



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:33 PM UTC

PDB ID : 3RZD / pdb_00003rzd
Title : RNA Polymerase II Initiation Complex with a 5-nt RNA
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-11
Resolution : 3.30 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

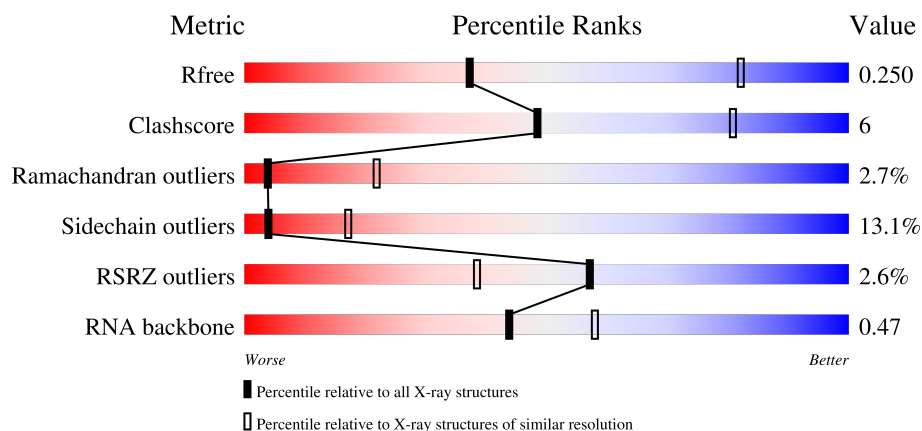
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

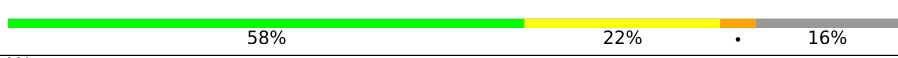
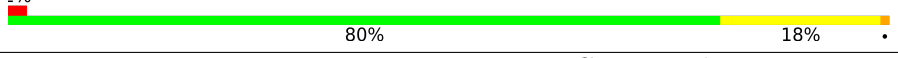
The reported resolution of this entry is 3.30 Å.

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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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	
2	B	1224	
3	C	318	
4	E	215	

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Mol	Chain	Length	Quality of chain
5	F	155	45% 9% • 45%
6	H	146	5% 65% 23% • 9%
7	I	122	% 80% 14% • •
8	J	70	% 60% 27% 6% 7%
9	K	120	% 74% 19% • 5%
10	L	70	7% 36% 21% 7% • 34%
11	R	5	60% 40%
12	T	29	21% 7% 72%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 28570 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	1405	Total	C	N	O	S	0	0	0
			11043	6965	1936	2081	61			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	5	Total	C	N	O	P	0	0	0
			110	50	25	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*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3').

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

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		

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

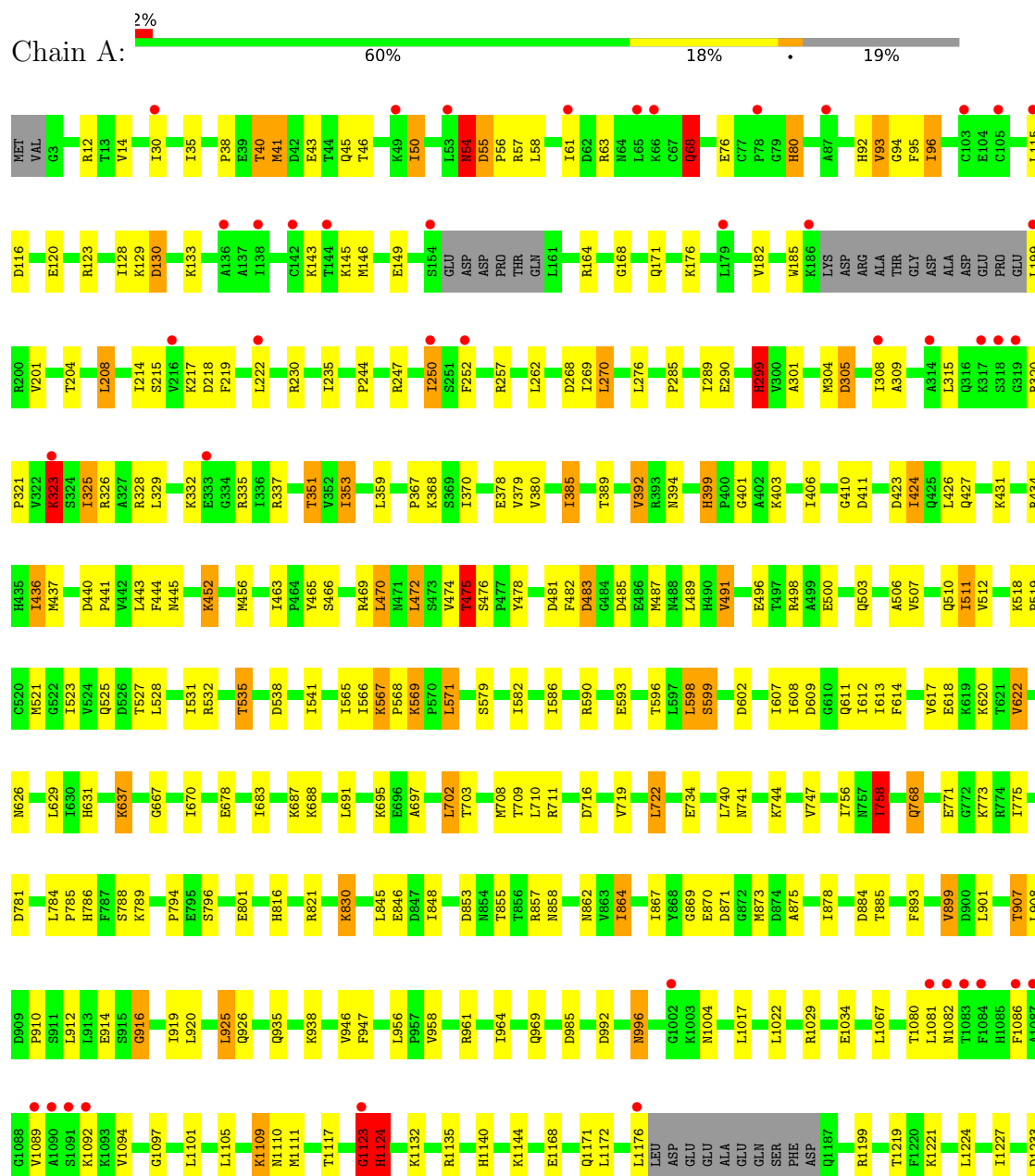
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

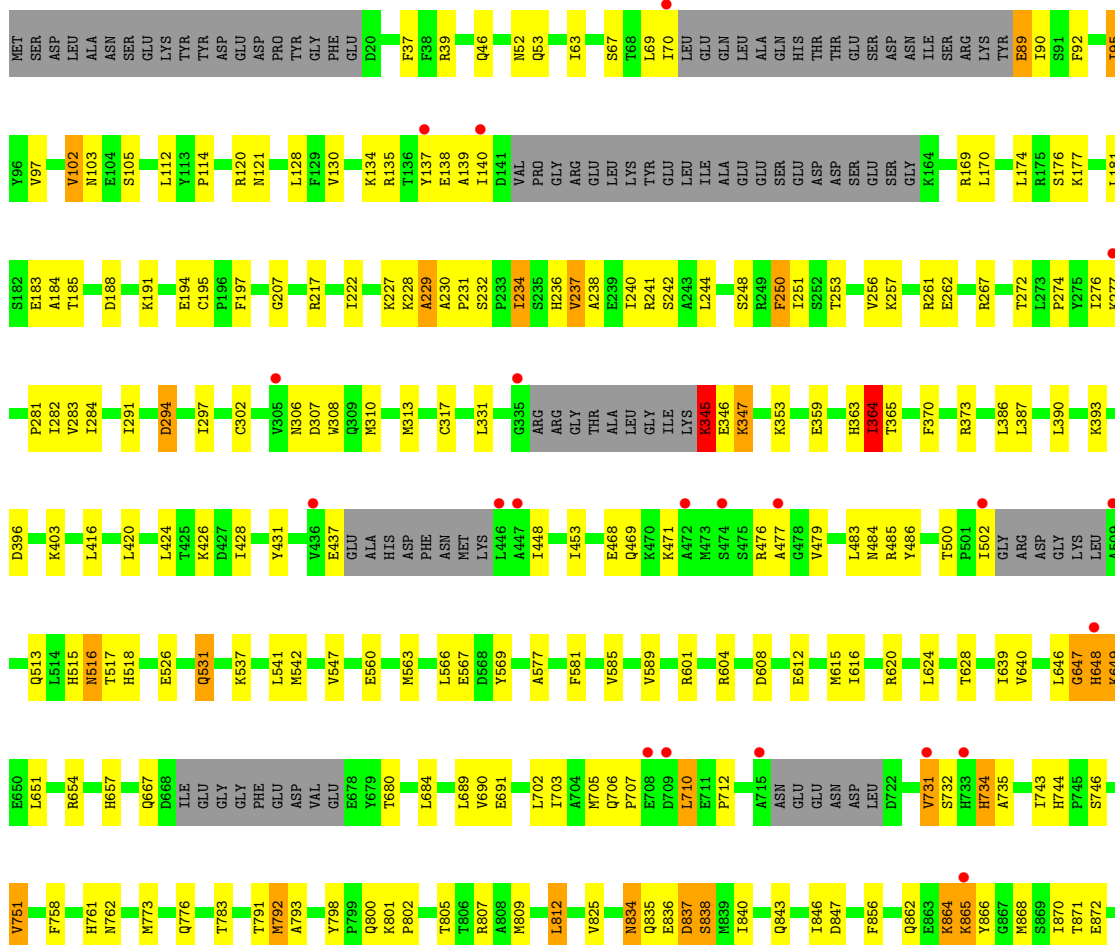
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

