



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:01 PM UTC

PDB ID : 5C4A / pdb_00005c4a
Title : Crystal structure of a transcribing RNA Polymerase II complex reveals a complete transcription bubble
Authors : Barnes, C.O.; Calero, M.; Malik, I.; Saphr, H.; Zhang, Q.; Pullara, F.; Kaplan, C.D.; Calero, G.
Deposited on : 2015-06-17
Resolution : 4.20 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

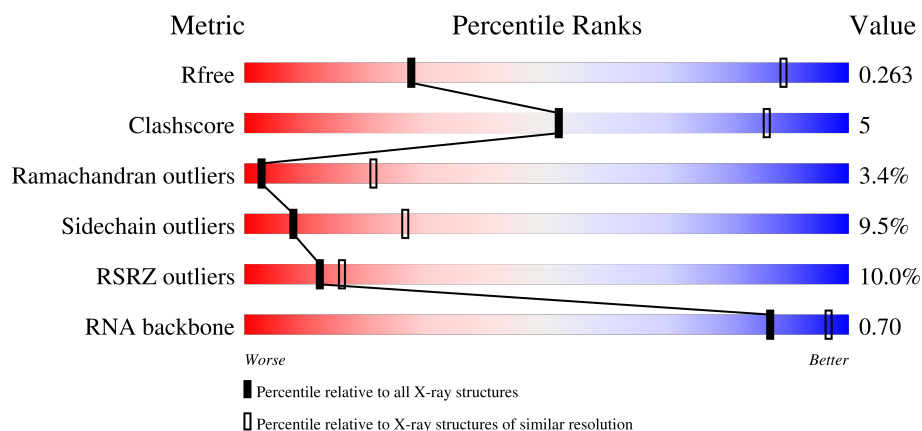
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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}	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)
RNA backbone	3983	1026 (5.04-3.10)

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 $\leq 5\%$. 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	1733	5% 62% 17% • 18%
2	B	1224	11% 70% 20% • 5%
3	C	318	6% 66% 15% • 17%
4	D	221	21% 63% 13% 24%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	179	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	R	9	
14	S	56	
15	U	56	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 32574 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1425	Total	C	N	O	S	0	0	0
			11206	7057	1960	2127	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1162	Total	C	N	O	S	0	0	0
			9215	5816	1617	1726	56			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2086	1312	347	414	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	168	Total	C	N	O	S	0	0	0
			1331	822	237	270	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	170	Total	C	N	O	S	0	0	0
			1331	857	220	246	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	172	LEU	-	expression tag	UNP P34087
G	173	GLU	-	expression tag	UNP P34087
G	174	HIS	-	expression tag	UNP P34087
G	175	HIS	-	expression tag	UNP P34087
G	176	HIS	-	expression tag	UNP P34087
G	177	HIS	-	expression tag	UNP P34087
G	178	HIS	-	expression tag	UNP P34087
G	179	HIS	-	expression tag	UNP P34087

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	135	Total	C	N	O	S	0	0	0
			1080	679	182	214	5			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	114	Total	C	N	O	S	0	0	0
			927	571	168	178	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	66	Total	C	N	O	S	0	0	0
			540	345	94	95	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	0
			924	593	157	172	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			352	217	70	61	4			

- Molecule 13 is a RNA chain called RNA (5'-R(P*UP*CP*GP*AP*GP*AP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	9	Total	C	N	O	P	0	0	0
			197	88	40	60	9			

- Molecule 14 is a DNA chain called Scaffold 2 Non-template Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	S	16	Total	C	N	O	P	0	0	0
			331	158	58	99	16			

- Molecule 15 is a DNA chain called Scaffold 2 Template Strand.

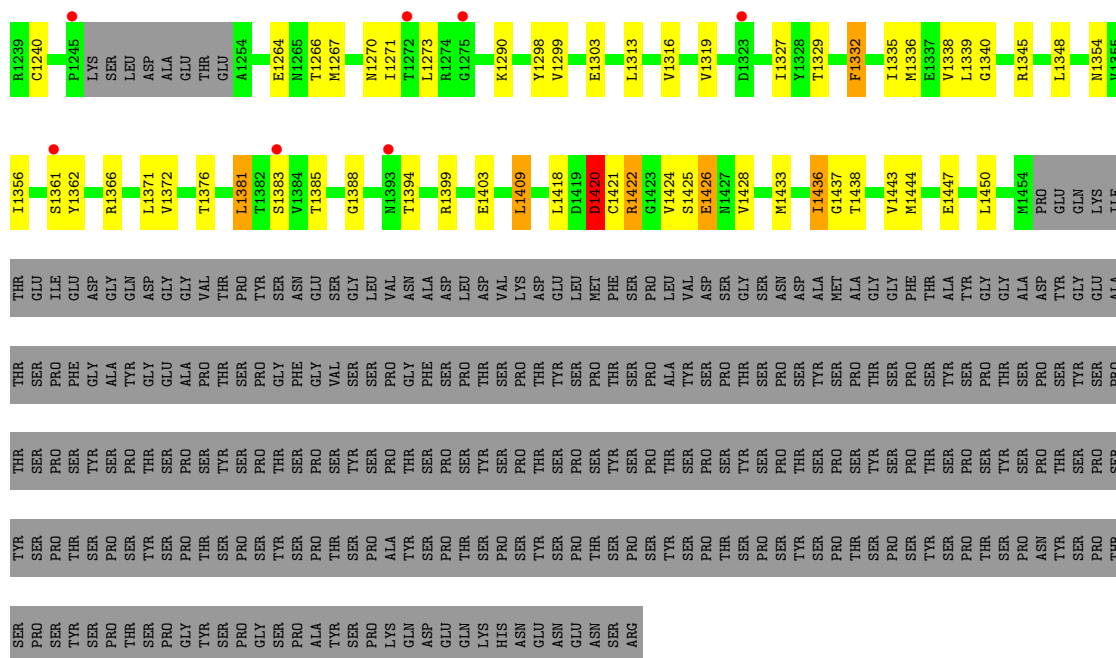
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	29	Total	C	N	O	P	0	0	0
			587	280	107	171	29			

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

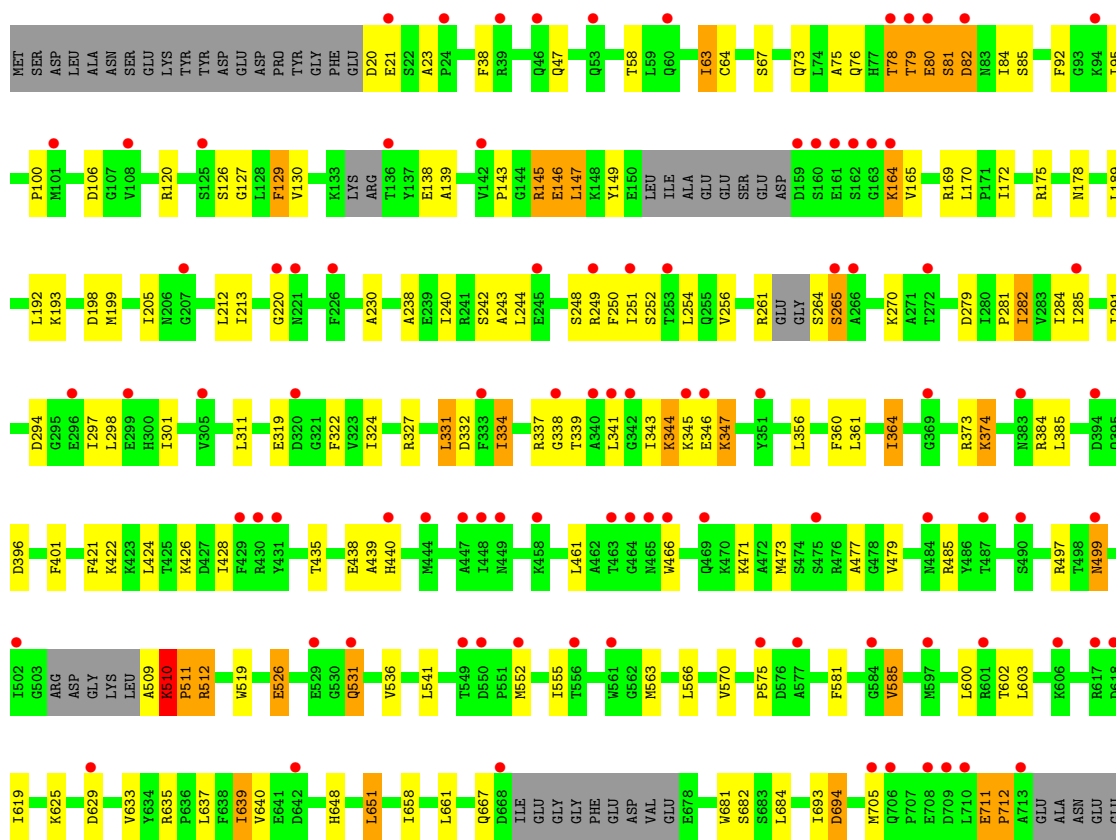
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total	Zn	0	0
			2	2		
16	B	1	Total	Zn	0	0
			1	1		
16	C	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	J	1	Total	Zn	0	0
			1	1		
16	L	1	Total	Zn	0	0
			1	1		

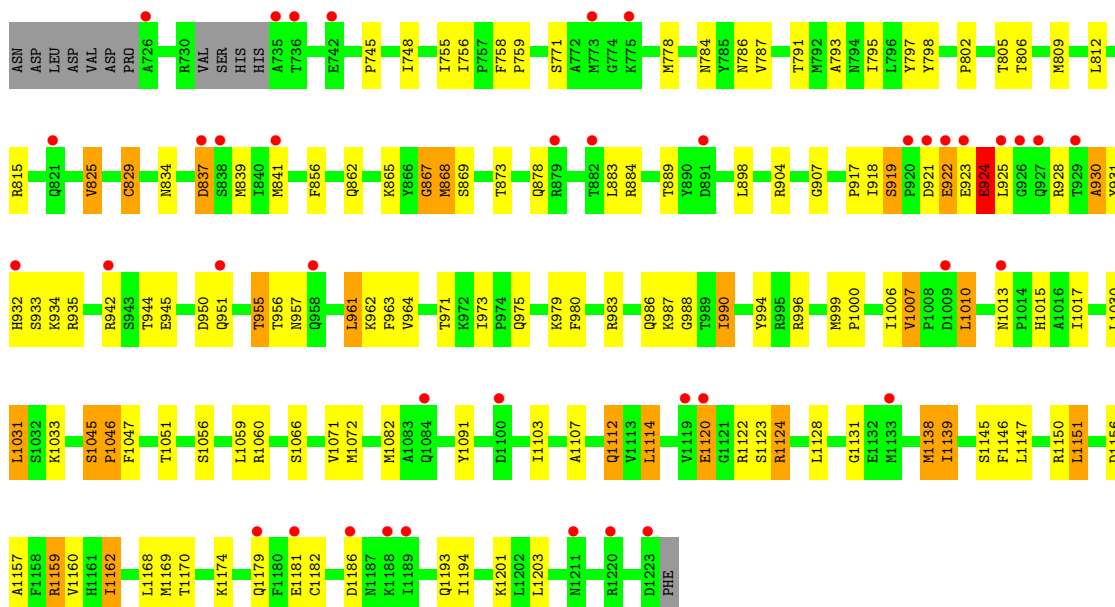
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total	Mg	0	0
			2	2		

