



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:08 PM GMT

PDB ID : 3S1R
Title : RNA Polymerase II Initiation Complex with a 5-nt 3'-deoxy RNA soaked with GTP
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-16
Resolution : 3.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

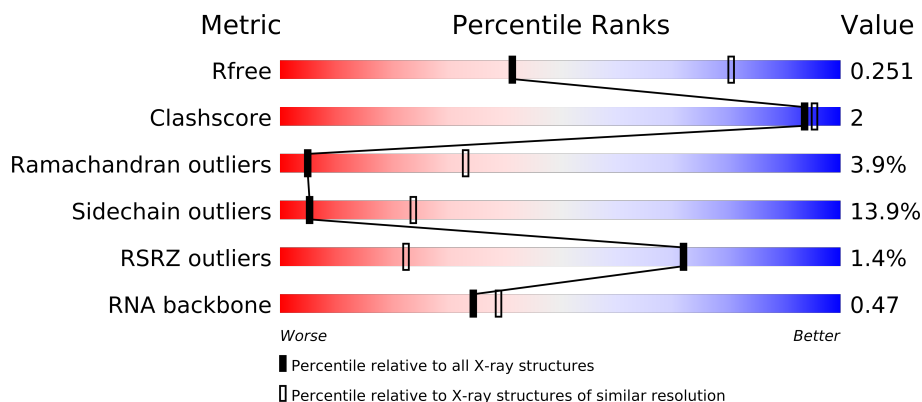
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	E	215	
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	5	
12	T	29	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
13	GTP	R	100	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 28601 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	1405	Total	C	N	O	S	0	0	0
			11043	6965	1936	2081	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0	0
			8861	5610	1549	1647	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	85	Total	C	N	O	S	0	0	0
			688	439	116	130	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

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

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

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

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

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

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

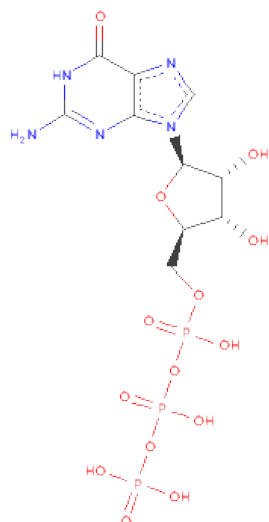
- Molecule 11 is a RNA chain called RNA (5'-R(*AP*GP*AP*GP*G*)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	5	Total	C	N	O	P	0	0	0
			109	50	25	30	4			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	8	Total	C	N	O	P	0	0	0
			159	76	26	49	8			

- Molecule 13 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	R	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