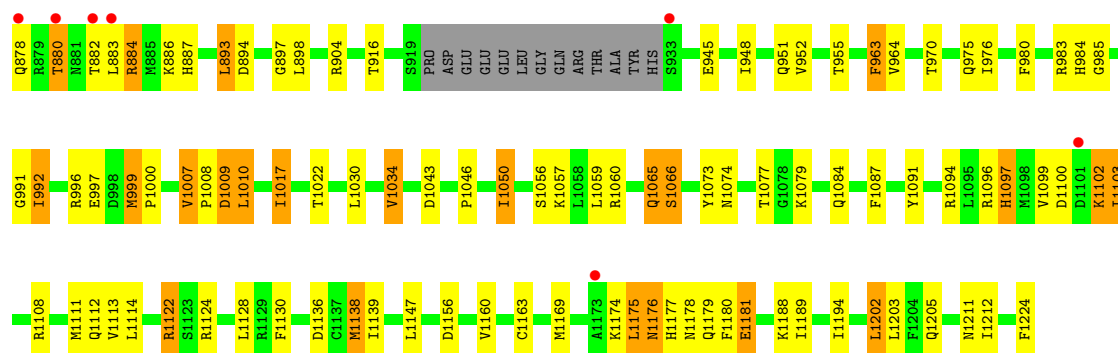
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

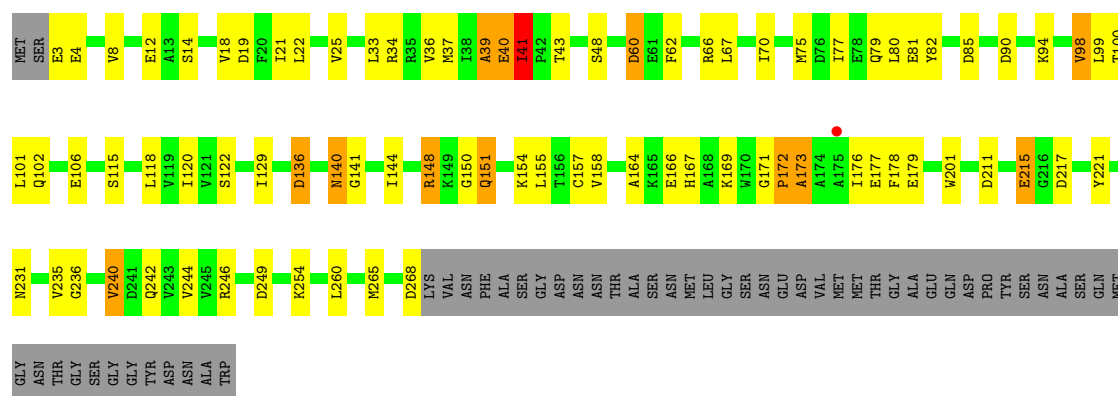






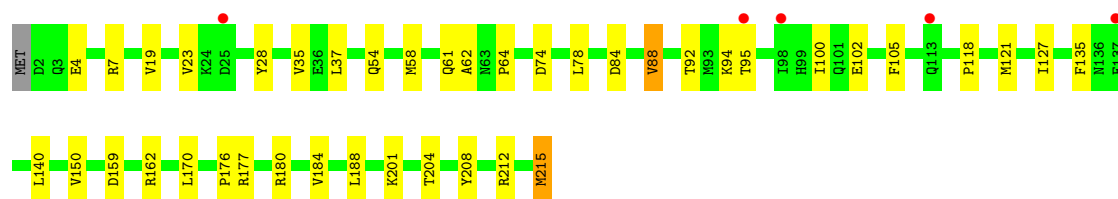
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 58% 22% 16%



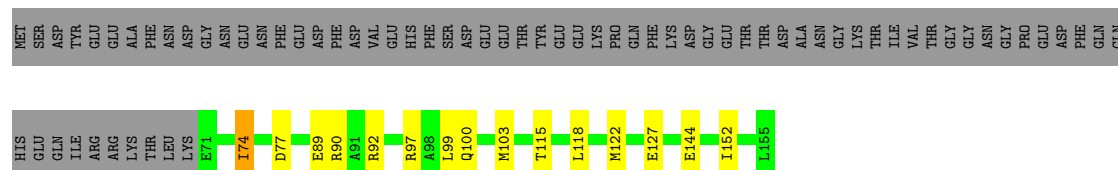
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 2% 80% 18%



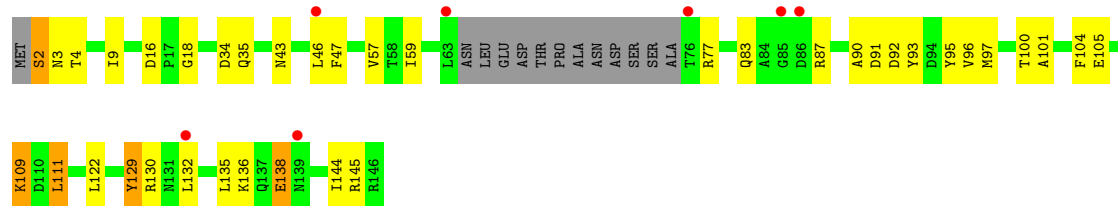
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 45% 9% 45%

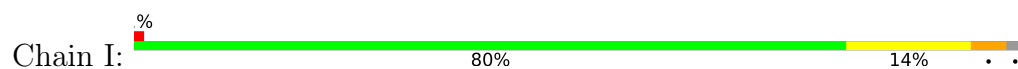


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

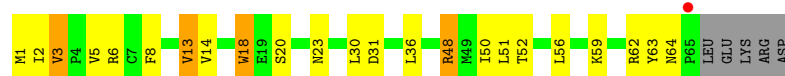
Chain H: 5% 65% 23% 9%



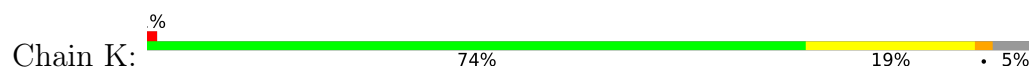
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



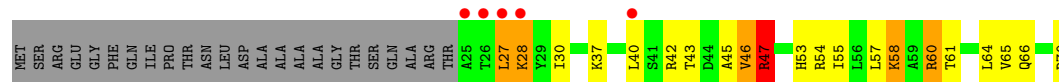
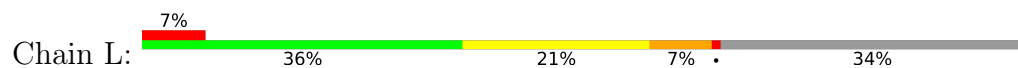
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- 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(*AP*GP*AP*GP*G)-3')



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



DC	DT	DA	DC	DC	DG	DA	DT	DA	DA	DG	DC	DA	DG	DA	C16	C21	T22	C23	DT	DC	DG	DA	DT	DG
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.54Å 221.27Å 192.18Å 90.00° 97.44° 90.00°	Depositor
Resolution (Å)	45.14 – 3.30 45.14 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.14-3.30) 99.2 (45.14-3.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 3.32Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.188 , 0.230 0.206 , 0.250	Depositor DCC
R_{free} test set	4848 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 85.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28570	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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	0.76	0/11241	1.41	40/15199 (0.3%)
2	B	0.75	0/9033	1.38	44/12181 (0.4%)
3	C	0.71	0/2133	1.39	19/2891 (0.7%)
4	E	0.74	0/1788	1.34	4/2406 (0.2%)
5	F	0.75	0/700	1.30	0/945
6	H	0.75	0/1086	1.27	10/1470 (0.7%)
7	I	0.70	0/989	1.32	5/1331 (0.4%)
8	J	0.72	0/541	1.43	4/727 (0.6%)
9	K	0.66	0/937	1.29	1/1265 (0.1%)
10	L	0.82	0/365	1.50	7/485 (1.4%)
11	R	0.41	0/124	0.80	0/193
12	T	0.45	0/176	1.26	1/268 (0.4%)
All	All	0.74	0/29113	1.38	135/39361 (0.3%)

There are no bond length outliers.