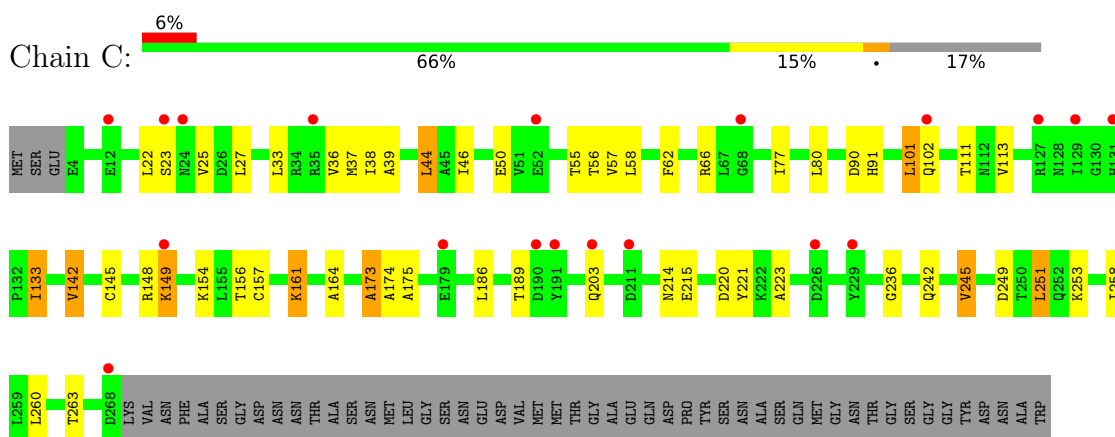


● Molecule 2: DNA-directed RNA polymerase II subunit RPB2

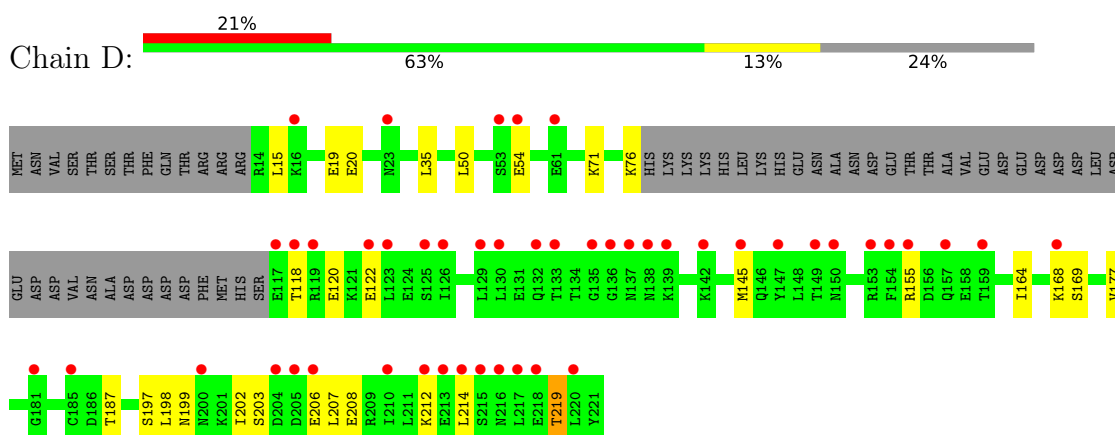




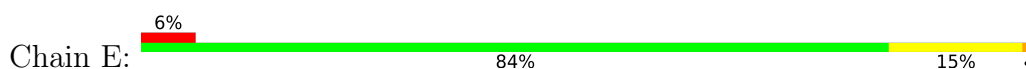
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

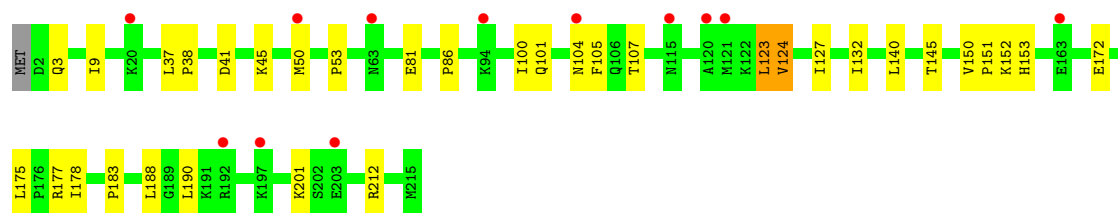


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

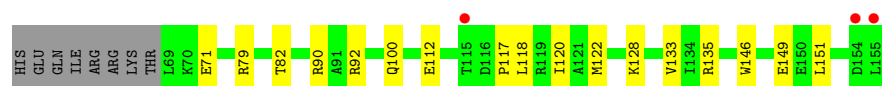
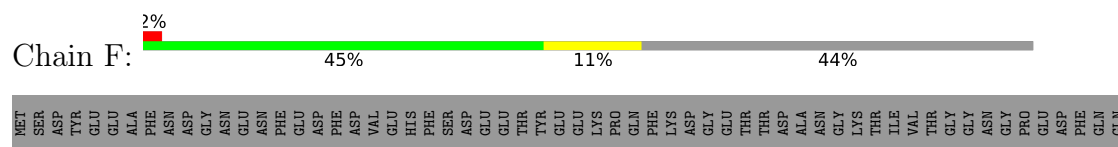


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

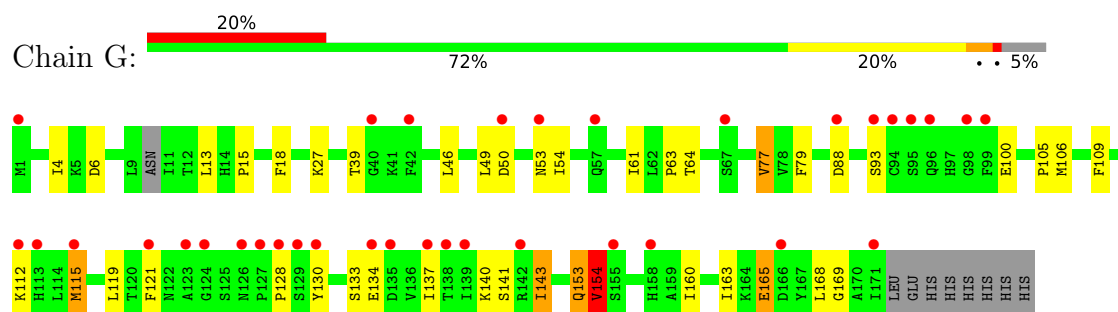




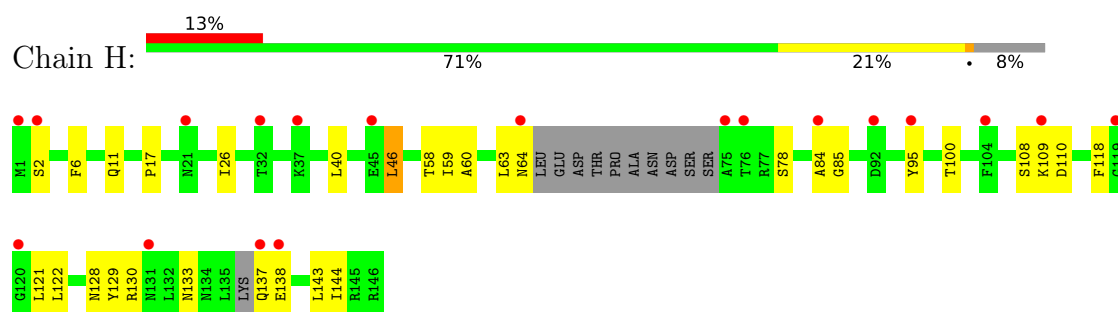
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



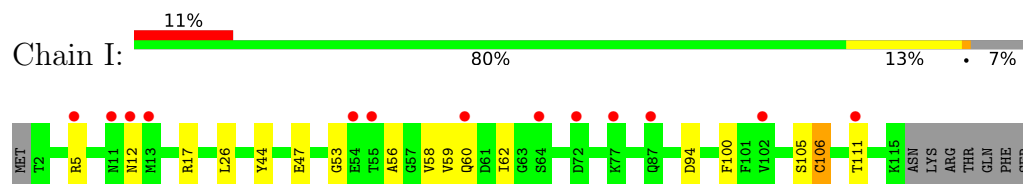
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

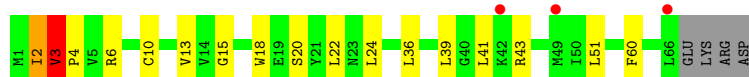


- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

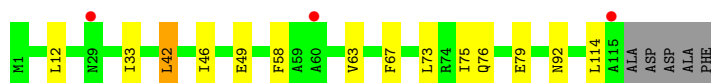
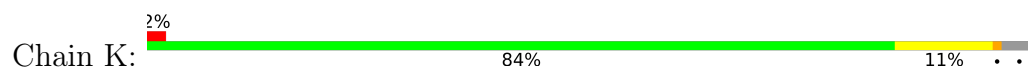


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

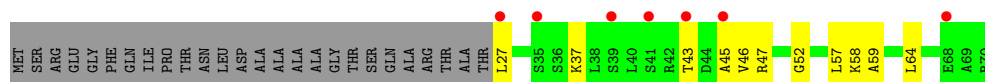




- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



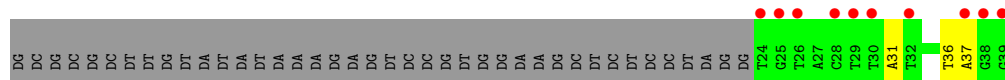
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