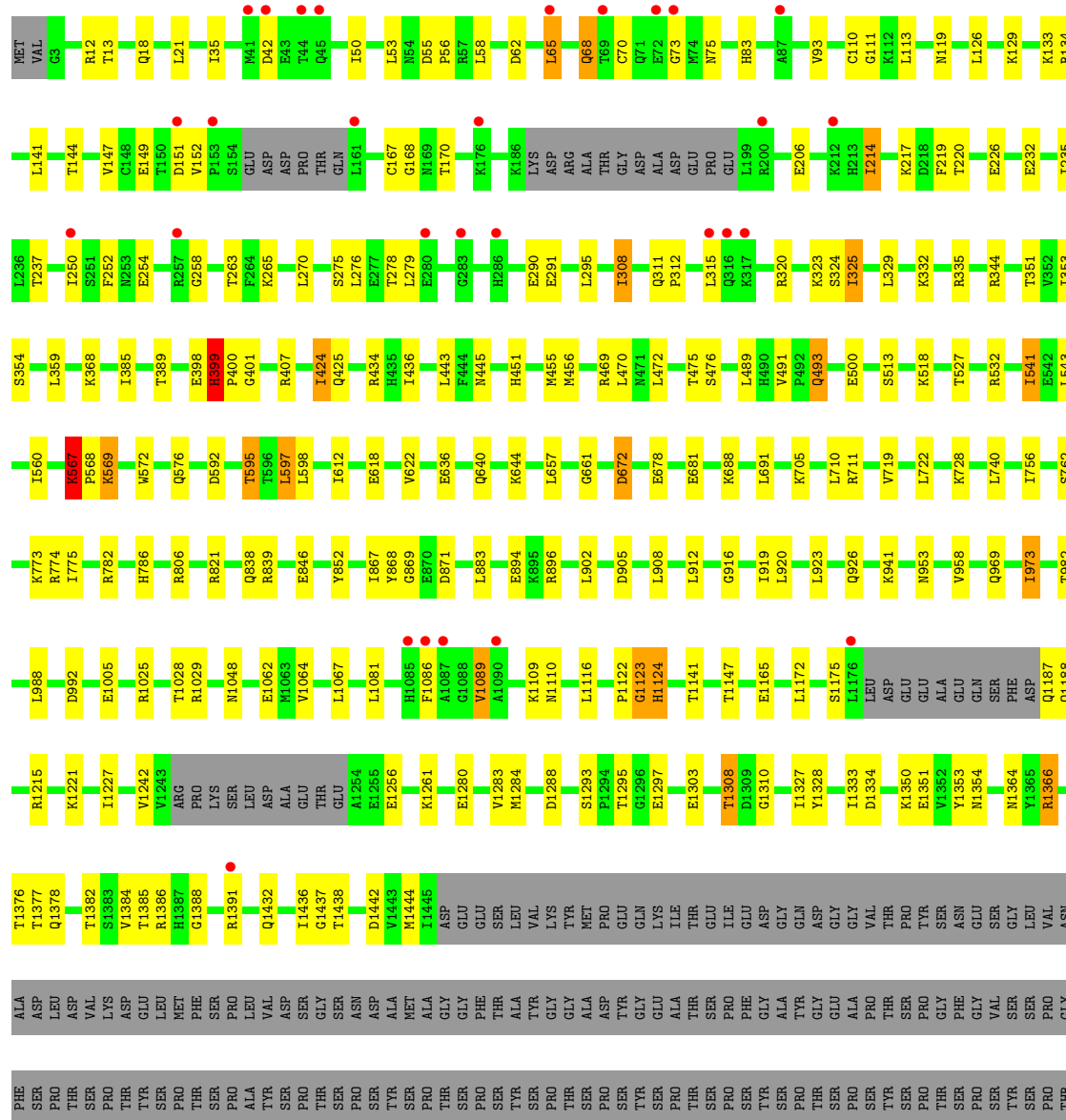
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 

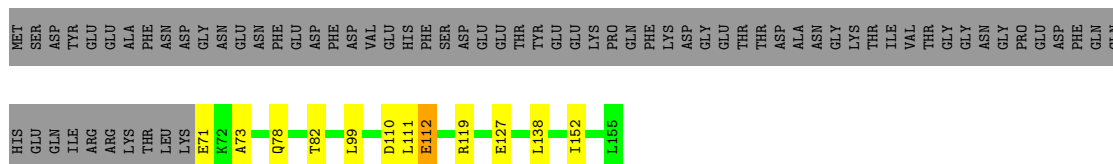


Chain E: 



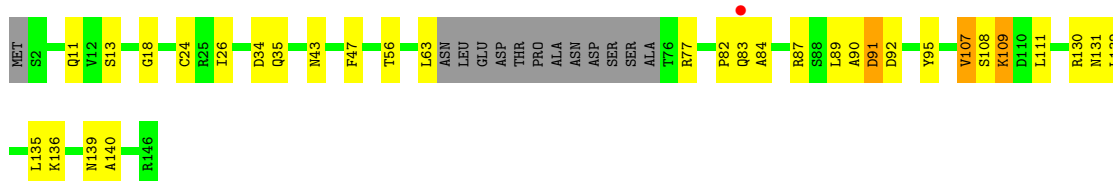
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

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: 



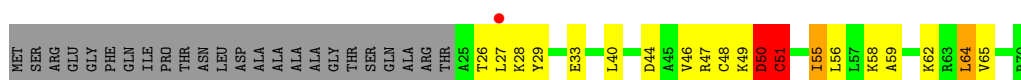
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 



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

Chain L: 



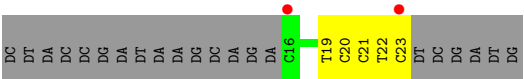
- Molecule 11: RNA (5'-R(*AP*GP*AP*GP*G*)-3')

Chain R: 



● Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3')