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	647	GLY	CA-C-N	10.62	140.81	121.70
2	B	647	GLY	C-N-CA	10.62	140.81	121.70
3	C	39	ALA	N-CA-C	9.02	124.67	112.68
10	L	58	LYS	N-CA-C	8.83	123.06	111.75
6	H	92	ASP	N-CA-C	-8.10	100.44	111.87
1	A	466	SER	N-CA-C	7.97	122.27	112.54
3	C	172	PRO	CA-C-N	7.72	136.29	121.54
3	C	172	PRO	C-N-CA	7.72	136.29	121.54
1	A	1123	GLY	CA-C-N	7.68	135.52	121.70
1	A	1123	GLY	C-N-CA	7.68	135.52	121.70
1	A	1097	GLY	CA-C-N	7.60	126.41	120.33
1	A	1097	GLY	C-N-CA	7.60	126.41	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	2	SER	CA-C-N	7.28	134.81	121.70
6	H	2	SER	C-N-CA	7.28	134.81	121.70
4	E	150	VAL	N-CA-C	7.19	114.11	107.56
1	A	54	ASN	CA-CB-CG	7.05	119.65	112.60
1	A	947	PHE	CA-C-N	6.91	129.52	120.60
1	A	947	PHE	C-N-CA	6.91	129.52	120.60
6	H	91	ASP	N-CA-C	6.85	120.34	108.76
2	B	1156	ASP	N-CA-C	6.84	119.63	110.88
2	B	345	LYS	CA-C-N	6.74	133.84	121.70
2	B	345	LYS	C-N-CA	6.74	133.84	121.70
1	A	1004	ASN	CA-C-N	6.65	129.51	120.54
1	A	1004	ASN	C-N-CA	6.65	129.51	120.54
2	B	37	PHE	N-CA-C	-6.59	102.31	110.41
3	C	41	ILE	N-CA-CB	6.53	117.22	110.23
3	C	82	TYR	N-CA-C	-6.37	99.63	109.76
3	C	40	GLU	N-CA-C	6.35	121.17	113.17
2	B	184	ALA	N-CA-C	6.32	119.14	110.24
2	B	648	HIS	CA-C-N	6.29	129.63	120.71
2	B	648	HIS	C-N-CA	6.29	129.63	120.71
3	C	41	ILE	CB-CA-C	6.28	116.78	110.94
4	E	102	GLU	N-CA-C	6.27	117.78	111.07
2	B	945	GLU	N-CA-C	6.18	119.61	110.46
1	A	506	ALA	CA-C-N	6.08	125.19	120.33
1	A	506	ALA	C-N-CA	6.08	125.19	120.33
1	A	1269	GLU	N-CA-C	6.08	118.82	111.40
1	A	602	ASP	CA-CB-CG	6.07	118.67	112.60
2	B	628	THR	CA-C-N	6.03	133.06	121.54
2	B	628	THR	C-N-CA	6.03	133.06	121.54
8	J	18	TRP	N-CA-C	6.03	117.52	111.07
3	C	136	ASP	CA-C-N	6.01	128.62	120.38
3	C	136	ASP	C-N-CA	6.01	128.62	120.38
9	K	71	PHE	CA-CB-CG	6.01	119.81	113.80
2	B	228	LYS	N-CA-C	5.99	118.28	108.52
1	A	452	LYS	N-CA-C	-5.80	104.92	112.23
3	C	172	PRO	N-CA-C	-5.77	107.27	114.20
1	A	481	ASP	CA-CB-CG	5.76	118.36	112.60
7	I	31	THR	N-CA-C	-5.75	107.26	114.56
1	A	483	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	426	LEU	N-CA-C	5.73	117.94	110.43
1	A	864	ILE	N-CA-C	-5.72	106.23	111.67
1	A	244	PRO	N-CA-C	5.71	117.66	110.70
1	A	758	ILE	CA-C-N	5.70	128.23	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	758	ILE	C-N-CA	5.70	128.23	120.54
1	A	323	LYS	N-CA-C	5.69	117.29	111.14
6	H	16	ASP	N-CA-C	5.64	118.57	109.15
1	A	884	ASP	N-CA-C	5.62	119.23	112.38
2	B	1169	MET	CA-C-N	5.61	127.80	120.28
2	B	1169	MET	C-N-CA	5.61	127.80	120.28
8	J	8	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	475	THR	CA-C-N	5.59	127.75	120.26
1	A	475	THR	C-N-CA	5.59	127.75	120.26
1	A	445	ASN	CA-CB-CG	5.57	118.17	112.60
2	B	294	ASP	CA-CB-CG	5.57	118.17	112.60
2	B	884	ARG	CA-C-N	5.57	128.75	120.90
2	B	884	ARG	C-N-CA	5.57	128.75	120.90
10	L	40	LEU	N-CA-C	5.55	118.50	109.24
2	B	1176	ASN	CA-CB-CG	5.52	118.12	112.60
3	C	236	GLY	CA-C-N	5.50	127.96	120.54
3	C	236	GLY	C-N-CA	5.50	127.96	120.54
3	C	240	VAL	N-CA-CB	5.46	116.36	110.62
1	A	1034	GLU	CA-C-N	5.46	127.60	120.28
1	A	1034	GLU	C-N-CA	5.46	127.60	120.28
6	H	129	TYR	CA-C-N	5.45	127.85	120.65
6	H	129	TYR	C-N-CA	5.45	127.85	120.65
1	A	1424	VAL	CA-C-N	5.42	127.81	120.38
1	A	1424	VAL	C-N-CA	5.42	127.81	120.38
3	C	120	ILE	CA-C-N	5.42	127.91	122.66
3	C	120	ILE	C-N-CA	5.42	127.91	122.66
3	C	150	GLY	CA-C-N	5.41	128.40	120.71
3	C	150	GLY	C-N-CA	5.41	128.40	120.71
7	I	97	MET	CA-C-N	5.41	127.75	120.50
7	I	97	MET	C-N-CA	5.41	127.75	120.50
2	B	250	PHE	CA-CB-CG	5.34	119.14	113.80
7	I	116	ASN	N-CA-C	5.33	117.92	109.50
1	A	716	ASP	CA-CB-CG	5.32	117.92	112.60
4	E	88	VAL	N-CA-C	5.32	116.23	108.58
3	C	60	ASP	CA-CB-CG	5.31	117.91	112.60
2	B	569	TYR	CA-C-N	5.29	127.46	122.85
2	B	569	TYR	C-N-CA	5.29	127.46	122.85
10	L	40	LEU	CA-C-N	5.29	130.37	120.95
10	L	40	LEU	C-N-CA	5.29	130.37	120.95
2	B	1009	ASP	N-CA-C	-5.29	105.98	112.90
1	A	305	ASP	CA-CB-CG	5.28	117.88	112.60
8	J	5	VAL	N-CA-C	-5.28	102.03	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	178	PHE	CA-CB-CG	5.25	119.05	113.80
2	B	847	ASP	CA-CB-CG	5.23	117.83	112.60
10	L	60	ARG	N-CA-C	5.23	117.67	110.35
1	A	996	ASN	N-CA-C	5.22	118.67	112.72
2	B	648	HIS	N-CA-CB	5.22	119.37	110.50
1	A	491	VAL	N-CA-C	5.21	113.67	107.73
6	H	138	GLU	N-CA-C	-5.20	106.77	113.01
1	A	485	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	708	MET	N-CA-C	5.20	117.28	109.23
2	B	776	GLN	CA-C-N	5.18	128.20	120.90
2	B	776	GLN	C-N-CA	5.18	128.20	120.90
8	J	64	ASN	N-CA-C	5.18	121.25	109.81
2	B	176	SER	CA-C-N	5.17	127.52	120.54
2	B	176	SER	C-N-CA	5.17	127.52	120.54
2	B	308	TRP	CA-C-N	5.15	127.14	120.44
2	B	308	TRP	C-N-CA	5.15	127.14	120.44
2	B	807	ARG	CA-C-N	5.14	127.16	120.28
2	B	807	ARG	C-N-CA	5.14	127.16	120.28
12	T	22	DT	P-O5'-C5'	5.13	127.69	120.00
10	L	57	LEU	CA-C-N	5.13	127.87	120.38
10	L	57	LEU	C-N-CA	5.13	127.87	120.38
1	A	351	THR	CA-C-N	5.11	127.42	120.63
1	A	351	THR	C-N-CA	5.11	127.42	120.63
2	B	834	ASN	CA-CB-CG	5.09	117.69	112.60
6	H	91	ASP	CA-C-N	5.08	131.07	122.79
6	H	91	ASP	C-N-CA	5.08	131.07	122.79
2	B	581	PHE	CA-CB-CG	5.07	118.87	113.80
7	I	10	CYS	N-CA-C	5.06	116.80	111.28
2	B	1065	GLN	CB-CA-C	5.05	117.84	110.26
2	B	680	THR	CA-C-N	5.03	127.44	120.29
2	B	680	THR	C-N-CA	5.03	127.44	120.29
1	A	985	ASP	CA-CB-CG	5.03	117.63	112.60
2	B	307	ASP	CA-CB-CG	5.02	117.62	112.60
4	E	94	LYS	N-CA-C	5.02	117.41	111.33
2	B	541	LEU	N-CA-C	5.01	117.40	111.33
2	B	183	GLU	CA-C-N	5.01	127.97	120.90
2	B	183	GLU	C-N-CA	5.01	127.97	120.90
2	B	431	TYR	CA-C-N	5.01	126.95	120.44
2	B	431	TYR	C-N-CA	5.01	126.95	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11043	0	11133	138	0
2	B	8861	0	8884	115	0
3	C	2095	0	2051	30	0
4	E	1752	0	1776	17	0
5	F	688	0	707	6	0
6	H	1068	0	1040	15	0
7	I	971	0	927	5	0
8	J	532	0	542	10	0
9	K	919	0	929	8	0
10	L	363	0	386	6	0
11	R	110	0	56	1	0
12	T	159	0	91	1	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	28522	314	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 6.

