



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:06 PM GMT

PDB ID : 3S14
Title : RNA Polymerase II Initiation Complex with a 6-nt RNA
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-14
Resolution : 2.85 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>

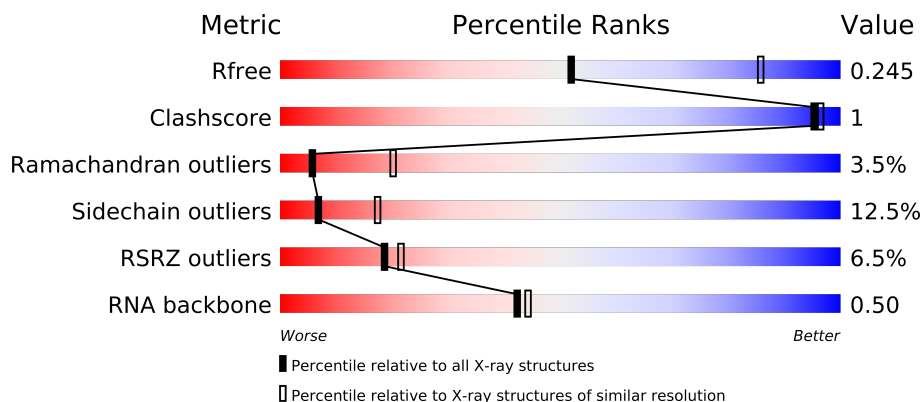
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.85 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	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)
RNA backbone	1838	1014 (3.32-2.40)

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	6	
12	T	29	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28695 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(*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	6	Total	C	N	O	P	0	0	0
			133	60	30	38	5			

- 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	13	Total	C	N	O	P	0	0	0
			261	125	43	80	13			

- 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

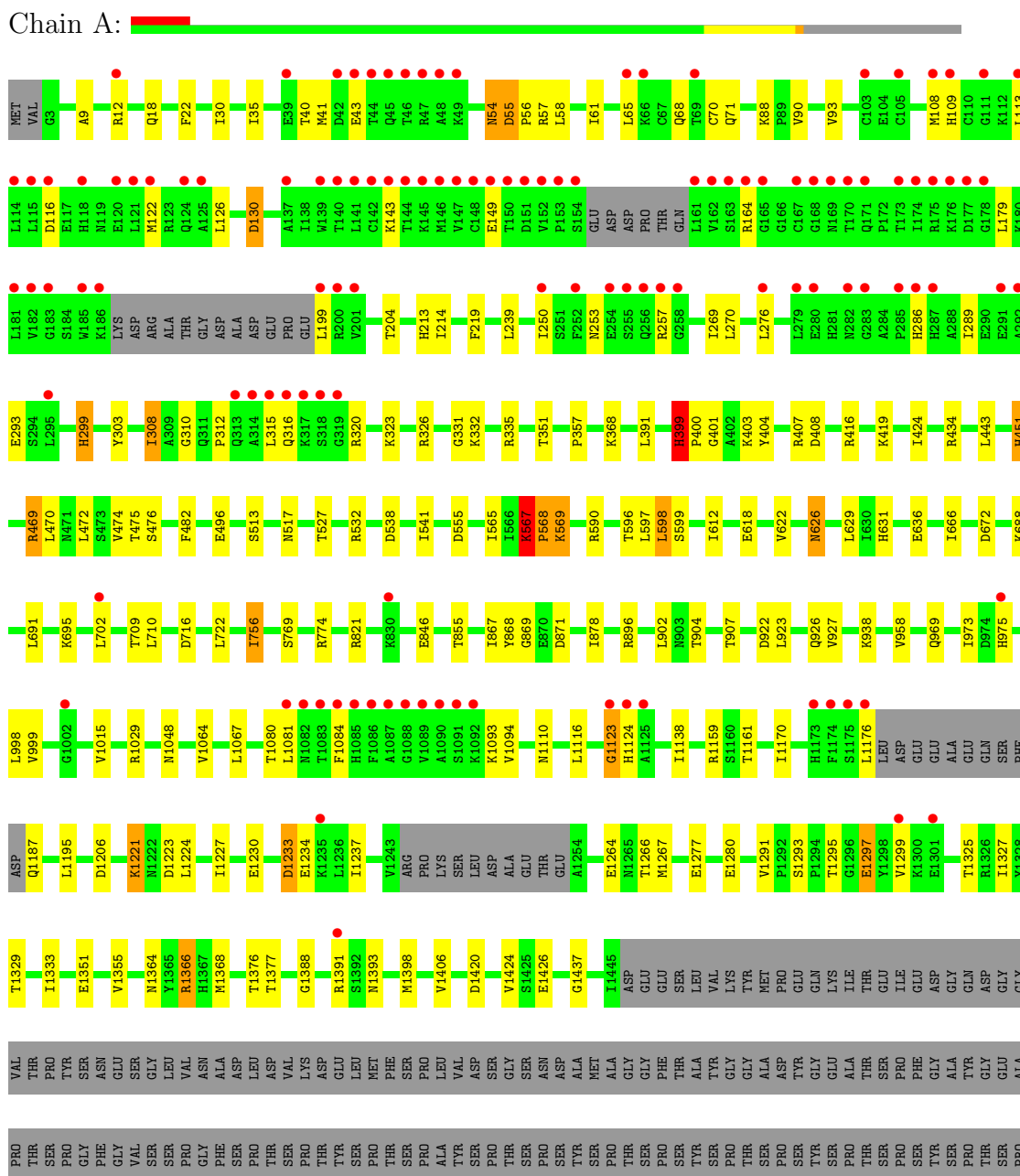
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots

