Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 04:46 PM JST

PDB ID	:	5ZX2
Title	:	Mycobacterium tuberculosis RNA polymerase transcription initiation complex with ECF sigma factor sigma H and 7nt RNA
Authors	:	Li, L.; Zhang, Y.
Deposited on	:	2018-05-17
Resolution	:	2.80 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:

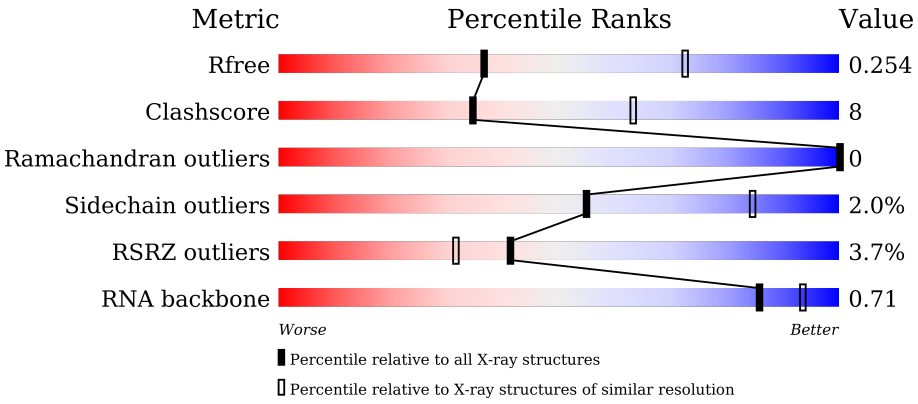
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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	368	48% 10% 42%
1	B	368	2% 46% 17% 36%
2	C	1174	4% 79% 18%
3	D	1317	3% 78% 17%

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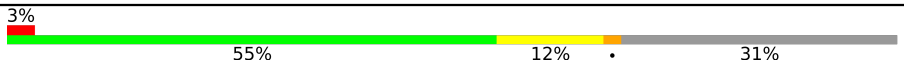
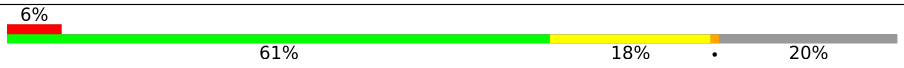
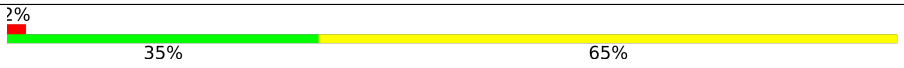
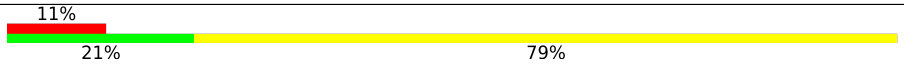
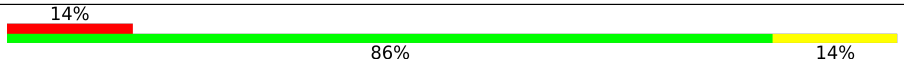
Mol	Chain	Length	Quality of chain
4	E	110	
5	F	218	
6	G	48	
7	H	47	
8	I	7	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 25858 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1622	1024	278	318	2			
1	B	234	Total	C	N	O	S	0	0	0
			1761	1108	304	346	3			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P9WGZ1
A	-19	GLY	-	expression tag	UNP P9WGZ1
A	-18	HIS	-	expression tag	UNP P9WGZ1
A	-17	HIS	-	expression tag	UNP P9WGZ1
A	-16	HIS	-	expression tag	UNP P9WGZ1
A	-15	HIS	-	expression tag	UNP P9WGZ1
A	-14	HIS	-	expression tag	UNP P9WGZ1
A	-13	HIS	-	expression tag	UNP P9WGZ1
A	-12	HIS	-	expression tag	UNP P9WGZ1
A	-11	HIS	-	expression tag	UNP P9WGZ1
A	-10	HIS	-	expression tag	UNP P9WGZ1
A	-9	HIS	-	expression tag	UNP P9WGZ1
A	-8	SER	-	expression tag	UNP P9WGZ1
A	-7	SER	-	expression tag	UNP P9WGZ1
A	-6	GLY	-	expression tag	UNP P9WGZ1
A	-5	HIS	-	expression tag	UNP P9WGZ1
A	-4	ILE	-	expression tag	UNP P9WGZ1
A	-3	GLU	-	expression tag	UNP P9WGZ1
A	-2	GLY	-	expression tag	UNP P9WGZ1
A	-1	ARG	-	expression tag	UNP P9WGZ1
A	0	HIS	-	expression tag	UNP P9WGZ1
B	-20	MET	-	expression tag	UNP P9WGZ1
B	-19	GLY	-	expression tag	UNP P9WGZ1
B	-18	HIS	-	expression tag	UNP P9WGZ1
B	-17	HIS	-	expression tag	UNP P9WGZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP P9WGZ1
B	-15	HIS	-	expression tag	UNP P9WGZ1
B	-14	HIS	-	expression tag	UNP P9WGZ1
B	-13	HIS	-	expression tag	UNP P9WGZ1
B	-12	HIS	-	expression tag	UNP P9WGZ1
B	-11	HIS	-	expression tag	UNP P9WGZ1
B	-10	HIS	-	expression tag	UNP P9WGZ1
B	-9	HIS	-	expression tag	UNP P9WGZ1
B	-8	SER	-	expression tag	UNP P9WGZ1
B	-7	SER	-	expression tag	UNP P9WGZ1
B	-6	GLY	-	expression tag	UNP P9WGZ1
B	-5	HIS	-	expression tag	UNP P9WGZ1
B	-4	ILE	-	expression tag	UNP P9WGZ1
B	-3	GLU	-	expression tag	UNP P9WGZ1
B	-2	GLY	-	expression tag	UNP P9WGZ1
B	-1	ARG	-	expression tag	UNP P9WGZ1
B	0	HIS	-	expression tag	UNP P9WGZ1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1137	Total	C	N	O	S	0	0	0
			8611	5393	1512	1667	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	MET	-	expression tag	UNP P9WGY9
C	6	VAL	-	expression tag	UNP P9WGY9

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1260	Total	C	N	O	S	0	0	0
			9769	6123	1774	1832	40			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	expression tag	UNP P9WGY7
D	1	VAL	-	expression tag	UNP P9WGY7

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	76	Total	C	N	O	0	0	0
			600	383	101	116			

- Molecule 5 is a protein called ECF RNA polymerase sigma factor SigH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	175	Total	C	N	O	S	0	0	0
			1381	866	244	266	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP P9WGH9
F	0	ALA	-	expression tag	UNP P9WGH9

- Molecule 6 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	48	Total	C	N	O	P	0	0	0
			976	464	177	288	47			

- Molecule 7 is a DNA chain called DNA (47-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	47	Total	C	N	O	P	0	0	0
			948	450	175	277	46			

- Molecule 8 is a RNA chain called RNA (5'-R(*CP*CP*CP*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	7	Total	C	N	O	P	0	0	0
			141	65	24	46	6			

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		

- Molecule 10 is water.

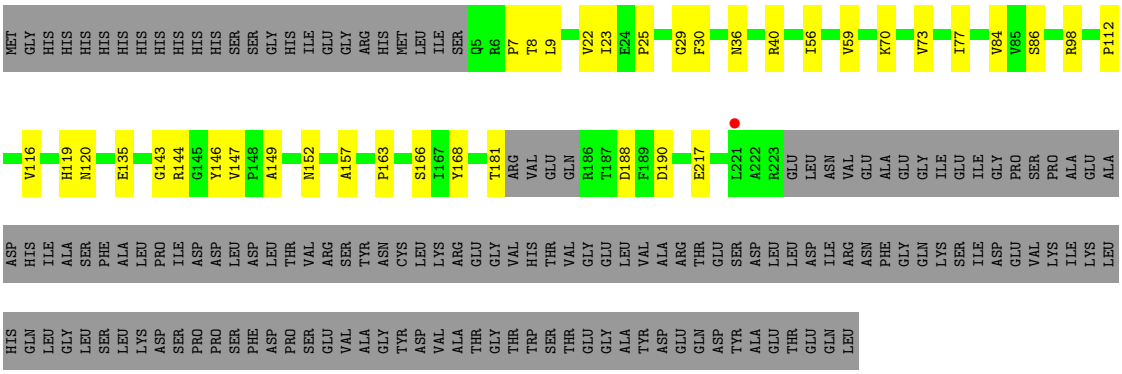
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	2	Total O 2 2	0	0
10	C	24	Total O 24 24	0	0
10	D	17	Total O 17 17	0	0
10	E	1	Total O 1 1	0	0
10	F	3	Total O 3 3	0	0

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.