All (314) 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:1123:GLY:HA3	1:A:1124:HIS:HB2	1.33	1.07
8:J:48:ARG:O	8:J:52:THR:HB	1.79	0.83
1:A:1123:GLY:CA	1:A:1124:HIS:HB2	2.10	0.80
7:I:63:GLY:HA3	7:I:104:LEU:HD11	1.63	0.80
1:A:285:PRO:HD2	1:A:289:ILE:HD11	1.65	0.79
1:A:935:GLN:HE22	1:A:938:LYS:HD3	1.46	0.78
2:B:984:HIS:HB3	2:B:1022:THR:CG2	2.17	0.74
1:A:535:THR:HG21	1:A:617:VAL:H	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.70	0.72
2:B:654:ARG:H	2:B:657:HIS:HD2	1.37	0.71
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.39	0.70
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.74	0.70
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.72	0.70
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.23	0.69
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.40	0.68
1:A:567:LYS:HB3	6:H:96:VAL:H	1.57	0.68
1:A:456:MET:HE3	1:A:510:GLN:HB2	1.76	0.67
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.75	0.67
3:C:167:HIS:HD2	3:C:169:LYS:H	1.40	0.67
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.77	0.67
5:F:74:ILE:HG21	5:F:144:GLU:HG2	1.76	0.66
9:K:65:HIS:HD2	9:K:67:PHE:H	1.41	0.66
2:B:984:HIS:HB3	2:B:1022:THR:HG21	1.75	0.66
2:B:1097:HIS:HB2	2:B:1102:LYS:HE3	1.78	0.66
1:A:14:VAL:HG12	1:A:1432:GLN:HE22	1.59	0.65
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.77	0.65
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.79	0.65
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	1.78	0.64
1:A:511:ILE:HA	1:A:521:MET:HE3	1.78	0.64
1:A:472:LEU:O	1:A:475:THR:HB	1.98	0.64
2:B:706:GLN:O	2:B:710:LEU:HB2	1.99	0.63
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.63	0.63
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.81	0.63
1:A:1276:VAL:HG21	1:A:1316:VAL:HG22	1.80	0.63
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.80	0.62
3:C:115:SER:HB3	3:C:141:GLY:HA3	1.81	0.62
1:A:215:SER:O	1:A:219:PHE:HB2	1.99	0.62
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.81	0.62
1:A:323:LYS:HE2	1:A:328:ARG:HE	1.65	0.61
2:B:234:ILE:HD11	2:B:237:VAL:HG23	1.82	0.61
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.80	0.61
10:L:27:LEU:HB3	10:L:37:LYS:HD2	1.81	0.61
3:C:41:ILE:HG12	3:C:172:PRO:HG3	1.83	0.61
6:H:2:SER:HB2	6:H:3:ASN:HB2	1.82	0.61
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.80	0.61
2:B:1074:ASN:HD22	2:B:1077:THR:H	1.49	0.60
2:B:798:TYR:HE2	3:C:66:ARG:HH21	1.50	0.58
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.37	0.58
2:B:1034:VAL:HG22	2:B:1059:LEU:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:PHE:HB3	1:A:1092:LYS:HE2	1.86	0.58
1:A:95:PHE:HE2	1:A:1414:ALA:HB2	1.67	0.58
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.49	0.58
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.85	0.58
1:A:535:THR:HG21	1:A:617:VAL:N	2.19	0.58
2:B:744:HIS:HD2	2:B:746:SER:H	1.52	0.58
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.84	0.58
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.86	0.57
1:A:579:SER:HB3	1:A:611:GLN:HA	1.86	0.57
1:A:1089:VAL:HB	1:A:1092:LYS:HD3	1.85	0.57
2:B:234:ILE:HG13	2:B:257:LYS:HB3	1.86	0.57
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.40	0.57
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.86	0.57
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.86	0.57
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.69	0.56
1:A:535:THR:CG2	1:A:617:VAL:H	2.17	0.56
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.87	0.56
1:A:483:ASP:HB3	2:B:837:ASP:HB2	1.87	0.56
3:C:171:GLY:C	3:C:173:ALA:H	2.14	0.56
1:A:1239:ARG:HH12	1:A:1241:ARG:HH12	1.54	0.56
4:E:118:PRO:HA	4:E:121:MET:HB2	1.88	0.55
1:A:219:PHE:HZ	1:A:230:ARG:HG2	1.71	0.55
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.87	0.55
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.07	0.55
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.88	0.55
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.88	0.55
9:K:32:VAL:HG22	9:K:74:ARG:HG3	1.87	0.55
1:A:579:SER:HA	1:A:582:ILE:HD12	1.88	0.55
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.87	0.55
2:B:864:LYS:HG2	2:B:871:THR:HA	1.88	0.55
4:E:19:VAL:O	4:E:23:VAL:HG23	2.07	0.55
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.89	0.55
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.90	0.54
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.87	0.54
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.89	0.54
1:A:596:THR:C	1:A:598:LEU:H	2.14	0.54
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.89	0.54
1:A:567:LYS:HB3	6:H:95:TYR:HA	1.89	0.54
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.88	0.54
1:A:1377:THR:HG22	4:E:176:PRO:HB3	1.89	0.54
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.89	0.54
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.72	0.54
2:B:89:GLU:HB3	2:B:135:ARG:HB3	1.91	0.53
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.90	0.53
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.91	0.53
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.90	0.53
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.91	0.53
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.38	0.53
6:H:109:LYS:HZ1	6:H:111:LEU:HD12	1.74	0.53
11:R:8:A:H61	12:T:21:DC:H42	1.56	0.53
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.74	0.52
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.91	0.52
1:A:567:LYS:NZ	6:H:46:LEU:HB2	2.23	0.52
1:A:871:ASP:HB3	4:E:204:THR:HG22	1.92	0.52
1:A:1111:MET:HE1	1:A:1330:ASN:CG	2.35	0.52
1:A:1281:ARG:HB2	1:A:1309:ASP:HB3	1.92	0.52
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.91	0.52
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.92	0.52
1:A:304:MET:HG2	1:A:325:ILE:HD12	1.92	0.52
2:B:283:VAL:HG12	2:B:297:ILE:HG21	1.90	0.52
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.91	0.52
1:A:441:PRO:HG2	1:A:498:ARG:HB2	1.92	0.52
3:C:12:GLU:HB3	3:C:19:ASP:HB3	1.92	0.52
2:B:302:CYS:HA	2:B:310:MET:HE3	1.92	0.52
1:A:569:LYS:HG2	1:A:571:LEU:HD13	1.91	0.51
3:C:36:VAL:HG23	3:C:40:GLU:HB2	1.91	0.51
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.76	0.51
2:B:486:TYR:OH	2:B:1096:ARG:HB3	2.10	0.51
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.93	0.51
1:A:392:VAL:HG13	1:A:424:ILE:HD12	1.93	0.51
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.93	0.50
1:A:55:ASP:O	1:A:57:ARG:N	2.43	0.50
1:A:626:ASN:O	1:A:631:HIS:HD2	1.94	0.50
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.11	0.50
1:A:1105:LEU:HB3	1:A:1384:VAL:HG22	1.93	0.50
2:B:1030:LEU:O	2:B:1034:VAL:HG23	2.11	0.50
1:A:469:ARG:NH2	2:B:991:GLY:O	2.44	0.50
2:B:313:MET:HE2	2:B:390:LEU:HG	1.93	0.50
1:A:709:THR:HG22	1:A:711:ARG:H	1.76	0.50
3:C:136:ASP:HB3	3:C:140:ASN:O	2.12	0.50
1:A:120:GLU:HA	1:A:123:ARG:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:176:PRO:O	4:E:212:ARG:HA	2.12	0.49
1:A:586:ILE:HD11	1:A:637:LYS:HG3	1.93	0.49
7:I:47:GLU:HB3	7:I:50:THR:HG23	1.94	0.48
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.77	0.48
1:A:68:GLN:HG2	1:A:80:HIS:CE1	2.48	0.48
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.94	0.48
5:F:97:ARG:HH11	5:F:100:GLN:HG3	1.79	0.48
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.78	0.48
2:B:809:MET:HE1	2:B:983:ARG:HH21	1.78	0.48
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.95	0.48
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.94	0.48
2:B:516:ASN:H	2:B:516:ASN:HD22	1.60	0.48
3:C:48:SER:HB3	3:C:158:VAL:HB	1.96	0.48
1:A:92:HIS:HD2	1:A:94:GLY:H	1.61	0.48
1:A:741:ASN:HD22	1:A:744:LYS:H	1.62	0.48
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.96	0.48
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.95	0.48
2:B:345:LYS:HA	2:B:347:LYS:H	1.78	0.48
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.78	0.48
1:A:869:GLY:O	4:E:204:THR:HG21	2.13	0.48
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.79	0.48
2:B:516:ASN:H	2:B:516:ASN:ND2	2.12	0.48
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.94	0.48
3:C:98:VAL:H	3:C:122:SER:HB2	1.77	0.48
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.96	0.48
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.96	0.47