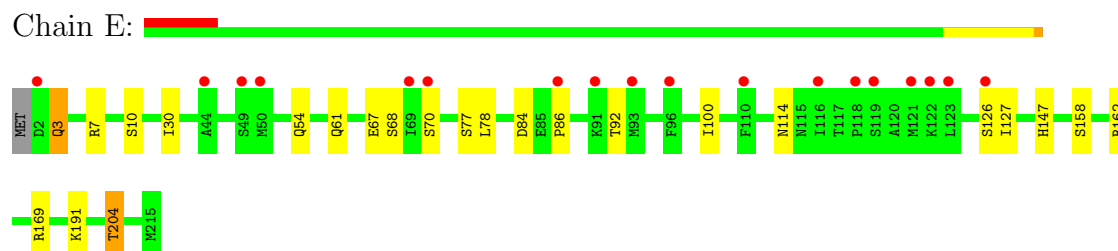
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

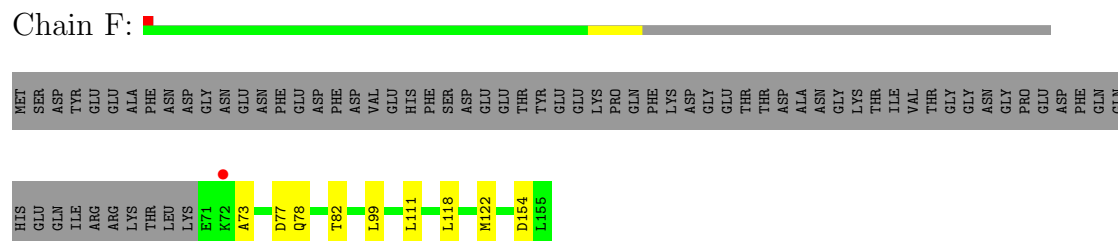




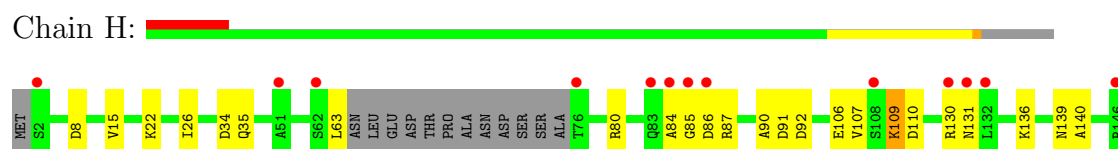
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



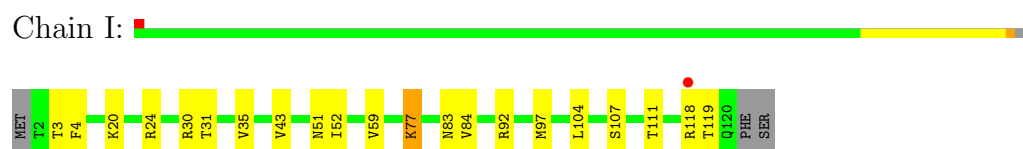
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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



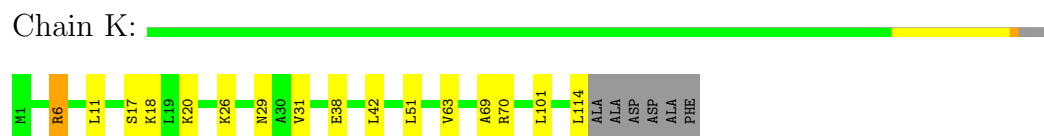
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



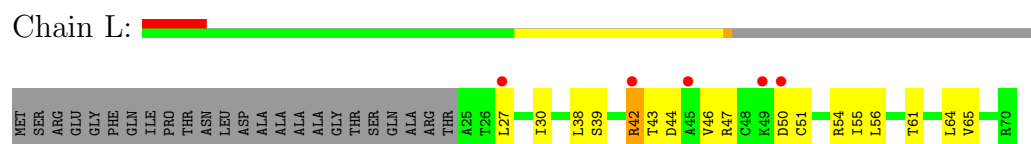
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



