



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:38 AM GMT

PDB ID : 3S1N
Title : RNA Polymerase II Initiation Complex with a 5-nt RNA (variant 2)
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-15
Resolution : 3.10 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>

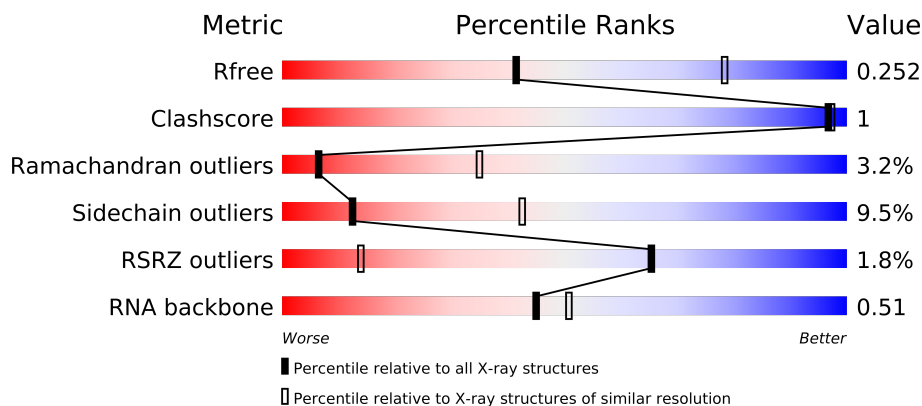
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 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	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28570 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*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	5	Total	C	N	O	P	0	0	0
			107	49	23	31	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*GP*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
			162	77	28	49	8			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

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

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

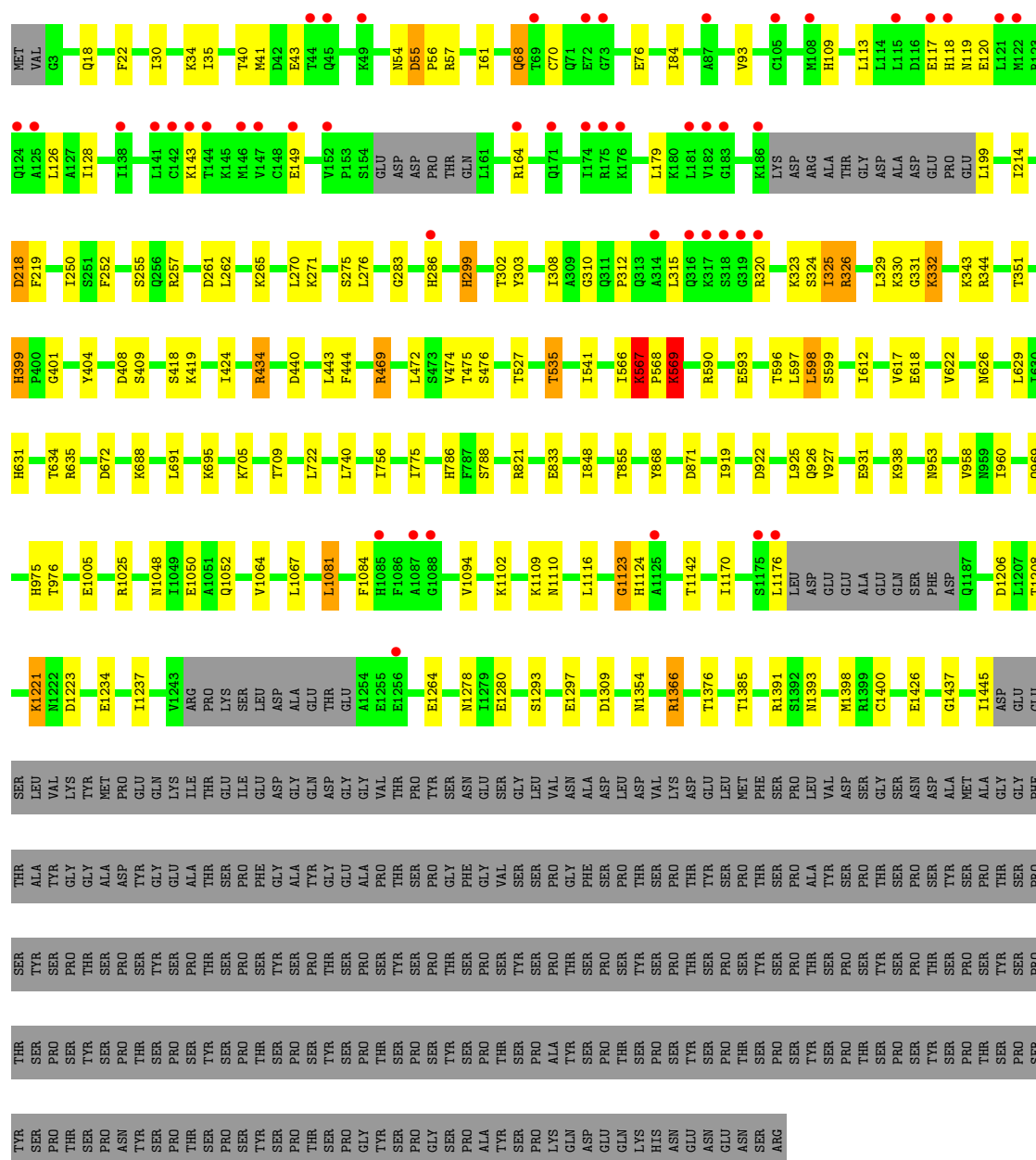
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

