



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:05 AM UTC

PDB ID : 3RZO / pdb_00003rzo
Title : RNA Polymerase II Initiation Complex with a 4-nt RNA
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-12
Resolution : 3.00 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

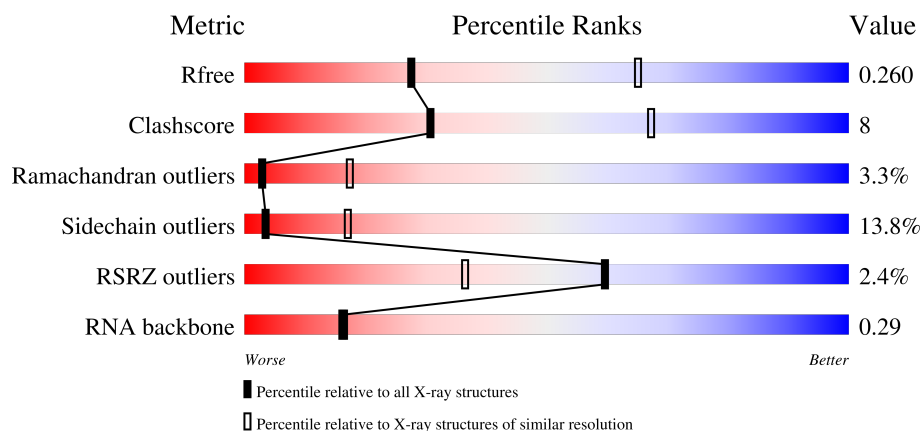
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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% 56% 21% • • 19%
2	B	1224	3% 58% 26% 6% • • 9%
3	C	318	53% 26% • • 16%
4	E	215	74% 22% •

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Mol	Chain	Length	Quality of chain
5	F	155	42%12%45%
6	H	146	2% 58%27%6%9%
7	I	122	2% 73%22%. .
8	J	70	% 53%23%16%. 7%
9	K	120	% 76%14%5%5%
10	L	70	9% 26%24%14%. 34%
11	R	4	100%
12	T	29	7% 21%7%72%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28547 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(*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	4	Total	C	N	O	P	0	0	0
			88	40	20	25	3			

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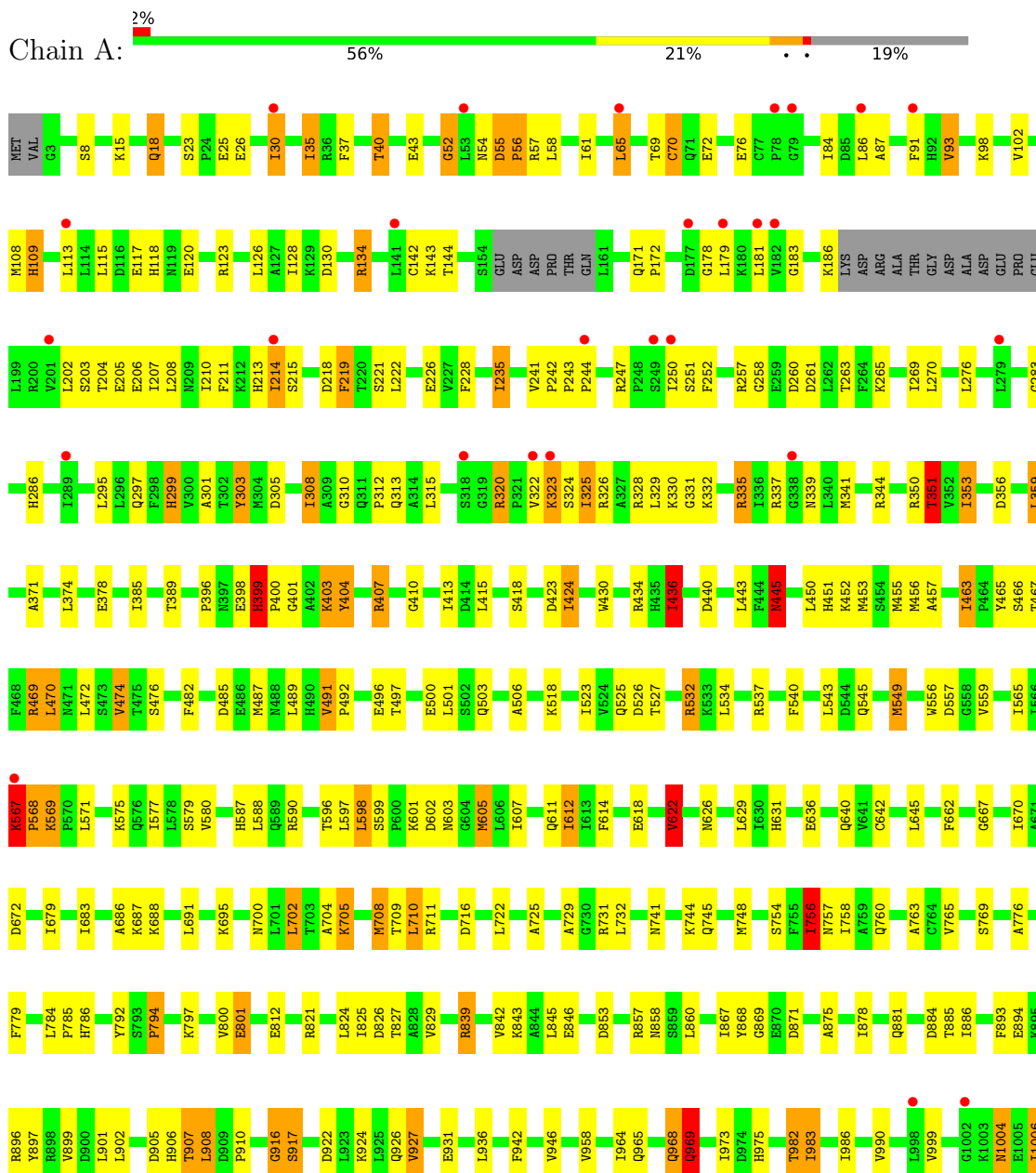
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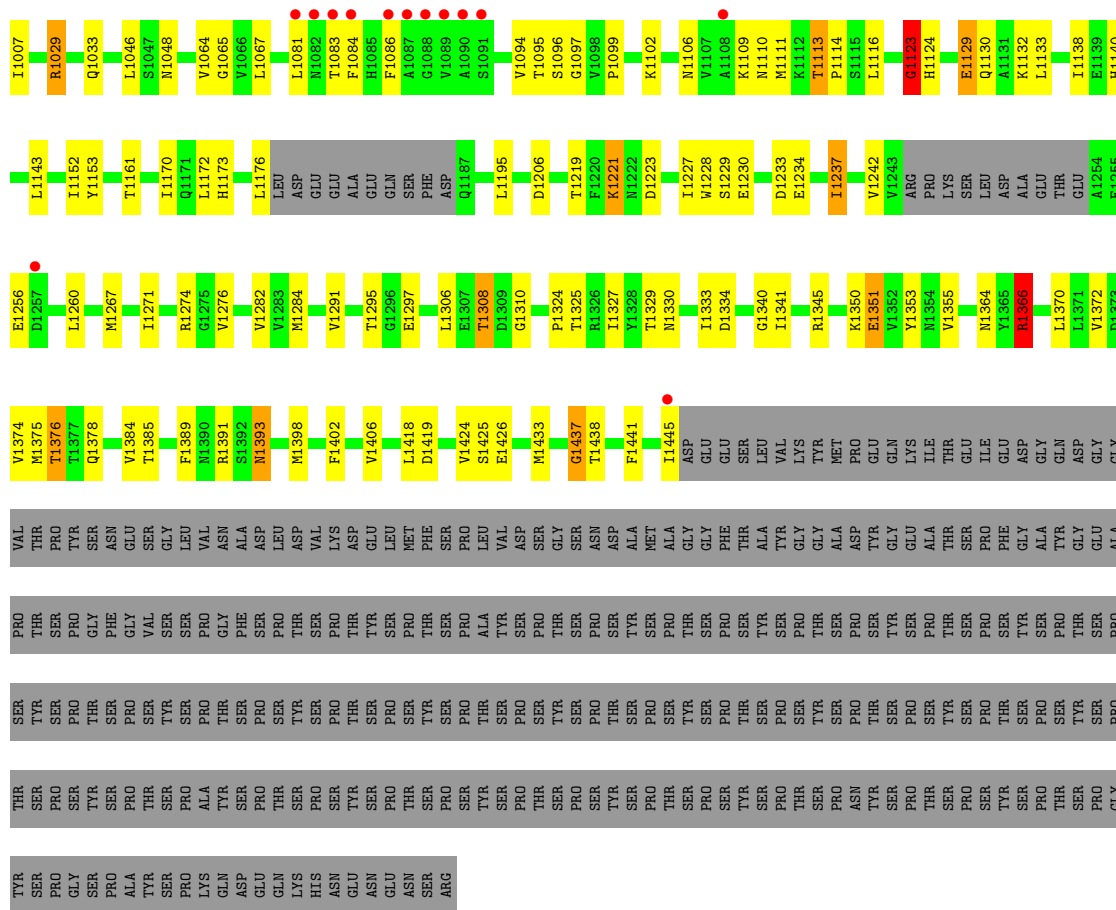
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Zn 1	0	0
13	C	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	J	1	Total 1	Zn 1	0	0
13	L	1	Total 1	Zn 1	0	0

3 Residue-property plots

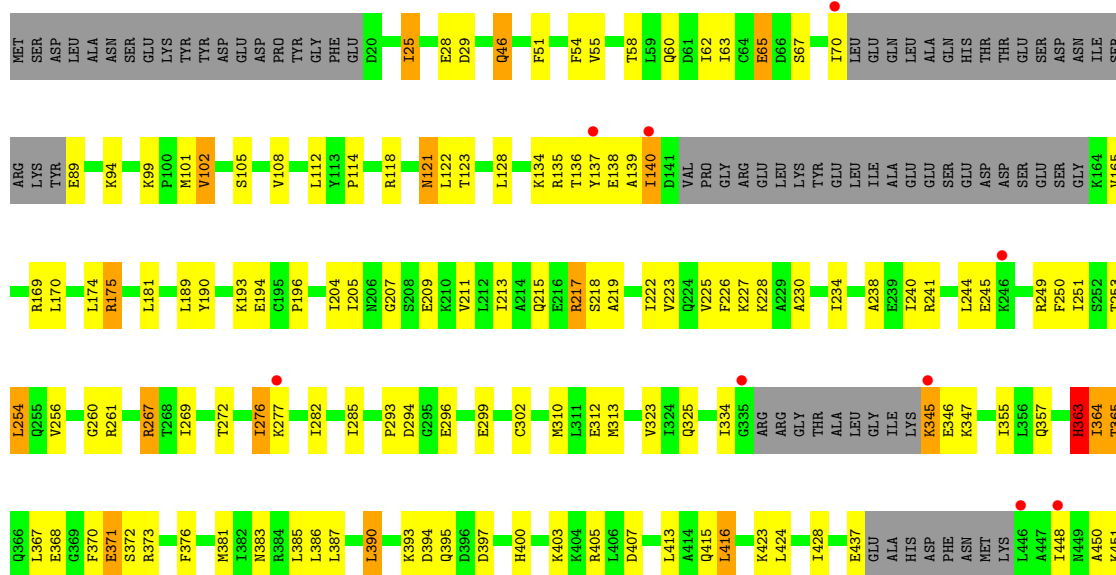
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