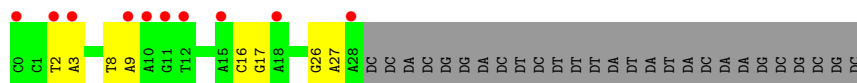
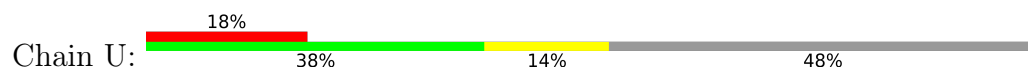
- Molecule 13: RNA (5'-R(P*UP*CP*GP*AP*GP*AP*GP*GP*A)-3')



- Molecule 14: Scaffold 2 Non-template Strand



- Molecule 15: Scaffold 2 Template Strand



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	219.83Å 396.71Å 273.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 4.20 39.91 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.91-4.20) 99.6 (39.91-4.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 4.13Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.224 , 0.242 0.245 , 0.263	Depositor DCC
R_{free} test set	6719 reflections (7.74%)	wwPDB-VP
Wilson B-factor (Å ²)	100.3	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 134.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.019 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	32574	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, 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	0.95	2/11407 (0.0%)	1.25	17/15428 (0.1%)
2	B	0.96	4/9390 (0.0%)	1.22	27/12662 (0.2%)
3	C	0.91	0/2124	1.18	1/2879 (0.0%)
4	D	0.89	0/1339	1.25	0/1793
5	E	0.92	1/1788 (0.1%)	1.17	2/2406 (0.1%)
6	F	0.92	0/717	1.17	0/967
7	G	0.93	0/1358	1.19	5/1830 (0.3%)
8	H	0.87	0/1097	1.09	1/1484 (0.1%)
9	I	0.88	0/945	1.13	0/1273
10	J	0.87	0/549	1.17	1/738 (0.1%)
11	K	0.86	0/942	1.19	1/1272 (0.1%)
12	L	0.93	0/354	1.14	0/468
13	R	0.51	0/221	0.62	0/343
14	S	0.40	0/370	0.65	0/570
15	U	0.43	0/657	0.57	0/1009
All	All	0.92	7/33258 (0.0%)	1.19	55/45122 (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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	264	SER	C-N	15.25	1.51	1.33
2	B	924	GLU	CA-C	11.95	1.58	1.52
1	A	417	TYR	CA-C	7.57	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	265	SER	C-N	6.13	1.42	1.33
5	E	124	VAL	CA-CB	5.53	1.57	1.54
1	A	50	ILE	CA-CB	5.34	1.59	1.54
2	B	78	THR	CA-C	5.11	1.59	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	934	LYS	N-CA-C	7.72	119.39	110.97
2	B	1139	ILE	N-CA-C	-7.57	103.47	110.82
1	A	864	ILE	N-CA-C	-6.83	105.18	111.67
2	B	129	PHE	CA-CB-CG	6.49	120.29	113.80
2	B	918	ILE	CA-C-N	6.48	133.37	121.70
2	B	918	ILE	C-N-CA	6.48	133.37	121.70
1	A	1015	VAL	N-CA-CB	6.40	118.32	110.64
2	B	145	ARG	CA-C-N	6.21	132.88	121.70
2	B	145	ARG	C-N-CA	6.21	132.88	121.70
1	A	219	PHE	CA-CB-CG	6.19	119.99	113.80
1	A	417	TYR	CA-C-O	-6.17	116.25	119.77
1	A	641	VAL	N-CA-C	-6.16	104.34	110.62
2	B	165	VAL	N-CA-CB	6.14	117.55	110.49
2	B	79	THR	CA-C-N	6.10	132.69	121.70
2	B	79	THR	C-N-CA	6.10	132.69	121.70
1	A	445	ASN	CA-CB-CG	6.08	118.68	112.60
2	B	1186	ASP	CA-CB-CG	6.04	118.64	112.60
2	B	364	ILE	N-CA-CB	6.00	121.13	111.23
2	B	344	LYS	CA-C-N	5.98	132.96	121.54
2	B	344	LYS	C-N-CA	5.98	132.96	121.54
1	A	1106	ASN	N-CA-C	5.96	117.58	111.14
7	G	77	VAL	N-CA-CB	5.96	118.42	110.26
8	H	133	ASN	CA-CB-CG	5.95	118.55	112.60
7	G	61	ILE	N-CA-CB	5.93	117.31	110.49
2	B	639	ILE	N-CA-CB	5.88	117.70	111.00
7	G	18	PHE	CA-CB-CG	5.87	119.67	113.80
7	G	53	ASN	CA-CB-CG	5.86	118.46	112.60
11	K	63	VAL	N-CA-CB	5.82	117.70	112.06
2	B	867	GLY	CA-C-N	5.54	131.66	121.70
2	B	867	GLY	C-N-CA	5.54	131.66	121.70
2	B	1071	VAL	N-CA-CB	5.53	116.95	110.82
1	A	91	PHE	CA-CB-CG	5.47	119.27	113.80
2	B	930	ALA	CA-C-N	5.45	131.50	121.70
2	B	930	ALA	C-N-CA	5.45	131.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	ILE	N-CA-CB	5.42	121.19	110.95
2	B	922	GLU	CA-C-N	5.42	131.88	121.54
2	B	922	GLU	C-N-CA	5.42	131.88	121.54
5	E	123	LEU	CA-C-N	5.33	124.59	120.33
5	E	123	LEU	C-N-CA	5.33	124.59	120.33
2	B	511	PRO	CA-C-N	5.31	131.68	121.54
2	B	511	PRO	C-N-CA	5.31	131.68	121.54
2	B	428	ILE	N-CA-C	-5.30	105.37	110.72
3	C	173	ALA	N-CA-C	5.30	117.74	111.33
1	A	96	ILE	N-CA-C	-5.25	106.69	111.67
2	B	694	ASP	CA-CB-CG	5.24	117.83	112.60
10	J	3	VAL	N-CA-CB	5.23	118.53	111.21
7	G	88	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	739	ASP	CA-C-N	5.17	127.72	120.28
1	A	739	ASP	C-N-CA	5.17	127.72	120.28
1	A	999	VAL	N-CA-C	-5.14	106.65	111.48
1	A	48	ALA	CA-C-N	5.13	131.34	121.54
1	A	48	ALA	C-N-CA	5.13	131.34	121.54
2	B	784	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	298	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	1420	ASP	CA-CB-CG	5.09	117.69	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	265	SER	Mainchain

5.2 Too-close contacts [i](#)

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	11206	0	11265	140	0
2	B	9215	0	9210	114	0
3	C	2086	0	2045	24	0
4	D	1331	0	1345	8	0
5	E	1752	0	1776	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	705	0	731	8	0
7	G	1331	0	1350	20	0
8	H	1080	0	1049	10	0
9	I	927	0	883	7	0
10	J	540	0	555	9	0
11	K	924	0	934	3	0
12	L	352	0	377	2	0
13	R	197	0	96	4	0
14	S	331	0	183	2	0
15	U	587	0	326	6	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	2	0	0	0	0
All	All	32574	0	32125	328	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 5.