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



- Molecule 11: RNA (5'-R(*GP*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*C
P*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	159.34Å 221.34Å 192.37Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	39.46 – 2.85 39.46 – 2.84	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.46-2.85) 99.5 (39.46-2.84)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.189 , 0.227 0.206 , 0.245	Depositor DCC
R_{free} test set	7772 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.8	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 154852 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28695	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: 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	0.51	0/11241	0.79	3/15199 (0.0%)
2	B	0.53	0/9033	0.82	3/12181 (0.0%)
3	C	0.49	0/2133	0.83	1/2891 (0.0%)
4	E	0.45	0/1788	0.72	0/2406
5	F	0.48	0/700	0.70	0/945
6	H	0.50	0/1086	0.84	0/1470
7	I	0.54	0/989	0.87	1/1331 (0.1%)
8	J	0.56	0/541	0.87	0/727
9	K	0.45	0/937	0.74	0/1265
10	L	0.56	0/365	0.94	0/485
11	R	1.08	0/150	1.55	1/234 (0.4%)
12	T	1.18	0/290	2.30	22/444 (5.0%)
All	All	0.53	0/29253	0.84	31/39578 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	24	DT	O4'-C1'-N1	11.54	116.08	108.00
12	T	16	DC	P-O3'-C3'	11.48	133.47	119.70
12	T	21	DC	O4'-C4'-C3'	-11.25	99.25	106.00
12	T	22	DT	O4'-C4'-C3'	-9.49	100.31	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	17	DG	O4'-C1'-N9	8.94	114.26	108.00
2	B	647	GLY	C-N-CA	8.52	143.01	121.70
12	T	22	DT	C4'-C3'-C2'	-7.87	96.02	103.10
12	T	27	DA	O4'-C1'-N9	7.86	113.50	108.00
12	T	17	DG	O4'-C4'-C3'	-7.86	101.29	106.00
12	T	20	DC	O4'-C1'-N1	7.74	113.42	108.00
12	T	16	DC	O4'-C1'-N1	7.51	113.26	108.00
2	B	648	HIS	N-CA-CB	7.08	123.34	110.60
12	T	25	DC	O4'-C1'-N1	6.80	112.76	108.00
12	T	21	DC	C4'-C3'-C2'	-6.69	97.08	103.10
3	C	172	PRO	C-N-CA	6.54	138.06	121.70
12	T	20	DC	O4'-C4'-C3'	-6.15	102.04	104.50
1	A	1123	GLY	C-N-CA	6.12	137.00	121.70
1	A	451	HIS	CB-CA-C	-5.86	98.68	110.40
11	R	6	A	P-O3'-C3'	5.82	126.69	119.70
12	T	22	DT	O4'-C1'-N1	5.77	112.04	108.00
12	T	19	DT	C4-C5-C7	5.75	122.45	119.00
12	T	27	DA	C1'-O4'-C4'	-5.58	104.52	110.10
12	T	22	DT	C4-C5-C7	5.51	122.31	119.00
12	T	19	DT	C4'-C3'-C2'	-5.40	98.24	103.10
1	A	399	HIS	N-CA-CB	5.40	120.32	110.60
12	T	19	DT	C6-C5-C7	-5.31	119.71	122.90
2	B	140	ILE	C-N-CA	5.26	134.85	121.70
12	T	28	DT	C4-C5-C7	5.22	122.13	119.00
12	T	27	DA	P-O3'-C3'	5.14	125.87	119.70
12	T	23	DC	O4'-C4'-C3'	-5.08	102.47	104.50
7	I	59	VAL	N-CA-CB	-5.01	100.48	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	647	GLY	Peptide