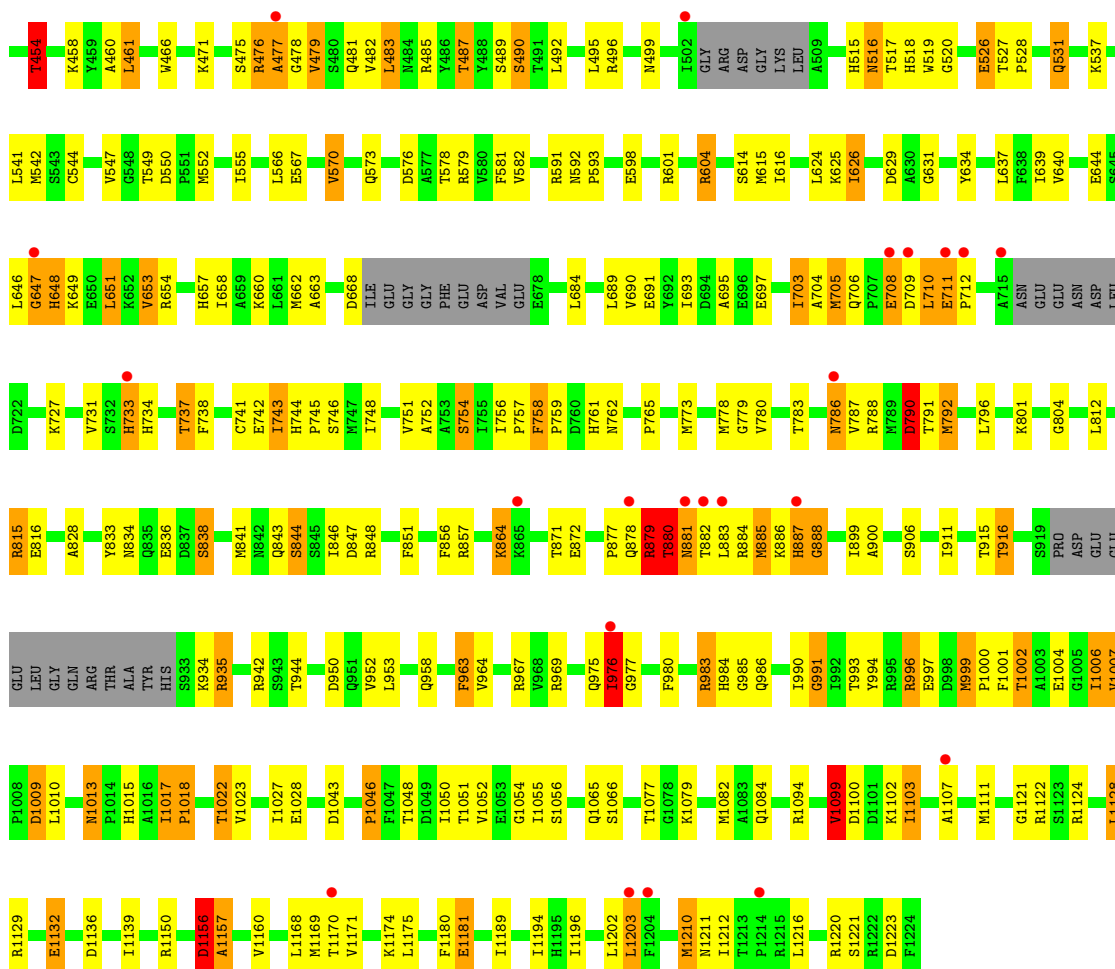
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1





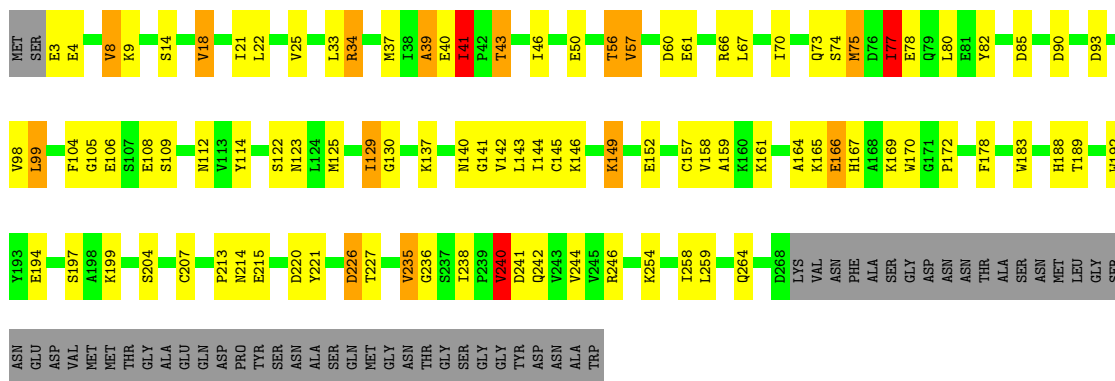
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2





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

Chain C: 53% 26% 16%



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

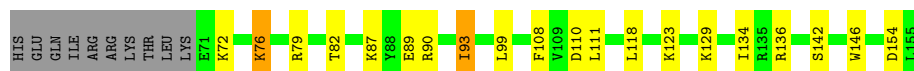
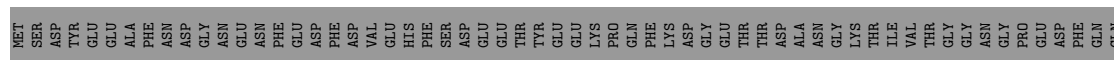
Chain E: 74% 22%





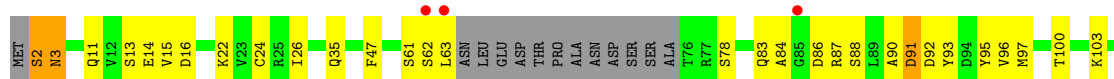
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 42% 12% 45%



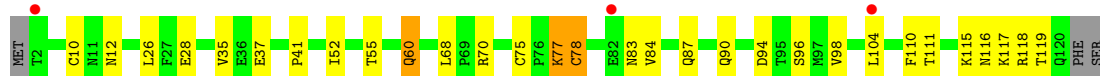
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 2% 58% 27% 6% 9%



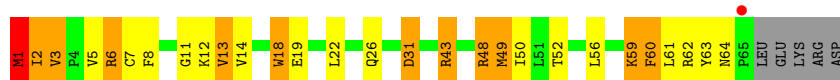
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 2% 73% 22% 5%



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

Chain J: 53% 23% 16% 7%



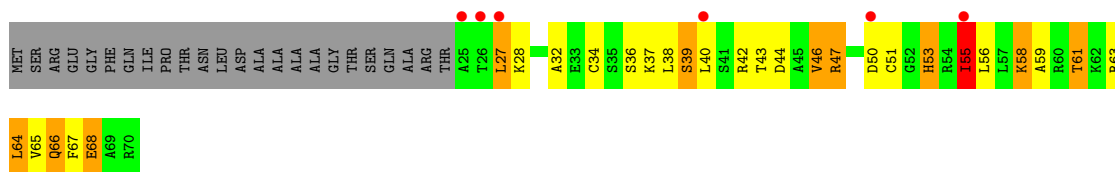
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 76% 14% 5% 5%



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

Chain L: 9% 26% 24% 14% 34%



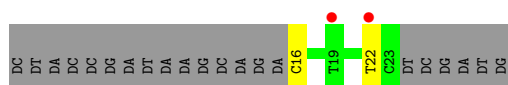
- Molecule 11: RNA (5'-R(*GP*AP*GP*G)-3')

Chain R: 100%

There are no outlier residues recorded for this chain.

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

Chain T:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.04Å 221.15Å 192.88Å 90.00° 98.34° 90.00°	Depositor
Resolution (Å)	40.01 – 3.00 40.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.01-3.00) 99.4 (40.01-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.188 , 0.236 0.211 , 0.260	Depositor DCC
R_{free} test set	6685 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.793	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 95.1	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	0.95	EDS
Total number of atoms	28547	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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

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	0.85	2/11241 (0.0%)	1.47	85/15199 (0.6%)
2	B	0.88	2/9033 (0.0%)	1.47	81/12181 (0.7%)
3	C	0.81	0/2133	1.44	22/2891 (0.8%)
4	E	0.80	0/1788	1.43	10/2406 (0.4%)
5	F	0.78	0/700	1.30	0/945
6	H	0.79	0/1086	1.38	21/1470 (1.4%)
7	I	0.80	0/989	1.40	11/1331 (0.8%)
8	J	0.95	2/541 (0.4%)	1.59	9/727 (1.2%)
9	K	0.77	0/937	1.36	2/1265 (0.2%)
10	L	0.90	0/365	1.50	5/485 (1.0%)
11	R	0.47	0/99	1.03	0/154
12	T	0.50	0/176	1.42	2/268 (0.7%)
All	All	0.85	6/29088 (0.0%)	1.45	248/39322 (0.6%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	756	ILE	CG1-CD1	6.57	1.77	1.51
1	A	605	MET	SD-CE	-6.17	1.64	1.79
8	J	1	MET	SD-CE	6.12	1.94	1.79
2	B	705	MET	SD-CE	-5.87	1.64	1.79
8	J	49	MET	SD-CE	-5.83	1.65	1.79
2	B	991	GLY	C-N	5.13	1.36	1.33