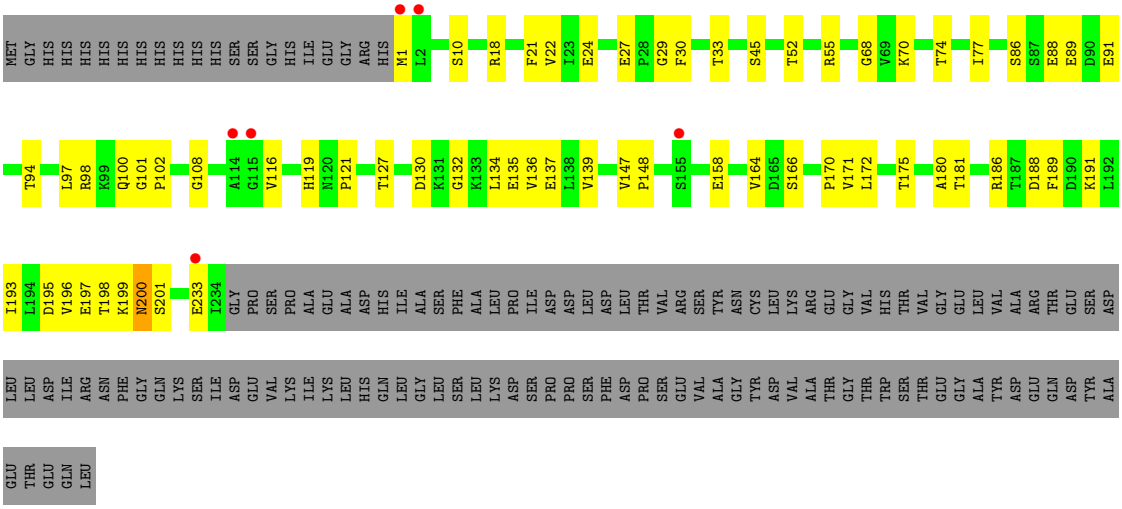
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



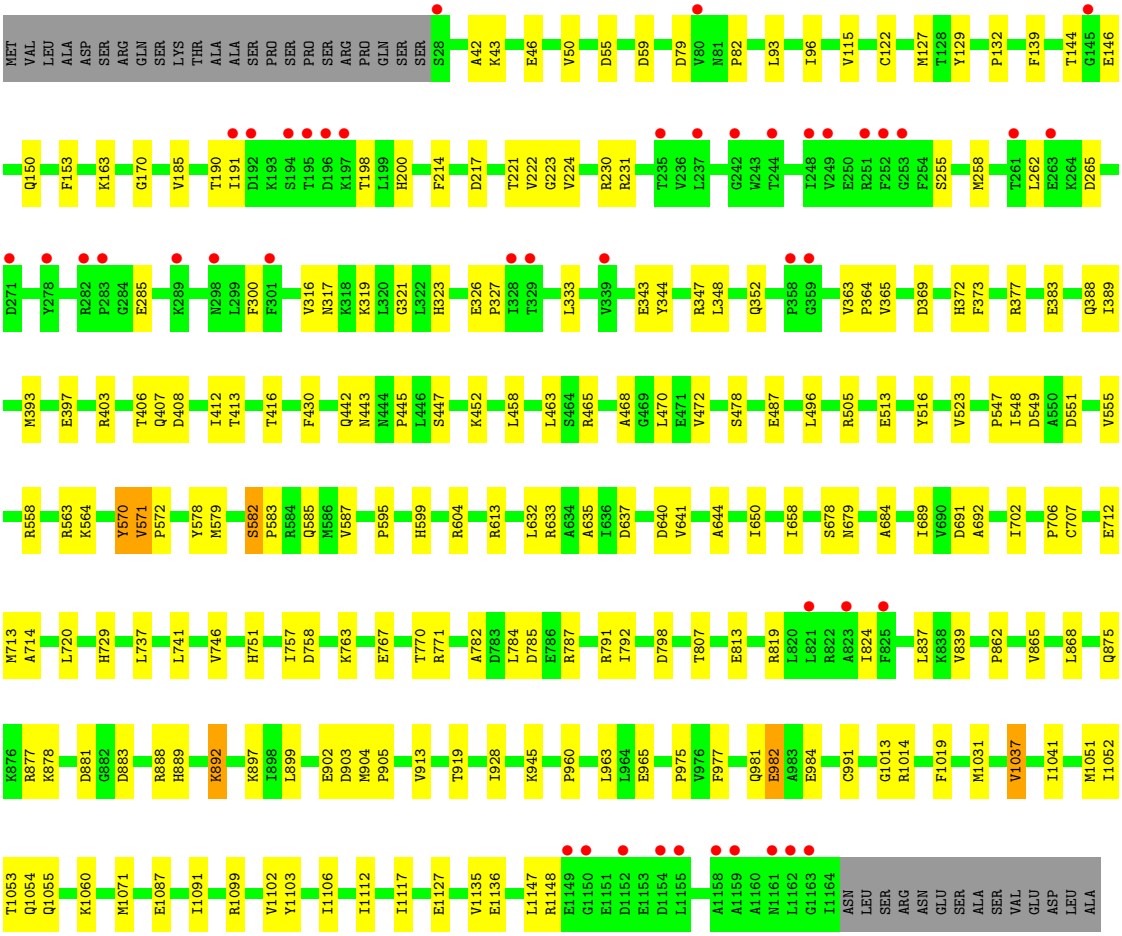
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



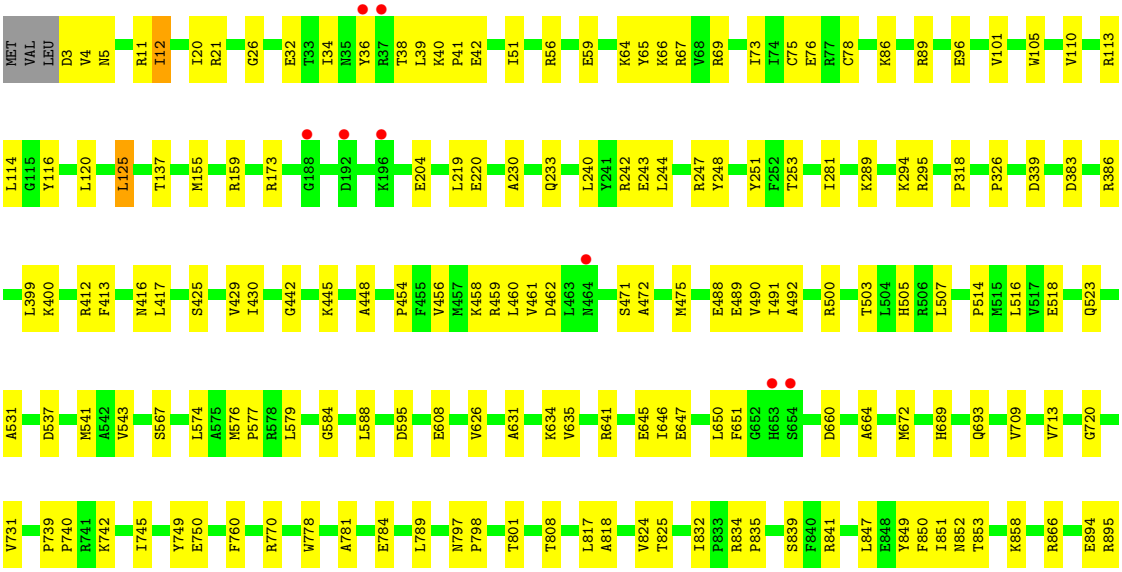
• Molecule 2: DNA-directed RNA polymerase subunit beta

