



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:53 AM UTC

PDB ID : 3S1M / pdb_00003s1m
Title : RNA Polymerase II Initiation Complex with a 5-nt RNA (variant 1)
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-15
Resolution : 3.13 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

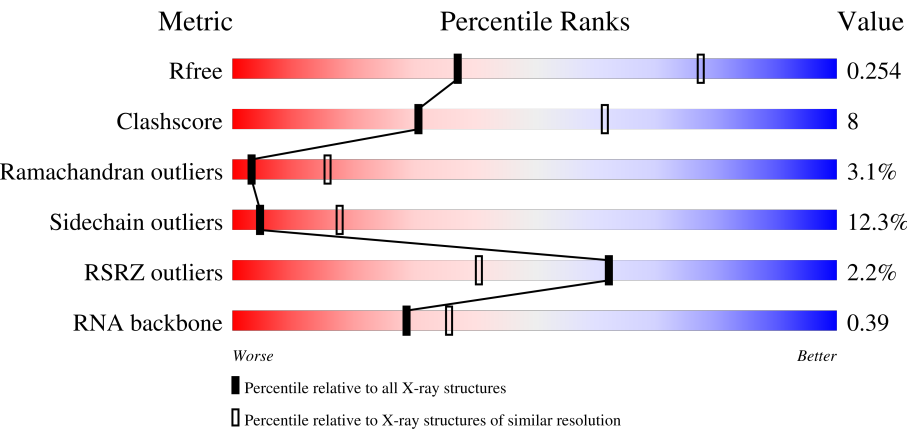
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)
RNA backbone	3983	1040 (3.38-2.90)

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% 57%19%19%
2	B	1224	2% 60%25%6%9%
3	C	318	% 56%22%5%16%
4	E	215	% 75%22%

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Mol	Chain	Length	Quality of chain
5	F	155	45%10%45%
6	H	146	5% 58%26%7%9%
7	I	122	2% 70%20%7%
8	J	70	% 57%27%7%7%
9	K	120	% 68%20%7%5%
10	L	70	9% 27%30%9%34%
11	R	5	80%20%
12	T	29	28%72%

2 Entry composition

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*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	5	Total	C	N	O	P	0	0	0
			107	49	23	31	4			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*GP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	8	Total	C	N	O	P	0	0	0
			162	77	28	49	8			

- Molecule 13 is ZINC ION (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

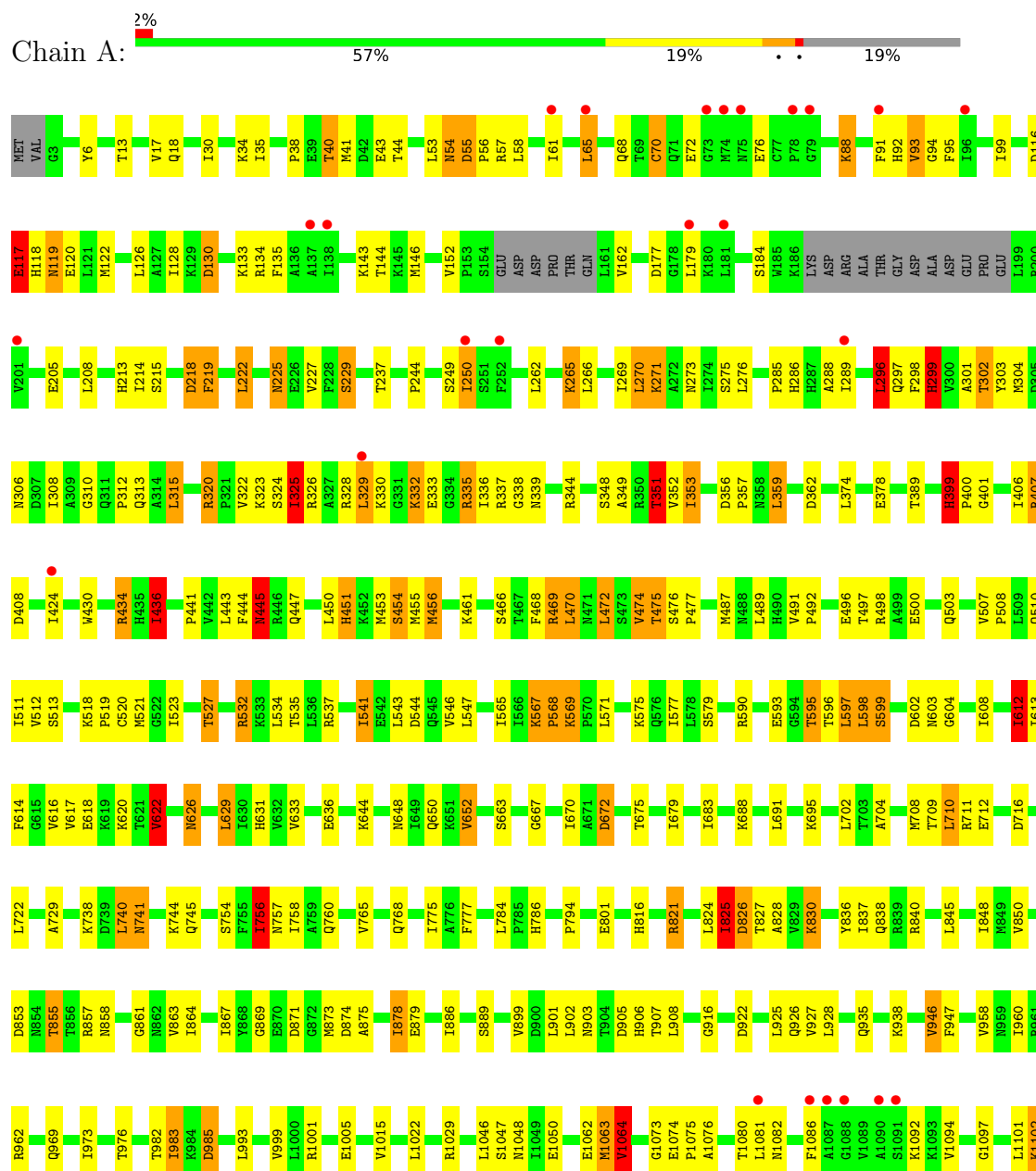
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