All (328) 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)
1:A:869:GLY:HA3	1:A:1366:ARG:HG2	1.46	0.98
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.64	0.80
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.64	0.79
1:A:311:GLN:HB2	1:A:312:PRO:HD3	1.67	0.77
1:A:1107:VAL:HA	1:A:1108:ALA:HB3	1.68	0.75
1:A:508:PRO:HB3	1:A:643:ALA:HB2	1.70	0.74
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.71	0.70
2:B:145:ARG:HA	2:B:146:GLU:CB	2.22	0.69
3:C:50:GLU:HB2	3:C:156:THR:HB	1.77	0.66
2:B:1138:MET:HB3	2:B:1147:LEU:HD12	1.77	0.66
1:A:394:ASN:HB3	1:A:398:GLU:HB3	1.78	0.65
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.26	0.65
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.79	0.65
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.78	0.65
2:B:980:PHE:HE2	2:B:990:ILE:HD11	1.61	0.64
15:U:8:DT:H2"	15:U:9:DA:H5"	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:ILE:HG13	3:C:161:LYS:HE3	1.78	0.63
1:A:27:VAL:HA	1:A:30:ILE:HG22	1.80	0.63
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.28	0.63
1:A:72:GLU:HB3	1:A:76:GLU:HG3	1.81	0.62
1:A:899:VAL:HG22	1:A:1029:ARG:HG3	1.81	0.62
1:A:662:PHE:HB3	2:B:829:CYS:SG	2.39	0.62
1:A:1107:VAL:CA	1:A:1108:ALA:HB3	2.29	0.62
1:A:105:CYS:SG	1:A:139:TRP:HA	2.39	0.62
2:B:921:ASP:HB3	2:B:928:ARG:HG3	1.81	0.61
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.82	0.61
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.81	0.61
2:B:20:ASP:HB3	2:B:23:ALA:HB2	1.82	0.61
2:B:994:TYR:HB2	2:B:999:MET:HE3	1.81	0.61
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.30	0.61
11:K:42:LEU:HD23	11:K:46:ILE:HD11	1.81	0.61
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.83	0.60
2:B:825:VAL:HG23	2:B:1010:LEU:HD12	1.83	0.60
1:A:567:LYS:HG2	1:A:568:PRO:HD3	1.83	0.60
1:A:842:VAL:HA	1:A:1069:ALA:HB1	1.84	0.60
2:B:640:VAL:HA	2:B:651:LEU:HA	1.83	0.60
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.84	0.60
2:B:364:ILE:HD11	2:B:374:LYS:HG3	1.83	0.59
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.82	0.59
1:A:810:PRO:HB3	2:B:745:PRO:HB3	1.84	0.58
7:G:153:GLN:HG2	7:G:154:VAL:HG23	1.84	0.58
1:A:247:ARG:HD3	1:A:266:LEU:HD13	1.86	0.58
1:A:483:ASP:HB3	2:B:837:ASP:HB3	1.86	0.58
1:A:316:GLN:HG2	1:A:322:VAL:HB	1.85	0.58
1:A:512:VAL:HA	1:A:519:PRO:HA	1.86	0.57
6:F:118:LEU:HG	6:F:122:MET:HE2	1.85	0.57
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.03	0.57
2:B:84:ILE:HG22	2:B:138:GLU:HB3	1.85	0.57
1:A:508:PRO:HB2	1:A:639:PRO:O	2.04	0.57
2:B:661:LEU:HD21	2:B:684:LEU:HD11	1.85	0.57
7:G:130:TYR:HB2	7:G:137:ILE:HB	1.87	0.57
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.86	0.57
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.86	0.56
2:B:422:LYS:HG2	2:B:426:LYS:HE2	1.86	0.56
1:A:1063:MET:HG3	2:B:1139:ILE:HG22	1.87	0.56
3:C:186:LEU:HG	3:C:223:ALA:HB1	1.86	0.56
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:LYS:HD2	2:B:1015:HIS:HB3	1.88	0.56
2:B:145:ARG:HA	2:B:146:GLU:HB3	1.87	0.56
2:B:711:GLU:HB3	2:B:712:PRO:HD3	1.88	0.56
2:B:477:ALA:HB3	13:R:6:G:H5'	1.86	0.55
2:B:806:THR:HG23	2:B:1045:SER:HA	1.87	0.55
9:I:105:SER:O	9:I:106:CYS:HB3	2.06	0.55
1:A:150:THR:O	1:A:163:SER:HA	2.07	0.55
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	1.88	0.54
2:B:145:ARG:HA	2:B:146:GLU:HB2	1.89	0.54
1:A:317:LYS:HA	1:A:318:SER:C	2.31	0.54
3:C:102:GLN:HG3	3:C:154:LYS:HE2	1.88	0.54
7:G:143:ILE:HG13	7:G:169:GLY:O	2.07	0.54
2:B:298:LEU:HD12	2:B:311:LEU:HD23	1.90	0.54
1:A:179:LEU:HD22	1:A:297:GLN:HG3	1.90	0.54
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.90	0.54
1:A:1107:VAL:CA	1:A:1108:ALA:CB	2.85	0.54
2:B:80:GLU:O	2:B:81:SER:HB3	2.07	0.53
2:B:346:GLU:O	2:B:347:LYS:HB2	2.08	0.53
1:A:1193:LEU:HD11	1:A:1264:GLU:HB2	1.90	0.53
2:B:79:THR:HG22	2:B:82:ASP:O	2.09	0.53
2:B:213:ILE:HG23	2:B:497:ARG:HB3	1.91	0.53
2:B:980:PHE:CE2	2:B:990:ILE:HD11	2.42	0.53
1:A:1107:VAL:N	1:A:1108:ALA:CB	2.71	0.53
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.91	0.53
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.91	0.53
2:B:1168:LEU:HB2	2:B:1170:THR:HG23	1.91	0.53
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.90	0.52
2:B:509:ALA:C	2:B:511:PRO:HA	2.34	0.52
6:F:128:LYS:HD2	6:F:149:GLU:HA	1.91	0.52
1:A:365:GLY:HA3	1:A:469:ARG:HB3	1.92	0.52
2:B:100:PRO:HG3	2:B:172:ILE:HG21	1.91	0.52
10:J:36:LEU:HD22	10:J:41:LEU:HG	1.92	0.52
1:A:908:LEU:HD21	1:A:1029:ARG:HG2	1.92	0.52
1:A:443:LEU:HD12	2:B:1146:PHE:CE1	2.45	0.52
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.91	0.52
1:A:342:GLY:HA3	2:B:1131:GLY:HA2	1.92	0.52
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.91	0.52
1:A:1118:VAL:HG13	1:A:1327:ILE:HD12	1.92	0.52
1:A:842:VAL:HA	1:A:1069:ALA:CB	2.41	0.52
1:A:1290:LYS:HG2	1:A:1298:TYR:HB3	1.91	0.51
1:A:1421:CYS:HA	1:A:1426:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:MET:HG3	1:A:1381:LEU:HD12	1.92	0.51
15:U:26:DG:H4'	15:U:27:DA:OP1	2.09	0.51
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.90	0.51
1:A:451:HIS:CD2	1:A:453:MET:HB2	2.46	0.51
1:A:513:SER:HB2	1:A:520:CYS:HB3	1.92	0.51
1:A:182:VAL:HG12	1:A:201:VAL:HA	1.92	0.51
2:B:364:ILE:HG23	2:B:585:VAL:HG22	1.92	0.51
8:H:58:THR:HB	8:H:143:LEU:HB2	1.91	0.51
1:A:549:MET:HG2	1:A:577:ILE:HD12	1.92	0.51
2:B:930:ALA:HA	2:B:931:TYR:C	2.36	0.51
3:C:46:ILE:HG12	3:C:157:CYS:HB3	1.92	0.51
5:E:9:ILE:HG12	5:E:53:PRO:HG3	1.93	0.51
3:C:148:ARG:HG2	3:C:149:LYS:HG3	1.92	0.50
7:G:93:SER:HB2	7:G:100:GLU:HB2	1.92	0.50
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.92	0.50
1:A:341:MET:HE1	1:A:1425:SER:HA	1.94	0.50
3:C:58:LEU:HD23	3:C:145:CYS:HB2	1.94	0.50
5:E:145:THR:HA	5:E:150:VAL:HG11	1.94	0.50
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.94	0.50
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.77	0.50
1:A:1101:LEU:HA	1:A:1104:ILE:HD12	1.93	0.50
2:B:640:VAL:HG22	2:B:651:LEU:HB3	1.93	0.50
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.93	0.50
1:A:103:CYS:HB3	1:A:108:MET:HE1	1.94	0.50
1:A:1107:VAL:N	1:A:1108:ALA:HB2	2.27	0.50
7:G:46:LEU:HD11	7:G:79:PHE:HB2	1.94	0.50
1:A:374:LEU:HA	2:B:1107:ALA:HB2	1.94	0.49
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.45	0.49
5:E:38:PRO:HD2	5:E:41:ASP:HB2	1.94	0.49
1:A:1420:ASP:HB2	1:A:1422:ARG:HG2	1.94	0.49
2:B:319:GLU:HA	2:B:322:PHE:HB2	1.93	0.49
6:F:117:PRO:HA	6:F:120:ILE:HD12	1.94	0.49
1:A:467:THR:HG23	1:A:469:ARG:HH12	1.78	0.49
1:A:761:MET:HA	1:A:804:TYR:HB2	1.95	0.49
8:H:110:ASP:HB3	8:H:128:ASN:HD22	1.76	0.49
3:C:62:PHE:O	3:C:66:ARG:HG3	2.13	0.49
1:A:464:PRO:HD2	11:K:67:PHE:CD2	2.48	0.49
1:A:540:PHE:HB2	1:A:571:LEU:HD23	1.94	0.49
2:B:294:ASP:HB2	9:I:12:ASN:HA	1.93	0.49
1:A:405:VAL:HG22	1:A:432:VAL:HG13	1.95	0.49
7:G:163:ILE:HD12	7:G:169:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:LEU:HD11	1:A:982:THR:HA	1.94	0.48
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.95	0.48
13:R:2:U:O2	13:R:3:C:C2	2.65	0.48
1:A:1224:LEU:HD21	1:A:1240:CYS:HB3	1.94	0.48
2:B:924:GLU:HG2	2:B:925:LEU:H	1.78	0.48
15:U:2:DT:H2"	15:U:3:DA:N7	2.29	0.48
1:A:849:MET:HG3	1:A:1063:MET:SD	2.54	0.48
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.77	0.48
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.95	0.48
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.95	0.48
2:B:373:ARG:HG2	2:B:566:LEU:HB3	1.95	0.48
2:B:805:THR:HG21	2:B:815:ARG:HD3	1.95	0.48
7:G:46:LEU:HD21	7:G:105:PRO:HG3	1.95	0.48
4:D:208:GLU:HG3	4:D:212:LYS:HE3	1.94	0.48
1:A:508:PRO:CB	1:A:643:ALA:HB2	2.41	0.48
4:D:155:ARG:HG3	4:D:219:THR:HG21	1.96	0.48
8:H:6:PHE:HB3	8:H:59:ILE:HD12	1.94	0.48
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.49	0.47
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.79	0.47
2:B:499:ASN:HA	2:B:536:VAL:HG22	1.95	0.47
2:B:509:ALA:O	2:B:510:LYS:HB2	2.12	0.47
2:B:238:ALA:HB2	2:B:385:LEU:HB2	1.96	0.47
10:J:3:VAL:HG23	10:J:15:GLY:HA2	1.95	0.47
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.97	0.47
1:A:451:HIS:ND1	1:A:1074:GLU:HG3	2.29	0.47
1:A:709:THR:HG21	9:I:94:ASP:HA	1.95	0.47
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.96	0.47