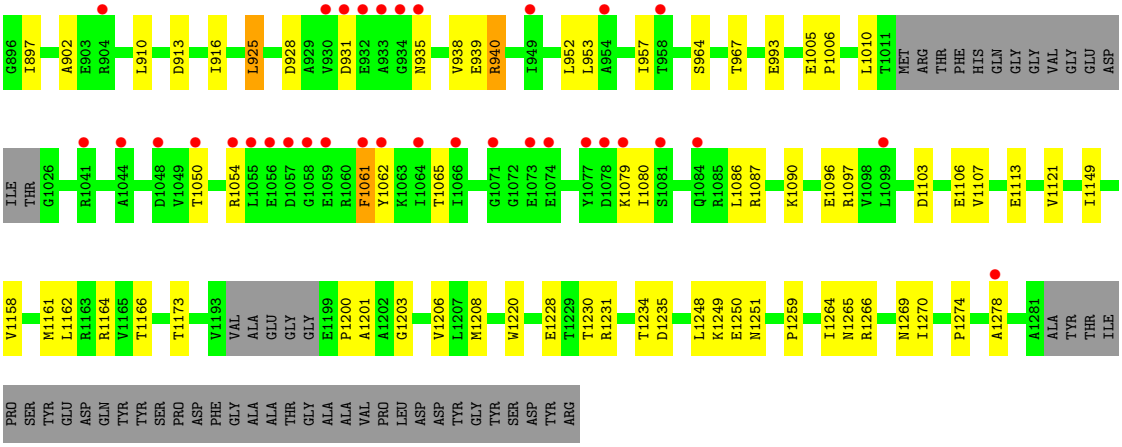
Chain C:



• Molecule 3: DNA-directed RNA polymerase subunit beta'

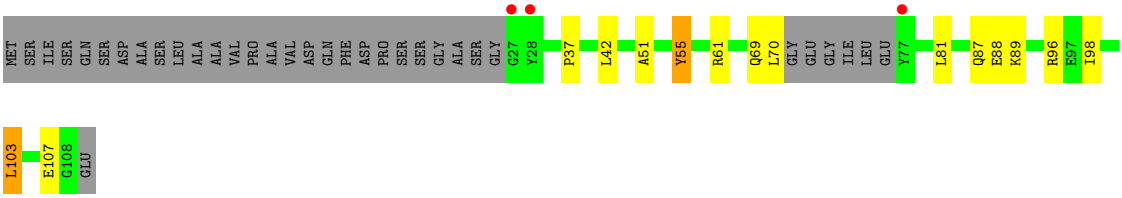
Chain D:





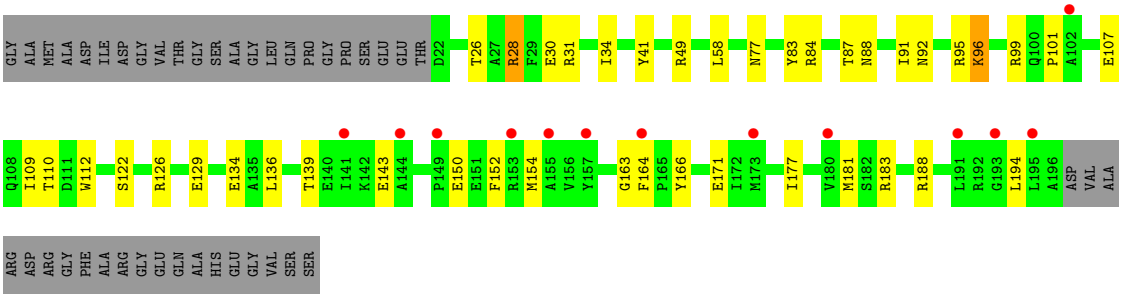
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



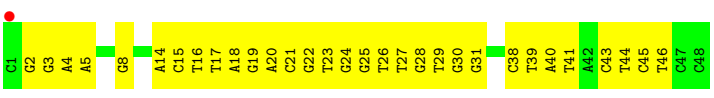
• Molecule 5: ECF RNA polymerase sigma factor SigH

Chain F:



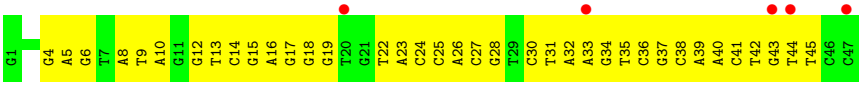
• Molecule 6: DNA (48-MER)

Chain G:

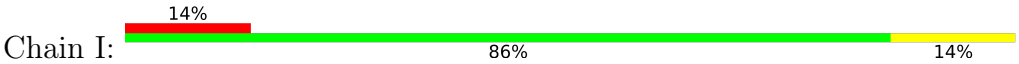


• Molecule 7: DNA (47-MER)

Chain H:



• Molecule 8: RNA (5'-R(*CP*CP*CP*UP*CP*GP*A)-3')



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	129.82Å 164.03Å 214.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.94 – 2.80 49.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.94-2.80) 99.7 (49.53-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.220 , 0.255 0.221 , 0.254	Depositor DCC
R_{free} test set	2290 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 33.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	25858	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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	0.27	0/1647	0.47	0/2241
1	B	0.26	0/1787	0.46	0/2433
2	C	0.27	0/8768	0.46	0/11909
3	D	0.26	0/9932	0.45	0/13435
4	E	0.25	0/612	0.45	0/833
5	F	0.24	0/1409	0.40	0/1909
6	G	0.58	0/1094	0.98	0/1688
7	H	0.54	0/1064	0.90	0/1641
8	I	0.25	0/156	0.95	0/241
All	All	0.30	0/26469	0.52	0/36330

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	1622	0	1651	24	0
1	B	1761	0	1783	38	0
2	C	8611	0	8396	141	0
3	D	9769	0	9792	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	600	0	592	13	0
5	F	1381	0	1319	29	0
6	G	976	0	537	40	0
7	H	948	0	519	35	0
8	I	141	0	75	1	0
9	D	2	0	0	0	0
10	A	2	0	0	0	0
10	C	24	0	0	0	0
10	D	17	0	0	0	0
10	E	1	0	0	0	0
10	F	3	0	0	0	0
All	All	25858	0	24664	420	0