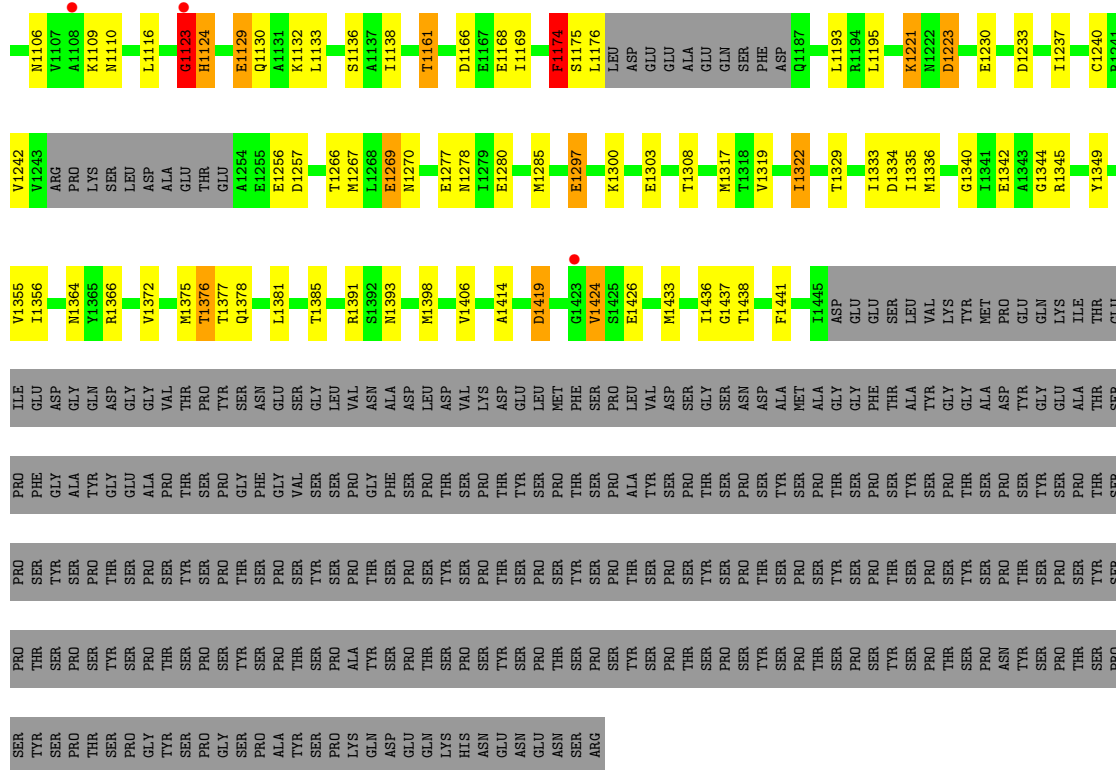
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