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	20	0
2	B	8861	0	0	17	0
3	C	2095	0	0	3	0
4	E	1752	0	0	2	0
5	F	688	0	5	0	0
6	H	1068	0	0	0	0
7	I	971	0	0	0	0
8	J	532	0	0	2	0
9	K	919	0	0	3	0
10	L	363	0	0	0	0
11	R	133	0	0	0	0
12	T	261	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	28695	0	28	38	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 (38) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:867:ILE:CD1	1:A:867:ILE:CG1	1.77	1.57
1:A:756:ILE:CD1	1:A:756:ILE:CG1	1.83	1.55
1:A:399:HIS:O	1:A:401:GLY:N	2.22	0.72
2:B:976:ILE:O	2:B:990:ILE:O	2.08	0.72
3:C:66:ARG:NH2	8:J:3:VAL:O	2.26	0.68
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.31	0.63
2:B:950:ASP:OD2	2:B:967:ARG:NH1	2.31	0.63
2:B:1094:ARG:CG	2:B:1094:ARG:NH1	2.62	0.62
1:A:469:ARG:NH2	2:B:991:GLY:O	2.32	0.62
1:A:55:ASP:O	1:A:57:ARG:N	2.33	0.61
1:A:567:LYS:O	1:A:569:LYS:N	2.33	0.61
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.36	0.58
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.58	0.57
1:A:626:ASN:O	1:A:631:HIS:CD2	2.59	0.56
3:C:165:LYS:O	9:K:6:ARG:NH1	2.39	0.55
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.42	0.53
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.92	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:476:ARG:O	2:B:478:GLY:N	2.43	0.52
9:K:38:GLU:O	9:K:69:ALA:O	2.28	0.52
2:B:708:GLU:O	2:B:710:LEU:N	2.43	0.51
2:B:882:THR:O	2:B:884:ARG:N	2.45	0.50
1:A:596:THR:O	1:A:598:LEU:N	2.45	0.50
3:C:173:ALA:O	3:C:233:GLU:O	2.31	0.48
2:B:209:GLU:OE1	2:B:788:ARG:NH2	2.47	0.48
1:A:565:ILE:CG2	1:A:567:LYS:CD	2.93	0.47
1:A:1364:ASN:ND2	1:A:1366:ARG:CD	2.79	0.46
2:B:1013:ASN:OD1	2:B:1015:HIS:CD2	2.69	0.46
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.34	0.46
1:A:567:LYS:CG	1:A:568:PRO:CD	2.94	0.45
2:B:728:ARG:NH1	2:B:760:ASP:OD2	2.49	0.45
1:A:567:LYS:CB	1:A:568:PRO:CD	2.96	0.44
1:A:517:ASN:ND2	1:A:1364:ASN:OD1	2.51	0.43
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.51	0.43
1:A:482:PHE:N	2:B:836:GLU:O	2.52	0.42
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.53	0.42
1:A:1327:ILE:O	4:E:147:HIS:CE1	2.74	0.41
1:A:869:GLY:O	4:E:204:THR:CG2	2.69	0.41
1:A:9:ALA:O	2:B:1193:GLN:NE2	2.55	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%)	1251 (90%)	100 (7%)	44 (3%)	6	22
2	B	1096/1224 (90%)	963 (88%)	86 (8%)	47 (4%)	4	13
3	C	264/318 (83%)	243 (92%)	13 (5%)	8 (3%)	7	24
4	E	212/215 (99%)	199 (94%)	10 (5%)	3 (1%)	16	49
5	F	83/155 (54%)	77 (93%)	3 (4%)	3 (4%)	5	19
6	H	129/146 (88%)	106 (82%)	17 (13%)	6 (5%)	4	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	I	117/122 (96%)	103 (88%)	9 (8%)	5 (4%)	4	13
8	J	63/70 (90%)	59 (94%)	2 (3%)	2 (3%)	6	22
9	K	112/120 (93%)	106 (95%)	5 (4%)	1 (1%)	25	62
10	L	44/70 (63%)	32 (73%)	7 (16%)	5 (11%)	1	1
All	All	3515/4173 (84%)	3139 (89%)	252 (7%)	124 (4%)	6	20

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	54	ASN
1	A	55	ASP
1	A	109	HIS
1	A	257	ARG
1	A	399	HIS
1	A	424	ILE
1	A	567	LYS
1	A	923	LEU
1	A	1234	GLU
2	B	67	SER
2	B	137	TYR
2	B	371	GLU
2	B	469	GLN
2	B	477	ALA
2	B	592	ASN
2	B	709	ASP
2	B	712	PRO
2	B	732	SER
2	B	734	HIS
2	B	883	LEU
2	B	887	HIS
2	B	1046	PRO
2	B	1156	ASP
2	B	1181	GLU
2	B	1223	ASP
3	C	173	ALA
3	C	227	THR
5	F	73	ALA
5	F	78	GLN
6	H	131	ASN
6	H	140	ALA

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Mol	Chain	Res	Type
7	I	118	ARG
8	J	2	ILE
1	A	56	PRO
1	A	214	ILE
1	A	250	ILE
1	A	1123	GLY
1	A	1124	HIS
1	A	1221	LYS
1	A	1437	GLY
2	B	138	GLU
2	B	368	GLU
2	B	465	ASN
2	B	483	LEU
2	B	526	GLU
2	B	531	GLN
2	B	648	HIS
2	B	888	GLY
2	B	1221	SER
3	C	141	GLY
3	C	142	VAL
6	H	90	ALA
6	H	109	LYS
8	J	6	ARG
10	L	46	VAL
10	L	51	CYS
1	A	310	GLY
1	A	312	PRO
1	A	331	GLY
1	A	332	LYS
1	A	597	LEU
1	A	672	ASP
1	A	1377	THR
2	B	139	ALA
2	B	249	ARG
2	B	474	SER
2	B	563	MET
2	B	646	LEU
2	B	882	THR
3	C	4	GLU
4	E	126	SER
10	L	42	ARG
10	L	56	LEU

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Mol	Chain	Res	Type
10	L	64	LEU
1	A	130	ASP
1	A	568	PRO
1	A	569	LYS
1	A	958	VAL
1	A	1081	LEU
1	A	1233	ASP
2	B	346	GLU
3	C	5	GLY
7	I	3	THR
7	I	20	LYS
7	I	77	LYS
9	K	70	ARG
1	A	65	LEU
1	A	286	HIS
1	A	299	HIS
1	A	400	PRO
1	A	404	TYR
1	A	975	HIS
1	A	1093	LYS
2	B	230	ALA
2	B	482	VAL
2	B	707	PRO
2	B	708	GLU
2	B	713	ALA
2	B	943	SER
2	B	1178	ASN
3	C	90	ASP
3	C	149	LYS
4	E	3	GLN
5	F	154	ASP
6	H	84	ALA
7	I	107	SER
1	A	35	ILE
1	A	149	GLU
1	A	213	HIS
1	A	308	ILE
1	A	846	GLU
2	B	647	GLY
2	B	792	MET
2	B	1171	VAL
2	B	1173	ALA