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	647	GLY	CA-C-N	11.56	142.50	121.70
2	B	647	GLY	C-N-CA	11.56	142.50	121.70
1	A	1097	GLY	CA-C-N	9.77	126.40	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1097	GLY	C-N-CA	9.77	126.40	120.24
6	H	92	ASP	N-CA-C	-8.89	101.75	112.59
3	C	39	ALA	N-CA-C	8.86	124.40	113.50
2	B	99	LYS	N-CA-C	-8.32	99.58	110.39
1	A	445	ASN	CA-CB-CG	8.04	120.64	112.60
2	B	1028	GLU	CB-CG-CD	7.69	125.67	112.60
7	I	78	CYS	CA-C-N	-7.52	111.35	122.86
7	I	78	CYS	C-N-CA	-7.52	111.35	122.86
6	H	2	SER	CA-C-N	7.46	135.13	121.70
6	H	2	SER	C-N-CA	7.46	135.13	121.70
2	B	879	ARG	N-CA-C	7.42	120.02	111.11
1	A	526	ASP	CA-CB-CG	7.42	120.02	112.60
2	B	743	ILE	N-CA-CB	7.39	118.38	110.62
2	B	245	GLU	N-CA-C	7.37	119.21	111.03
2	B	140	ILE	CA-C-N	7.28	134.81	121.70
2	B	140	ILE	C-N-CA	7.28	134.81	121.70
2	B	648	HIS	N-CA-CB	7.28	122.87	110.50
4	E	48	ASP	CA-CB-CG	7.28	119.88	112.60
2	B	363	HIS	N-CA-C	-7.23	99.58	110.28
6	H	91	ASP	N-CA-C	7.19	120.20	108.26
1	A	922	ASP	N-CA-C	7.10	119.92	111.33
1	A	463	ILE	N-CA-C	7.09	116.96	108.45
2	B	1018	PRO	CA-C-N	7.04	130.02	120.38
2	B	1018	PRO	C-N-CA	7.04	130.02	120.38
1	A	983	ILE	N-CA-C	-6.94	104.01	110.53
10	L	50	ASP	CA-C-N	6.86	134.65	121.54
10	L	50	ASP	C-N-CA	6.86	134.65	121.54
1	A	436	ILE	CB-CA-C	6.84	120.49	111.33
2	B	916	THR	CB-CA-C	6.73	117.89	110.15
1	A	1375	MET	CA-C-N	6.72	129.58	120.44
1	A	1375	MET	C-N-CA	6.72	129.58	120.44
2	B	476	ARG	CA-C-N	6.71	134.36	121.54
2	B	476	ARG	C-N-CA	6.71	134.36	121.54
8	J	5	VAL	N-CA-C	-6.68	100.96	109.58
1	A	886	ILE	N-CA-C	6.64	117.43	110.72
8	J	18	TRP	N-CA-C	6.64	118.17	111.07
1	A	525	GLN	N-CA-C	6.60	118.34	108.31
2	B	345	LYS	CA-C-N	6.60	133.57	121.70
2	B	345	LYS	C-N-CA	6.60	133.57	121.70
1	A	853	ASP	CA-CB-CG	6.51	119.11	112.60
8	J	1	MET	CA-C-N	6.51	133.69	121.97
8	J	1	MET	C-N-CA	6.51	133.69	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	282	ILE	N-CA-C	6.48	117.16	110.36
1	A	1437	GLY	CA-C-N	6.48	128.96	120.28
1	A	1437	GLY	C-N-CA	6.48	128.96	120.28
2	B	550	ASP	CA-CB-CG	6.44	119.04	112.60
1	A	1123	GLY	CA-C-N	6.43	133.28	121.70
1	A	1123	GLY	C-N-CA	6.43	133.28	121.70
1	A	557	ASP	CA-CB-CG	6.41	119.00	112.60
1	A	622	VAL	N-CA-CB	-6.37	104.04	112.26
2	B	963	PHE	CA-CB-CG	6.36	120.16	113.80
1	A	303	TYR	N-CA-C	-6.32	105.72	113.50
1	A	917	SER	CA-C-N	6.31	129.59	120.38
1	A	917	SER	C-N-CA	6.31	129.59	120.38
2	B	629	ASP	CA-CB-CG	6.31	118.91	112.60
7	I	55	THR	CB-CA-C	6.26	120.54	110.09
1	A	1233	ASP	CA-C-N	6.24	130.19	120.82
1	A	1233	ASP	C-N-CA	6.24	130.19	120.82
1	A	351	THR	CA-C-N	6.21	129.76	120.69
1	A	351	THR	C-N-CA	6.21	129.76	120.69
2	B	1022	THR	CB-CA-C	6.21	120.25	111.74
12	T	16	DC	N1-C1'-C2'	6.21	122.82	113.50
2	B	663	ALA	N-CA-C	-6.20	104.61	111.36
3	C	77	ILE	N-CA-C	6.18	116.97	110.72
2	B	737	THR	CA-C-N	6.16	129.59	120.90
2	B	737	THR	C-N-CA	6.16	129.59	120.90
1	A	827	THR	N-CA-C	-6.11	104.53	111.07
1	A	708	MET	N-CA-C	6.09	118.67	109.23
7	I	116	ASN	CA-CB-CG	6.04	118.64	112.60
10	L	40	LEU	CA-C-N	6.02	129.85	120.75
10	L	40	LEU	C-N-CA	6.02	129.85	120.75
1	A	474	VAL	CB-CA-C	6.01	117.11	110.62
3	C	85	ASP	CA-CB-CG	6.00	118.61	112.60
1	A	794	PRO	CA-C-N	6.00	128.60	120.38
1	A	794	PRO	C-N-CA	6.00	128.60	120.38
4	E	177	ARG	N-CA-C	6.00	119.32	109.72
3	C	82	TYR	N-CA-C	-6.00	100.23	109.76
2	B	756	ILE	N-CA-C	5.95	114.78	108.95
6	H	137	GLN	N-CA-C	5.95	118.63	110.24
2	B	1006	ILE	N-CA-CB	5.95	118.77	110.56
1	A	474	VAL	CA-C-N	5.94	128.49	120.65
1	A	474	VAL	C-N-CA	5.94	128.49	120.65
1	A	485	ASP	CA-CB-CG	5.93	118.53	112.60
2	B	786	ASN	CA-CB-CG	5.89	118.49	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	786	ASN	CA-C-N	5.88	129.90	121.55
2	B	786	ASN	C-N-CA	5.88	129.90	121.55
2	B	1009	ASP	N-CA-C	-5.86	105.23	112.90
1	A	466	SER	N-CA-C	5.85	120.04	113.02
3	C	78	GLU	CB-CG-CD	5.84	122.52	112.60
6	H	136	LYS	CA-C-N	5.83	129.13	120.90
6	H	136	LYS	C-N-CA	5.83	129.13	120.90
2	B	828	ALA	N-CA-C	5.83	117.97	108.76
3	C	240	VAL	N-CA-C	5.83	117.27	110.62
3	C	197	SER	CA-C-N	5.83	128.01	120.44
3	C	197	SER	C-N-CA	5.83	128.01	120.44
3	C	40	GLU	N-CA-C	5.79	121.10	112.94
6	H	139	ASN	CA-C-N	5.76	132.55	121.54
6	H	139	ASN	C-N-CA	5.76	132.55	121.54
2	B	711	GLU	N-CA-C	5.76	122.54	109.81
1	A	1366	ARG	N-CA-C	5.75	119.11	111.75
12	T	22	DT	P-O3'-C3'	5.74	128.82	120.20
8	J	64	ASN	N-CA-C	5.74	122.50	109.81
6	H	130	ARG	CA-C-N	5.74	132.50	121.54
6	H	130	ARG	C-N-CA	5.74	132.50	121.54
1	A	1256	GLU	N-CA-C	5.73	118.39	111.40
7	I	10	CYS	N-CA-C	5.66	117.53	111.36
1	A	763	ALA	N-CA-C	5.62	119.84	112.13
1	A	117	GLU	CA-C-N	5.61	129.67	120.63
1	A	117	GLU	C-N-CA	5.61	129.67	120.63
2	B	986	GLN	CA-C-N	5.61	128.84	120.87
2	B	986	GLN	C-N-CA	5.61	128.84	120.87
1	A	1389	PHE	N-CA-C	5.61	117.39	111.28
6	H	122	LEU	N-CA-C	5.60	118.81	110.52
1	A	1161	THR	CB-CA-C	5.60	118.99	109.53
2	B	847	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	228	PHE	N-CA-C	5.58	120.10	112.68
1	A	580	VAL	N-CA-C	-5.58	105.08	110.72
2	B	733	HIS	N-CA-C	-5.57	105.11	111.07
1	A	906	HIS	N-CA-C	5.56	119.38	112.59
8	J	2	ILE	N-CA-C	5.56	120.90	109.34
1	A	244	PRO	N-CA-C	5.56	117.48	110.70
3	C	240	VAL	N-CA-CB	5.53	117.38	110.47
2	B	593	PRO	CA-C-N	5.52	127.68	120.28
2	B	593	PRO	C-N-CA	5.52	127.68	120.28
2	B	1169	MET	CA-C-N	5.51	127.93	120.38
2	B	1169	MET	C-N-CA	5.51	127.93	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	703	ILE	N-CA-C	5.50	115.87	108.17
1	A	1419	ASP	CA-C-N	5.49	127.90	120.38
1	A	1419	ASP	C-N-CA	5.49	127.90	120.38
7	I	52	ILE	N-CA-C	5.48	116.66	108.54
2	B	415	GLN	CA-C-N	5.41	127.47	120.44
2	B	415	GLN	C-N-CA	5.41	127.47	120.44
1	A	758	ILE	CA-C-N	5.41	127.47	120.44
1	A	758	ILE	C-N-CA	5.41	127.47	120.44
2	B	758	PHE	CA-CB-CG	5.41	119.21	113.80
4	E	92	THR	CA-C-N	5.41	127.47	120.44
4	E	92	THR	C-N-CA	5.41	127.47	120.44
1	A	602	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	305	ASP	N-CA-C	5.39	116.83	107.93
1	A	881	GLN	CA-C-N	5.39	129.00	121.02
1	A	881	GLN	C-N-CA	5.39	129.00	121.02
2	B	60	GLN	CA-C-N	5.39	127.44	120.44
2	B	60	GLN	C-N-CA	5.39	127.44	120.44
2	B	738	PHE	N-CA-C	5.38	117.83	110.24
3	C	34	ARG	CA-C-N	5.38	127.75	120.65
3	C	34	ARG	C-N-CA	5.38	127.75	120.65
1	A	1393	ASN	CA-CB-CG	5.36	117.96	112.60
7	I	110	PHE	CA-CB-CG	5.36	119.16	113.80
3	C	236	GLY	CA-C-N	5.34	127.70	120.38
3	C	236	GLY	C-N-CA	5.34	127.70	120.38
2	B	1121	GLY	CA-C-N	5.32	127.41	120.28
2	B	1121	GLY	C-N-CA	5.32	127.41	120.28
1	A	399	HIS	N-CA-CB	5.31	119.82	110.37
2	B	1022	THR	CA-C-N	5.30	129.31	120.62
2	B	1022	THR	C-N-CA	5.30	129.31	120.62
9	K	93	SER	CA-C-N	5.29	127.31	120.70
9	K	93	SER	C-N-CA	5.29	127.31	120.70
4	E	160	GLU	CA-C-N	5.28	127.63	120.44
4	E	160	GLU	C-N-CA	5.28	127.63	120.44
2	B	479	VAL	N-CA-C	-5.26	102.06	109.21
3	C	226	ASP	CA-C-N	5.26	131.58	121.54
3	C	226	ASP	C-N-CA	5.26	131.58	121.54
4	E	46	TYR	N-CA-C	5.25	121.42	114.12
2	B	454	THR	CA-C-N	5.25	127.75	120.29
2	B	454	THR	C-N-CA	5.25	127.75	120.29
1	A	884	ASP	N-CA-C	5.25	119.44	113.19
3	C	41	ILE	N-CA-CB	5.25	118.56	111.21
2	B	881	ASN	CA-C-N	5.25	131.56	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	881	ASN	C-N-CA	5.25	131.56	121.54
1	A	537	ARG	CA-C-N	5.24	128.28	120.31
1	A	537	ARG	C-N-CA	5.24	128.28	120.31
1	A	1228	TRP	N-CA-C	5.23	116.80	108.79
2	B	136	THR	CA-C-N	5.23	131.53	121.54
2	B	136	THR	C-N-CA	5.23	131.53	121.54
6	H	129	TYR	CA-C-N	5.23	127.54	120.38
6	H	129	TYR	C-N-CA	5.23	127.54	120.38
6	H	91	ASP	CA-C-N	5.22	130.98	122.67
6	H	91	ASP	C-N-CA	5.22	130.98	122.67
1	A	857	ARG	N-CA-C	5.22	117.33	109.23
4	E	115	ASN	N-CA-C	5.22	116.22	108.60
2	B	450	ALA	CA-C-N	5.22	127.53	120.38
2	B	450	ALA	C-N-CA	5.22	127.53	120.38
6	H	16	ASP	N-CA-C	5.21	118.59	107.91
1	A	1086	PHE	CA-C-N	5.20	128.92	120.60
1	A	1086	PHE	C-N-CA	5.20	128.92	120.60
1	A	235	ILE	N-CA-CB	5.20	116.38	110.72
1	A	399	HIS	CA-C-O	-5.19	113.04	120.16
2	B	790	ASP	CA-CB-CG	5.19	117.79	112.60
8	J	60	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	1004	ASN	CA-C-N	5.18	127.54	120.54
1	A	1004	ASN	C-N-CA	5.18	127.54	120.54
1	A	969	GLN	CA-C-N	5.18	127.54	120.54
1	A	969	GLN	C-N-CA	5.18	127.54	120.54
1	A	525	GLN	CA-C-N	5.18	127.22	120.28
1	A	525	GLN	C-N-CA	5.18	127.22	120.28
1	A	1237	ILE	N-CA-C	5.18	115.94	108.48
1	A	134	ARG	CA-C-N	5.17	127.21	120.28
1	A	134	ARG	C-N-CA	5.17	127.21	120.28
2	B	397	ASP	CA-CB-CG	5.16	117.76	112.60
2	B	833	TYR	N-CA-C	-5.16	106.30	112.59
7	I	83	ASN	CA-C-N	5.15	129.87	122.45
7	I	83	ASN	C-N-CA	5.15	129.87	122.45
1	A	612	ILE	N-CA-CB	5.14	116.71	110.95
8	J	31	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	143	LYS	CA-C-N	5.13	127.66	120.28
1	A	143	LYS	C-N-CA	5.13	127.66	120.28
2	B	230	ALA	N-CA-C	5.12	121.11	109.81
1	A	398	GLU	N-CA-C	-5.11	101.37	109.96
2	B	490	SER	CA-C-N	5.11	127.40	120.65
2	B	490	SER	C-N-CA	5.11	127.40	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	754	SER	CA-C-N	5.11	129.08	120.29
2	B	754	SER	C-N-CA	5.11	129.08	120.29
1	A	84	ILE	CB-CA-C	5.10	116.23	110.41
1	A	1351	GLU	CB-CG-CD	5.10	121.27	112.60
3	C	220	ASP	CA-CB-CG	5.10	117.70	112.60
6	H	3	ASN	CA-C-N	5.08	128.91	120.94
6	H	3	ASN	C-N-CA	5.08	128.91	120.94
6	H	62	SER	CA-C-N	5.08	130.83	121.70
6	H	62	SER	C-N-CA	5.08	130.83	121.70
1	A	776	ALA	N-CA-C	5.07	117.40	110.55
1	A	491	VAL	N-CA-C	5.07	113.51	107.73
2	B	29	ASP	CA-C-N	5.07	127.07	120.28
2	B	29	ASP	C-N-CA	5.07	127.07	120.28
8	J	8	PHE	CA-CB-CG	5.07	118.86	113.80
7	I	117	LYS	CA-C-N	5.06	131.21	121.54
7	I	117	LYS	C-N-CA	5.06	131.21	121.54
2	B	1054	GLY	CA-C-N	5.06	126.94	120.56
2	B	1054	GLY	C-N-CA	5.06	126.94	120.56
2	B	1156	ASP	N-CA-C	5.06	121.58	110.80
10	L	68	GLU	N-CA-C	-5.06	102.21	110.20
3	C	194	GLU	N-CA-C	-5.05	105.35	112.12
2	B	477	ALA	N-CA-C	5.05	121.56	110.80
3	C	108	GLU	N-CA-C	-5.04	105.87	111.36
2	B	838	SER	N-CA-C	-5.03	103.02	110.46
3	C	166	GLU	CB-CG-CD	5.03	121.14	112.60
1	A	1308	THR	N-CA-C	5.02	117.76	109.72
2	B	668	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	445	ASN	N-CA-C	5.02	117.43	109.50
1	A	1341	ILE	N-CA-C	5.02	115.63	110.36
2	B	228	LYS	CA-C-N	5.01	131.12	121.54
2	B	228	LYS	C-N-CA	5.01	131.12	121.54
3	C	130	GLY	N-CA-C	5.01	121.79	115.42
2	B	1013	ASN	N-CA-C	5.01	116.14	109.93
4	E	94	LYS	CA-C-N	5.01	126.99	120.28
4	E	94	LYS	C-N-CA	5.01	126.99	120.28