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.96	0.47
15:U:2:DT:H2"	15:U:3:DA:C8	2.49	0.47
1:A:567:LYS:CB	1:A:568:PRO:CD	2.91	0.46
2:B:64:CYS:HA	2:B:67:SER:HB2	1.96	0.46
2:B:270:LYS:HB3	2:B:279:ASP:HB3	1.96	0.46
4:D:168:LYS:HG3	4:D:177:VAL:HG11	1.97	0.46
1:A:883:LEU:HD22	1:A:943:LEU:HD21	1.97	0.46
2:B:841:MET:HE2	2:B:1010:LEU:HD22	1.97	0.46
2:B:1082:MET:HA	3:C:189:THR:HA	1.97	0.46
7:G:46:LEU:HB2	7:G:77:VAL:HG23	1.98	0.46
1:A:456:MET:HE2	1:A:507:VAL:HG22	1.97	0.46
8:H:100:THR:HG23	8:H:138:GLU:HB2	1.98	0.46
1:A:214:ILE:HG23	1:A:218:ASP:HB2	1.98	0.46
2:B:84:ILE:CG2	2:B:138:GLU:HB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.98	0.46
8:H:110:ASP:HB3	8:H:128:ASN:ND2	2.31	0.46
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.97	0.46
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.97	0.46
2:B:63:ILE:HG23	2:B:92:PHE:HB2	1.97	0.46
1:A:1095:THR:HG21	1:A:1112:LYS:HD2	1.97	0.46
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.51	0.45
2:B:745:PRO:HB2	2:B:1047:PHE:CD2	2.52	0.45
3:C:57:VAL:HG21	10:J:60:PHE:HB2	1.99	0.45
2:B:619:ILE:HD13	9:I:62:ILE:HA	1.99	0.45
6:F:100:GLN:HG2	7:G:15:PRO:HB3	1.97	0.45
2:B:1112:GLN:HG3	13:R:2:U:OP1	2.17	0.45
2:B:1124:ARG:NH2	13:R:2:U:OP2	2.49	0.45
2:B:38:PHE:HZ	2:B:541:LEU:HB3	1.81	0.45
2:B:81:SER:HA	2:B:82:ASP:HA	1.68	0.45
2:B:85:SER:HB3	2:B:139:ALA:HB3	1.98	0.45
2:B:600:LEU:HA	2:B:603:LEU:HD12	1.97	0.45
2:B:327:ARG:HG2	2:B:331:LEU:HD12	1.99	0.45
15:U:16:DC:H2"	15:U:17:DG:OP1	2.16	0.45
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	1.98	0.44
1:A:880:LYS:HA	1:A:955:PRO:HA	1.99	0.44
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.99	0.44
7:G:49:LEU:HD11	7:G:77:VAL:HG13	1.99	0.44
1:A:380:VAL:HG21	1:A:426:LEU:HD22	1.99	0.44
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.99	0.44
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.99	0.44
3:C:33:LEU:HG	3:C:37:MET:HE2	1.98	0.44
4:D:203:SER:HB2	4:D:206:GLU:HB2	1.99	0.44
1:A:335:ARG:NH2	2:B:1114:LEU:HD21	2.33	0.44
1:A:523:ILE:HD13	1:A:622:VAL:HG22	2.00	0.44
11:K:58:PHE:HB3	11:K:76:GLN:HB3	2.00	0.44
4:D:202:ILE:HG21	4:D:207:LEU:HD13	2.00	0.43
12:L:47:ARG:HD3	12:L:52:GLY:HA2	2.00	0.43
2:B:230:ALA:HA	2:B:261:ARG:CZ	2.47	0.43
1:A:850:VAL:HG12	1:A:1060:PRO:HA	2.01	0.43
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	2.01	0.43
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.18	0.43
1:A:344:ARG:CZ	2:B:1120:GLU:HA	2.49	0.43
2:B:999:MET:HG3	2:B:1000:PRO:HD2	2.01	0.43
14:S:31:DA:H61	15:U:8:DT:H3	1.66	0.43
1:A:859:SER:O	1:A:1422:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1394:THR:HB	1:A:1399:ARG:HD3	2.00	0.43
2:B:193:LYS:HB3	2:B:787:VAL:HG11	2.01	0.43
2:B:332:ASP:OD1	2:B:346:GLU:HB3	2.18	0.43
2:B:758:PHE:HZ	2:B:1031:LEU:HD13	1.83	0.43
5:E:101:GLN:HB2	5:E:127:ILE:HD13	1.99	0.43
9:I:100:PHE:HD1	9:I:111:THR:HG22	1.84	0.43
2:B:80:GLU:O	2:B:81:SER:CB	2.67	0.43
3:C:220:ASP:HB3	3:C:223:ALA:HB2	2.01	0.43
2:B:127:GLY:HA2	2:B:169:ARG:HG2	1.99	0.43
2:B:205:ILE:HD11	2:B:461:LEU:HD23	2.01	0.43
3:C:50:GLU:HB3	12:L:64:LEU:HD21	2.01	0.43
3:C:242:GLN:HA	3:C:245:VAL:HG12	2.00	0.43
7:G:79:PHE:HE2	7:G:106:MET:HB3	1.83	0.43
7:G:121:PHE:HE1	7:G:128:PRO:HB3	1.84	0.43
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.00	0.43
2:B:63:ILE:HG13	2:B:421:PHE:CZ	2.54	0.43
1:A:1313:LEU:HD23	1:A:1338:VAL:HG11	2.01	0.42
3:C:36:VAL:HG11	3:C:251:LEU:HD12	2.00	0.42
8:H:2:SER:HB2	8:H:64:ASN:HB2	1.99	0.42
1:A:44:THR:N	1:A:45:GLN:HA	2.35	0.42
1:A:451:HIS:HD2	1:A:453:MET:HB2	1.84	0.42
1:A:760:GLN:HG2	1:A:765:VAL:HA	2.00	0.42
1:A:1444:MET:HE2	6:F:133:VAL:HG23	2.01	0.42
10:J:3:VAL:HG21	10:J:18:TRP:HB2	2.01	0.42
1:A:919:ILE:HG13	1:A:925:LEU:HD13	2.01	0.42
2:B:1174:LYS:HD2	2:B:1179:GLN:HB2	2.00	0.42
5:E:100:ILE:HG23	5:E:105:PHE:HB2	2.01	0.42
1:A:381:THR:HB	1:A:382:PRO:HD2	2.00	0.42
2:B:338:GLY:HA2	2:B:339:THR:HA	1.72	0.42
2:B:526:GLU:HG3	2:B:771:SER:HB2	2.01	0.42
2:B:1162:ILE:HG22	2:B:1169:MET:HG3	2.00	0.42
1:A:606:LEU:HD23	1:A:613:ILE:HG13	2.02	0.42
6:F:146:TRP:HB3	6:F:151:LEU:HD11	2.01	0.42
7:G:100:GLU:HG3	7:G:109:PHE:HD1	1.84	0.42
1:A:446:ARG:NE	1:A:480:ALA:HB2	2.34	0.42
1:A:940:ARG:HG2	1:A:941:LYS:HE2	2.02	0.42
4:D:50:LEU:HB3	4:D:54:GLU:HB3	2.01	0.42
5:E:151:PRO:HD2	5:E:153:HIS:HE1	1.85	0.42
1:A:319:GLY:HA3	2:B:471:LYS:HB2	2.01	0.42
1:A:1409:LEU:HD12	1:A:1409:LEU:HA	1.91	0.42
10:J:6:ARG:HG2	10:J:13:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:HG2	1:A:232:GLU:HG2	2.02	0.42
1:A:483:ASP:HA	2:B:988:GLY:HA2	2.01	0.42
7:G:163:ILE:HA	7:G:168:LEU:HD13	2.01	0.42
1:A:242:PRO:HB2	1:A:246:VAL:HB	2.02	0.41
1:A:981:LEU:HD13	1:A:986:ILE:HD11	2.01	0.41
2:B:1033:LYS:HE3	2:B:1059:LEU:HD11	2.02	0.41
1:A:75:ASN:O	1:A:76:GLU:HB2	2.21	0.41
1:A:335:ARG:HA	1:A:339:ASN:HB2	2.02	0.41
1:A:389:THR:O	1:A:393:ARG:HG2	2.21	0.41
3:C:101:LEU:HD21	3:C:113:VAL:HG11	2.01	0.41
7:G:112:LYS:HD2	7:G:115:MET:HE2	2.01	0.41
1:A:1383:SER:HB2	1:A:1388:GLY:HA3	2.02	0.41
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.55	0.41
2:B:581:PHE:HB2	2:B:625:LYS:HG2	2.01	0.41
2:B:798:TYR:CG	10:J:4:PRO:HG3	2.55	0.41
2:B:809:MET:HA	2:B:812:LEU:HD12	2.02	0.41
1:A:1116:LEU:HB2	1:A:1329:THR:HA	2.02	0.41
1:A:1228:TRP:HB3	1:A:1238:ILE:HG23	2.03	0.41
3:C:221:TYR:HB3	8:H:46:LEU:HD22	2.02	0.41
8:H:95:TYR:HB3	8:H:144:ILE:HB	2.02	0.41
8:H:118:PHE:HB2	8:H:121:LEU:HB2	2.02	0.41
1:A:722:LEU:HD21	1:A:794:PRO:HB3	2.02	0.41
2:B:868:MET:HG3	2:B:869:SER:N	2.35	0.41
2:B:961:LEU:HB3	2:B:962:LYS:H	1.74	0.41
5:E:124:VAL:HG13	5:E:132:ILE:HB	2.02	0.41
1:A:106:VAL:HG11	1:A:214:ILE:HG12	2.02	0.41
1:A:252:PHE:O	1:A:256:GLN:HB2	2.21	0.41
1:A:354:SER:HB2	1:A:469:ARG:HD3	2.02	0.41
3:C:44:LEU:HB2	3:C:77:ILE:HD13	2.03	0.41
1:A:469:ARG:HD3	1:A:469:ARG:HA	1.91	0.41
1:A:506:ALA:HB3	1:A:509:LEU:HB2	2.01	0.41
1:A:722:LEU:HD23	1:A:767:GLN:HB2	2.03	0.41
1:A:1063:MET:O	1:A:1065:GLY:N	2.54	0.41
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	2.03	0.41
1:A:1438:THR:HG22	6:F:92:ARG:HD3	2.03	0.41
2:B:139:ALA:HB2	2:B:149:TYR:HA	2.02	0.41
7:G:121:PHE:CE1	7:G:128:PRO:HB3	2.56	0.41
1:A:88:LYS:HD3	1:A:293:GLU:HG3	2.03	0.41
1:A:384:ASN:O	1:A:386:ASP:N	2.54	0.41
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.01	0.41
1:A:567:LYS:HE2	1:A:568:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	2.03	0.41
1:A:1267:MET:HA	1:A:1271:ILE:HD12	2.02	0.41
1:A:1345:ARG:HB3	1:A:1376:THR:HG21	2.01	0.41
2:B:438:GLU:HB2	2:B:439:ALA:HA	2.03	0.41
2:B:802:PRO:HG2	2:B:805:THR:HG22	2.01	0.41
3:C:38:ILE:HA	3:C:173:ALA:HB2	2.02	0.41
3:C:133:ILE:HG21	3:C:236:GLY:HA3	2.02	0.41
3:C:249:ASP:O	3:C:253:LYS:HG2	2.21	0.41
1:A:1332:PHE:HA	1:A:1335:ILE:HD12	2.03	0.41
2:B:867:GLY:HA3	2:B:868:MET:HG2	2.03	0.41
1:A:1266:THR:O	1:A:1270:ASN:HB3	2.20	0.40
14:S:36:DT:H2''	14:S:37:DA:O4'	2.20	0.40
1:A:1361:SER:HA	1:A:1362:TYR:HA	1.91	0.40
5:E:178:ILE:HB	5:E:212:ARG:HD3	2.04	0.40
9:I:58:VAL:HG12	9:I:62:ILE:HD12	2.02	0.40
1:A:139:TRP:O	1:A:143:LYS:HB2	2.20	0.40
2:B:220:GLY:HA3	2:B:243:ALA:HB2	2.03	0.40
2:B:681:TRP:HA	2:B:684:LEU:HD12	2.03	0.40
2:B:756:ILE:O	2:B:759:PRO:HD3	2.20	0.40
2:B:917:PRO:HA	2:B:933:SER:O	2.21	0.40
4:D:50:LEU:HD11	7:G:4:ILE:CD1	2.51	0.40
2:B:1006:ILE:HD11	10:J:43:ARG:HB3	2.03	0.40
10:J:20:SER:HB2	10:J:39:LEU:HD21	2.03	0.40
1:A:1383:SER:HB3	1:A:1385:THR:HG22	2.04	0.40
9:I:53:GLY:HA2	9:I:56:ALA:HB2	2.04	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	1417/1733 (82%)	1222 (86%)	147 (10%)	48 (3%)	3 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1146/1224 (94%)	977 (85%)	124 (11%)	45 (4%)	2	19
3	C	263/318 (83%)	235 (89%)	20 (8%)	8 (3%)	3	23
4	D	164/221 (74%)	150 (92%)	8 (5%)	6 (4%)	2	20
5	E	212/215 (99%)	197 (93%)	9 (4%)	6 (3%)	4	25
6	F	85/155 (55%)	74 (87%)	10 (12%)	1 (1%)	10	42
7	G	166/179 (93%)	147 (89%)	14 (8%)	5 (3%)	3	23
8	H	129/146 (88%)	111 (86%)	10 (8%)	8 (6%)	1	13
9	I	112/122 (92%)	100 (89%)	10 (9%)	2 (2%)	6	33
10	J	64/70 (91%)	57 (89%)	6 (9%)	1 (2%)	7	37
11	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
12	L	42/70 (60%)	31 (74%)	9 (21%)	2 (5%)	2	17
All	All	3913/4573 (86%)	3410 (87%)	371 (10%)	132 (3%)	3	21