3 Residue-property plots [i](#)

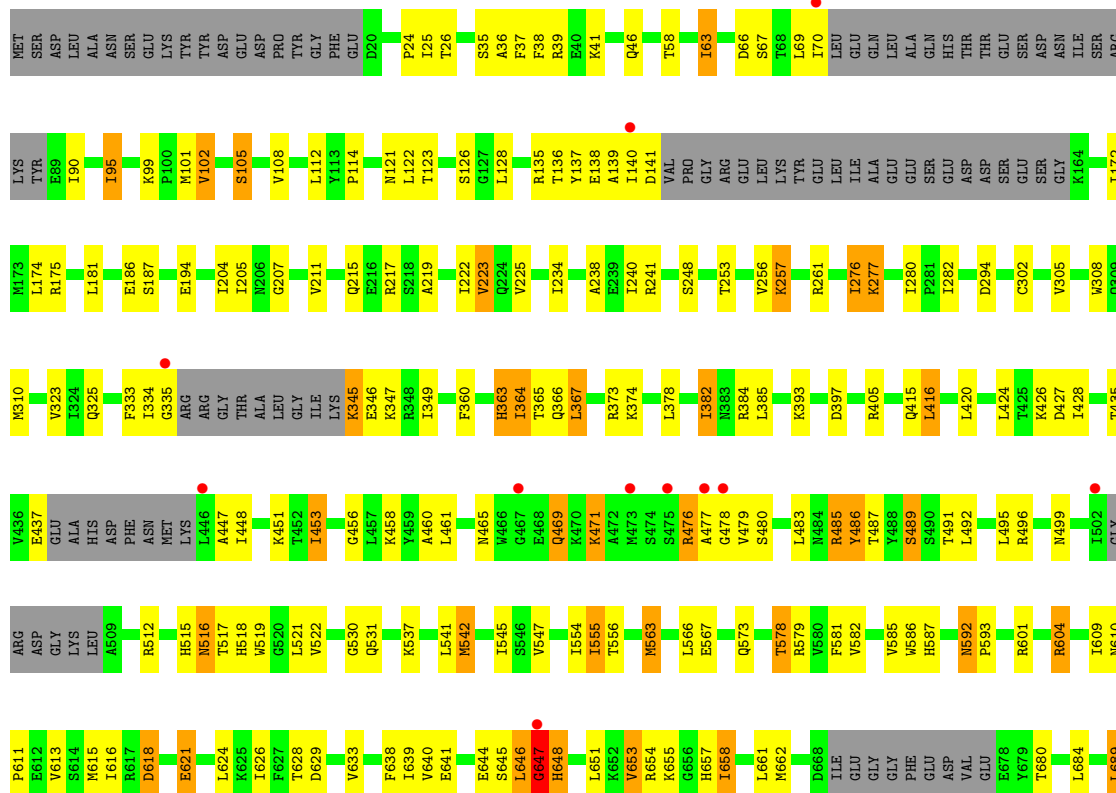
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

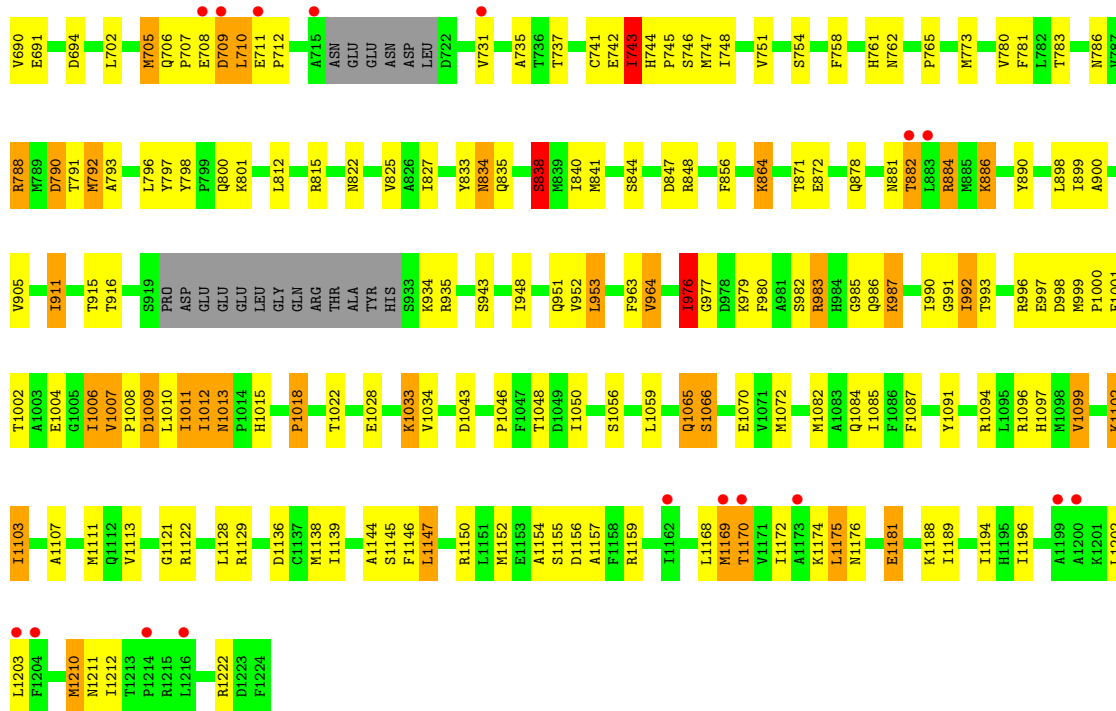
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