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Mol	Chain	Res	Type
2	B	1176	ASN
4	E	86	PRO
1	A	599	SER
1	A	1388	GLY
6	H	85	GLY
2	B	731	VAL
2	B	751	VAL
2	B	1017	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%)	1073 (88%)	152 (12%)	7	17
2	B	967/1061 (91%)	855 (88%)	112 (12%)	8	21
3	C	234/274 (85%)	205 (88%)	29 (12%)	7	17
4	E	196/197 (100%)	175 (89%)	21 (11%)	10	26
5	F	75/137 (55%)	69 (92%)	6 (8%)	17	44
6	H	117/128 (91%)	98 (84%)	19 (16%)	3	9
7	I	113/116 (97%)	97 (86%)	16 (14%)	5	12
8	J	60/65 (92%)	49 (82%)	11 (18%)	2	6
9	K	99/102 (97%)	86 (87%)	13 (13%)	6	15
10	L	40/57 (70%)	27 (68%)	13 (32%)	0	0
All	All	3126/3657 (86%)	2734 (88%)	392 (12%)	7	17

All (392) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	18	GLN
1	A	22	PHE
1	A	30	ILE
1	A	41	MET
1	A	43	GLU

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Mol	Chain	Res	Type
1	A	54	ASN
1	A	58	LEU
1	A	61	ILE
1	A	68	GLN
1	A	70	CYS
1	A	71	GLN
1	A	88	LYS
1	A	90	VAL
1	A	93	VAL
1	A	108	MET
1	A	113	LEU
1	A	116	ASP
1	A	122	MET
1	A	126	LEU
1	A	130	ASP
1	A	143	LYS
1	A	164	ARG
1	A	179	LEU
1	A	199	LEU
1	A	204	THR
1	A	219	PHE
1	A	239	LEU
1	A	253	ASN
1	A	269	ILE
1	A	270	LEU
1	A	276	LEU
1	A	289	ILE
1	A	293	GLU
1	A	299	HIS
1	A	303	TYR
1	A	308	ILE
1	A	315	LEU
1	A	316	GLN
1	A	320	ARG
1	A	323	LYS
1	A	326	ARG
1	A	335	ARG
1	A	351	THR
1	A	357	PRO
1	A	368	LYS
1	A	391	LEU
1	A	403	LYS

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Mol	Chain	Res	Type
1	A	407	ARG
1	A	408	ASP
1	A	416	ARG
1	A	419	LYS
1	A	434	ARG
1	A	443	LEU
1	A	451	HIS
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	496	GLU
1	A	513	SER
1	A	527	THR
1	A	532	ARG
1	A	538	ASP
1	A	541	ILE
1	A	555	ASP
1	A	567	LYS
1	A	590	ARG
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	626	ASN
1	A	629	LEU
1	A	636	GLU
1	A	666	ILE
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	702	LEU
1	A	709	THR
1	A	710	LEU
1	A	716	ASP
1	A	722	LEU
1	A	756	ILE
1	A	769	SER
1	A	774	ARG
1	A	821	ARG

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Mol	Chain	Res	Type
1	A	855	THR
1	A	878	ILE
1	A	896	ARG
1	A	902	LEU
1	A	904	THR
1	A	907	THR
1	A	922	ASP
1	A	926	GLN
1	A	927	VAL
1	A	938	LYS
1	A	969	GLN
1	A	973	ILE
1	A	998	LEU
1	A	999	VAL
1	A	1015	VAL
1	A	1029	ARG
1	A	1048	ASN
1	A	1067	LEU
1	A	1080	THR
1	A	1084	PHE
1	A	1094	VAL
1	A	1110	ASN
1	A	1116	LEU
1	A	1138	ILE
1	A	1159	ARG
1	A	1161	THR
1	A	1170	ILE
1	A	1176	LEU
1	A	1187	GLN
1	A	1195	LEU
1	A	1206	ASP
1	A	1221	LYS
1	A	1223	ASP
1	A	1224	LEU
1	A	1227	ILE
1	A	1230	GLU
1	A	1233	ASP
1	A	1237	ILE
1	A	1264	GLU
1	A	1266	THR
1	A	1267	MET
1	A	1277	GLU

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Mol	Chain	Res	Type
1	A	1280	GLU
1	A	1291	VAL
1	A	1293	SER
1	A	1297	GLU
1	A	1299	VAL
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1351	GLU
1	A	1355	VAL
1	A	1366	ARG
1	A	1368	MET
1	A	1376	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1406	VAL
1	A	1420	ASP
1	A	1424	VAL
1	A	1426	GLU
2	B	25	ILE
2	B	28	GLU
2	B	30	SER
2	B	46	GLN
2	B	63	ILE
2	B	94	LYS
2	B	101	MET
2	B	102	VAL
2	B	106	ASP
2	B	108	VAL
2	B	133	LYS
2	B	134	LYS
2	B	135	ARG
2	B	178	ASN
2	B	183	GLU
2	B	187	SER
2	B	194	GLU
2	B	199	MET
2	B	208	SER
2	B	217	ARG
2	B	222	ILE
2	B	223	VAL