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	190	0
2	B	8861	0	8884	205	0
3	C	2095	0	2051	52	0
4	E	1752	0	1776	18	0
5	F	688	0	707	9	0
6	H	1068	0	1040	12	0
7	I	971	0	927	7	0
8	J	532	0	542	22	0
9	K	919	0	929	16	0
10	L	363	0	386	13	0
11	R	88	0	46	0	0
12	T	159	0	91	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
All	All	28547	0	28512	476	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 8.

All (476) 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:756:ILE:CG1	1:A:756:ILE:CD1	1.77	1.56
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.90	1.06
1:A:869:GLY:O	4:E:204:THR:HG21	1.63	0.96
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.89	0.88
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.39	0.88
6:H:2:SER:HB2	6:H:3:ASN:HB2	1.56	0.88
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.42	0.84
8:J:48:ARG:O	8:J:52:THR:HG22	1.76	0.84
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.22	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:THR:HG21	3:C:145:CYS:SG	2.20	0.82
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.61	0.82
1:A:901:LEU:HA	1:A:907:THR:HG23	1.60	0.82
2:B:313:MET:HE2	2:B:390:LEU:HG	1.62	0.81
1:A:741:ASN:HD22	1:A:744:LYS:H	1.29	0.81
5:F:110:ASP:O	5:F:123:LYS:HE2	1.81	0.80
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.63	0.79
1:A:605:MET:HE2	1:A:607:ILE:HG13	1.65	0.79
1:A:754:SER:H	1:A:757:ASN:HD22	1.30	0.77
2:B:1100:ASP:HA	2:B:1103:ILE:HD11	1.66	0.76
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.68	0.76
2:B:276:ILE:HG13	2:B:334:ILE:HG23	1.68	0.76
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.23	0.74
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.69	0.74
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.69	0.74
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.72	0.72
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.54	0.72
3:C:167:HIS:HD2	3:C:169:LYS:H	1.36	0.71
2:B:999:MET:HE3	2:B:999:MET:HA	1.71	0.71
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.74	0.69
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.58	0.69
2:B:744:HIS:HD2	2:B:746:SER:H	1.38	0.69
1:A:756:ILE:HD13	1:A:756:ILE:H	1.58	0.69
4:E:77:SER:HB3	4:E:105:PHE:HA	1.74	0.68
1:A:37:PHE:HD1	1:A:52:GLY:HA3	1.58	0.68
1:A:72:GLU:HB3	1:A:76:GLU:HG2	1.76	0.67
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.77	0.67
1:A:399:HIS:O	1:A:401:GLY:N	2.27	0.67
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.43	0.66
2:B:706:GLN:O	2:B:710:LEU:HB2	1.95	0.66
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.60	0.65
1:A:1364:ASN:HD21	1:A:1366:ARG:HD2	1.61	0.65
2:B:884:ARG:HG3	2:B:935:ARG:HE	1.62	0.65
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.79	0.64
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.79	0.64
2:B:848:ARG:HH22	2:B:996:ARG:NH1	1.95	0.64
1:A:378:GLU:OE2	1:A:434:ARG:HD3	1.97	0.64
2:B:516:ASN:H	2:B:516:ASN:HD22	1.46	0.64
2:B:834:ASN:HA	2:B:838:SER:HB2	1.78	0.64
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.80	0.63
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:VAL:HG13	4:E:201:LYS:HB3	1.81	0.63
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.79	0.63
2:B:916:THR:HG23	2:B:935:ARG:HB3	1.80	0.63
2:B:54:PHE:HA	2:B:58:THR:HB	1.80	0.63
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.81	0.63
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.81	0.63
2:B:864:LYS:HB3	2:B:872:GLU:H	1.61	0.62
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.64	0.62
1:A:469:ARG:NH2	2:B:991:GLY:O	2.32	0.62
2:B:877:PRO:HB2	2:B:885:MET:HE1	1.80	0.62
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.14	0.62
1:A:567:LYS:HB3	6:H:96:VAL:H	1.63	0.62
2:B:887:HIS:HA	2:B:888:GLY:C	2.24	0.62
1:A:705:LYS:HE3	1:A:705:LYS:H	1.65	0.62
3:C:165:LYS:O	9:K:6:ARG:NH1	2.33	0.62
2:B:260:GLY:O	2:B:267:ARG:HD3	1.99	0.62
3:C:18:VAL:HG22	3:C:240:VAL:HB	1.82	0.61
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.81	0.61
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.81	0.61
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.81	0.61
3:C:73:GLN:HE21	3:C:75:MET:H	1.49	0.61
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.54	0.60
2:B:1100:ASP:HA	2:B:1103:ILE:CD1	2.31	0.60
1:A:1206:ASP:HB2	1:A:1274:ARG:HH12	1.67	0.60
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.84	0.60
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.84	0.60
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.83	0.60
1:A:596:THR:C	1:A:598:LEU:H	2.10	0.59
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.84	0.59
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.83	0.59
7:I:26:LEU:HD23	7:I:37:GLU:HA	1.84	0.59
1:A:404:TYR:HA	1:A:413:ILE:O	2.03	0.59
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.48	0.59
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.84	0.59
2:B:345:LYS:HA	2:B:347:LYS:H	1.67	0.59
1:A:545:GLN:HG2	1:A:549:MET:HE2	1.84	0.58
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.51	0.58
2:B:887:HIS:HA	2:B:888:GLY:O	2.03	0.58
4:E:88:VAL:HB	4:E:116:ILE:HD13	1.84	0.58
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.39	0.58
8:J:48:ARG:O	8:J:52:THR:CG2	2.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.03	0.58
3:C:41:ILE:HD12	3:C:246:ARG:HB2	1.86	0.58
9:K:65:HIS:CD2	9:K:67:PHE:H	2.22	0.58
1:A:596:THR:O	1:A:598:LEU:N	2.36	0.58
2:B:416:LEU:HD11	2:B:460:ALA:HB3	1.86	0.57
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.85	0.57
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.86	0.57
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.40	0.57
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.85	0.57
8:J:6:ARG:HG3	8:J:13:VAL:HG13	1.87	0.57
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.86	0.57
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.85	0.57
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.20	0.56
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.86	0.56
2:B:254:LEU:HD22	2:B:381:MET:HE1	1.87	0.56
2:B:999:MET:HB3	2:B:1007:VAL:HG22	1.87	0.56
2:B:219:ALA:HB3	2:B:222:ILE:HD12	1.87	0.56
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.88	0.56
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.89	0.56
2:B:843:GLN:HB2	2:B:993:THR:HB	1.86	0.56
1:A:924:LYS:O	1:A:927:VAL:HG12	2.06	0.56
2:B:975:GLN:HG2	2:B:976:ILE:H	1.69	0.56
1:A:588:LEU:HD23	1:A:605:MET:HG2	1.88	0.55
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.88	0.55
2:B:1099:VAL:O	2:B:1103:ILE:HG13	2.05	0.55
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.35	0.55
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.89	0.55
2:B:363:HIS:O	2:B:364:ILE:HB	2.07	0.55
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.31	0.54
2:B:705:MET:H	2:B:710:LEU:HG	1.73	0.54
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.88	0.54
1:A:313:GLN:HG2	1:A:322:VAL:HG22	1.88	0.54
1:A:567:LYS:O	1:A:569:LYS:N	2.40	0.54
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.43	0.54
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.54	0.54
2:B:357:GLN:HG2	2:B:368:GLU:HA	1.89	0.54
9:K:7:PHE:HA	9:K:10:PHE:CZ	2.43	0.54
1:A:741:ASN:ND2	1:A:744:LYS:H	2.00	0.54
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.71	0.54
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.90	0.54
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:7:CYS:HA	8:J:49:MET:HG2	1.89	0.54
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.88	0.54
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.43	0.54
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.72	0.54
1:A:30:ILE:HG12	2:B:1170:THR:HG21	1.89	0.54
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.90	0.53
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.89	0.53
2:B:915:THR:HG21	2:B:934:LYS:HD2	1.89	0.53
1:A:1006:ILE:HD11	4:E:163:GLU:HG3	1.88	0.53
2:B:213:ILE:HG12	2:B:481:GLN:HG3	1.90	0.53
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.90	0.53
2:B:222:ILE:HD13	2:B:403:LYS:HG3	1.90	0.53
2:B:1079:LYS:HE3	3:C:188:HIS:CE1	2.44	0.53
8:J:6:ARG:HG2	8:J:11:GLY:O	2.09	0.53
2:B:983:ARG:HH11	2:B:983:ARG:HB2	1.74	0.52
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.90	0.52