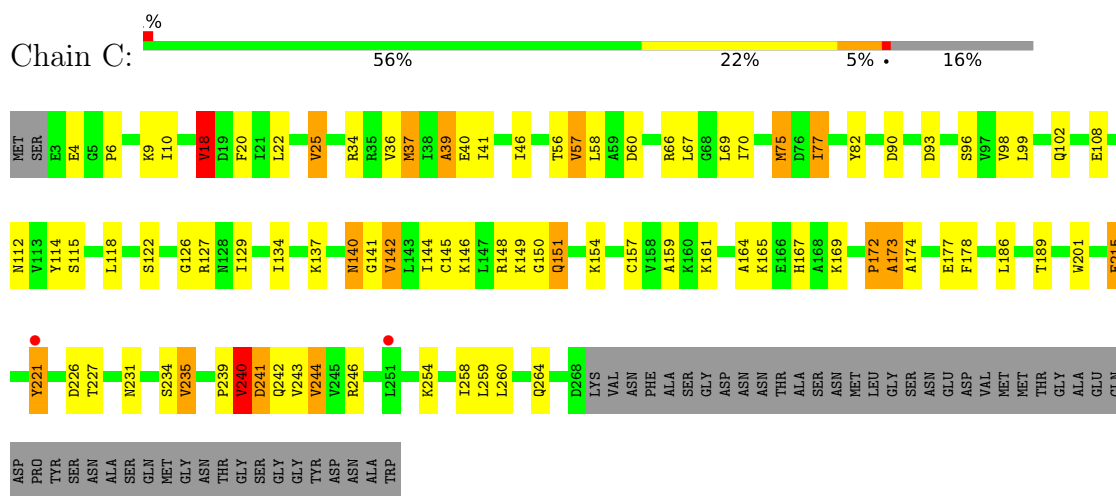


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

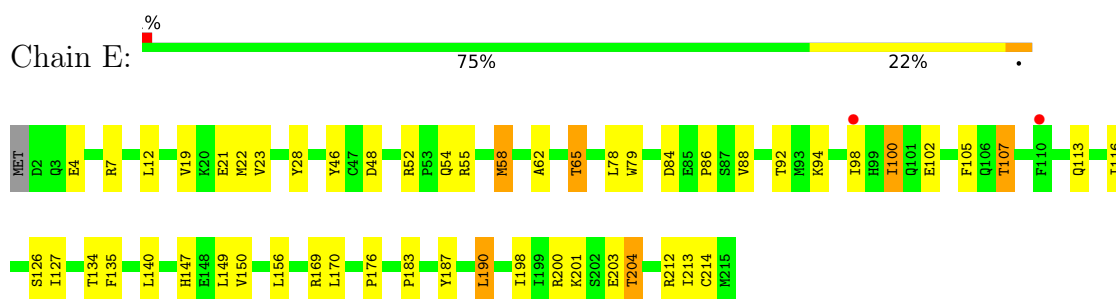




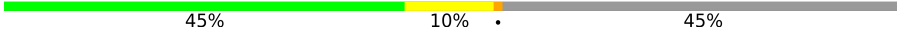
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

