	1485	MET	3.1
8	H	134	ASN	3.1
13	M	54	HIS	3.1
11	K	41	GLU	3.0
4	D	36	VAL	3.0
2	B	153	PHE	3.0
1	A	1513	GLU	3.0
1	A	1472	PHE	3.0
8	H	75	ALA	3.0
8	H	112	ILE	3.0
2	B	861	TYR	3.0
3	C	253	PRO	3.0
14	N	137	PHE	3.0
1	A	675	SER	3.0
1	A	891	ILE	3.0
2	B	225	ARG	3.0
2	B	424	ILE	2.9
14	N	145	ILE	2.9
14	N	34	HIS	2.9
2	B	871	ILE	2.9
13	M	60	LEU	2.9
2	B	1043	LYS	2.9
3	C	247	PHE	2.9
11	K	49	LEU	2.9
4	D	92	ILE	2.9
11	K	117	LEU	2.9
14	N	106	ASN	2.9
13	M	43	LYS	2.8
2	B	13	THR	2.8
2	B	811	LEU	2.8
7	G	128	GLN	2.8
13	M	41	TYR	2.8
2	B	450	LEU	2.8
13	M	92	LYS	2.8
1	A	328	PHE	2.8
13	M	72	ALA	2.8
13	M	52	VAL	2.8
2	B	579	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
8	H	114	VAL	2.8
14	N	76	SER	2.8
2	B	858	ILE	2.7
7	G	170	HIS	2.7
2	B	865	THR	2.7
1	A	1349	PRO	2.7
8	H	126	GLU	2.7
7	G	262	SER	2.7
13	M	58	GLU	2.7
8	H	116	TYR	2.7
2	B	1069	ILE	2.7
14	N	51	GLN	2.7
2	B	143	TRP	2.7
1	A	100	ALA	2.7
8	H	96	VAL	2.7
1	A	972	TYR	2.7
8	H	127	GLY	2.7
1	A	108	PHE	2.7
14	N	116	LYS	2.7
2	B	80	ASN	2.6
2	B	590	GLY	2.6
3	C	261	GLY	2.6
1	A	375	GLU	2.6
7	G	142	ALA	2.6
8	H	142	LEU	2.6
2	B	864	ASP	2.6
2	B	438	ILE	2.6
7	G	82	LEU	2.6
2	B	620	LEU	2.6
2	B	1021	GLU	2.6
9	I	41	GLN	2.6
3	C	279	VAL	2.6
2	B	827	PHE	2.6
2	B	829	ASN	2.6
11	K	107	THR	2.6
4	D	40	LEU	2.6
14	N	55	LEU	2.6
5	E	50	MET	2.6
2	B	786	ALA	2.5
2	B	139	LEU	2.5
1	A	176	THR	2.5
2	B	511	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
13	M	19	PRO	2.5
3	C	289	VAL	2.5
3	C	67	PHE	2.5
9	I	39	LYS	2.5
1	A	141	LEU	2.5
2	B	933	THR	2.5
2	B	91	LEU	2.5
2	B	823	GLN	2.5
3	C	268	LYS	2.5
7	G	241	ARG	2.5
14	N	94	ASP	2.5
5	E	123	LEU	2.5
9	I	125	ASN	2.5
2	B	409	TYR	2.4
11	K	61	ALA	2.4
1	A	1474	LEU	2.4
14	N	40	LEU	2.4
1	A	118	TYR	2.4
2	B	809	VAL	2.4
7	G	168	PHE	2.4
7	G	269	SER	2.4
8	H	140	ALA	2.4
1	A	1131	LYS	2.4
7	G	245	VAL	2.4
3	C	54	PHE	2.4
7	G	265	SER	2.4
11	K	47	ILE	2.4
2	B	140	LYS	2.4
5	E	16	PHE	2.4
8	H	36	CYS	2.4
8	H	6	PHE	2.4
8	H	95	TYR	2.4
1	A	1398	ALA	2.4
8	H	132	LEU	2.4
13	M	20	SER	2.4
8	H	143	LEU	2.4
2	B	369	ASP	2.3
13	M	12	ILE	2.3
13	M	80	LEU	2.3
13	M	26	PHE	2.3
1	A	720	PHE	2.3
1	A	334	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1608	SER	2.3
7	G	149	ILE	2.3
5	E	51	GLY	2.3
7	G	264	ARG	2.3
2	B	767	ASN	2.3
2	B	1124	SER	2.3
7	G	231	PHE	2.3
11	K	40	GLU	2.3
13	M	90	LEU	2.3
8	H	35	GLN	2.3
11	K	86	VAL	2.3
1	A	1	MET	2.3
13	M	97	VAL	2.3
1	A	705	GLY	2.2
13	M	21	VAL	2.2
2	B	368	GLN	2.2
1	A	1270	VAL	2.2
2	B	154	GLU	2.2
2	B	975	HIS	2.2
7	G	270	LEU	2.2
2	B	845	LEU	2.2
3	C	134	LEU	2.2
2	B	860	ALA	2.2
3	C	270	ALA	2.2
1	A	1292	ILE	2.2
5	E	126	SER	2.2
14	N	123	SER	2.2
3	C	274	THR	2.2
7	G	143	SER	2.2
14	N	179	ASP	2.2
7	G	166	TRP	2.2
3	C	132	ILE	2.2
7	G	226	ASP	2.2
1	A	1094	ALA	2.1
1	A	635	MET	2.1
8	H	130	ARG	2.1
5	E	110	PHE	2.1
2	B	19	LEU	2.1
1	A	1648	ASN	2.1
5	E	58	MET	2.1
11	K	42	PRO	2.1
1	A	1089	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	939	SER	2.1
3	C	263	ASP	2.1
1	A	128	GLY	2.1
13	M	36	THR	2.1
1	A	710	SER	2.1
7	G	89	ILE	2.1
1	A	1476	LEU	2.1
9	I	118	GLY	2.1
11	K	52	GLN	2.1
1	A	824	THR	2.1
1	A	1397	GLU	2.1
8	H	57	VAL	2.1
1	A	97	TYR	2.0
5	E	172	GLU	2.0
14	N	71	PRO	2.0
5	E	119	SER	2.0
14	N	52	GLN	2.0
14	N	58	PHE	2.0
2	B	887	LEU	2.0
1	A	1294	MET	2.0
1	A	536	ILE	2.0
2	B	870	LYS	2.0
1	A	403	LEU	2.0
14	N	38	PHE	2.0
1	A	1471	GLU	2.0
4	D	88	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	ZN	I	1126	1/1	0.95	0.16	195,195,195,195	0
15	ZN	A	2664	1/1	0.96	0.12	182,182,182,182	0
15	ZN	L	1071	1/1	0.97	0.14	178,178,178,178	0
15	ZN	A	2665	1/1	0.98	0.13	137,137,137,137	0
15	ZN	I	1127	1/1	0.98	0.12	136,136,136,136	0
15	ZN	B	2204	1/1	0.98	0.17	144,144,144,144	0
15	ZN	J	1070	1/1	1.00	0.26	148,148,148,148	0

6.5 Other polymers (i)

There are no such residues in this entry.