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

All (420) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:113:ARG:NH2	3:D:1235:ASP:OD1	2.15	0.80
2:C:300:PHE:HB3	2:C:333:LEU:HD11	1.66	0.77
3:D:1166:THR:O	3:D:1203:GLY:HA2	1.86	0.76
2:C:55:ASP:O	2:C:59:ASP:HB2	1.86	0.76
2:C:144:THR:HB	2:C:146:GLU:HG2	1.68	0.75
2:C:758:ASP:HB3	2:C:868:LEU:HD23	1.67	0.75
3:D:925:LEU:HB3	3:D:940:ARG:HA	1.66	0.75
7:H:25:DC:H2"	7:H:26:DA:C8	2.23	0.74
2:C:1054:GLN:HG3	2:C:1099:ARG:HH22	1.52	0.73
2:C:782:ALA:O	2:C:791:ARG:NH2	2.23	0.71
2:C:571:VAL:HG22	2:C:572:PRO:HD2	1.74	0.70
7:H:43:DG:H2'	7:H:44:DT:H71	1.74	0.69
6:G:23:DT:H2"	6:G:24:DG:C8	2.26	0.69
3:D:938:VAL:HG22	3:D:952:LEU:HD21	1.74	0.69
5:F:88:ASN:ND2	6:G:26:DT:O2	2.27	0.68
1:A:143:GLY:HA2	1:B:1:MET:HG2	1.74	0.68
2:C:903:ASP:HB2	2:C:1014:ARG:HG3	1.76	0.67
3:D:739:PRO:HG2	3:D:742:LYS:HB2	1.77	0.67
2:C:50:VAL:O	2:C:633:ARG:NH2	2.28	0.66
2:C:982:GLU:OE1	3:D:841:ARG:NH2	2.29	0.66
5:F:110:THR:HG22	5:F:112:TRP:H	1.60	0.66
2:C:200:HIS:HD2	2:C:348:LEU:HG	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1112:ILE:O	4:E:61:ARG:NH2	2.28	0.66
2:C:185:VAL:HG23	2:C:316:VAL:HG22	1.78	0.65
6:G:20:DA:H1'	6:G:21:DC:H5'	1.78	0.65
4:E:51:ALA:O	4:E:55:TYR:HB2	1.96	0.64
2:C:223:GLY:HA3	2:C:231:ARG:HD2	1.79	0.64
3:D:110:VAL:O	3:D:1231:ARG:NH1	2.31	0.64
3:D:114:LEU:HB3	3:D:125:LEU:HD21	1.80	0.64
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.80	0.64
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.80	0.64
1:B:55:ARG:HB2	1:B:137:GLU:HB3	1.80	0.63
7:H:26:DA:H2"	7:H:27:DC:H5"	1.78	0.63
7:H:9:DT:H2'	7:H:10:DA:C8	2.33	0.63
6:G:43:DC:H2"	6:G:44:DT:H71	1.80	0.63
2:C:658:ILE:HD13	2:C:702:ILE:HG22	1.81	0.62
1:B:186:ARG:NH2	1:B:188:ASP:OD2	2.25	0.62
2:C:403:ARG:NH1	2:C:416:THR:O	2.31	0.62
5:F:99:ARG:NH1	6:G:22:DG:OP2	2.32	0.62
3:D:1087:ARG:HA	3:D:1113:GLU:HG3	1.79	0.62
2:C:319:LYS:O	2:C:363:VAL:HG11	1.99	0.62
3:D:458:LYS:NZ	3:D:462:ASP:OD2	2.30	0.62
1:A:29:GLY:N	1:A:190:ASP:OD2	2.31	0.62
2:C:1136:GLU:OE1	3:D:11:ARG:NH2	2.30	0.62
2:C:919:THR:HG23	3:D:731:VAL:HG23	1.82	0.62
3:D:491:ILE:HG23	3:D:514:PRO:HG2	1.81	0.61
2:C:200:HIS:CD2	2:C:348:LEU:HG	2.35	0.61
3:D:281:ILE:O	3:D:289:LYS:NZ	2.34	0.61
7:H:44:DT:H2'	7:H:45:DT:H71	1.82	0.61
2:C:79:ASP:HB2	2:C:82:PRO:HD3	1.82	0.61
3:D:459:ARG:NE	3:D:489:GLU:OE2	2.33	0.61
3:D:739:PRO:HD3	3:D:789:LEU:HD13	1.83	0.60
2:C:635:ALA:HB2	2:C:713:MET:HG2	1.82	0.60
3:D:1265:ASN:OD1	3:D:1269:ASN:ND2	2.32	0.60
3:D:116:TYR:O	3:D:295:ARG:NH1	2.34	0.60
6:G:15:DC:H2'	6:G:16:DT:C6	2.37	0.60
2:C:388:GLN:HG3	2:C:430:PHE:HB2	1.82	0.60
2:C:389:ILE:O	2:C:393:MET:HB2	2.01	0.60
2:C:285:GLU:OE2	6:G:31:DG:N2	2.21	0.60
3:D:445:LYS:NZ	3:D:518:GLU:OE2	2.27	0.60
5:F:91:ILE:HD12	7:H:23:DA:H2"	1.82	0.60
3:D:1166:THR:O	3:D:1203:GLY:CA	2.51	0.59
6:G:38:DC:H2'	6:G:39:DT:C6	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.83	0.59
7:H:38:DC:H2"	7:H:39:DA:C8	2.37	0.59
3:D:400:LYS:HG3	5:F:107:GLU:HG3	1.83	0.59
7:H:31:DT:H2"	7:H:32:DA:C8	2.37	0.59
2:C:824:ILE:HG22	5:F:188:ARG:HG2	1.85	0.59
3:D:67:ARG:HG3	3:D:69:ARG:H	1.68	0.59
2:C:1117:ILE:HD13	3:D:3:ASP:HB3	1.83	0.59
3:D:448:ALA:HB1	3:D:491:ILE:HD11	1.85	0.59
6:G:2:DG:H2"	6:G:3:DG:C8	2.38	0.59
1:A:149:ALA:HB1	1:A:163:PRO:HB2	1.85	0.58
2:C:442:GLN:HE21	2:C:679:ASN:H	1.50	0.58
2:C:741:LEU:HA	2:C:746:VAL:HG13	1.84	0.58
3:D:1050:THR:HG22	3:D:1106:GLU:HA	1.86	0.58
4:E:37:PRO:HG2	4:E:42:LEU:HD11	1.86	0.58
1:B:94:THR:HG22	1:B:139:VAL:HG22	1.85	0.57
3:D:745:ILE:HD13	3:D:784:GLU:HG2	1.86	0.57
3:D:383:ASP:OD2	3:D:386:ARG:NH1	2.35	0.57
3:D:155:MET:HE1	3:D:219:LEU:HD22	1.85	0.57
1:A:36:ASN:O	1:A:40:ARG:HG2	2.05	0.56
2:C:217:ASP:N	2:C:221:THR:O	2.39	0.56
3:D:894:GLU:H	3:D:894:GLU:CD	2.08	0.56
3:D:20:ILE:HD13	3:D:318:PRO:HD3	1.87	0.56
3:D:243:GLU:HG3	3:D:247:ARG:HH21	1.69	0.56
3:D:240:LEU:O	3:D:244:LEU:HB2	2.05	0.55
6:G:14:DA:H2'	6:G:15:DC:C6	2.41	0.55
7:H:32:DA:H2"	7:H:33:DA:H5"	1.88	0.55
2:C:767:GLU:OE2	2:C:807:THR:OG1	2.23	0.55
6:G:45:DC:H2"	6:G:46:DT:C6	2.41	0.55
1:B:86:SER:OG	1:B:119:HIS:NE2	2.31	0.55
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.89	0.55
2:C:960:PRO:HD2	2:C:963:LEU:HD12	1.89	0.55
5:F:49:ARG:NH2	7:H:22:DT:O4	2.39	0.55
6:G:28:DG:H2"	6:G:29:DT:OP1	2.06	0.55
2:C:516:TYR:HB3	2:C:578:TYR:HB3	1.87	0.55
4:E:88:GLU:OE2	4:E:96:ARG:NH1	2.40	0.55
5:F:92:ASN:O	5:F:96:LYS:HB2	2.07	0.55
2:C:413:THR:O	2:C:416:THR:OG1	2.25	0.54
2:C:458:LEU:HD21	2:C:496:LEU:HD13	1.89	0.54
2:C:888:ARG:HG2	2:C:1031:MET:HE1	1.88	0.54
6:G:3:DG:H2"	6:G:4:DA:H5"	1.89	0.54
2:C:377:ARG:NH2	2:C:383:GLU:OE2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:505:HIS:ND1	3:D:1005:GLU:HG3	2.22	0.54
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.43	0.54