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.41	0.52
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.74	0.52
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.92	0.52
1:A:72:GLU:HB3	1:A:76:GLU:CG	2.39	0.52
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.41	0.52
2:B:880:THR:C	2:B:882:THR:H	2.17	0.52
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.44	0.52
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.92	0.52
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.90	0.52
6:H:137:GLN:HB3	6:H:139:ASN:HB2	1.92	0.52
9:K:65:HIS:HD2	9:K:67:PHE:H	1.56	0.52
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.92	0.52
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.92	0.51
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.09	0.51
1:A:1129:GLU:HA	1:A:1132:LYS:HE3	1.91	0.51
2:B:705:MET:HE3	2:B:742:GLU:HG2	1.91	0.51
2:B:999:MET:HA	2:B:999:MET:CE	2.39	0.51
2:B:516:ASN:H	2:B:516:ASN:ND2	2.08	0.51
2:B:1002:THR:HG21	2:B:1006:ILE:HG12	1.93	0.51
1:A:1096:SER:O	1:A:1099:PRO:HD2	2.11	0.51
2:B:58:THR:O	2:B:62:ILE:HG12	2.10	0.51
1:A:15:LYS:HB3	2:B:1220:ARG:HG2	1.92	0.51
8:J:12:LYS:HD2	8:J:43:ARG:HH12	1.76	0.51
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.93	0.50
3:C:46:ILE:HA	3:C:159:ALA:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:VAL:HG13	6:H:78:SER:HA	1.93	0.50
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.93	0.50
2:B:976:ILE:HG23	2:B:977:GLY:H	1.75	0.50
1:A:18:GLN:HE21	1:A:1418:LEU:HB2	1.75	0.50
5:F:111:LEU:HD12	5:F:111:LEU:H	1.77	0.50
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.92	0.50
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.75	0.50
1:A:756:ILE:CD1	1:A:756:ILE:H	2.23	0.50
2:B:705:MET:N	2:B:710:LEU:HG	2.27	0.50
2:B:804:GLY:O	2:B:983:ARG:NH2	2.45	0.50
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.94	0.50
2:B:639:ILE:HD11	2:B:691:GLU:HB3	1.93	0.50
1:A:826:ASP:HA	1:A:829:VAL:HB	1.94	0.50
2:B:570:VAL:HB	2:B:573:GLN:HG2	1.93	0.50
1:A:350:ARG:HD2	2:B:1128:LEU:HD21	1.94	0.49
3:C:235:VAL:HG11	8:J:6:ARG:HH21	1.77	0.49
6:H:135:LEU:C	6:H:137:GLN:H	2.20	0.49
1:A:315:LEU:HA	1:A:320:ARG:HB3	1.92	0.49
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.47	0.49
1:A:683:ILE:HG21	1:A:801:GLU:HG2	1.93	0.49
3:C:22:LEU:HD11	9:K:101:LEU:HD11	1.93	0.49
2:B:466:TRP:HB3	2:B:475:SER:HB3	1.93	0.49
2:B:651:LEU:HD21	2:B:741:CYS:HB3	1.93	0.49
4:E:65:THR:HG22	4:E:67:GLU:H	1.77	0.49
10:L:27:LEU:HB3	10:L:37:LYS:HG2	1.94	0.49
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.12	0.49
2:B:476:ARG:O	2:B:478:GLY:N	2.45	0.49
2:B:256:VAL:HG12	2:B:385:LEU:HD22	1.93	0.49
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.95	0.49
1:A:37:PHE:CD1	1:A:52:GLY:HA3	2.44	0.49
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.95	0.49
2:B:1002:THR:CG2	2:B:1006:ILE:H	2.25	0.49
1:A:371:ALA:HA	1:A:436:ILE:HG22	1.95	0.49
1:A:626:ASN:O	1:A:631:HIS:CD2	2.66	0.49
2:B:1082:MET:HA	3:C:189:THR:HA	1.95	0.49
3:C:57:VAL:CG1	8:J:60:PHE:HB3	2.37	0.49
1:A:128:ILE:HG23	1:A:134:ARG:HG3	1.94	0.48
2:B:783:THR:CG2	8:J:59:LYS:HB3	2.43	0.48
1:A:219:PHE:HZ	1:A:226:GLU:HA	1.78	0.48
1:A:396:PRO:HB3	1:A:403:LYS:HB3	1.94	0.48
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.95	0.48
10:L:32:ALA:HB3	10:L:55:ILE:HB	1.96	0.48
1:A:744:LYS:O	1:A:748:MET:HG3	2.13	0.48
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.77	0.48
3:C:167:HIS:CD2	3:C:169:LYS:H	2.24	0.48
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.39	0.48
2:B:640:VAL:HG13	2:B:649:LYS:HB3	1.95	0.48
2:B:708:GLU:O	2:B:710:LEU:N	2.46	0.48
2:B:801:LYS:O	8:J:52:THR:OG1	2.26	0.48
2:B:190:TYR:CD1	8:J:62:ARG:HG2	2.48	0.48
2:B:704:ALA:HB1	2:B:710:LEU:HB3	1.95	0.48
2:B:637:LEU:HD12	2:B:693:ILE:HG13	1.95	0.47
10:L:61:THR:HG21	10:L:63:ARG:HG3	1.96	0.47
1:A:1152:ILE:HG23	1:A:1260:LEU:HD23	1.96	0.47
1:A:1327:ILE:O	4:E:147:HIS:HE1	1.97	0.47
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.96	0.47
2:B:492:LEU:O	2:B:496:ARG:HG3	2.14	0.47
2:B:841:MET:O	2:B:993:THR:HA	2.14	0.47
3:C:105:GLY:O	3:C:149:LYS:O	2.32	0.47
1:A:55:ASP:O	1:A:57:ARG:N	2.47	0.47
1:A:115:LEU:HD12	1:A:142:CYS:HB3	1.97	0.47
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.96	0.47
1:A:323:LYS:HG3	1:A:328:ARG:HG3	1.96	0.47
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.97	0.47
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.96	0.47
3:C:123:ASN:HD22	3:C:125:MET:HG3	1.79	0.47
2:B:705:MET:CE	2:B:742:GLU:HG2	2.45	0.47
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.66	0.47
8:J:3:VAL:CG1	8:J:18:TRP:HB2	2.44	0.47
1:A:614:PHE:HB3	6:H:122:LEU:HD21	1.97	0.47
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.97	0.47
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.97	0.47
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.97	0.47
2:B:984:HIS:HB3	2:B:1022:THR:OG1	2.14	0.47
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.12	0.47
1:A:324:SER:O	1:A:326:ARG:N	2.40	0.47
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.96	0.47
2:B:792:MET:HA	2:B:856:PHE:O	2.14	0.47
2:B:1048:THR:OG1	2:B:1050:ILE:HD12	2.15	0.47
3:C:98:VAL:H	3:C:122:SER:HB2	1.80	0.47
1:A:899:VAL:HG22	1:A:1029:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:LEU:HD23	1:A:1267:MET:HB3	1.96	0.46
1:A:702:LEU:O	1:A:710:LEU:HD11	2.14	0.46
2:B:370:PHE:O	2:B:372:SER:N	2.39	0.46
2:B:424:LEU:O	2:B:428:ILE:HG12	2.15	0.46
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.51	0.46
2:B:128:LEU:HD11	2:B:170:LEU:HB2	1.96	0.46
2:B:487:THR:HG22	2:B:490:SER:HB3	1.98	0.46
1:A:350:ARG:HB2	2:B:1128:LEU:HD21	1.98	0.46
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.97	0.46
3:C:166:GLU:HG2	9:K:6:ARG:HB2	1.97	0.46
1:A:211:PHE:HA	1:A:214:ILE:HD11	1.97	0.46
1:A:467:THR:HG23	2:B:976:ILE:HG23	1.97	0.46
3:C:77:ILE:HG12	3:C:129:ILE:HD11	1.98	0.46
2:B:582:VAL:HG22	2:B:626:ILE:HD12	1.96	0.46
1:A:704:ALA:H	1:A:710:LEU:HD22	1.81	0.46
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.97	0.46
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.46	0.46
1:A:23:SER:HB3	1:A:26:GLU:HB2	1.99	0.45
1:A:203:SER:HB3	1:A:206:GLU:HB2	1.98	0.45
1:A:907:THR:HG22	1:A:908:LEU:H	1.81	0.45
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.98	0.45
7:I:68:LEU:HB3	7:I:84:VAL:HG22	1.97	0.45
1:A:800:VAL:HA	1:A:812:GLU:HG2	1.99	0.45
1:A:1102:LYS:HE2	1:A:1106:ASN:HD21	1.81	0.45
2:B:654:ARG:H	2:B:657:HIS:HD2	1.63	0.45
2:B:783:THR:HG23	8:J:59:LYS:HB3	1.97	0.45
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.51	0.45
5:F:93:ILE:HD13	5:F:134:ILE:HD11	1.98	0.45
1:A:942:PHE:O	1:A:946:VAL:HG23	2.17	0.45
2:B:102:VAL:HG11	2:B:122:LEU:HD13	1.99	0.45
1:A:575:LYS:HD2	6:H:120:GLY:HA3	1.98	0.45
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.98	0.45
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.50	0.45
2:B:1103:ILE:O	2:B:1122:ARG:HD2	2.16	0.45
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.99	0.45
3:C:8:VAL:HG12	9:K:108:GLU:HG3	1.97	0.45
5:F:72:LYS:HE2	5:F:142:SER:HB3	1.98	0.45
8:J:1:MET:H1	8:J:56:LEU:HB2	1.81	0.45
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.81	0.45
1:A:1138:ILE:HG13	1:A:1282:VAL:HG21	1.99	0.45
3:C:146:LYS:HB3	8:J:61:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:H	1:A:56:PRO:HD2	1.82	0.45
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.42	0.45
1:A:700:ASN:HD22	7:I:115:LYS:HB2	1.82	0.45
1:A:839:ARG:HH21	1:A:1402:PHE:HA	1.80	0.45
1:A:982:THR:HG22	1:A:983:ILE:H	1.82	0.45
2:B:254:LEU:CD2	2:B:381:MET:HE1	2.47	0.45
3:C:33:LEU:HG	3:C:37:MET:HE2	1.99	0.45
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.99	0.45
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.50	0.45
2:B:515:HIS:CD2	2:B:517:THR:H	2.35	0.45
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.52	0.45
1:A:341:MET:HE2	1:A:843:LYS:HZ1	1.82	0.44
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.42	0.44
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.99	0.44
4:E:64:PRO:HD3	4:E:76:GLY:CA	2.48	0.44
2:B:25:ILE:CD1	2:B:653:VAL:HB	2.47	0.44
2:B:581:PHE:HB2	2:B:625:LYS:HG2	2.00	0.44
2:B:778:MET:HB3	2:B:796:LEU:HD13	1.99	0.44
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.99	0.44
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.47	0.44