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Mol	Chain	Res	Type
2	B	234	ILE
2	B	242	SER
2	B	272	THR
2	B	276	ILE
2	B	277	LYS
2	B	278	GLN
2	B	299	GLU
2	B	323	VAL
2	B	345	LYS
2	B	361	LEU
2	B	366	GLN
2	B	382	ILE
2	B	393	LYS
2	B	416	LEU
2	B	418	LYS
2	B	436	VAL
2	B	437	GLU
2	B	451	LYS
2	B	458	LYS
2	B	469	GLN
2	B	471	LYS
2	B	485	ARG
2	B	489	SER
2	B	500	THR
2	B	513	GLN
2	B	522	VAL
2	B	537	LYS
2	B	547	VAL
2	B	549	THR
2	B	567	GLU
2	B	612	GLU
2	B	615	MET
2	B	624	LEU
2	B	646	LEU
2	B	653	VAL
2	B	658	ILE
2	B	690	VAL
2	B	708	GLU
2	B	732	SER
2	B	780	VAL
2	B	783	THR
2	B	786	ASN

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Mol	Chain	Res	Type
2	B	815	ARG
2	B	825	VAL
2	B	839	MET
2	B	864	LYS
2	B	868	MET
2	B	869	SER
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	895	ASP
2	B	898	LEU
2	B	916	THR
2	B	935	ARG
2	B	951	GLN
2	B	953	LEU
2	B	956	THR
2	B	963	PHE
2	B	964	VAL
2	B	976	ILE
2	B	992	ILE
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1010	LEU
2	B	1012	ILE
2	B	1065	GLN
2	B	1077	THR
2	B	1094	ARG
2	B	1096	ARG
2	B	1099	VAL
2	B	1103	ILE
2	B	1111	MET
2	B	1147	LEU
2	B	1151	LEU
2	B	1155	SER
2	B	1156	ASP
2	B	1160	VAL
2	B	1178	ASN
2	B	1181	GLU
2	B	1188	LYS

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Mol	Chain	Res	Type
2	B	1189	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1210	MET
2	B	1222	ARG
3	C	18	VAL
3	C	23	SER
3	C	34	ARG
3	C	41	ILE
3	C	57	VAL
3	C	66	ARG
3	C	69	LEU
3	C	75	MET
3	C	77	ILE
3	C	79	GLN
3	C	100	THR
3	C	106	GLU
3	C	116	LYS
3	C	121	VAL
3	C	129	ILE
3	C	149	LYS
3	C	197	SER
3	C	199	LYS
3	C	205	LYS
3	C	215	GLU
3	C	226	ASP
3	C	231	ASN
3	C	235	VAL
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	259	LEU
3	C	264	GLN
3	C	267	GLN
4	E	3	GLN
4	E	7	ARG
4	E	10	SER
4	E	30	ILE
4	E	54	GLN
4	E	61	GLN
4	E	67	GLU

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Mol	Chain	Res	Type
4	E	68	SER
4	E	70	SER
4	E	77	SER
4	E	78	LEU
4	E	84	ASP
4	E	92	THR
4	E	100	ILE
4	E	114	ASN
4	E	127	ILE
4	E	158	SER
4	E	162	ARG
4	E	169	ARG
4	E	191	LYS
4	E	204	THR
5	F	77	ASP
5	F	82	THR
5	F	99	LEU
5	F	111	LEU
5	F	118	LEU
5	F	122	MET
6	H	8	ASP
6	H	15	VAL
6	H	22	LYS
6	H	26	ILE
6	H	34	ASP
6	H	35	GLN
6	H	63	LEU
6	H	80	ARG
6	H	86	ASP
6	H	87	ARG
6	H	91	ASP
6	H	92	ASP
6	H	106	GLU
6	H	107	VAL
6	H	109	LYS
6	H	110	ASP
6	H	130	ARG
6	H	136	LYS
6	H	139	ASN
7	I	4	PHE
7	I	24	ARG
7	I	30	ARG

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Mol	Chain	Res	Type
7	I	31	THR
7	I	35	VAL
7	I	43	VAL
7	I	51	ASN
7	I	52	ILE
7	I	77	LYS
7	I	83	ASN
7	I	84	VAL
7	I	92	ARG
7	I	97	MET
7	I	104	LEU
7	I	111	THR
7	I	119	THR
8	J	1	MET
8	J	2	ILE
8	J	3	VAL
8	J	7	CYS
8	J	9	SER
8	J	13	VAL
8	J	31	ASP
8	J	48	ARG
8	J	52	THR
8	J	59	LYS
8	J	62	ARG
9	K	6	ARG
9	K	11	LEU
9	K	17	SER
9	K	18	LYS
9	K	20	LYS
9	K	26	LYS
9	K	29	ASN
9	K	31	VAL
9	K	42	LEU
9	K	51	LEU
9	K	63	VAL
9	K	101	LEU
9	K	114	LEU
10	L	27	LEU
10	L	30	ILE
10	L	38	LEU
10	L	39	SER
10	L	42	ARG