Chain T:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.67Å 221.32Å 193.21Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	29.97 – 3.20 29.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.97-3.20) 99.4 (29.97-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.18Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.177 , 0.226 0.201 , 0.251	Depositor DCC
R_{free} test set	5435 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 76.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 108691 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28601	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/11241	0.77	3/15199 (0.0%)
2	B	0.52	0/9033	0.80	2/12181 (0.0%)
3	C	0.49	0/2133	0.81	0/2891
4	E	0.45	0/1788	0.73	0/2406
5	F	0.51	0/700	0.76	0/945
6	H	0.50	0/1086	0.83	1/1470 (0.1%)
7	I	0.51	0/989	0.82	0/1331
8	J	0.55	0/541	0.88	0/727
9	K	0.45	0/937	0.71	0/1265
10	L	0.57	0/365	1.13	2/485 (0.4%)
11	R	0.93	0/123	1.64	0/191
12	T	1.29	0/176	1.87	5/268 (1.9%)
All	All	0.51	0/29112	0.81	13/39359 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	22	DT	O4'-C1'-N1	8.14	113.70	108.00
2	B	647	GLY	C-N-CA	7.65	140.83	121.70
10	L	50	ASP	C-N-CA	7.62	140.74	121.70
12	T	23	DC	O4'-C1'-N1	6.07	112.25	108.00
1	A	1123	GLY	C-N-CA	6.02	136.75	121.70
10	L	51	CYS	N-CA-C	-5.90	95.06	111.00
12	T	19	DT	O4'-C1'-N1	5.90	112.13	108.00
12	T	21	DC	O4'-C1'-N1	5.69	111.98	108.00
1	A	399	HIS	N-CA-CB	5.40	120.32	110.60
2	B	140	ILE	C-N-CA	5.33	135.04	121.70
12	T	20	DC	O4'-C1'-N1	5.29	111.70	108.00
1	A	451	HIS	CB-CA-C	-5.11	100.18	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	91	ASP	C-N-CA	5.02	134.25	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11043	0	23	16	0
2	B	8861	0	0	21	0
3	C	2095	0	0	6	0
4	E	1752	0	0	2	0
5	F	688	0	5	0	0
6	H	1068	0	0	4	0
7	I	971	0	0	2	0
8	J	532	0	0	4	0
9	K	919	0	0	1	0
10	L	363	0	0	1	0
11	R	109	0	0	0	0
12	T	159	0	0	0	0
13	R	32	0	0	0	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	28601	0	28	46	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (46) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:469:ARG:NH2	2:B:991:GLY:O	2.31	0.64
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.31	0.63
1:A:399:HIS:O	1:A:401:GLY:N	2.32	0.63
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.38	0.57
2:B:848:ARG:NH2	2:B:996:ARG:NH1	2.54	0.55
2:B:1094:ARG:NH1	2:B:1094:ARG:CG	2.72	0.53
3:C:66:ARG:NH2	8:J:3:VAL:O	2.43	0.52
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.45	0.50
2:B:708:GLU:O	2:B:711:GLU:N	2.45	0.50
3:C:46:ILE:O	3:C:169:LYS:NZ	2.45	0.50
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.46	0.49
3:C:93:ASP:O	3:C:127:ARG:NH2	2.45	0.49
1:A:1328:TYR:OH	1:A:1351:GLU:OE1	2.31	0.48
4:E:125:PRO:O	4:E:127:ILE:N	2.47	0.48
1:A:786:HIS:CE1	2:B:742:GLU:OE1	2.68	0.47
1:A:567:LYS:CB	1:A:568:PRO:CD	2.93	0.46
2:B:896:ASP:OD2	10:L:29:TYR:OH	2.34	0.46
1:A:869:GLY:O	4:E:204:THR:CG2	2.64	0.46
1:A:711:ARG:NH2	7:I:87:GLN:OE1	2.49	0.45
3:C:173:ALA:O	3:C:174:ALA:CB	2.65	0.45
2:B:1037:LEU:O	8:J:47:ARG:NH1	2.50	0.45
2:B:732:SER:O	2:B:734:HIS:N	2.50	0.44
6:H:82:PRO:O	6:H:84:ALA:N	2.51	0.44
2:B:804:GLY:O	2:B:983:ARG:NH2	2.51	0.44
2:B:363:HIS:O	2:B:364:ILE:CB	2.66	0.44
1:A:167:CYS:SG	1:A:168:GLY:N	2.91	0.44
2:B:96:TYR:N	2:B:129:PHE:O	2.51	0.44
6:H:43:ASN:N	6:H:95:TYR:OH	2.51	0.44
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.51	0.43
2:B:604:ARG:NH2	2:B:697:GLU:OE1	2.51	0.43
2:B:228:LYS:O	2:B:261:ARG:NH2	2.51	0.43
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	3.01	0.43
6:H:89:LEU:O	6:H:91:ASP:N	2.52	0.43
2:B:976:ILE:O	2:B:990:ILE:O	2.36	0.43
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.67	0.43
1:A:1353:TYR:CD2	1:A:1353:TYR:C	2.93	0.42
2:B:839:MET:O	2:B:991:GLY:N	2.52	0.42
1:A:351:THR:OG1	2:B:1103:ILE:CD1	2.68	0.42
2:B:822:ASN:O	8:J:48:ARG:NE	2.53	0.41
7:I:75:CYS:O	7:I:78:CYS:O	2.38	0.41
1:A:657:LEU:O	1:A:661:GLY:N	2.54	0.41
1:A:491:VAL:O	1:A:493:GLN:NE2	2.54	0.41
3:C:242:GLN:O	3:C:246:ARG:N	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:105:GLY:O	3:C:149:LYS:O	2.37	0.41
1:A:541:ILE:N	1:A:572:TRP:O	2.54	0.41
6:H:47:PHE:CB	6:H:95:TYR:CD1	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	1205 (86%)	137 (10%)	53 (4%)	5	34
2	B	1096/1224 (90%)	958 (87%)	90 (8%)	48 (4%)	4	29
3	C	264/318 (83%)	238 (90%)	19 (7%)	7 (3%)	8	46
4	E	212/215 (99%)	185 (87%)	22 (10%)	5 (2%)	9	51
5	F	83/155 (54%)	75 (90%)	6 (7%)	2 (2%)	9	51
6	H	129/146 (88%)	102 (79%)	18 (14%)	9 (7%)	2	13
7	I	117/122 (96%)	101 (86%)	14 (12%)	2 (2%)	14	62
8	J	63/70 (90%)	55 (87%)	7 (11%)	1 (2%)	14	63
9	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
10	L	44/70 (63%)	27 (61%)	7 (16%)	10 (23%)	0	0
All	All	3515/4173 (84%)	3053 (87%)	325 (9%)	137 (4%)	5	33