2:B:1051:THR:O	2:B:1055:ILE:HG12	2.17	0.44
3:C:258:ILE:HG23	9:K:19:LEU:HD11	1.98	0.44
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.83	0.44
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.83	0.44
2:B:879:ARG:NH1	2:B:879:ARG:HA	2.33	0.44
1:A:858:ASN:HD21	1:A:860:LEU:HD12	1.83	0.44
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.52	0.44
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.83	0.44
10:L:61:THR:HB	10:L:63:ARG:H	1.82	0.44
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.99	0.44
2:B:815:ARG:HG2	2:B:816:GLU:OE1	2.17	0.44
2:B:976:ILE:O	2:B:990:ILE:HB	2.17	0.44
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.83	0.44
1:A:642:CYS:O	1:A:645:LEU:HB3	2.17	0.44
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.99	0.44
1:A:341:MET:HB3	2:B:1132:GLU:HB3	2.00	0.44
1:A:702:LEU:HD12	1:A:710:LEU:HD13	2.00	0.44
2:B:169:ARG:HH22	2:B:958:GLN:HE22	1.64	0.44
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.99	0.44
2:B:515:HIS:HD2	2:B:517:THR:H	1.65	0.44
2:B:857:ARG:HH21	2:B:942:ARG:NH2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.53	0.44
1:A:729:ALA:O	1:A:732:LEU:HB2	2.17	0.44
5:F:108:PHE:HB3	5:F:129:LYS:HD2	1.99	0.44
1:A:579:SER:HB3	1:A:611:GLN:HA	1.99	0.43
2:B:51:PHE:O	2:B:55:VAL:HG23	2.18	0.43
1:A:687:LYS:HD2	1:A:794:PRO:HG2	2.00	0.43
2:B:244:LEU:HD12	2:B:250:PHE:HB2	2.00	0.43
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.18	0.43
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.51	0.43
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.53	0.43
2:B:123:THR:HA	2:B:204:ILE:O	2.18	0.43
3:C:41:ILE:HG12	3:C:172:PRO:HG3	2.01	0.43
2:B:102:VAL:HG13	2:B:112:LEU:HD22	2.01	0.43
2:B:370:PHE:CD2	2:B:373:ARG:HD2	2.53	0.43
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.99	0.43
5:F:76:LYS:HG2	5:F:79:ARG:HH12	1.82	0.43
7:I:75:CYS:O	7:I:78:CYS:O	2.35	0.43
2:B:302:CYS:HA	2:B:310:MET:HE3	1.99	0.43
2:B:848:ARG:NH2	2:B:996:ARG:NH1	2.66	0.43
1:A:709:THR:HG22	1:A:711:ARG:H	1.83	0.43
1:A:1353:TYR:CD2	1:A:1353:TYR:C	2.96	0.43
2:B:227:LYS:HG3	2:B:395:GLN:HB2	2.00	0.43
2:B:745:PRO:O	2:B:748:ILE:HG12	2.18	0.43
2:B:1001:PHE:CE1	3:C:178:PHE:HB3	2.54	0.43
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.99	0.43
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.19	0.43
10:L:28:LYS:HB2	10:L:39:SER:HB2	2.01	0.43
1:A:134:ARG:HH11	1:A:221:SER:HA	1.83	0.43
1:A:1297:GLU:H	1:A:1297:GLU:HG3	1.71	0.43
1:A:686:ALA:HB2	1:A:725:ALA:HB2	2.01	0.42
3:C:56:THR:HG22	3:C:57:VAL:H	1.83	0.42
10:L:27:LEU:HD13	10:L:59:ALA:HB1	2.01	0.42
1:A:98:LYS:O	1:A:102:VAL:HG23	2.19	0.42
1:A:181:LEU:HB2	1:A:202:LEU:HB2	2.01	0.42
1:A:786:HIS:HE1	2:B:742:GLU:OE1	2.02	0.42
2:B:190:TYR:CE1	8:J:62:ARG:HG2	2.55	0.42
2:B:238:ALA:HB3	2:B:256:VAL:HB	2.01	0.42
2:B:1210:MET:HB3	2:B:1212:ILE:HD12	2.00	0.42
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.99	0.42
3:C:60:ASP:HB3	10:L:67:PHE:CZ	2.53	0.42
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:TYR:HA	1:A:797:LYS:HD2	2.00	0.42
2:B:1156:ASP:HB3	2:B:1157:ALA:H	1.72	0.42
4:E:151:PRO:HD2	4:E:153:HIS:HE1	1.84	0.42
1:A:120:GLU:HA	1:A:123:ARG:HH11	1.84	0.42
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.52	0.42
1:A:667:GLY:HA2	1:A:670:ILE:HG12	2.01	0.42
1:A:779:PHE:CZ	2:B:517:THR:HA	2.54	0.42
1:A:1330:ASN:HB2	1:A:1351:GLU:OE2	2.20	0.42
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.49	0.42
3:C:14:SER:HA	9:K:114:LEU:HD22	2.01	0.42
3:C:241:ASP:HB3	9:K:109:TRP:CD2	2.55	0.42
1:A:134:ARG:HD2	1:A:221:SER:O	2.20	0.42
1:A:353:ILE:HD12	1:A:482:PHE:CD2	2.54	0.42
1:A:842:VAL:HG11	2:B:1136:ASP:CG	2.45	0.42
1:A:839:ARG:NH2	1:A:1402:PHE:HA	2.35	0.42
1:A:1173:HIS:CG	1:A:1227:ILE:HG23	2.55	0.42
1:A:1284:MET:HA	1:A:1306:LEU:HD23	2.02	0.42
2:B:759:PRO:HD2	2:B:1046:PRO:HG3	2.02	0.42
2:B:994:TYR:HD1	2:B:999:MET:HE1	1.85	0.42
1:A:567:LYS:HZ1	6:H:97:MET:HG2	1.85	0.42
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.55	0.42
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.20	0.42
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	2.01	0.42
2:B:241:ARG:HG2	2:B:253:THR:HG22	2.01	0.42
2:B:654:ARG:H	2:B:657:HIS:CD2	2.38	0.42
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	2.02	0.42
3:C:183:TRP:HB3	3:C:213:PRO:HD3	2.01	0.42
1:A:109:HIS:H	1:A:210:ILE:HD12	1.85	0.41
2:B:405:ARG:HB3	2:B:631:GLY:HA3	2.02	0.41
2:B:844:SER:HB2	2:B:996:ARG:H	1.85	0.41
2:B:880:THR:HB	2:B:934:LYS:HE2	2.01	0.41
10:L:34:CYS:SG	10:L:36:SER:HB2	2.60	0.41
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.56	0.41
2:B:189:LEU:HD13	2:B:196:PRO:HA	2.02	0.41
2:B:487:THR:HG22	2:B:490:SER:H	1.85	0.41
3:C:50:GLU:HG2	10:L:66:GLN:HG3	2.01	0.41
6:H:113:ALA:HB2	6:H:126:GLU:HG3	2.01	0.41
1:A:451:HIS:HB3	1:A:453:MET:H	1.85	0.41
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.55	0.41
1:A:577:ILE:H	1:A:577:ILE:HG13	1.76	0.41
1:A:1308:THR:HG22	1:A:1310:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:PRO:HB3	2:B:174:LEU:HD21	2.01	0.41
2:B:383:ASN:O	2:B:387:LEU:HB2	2.21	0.41
2:B:604:ARG:HH22	2:B:697:GLU:CD	2.28	0.41
3:C:43:THR:HG22	3:C:170:TRP:HD1	1.85	0.41
9:K:26:LYS:H	9:K:26:LYS:HG2	1.48	0.41
10:L:46:VAL:HG12	10:L:47:ARG:H	1.85	0.41
1:A:403:LYS:HA	1:A:415:LEU:HB2	2.02	0.41
1:A:821:ARG:HG3	1:A:825:ILE:CD1	2.50	0.41
2:B:520:GLY:HA2	2:B:748:ILE:HA	2.03	0.41
2:B:552:MET:HA	2:B:555:ILE:HD12	2.02	0.41
10:L:47:ARG:HA	10:L:53:HIS:O	2.20	0.41
1:A:172:PRO:HB2	1:A:183:GLY:HA3	2.02	0.41
1:A:251:SER:HB3	1:A:258:GLY:HA3	2.01	0.41
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.00	0.41
4:E:64:PRO:HG2	4:E:69:ILE:HD11	2.01	0.41
4:E:116:ILE:HG22	4:E:121:MET:HG2	2.03	0.41
2:B:345:LYS:N	2:B:346:GLU:HB3	2.36	0.41
2:B:757:PRO:HG3	2:B:983:ARG:NH1	2.36	0.41
2:B:1103:ILE:HG13	2:B:1103:ILE:H	1.61	0.41
2:B:555:ILE:H	2:B:555:ILE:HG13	1.71	0.41
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.89	0.41
1:A:1004:ASN:HD21	1:A:1007:ILE:HG12	1.86	0.41
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	2.02	0.41
2:B:950:ASP:HB3	2:B:967:ARG:HG2	2.03	0.41
3:C:98:VAL:HG22	3:C:158:VAL:HG22	2.03	0.41
1:A:353:ILE:HB	1:A:470:LEU:HD21	2.02	0.41
1:A:374:LEU:HA	2:B:1107:ALA:HB2	2.02	0.41
1:A:760:GLN:HG2	1:A:765:VAL:HA	2.01	0.41
2:B:209:GLU:HB3	2:B:483:LEU:HD23	2.02	0.41
2:B:400:HIS:CD2	2:B:517:THR:HG21	2.55	0.41
2:B:515:HIS:H	2:B:518:HIS:CD2	2.39	0.41
2:B:879:ARG:HA	2:B:879:ARG:HD3	1.93	0.41
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.45	0.41
4:E:107:THR:HA	4:E:131:THR:O	2.20	0.41
9:K:108:GLU:HA	9:K:111:LEU:HD12	2.02	0.41
1:A:897:TYR:HB3	1:A:936:LEU:HD13	2.03	0.41
2:B:175:ARG:NH2	2:B:181:LEU:O	2.54	0.41
2:B:706:GLN:H	2:B:710:LEU:HG	1.86	0.41
7:I:60:GLN:HE21	7:I:60:GLN:HA	1.85	0.41
9:K:21:ILE:HG13	9:K:33:ILE:HG12	2.03	0.41
1:A:91:PHE:H	1:A:297:GLN:HE22	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:PHE:HB3	1:A:571:LEU:HG	2.03	0.40
2:B:601:ARG:HA	2:B:615:MET:HE1	2.03	0.40
3:C:74:SER:O	3:C:77:ILE:HB	2.21	0.40
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.95	0.40
1:A:601:LYS:HE3	1:A:603:ASN:HD21	1.86	0.40
1:A:910:PRO:HA	1:A:916:GLY:HA3	2.03	0.40
1:A:986:ILE:O	1:A:990:VAL:HG23	2.21	0.40
1:A:587:HIS:HE1	1:A:969:GLN:HE21	1.70	0.40
1:A:964:ILE:HG22	1:A:968:GLN:OE1	2.21	0.40
1:A:965:GLN:HE21	1:A:965:GLN:HB2	1.71	0.40
2:B:950:ASP:OD2	2:B:967:ARG:NH1	2.54	0.40
2:B:952:VAL:HB	10:L:58:LYS:HB2	2.03	0.40
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.03	0.40
1:A:1153:TYR:HD2	7:I:41:PRO:HG2	1.86	0.40
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.54	0.40
2:B:1013:ASN:OD1	2:B:1015:HIS:CD2	2.74	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%)	1239 (89%)	110 (8%)	46 (3%)	3	17
2	B	1096/1224 (90%)	962 (88%)	91 (8%)	43 (4%)	2	14
3	C	264/318 (83%)	238 (90%)	22 (8%)	4 (2%)	8	35
4	E	212/215 (99%)	199 (94%)	11 (5%)	2 (1%)	14	48
5	F	83/155 (54%)	77 (93%)	5 (6%)	1 (1%)	10	40
6	H	129/146 (88%)	101 (78%)	21 (16%)	7 (5%)	1	9
7	I	117/122 (96%)	102 (87%)	13 (11%)	2 (2%)	7	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	63/70 (90%)	58 (92%)	2 (3%)	3 (5%)	2	11
9	K	112/120 (93%)	108 (96%)	3 (3%)	1 (1%)	14	48
10	L	44/70 (63%)	31 (70%)	7 (16%)	6 (14%)	0	1
All	All	3515/4173 (84%)	3115 (89%)	285 (8%)	115 (3%)	3	17