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.

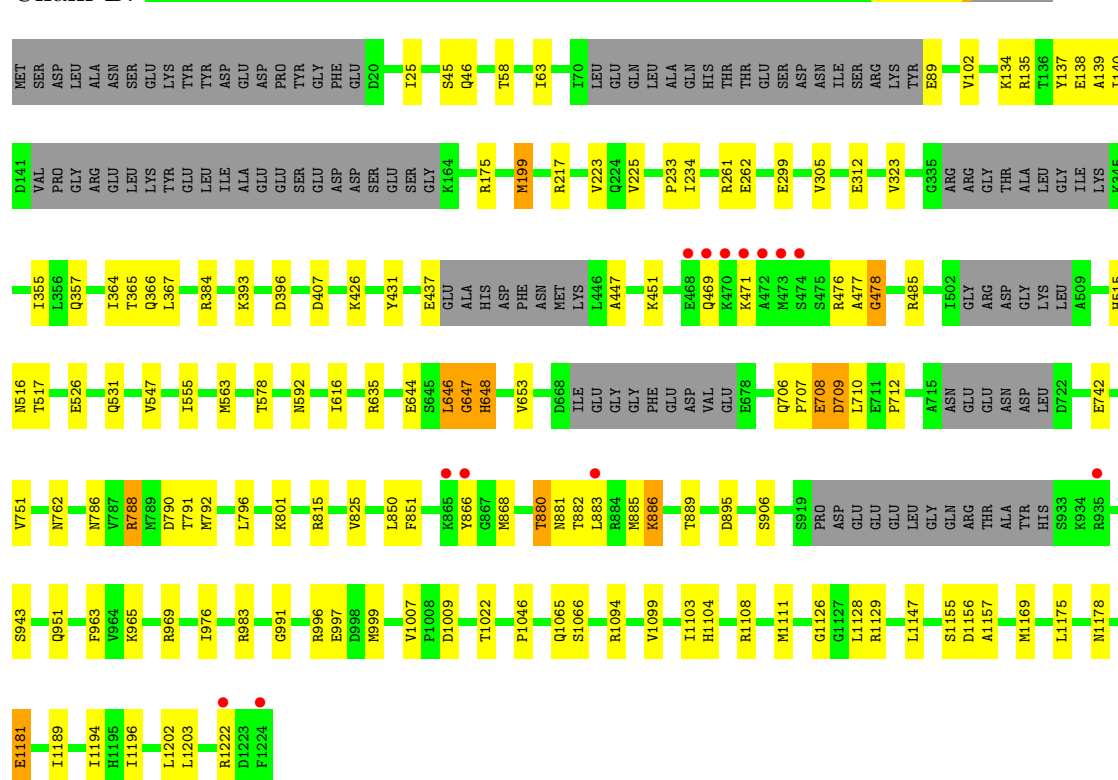
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A: 