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	66	LYS
1	A	76	GLU
1	A	194	ALA
1	A	286	HIS
1	A	385	ILE
1	A	418	SER
1	A	567	LYS
1	A	629	LEU
1	A	751	SER
1	A	775	ILE
1	A	1016	THR
1	A	1064	VAL
1	A	1108	ALA
1	A	1111	MET
2	B	81	SER
2	B	146	GLU
2	B	248	SER
2	B	252	SER
2	B	334	ILE
2	B	510	LYS
2	B	512	ARG

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Mol	Chain	Res	Type
2	B	712	PRO
2	B	889	THR
2	B	907	GLY
2	B	932	HIS
2	B	1157	ALA
3	C	142	VAL
4	D	20	GLU
7	G	141	SER
7	G	153	GLN
10	J	2	ILE
1	A	43	GLU
1	A	131	SER
1	A	311	GLN
1	A	319	GLY
1	A	335	ARG
1	A	593	GLU
1	A	595	THR
1	A	628	GLY
1	A	701	LEU
1	A	1003	LYS
1	A	1332	PHE
1	A	1437	GLY
2	B	58	THR
2	B	249	ARG
2	B	337	ARG
2	B	345	LYS
2	B	347	LYS
2	B	922	GLU
2	B	923	GLU
2	B	1181	GLU
3	C	214	ASN
4	D	19	GLU
4	D	118	THR
4	D	169	SER
4	D	199	ASN
5	E	3	GLN
5	E	172	GLU
6	F	71	GLU
8	H	109	LYS
8	H	129	TYR
9	I	106	CYS
12	L	45	ALA

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Mol	Chain	Res	Type
1	A	63	ARG
1	A	117	GLU
1	A	152	VAL
1	A	188	ASP
1	A	423	ASP
1	A	1115	SER
1	A	1221	LYS
1	A	1403	GLU
2	B	75	ALA
2	B	76	GLN
2	B	78	THR
2	B	164	LYS
2	B	199	MET
2	B	531	GLN
2	B	575	PRO
2	B	648	HIS
2	B	711	GLU
2	B	884	ARG
3	C	91	HIS
3	C	174	ALA
4	D	198	LEU
5	E	45	LYS
7	G	50	ASP
7	G	63	PRO
7	G	154	VAL
8	H	17	PRO
8	H	84	ALA
8	H	85	GLY
8	H	108	SER
9	I	47	GLU
1	A	67	CYS
1	A	158	PRO
1	A	314	ALA
1	A	424	ILE
1	A	568	PRO
1	A	779	PHE
1	A	958	VAL
1	A	1112	LYS
2	B	935	ARG
2	B	951	GLN
2	B	1017	ILE
2	B	1046	PRO

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Mol	Chain	Res	Type
2	B	1156	ASP
3	C	90	ASP
5	E	104	ASN
12	L	59	ALA
1	A	4	GLN
1	A	54	ASN
1	A	426	LEU
1	A	591	PHE
2	B	147	LEU
2	B	198	ASP
2	B	250	PHE
2	B	440	HIS
3	C	161	LYS
3	C	215	GLU
5	E	50	MET
8	H	60	ALA
8	H	78	SER
1	A	48	ALA
2	B	80	GLU
2	B	143	PRO
2	B	282	ILE
2	B	919	SER
3	C	149	LYS
2	B	1045	SER
5	E	86	PRO
2	B	343	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	1244/1520 (82%)	1116 (90%)	128 (10%)	7	23
2	B	1002/1061 (94%)	888 (89%)	114 (11%)	5	21
3	C	233/274 (85%)	217 (93%)	16 (7%)	14	37
4	D	146/200 (73%)	134 (92%)	12 (8%)	10	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	196/197 (100%)	185 (94%)	11 (6%)	19	42
6	F	77/137 (56%)	73 (95%)	4 (5%)	21	44
7	G	151/160 (94%)	138 (91%)	13 (9%)	10	30
8	H	118/128 (92%)	111 (94%)	7 (6%)	18	41
9	I	108/116 (93%)	102 (94%)	6 (6%)	19	42
10	J	61/65 (94%)	56 (92%)	5 (8%)	10	32
11	K	99/102 (97%)	90 (91%)	9 (9%)	9	29
12	L	39/57 (68%)	33 (85%)	6 (15%)	2	14
All	All	3474/4017 (86%)	3143 (90%)	331 (10%)	8	26

All (331) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	40	THR
1	A	43	GLU
1	A	44	THR
1	A	53	LEU
1	A	57	ARG
1	A	58	LEU
1	A	70	CYS
1	A	93	VAL
1	A	121	LEU
1	A	129	LYS
1	A	152	VAL
1	A	173	THR
1	A	187	LYS
1	A	204	THR
1	A	226	GLU
1	A	236	LEU
1	A	247	ARG
1	A	266	LEU
1	A	279	LEU
1	A	289	ILE
1	A	307	ASP
1	A	315	LEU
1	A	320	ARG
1	A	329	LEU
1	A	363	GLN

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Mol	Chain	Res	Type
1	A	459	ARG
1	A	461	LYS
1	A	467	THR
1	A	469	ARG
1	A	475	THR
1	A	485	ASP
1	A	498	ARG
1	A	509	LEU
1	A	518	LYS
1	A	521	MET
1	A	523	ILE
1	A	527	THR
1	A	528	LEU
1	A	536	LEU
1	A	546	VAL
1	A	588	LEU
1	A	595	THR
1	A	597	LEU
1	A	606	LEU
1	A	618	GLU
1	A	622	VAL
1	A	630	ILE
1	A	635	ARG
1	A	640	GLN
1	A	644	LYS
1	A	657	LEU
1	A	664	THR
1	A	666	ILE
1	A	672	ASP
1	A	701	LEU
1	A	702	LEU
1	A	710	LEU
1	A	732	LEU
1	A	738	LYS
1	A	746	MET
1	A	771	GLU
1	A	811	GLN
1	A	830	LYS
1	A	837	ILE
1	A	838	GLN
1	A	841	LEU
1	A	849	MET

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Mol	Chain	Res	Type
1	A	860	LEU
1	A	870	GLU
1	A	899	VAL
1	A	904	THR
1	A	913	LEU
1	A	919	ILE
1	A	920	LEU
1	A	932	GLU
1	A	936	LEU
1	A	938	LYS
1	A	961	ARG
1	A	963	ILE
1	A	980	ASP
1	A	981	LEU
1	A	983	ILE
1	A	988	LEU
1	A	998	LEU
1	A	1003	LYS
1	A	1009	ASN
1	A	1015	VAL
1	A	1016	THR
1	A	1045	VAL
1	A	1058	VAL
1	A	1067	LEU
1	A	1078	GLN
1	A	1096	SER
1	A	1100	ARG
1	A	1104	ILE
1	A	1109	LYS
1	A	1113	THR
1	A	1116	LEU
1	A	1120	LEU
1	A	1135	ARG
1	A	1143	LEU
1	A	1155	ASP
1	A	1166	ASP
1	A	1168	GLU
1	A	1186	ASP
1	A	1208	THR
1	A	1219	THR
1	A	1224	LEU
1	A	1238	ILE

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Mol	Chain	Res	Type
1	A	1273	LEU
1	A	1299	VAL
1	A	1303	GLU
1	A	1316	VAL
1	A	1354	ASN
1	A	1356	ILE
1	A	1371	LEU
1	A	1381	LEU
1	A	1409	LEU
1	A	1418	LEU
1	A	1420	ASP
1	A	1422	ARG
1	A	1426	GLU
1	A	1433	MET
1	A	1436	ILE
1	A	1443	VAL
1	A	1447	GLU
1	A	1450	LEU
2	B	21	GLU
2	B	47	GLN
2	B	63	ILE
2	B	73	GLN
2	B	82	ASP
2	B	95	ILE
2	B	106	ASP
2	B	126	SER
2	B	129	PHE
2	B	130	VAL
2	B	147	LEU
2	B	164	LYS
2	B	170	LEU
2	B	175	ARG
2	B	178	ASN
2	B	240	ILE
2	B	242	SER
2	B	244	LEU
2	B	251	ILE
2	B	254	LEU
2	B	301	ILE
2	B	324	ILE
2	B	331	LEU
2	B	334	ILE

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Mol	Chain	Res	Type
2	B	341	LEU
2	B	344	LYS
2	B	361	LEU
2	B	374	LYS
2	B	384	ARG
2	B	396	ASP
2	B	401	PHE
2	B	424	LEU
2	B	435	THR
2	B	473	MET
2	B	479	VAL
2	B	485	ARG
2	B	499	ASN
2	B	510	LYS
2	B	512	ARG
2	B	526	GLU
2	B	531	GLN
2	B	552	MET
2	B	555	ILE
2	B	563	MET
2	B	570	VAL
2	B	585	VAL
2	B	602	THR
2	B	629	ASP
2	B	633	VAL
2	B	635	ARG
2	B	639	ILE
2	B	651	LEU
2	B	658	ILE
2	B	667	GLN
2	B	682	SER
2	B	694	ASP
2	B	748	ILE
2	B	755	ILE
2	B	778	MET
2	B	786	ASN
2	B	791	THR
2	B	795	ILE
2	B	797	TYR
2	B	825	VAL
2	B	829	CYS
2	B	837	ASP