3:D:895:ARG:HB2	3:D:967:THR:HB	1.88	0.54
2:C:582:SER:OG	2:C:583:PRO:O	2.24	0.54
3:D:750:GLU:OE2	3:D:834:ARG:NH1	2.34	0.54
2:C:93:LEU:HD11	2:C:397:GLU:HB2	1.90	0.54
2:C:369:ASP:HB3	2:C:372:HIS:HB2	1.90	0.54
7:H:33:DA:H2'	7:H:34:DG:O4'	2.08	0.54
3:D:56:ARG:NH1	3:D:59:GLU:OE2	2.40	0.53
3:D:928:ASP:OD1	3:D:940:ARG:N	2.36	0.53
2:C:785:ASP:OD2	2:C:787:ARG:NH1	2.38	0.53
3:D:641:ARG:NH1	3:D:647:GLU:OE1	2.41	0.53
2:C:644:ALA:HB2	2:C:702:ILE:HD11	1.91	0.53
7:H:27:DC:H2"	7:H:28:DG:C8	2.43	0.53
1:A:40:ARG:HD3	2:C:1013:GLY:O	2.09	0.53
1:B:148:PRO:HG3	3:D:626:VAL:HG21	1.91	0.53
1:A:144:ARG:NH2	1:B:27:GLU:OE2	2.42	0.52
3:D:1270:ILE:HG12	4:E:107:GLU:HA	1.91	0.52
1:B:175:THR:HG22	1:B:195:ASP:HB3	1.90	0.52
3:D:709:VAL:O	3:D:713:VAL:HG23	2.10	0.52
1:B:171:VAL:HA	1:B:198:THR:HA	1.91	0.52
2:C:1053:THR:HG23	2:C:1055:GLN:H	1.75	0.52
3:D:248:TYR:HA	3:D:251:TYR:CD1	2.45	0.52
2:C:899:LEU:HB2	2:C:904:MET:HE1	1.92	0.52
2:C:1041:ILE:O	2:C:1060:LYS:NZ	2.43	0.52
6:G:19:DG:H2"	6:G:20:DA:C8	2.45	0.52
1:B:55:ARG:NH1	1:B:158:GLU:OE1	2.43	0.52
3:D:12:ILE:HD11	3:D:1220:TRP:CE3	2.44	0.52
3:D:21:ARG:HD3	3:D:96:GLU:OE2	2.10	0.52
5:F:181:MET:HB3	7:H:44:DT:H73	1.93	0.51
6:G:25:DG:H2'	6:G:26:DT:C6	2.45	0.51
6:G:40:DA:H2'	6:G:41:DT:H71	1.93	0.51
1:A:40:ARG:HD2	2:C:902:GLU:HB2	1.92	0.51
3:D:1230:THR:O	3:D:1234:THR:HG23	2.09	0.51
2:C:132:PRO:HB3	2:C:153:PHE:HE1	1.76	0.51
2:C:487:GLU:OE2	2:C:613:ARG:NH2	2.44	0.51
6:G:22:DG:H2"	6:G:23:DT:H5"	1.92	0.51
3:D:505:HIS:CD2	3:D:507:LEU:HB2	2.46	0.51
2:C:46:GLU:HG2	2:C:582:SER:HB2	1.91	0.51
1:B:97:LEU:HB3	1:B:136:VAL:HG13	1.92	0.51
3:D:1228:GLU:HG2	7:H:9:DT:H4'	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:166:TYR:HB3	5:F:177:ILE:HG23	1.92	0.51
2:C:632:LEU:HB2	2:C:712:GLU:HG2	1.92	0.51
6:G:17:DT:H2'	6:G:18:DA:N7	2.26	0.51
1:A:181:THR:O	1:A:188:ASP:HA	2.11	0.50
2:C:563:ARG:HG3	2:C:564:LYS:H	1.76	0.50
3:D:490:VAL:O	4:E:89:LYS:NZ	2.44	0.50
3:D:832:ILE:HD12	3:D:851:ILE:HG23	1.93	0.50
5:F:166:TYR:OH	7:H:43:DG:OP2	2.27	0.50
1:B:98:ARG:HG2	1:B:135:GLU:HG3	1.94	0.50
7:H:13:DT:H2'	7:H:14:DC:C6	2.46	0.50
3:D:4:VAL:HG22	3:D:5:ASN:H	1.76	0.50
3:D:248:TYR:HA	3:D:251:TYR:HD1	1.77	0.50
3:D:817:LEU:O	3:D:839:SER:HB2	2.11	0.50
7:H:16:DA:H2'	7:H:17:DG:C8	2.46	0.50
3:D:413:PHE:HA	3:D:417:LEU:HD12	1.94	0.50
3:D:1054:ARG:HB2	3:D:1065:THR:HB	1.94	0.50
1:A:152:ASN:HD22	1:A:157:ALA:HB3	1.77	0.49
2:C:150:GLN:NE2	2:C:413:THR:OG1	2.44	0.49
2:C:899:LEU:HB2	2:C:904:MET:CE	2.42	0.49
3:D:326:PRO:HG2	5:F:109:ILE:HD12	1.95	0.49
6:G:15:DC:H4'	6:G:16:DT:OP1	2.12	0.49
2:C:445:PRO:HD2	2:C:707:CYS:HB2	1.94	0.49
3:D:913:ASP:HB3	3:D:916:ILE:HG13	1.93	0.49
5:F:152:PHE:CE1	5:F:183:ARG:HG2	2.46	0.49
2:C:442:GLN:HE21	2:C:679:ASN:N	2.11	0.49
1:B:181:THR:O	1:B:189:PHE:HB2	2.12	0.49
6:G:23:DT:H2"	6:G:24:DG:H8	1.76	0.49
3:D:34:ILE:HG22	3:D:41:PRO:HA	1.95	0.49
3:D:339:ASP:HB3	3:D:399:LEU:HB3	1.94	0.49
2:C:191:ILE:HA	2:C:198:THR:HA	1.94	0.49
6:G:43:DC:H2"	6:G:44:DT:C7	2.42	0.49
2:C:881:ASP:O	2:C:1037:VAL:HG21	2.13	0.49
6:G:17:DT:H2'	6:G:18:DA:C8	2.48	0.49
6:G:46:DT:O2	7:H:4:DG:N2	2.46	0.49
1:A:146:TYR:OH	2:C:878:LYS:NZ	2.44	0.49
3:D:461:VAL:HG23	3:D:472:ALA:HB2	1.95	0.49
6:G:8:DG:N2	7:H:42:DT:O2	2.46	0.49
2:C:463:LEU:HD13	2:C:468:ALA:HB2	1.95	0.48
5:F:30:GLU:HA	5:F:34:ILE:HD13	1.96	0.48
6:G:39:DT:H2'	6:G:40:DA:C8	2.49	0.48
1:B:18:ARG:HG3	1:B:197:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:230:ALA:N	3:D:233:GLN:OE1	2.46	0.48
2:C:224:VAL:O	2:C:231:ARG:HA	2.14	0.48
7:H:40:DA:H1'	7:H:41:DC:H5'	1.96	0.48
2:C:96:ILE:HD12	2:C:397:GLU:HG3	1.96	0.48
5:F:126:ARG:NH2	5:F:134:GLU:OE1	2.36	0.48
7:H:30:DC:H2'	7:H:31:DT:C6	2.48	0.47
1:A:9:LEU:HA	1:A:22:VAL:O	2.14	0.47
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.97	0.47
3:D:76:GLU:CD	3:D:76:GLU:H	2.18	0.47
3:D:26:GLY:HA3	3:D:51:ILE:HG22	1.95	0.47
6:G:15:DC:H2"	6:G:16:DT:O5'	2.14	0.47
1:A:147:VAL:HG12	1:A:168:TYR:HE2	1.80	0.47
3:D:576:MET:HG2	3:D:577:PRO:HD2	1.97	0.47
7:H:5:DA:H4'	7:H:6:DG:OP1	2.13	0.47
2:C:403:ARG:O	2:C:407:GLN:HG3	2.14	0.47
2:C:1052:ILE:HG12	3:D:326:PRO:HG3	1.96	0.47
3:D:902:ALA:HB2	3:D:953:LEU:HD11	1.96	0.47
1:B:147:VAL:HG22	1:B:166:SER:HB2	1.95	0.47
2:C:792:ILE:HD12	2:C:792:ILE:H	1.80	0.47
2:C:892:LYS:HD2	3:D:537:ASP:HB2	1.96	0.47
2:C:1103:TYR:CE2	3:D:454:PRO:HG3	2.50	0.47
1:A:217:GLU:OE2	1:B:233:GLU:HG3	2.15	0.47
1:B:100:GLN:HG3	1:B:101:GLY:N	2.30	0.47
3:D:69:ARG:HG3	5:F:164:PHE:CZ	2.49	0.47
6:G:39:DT:H2'	6:G:40:DA:H8	1.80	0.47
3:D:1274:PRO:HA	4:E:103:LEU:HB3	1.97	0.47
1:B:102:PRO:HG3	1:B:130:ASP:HB3	1.96	0.47
2:C:447:SER:HB3	2:C:613:ARG:HB3	1.97	0.47
7:H:8:DA:H2'	7:H:9:DT:C6	2.50	0.47
7:H:36:DC:H2"	7:H:37:DG:C8	2.49	0.47
2:C:122:CYS:HA	2:C:127:MET:HB2	1.98	0.46