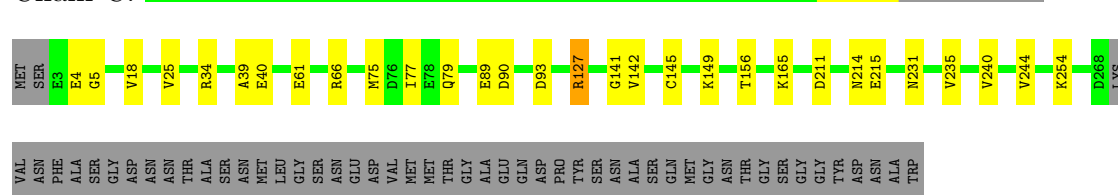
- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:



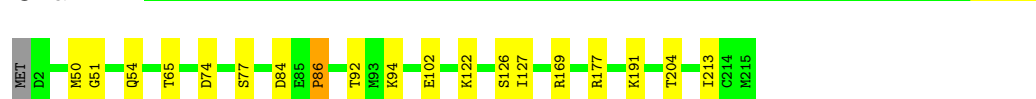
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



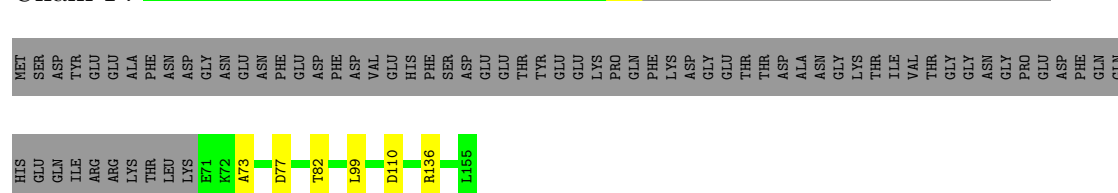
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



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

Chain F:



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

Chain H: 



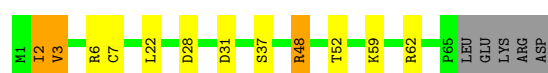
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 



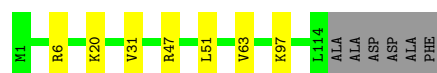
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 



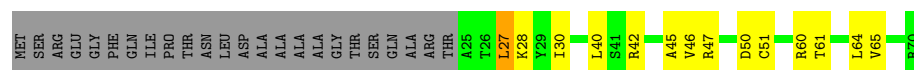
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 



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

Chain L: 



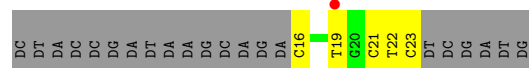
- Molecule 11: RNA (5'-R(*AP*GP*AP*GP*C)-3')

Chain R: 



- Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*C
P*GP*AP*TP*GP*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	157.30Å 221.13Å 191.94Å 90.00° 97.52° 90.00°	Depositor
Resolution (Å)	47.80 – 3.10 47.80 – 3.08	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.80-3.10) 99.0 (47.80-3.08)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.191 , 0.232 0.208 , 0.252	Depositor DCC
R_{free} test set	5960 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 118893 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28570	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	0/11241	0.72	3/15199 (0.0%)
2	B	0.43	0/9033	0.71	3/12181 (0.0%)
3	C	0.40	0/2133	0.71	1/2891 (0.0%)
4	E	0.41	0/1788	0.66	0/2406
5	F	0.42	0/700	0.64	0/945
6	H	0.42	0/1086	0.74	0/1470
7	I	0.41	0/989	0.74	0/1331
8	J	0.47	0/541	0.78	0/727
9	K	0.38	0/937	0.62	0/1265
10	L	0.48	0/365	0.82	0/485
11	R	0.92	0/120	1.45	1/186 (0.5%)
12	T	1.15	0/180	1.93	6/275 (2.2%)
All	All	0.44	0/29113	0.73	14/39361 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	22	DT	O4'-C1'-N1	8.29	113.80	108.00
2	B	647	GLY	C-N-CA	8.15	142.07	121.70
1	A	218	ASP	C-N-CA	7.05	139.32	121.70
12	T	19	DT	O4'-C1'-N1	6.59	112.61	108.00
12	T	16	DC	O4'-C1'-N1	6.19	112.33	108.00
1	A	1123	GLY	C-N-CA	5.99	136.68	121.70
2	B	648	HIS	N-CA-CB	5.80	121.05	110.60
1	A	117	GLU	C-N-CA	5.54	135.55	121.70
11	R	10	C	O4'-C1'-N1	5.38	112.50	108.20
3	C	39	ALA	N-CA-C	5.32	125.37	111.00
2	B	140	ILE	C-N-CA	5.26	134.85	121.70
12	T	23	DC	O4'-C1'-N1	5.15	111.60	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	21	DC	O4'-C1'-N1	5.13	111.59	108.00
12	T	19	DT	P-O3'-C3'	5.05	125.76	119.70

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	12	0
2	B	8861	0	0	14	0
3	C	2095	0	0	4	0
4	E	1752	0	0	0	0
5	F	688	0	5	1	0
6	H	1068	0	0	0	0
7	I	971	0	0	0	0
8	J	532	0	0	3	0
9	K	919	0	0	1	0
10	L	363	0	0	0	0
11	R	107	0	0	0	0
12	T	162	0	0	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	28570	0	28	28	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 1.

All (28) 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	2.24	0.70
3:C:66:ARG:NH2	8:J:3:VAL:O	2.31	0.63
1:A:399:HIS:O	1:A:401:GLY:N	2.32	0.62
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.33	0.60
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.36	0.58
3:C:93:ASP:O	3:C:127:ARG:NH2	2.36	0.57
3:C:165:LYS:O	9:K:6:ARG:NH1	2.40	0.55
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.43	0.52
1:A:626:ASN:O	1:A:631:HIS:CD2	2.63	0.51
1:A:324:SER:O	1:A:326:ARG:N	2.43	0.51
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.44	0.51
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.94	0.50
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.65	0.50
1:A:567:LYS:O	1:A:569:LYS:N	2.45	0.50
2:B:801:LYS:O	8:J:52:THR:CG2	2.60	0.48
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.48	0.47
5:F:82:THR:O	5:F:136:ARG:NH1	2.49	0.46
2:B:199:MET:N	2:B:199:MET:SD	2.89	0.46
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.48	0.46
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.49	0.46
2:B:880:THR:O	2:B:882:THR:N	2.49	0.45
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.50	0.44
1:A:596:THR:O	1:A:598:LEU:N	2.51	0.44
1:A:55:ASP:O	1:A:57:ARG:N	2.51	0.44
2:B:476:ARG:O	2:B:478:GLY:N	2.51	0.43
1:A:535:THR:CG2	1:A:617:VAL:N	2.82	0.43
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.52	0.42
1:A:786:HIS:CE1	2:B:742:GLU:OE1	2.74	0.41