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Mol	Chain	Res	Type
10	L	43	THR
10	L	44	ASP
10	L	47	ARG
10	L	50	ASP
10	L	54	ARG
10	L	55	ILE
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	5/6 (83%)	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 ⓘ

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%)	0.26	121 (8%) 11 12	37, 78, 167, 219	0
2	B	1114/1224 (91%)	0.14	65 (5%) 22 26	39, 70, 132, 181	0
3	C	266/318 (83%)	-0.20	5 (1%) 64 72	46, 65, 106, 158	0
4	E	214/215 (99%)	0.32	18 (8%) 11 13	53, 107, 156, 168	0
5	F	85/155 (54%)	0.11	1 (1%) 75 83	57, 86, 127, 151	0
6	H	133/146 (91%)	0.46	13 (9%) 8 10	68, 112, 147, 158	0
7	I	119/122 (97%)	-0.09	1 (0%) 83 89	53, 84, 122, 136	0
8	J	65/70 (92%)	-0.11	2 (3%) 47 56	44, 60, 95, 105	0
9	K	114/120 (95%)	-0.29	0 100 100	42, 73, 96, 113	0
10	L	46/70 (65%)	0.42	5 (10%) 6 8	56, 101, 135, 144	0
11	R	6/6 (100%)	-0.02	0 100 100	66, 78, 114, 130	0
12	T	13/29 (44%)	0.43	2 (15%) 3 3	84, 103, 163, 171	0
All	All	3580/4208 (85%)	0.16	233 (6%) 18 21	37, 77, 150, 219	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	18.0
2	B	883	LEU	10.5
1	A	44	THR	9.7
1	A	1087	ALA	9.2
2	B	474	SER	8.6
2	B	1224	PHE	8.4
1	A	317	LYS	8.4
1	A	147	VAL	8.0
1	A	144	THR	7.9
1	A	1086	PHE	7.9
6	H	132	LEU	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	7.6
1	A	255	SER	7.5
1	A	152	VAL	7.4
1	A	319	GLY	7.0
1	A	149	GLU	6.8
1	A	161	LEU	6.7
1	A	1082	ASN	6.6
1	A	49	LYS	6.6
2	B	866	TYR	6.6
1	A	316	GLN	6.5
1	A	182	VAL	6.4
2	B	477	ALA	6.1
2	B	1222	ARG	6.0
2	B	473	MET	5.9
6	H	86	ASP	5.9
1	A	183	GLY	5.8
1	A	114	LEU	5.8
2	B	1223	ASP	5.7
1	A	250	ILE	5.7
1	A	141	LEU	5.6
1	A	162	VAL	5.5
2	B	136	THR	5.5
2	B	865	LYS	5.3
1	A	1083	THR	5.3
1	A	283	GLY	5.2
1	A	318	SER	5.2
6	H	85	GLY	5.1
1	A	163	SER	5.1
1	A	1175	SER	5.0
1	A	257	ARG	5.0
1	A	1090	ALA	4.9
1	A	287	HIS	4.8
1	A	45	GLN	4.8
1	A	199	LEU	4.8
1	A	146	MET	4.7
1	A	103	CYS	4.7
6	H	83	GLN	4.6
1	A	171	GLN	4.6
10	L	50	ASP	4.6
6	H	84	ALA	4.5
2	B	882	THR	4.5
4	E	2	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	122	MET	4.5
1	A	186	LYS	4.4
2	B	106	ASP	4.4
1	A	1089	VAL	4.4
1	A	170	THR	4.3
1	A	153	PRO	4.3
2	B	472	ALA	4.3
1	A	118	HIS	4.2
1	A	116	ASP	4.2
2	B	868	MET	4.2
2	B	935	ARG	4.1
1	A	168	GLY	4.1
1	A	65	LEU	4.1
1	A	1085	HIS	4.1
2	B	709	ASP	4.1
1	A	115	LEU	4.1
2	B	933	SER	4.1
4	E	93	MET	4.0
2	B	470	LYS	4.0
2	B	250	PHE	3.9
2	B	870	ILE	3.9
1	A	164	ARG	3.9
1	A	148	CYS	3.9
1	A	1173	HIS	3.9
2	B	135	ARG	3.9
2	B	867	GLY	3.8
2	B	888	GLY	3.8
2	B	429	PHE	3.8
1	A	1091	SER	3.8
2	B	645	SER	3.8
4	E	118	PRO	3.7
1	A	108	MET	3.7
1	A	154	SER	3.7
1	A	42	ASP	3.7
10	L	27	LEU	3.7
2	B	468	GLU	3.7
1	A	176	LYS	3.6
1	A	167	CYS	3.6
1	A	165	GLY	3.6
1	A	185	TRP	3.6
1	A	286	HIS	3.6
2	B	471	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
10	L	45	ALA	3.5
2	B	140	ILE	3.5
1	A	109	HIS	3.5
4	E	126	SER	3.5