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	55	ASP
1	A	56	PRO
1	A	109	HIS
1	A	260	ASP
1	A	286	HIS
1	A	399	HIS
1	A	418	SER
1	A	424	ILE
1	A	569	LYS
1	A	597	LEU
2	B	67	SER
2	B	137	TYR
2	B	139	ALA
2	B	364	ILE
2	B	367	LEU
2	B	477	ALA
2	B	648	HIS
2	B	709	ASP
2	B	731	VAL
2	B	734	HIS
2	B	751	VAL
2	B	880	THR
2	B	883	LEU
2	B	976	ILE
2	B	1046	PRO
2	B	1156	ASP
3	C	227	THR
6	H	90	ALA
6	H	109	LYS
6	H	131	ASN
7	I	118	ARG
8	J	2	ILE

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Mol	Chain	Res	Type
8	J	6	ARG
1	A	250	ILE
1	A	283	GLY
1	A	312	PRO
1	A	325	ILE
1	A	556	TRP
1	A	846	GLU
1	A	1083	THR
1	A	1123	GLY
1	A	1221	LYS
1	A	1437	GLY
2	B	138	GLU
2	B	371	GLU
2	B	483	LEU
2	B	531	GLN
2	B	695	ALA
2	B	712	PRO
2	B	881	ASN
2	B	888	GLY
2	B	1124	ARG
2	B	1157	ALA
2	B	1180	PHE
2	B	1181	GLU
3	C	141	GLY
4	E	126	SER
10	L	51	CYS
10	L	64	LEU
1	A	332	LYS
1	A	410	GLY
1	A	662	PHE
1	A	975	HIS
2	B	65	GLU
2	B	737	THR
2	B	887	HIS
2	B	1171	VAL
2	B	1223	ASP
3	C	90	ASP
6	H	140	ALA
7	I	77	LYS
10	L	39	SER
10	L	56	LEU
1	A	35	ILE

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Mol	Chain	Res	Type
1	A	52	GLY
1	A	65	LEU
1	A	214	ILE
1	A	257	ARG
1	A	308	ILE
1	A	310	GLY
1	A	404	TYR
2	B	526	GLU
2	B	644	GLU
2	B	1221	SER
5	F	154	ASP
6	H	84	ALA
8	J	26	GLN
9	K	18	LYS
10	L	46	VAL
10	L	55	ILE
1	A	213	HIS
1	A	299	HIS
1	A	400	PRO
1	A	567	LYS
1	A	958	VAL
2	B	646	LEU
2	B	647	GLY
2	B	792	MET
3	C	142	VAL
6	H	108	SER
1	A	331	GLY
1	A	385	ILE
1	A	543	LEU
1	A	599	SER
4	E	3	GLN
6	H	61	SER
1	A	568	PRO
2	B	592	ASN
2	B	1017	ILE
2	B	711	GLU
2	B	1099	VAL
1	A	178	GLY
1	A	916	GLY
1	A	1384	VAL

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	1212/1520 (80%)	1057 (87%)	155 (13%)	4	19
2	B	967/1061 (91%)	828 (86%)	139 (14%)	3	15
3	C	234/274 (85%)	200 (86%)	34 (14%)	3	15
4	E	196/197 (100%)	170 (87%)	26 (13%)	4	18
5	F	75/137 (55%)	69 (92%)	6 (8%)	11	38
6	H	117/128 (91%)	95 (81%)	22 (19%)	1	9
7	I	113/116 (97%)	100 (88%)	13 (12%)	5	24
8	J	60/65 (92%)	51 (85%)	9 (15%)	3	14
9	K	99/102 (97%)	87 (88%)	12 (12%)	5	21
10	L	40/57 (70%)	26 (65%)	14 (35%)	0	1
All	All	3113/3657 (85%)	2683 (86%)	430 (14%)	3	17

All (430) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	18	GLN
1	A	25	GLU
1	A	30	ILE
1	A	40	THR
1	A	43	GLU
1	A	58	LEU
1	A	61	ILE
1	A	65	LEU
1	A	69	THR
1	A	70	CYS
1	A	86	LEU
1	A	93	VAL
1	A	108	MET
1	A	113	LEU
1	A	118	HIS

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Mol	Chain	Res	Type
1	A	126	LEU
1	A	130	ASP
1	A	144	THR
1	A	171	GLN
1	A	179	LEU
1	A	186	LYS
1	A	204	THR
1	A	205	GLU
1	A	208	LEU
1	A	219	PHE
1	A	222	LEU
1	A	235	ILE
1	A	252	PHE
1	A	261	ASP
1	A	263	THR
1	A	265	LYS
1	A	270	LEU
1	A	295	LEU
1	A	303	TYR
1	A	308	ILE
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	351	THR
1	A	353	ILE
1	A	359	LEU
1	A	389	THR
1	A	403	LYS
1	A	407	ARG
1	A	423	ASP
1	A	424	ILE
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	456	MET
1	A	463	ILE

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Mol	Chain	Res	Type
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	476	SER
1	A	489	LEU
1	A	496	GLU
1	A	500	GLU
1	A	501	LEU
1	A	518	LYS
1	A	527	THR
1	A	532	ARG
1	A	549	MET
1	A	567	LYS
1	A	590	ARG
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	636	GLU
1	A	640	GLN
1	A	672	ASP
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	702	LEU
1	A	705	LYS
1	A	708	MET
1	A	710	LEU
1	A	716	ASP
1	A	722	LEU
1	A	731	ARG
1	A	756	ILE
1	A	769	SER
1	A	801	GLU
1	A	839	ARG
1	A	867	ILE
1	A	878	ILE
1	A	894	GLU
1	A	896	ARG
1	A	905	ASP

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Mol	Chain	Res	Type
1	A	907	THR
1	A	908	LEU
1	A	917	SER
1	A	927	VAL
1	A	931	GLU
1	A	968	GLN
1	A	969	GLN
1	A	973	ILE
1	A	982	THR
1	A	999	VAL
1	A	1006	ILE
1	A	1029	ARG
1	A	1033	GLN
1	A	1046	LEU
1	A	1048	ASN
1	A	1067	LEU
1	A	1081	LEU
1	A	1084	PHE
1	A	1095	THR
1	A	1109	LYS
1	A	1110	ASN
1	A	1113	THR
1	A	1129	GLU
1	A	1170	ILE
1	A	1172	LEU
1	A	1176	LEU
1	A	1195	LEU
1	A	1221	LYS
1	A	1223	ASP
1	A	1229	SER
1	A	1230	GLU
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1291	VAL
1	A	1295	THR
1	A	1325	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1350	LYS
1	A	1355	VAL
1	A	1366	ARG

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Mol	Chain	Res	Type
1	A	1376	THR
1	A	1378	GLN
1	A	1385	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1406	VAL
1	A	1424	VAL
1	A	1425	SER
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1445	ILE
2	B	25	ILE
2	B	28	GLU
2	B	46	GLN
2	B	63	ILE
2	B	65	GLU
2	B	70	ILE
2	B	89	GLU
2	B	94	LYS
2	B	101	MET
2	B	102	VAL
2	B	105	SER
2	B	108	VAL
2	B	121	ASN
2	B	134	LYS
2	B	135	ARG
2	B	140	ILE
2	B	165	VAL
2	B	175	ARG
2	B	194	GLU
2	B	217	ARG
2	B	218	SER
2	B	223	VAL
2	B	225	VAL
2	B	234	ILE
2	B	240	ILE
2	B	249	ARG
2	B	251	ILE
2	B	254	LEU
2	B	261	ARG

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Mol	Chain	Res	Type
2	B	267	ARG
2	B	272	THR
2	B	276	ILE
2	B	277	LYS
2	B	285	ILE
2	B	299	GLU
2	B	312	GLU
2	B	323	VAL
2	B	325	GLN
2	B	355	ILE
2	B	363	HIS
2	B	365	THR
2	B	371	GLU
2	B	376	PHE
2	B	390	LEU
2	B	393	LYS
2	B	394	ASP
2	B	413	LEU
2	B	416	LEU
2	B	423	LYS
2	B	437	GLU
2	B	448	ILE
2	B	451	LYS
2	B	454	THR
2	B	458	LYS
2	B	461	LEU
2	B	471	LYS
2	B	479	VAL
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	489	SER
2	B	516	ASN
2	B	531	GLN
2	B	537	LYS
2	B	541	LEU
2	B	542	MET
2	B	547	VAL
2	B	549	THR
2	B	567	GLU
2	B	570	VAL
2	B	576	ASP