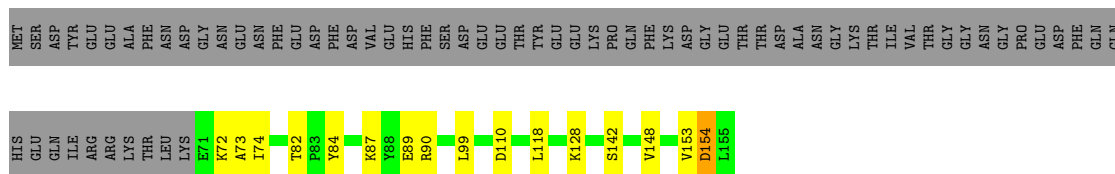


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



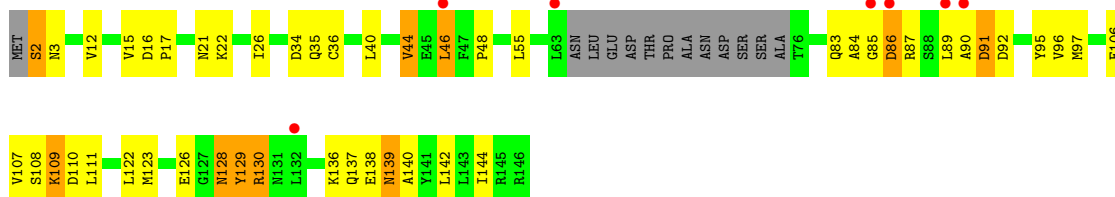
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



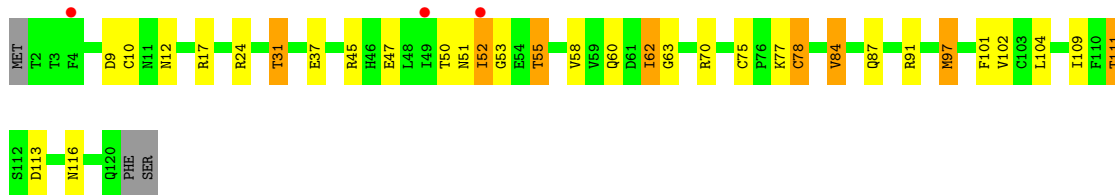
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



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

Chain I: 



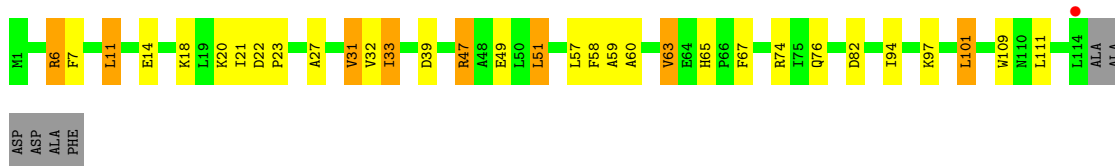
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 



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

Chain K: 

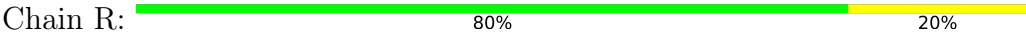


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

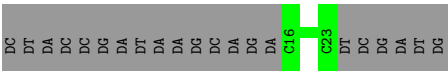
Chain L: 



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.92Å 220.71Å 191.77Å 90.00° 97.48° 90.00°	Depositor
Resolution (Å)	47.72 – 3.13 47.72 – 3.13	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.72-3.13) 99.1 (47.72-3.13)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 3.12Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.183 , 0.233 0.205 , 0.254	Depositor DCC
R_{free} test set	5668 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 101.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28570	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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	0.83	3/11241 (0.0%)	1.47	80/15199 (0.5%)
2	B	0.84	3/9033 (0.0%)	1.44	76/12181 (0.6%)
3	C	0.79	0/2133	1.44	21/2891 (0.7%)
4	E	0.78	0/1788	1.40	11/2406 (0.5%)
5	F	0.77	0/700	1.37	5/945 (0.5%)
6	H	0.76	0/1086	1.32	12/1470 (0.8%)
7	I	0.80	0/989	1.47	10/1331 (0.8%)
8	J	0.83	0/541	1.60	6/727 (0.8%)
9	K	0.74	0/937	1.38	5/1265 (0.4%)
10	L	0.90	0/365	1.51	8/485 (1.6%)
11	R	0.59	0/120	0.90	0/186
12	T	0.48	0/180	1.16	0/275
All	All	0.82	6/29113 (0.0%)	1.44	234/39361 (0.6%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	705	MET	SD-CE	-6.78	1.62	1.79
2	B	563	MET	SD-CE	-6.03	1.64	1.79
1	A	756	ILE	CG1-CD1	5.90	1.74	1.51
1	A	249	SER	CA-C	5.51	1.55	1.52
2	B	542	MET	SD-CE	-5.14	1.66	1.79
1	A	456	MET	SD-CE	-5.02	1.67	1.79