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%)	1237 (89%)	112 (8%)	46 (3%)	6 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1096/1224 (90%)	966 (88%)	94 (9%)	36 (3%)	6	33
3	C	264/318 (83%)	247 (94%)	11 (4%)	6 (2%)	10	45
4	E	212/215 (99%)	201 (95%)	7 (3%)	4 (2%)	12	51
5	F	83/155 (54%)	74 (89%)	8 (10%)	1 (1%)	19	62
6	H	129/146 (88%)	99 (77%)	22 (17%)	8 (6%)	2	16
7	I	117/122 (96%)	101 (86%)	14 (12%)	2 (2%)	14	54
8	J	63/70 (90%)	59 (94%)	2 (3%)	2 (3%)	6	35
9	K	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
10	L	44/70 (63%)	31 (70%)	6 (14%)	7 (16%)	0	1
All	All	3515/4173 (84%)	3124 (89%)	279 (8%)	112 (3%)	6	35

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	ASP
1	A	109	HIS
1	A	325	ILE
1	A	567	LYS
1	A	1223	ASP
2	B	139	ALA
2	B	367	LEU
2	B	469	GLN
2	B	477	ALA
2	B	648	HIS
2	B	712	PRO
2	B	751	VAL
2	B	880	THR
2	B	1046	PRO
2	B	1156	ASP
3	C	4	GLU
4	E	77	SER
6	H	85	GLY
6	H	109	LYS
6	H	131	ASN
6	H	140	ALA
8	J	2	ILE
10	L	28	LYS
10	L	46	VAL

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Mol	Chain	Res	Type
10	L	50	ASP
10	L	60	ARG
1	A	40	THR
1	A	219	PHE
1	A	286	HIS
1	A	299	HIS
1	A	409	SER
1	A	418	SER
1	A	569	LYS
1	A	597	LEU
1	A	1081	LEU
1	A	1123	GLY
1	A	1124	HIS
1	A	1437	GLY
2	B	137	TYR
2	B	707	PRO
2	B	709	ASP
2	B	850	LEU
2	B	881	ASN
2	B	883	LEU
2	B	1066	SER
3	C	5	GLY
3	C	141	GLY
4	E	86	PRO
6	H	90	ALA
10	L	64	LEU
1	A	68	GLN
1	A	76	GLU
1	A	118	HIS
1	A	250	ILE
1	A	312	PRO
1	A	332	LYS
1	A	922	ASP
1	A	1221	LYS
2	B	138	GLU
2	B	526	GLU
2	B	563	MET
2	B	792	MET
2	B	886	LYS
3	C	90	ASP
4	E	126	SER
6	H	108	SER

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Mol	Chain	Res	Type
8	J	6	ARG
1	A	214	ILE
1	A	255	SER
1	A	275	SER
1	A	424	ILE
1	A	775	ILE
1	A	1278	ASN
2	B	478	GLY
2	B	646	LEU
2	B	647	GLY
2	B	708	GLU
2	B	943	SER
2	B	1155	SER
2	B	1181	GLU
3	C	142	VAL
7	I	3	THR
7	I	77	LYS
1	A	257	ARG
1	A	593	GLU
1	A	958	VAL
1	A	975	HIS
2	B	364	ILE
2	B	447	ALA
2	B	592	ASN
2	B	1157	ALA
2	B	1169	MET
3	C	214	ASN
5	F	73	ALA
6	H	17	PRO
10	L	27	LEU
10	L	45	ALA
1	A	35	ILE
1	A	56	PRO
1	A	119	ASN
1	A	399	HIS
1	A	404	TYR
2	B	1108	ARG
1	A	283	GLY
1	A	310	GLY
6	H	18	GLY
1	A	331	GLY
1	A	568	PRO

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Mol	Chain	Res	Type
2	B	976	ILE
1	A	599	SER
4	E	51	GLY