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Mol	Chain	Res	Type
2	B	578	THR
2	B	579	ARG
2	B	591	ARG
2	B	598	GLU
2	B	604	ARG
2	B	614	SER
2	B	616	ILE
2	B	624	LEU
2	B	626	ILE
2	B	651	LEU
2	B	653	VAL
2	B	660	LYS
2	B	690	VAL
2	B	708	GLU
2	B	710	LEU
2	B	727	LYS
2	B	733	HIS
2	B	743	ILE
2	B	762	ASN
2	B	780	VAL
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	815	ARG
2	B	844	SER
2	B	864	LYS
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	885	MET
2	B	886	LYS
2	B	906	SER
2	B	935	ARG
2	B	944	THR
2	B	953	LEU
2	B	963	PHE
2	B	964	VAL
2	B	976	ILE
2	B	983	ARG
2	B	996	ARG
2	B	997	GLU
2	B	999	MET

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Mol	Chain	Res	Type
2	B	1002	THR
2	B	1007	VAL
2	B	1010	LEU
2	B	1052	VAL
2	B	1065	GLN
2	B	1077	THR
2	B	1099	VAL
2	B	1102	LYS
2	B	1103	ILE
2	B	1111	MET
2	B	1128	LEU
2	B	1129	ARG
2	B	1132	GLU
2	B	1150	ARG
2	B	1160	VAL
2	B	1168	LEU
2	B	1175	LEU
2	B	1181	GLU
2	B	1189	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1203	LEU
2	B	1210	MET
2	B	1211	ASN
2	B	1216	LEU
3	C	3	GLU
3	C	4	GLU
3	C	8	VAL
3	C	9	LYS
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	56	THR
3	C	57	VAL
3	C	66	ARG
3	C	75	MET
3	C	77	ILE
3	C	80	LEU

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Mol	Chain	Res	Type
3	C	93	ASP
3	C	99	LEU
3	C	106	GLU
3	C	109	SER
3	C	129	ILE
3	C	137	LYS
3	C	149	LYS
3	C	199	LYS
3	C	204	SER
3	C	214	ASN
3	C	215	GLU
3	C	226	ASP
3	C	235	VAL
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	259	LEU
3	C	264	GLN
4	E	30	ILE
4	E	40	GLU
4	E	52	ARG
4	E	54	GLN
4	E	75	MET
4	E	78	LEU
4	E	84	ASP
4	E	92	THR
4	E	94	LYS
4	E	95	THR
4	E	100	ILE
4	E	104	ASN
4	E	106	GLN
4	E	107	THR
4	E	114	ASN
4	E	123	LEU
4	E	127	ILE
4	E	131	THR
4	E	132	ILE
4	E	144	ILE
4	E	149	LEU
4	E	156	LEU
4	E	169	ARG
4	E	178	ILE

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Mol	Chain	Res	Type
4	E	200	ARG
4	E	204	THR
5	F	76	LYS
5	F	82	THR
5	F	87	LYS
5	F	93	ILE
5	F	99	LEU
5	F	118	LEU
6	H	11	GLN
6	H	13	SER
6	H	14	GLU
6	H	15	VAL
6	H	22	LYS
6	H	24	CYS
6	H	26	ILE
6	H	35	GLN
6	H	63	LEU
6	H	83	GLN
6	H	86	ASP
6	H	87	ARG
6	H	88	SER
6	H	91	ASP
6	H	100	THR
6	H	103	LYS
6	H	106	GLU
6	H	109	LYS
6	H	110	ASP
6	H	130	ARG
6	H	132	LEU
6	H	136	LYS
7	I	28	GLU
7	I	35	VAL
7	I	60	GLN
7	I	70	ARG
7	I	77	LYS
7	I	87	GLN
7	I	90	GLN
7	I	94	ASP
7	I	96	SER
7	I	98	VAL
7	I	104	LEU
7	I	111	THR

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Mol	Chain	Res	Type
7	I	119	THR
8	J	1	MET
8	J	3	VAL
8	J	13	VAL
8	J	19	GLU
8	J	22	LEU
8	J	31	ASP
8	J	43	ARG
8	J	48	ARG
8	J	59	LYS
9	K	11	LEU
9	K	16	GLU
9	K	18	LYS
9	K	20	LYS
9	K	21	ILE
9	K	26	LYS
9	K	31	VAL
9	K	33	ILE
9	K	51	LEU
9	K	63	VAL
9	K	74	ARG
9	K	114	LEU
10	L	27	LEU
10	L	38	LEU
10	L	42	ARG
10	L	43	THR
10	L	44	ASP
10	L	47	ARG
10	L	53	HIS
10	L	55	ILE
10	L	58	LYS
10	L	61	THR
10	L	64	LEU
10	L	65	VAL
10	L	66	GLN
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	71	GLN
1	A	118	HIS
1	A	119	ASN
1	A	209	ASN
1	A	256	GLN
1	A	297	GLN
1	A	339	ASN
1	A	503	GLN
1	A	517	ASN
1	A	587	HIS
1	A	603	ASN
1	A	631	HIS
1	A	700	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	760	GLN
1	A	786	HIS
1	A	906	HIS
1	A	926	GLN
1	A	965	GLN
1	A	966	ASN
1	A	969	GLN
1	A	1033	GLN
1	A	1085	HIS
1	A	1110	ASN
1	A	1130	GLN
1	A	1140	HIS
1	A	1211	GLN
1	A	1258	HIS
1	A	1364	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	53	GLN
2	B	103	ASN
2	B	215	GLN
2	B	363	HIS
2	B	395	GLN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS

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Mol	Chain	Res	Type
2	B	587	HIS
2	B	657	HIS
2	B	744	HIS
2	B	762	ASN
2	B	843	GLN
2	B	881	ASN
2	B	958	GLN
2	B	984	HIS
2	B	1015	HIS
2	B	1065	GLN
2	B	1074	ASN
2	B	1084	GLN
2	B	1097	HIS
2	B	1141	HIS
2	B	1161	HIS
2	B	1179	GLN
3	C	17	ASN
3	C	54	ASN
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	151	GLN
3	C	231	ASN
3	C	242	GLN
3	C	267	GLN
4	E	5	ASN
4	E	8	ASN
4	E	54	GLN
4	E	147	HIS
4	E	179	GLN
6	H	128	ASN
6	H	131	ASN
7	I	60	GLN
7	I	89	GLN
8	J	64	ASN
9	K	65	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	3/4 (75%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1405/1733 (81%)	0.14	40 (2%) 55 32	63, 111, 202, 234	0
2	B	1114/1224 (91%)	0.06	31 (2%) 55 32	62, 96, 166, 219	0
3	C	266/318 (83%)	-0.13	0 100 100	67, 94, 132, 186	0
4	E	214/215 (99%)	0.08	0 100 100	81, 139, 193, 210	0
5	F	85/155 (54%)	-0.07	0 100 100	81, 115, 159, 172	0
6	H	133/146 (91%)	0.31	3 (2%) 61 38	109, 151, 177, 187	0
7	I	119/122 (97%)	0.12	3 (2%) 58 35	78, 114, 150, 167	0
8	J	65/70 (92%)	-0.24	1 (1%) 72 49	65, 83, 114, 130	0
9	K	114/120 (95%)	-0.18	1 (0%) 81 61	66, 102, 126, 149	0
10	L	46/70 (65%)	0.74	6 (13%) 7 4	82, 119, 152, 176	0
11	R	4/4 (100%)	0.60	0 100 100	210, 216, 218, 219	0
12	T	8/29 (27%)	1.33	2 (25%) 2 1	200, 204, 210, 211	0
All	All	3573/4206 (84%)	0.09	87 (2%) 59 36	62, 106, 192, 234	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1087	ALA	6.1
2	B	715	ALA	5.9
2	B	335	GLY	4.9
10	L	27	LEU	4.8
7	I	104	LEU	4.6
1	A	1090	ALA	4.6
1	A	1081	LEU	4.5
2	B	1214	PRO	4.4
1	A	179	LEU	4.3
2	B	883	LEU	4.1
1	A	250	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	65	LEU	4.0
1	A	289	ILE	3.9
2	B	446	LEU	3.9
6	H	63	LEU	3.9
6	H	85	GLY	3.8
2	B	502	ILE	3.6
2	B	882	THR	3.6
1	A	1091	SER	3.5
2	B	1204	PHE	3.5
2	B	708	GLU	3.4
10	L	26	THR	3.4
1	A	86	LEU	3.3
2	B	477	ALA	3.3
1	A	1002	GLY	3.2
1	A	1083	THR	3.2
1	A	1088	GLY	3.1
1	A	1108	ALA	3.1
9	K	114	LEU	3.1
10	L	25	ALA	3.0
2	B	246	LYS	2.9
1	A	323	LYS	2.8
1	A	1089	VAL	2.8
1	A	1086	PHE	2.8
1	A	181	LEU	2.8
1	A	79	GLY	2.7
12	T	19	DT	2.7
2	B	709	ASP	2.7
1	A	30	ILE	2.7
2	B	70	ILE	2.7
1	A	141	LEU	2.7
1	A	318	SER	2.6
1	A	53	LEU	2.6
1	A	567	LYS	2.5
1	A	113	LEU	2.5
2	B	976	ILE	2.5
2	B	647	GLY	2.4
10	L	55	ILE	2.4
8	J	65	PRO	2.4
2	B	881	ASN	2.4
2	B	345	LYS	2.4
1	A	182	VAL	2.4
1	A	177	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	712	PRO	2.3
1	A	1082	ASN	2.3
10	L	50	ASP	2.3
1	A	201	VAL	2.3
1	A	322	VAL	2.3
1	A	244	PRO	2.2
1	A	279	LEU	2.2
2	B	865	LYS	2.2
1	A	214	ILE	2.2
2	B	140	ILE	2.2
1	A	1084	PHE	2.2
2	B	448	ILE	2.2
1	A	998	LEU	2.2
7	I	2	THR	2.2
1	A	1445	ILE	2.2
7	I	82	GLU	2.2
6	H	62	SER	2.1
2	B	733	HIS	2.1
2	B	887	HIS	2.1
2	B	878	GLN	2.1
1	A	78	PRO	2.1
2	B	786	ASN	2.1
2	B	711	GLU	2.1
1	A	91	PHE	2.1
1	A	249	SER	2.1
2	B	1170	THR	2.1
2	B	1107	ALA	2.1
2	B	277	LYS	2.0
10	L	40	LEU	2.0
1	A	338	GLY	2.0
2	B	1203	LEU	2.0
12	T	22	DT	2.0
2	B	137	TYR	2.0
1	A	1257	ASP	2.0

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

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

6.3 Carbohydrates [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	0.86	0.08	300,300,300,300	0
13	ZN	B	1307	1/1	0.89	0.08	206,206,206,206	0
13	ZN	A	1735	1/1	0.97	0.05	177,177,177,177	0
13	ZN	C	319	1/1	0.99	0.02	79,79,79,79	0
13	ZN	I	203	1/1	0.99	0.03	113,113,113,113	0
13	ZN	L	105	1/1	0.99	0.02	111,111,111,111	0
13	ZN	J	101	1/1	1.00	0.03	88,88,88,88	0
13	ZN	I	204	1/1	1.00	0.02	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.