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Mol	Chain	Res	Type
2	B	839	MET
2	B	865	LYS
2	B	868	MET
2	B	873	THR
2	B	878	GLN
2	B	883	LEU
2	B	904	ARG
2	B	919	SER
2	B	924	GLU
2	B	942	ARG
2	B	944	THR
2	B	945	GLU
2	B	950	ASP
2	B	955	THR
2	B	956	THR
2	B	957	ASN
2	B	961	LEU
2	B	971	THR
2	B	973	ILE
2	B	975	GLN
2	B	979	LYS
2	B	986	GLN
2	B	990	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1031	LEU
2	B	1051	THR
2	B	1060	ARG
2	B	1072	MET
2	B	1103	ILE
2	B	1112	GLN
2	B	1114	LEU
2	B	1120	GLU
2	B	1122	ARG
2	B	1123	SER
2	B	1124	ARG
2	B	1128	LEU
2	B	1138	MET
2	B	1145	SER
2	B	1150	ARG
2	B	1151	LEU
2	B	1159	ARG

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Mol	Chain	Res	Type
2	B	1160	VAL
2	B	1162	ILE
2	B	1182	CYS
2	B	1194	ILE
2	B	1201	LYS
2	B	1203	LEU
3	C	23	SER
3	C	27	LEU
3	C	44	LEU
3	C	55	THR
3	C	56	THR
3	C	80	LEU
3	C	101	LEU
3	C	111	THR
3	C	133	ILE
3	C	142	VAL
3	C	203	GLN
3	C	245	VAL
3	C	251	LEU
3	C	258	ILE
3	C	260	LEU
3	C	263	THR
4	D	15	LEU
4	D	35	LEU
4	D	71	LYS
4	D	76	LYS
4	D	120	GLU
4	D	122	GLU
4	D	145	MET
4	D	164	ILE
4	D	187	THR
4	D	197	SER
4	D	214	LEU
4	D	219	THR
5	E	37	LEU
5	E	81	GLU
5	E	107	THR
5	E	123	LEU
5	E	140	LEU
5	E	152	LYS
5	E	175	LEU
5	E	177	ARG

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Mol	Chain	Res	Type
5	E	188	LEU
5	E	190	LEU
5	E	201	LYS
6	F	79	ARG
6	F	82	THR
6	F	90	ARG
6	F	112	GLU
7	G	6	ASP
7	G	13	LEU
7	G	39	THR
7	G	64	THR
7	G	115	MET
7	G	119	LEU
7	G	133	SER
7	G	134	GLU
7	G	140	LYS
7	G	143	ILE
7	G	154	VAL
7	G	160	ILE
7	G	165	GLU
8	H	11	GLN
8	H	26	ILE
8	H	40	LEU
8	H	46	LEU
8	H	63	LEU
8	H	130	ARG
8	H	137	GLN
9	I	5	ARG
9	I	17	ARG
9	I	26	LEU
9	I	44	TYR
9	I	59	VAL
9	I	60	GLN
10	J	2	ILE
10	J	3	VAL
10	J	22	LEU
10	J	24	LEU
10	J	51	LEU
11	K	12	LEU
11	K	33	ILE
11	K	42	LEU
11	K	49	GLU

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Mol	Chain	Res	Type
11	K	73	LEU
11	K	75	ILE
11	K	79	GLU
11	K	92	ASN
11	K	114	LEU
12	L	27	LEU
12	L	37	LYS
12	L	43	THR
12	L	46	VAL
12	L	57	LEU
12	L	58	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	311	GLN
1	A	445	ASN
1	A	479	ASN
1	A	525	GLN
1	A	603	ASN
1	A	611	GLN
1	A	626	ASN
1	A	648	ASN
1	A	717	ASN
1	A	767	GLN
1	A	881	GLN
1	A	994	GLN
1	A	1048	ASN
1	A	1052	GLN
1	A	1078	GLN
1	A	1128	GLN
1	A	1222	ASN
1	A	1258	HIS
1	A	1312	ASN
1	A	1330	ASN
1	A	1364	ASN
2	B	73	GLN
2	B	103	ASN
2	B	121	ASN
2	B	300	HIS
2	B	357	GLN

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Mol	Chain	Res	Type
2	B	366	GLN
2	B	481	GLN
2	B	499	ASN
2	B	572	HIS
2	B	587	HIS
2	B	592	ASN
2	B	800	GLN
2	B	862	GLN
2	B	951	GLN
2	B	1193	GLN
2	B	1205	GLN
2	B	1211	ASN
3	C	7	GLN
3	C	131	HIS
3	C	231	ASN
4	D	37	GLN
4	D	41	GLN
5	E	8	ASN
5	E	106	GLN
7	G	57	GLN
7	G	96	GLN
8	H	11	GLN
8	H	21	ASN
8	H	131	ASN
8	H	137	GLN
9	I	11	ASN
11	K	2	ASN
11	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	7/9 (77%)	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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, 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	1425/1733 (82%)	0.66	87 (6%) 27 27	50, 116, 208, 300	0
2	B	1162/1224 (94%)	0.90	133 (11%) 10 14	50, 131, 241, 300	0
3	C	265/318 (83%)	0.77	19 (7%) 21 23	50, 121, 191, 240	0
4	D	168/221 (76%)	1.53	47 (27%) 1 4	78, 178, 284, 300	0
5	E	214/215 (99%)	0.70	12 (5%) 30 28	65, 148, 226, 282	0
6	F	87/155 (56%)	0.49	3 (3%) 48 38	51, 94, 173, 238	0
7	G	170/179 (94%)	1.11	35 (20%) 2 6	57, 128, 270, 300	0
8	H	135/146 (92%)	1.00	19 (14%) 6 10	99, 164, 236, 292	0
9	I	114/122 (93%)	0.98	13 (11%) 10 14	78, 155, 214, 280	0
10	J	66/70 (94%)	0.61	3 (4%) 38 33	67, 121, 194, 218	0
11	K	115/120 (95%)	0.54	3 (2%) 57 43	50, 116, 179, 237	0
12	L	44/70 (62%)	1.15	7 (15%) 5 8	82, 157, 207, 241	0
13	R	9/9 (100%)	0.69	0 100 100	158, 185, 278, 293	0
14	S	16/56 (28%)	2.28	10 (62%) 0 1	111, 278, 300, 300	0
15	U	29/56 (51%)	1.82	10 (34%) 1 3	111, 262, 300, 300	0
All	All	4019/4694 (85%)	0.83	401 (9%) 12 16	50, 129, 238, 300	0