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%)	1098 (90%)	127 (10%)	10	36
2	B	967/1061 (91%)	881 (91%)	86 (9%)	14	47
3	C	234/274 (85%)	215 (92%)	19 (8%)	17	53
4	E	196/197 (100%)	180 (92%)	16 (8%)	17	53
5	F	75/137 (55%)	72 (96%)	3 (4%)	42	82
6	H	117/128 (91%)	101 (86%)	16 (14%)	5	21
7	I	113/116 (97%)	106 (94%)	7 (6%)	26	66
8	J	60/65 (92%)	50 (83%)	10 (17%)	3	11
9	K	99/102 (97%)	93 (94%)	6 (6%)	26	67
10	L	40/57 (70%)	32 (80%)	8 (20%)	2	8
All	All	3126/3657 (86%)	2828 (90%)	298 (10%)	12	42

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	22	PHE
1	A	30	ILE
1	A	34	LYS
1	A	41	MET
1	A	43	GLU
1	A	61	ILE
1	A	68	GLN
1	A	70	CYS
1	A	84	ILE
1	A	93	VAL

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Mol	Chain	Res	Type
1	A	113	LEU
1	A	120	GLU
1	A	126	LEU
1	A	128	ILE
1	A	143	LYS
1	A	149	GLU
1	A	164	ARG
1	A	179	LEU
1	A	199	LEU
1	A	218	ASP
1	A	252	PHE
1	A	261	ASP
1	A	262	LEU
1	A	265	LYS
1	A	270	LEU
1	A	271	LYS
1	A	276	LEU
1	A	299	HIS
1	A	302	THR
1	A	303	TYR
1	A	308	ILE
1	A	315	LEU
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	326	ARG
1	A	329	LEU
1	A	330	LYS
1	A	332	LYS
1	A	343	LYS
1	A	344	ARG
1	A	351	THR
1	A	408	ASP
1	A	419	LYS
1	A	434	ARG
1	A	443	LEU
1	A	444	PHE
1	A	469	ARG
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER

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Mol	Chain	Res	Type
1	A	527	THR
1	A	535	THR
1	A	541	ILE
1	A	566	ILE
1	A	567	LYS
1	A	569	LYS
1	A	590	ARG
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	672	ASP
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	705	LYS
1	A	709	THR
1	A	722	LEU
1	A	740	LEU
1	A	756	ILE
1	A	788	SER
1	A	821	ARG
1	A	833	GLU
1	A	848	ILE
1	A	855	THR
1	A	919	ILE
1	A	925	LEU
1	A	926	GLN
1	A	927	VAL
1	A	931	GLU
1	A	938	LYS
1	A	953	ASN
1	A	960	ILE
1	A	969	GLN
1	A	976	THR
1	A	1005	GLU
1	A	1025	ARG
1	A	1048	ASN
1	A	1050	GLU

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Mol	Chain	Res	Type
1	A	1052	GLN
1	A	1067	LEU
1	A	1081	LEU
1	A	1084	PHE
1	A	1094	VAL
1	A	1102	LYS
1	A	1109	LYS
1	A	1110	ASN
1	A	1116	LEU
1	A	1142	THR
1	A	1170	ILE
1	A	1176	LEU
1	A	1206	ASP
1	A	1208	THR
1	A	1221	LYS
1	A	1234	GLU
1	A	1237	ILE
1	A	1264	GLU
1	A	1280	GLU
1	A	1293	SER
1	A	1297	GLU
1	A	1309	ASP
1	A	1354	ASN
1	A	1366	ARG
1	A	1376	THR
1	A	1385	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1400	CYS
1	A	1426	GLU
1	A	1445	ILE
2	B	25	ILE
2	B	45	SER
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	89	GLU
2	B	102	VAL
2	B	134	LYS
2	B	135	ARG
2	B	175	ARG