1:A:858:ASN:HD22	1:A:864:ILE:HD11	1.79	0.47
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.78	0.47
3:C:33:LEU:HG	3:C:37:MET:HE2	1.95	0.47
1:A:250:ILE:HD13	2:B:1113:VAL:HG11	1.95	0.47
2:B:53:GLN:HG2	2:B:547:VAL:HB	1.96	0.47
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.80	0.47
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.96	0.47
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.95	0.47
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.96	0.47
1:A:399:HIS:O	1:A:401:GLY:N	2.47	0.46
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.97	0.46
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.48	0.46
2:B:801:LYS:O	8:J:52:THR:HG23	2.15	0.46
2:B:825:VAL:HG23	2:B:1010:LEU:HB3	1.97	0.46
1:A:711:ARG:HH12	7:I:95:THR:HG22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.80	0.46
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.97	0.46
1:A:1144:LYS:HG3	7:I:48:LEU:HD22	1.97	0.46
2:B:980:PHE:CE2	2:B:1094:ARG:HD2	2.50	0.46
2:B:893:LEU:HD13	2:B:897:GLY:HA2	1.98	0.46
4:E:159:ASP:HA	4:E:162:ARG:HD3	1.98	0.46
2:B:862:GLN:HG2	2:B:963:PHE:HB2	1.98	0.46
3:C:3:GLU:HG3	3:C:4:GLU:HG2	1.98	0.46
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.98	0.45
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.51	0.45
9:K:7:PHE:O	9:K:11:LEU:HB2	2.17	0.45
2:B:486:TYR:CZ	2:B:1096:ARG:HB3	2.51	0.45
1:A:456:MET:HE2	1:A:507:VAL:HA	1.99	0.45
1:A:899:VAL:HG13	1:A:1029:ARG:HD3	1.98	0.45
6:H:101:ALA:HB1	6:H:104:PHE:HE1	1.80	0.45
1:A:367:PRO:HB3	1:A:465:TYR:O	2.16	0.45
1:A:830:LYS:HE3	1:A:1082:ASN:HB3	1.97	0.45
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.81	0.45
2:B:1122:ARG:C	2:B:1124:ARG:H	2.25	0.45
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.82	0.45
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.99	0.45
2:B:835:GLN:O	2:B:838:SER:HB2	2.17	0.45
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.99	0.45
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.52	0.45
1:A:919:ILE:HD11	1:A:925:LEU:HG	1.97	0.45
2:B:428:ILE:HD11	2:B:448:ILE:HG23	1.98	0.45
1:A:456:MET:HB2	1:A:478:TYR:OH	2.17	0.44
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.97	0.44
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.50	0.44
2:B:601:ARG:HA	2:B:615:MET:HE1	1.99	0.44
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.98	0.44
2:B:232:SER:HB3	2:B:261:ARG:HH22	1.83	0.44
1:A:406:ILE:HB	1:A:431:LYS:HB2	2.00	0.44
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.47	0.44
4:E:61:GLN:HG3	4:E:105:PHE:HE2	1.82	0.44
9:K:7:PHE:HB2	9:K:11:LEU:HD22	2.00	0.44
2:B:291:ILE:HG22	2:B:297:ILE:HG13	2.00	0.44
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	2.16	0.44
3:C:171:GLY:C	3:C:173:ALA:N	2.76	0.44
1:A:567:LYS:C	1:A:569:LYS:H	2.26	0.44
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:LEU:HD11	9:K:101:LEU:HD21	2.00	0.44
6:H:100:THR:HG23	6:H:138:GLU:HA	1.98	0.44
1:A:910:PRO:HA	1:A:916:GLY:HA3	2.00	0.44
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.98	0.44
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.50	0.44
2:B:1100:ASP:HA	2:B:1103:ILE:HG12	1.99	0.44
3:C:166:GLU:HG2	10:L:70:ARG:HH21	1.83	0.44
1:A:567:LYS:NZ	6:H:43:ASN:HB3	2.33	0.43
1:A:1199:ARG:NH2	1:A:1233:ASP:O	2.50	0.43
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.18	0.43
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	2.01	0.43
2:B:1181:GLU:HA	2:B:1188:LYS:HA	2.01	0.43
1:A:528:LEU:O	1:A:531:ILE:HG22	2.18	0.43
1:A:614:PHE:HB3	6:H:122:LEU:HD21	2.00	0.43
3:C:101:LEU:HB2	3:C:118:LEU:HD23	2.00	0.43
4:E:28:TYR:HA	4:E:64:PRO:HA	2.01	0.43
1:A:781:ASP:HB2	1:A:789:LYS:HG2	2.00	0.43
2:B:880:THR:C	2:B:882:THR:H	2.27	0.43
2:B:1056:SER:HB3	2:B:1066:SER:HB2	2.00	0.43
2:B:515:HIS:HD2	2:B:517:THR:OG1	2.01	0.43
2:B:834:ASN:HA	2:B:838:SER:HB3	2.01	0.43
2:B:744:HIS:CD2	2:B:746:SER:OG	2.72	0.43
1:A:353:ILE:HG21	1:A:487:MET:HE3	2.00	0.42
1:A:845:LEU:HA	1:A:848:ILE:HD12	2.01	0.42
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.53	0.42
2:B:1175:LEU:C	2:B:1177:HIS:H	2.27	0.42
2:B:542:MET:HE1	2:B:743:ILE:HB	2.00	0.42
4:E:177:ARG:HB3	4:E:215:MET:HG3	2.00	0.42
1:A:208:LEU:HD23	1:A:235:ILE:HD11	2.01	0.42
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.52	0.42
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	2.00	0.42
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.99	0.42
2:B:684:LEU:HA	2:B:689:LEU:HD12	2.01	0.42
6:H:93:TYR:HA	6:H:145:ARG:HB3	2.00	0.42
1:A:182:VAL:HG12	1:A:201:VAL:HA	2.01	0.42
1:A:512:VAL:HA	1:A:519:PRO:HA	2.01	0.42
1:A:567:LYS:HD2	1:A:568:PRO:HD2	2.00	0.42
2:B:955:THR:HG23	10:L:54:ARG:O	2.18	0.42
2:B:1174:LYS:HB2	2:B:1179:GLN:O	2.19	0.42
2:B:515:HIS:H	2:B:518:HIS:HD2	1.68	0.42
2:B:751:VAL:HA	2:B:812:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.20	0.42
1:A:185:TRP:HB2	1:A:199:LEU:HD12	2.01	0.42
1:A:747:VAL:HG21	1:A:758:ILE:HD11	2.00	0.42
1:A:875:ALA:HA	1:A:878:ILE:HD12	2.02	0.42
2:B:95:ILE:HD12	2:B:130:VAL:HB	2.00	0.42
3:C:167:HIS:CD2	3:C:169:LYS:H	2.29	0.42
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.55	0.42
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.20	0.42
2:B:188:ASP:HA	2:B:191:LYS:HE3	2.02	0.42
1:A:567:LYS:CB	1:A:568:PRO:CD	2.96	0.42
1:A:697:ALA:HA	1:A:702:LEU:HB2	2.02	0.42
1:A:1279:ILE:HG13	1:A:1308:THR:HG21	2.02	0.42
2:B:229:ALA:HB1	2:B:231:PRO:HD2	2.01	0.41
10:L:27:LEU:HB2	10:L:28:LYS:H	1.73	0.41
3:C:14:SER:HA	9:K:114:LEU:HB3	2.02	0.41
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.56	0.41
1:A:1109:LYS:HE2	1:A:1109:LYS:H	1.85	0.41
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	2.02	0.41
4:E:61:GLN:HG3	4:E:105:PHE:CE2	2.55	0.41
1:A:503:GLN:HE21	5:F:90:ARG:NH1	2.11	0.41
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.24	0.41
2:B:52:ASN:OD1	2:B:177:LYS:HB2	2.20	0.41
2:B:241:ARG:HA	2:B:253:THR:HG22	2.02	0.41
2:B:420:LEU:HB3	2:B:453:ILE:HD13	2.02	0.41
1:A:40:THR:HG22	1:A:41:MET:HG3	2.03	0.41
1:A:96:ILE:HD12	1:A:176:LYS:HE3	2.03	0.41
1:A:1338:VAL:HG12	1:A:1339:LEU:HG	2.03	0.41
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.86	0.41
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.21	0.41
9:K:47:ARG:HD2	9:K:60:ALA:HA	2.02	0.41
1:A:531:ILE:HG21	1:A:622:VAL:HG11	2.03	0.41
1:A:855:THR:HG23	1:A:857:ARG:HG3	2.01	0.41
1:A:1438:THR:HG23	5:F:92:ARG:HD3	2.02	0.41
2:B:128:LEU:HD11	2:B:170:LEU:HB2	2.02	0.41
2:B:373:ARG:HA	2:B:566:LEU:HD23	2.03	0.41
2:B:999:MET:HG2	2:B:1007:VAL:HG13	2.02	0.41
3:C:62:PHE:O	3:C:66:ARG:HG2	2.21	0.41
6:H:57:VAL:HG22	6:H:144:ILE:HG12	2.03	0.41
10:L:47:ARG:HD2	10:L:54:ARG:HG3	2.03	0.41
1:A:901:LEU:HA	1:A:907:THR:HG23	2.01	0.41
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:577:ALA:HB1	2:B:589:VAL:HB	2.02	0.40
2:B:882:THR:C	2:B:884:ARG:H	2.28	0.40
3:C:148:ARG:HB3	3:C:151:GLN:HG3	2.02	0.40
2:B:363:HIS:O	2:B:364:ILE:HB	2.21	0.40
2:B:802:PRO:HG2	2:B:805:THR:HG22	2.03	0.40
2:B:904:ARG:HG2	2:B:948:ILE:HG12	2.04	0.40
1:A:567:LYS:HE3	6:H:46:LEU:HD13	2.02	0.40
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.61	0.40
1:A:367:PRO:HG2	1:A:370:ILE:HD12	2.03	0.40
1:A:858:ASN:HD21	1:A:862:ASN:HB2	1.86	0.40
1:A:1105:LEU:HB3	1:A:1384:VAL:CG2	2.50	0.40
1:A:1286:LYS:HE2	1:A:1302:PRO:HB2	2.02	0.40
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.56	0.40
2:B:244:LEU:HD12	2:B:250:PHE:HB2	2.04	0.40
2:B:640:VAL:HG12	2:B:649:LYS:HB3	2.04	0.40
8:J:1:MET:H2	8:J:56:LEU:H	1.70	0.40
1:A:571:LEU:HD12	1:A:571:LEU:HA	1.93	0.40
2:B:69:LEU:HD12	2:B:90:ILE:HB	2.04	0.40
2:B:898:LEU:HD21	2:B:964:VAL:HG11	2.03	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%)	1252 (90%)	103 (7%)	40 (3%)	3	21
2	B	1096/1224 (90%)	969 (88%)	88 (8%)	39 (4%)	2	17
3	C	264/318 (83%)	241 (91%)	19 (7%)	4 (2%)	8	32
4	E	212/215 (99%)	201 (95%)	11 (5%)	0	100	100
5	F	83/155 (54%)	73 (88%)	10 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	H	129/146 (88%)	105 (81%)	20 (16%)	4 (3%)	3	20
7	I	117/122 (96%)	103 (88%)	13 (11%)	1 (1%)	14	43
8	J	63/70 (90%)	59 (94%)	1 (2%)	3 (5%)	2	12
9	K	112/120 (93%)	108 (96%)	4 (4%)	0	100	100
10	L	44/70 (63%)	30 (68%)	9 (20%)	5 (11%)	0	2
All	All	3515/4173 (84%)	3141 (89%)	278 (8%)	96 (3%)	4	22