2:C:214:PHE:CD1	2:C:224:VAL:HG22	2.49	0.46
5:F:139:THR:O	5:F:143:GLU:HG3	2.15	0.46
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.97	0.46
2:C:599:HIS:HB3	2:C:928:ILE:HG22	1.97	0.46
2:C:1051:MET:O	3:D:89:ARG:NH2	2.48	0.46
2:C:1135:VAL:HA	3:D:11:ARG:O	2.16	0.46
3:D:567:SER:HB2	3:D:574:LEU:HD13	1.98	0.46
1:B:74:THR:HA	1:B:77:ILE:HD12	1.97	0.46
1:B:200:ASN:OD1	1:B:200:ASN:N	2.41	0.46
3:D:492:ALA:O	4:E:89:LYS:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:634:LYS:HA	3:D:664:ALA:O	2.16	0.46
6:G:18:DA:H4'	6:G:19:DG:OP1	2.15	0.46
2:C:230:ARG:HA	2:C:230:ARG:HD3	1.67	0.46
2:C:317:ASN:O	2:C:321:GLY:N	2.48	0.46
7:H:34:DG:H2'	7:H:35:DT:C7	2.45	0.46
2:C:43:LYS:NZ	2:C:984:GLU:OE1	2.49	0.46
2:C:344:TYR:OH	2:C:364:PRO:O	2.22	0.46
2:C:548:ILE:HD11	2:C:579:MET:SD	2.55	0.46
2:C:945:LYS:HD2	2:C:965:GLU:HB3	1.97	0.46
2:C:763:LYS:HE3	3:D:39:LEU:O	2.16	0.46
3:D:798:PRO:HA	3:D:801:THR:HG22	1.98	0.46
1:A:84:VAL:HG13	1:A:119:HIS:HB2	1.97	0.46
2:C:326:GLU:N	2:C:327:PRO:HD3	2.31	0.46
2:C:1127:GLU:OE1	3:D:412:ARG:HG3	2.15	0.46
2:C:214:PHE:HD1	2:C:224:VAL:HG22	1.80	0.46
3:D:430:ILE:HD13	3:D:541:MET:HG3	1.98	0.46
3:D:866:ARG:HD3	3:D:1010:LEU:O	2.16	0.46
1:B:180:ALA:HA	1:B:189:PHE:O	2.16	0.46
3:D:456:VAL:O	3:D:460:LEU:HG	2.16	0.45
3:D:1158:VAL:HG22	3:D:1161:MET:HE3	1.97	0.45
5:F:87:THR:O	5:F:91:ILE:HG12	2.16	0.45
3:D:847:LEU:HD12	3:D:847:LEU:HA	1.73	0.45
6:G:16:DT:H2"	6:G:17:DT:H5"	1.97	0.45
1:A:86:SER:OG	1:A:119:HIS:NE2	2.29	0.45
6:G:15:DC:H2'	6:G:16:DT:H6	1.81	0.45
1:B:74:THR:HG21	3:D:608:GLU:OE1	2.15	0.45
1:B:100:GLN:HG3	1:B:101:GLY:H	1.80	0.45
3:D:38:THR:HB	3:D:40:LYS:HG3	1.98	0.45
6:G:44:DT:H2"	6:G:45:DC:C6	2.50	0.45
1:B:24:GLU:HB2	1:B:191:LYS:HG3	1.98	0.45
6:G:21:DC:H2"	6:G:22:DG:C8	2.51	0.45
7:H:12:DG:H2'	7:H:13:DT:C6	2.52	0.45
2:C:344:TYR:CZ	2:C:365:VAL:HA	2.52	0.45
2:C:650:ILE:HG22	2:C:692:ALA:HA	1.97	0.45
5:F:41:TYR:HB2	5:F:58:LEU:HD22	1.98	0.45
1:B:68:GLY:HA3	1:B:132:GLY:HA3	1.98	0.45
2:C:729:HIS:CE1	2:C:897:LYS:HD2	2.51	0.45
3:D:459:ARG:NH2	4:E:87:GLN:OE1	2.49	0.45
1:A:112:PRO:HB2	1:A:116:VAL:HG13	1.98	0.45
3:D:760:PHE:CG	3:D:770:ARG:HD3	2.52	0.45
3:D:1251:ASN:ND2	3:D:1259:PRO:HD3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:28:ARG:HA	5:F:31:ARG:HG2	1.98	0.45
1:B:98:ARG:HA	1:B:134:LEU:O	2.17	0.45
2:C:505:ARG:NH2	2:C:513:GLU:OE1	2.39	0.45
3:D:159:ARG:HH12	3:D:220:GLU:HB2	1.82	0.45
3:D:173:ARG:NE	3:D:204:GLU:OE1	2.37	0.45
3:D:574:LEU:HD12	3:D:574:LEU:HA	1.71	0.45
7:H:41:DC:H2"	7:H:42:DT:C6	2.52	0.45
1:B:29:GLY:O	1:B:33:THR:HG23	2.17	0.44
2:C:139:PHE:CZ	2:C:412:ILE:HD11	2.52	0.44
2:C:323:HIS:HB3	2:C:327:PRO:HD2	1.99	0.44
3:D:137:THR:OG1	3:D:253:THR:OG1	2.34	0.44
3:D:925:LEU:HD11	3:D:938:VAL:HG23	1.99	0.44
1:B:22:VAL:HG12	1:B:193:ILE:HG12	2.00	0.44
2:C:1037:VAL:HG13	3:D:429:VAL:HG12	1.98	0.44
3:D:850:PHE:O	3:D:853:THR:OG1	2.29	0.44
2:C:689:ILE:HG12	2:C:702:ILE:O	2.17	0.44
2:C:1091:ILE:HD12	2:C:1102:VAL:HG21	1.99	0.44
3:D:579:LEU:HD23	3:D:808:THR:HB	1.99	0.44
3:D:1248:LEU:HD12	3:D:1249:LYS:N	2.33	0.44
4:E:69:GLN:O	4:E:70:LEU:HG	2.17	0.44
1:B:170:PRO:HA	1:B:199:LYS:HE3	1.98	0.44
2:C:262:LEU:O	2:C:265:ASP:HB3	2.18	0.44
2:C:1037:VAL:HG13	3:D:429:VAL:CG1	2.48	0.44
3:D:66:LYS:O	3:D:67:ARG:HB2	2.17	0.44
3:D:797:ASN:O	3:D:801:THR:HG22	2.17	0.44
2:C:408:ASP:O	2:C:412:ILE:HG23	2.18	0.44
2:C:982:GLU:H	2:C:982:GLU:HG3	1.58	0.44
3:D:789:LEU:HD21	3:D:818:ALA:HB3	1.99	0.44
6:G:4:DA:H2"	6:G:5:DA:H8	1.82	0.44
2:C:343:GLU:O	2:C:347:ARG:HG3	2.18	0.44
3:D:36:TYR:CD1	5:F:101:PRO:HG3	2.53	0.44
3:D:931:ASP:HA	3:D:957:ILE:HG12	1.99	0.44
3:D:953:LEU:HD12	3:D:953:LEU:HA	1.85	0.44
3:D:1264:ILE:HG22	3:D:1266:ARG:H	1.82	0.44
2:C:1037:VAL:O	2:C:1041:ILE:HG22	2.18	0.44
3:D:1097:ARG:NH1	3:D:1103:ASP:OD1	2.50	0.44
3:D:69:ARG:NH2	5:F:163:GLY:O	2.51	0.44
2:C:255:SER:HB2	2:C:258:MET:HB2	1.99	0.43
2:C:819:ARG:HD2	3:D:67:ARG:HH12	1.81	0.43
3:D:471:SER:O	3:D:475:MET:HB2	2.18	0.43
3:D:588:LEU:HD11	3:D:672:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:377:ARG:HH22	2:C:383:GLU:CD	2.20	0.43
2:C:1103:TYR:OH	5:F:129:GLU:OE2	2.35	0.43
3:D:500:ARG:HB2	3:D:541:MET:HG2	2.00	0.43
6:G:25:DG:H2"	6:G:26:DT:O5'	2.19	0.43
2:C:862:PRO:HG2	2:C:865:VAL:HG21	1.99	0.43
1:A:7:PRO:HB3	1:A:25:PRO:O	2.18	0.43
1:B:108:GLY:N	1:B:121:PRO:O	2.51	0.43
2:C:707:CYS:O	2:C:714:ALA:N	2.37	0.43
5:F:84:ARG:HG2	6:G:27:DT:OP1	2.18	0.43
1:B:171:VAL:HG12	1:B:198:THR:HG22	2.00	0.43
2:C:737:LEU:HD22	2:C:741:LEU:HD12	2.00	0.43
3:D:1090:LYS:HG3	3:D:1096:GLU:HG2	2.00	0.43
2:C:771:ARG:NH1	2:C:784:LEU:O	2.51	0.43
3:D:1050:THR:HG23	3:D:1107:VAL:HG22	2.01	0.43
1:B:88:GLU:N	1:B:88:GLU:OE1	2.51	0.43
3:D:897:ILE:HD13	3:D:964:SER:HB3	2.00	0.43
1:A:120:ASN:OD1	1:A:120:ASN:N	2.50	0.43