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Mol	Chain	Res	Type
2	B	199	MET
2	B	223	VAL
2	B	225	VAL
2	B	233	PRO
2	B	234	ILE
2	B	261	ARG
2	B	262	GLU
2	B	299	GLU
2	B	305	VAL
2	B	312	GLU
2	B	323	VAL
2	B	355	ILE
2	B	357	GLN
2	B	365	THR
2	B	366	GLN
2	B	384	ARG
2	B	393	LYS
2	B	396	ASP
2	B	426	LYS
2	B	431	TYR
2	B	437	GLU
2	B	451	LYS
2	B	471	LYS
2	B	485	ARG
2	B	516	ASN
2	B	531	GLN
2	B	547	VAL
2	B	555	ILE
2	B	578	THR
2	B	616	ILE
2	B	644	GLU
2	B	646	LEU
2	B	653	VAL
2	B	706	GLN
2	B	708	GLU
2	B	709	ASP
2	B	710	LEU
2	B	762	ASN
2	B	786	ASN
2	B	788	ARG
2	B	791	THR
2	B	796	LEU

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Mol	Chain	Res	Type
2	B	815	ARG
2	B	825	VAL
2	B	866	TYR
2	B	868	MET
2	B	885	MET
2	B	886	LYS
2	B	889	THR
2	B	895	ASP
2	B	906	SER
2	B	951	GLN
2	B	963	PHE
2	B	965	LYS
2	B	983	ARG
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1022	THR
2	B	1065	GLN
2	B	1099	VAL
2	B	1103	ILE
2	B	1111	MET
2	B	1128	LEU
2	B	1129	ARG
2	B	1147	LEU
2	B	1175	LEU
2	B	1178	ASN
2	B	1181	GLU
2	B	1189	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1203	LEU
2	B	1222	ARG
3	C	18	VAL
3	C	25	VAL
3	C	34	ARG
3	C	40	GLU
3	C	75	MET
3	C	77	ILE
3	C	79	GLN
3	C	89	GLU

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Mol	Chain	Res	Type
3	C	127	ARG
3	C	145	CYS
3	C	149	LYS
3	C	156	THR
3	C	211	ASP
3	C	215	GLU
3	C	231	ASN
3	C	235	VAL
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
4	E	50	MET
4	E	54	GLN
4	E	65	THR
4	E	74	ASP
4	E	84	ASP
4	E	86	PRO
4	E	92	THR
4	E	94	LYS
4	E	102	GLU
4	E	122	LYS
4	E	127	ILE
4	E	169	ARG
4	E	177	ARG
4	E	191	LYS
4	E	204	THR
4	E	213	ILE
5	F	77	ASP
5	F	99	LEU
5	F	110	ASP
6	H	5	LEU
6	H	16	ASP
6	H	21	ASN
6	H	22	LYS
6	H	26	ILE
6	H	35	GLN
6	H	42	ILE
6	H	46	LEU
6	H	86	ASP
6	H	87	ARG
6	H	94	ASP
6	H	107	VAL

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Mol	Chain	Res	Type
6	H	130	ARG
6	H	136	LYS
6	H	139	ASN
6	H	142	LEU
7	I	35	VAL
7	I	50	THR
7	I	52	ILE
7	I	77	LYS
7	I	84	VAL
7	I	111	THR
7	I	117	LYS
8	J	2	ILE
8	J	3	VAL
8	J	7	CYS
8	J	22	LEU
8	J	28	ASP
8	J	31	ASP
8	J	37	SER
8	J	48	ARG
8	J	59	LYS
8	J	62	ARG
9	K	20	LYS
9	K	31	VAL
9	K	47	ARG
9	K	51	LEU
9	K	63	VAL
9	K	97	LYS
10	L	27	LEU
10	L	30	ILE
10	L	40	LEU
10	L	42	ARG
10	L	47	ARG
10	L	51	CYS
10	L	61	THR
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	4/5 (80%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	7	G

There are no RNA pucker outliers to report.