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	ASP
1	A	56	PRO
1	A	257	ARG
1	A	423	ASP
1	A	424	ILE
1	A	567	LYS
1	A	1221	LYS
2	B	137	TYR
2	B	469	GLN
2	B	477	ALA
2	B	531	GLN
2	B	648	HIS
2	B	712	PRO
2	B	731	VAL
2	B	732	SER
2	B	751	VAL
2	B	880	THR
2	B	883	LEU
2	B	1046	PRO
2	B	1180	PHE
3	C	173	ALA
3	C	215	GLU
8	J	2	ILE
8	J	6	ARG
10	L	28	LYS
1	A	40	THR
1	A	50	ILE
1	A	214	ILE
1	A	299	HIS

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Mol	Chain	Res	Type
1	A	410	GLY
1	A	846	GLU
1	A	1123	GLY
1	A	1124	HIS
1	A	1437	GLY
2	B	364	ILE
2	B	646	LEU
2	B	887	HIS
6	H	18	GLY
6	H	90	ALA
6	H	136	LYS
10	L	64	LEU
1	A	68	GLN
1	A	130	ASP
1	A	958	VAL
1	A	1393	ASN
2	B	105	SER
2	B	138	GLU
2	B	139	ALA
2	B	229	ALA
2	B	248	SER
2	B	346	GLU
2	B	468	GLU
2	B	483	LEU
2	B	563	MET
2	B	707	PRO
2	B	734	HIS
2	B	1066	SER
2	B	1097	HIS
3	C	148	ARG
6	H	135	LEU
7	I	77	LYS
10	L	45	ALA
10	L	46	VAL
1	A	46	THR
1	A	76	GLU
1	A	168	GLY
1	A	309	ALA
1	A	332	LYS
1	A	775	ILE
1	A	907	THR
1	A	1278	ASN

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Mol	Chain	Res	Type
2	B	306	ASN
2	B	526	GLU
2	B	792	MET
2	B	1017	ILE
2	B	1108	ARG
3	C	90	ASP
1	A	45	GLN
1	A	399	HIS
2	B	1103	ILE
2	B	1181	GLU
8	J	13	VAL
10	L	47	ARG
1	A	149	GLU
1	A	250	ILE
1	A	511	ILE
1	A	599	SER
2	B	865	LYS
1	A	35	ILE
1	A	385	ILE
1	A	569	LYS
2	B	647	GLY
1	A	916	GLY
2	B	230	ALA
1	A	321	PRO

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%)	1061 (87%)	164 (13%)	4	16
2	B	967/1061 (91%)	847 (88%)	120 (12%)	4	19
3	C	234/274 (85%)	200 (86%)	34 (14%)	3	14
4	E	196/197 (100%)	179 (91%)	17 (9%)	9	32
5	F	75/137 (55%)	66 (88%)	9 (12%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	H	117/128 (91%)	103 (88%)	14 (12%)	5	20
7	I	113/116 (97%)	98 (87%)	15 (13%)	4	17
8	J	60/65 (92%)	51 (85%)	9 (15%)	3	13
9	K	99/102 (97%)	84 (85%)	15 (15%)	3	13
10	L	40/57 (70%)	28 (70%)	12 (30%)	0	1
All	All	3126/3657 (86%)	2717 (87%)	409 (13%)	4	17