2:C:403:ARG:HA	2:C:406:THR:HG22	1.99	0.43
2:C:442:GLN:HG3	2:C:678:SER:HB2	2.00	0.43
2:C:583:PRO:C	2:C:585:GLN:H	2.21	0.43
3:D:1061:PHE:CE1	3:D:1079:LYS:HG3	2.54	0.43
7:H:34:DG:H2'	7:H:35:DT:H71	1.99	0.43
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.54	0.42
5:F:150:GLU:O	5:F:154:MET:HG2	2.19	0.42
6:G:29:DT:H2'	6:G:30:DG:C8	2.54	0.42
2:C:549:ASP:HB3	2:C:551:ASP:OD1	2.19	0.42
2:C:633:ARG:NH1	2:C:637:ASP:OD2	2.52	0.42
7:H:38:DC:H2"	7:H:39:DA:H5"	2.01	0.42
2:C:595:PRO:O	2:C:889:HIS:HE1	2.02	0.42
3:D:595:ASP:HB3	3:D:631:ALA:HB2	2.01	0.42
3:D:1086:LEU:H	3:D:1086:LEU:HD12	1.84	0.42
3:D:1278:ALA:HB1	4:E:81:LEU:HD13	2.00	0.42
2:C:757:ILE:HB	2:C:837:LEU:HD22	2.01	0.42
7:H:24:DC:P	7:H:24:DC:H3'	2.59	0.42
2:C:583:PRO:HB2	2:C:977:PHE:HB2	2.01	0.42
2:C:798:ASP:HA	2:C:839:VAL:HB	2.01	0.42
3:D:75:CYS:HB3	3:D:78:CYS:SG	2.59	0.42
2:C:547:PRO:HG2	2:C:555:VAL:HB	2.01	0.42
3:D:86:LYS:O	3:D:89:ARG:HG2	2.20	0.42
5:F:95:ARG:O	5:F:99:ARG:HG3	2.19	0.42
6:G:44:DT:H2"	6:G:45:DC:H5"	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:470:LEU:HD13	3:D:858:LYS:HE2	2.00	0.42
2:C:558:ARG:HB3	2:C:570:TYR:CD1	2.55	0.42
3:D:1248:LEU:HB3	3:D:1259:PRO:HD2	2.01	0.42
1:A:73:VAL:O	1:A:77:ILE:HG13	2.20	0.42
1:B:188:ASP:OD1	1:B:188:ASP:N	2.38	0.42
2:C:751:HIS:CD2	2:C:877:ARG:HG3	2.54	0.42
2:C:903:ASP:HA	2:C:1013:GLY:HA3	2.01	0.42
3:D:64:LYS:HG2	3:D:65:TYR:CE2	2.54	0.42
3:D:425:SER:HA	3:D:543:VAL:O	2.19	0.42
3:D:584:GLY:HA3	3:D:720:GLY:O	2.19	0.42
7:H:26:DA:H1'	7:H:27:DC:O4'	2.20	0.42
3:D:116:TYR:HE2	3:D:294:LYS:HB3	1.84	0.42
3:D:739:PRO:HA	3:D:740:PRO:HD3	1.88	0.42
1:B:89:GLU:C	1:B:91:GLU:H	2.23	0.41
3:D:459:ARG:HD2	3:D:459:ARG:HA	1.78	0.41
3:D:646:ILE:O	3:D:650:LEU:HB2	2.20	0.41
6:G:27:DT:H4'	6:G:28:DG:OP1	2.20	0.41
2:C:465:ARG:HH21	8:I:3:C:P	2.42	0.41
3:D:412:ARG:NH1	3:D:416:ASN:OD1	2.52	0.41
3:D:1173:THR:OG1	3:D:1201:ALA:HB2	2.20	0.41
7:H:16:DA:H2'	7:H:17:DG:H8	1.85	0.41
3:D:938:VAL:CG2	3:D:952:LEU:HD21	2.46	0.41
2:C:347:ARG:HD3	2:C:352:GLN:OE1	2.19	0.41
2:C:604:ARG:HA	2:C:604:ARG:HD2	1.92	0.41
3:D:1062:TYR:HB2	3:D:1080:ILE:HB	2.01	0.41
2:C:127:MET:O	2:C:170:GLY:N	2.54	0.41
2:C:813:GLU:CD	5:F:122:SER:HG	2.24	0.41
2:C:904:MET:HG2	2:C:913:VAL:O	2.20	0.41
3:D:1006:PRO:HG3	3:D:1149:ILE:HD11	2.01	0.41
1:B:27:GLU:HB2	1:B:30:PHE:HD2	1.85	0.41
2:C:1071:MET:HE3	3:D:503:THR:H	1.84	0.41
3:D:689:HIS:O	3:D:693:GLN:HG3	2.21	0.41
3:D:849:TYR:O	3:D:853:THR:HG23	2.21	0.41
3:D:1164:ARG:HD2	3:D:1208:MET:SD	2.60	0.41
6:G:16:DT:H2"	6:G:17:DT:O4'	2.20	0.41
2:C:373:PHE:HB2	2:C:478:SER:HB2	2.02	0.41
3:D:749:TYR:CG	3:D:781:ALA:HB2	2.56	0.41
5:F:26:THR:O	5:F:30:GLU:HG3	2.21	0.41
2:C:222:VAL:HG21	2:C:258:MET:SD	2.61	0.41
3:D:32:GLU:HB3	3:D:42:GLU:HG3	2.02	0.41
3:D:120:LEU:HD23	3:D:125:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:34:DG:H2'	7:H:35:DT:C5	2.56	0.41
1:B:10:SER:O	1:B:21:PHE:HA	2.21	0.41
1:B:70:LYS:HB3	1:B:127:THR:HG23	2.03	0.41
2:C:905:PRO:HB3	2:C:1019:PHE:HE2	1.86	0.41
3:D:651:PHE:CE2	3:D:660:ASP:HB3	2.56	0.41
7:H:15:DG:H2'	7:H:16:DA:C8	2.56	0.41
2:C:163:LYS:O	2:C:452:LYS:NZ	2.40	0.41
3:D:1250:GLU:OE1	3:D:1250:GLU:N	2.47	0.41
4:E:98:ILE:HG12	4:E:103:LEU:HD11	2.04	0.41
3:D:507:LEU:HB3	3:D:531:ALA:HB1	2.03	0.40
2:C:883:ASP:OD1	2:C:1037:VAL:HG23	2.21	0.40
2:C:1147:LEU:O	2:C:1148:ARG:HG3	2.21	0.40
3:D:516:LEU:HD23	3:D:516:LEU:HA	1.90	0.40
1:A:8:THR:O	1:A:23:ILE:HA	2.21	0.40
1:A:40:ARG:HE	2:C:902:GLU:HG3	1.85	0.40
1:A:98:ARG:HG2	1:A:135:GLU:HG3	2.02	0.40
2:C:684:ALA:HA	2:C:706:PRO:HG3	2.02	0.40
3:D:489:GLU:OE2	4:E:87:GLN:HG2	2.21	0.40
3:D:505:HIS:NE2	3:D:507:LEU:HB2	2.36	0.40
3:D:1173:THR:HG23	3:D:1200:PRO:HB2	2.04	0.40
5:F:136:LEU:HD23	5:F:136:LEU:HA	1.95	0.40
6:G:22:DG:C8	6:G:23:DT:H72	2.56	0.40
7:H:18:DG:H2'	7:H:19:DG:C8	2.56	0.40
3:D:105:TRP:CE3	3:D:1234:THR:HG22	2.57	0.40
3:D:242:ARG:HA	3:D:242:ARG:HD3	1.73	0.40
3:D:939:GLU:H	3:D:939:GLU:HG2	1.54	0.40
1:A:70:LYS:NZ	2:C:691:ASP:OD1	2.50	0.40
1:B:52:THR:O	1:B:164:VAL:HG22	2.21	0.40
2:C:1106:ILE:HG21	3:D:454:PRO:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/368 (57%)	205 (97%)	6 (3%)	0	100	100
1	B	232/368 (63%)	225 (97%)	7 (3%)	0	100	100
2	C	1135/1174 (97%)	1105 (97%)	30 (3%)	0	100	100
3	D	1254/1317 (95%)	1223 (98%)	31 (2%)	0	100	100
4	E	72/110 (66%)	69 (96%)	3 (4%)	0	100	100
5	F	173/218 (79%)	170 (98%)	3 (2%)	0	100	100
All	All	3077/3555 (87%)	2997 (97%)	80 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	181/315 (58%)	179 (99%)	2 (1%)	73	92
1	B	194/315 (62%)	188 (97%)	6 (3%)	40	74
2	C	907/995 (91%)	890 (98%)	17 (2%)	57	85
3	D	1024/1096 (93%)	1007 (98%)	17 (2%)	60	87
4	E	64/90 (71%)	62 (97%)	2 (3%)	40	74
5	F	137/175 (78%)	131 (96%)	6 (4%)	28	61
All	All	2507/2986 (84%)	2457 (98%)	50 (2%)	55	84