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

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 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	0.05	48 (3%)	43	6	42, 82, 183, 220	0
2	B	1114/1224 (91%)	-0.10	13 (1%)	75	20	39, 77, 146, 186	0
3	C	266/318 (83%)	-0.25	0	100	100	46, 72, 108, 145	0
4	E	214/215 (99%)	-0.06	0	100	100	52, 112, 155, 167	0
5	F	85/155 (54%)	-0.26	0	100	100	60, 90, 128, 150	0
6	H	133/146 (91%)	0.10	2 (1%)	70	16	72, 113, 146, 159	0
7	I	119/122 (97%)	-0.26	0	100	100	55, 84, 120, 131	0
8	J	65/70 (92%)	-0.22	0	100	100	46, 66, 98, 109	0
9	K	114/120 (95%)	-0.21	0	100	100	44, 74, 100, 118	0
10	L	46/70 (65%)	-0.01	0	100	100	53, 108, 135, 156	0
11	R	5/5 (100%)	0.73	0	100	100	170, 176, 182, 183	0
12	T	8/29 (27%)	0.55	1 (12%)	5	1	158, 164, 180, 181	0
All	All	3574/4207 (84%)	-0.05	64 (1%)	65	14	39, 82, 167, 220	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	LYS	5.1
1	A	1176	LEU	4.7
2	B	865	LYS	3.8
1	A	1087	ALA	3.8
2	B	883	LEU	3.7
1	A	87	ALA	3.7
1	A	118	HIS	3.6
1	A	316	GLN	3.6
1	A	319	GLY	3.5
6	H	85	GLY	3.3
1	A	49	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	469	GLN	3.2
1	A	45	GLN	3.1
2	B	470	LYS	3.1
1	A	73	GLY	3.0
1	A	144	THR	3.0
1	A	1085	HIS	3.0
1	A	141	LEU	3.0
1	A	183	GLY	3.0
1	A	44	THR	3.0
1	A	121	LEU	2.9
1	A	171	GLN	2.9
2	B	866	TYR	2.9
1	A	69	THR	2.8
1	A	72	GLU	2.8
2	B	472	ALA	2.8
2	B	471	LYS	2.7
1	A	146	MET	2.7
1	A	320	ARG	2.6
1	A	176	LYS	2.6
1	A	115	LEU	2.6
1	A	125	ALA	2.5
1	A	142	CYS	2.5
1	A	117	GLU	2.5
1	A	314	ALA	2.5
2	B	468	GLU	2.4
1	A	122	MET	2.4
1	A	143	LYS	2.4
1	A	105	CYS	2.4
1	A	108	MET	2.4
1	A	318	SER	2.4
6	H	132	LEU	2.3
2	B	473	MET	2.3
1	A	1256	GLU	2.3
1	A	182	VAL	2.3
2	B	1222	ARG	2.3
1	A	138	ILE	2.3
1	A	1125	ALA	2.2
1	A	149	GLU	2.2
1	A	1088	GLY	2.2
1	A	175	ARG	2.2
1	A	181	LEU	2.1
12	T	19	DT	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	147	VAL	2.1
1	A	124	GLN	2.1
1	A	152	VAL	2.1
1	A	186	LYS	2.1
1	A	286	HIS	2.0
1	A	174	ILE	2.0
2	B	1224	PHE	2.0
1	A	164	ARG	2.0
2	B	935	ARG	2.0
1	A	1175	SER	2.0
2	B	474	SER	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	ZN	I	204	1/1	0.11	-0.74	63,63,63,63	0
13	ZN	I	203	1/1	0.10	-0.94	94,94,94,94	0
13	ZN	A	1734	1/1	0.26	-0.96	300,300,300,300	0
13	ZN	C	319	1/1	0.10	-1.06	66,66,66,66	0
13	ZN	J	101	1/1	0.20	-1.36	57,57,57,57	0
13	ZN	B	1307	1/1	0.07	-1.42	159,159,159,159	0
13	ZN	L	105	1/1	0.09	-1.64	102,102,102,102	0
14	MG	A	2001	1/1	0.11	-2.38	42,42,42,42	0
13	ZN	A	1735	1/1	0.06	-2.64	146,146,146,146	0

6.5 Other polymers ⓘ

There are no such residues in this entry.