All (409) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	30	ILE
1	A	41	MET
1	A	43	GLU
1	A	50	ILE
1	A	54	ASN
1	A	58	LEU
1	A	61	ILE
1	A	63	ARG
1	A	68	GLN
1	A	80	HIS
1	A	93	VAL
1	A	96	ILE
1	A	115	LEU
1	A	116	ASP
1	A	128	ILE
1	A	129	LYS
1	A	143	LYS
1	A	145	LYS
1	A	146	MET
1	A	164	ARG
1	A	171	GLN
1	A	204	THR
1	A	208	LEU
1	A	217	LYS
1	A	222	LEU
1	A	252	PHE
1	A	262	LEU
1	A	268	ASP
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	276	LEU
1	A	290	GLU
1	A	299	HIS
1	A	305	ASP
1	A	308	ILE
1	A	315	LEU
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	329	LEU
1	A	335	ARG
1	A	337	ARG
1	A	351	THR
1	A	353	ILE
1	A	359	LEU
1	A	368	LYS
1	A	378	GLU
1	A	380	VAL
1	A	385	ILE
1	A	389	THR
1	A	392	VAL
1	A	394	ASN
1	A	403	LYS
1	A	411	ASP
1	A	427	GLN
1	A	436	ILE
1	A	437	MET
1	A	443	LEU
1	A	452	LYS
1	A	463	ILE
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	496	GLU
1	A	518	LYS
1	A	523	ILE
1	A	525	GLN
1	A	527	THR
1	A	532	ARG

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Mol	Chain	Res	Type
1	A	535	THR
1	A	538	ASP
1	A	541	ILE
1	A	566	ILE
1	A	571	LEU
1	A	590	ARG
1	A	593	GLU
1	A	598	LEU
1	A	599	SER
1	A	609	ASP
1	A	618	GLU
1	A	620	LYS
1	A	622	VAL
1	A	629	LEU
1	A	637	LYS
1	A	678	GLU
1	A	687	LYS
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	702	LEU
1	A	703	THR
1	A	710	LEU
1	A	719	VAL
1	A	722	LEU
1	A	734	GLU
1	A	740	LEU
1	A	756	ILE
1	A	758	ILE
1	A	768	GLN
1	A	771	GLU
1	A	773	LYS
1	A	788	SER
1	A	796	SER
1	A	821	ARG
1	A	830	LYS
1	A	867	ILE
1	A	899	VAL
1	A	908	LEU
1	A	912	LEU
1	A	914	GLU
1	A	920	LEU

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Mol	Chain	Res	Type
1	A	925	LEU
1	A	926	GLN
1	A	961	ARG
1	A	964	ILE
1	A	969	GLN
1	A	992	ASP
1	A	996	ASN
1	A	1022	LEU
1	A	1067	LEU
1	A	1080	THR
1	A	1081	LEU
1	A	1094	VAL
1	A	1109	LYS
1	A	1110	ASN
1	A	1117	THR
1	A	1124	HIS
1	A	1132	LYS
1	A	1135	ARG
1	A	1168	GLU
1	A	1171	GLN
1	A	1172	LEU
1	A	1176	LEU
1	A	1224	LEU
1	A	1227	ILE
1	A	1237	ILE
1	A	1242	VAL
1	A	1261	LYS
1	A	1277	GLU
1	A	1280	GLU
1	A	1291	VAL
1	A	1319	VAL
1	A	1334	ASP
1	A	1351	GLU
1	A	1354	ASN
1	A	1356	ILE
1	A	1366	ARG
1	A	1376	THR
1	A	1382	THR
1	A	1387	HIS
1	A	1391	ARG
1	A	1393	ASN
1	A	1394	THR

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Mol	Chain	Res	Type
1	A	1398	MET
1	A	1403	GLU
1	A	1420	ASP
1	A	1425	SER
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1445	ILE
2	B	39	ARG
2	B	46	GLN
2	B	63	ILE
2	B	70	ILE
2	B	89	GLU
2	B	95	ILE
2	B	97	VAL
2	B	102	VAL
2	B	134	LYS
2	B	140	ILE
2	B	174	LEU
2	B	185	THR
2	B	194	GLU
2	B	217	ARG
2	B	222	ILE
2	B	234	ILE
2	B	237	VAL
2	B	240	ILE
2	B	242	SER
2	B	251	ILE
2	B	262	GLU
2	B	267	ARG
2	B	272	THR
2	B	276	ILE
2	B	277	LYS
2	B	282	ILE
2	B	317	CYS
2	B	331	LEU
2	B	345	LYS
2	B	347	LYS
2	B	353	LYS
2	B	364	ILE
2	B	387	LEU
2	B	393	LYS

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Mol	Chain	Res	Type
2	B	396	ASP
2	B	403	LYS
2	B	416	LEU
2	B	424	LEU
2	B	426	LYS
2	B	437	GLU
2	B	471	LYS
2	B	476	ARG
2	B	479	VAL
2	B	484	ASN
2	B	485	ARG
2	B	500	THR
2	B	502	ILE
2	B	513	GLN
2	B	516	ASN
2	B	531	GLN
2	B	537	LYS
2	B	560	GLU
2	B	567	GLU
2	B	604	ARG
2	B	608	ASP
2	B	612	GLU
2	B	616	ILE
2	B	620	ARG
2	B	624	LEU
2	B	649	LYS
2	B	667	GLN
2	B	690	VAL
2	B	705	MET
2	B	710	LEU
2	B	731	VAL
2	B	734	HIS
2	B	762	ASN
2	B	791	THR
2	B	792	MET
2	B	812	LEU
2	B	837	ASP
2	B	838	SER
2	B	864	LYS
2	B	865	LYS
2	B	866	TYR
2	B	868	MET

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Mol	Chain	Res	Type
2	B	870	ILE
2	B	878	GLN
2	B	886	LYS
2	B	893	LEU
2	B	894	ASP
2	B	951	GLN
2	B	963	PHE
2	B	970	THR
2	B	975	GLN
2	B	976	ILE
2	B	992	ILE
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1010	LEU
2	B	1017	ILE
2	B	1034	VAL
2	B	1050	ILE
2	B	1057	LYS
2	B	1060	ARG
2	B	1065	GLN
2	B	1079	LYS
2	B	1099	VAL
2	B	1102	LYS
2	B	1111	MET
2	B	1112	GLN
2	B	1122	ARG
2	B	1128	LEU
2	B	1138	MET
2	B	1147	LEU
2	B	1160	VAL
2	B	1163	CYS
2	B	1175	LEU
2	B	1176	ASN
2	B	1178	ASN
2	B	1189	ILE
2	B	1194	ILE
2	B	1202	LEU
2	B	1203	LEU
2	B	1205	GLN
2	B	1211	ASN

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Mol	Chain	Res	Type
2	B	1212	ILE
2	B	1224	PHE
3	C	18	VAL
3	C	21	ILE
3	C	25	VAL
3	C	34	ARG
3	C	41	ILE
3	C	43	THR
3	C	60	ASP
3	C	75	MET
3	C	77	ILE
3	C	79	GLN
3	C	80	LEU
3	C	81	GLU
3	C	85	ASP
3	C	94	LYS
3	C	98	VAL
3	C	100	THR
3	C	106	GLU
3	C	129	ILE
3	C	140	ASN
3	C	151	GLN
3	C	155	LEU
3	C	176	ILE
3	C	211	ASP
3	C	215	GLU
3	C	217	ASP
3	C	221	TYR
3	C	235	VAL
3	C	240	VAL
3	C	244	VAL
3	C	249	ASP
3	C	254	LYS
3	C	260	LEU
3	C	265	MET
3	C	268	ASP
4	E	4	GLU
4	E	7	ARG
4	E	35	VAL
4	E	37	LEU
4	E	54	GLN
4	E	58	MET

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Mol	Chain	Res	Type
4	E	74	ASP
4	E	84	ASP
4	E	88	VAL
4	E	92	THR
4	E	95	THR
4	E	100	ILE
4	E	127	ILE
4	E	170	LEU
4	E	184	VAL
4	E	188	LEU
4	E	215	MET
5	F	74	ILE
5	F	77	ASP
5	F	99	LEU
5	F	103	MET
5	F	115	THR
5	F	118	LEU
5	F	122	MET
5	F	127	GLU
5	F	152	ILE
6	H	4	THR
6	H	9	ILE
6	H	34	ASP
6	H	35	GLN
6	H	59	ILE
6	H	77	ARG
6	H	83	GLN
6	H	87	ARG
6	H	105	GLU
6	H	109	LYS
6	H	111	LEU
6	H	129	TYR
6	H	130	ARG
6	H	132	LEU
7	I	28	GLU
7	I	49	ILE
7	I	50	THR
7	I	60	GLN
7	I	70	ARG
7	I	77	LYS
7	I	84	VAL
7	I	90	GLN