All (137) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	65	LEU
1	A	119	ASN
1	A	399	HIS
1	A	424	ILE
1	A	567	LYS
1	A	597	LEU

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Mol	Chain	Res	Type
1	A	846	GLU
1	A	1123	GLY
1	A	1221	LYS
1	A	1378	GLN
1	A	1437	GLY
2	B	137	TYR
2	B	476	ARG
2	B	510	LYS
2	B	648	HIS
2	B	709	ASP
2	B	712	PRO
2	B	733	HIS
2	B	751	VAL
2	B	1046	PRO
2	B	1156	ASP
3	C	40	GLU
3	C	215	GLU
3	C	227	THR
4	E	126	SER
5	F	73	ALA
6	H	83	GLN
6	H	131	ASN
7	I	91	ARG
8	J	6	ARG
10	L	50	ASP
1	A	68	GLN
1	A	250	ILE
1	A	312	PRO
1	A	332	LYS
1	A	385	ILE
1	A	672	ASP
1	A	1124	HIS
1	A	1188	GLN
1	A	1377	THR
2	B	67	SER
2	B	138	GLU
2	B	168	GLY
2	B	176	SER
2	B	277	LYS
2	B	364	ILE
2	B	480	SER
2	B	531	GLN

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Mol	Chain	Res	Type
2	B	708	GLU
2	B	891	ASP
2	B	1171	VAL
2	B	1181	GLU
3	C	174	ALA
6	H	90	ALA
7	I	115	LYS
10	L	49	LYS
10	L	51	CYS
10	L	64	LEU
1	A	42	ASP
1	A	308	ILE
1	A	324	SER
1	A	592	ASP
1	A	595	THR
1	A	1089	VAL
2	B	250	PHE
2	B	367	LEU
2	B	468	GLU
2	B	792	MET
2	B	864	LYS
2	B	865	LYS
2	B	879	ARG
2	B	887	HIS
2	B	974	PRO
2	B	1157	ALA
2	B	1180	PHE
2	B	1223	ASP
3	C	4	GLU
4	E	3	GLN
4	E	99	HIS
5	F	112	GLU
6	H	18	GLY
6	H	108	SER
10	L	40	LEU
1	A	53	LEU
1	A	56	PRO
1	A	110	CYS
1	A	111	GLY
1	A	149	GLU
1	A	214	ILE
1	A	275	SER