All (401) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	245	GLU	8.2
7	G	94	CYS	6.9
2	B	735	ALA	6.0
4	D	217	LEU	5.6
4	D	149	THR	5.5
2	B	463	THR	5.0
7	G	171	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
4	D	200	ASN	4.9
2	B	601	ARG	4.9
4	D	213	GLU	4.9
4	D	125	SER	4.7
1	A	65	LEU	4.6
2	B	713	ALA	4.6
4	D	138	ASN	4.5
2	B	837	ASP	4.5
8	H	76	THR	4.4
2	B	932	HIS	4.3
2	B	346	GLU	4.3
14	S	24	DT	4.3
4	D	145	MET	4.2
2	B	265	SER	4.2
4	D	153	ARG	4.2
4	D	117	GLU	4.1
4	D	218	GLU	4.1
4	D	53	SER	4.1
1	A	66	LYS	4.1
3	C	23	SER	4.0
2	B	296	GLU	3.9
3	C	179	GLU	3.9
2	B	926	GLY	3.9
1	A	587	HIS	3.8
2	B	465	ASN	3.8
2	B	1120	GLU	3.8
4	D	205	ASP	3.8
11	K	115	ALA	3.8
4	D	54	GLU	3.8
2	B	394	ASP	3.7
4	D	135	GLY	3.7
2	B	531	GLN	3.7
7	G	123	ALA	3.7
1	A	251	SER	3.7
6	F	155	LEU	3.7
1	A	44	THR	3.7
2	B	207	GLY	3.7
1	A	277	GLU	3.7
1	A	918	GLU	3.7
2	B	550	ASP	3.7
8	H	1	MET	3.6
8	H	75	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
4	D	133	THR	3.6
8	H	119	GLY	3.6
7	G	112	LYS	3.6
2	B	108	VAL	3.6
4	D	126	ILE	3.5
7	G	98	GLY	3.5
15	U	11	DG	3.5
1	A	1108	ALA	3.5
7	G	138	THR	3.5
15	U	28	DA	3.5
1	A	1081	LEU	3.5
4	D	123	LEU	3.5
15	U	10	DA	3.5
14	S	30	DT	3.5
3	C	102	GLN	3.5
1	A	1393	ASN	3.4
12	L	27	LEU	3.4
10	J	66	LEU	3.4
7	G	135	ASP	3.4
15	U	9	DA	3.4
3	C	52	GLU	3.3
4	D	154	PHE	3.3
9	I	13	MET	3.3
2	B	951	GLN	3.3
8	H	21	ASN	3.3
1	A	1245	PRO	3.3
2	B	251	ILE	3.3
2	B	575	PRO	3.2
4	D	204	ASP	3.2
2	B	775	LYS	3.2
15	U	3	DA	3.2
12	L	39	SER	3.2
2	B	345	LYS	3.2
2	B	475	SER	3.2
2	B	502	ILE	3.2
3	C	190	ASP	3.2
2	B	838	SER	3.1
2	B	1100	ASP	3.1
7	G	121	PHE	3.1
1	A	166	GLY	3.1
4	D	142	LYS	3.1
7	G	139	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	159	THR	3.1
4	D	61	GLU	3.1
1	A	256	GLN	3.1
7	G	96	GLN	3.1
2	B	549	THR	3.1
2	B	499	ASN	3.1
7	G	127	PRO	3.1
2	B	448	ILE	3.1
4	D	122	GLU	3.1
1	A	310	GLY	3.0
3	C	68	GLY	3.0
2	B	925	LEU	3.0
7	G	142	ARG	3.0
4	D	206	GLU	3.0
4	D	130	LEU	3.0
1	A	169	ASN	3.0
14	S	28	DC	3.0
7	G	130	TYR	3.0
7	G	1	MET	3.0
2	B	163	GLY	3.0
1	A	145	LYS	3.0
1	A	69	THR	3.0
12	L	35	SER	3.0
2	B	320	ASP	3.0
2	B	164	LYS	3.0
2	B	80	GLU	2.9
4	D	129	LEU	2.9
7	G	115	MET	2.9
8	H	2	SER	2.9
1	A	28	ARG	2.9
14	S	29	DT	2.9
5	E	197	LYS	2.9
1	A	1156	PRO	2.9
5	E	50	MET	2.9
14	S	39	DG	2.9
1	A	1175	SER	2.9
2	B	736	THR	2.9
8	H	92	ASP	2.9
2	B	449	ASN	2.9
4	D	216	ASN	2.9
1	A	71	GLN	2.9
2	B	706	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	139	LYS	2.9
7	G	88	ASP	2.9
1	A	252	PHE	2.9
8	H	104	PHE	2.8
12	L	68	GLU	2.8
1	A	316	GLN	2.8
3	C	24	ASN	2.8
1	A	1125	ALA	2.8
1	A	788	SER	2.8
5	E	163	GLU	2.8
14	S	38	DG	2.8
7	G	155	SER	2.8
1	A	257	ARG	2.8
2	B	921	ASP	2.8
7	G	124	GLY	2.8
8	H	138	GLU	2.8
1	A	2	VAL	2.8
2	B	1186	ASP	2.8
4	D	220	LEU	2.8
2	B	266	ALA	2.8
2	B	220	GLY	2.8
1	A	1080	THR	2.8
2	B	708	GLU	2.8
2	B	1084	GLN	2.8
4	D	210	ILE	2.7
9	I	11	ASN	2.7
5	E	203	GLU	2.7
4	D	168	LYS	2.7
4	D	181	GLY	2.7
1	A	1323	ASP	2.7
4	D	212	LYS	2.7
9	I	5	ARG	2.7
9	I	77	LYS	2.7
1	A	1275	GLY	2.7
4	D	136	GLY	2.7
2	B	920	PRO	2.7
1	A	85	ASP	2.7
4	D	150	ASN	2.7
1	A	1093	LYS	2.7
2	B	1181	GLU	2.7
2	B	469	GLN	2.7
2	B	742	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	929	THR	2.6
2	B	1189	ILE	2.6
3	C	229	TYR	2.6
2	B	529	GLU	2.6
2	B	226	PHE	2.6
2	B	584	GLY	2.6
2	B	253	THR	2.6
7	G	95	SER	2.6
9	I	64	SER	2.6
2	B	82	ASP	2.6
2	B	709	ASP	2.6
2	B	1179	GLN	2.6
3	C	203	GLN	2.6
5	E	120	ALA	2.6
4	D	147	TYR	2.6
2	B	927	GLN	2.6
11	K	29	ASN	2.6
1	A	1076	ALA	2.6
1	A	194	ALA	2.6
9	I	55	THR	2.6
2	B	642	ASP	2.5
1	A	1196	GLU	2.5
7	G	57	GLN	2.5
2	B	221	ASN	2.5
9	I	111	THR	2.5
1	A	167	CYS	2.5
1	A	253	ASN	2.5
2	B	1013	ASN	2.5
15	U	15	DA	2.5
1	A	3	GLY	2.5
1	A	537	ARG	2.5
2	B	369	GLY	2.5
1	A	466	SER	2.5
2	B	161	GLU	2.5
2	B	629	ASP	2.5
3	C	149	LYS	2.5
3	C	268	ASP	2.5
1	A	703	THR	2.5
2	B	299	GLU	2.5
2	B	1188	LYS	2.5
8	H	95	TYR	2.5
3	C	35	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
7	G	53	ASN	2.5
2	B	464	GLY	2.5
1	A	830	LYS	2.5
2	B	490	SER	2.5
9	I	54	GLU	2.5
1	A	1186	ASP	2.5
2	B	94	LYS	2.5
1	A	150	THR	2.4
1	A	75	ASN	2.4
2	B	340	ALA	2.4
2	B	136	THR	2.4
4	D	118	THR	2.4
4	D	185	CYS	2.4
2	B	458	LYS	2.4
2	B	333	PHE	2.4
5	E	104	ASN	2.4
1	A	425	GLN	2.4
7	G	67	SER	2.4
9	I	102	VAL	2.4
2	B	726	ALA	2.4
2	B	429	PHE	2.4
2	B	78	THR	2.4
2	B	552	MET	2.4
8	H	137	GLN	2.4
1	A	143	LYS	2.4
6	F	154	ASP	2.4
2	B	338	GLY	2.4
3	C	191	TYR	2.4
9	I	60	GLN	2.4
1	A	320	ARG	2.4
5	E	94	LYS	2.4
7	G	158	HIS	2.4
8	H	109	LYS	2.4
7	G	42	PHE	2.3
2	B	466	TRP	2.3
1	A	1109	LYS	2.3
2	B	1223	ASP	2.3
1	A	141	LEU	2.3
15	U	18	DA	2.3
1	A	612	ILE	2.3
1	A	1383	SER	2.3
1	A	914	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	115	ASN	2.3
8	H	37	LYS	2.3
2	B	891	ASP	2.3
2	B	46	GLN	2.3
2	B	484	ASN	2.3
4	D	23	ASN	2.3
7	G	126	ASN	2.3
5	E	192	ARG	2.3
15	U	12	DT	2.3
2	B	879	ARG	2.3
7	G	40	GLY	2.3
5	E	63	ASN	2.3
1	A	283	GLY	2.3
2	B	606	LYS	2.3
2	B	440	HIS	2.3
2	B	101	MET	2.3
7	G	93	SER	2.2
1	A	74	MET	2.2
10	J	49	MET	2.2
1	A	43	GLU	2.2
1	A	1272	THR	2.2
2	B	705	MET	2.2
14	S	32	DT	2.2
7	G	50	ASP	2.2
7	G	99	PHE	2.2
9	I	12	ASN	2.2
1	A	41	MET	2.2
3	C	127	ARG	2.2
1	A	589	GLN	2.2
2	B	53	GLN	2.2
2	B	285	ILE	2.2
2	B	1009	ASP	2.2
1	A	1098	VAL	2.2
2	B	617	ARG	2.2
4	D	119	ARG	2.2
8	H	120	GLY	2.2
2	B	556	THR	2.2
1	A	1361	SER	2.2
15	U	2	DT	2.2
3	C	131	HIS	2.2
4	D	16	LYS	2.2
2	B	431	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	457	ALA	2.2
2	B	444	MET	2.2
4	D	215	SER	2.2
1	A	503	GLN	2.2
2	B	60	GLN	2.2
4	D	155	ARG	2.2
4	D	137	ASN	2.2
14	S	26	DT	2.2
2	B	487	THR	2.2
8	H	32	THR	2.2
15	U	0	DC	2.2
4	D	157	GLN	2.2
2	B	249	ARG	2.2
3	C	12	GLU	2.2
2	B	668	ASP	2.1
7	G	128	PRO	2.1
2	B	272	THR	2.1
1	A	1173	HIS	2.1
2	B	430	ARG	2.1
2	B	958	GLN	2.1
1	A	120	GLU	2.1
7	G	134	GLU	2.1
7	G	137	ILE	2.1
12	L	43	THR	2.1
2	B	142	VAL	2.1
2	B	341	LEU	2.1
1	A	980	ASP	2.1
2	B	942	ARG	2.1
2	B	21	GLU	2.1
2	B	342	GLY	2.1
2	B	577	ALA	2.1
14	S	25	DG	2.1
1	A	521	MET	2.1
2	B	597	MET	2.1
1	A	109	HIS	2.1
2	B	79	THR	2.1
1	A	311	GLN	2.1
1	A	889	SER	2.1
11	K	60	ALA	2.1
1	A	790	ASP	2.1
3	C	211	ASP	2.1
14	S	37	DA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	103	CYS	2.1
2	B	39	ARG	2.1
5	E	121	MET	2.1
1	A	140	THR	2.1
2	B	1211	ASN	2.1
10	J	42	LYS	2.1
2	B	125	SER	2.1
2	B	160	SER	2.1
2	B	561	TRP	2.1
2	B	1220	ARG	2.1
1	A	70	CYS	2.1
1	A	83	HIS	2.1
4	D	214	LEU	2.1
1	A	410	GLY	2.1
1	A	627	GLY	2.1
1	A	13	THR	2.1
8	H	64	ASN	2.1
1	A	171	GLN	2.1
1	A	1218	GLN	2.1
2	B	162	SER	2.1
2	B	923	GLU	2.1
8	H	45	GLU	2.1
12	L	41	SER	2.1
2	B	305	VAL	2.1
2	B	1119	VAL	2.1
1	A	175	ARG	2.0
2	B	841	MET	2.0
2	B	1133	MET	2.0
1	A	62	ASP	2.0
1	A	791	ASP	2.0
3	C	226	ASP	2.0
1	A	975	HIS	2.0
8	H	84	ALA	2.0
6	F	115	THR	2.0
8	H	131	ASN	2.0
2	B	159	ASP	2.0
2	B	447	ALA	2.0
7	G	166	ASP	2.0
12	L	45	ALA	2.0
7	G	113	HIS	2.0
2	B	821	GLN	2.0
1	A	951	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	882	THR	2.0
4	D	132	GLN	2.0
2	B	773	MET	2.0
1	A	294	SER	2.0
2	B	710	LEU	2.0
7	G	129	SER	2.0
2	B	351	TYR	2.0
3	C	129	ILE	2.0
2	B	618	ASP	2.0
9	I	72	ASP	2.0
2	B	24	PRO	2.0
1	A	344	ARG	2.0
9	I	87	GLN	2.0
2	B	383	ASN	2.0
2	B	922	GLU	2.0
5	E	20	LYS	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 oligosaccharides 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, 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	MG	A	1804	1/1	0.62	0.28	71,71,71,71	0
17	MG	A	1803	1/1	0.96	0.07	54,54,54,54	0
16	ZN	A	1802	1/1	0.98	0.10	68,68,68,68	0
16	ZN	I	202	1/1	0.98	0.10	155,155,155,155	0
16	ZN	A	1801	1/1	0.99	0.05	101,101,101,101	0
16	ZN	J	101	1/1	0.99	0.10	90,90,90,90	0
16	ZN	L	101	1/1	0.99	0.08	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	ZN	B	1301	1/1	0.99	0.07	60,60,60,60	0
16	ZN	I	201	1/1	0.99	0.07	115,115,115,115	0
16	ZN	C	401	1/1	1.00	0.06	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.