1	A	150	THR	3.5
1	A	200	ARG	3.4
1	A	43	GLU	3.4
1	A	174	ILE	3.4
2	B	138	GLU	3.4
2	B	869	SER	3.4
4	E	121	MET	3.4
1	A	47	ARG	3.4
2	B	666	TYR	3.4
1	A	121	LEU	3.4
1	A	280	GLU	3.4
2	B	469	GLN	3.4
1	A	145	LYS	3.4
2	B	919	SER	3.3
1	A	285	PRO	3.3
1	A	120	GLU	3.3
1	A	314	ALA	3.3
1	A	1084	PHE	3.3
4	E	50	MET	3.3
1	A	1092	LYS	3.3
2	B	475	SER	3.3
2	B	918	ILE	3.2
1	A	125	ALA	3.2
4	E	123	LEU	3.2
1	A	105	CYS	3.2
1	A	111	GLY	3.2
2	B	434	ARG	3.1
4	E	49	SER	3.1
2	B	1217	TYR	3.1
2	B	708	GLU	3.1
2	B	89	GLU	3.0
2	B	139	ALA	3.0
10	L	42	ARG	3.0
2	B	887	HIS	3.0
1	A	1124	HIS	3.0
1	A	295	LEU	2.9
1	A	201	VAL	2.9
1	A	256	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	433	GLN	2.9
1	A	143	LYS	2.9
1	A	173	THR	2.8
1	A	175	ARG	2.8
7	I	118	ARG	2.8
1	A	1123	GLY	2.8
4	E	116	ILE	2.8
1	A	139	TRP	2.8
1	A	252	PHE	2.8
1	A	140	THR	2.7
4	E	110	PHE	2.7
1	A	258	GLY	2.7
1	A	46	THR	2.7
2	B	1186	ASP	2.7
2	B	432	MET	2.7
2	B	476	ARG	2.7
1	A	1301	GLU	2.7
4	E	119	SER	2.7
1	A	177	ASP	2.7
2	B	1189	ILE	2.6
3	C	268	ASP	2.6
2	B	430	ARG	2.6
2	B	351	TYR	2.6
2	B	437	GLU	2.6
1	A	292	ALA	2.5
1	A	975	HIS	2.5
1	A	315	LEU	2.5
3	C	215	GLU	2.5
2	B	1190	ASP	2.5
1	A	313	GLN	2.5
2	B	230	ALA	2.5
1	A	39	GLU	2.5
6	H	130	ARG	2.4
12	T	28	DT	2.4
1	A	1299	VAL	2.4
2	B	884	ARG	2.4
1	A	1174	PHE	2.4
1	A	830	LYS	2.4
4	E	122	LYS	2.4
4	E	96	PHE	2.4
1	A	113	LEU	2.4
1	A	254	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	169	ASN	2.3
6	H	131	ASN	2.3
2	B	1162	ILE	2.3
6	H	76	THR	2.3
1	A	137	ALA	2.3
8	J	26	GLN	2.3
1	A	66	LYS	2.3
2	B	1187	ASN	2.3
12	T	17	DG	2.3
1	A	291	GLU	2.3
4	E	70	SER	2.2
1	A	1002	GLY	2.2
4	E	91	LYS	2.2
10	L	49	LYS	2.2
1	A	276	LEU	2.2
1	A	1088	GLY	2.2
1	A	124	GLN	2.2
2	B	591	ARG	2.2
1	A	48	ALA	2.2
1	A	282	ASN	2.2
2	B	133	LYS	2.2
2	B	431	TYR	2.2
2	B	662	MET	2.2
1	A	12	ARG	2.2
2	B	881	ASN	2.2
1	A	1235	LYS	2.2
2	B	132	VAL	2.2
1	A	279	LEU	2.2
1	A	702	LEU	2.2
4	E	69	ILE	2.2
2	B	1221	SER	2.1
6	H	2	SER	2.1
1	A	1391	ARG	2.1
1	A	181	LEU	2.1
1	A	1125	ALA	2.1
1	A	1081	LEU	2.1
2	B	231	PRO	2.1
2	B	509	ALA	2.1
3	C	4	GLU	2.1
6	H	62	SER	2.1
2	B	478	GLY	2.1
6	H	146	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	151	ASP	2.1
1	A	142	CYS	2.1
6	H	108	SER	2.1
2	B	1175	LEU	2.1
3	C	264	GLN	2.0
3	C	265	MET	2.0
5	F	72	LYS	2.0
4	E	44	ALA	2.0
6	H	51	ALA	2.0
8	J	27	GLU	2.0
1	A	178	GLY	2.0
4	E	86	PRO	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
14	MG	A	2001	1/1	0.16	1.13	55,55,55,55	0
13	ZN	I	203	1/1	0.12	-0.02	102,102,102,102	0
13	ZN	J	101	1/1	0.17	-0.58	57,57,57,57	0
13	ZN	I	204	1/1	0.09	-0.81	60,60,60,60	0
13	ZN	B	1307	1/1	0.09	-0.95	123,123,123,123	0
13	ZN	L	105	1/1	0.07	-1.00	95,95,95,95	0
13	ZN	C	319	1/1	0.09	-1.01	59,59,59,59	0
13	ZN	A	1735	1/1	0.11	-1.34	106,106,106,106	0
13	ZN	A	1734	1/1	0.06	-2.13	220,220,220,220	0

6.5 Other polymers ⓘ

There are no such residues in this entry.