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Mol	Chain	Res	Type
1	A	569	LYS
1	A	852	TYR
2	B	474	SER
2	B	943	SER
2	B	1017	ILE
3	C	90	ASP
4	E	51	GLY
6	H	109	LYS
6	H	136	LYS
6	H	140	ALA
10	L	47	ARG
10	L	55	ILE
10	L	56	LEU
1	A	217	LYS
1	A	400	PRO
1	A	576	GLN
1	A	916	GLY
1	A	958	VAL
1	A	1376	THR
2	B	139	ALA
2	B	1099	VAL
10	L	46	VAL
10	L	59	ALA
1	A	543	LEU
1	A	1028	THR
2	B	177	LYS
2	B	447	ALA
2	B	471	LYS
4	E	37	LEU
1	A	73	GLY
1	A	258	GLY
1	A	325	ILE
2	B	647	GLY
3	C	5	GLY
1	A	35	ILE
1	A	1122	PRO
1	A	1388	GLY
2	B	592	ASN
2	B	479	VAL
2	B	711	GLU
2	B	907	GLY
2	B	1119	VAL

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Mol	Chain	Res	Type
6	H	107	VAL
1	A	973	ILE
1	A	1384	VAL
1	A	775	ILE

5.3.2 Protein sidechains ⓘ

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%)	1046 (85%)	179 (15%)	5	21
2	B	967/1061 (91%)	840 (87%)	127 (13%)	6	28
3	C	234/274 (85%)	208 (89%)	26 (11%)	9	36
4	E	196/197 (100%)	174 (89%)	22 (11%)	9	36
5	F	75/137 (55%)	64 (85%)	11 (15%)	4	21
6	H	117/128 (91%)	99 (85%)	18 (15%)	4	18
7	I	113/116 (97%)	101 (89%)	12 (11%)	10	38
8	J	60/65 (92%)	49 (82%)	11 (18%)	2	12
9	K	99/102 (97%)	83 (84%)	16 (16%)	3	15
10	L	40/57 (70%)	27 (68%)	13 (32%)	0	0
All	All	3126/3657 (86%)	2691 (86%)	435 (14%)	5	24

All (435) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	THR
1	A	18	GLN
1	A	21	LEU
1	A	50	ILE
1	A	58	LEU
1	A	62	ASP
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS

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Mol	Chain	Res	Type
1	A	75	ASN
1	A	83	HIS
1	A	93	VAL
1	A	113	LEU
1	A	126	LEU
1	A	129	LYS
1	A	133	LYS
1	A	134	ARG
1	A	141	LEU
1	A	144	THR
1	A	147	VAL
1	A	151	ASP
1	A	152	VAL
1	A	170	THR
1	A	206	GLU
1	A	214	ILE
1	A	219	PHE
1	A	220	THR
1	A	226	GLU
1	A	232	GLU
1	A	235	ILE
1	A	237	THR
1	A	252	PHE
1	A	254	GLU
1	A	263	THR
1	A	265	LYS
1	A	270	LEU
1	A	276	LEU
1	A	278	THR
1	A	279	LEU
1	A	290	GLU
1	A	291	GLU
1	A	295	LEU
1	A	308	ILE
1	A	311	GLN
1	A	315	LEU
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	329	LEU
1	A	335	ARG
1	A	344	ARG

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Mol	Chain	Res	Type
1	A	353	ILE
1	A	354	SER
1	A	359	LEU
1	A	368	LYS
1	A	389	THR
1	A	398	GLU
1	A	407	ARG
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	455	MET
1	A	456	MET
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	493	GLN
1	A	500	GLU
1	A	513	SER
1	A	518	LYS
1	A	527	THR
1	A	532	ARG
1	A	541	ILE
1	A	560	ILE
1	A	567	LYS
1	A	569	LYS
1	A	595	THR
1	A	597	LEU
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	636	GLU
1	A	640	GLN
1	A	644	LYS
1	A	672	ASP
1	A	678	GLU
1	A	681	GLU

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Mol	Chain	Res	Type
1	A	688	LYS
1	A	691	LEU
1	A	705	LYS
1	A	710	LEU
1	A	719	VAL
1	A	722	LEU
1	A	728	LYS
1	A	740	LEU
1	A	756	ILE
1	A	762	SER
1	A	773	LYS
1	A	774	ARG
1	A	782	ARG
1	A	806	ARG
1	A	821	ARG
1	A	838	GLN
1	A	839	ARG
1	A	867	ILE
1	A	883	LEU
1	A	894	GLU
1	A	896	ARG
1	A	902	LEU
1	A	905	ASP
1	A	908	LEU
1	A	912	LEU
1	A	919	ILE
1	A	920	LEU
1	A	923	LEU
1	A	926	GLN
1	A	941	LYS
1	A	953	ASN
1	A	969	GLN
1	A	973	ILE
1	A	982	THR
1	A	988	LEU
1	A	992	ASP
1	A	1005	GLU
1	A	1025	ARG
1	A	1029	ARG
1	A	1048	ASN
1	A	1062	GLU
1	A	1067	LEU