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Mol	Chain	Res	Type
7	I	94	ASP
7	I	95	THR
7	I	97	MET
7	I	104	LEU
7	I	107	SER
7	I	111	THR
7	I	120	GLN
8	J	3	VAL
8	J	13	VAL
8	J	20	SER
8	J	23	ASN
8	J	30	LEU
8	J	31	ASP
8	J	48	ARG
8	J	59	LYS
8	J	62	ARG
9	K	5	ASP
9	K	17	SER
9	K	18	LYS
9	K	20	LYS
9	K	21	ILE
9	K	22	ASP
9	K	31	VAL
9	K	33	ILE
9	K	41	THR
9	K	49	GLU
9	K	50	LEU
9	K	101	LEU
9	K	108	GLU
9	K	113	THR
9	K	114	LEU
10	L	27	LEU
10	L	30	ILE
10	L	42	ARG
10	L	43	THR
10	L	46	VAL
10	L	47	ARG
10	L	53	HIS
10	L	55	ILE
10	L	60	ARG
10	L	61	THR
10	L	65	VAL

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Mol	Chain	Res	Type
10	L	66	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	18	GLN
1	A	64	ASN
1	A	68	GLN
1	A	75	ASN
1	A	80	HIS
1	A	92	HIS
1	A	171	GLN
1	A	306	ASN
1	A	316	GLN
1	A	390	GLN
1	A	503	GLN
1	A	517	ASN
1	A	525	GLN
1	A	545	GLN
1	A	589	GLN
1	A	631	HIS
1	A	640	GLN
1	A	717	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	926	GLN
1	A	935	GLN
1	A	1082	ASN
1	A	1085	HIS
1	A	1140	HIS
1	A	1188	GLN
1	A	1265	ASN
1	A	1312	ASN
1	A	1364	ASN
1	A	1387	HIS
1	A	1390	ASN
1	A	1427	ASN
1	A	1432	GLN
2	B	46	GLN

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Mol	Chain	Res	Type
2	B	47	GLN
2	B	110	HIS
2	B	121	ASN
2	B	215	GLN
2	B	224	GLN
2	B	357	GLN
2	B	366	GLN
2	B	433	GLN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	657	HIS
2	B	706	GLN
2	B	744	HIS
2	B	762	ASN
2	B	763	GLN
2	B	767	ASN
2	B	770	GLN
2	B	822	ASN
2	B	842	ASN
2	B	862	GLN
2	B	958	GLN
2	B	984	HIS
2	B	1015	HIS
2	B	1074	ASN
2	B	1084	GLN
2	B	1093	GLN
2	B	1161	HIS
2	B	1195	HIS
2	B	1205	GLN
2	B	1211	ASN
3	C	54	ASN
3	C	112	ASN
3	C	151	GLN
3	C	195	GLN
3	C	242	GLN
3	C	267	GLN
4	E	32	GLN
4	E	54	GLN
4	E	99	HIS

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Mol	Chain	Res	Type
4	E	106	GLN
4	E	113	GLN
4	E	146	HIS
4	E	174	GLN
6	H	3	ASN
7	I	46	HIS
7	I	60	GLN
7	I	116	ASN
8	J	23	ASN
9	K	29	ASN
9	K	65	HIS
9	K	89	ASN
9	K	110	ASN

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 oligosaccharides 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.

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	1405/1733 (81%)	0.17	43 (3%) 51 35	40, 85, 170, 224	0
2	B	1114/1224 (91%)	0.11	28 (2%) 58 39	42, 82, 148, 194	0
3	C	266/318 (83%)	-0.00	1 (0%) 88 79	52, 79, 120, 144	0
4	E	214/215 (99%)	0.31	5 (2%) 61 42	63, 117, 165, 185	0
5	F	85/155 (54%)	-0.03	0 100 100	65, 96, 135, 155	0
6	H	133/146 (91%)	0.50	7 (5%) 32 22	83, 126, 152, 165	0
7	I	119/122 (97%)	0.27	1 (0%) 82 68	57, 89, 122, 131	0
8	J	65/70 (92%)	-0.12	1 (1%) 72 53	51, 74, 110, 122	0
9	K	114/120 (95%)	-0.15	1 (0%) 81 65	45, 79, 110, 132	0
10	L	46/70 (65%)	0.78	5 (10%) 10 9	66, 114, 132, 143	0
11	R	5/5 (100%)	0.50	0 100 100	133, 136, 153, 156	0
12	T	8/29 (27%)	1.13	0 100 100	125, 134, 149, 156	0
All	All	3574/4207 (84%)	0.15	92 (2%) 57 38	40, 86, 160, 224	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	5.4
6	H	63	LEU	5.2
2	B	70	ILE	4.8
1	A	1082	ASN	4.6
6	H	86	ASP	4.5
1	A	250	ILE	4.4
1	A	1081	LEU	4.3
2	B	305	VAL	4.2
2	B	715	ALA	4.1
2	B	882	THR	4.0
1	A	1086	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
4	E	95	THR	3.9
2	B	335	GLY	3.9
2	B	709	ASP	3.8
1	A	179	LEU	3.7
4	E	98	ILE	3.6
6	H	132	LEU	3.5
1	A	1084	PHE	3.4
1	A	216	VAL	3.4
1	A	1091	SER	3.4
2	B	708	GLU	3.3
1	A	1087	ALA	3.3
9	K	114	LEU	3.3
10	L	25	ALA	3.3
1	A	323	LYS	3.3
1	A	1083	THR	3.2
1	A	1002	GLY	3.1
1	A	1089	VAL	3.1
1	A	1176	LEU	3.0
1	A	65	LEU	2.9
10	L	40	LEU	2.9
6	H	85	GLY	2.9
1	A	318	SER	2.8
10	L	26	THR	2.8
2	B	502	ILE	2.8
1	A	1090	ALA	2.7
2	B	446	LEU	2.7
1	A	1092	LYS	2.7
1	A	142	CYS	2.6
2	B	140	ILE	2.6
1	A	78	PRO	2.6
2	B	477	ALA	2.6
6	H	139	ASN	2.6
1	A	154	SER	2.6
1	A	199	LEU	2.6
4	E	137	GLU	2.6
1	A	103	CYS	2.5
1	A	186	LYS	2.5
2	B	277	LYS	2.5
4	E	25	ASP	2.5
7	I	104	LEU	2.5
1	A	105	CYS	2.5
1	A	115	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
4	E	113	GLN	2.4
10	L	27	LEU	2.4
1	A	61	ILE	2.4
2	B	509	ALA	2.4
2	B	733	HIS	2.3
2	B	1173	ALA	2.3
2	B	474	SER	2.3
1	A	138	ILE	2.3
1	A	1123	GLY	2.3
6	H	76	THR	2.3
2	B	137	TYR	2.3
1	A	317	LYS	2.3
1	A	314	ALA	2.3
1	A	53	LEU	2.3
1	A	222	LEU	2.3
1	A	30	ILE	2.2
2	B	731	VAL	2.2
10	L	28	LYS	2.2
2	B	648	HIS	2.2
2	B	933	SER	2.2
2	B	878	GLN	2.2
1	A	87	ALA	2.2
1	A	136	ALA	2.2
1	A	319	GLY	2.2
1	A	144	THR	2.2
2	B	472	ALA	2.2
3	C	175	ALA	2.2
2	B	1101	ASP	2.2
2	B	436	VAL	2.1
1	A	66	LYS	2.1
2	B	865	LYS	2.1
2	B	447	ALA	2.1
8	J	65	PRO	2.1
1	A	49	LYS	2.1
2	B	880	THR	2.0
1	A	252	PHE	2.0
1	A	308	ILE	2.0
1	A	333	GLU	2.0
6	H	46	LEU	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
13	ZN	A	1734	1/1	0.90	0.08	274,274,274,274	0
13	ZN	A	1735	1/1	0.97	0.05	116,116,116,116	0
13	ZN	B	1307	1/1	0.98	0.04	146,146,146,146	0
13	ZN	I	203	1/1	0.99	0.03	94,94,94,94	0
14	MG	A	2001	1/1	0.99	0.04	38,38,38,38	0
13	ZN	I	204	1/1	1.00	0.02	67,67,67,67	0
13	ZN	J	101	1/1	1.00	0.02	63,63,63,63	0
13	ZN	L	105	1/1	1.00	0.02	96,96,96,96	0
13	ZN	C	319	1/1	1.00	0.02	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.