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	PHE
1	A	166	SER
1	B	45	SER
1	B	116	VAL
1	B	172	LEU
1	B	196	VAL
1	B	200	ASN

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Mol	Chain	Res	Type
1	B	201	SER
2	C	190	THR
2	C	443	ASN
2	C	472	VAL
2	C	523	VAL
2	C	570	TYR
2	C	571	VAL
2	C	582	SER
2	C	587	VAL
2	C	640	ASP
2	C	641	VAL
2	C	770	THR
2	C	875	GLN
2	C	892	LYS
2	C	981	GLN
2	C	982	GLU
2	C	991	CYS
2	C	1037	VAL
3	D	12	ILE
3	D	73	ILE
3	D	101	VAL
3	D	125	LEU
3	D	488	GLU
3	D	635	VAL
3	D	645	GLU
3	D	825	THR
3	D	910	LEU
3	D	925	LEU
3	D	935	ASN
3	D	940	ARG
3	D	993	GLU
3	D	1061	PHE
3	D	1121	VAL
3	D	1162	LEU
3	D	1206	VAL
4	E	55	TYR
4	E	103	LEU
5	F	28	ARG
5	F	77	ASN
5	F	83	TYR
5	F	96	LYS
5	F	171	GLU

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Mol	Chain	Res	Type
5	F	194	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	151	GLN
1	B	100	GLN
2	C	200	HIS
2	C	349	HIS
2	C	442	GLN
2	C	1129	GLN
3	D	175	GLN
3	D	304	GLN
3	D	892	GLN
3	D	1139	GLN
5	F	77	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	6/7 (85%)	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	215/368 (58%)	-0.13	1 (0%) 91 88	33, 47, 75, 102	0
1	B	234/368 (63%)	0.08	6 (2%) 56 46	43, 63, 85, 99	0
2	C	1137/1174 (96%)	0.13	45 (3%) 38 28	26, 49, 125, 152	0
3	D	1260/1317 (95%)	0.01	42 (3%) 46 36	29, 51, 97, 134	0
4	E	76/110 (69%)	0.02	3 (3%) 39 29	40, 60, 82, 91	0
5	F	175/218 (80%)	0.47	13 (7%) 14 8	42, 84, 110, 120	0
6	G	48/48 (100%)	0.30	1 (2%) 63 54	91, 124, 196, 205	0
7	H	47/47 (100%)	0.52	5 (10%) 6 3	80, 135, 207, 214	0
8	I	7/7 (100%)	0.99	1 (14%) 2 1	85, 92, 114, 117	0
All	All	3199/3657 (87%)	0.09	117 (3%) 41 31	26, 54, 118, 214	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1056	GLU	4.9
3	D	1057	ASP	4.7
5	F	102	ALA	4.6
3	D	1050	THR	4.1
2	C	252	PHE	4.1
3	D	1074	GLU	4.0
2	C	821	LEU	3.9
3	D	958	THR	3.9
3	D	1084	GLN	3.9
2	C	339	VAL	3.9
4	E	28	TYR	3.9
2	C	235	THR	3.9
1	B	1	MET	3.9
2	C	248	ILE	3.8
2	C	1161	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	194	SER	3.7
2	C	197	LYS	3.7
2	C	289	LYS	3.7
3	D	1071	GLY	3.7
1	A	221	LEU	3.7
3	D	653	HIS	3.6
2	C	825	PHE	3.6
2	C	1162	LEU	3.6
2	C	1149	GLU	3.6
2	C	196	ASP	3.5
2	C	1150	GLY	3.5
3	D	1055	LEU	3.4
2	C	263	GLU	3.4
5	F	195	LEU	3.4
5	F	180	VAL	3.4
3	D	932	GLU	3.3
3	D	1077	TYR	3.3
3	D	1061	PHE	3.3
2	C	282	ARG	3.3
2	C	1158	ALA	3.3
2	C	251	ARG	3.3
2	C	1154	ASP	3.3
5	F	191	LEU	3.3
2	C	1159	ALA	3.3
6	G	1	DC	3.2
7	H	47	DC	3.2
3	D	36	TYR	3.2
3	D	954	ALA	3.2
3	D	1064	ILE	3.1
2	C	329	THR	3.1
3	D	654	SER	3.1
3	D	930	VAL	3.1
2	C	1163	GLY	3.0
4	E	77	TYR	3.0
3	D	1041	ARG	3.0
3	D	931	ASP	3.0
3	D	192	ASP	3.0
5	F	155	ALA	3.0
2	C	298	ASN	3.0
2	C	244	THR	2.9
2	C	28	SER	2.9
2	C	823	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	1066	ILE	2.8
5	F	157	TYR	2.8
3	D	1058	GLY	2.7
1	B	115	GLY	2.7
2	C	80	VAL	2.7
3	D	1081	SER	2.6
2	C	283	PRO	2.6
4	E	27	GLY	2.6
3	D	1054	ARG	2.6
3	D	1278	ALA	2.6
2	C	192	ASP	2.6
2	C	249	VAL	2.6
3	D	935	ASN	2.5
3	D	1073	GLU	2.5
5	F	153	ARG	2.5
2	C	253	GLY	2.5
2	C	301	PHE	2.5
3	D	196	LYS	2.5
5	F	193	GLY	2.4
1	B	155	SER	2.4
2	C	145	GLY	2.4
5	F	173	MET	2.4
2	C	1152	ASP	2.3
3	D	1044	ALA	2.3
3	D	904	ARG	2.3
2	C	237	LEU	2.3
3	D	1078	ASP	2.3
2	C	278	TYR	2.3
3	D	1099	LEU	2.3
1	B	2	LEU	2.3
3	D	188	GLY	2.3
5	F	141	ILE	2.3
3	D	1048	ASP	2.2
5	F	149	PRO	2.2
2	C	359	GLY	2.2
3	D	1079	LYS	2.2
7	H	33	DA	2.2
3	D	949	ILE	2.2
5	F	164	PHE	2.2
2	C	271	ASP	2.2
2	C	195	THR	2.2
2	C	358	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
8	I	1	C	2.1
3	D	934	GLY	2.1
3	D	933	ALA	2.1
7	H	43	DG	2.1
3	D	464	ASN	2.1
1	B	233	GLU	2.1
3	D	1062	TYR	2.1
2	C	1155	LEU	2.1
7	H	44	DT	2.1
2	C	191	ILE	2.1
2	C	328	ILE	2.1
2	C	261	THR	2.0
3	D	1059	GLU	2.0
1	B	114	ALA	2.0
2	C	242	GLY	2.0
7	H	20	DT	2.0
3	D	37	ARG	2.0
5	F	144	ALA	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
9	ZN	D	2001	1/1	0.98	0.09	72,72,72,72	0
9	ZN	D	2002	1/1	0.99	0.10	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.