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Mol	Chain	Res	Type
1	A	1081	LEU
1	A	1086	PHE
1	A	1089	VAL
1	A	1109	LYS
1	A	1110	ASN
1	A	1116	LEU
1	A	1124	HIS
1	A	1141	THR
1	A	1147	THR
1	A	1165	GLU
1	A	1172	LEU
1	A	1175	SER
1	A	1187	GLN
1	A	1215	ARG
1	A	1227	ILE
1	A	1242	VAL
1	A	1256	GLU
1	A	1261	LYS
1	A	1280	GLU
1	A	1283	VAL
1	A	1284	MET
1	A	1288	ASP
1	A	1293	SER
1	A	1295	THR
1	A	1297	GLU
1	A	1303	GLU
1	A	1308	THR
1	A	1327	ILE
1	A	1333	ILE
1	A	1334	ASP
1	A	1350	LYS
1	A	1354	ASN
1	A	1364	ASN
1	A	1366	ARG
1	A	1382	THR
1	A	1385	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1432	GLN
1	A	1436	ILE
1	A	1438	THR
1	A	1442	ASP

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Mol	Chain	Res	Type
1	A	1444	MET
2	B	28	GLU
2	B	41	LYS
2	B	45	SER
2	B	46	GLN
2	B	63	ILE
2	B	89	GLU
2	B	101	MET
2	B	102	VAL
2	B	128	LEU
2	B	130	VAL
2	B	134	LYS
2	B	135	ARG
2	B	165	VAL
2	B	167	ILE
2	B	175	ARG
2	B	178	ASN
2	B	187	SER
2	B	194	GLU
2	B	208	SER
2	B	217	ARG
2	B	221	ASN
2	B	234	ILE
2	B	245	GLU
2	B	261	ARG
2	B	265	SER
2	B	267	ARG
2	B	277	LYS
2	B	292	ILE
2	B	306	ASN
2	B	323	VAL
2	B	325	GLN
2	B	333	PHE
2	B	350	GLN
2	B	367	LEU
2	B	373	ARG
2	B	376	PHE
2	B	384	ARG
2	B	392	ARG
2	B	393	LYS
2	B	394	ASP
2	B	398	ARG

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Mol	Chain	Res	Type
2	B	401	PHE
2	B	418	LYS
2	B	433	GLN
2	B	437	GLU
2	B	448	ILE
2	B	458	LYS
2	B	461	LEU
2	B	466	TRP
2	B	468	GLU
2	B	471	LYS
2	B	479	VAL
2	B	485	ARG
2	B	486	TYR
2	B	537	LYS
2	B	547	VAL
2	B	554	ILE
2	B	574	SER
2	B	591	ARG
2	B	598	GLU
2	B	604	ARG
2	B	616	ILE
2	B	620	ARG
2	B	629	ASP
2	B	642	ASP
2	B	643	ASP
2	B	645	SER
2	B	649	LYS
2	B	653	VAL
2	B	655	LYS
2	B	690	VAL
2	B	694	ASP
2	B	696	GLU
2	B	706	GLN
2	B	711	GLU
2	B	737	THR
2	B	776	GLN
2	B	780	VAL
2	B	786	ASN
2	B	788	ARG
2	B	790	ASP
2	B	791	THR
2	B	797	TYR

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Mol	Chain	Res	Type
2	B	807	ARG
2	B	815	ARG
2	B	835	GLN
2	B	838	SER
2	B	844	SER
2	B	866	TYR
2	B	870	ILE
2	B	875	GLU
2	B	880	THR
2	B	883	LEU
2	B	886	LYS
2	B	906	SER
2	B	945	GLU
2	B	959	ASP
2	B	961	LEU
2	B	963	PHE
2	B	973	ILE
2	B	983	ARG
2	B	987	LYS
2	B	993	THR
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1010	LEU
2	B	1065	GLN
2	B	1067	ARG
2	B	1094	ARG
2	B	1096	ARG
2	B	1099	VAL
2	B	1106	ARG
2	B	1108	ARG
2	B	1111	MET
2	B	1122	ARG
2	B	1128	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1172	ILE
2	B	1181	GLU
2	B	1195	HIS

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Mol	Chain	Res	Type
2	B	1202	LEU
2	B	1211	ASN
3	C	9	LYS
3	C	12	GLU
3	C	43	THR
3	C	53	THR
3	C	75	MET
3	C	77	ILE
3	C	80	LEU
3	C	100	THR
3	C	109	SER
3	C	119	VAL
3	C	129	ILE
3	C	136	ASP
3	C	137	LYS
3	C	151	GLN
3	C	156	THR
3	C	157	CYS
3	C	215	GLU
3	C	222	LYS
3	C	231	ASN
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	259	LEU
3	C	265	MET
3	C	266	ASP
3	C	268	ASP
4	E	7	ARG
4	E	30	ILE
4	E	52	ARG
4	E	54	GLN
4	E	55	ARG
4	E	61	GLN
4	E	65	THR
4	E	75	MET
4	E	78	LEU
4	E	90	VAL
4	E	95	THR
4	E	100	ILE
4	E	104	ASN
4	E	127	ILE

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Mol	Chain	Res	Type
4	E	142	VAL
4	E	156	LEU
4	E	158	SER
4	E	162	ARG
4	E	169	ARG
4	E	204	THR
4	E	213	ILE
4	E	215	MET
5	F	71	GLU
5	F	78	GLN
5	F	82	THR
5	F	99	LEU
5	F	110	ASP
5	F	111	LEU
5	F	112	GLU
5	F	119	ARG
5	F	127	GLU
5	F	138	LEU
5	F	152	ILE
6	H	11	GLN
6	H	13	SER
6	H	24	CYS
6	H	26	ILE
6	H	34	ASP
6	H	35	GLN
6	H	56	THR
6	H	63	LEU
6	H	77	ARG
6	H	87	ARG
6	H	92	ASP
6	H	107	VAL
6	H	109	LYS
6	H	111	LEU
6	H	130	ARG
6	H	132	LEU
6	H	135	LEU
6	H	139	ASN
7	I	12	ASN
7	I	17	ARG
7	I	31	THR
7	I	35	VAL
7	I	37	GLU

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Mol	Chain	Res	Type
7	I	61	ASP
7	I	62	ILE
7	I	70	ARG
7	I	88	SER
7	I	90	GLN
7	I	97	MET
7	I	118	ARG
8	J	1	MET
8	J	3	VAL
8	J	7	CYS
8	J	13	VAL
8	J	19	GLU
8	J	22	LEU
8	J	37	SER
8	J	43	ARG
8	J	48	ARG
8	J	62	ARG
8	J	64	ASN
9	K	1	MET
9	K	11	LEU
9	K	12	LEU
9	K	14	GLU
9	K	20	LYS
9	K	26	LYS
9	K	31	VAL
9	K	54	ARG
9	K	63	VAL
9	K	74	ARG
9	K	75	ILE
9	K	78	THR
9	K	81	TYR
9	K	85	ASP
9	K	97	LYS
9	K	101	LEU
10	L	26	THR
10	L	27	LEU
10	L	28	LYS
10	L	33	GLU
10	L	44	ASP
10	L	48	CYS
10	L	50	ASP
10	L	51	CYS

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Mol	Chain	Res	Type
10	L	55	ILE
10	L	58	LYS
10	L	62	LYS
10	L	64	LEU
10	L	65	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	3/5 (60%)	1 (33%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	8	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
13	GTP	R	100	-	34,34,34	1.59	7 (20%)	51,54,54	2.14	11 (21%)

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
13	GTP	R	100	-	-	0/22/38/38	0/1/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R	100	GTP	PA-O3A	3.40	1.66	1.59
13	R	100	GTP	PB-O3A	3.29	1.65	1.59
13	R	100	GTP	C2-N2	3.08	1.37	1.32
13	R	100	GTP	PB-O3B	2.80	1.65	1.59
13	R	100	GTP	O4'-C1'	2.59	1.45	1.41
13	R	100	GTP	PG-O3B	2.40	1.64	1.60
13	R	100	GTP	C8-N7	-2.40	1.29	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R	100	GTP	C6-C5-N7	7.83	135.19	134.14
13	R	100	GTP	PB-O3B-PG	-4.68	117.97	131.68
13	R	100	GTP	N3-C4-N9	4.60	133.66	126.91
13	R	100	GTP	O3A-PB-O3B	4.52	110.85	101.66
13	R	100	GTP	C2-N3-C4	4.29	121.12	115.09
13	R	100	GTP	C5-C4-N3	-3.90	120.30	125.94
13	R	100	GTP	PA-O3A-PB	-3.81	120.51	131.68
13	R	100	GTP	C4-C5-N7	-3.38	106.62	109.52
13	R	100	GTP	O4'-C1'-N9	3.03	111.26	108.44
13	R	100	GTP	C4'-O4'-C1'	-2.47	107.06	109.75
13	R	100	GTP	C3'-C2'-C1'	-2.17	97.51	100.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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%)	-0.10	29 (2%)	60	15	49, 97, 192, 214	0
2	B	1114/1224 (91%)	-0.21	14 (1%)	74	24	48, 84, 152, 204	0
3	C	266/318 (83%)	-0.32	0	100	100	58, 81, 117, 175	0
4	E	214/215 (99%)	-0.17	0	100	100	69, 124, 172, 182	0
5	F	85/155 (54%)	-0.27	0	100	100	73, 103, 140, 156	0
6	H	133/146 (91%)	0.02	1 (0%)	83	35	97, 131, 163, 178	0
7	I	119/122 (97%)	-0.25	0	100	100	61, 101, 141, 156	0
8	J	65/70 (92%)	-0.30	0	100	100	55, 73, 107, 123	0
9	K	114/120 (95%)	-0.32	0	100	100	59, 91, 118, 133	0
10	L	46/70 (65%)	-0.06	1 (2%)	59	14	70, 116, 147, 156	0
11	R	5/5 (100%)	2.40	3 (60%)	0	0	202, 206, 209, 212	0
12	T	8/29 (27%)	1.12	2 (25%)	1	1	169, 178, 191, 196	0
All	All	3574/4207 (84%)	-0.16	50 (1%)	72	22	48, 94, 180, 214	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	4.9
2	B	1222	ARG	4.0
2	B	883	LEU	4.0
11	R	6	A	3.8
1	A	72	GLU	3.7
11	R	8	A	3.7
1	A	161	LEU	3.7
1	A	316	GLN	3.7
1	A	73	GLY	3.2
1	A	317	LYS	3.0
1	A	1085	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	2.8
1	A	87	ALA	2.8
1	A	41	MET	2.8
12	T	16	DC	2.7
2	B	471	LYS	2.7
2	B	477	ALA	2.6
2	B	1169	MET	2.6
1	A	315	LEU	2.6
1	A	1087	ALA	2.6
1	A	45	GLN	2.6
1	A	1086	PHE	2.5
11	R	7	G	2.5
2	B	865	LYS	2.5
1	A	44	THR	2.5
1	A	151	ASP	2.5
1	A	286	HIS	2.5
12	T	23	DC	2.5
1	A	42	ASP	2.4
1	A	212	LYS	2.3
2	B	470	LYS	2.3
1	A	200	ARG	2.3
2	B	1224	PHE	2.3
2	B	882	THR	2.3
10	L	27	LEU	2.2
2	B	246	LYS	2.2
2	B	866	TYR	2.2
2	B	468	GLU	2.2
1	A	176	LYS	2.2
2	B	1223	ASP	2.1
1	A	283	GLY	2.1
1	A	153	PRO	2.1
1	A	65	LEU	2.1
1	A	1391	ARG	2.1
1	A	1090	ALA	2.1
2	B	474	SER	2.1
1	A	280	GLU	2.0
6	H	83	GLN	2.0
1	A	257	ARG	2.0
1	A	250	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
13	GTP	R	100	32/32	0.36	3.60	249,251,254,256	0
14	ZN	C	319	1/1	0.11	-0.62	89,89,89,89	0
14	ZN	J	101	1/1	0.17	-0.98	78,78,78,78	0
14	ZN	I	204	1/1	0.08	-1.13	82,82,82,82	0
14	ZN	B	1307	1/1	0.10	-1.21	183,183,183,183	0
14	ZN	I	203	1/1	0.06	-1.22	102,102,102,102	0
14	ZN	A	1735	1/1	0.16	-1.57	176,176,176,176	0
15	MG	A	2001	1/1	0.06	-2.19	60,60,60,60	0
14	ZN	L	105	1/1	0.05	-2.22	99,99,99,99	0
14	ZN	A	1734	1/1	0.06	-2.76	289,289,289,289	0

6.5 Other polymers ⓘ

There are no such residues in this entry.