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	ASP	CA-C-N	9.65	139.08	121.70
1	A	218	ASP	C-N-CA	9.65	139.08	121.70
2	B	37	PHE	N-CA-C	-9.10	99.22	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	39	ALA	N-CA-C	8.79	124.10	113.12
1	A	1097	GLY	CA-C-N	8.49	125.59	120.24
1	A	1097	GLY	C-N-CA	8.49	125.59	120.24
8	J	5	VAL	N-CA-C	-8.47	97.70	109.21
8	J	64	ASN	N-CA-C	8.02	124.35	113.77
1	A	445	ASN	CA-CB-CG	7.97	120.57	112.60
2	B	363	HIS	N-CA-C	-7.95	99.28	110.50
1	A	1375	MET	CA-C-N	7.68	131.19	120.29
1	A	1375	MET	C-N-CA	7.68	131.19	120.29
10	L	62	LYS	N-CA-C	-7.62	103.71	113.16
1	A	886	ILE	N-CA-C	7.34	117.47	110.42
2	B	140	ILE	CA-C-N	7.21	134.68	121.70
2	B	140	ILE	C-N-CA	7.21	134.68	121.70
1	A	827	THR	N-CA-C	-7.09	103.48	111.14
7	I	31	THR	N-CA-C	-7.08	104.77	113.41
6	H	91	ASP	N-CA-C	7.08	120.44	107.99
2	B	882	THR	N-CA-C	7.04	119.61	111.02
6	H	2	SER	CA-C-N	7.04	134.37	121.70
6	H	2	SER	C-N-CA	7.04	134.37	121.70
6	H	138	GLU	N-CA-C	-6.99	104.01	112.54
1	A	1082	ASN	N-CA-C	-6.93	104.97	113.50
1	A	1174	PHE	CA-CB-CG	6.90	120.70	113.80
2	B	99	LYS	N-CA-C	-6.89	101.13	110.36
1	A	466	SER	N-CA-C	6.85	121.47	113.18
3	C	240	VAL	N-CA-C	6.83	116.98	110.42
1	A	474	VAL	CA-C-N	6.83	129.31	120.44
1	A	474	VAL	C-N-CA	6.83	129.31	120.44
1	A	1063	MET	CA-C-N	6.82	134.25	121.97
1	A	1063	MET	C-N-CA	6.82	134.25	121.97
1	A	947	PHE	CA-C-N	6.80	129.37	120.60
1	A	947	PHE	C-N-CA	6.80	129.37	120.60
7	I	78	CYS	CA-C-N	-6.79	112.47	122.86
7	I	78	CYS	C-N-CA	-6.79	112.47	122.86
1	A	296	LEU	N-CA-C	-6.79	105.56	114.31
3	C	145	CYS	N-CA-C	6.78	117.19	108.24
1	A	117	GLU	CA-C-N	6.78	133.89	121.70
1	A	117	GLU	C-N-CA	6.78	133.89	121.70
2	B	647	GLY	CA-C-N	6.76	133.87	121.70
2	B	647	GLY	C-N-CA	6.76	133.87	121.70
2	B	1018	PRO	CA-C-N	6.74	129.61	120.38
2	B	1018	PRO	C-N-CA	6.74	129.61	120.38
2	B	541	LEU	N-CA-C	6.68	119.13	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	PHE	CA-C-N	6.67	133.70	121.70
1	A	298	PHE	C-N-CA	6.67	133.70	121.70
9	K	39	ASP	CA-CB-CG	6.66	119.26	112.60
2	B	1007	VAL	CB-CA-C	6.64	115.84	109.33
6	H	92	ASP	N-CA-C	-6.63	102.41	111.56
1	A	906	HIS	N-CA-C	6.58	120.30	112.93
1	A	532	ARG	CA-C-N	6.55	129.06	120.28
1	A	532	ARG	C-N-CA	6.55	129.06	120.28
1	A	603	ASN	CA-CB-CG	6.49	119.09	112.60
2	B	66	ASP	CA-C-N	6.48	129.28	120.54
2	B	66	ASP	C-N-CA	6.48	129.28	120.54
1	A	622	VAL	CB-CA-C	6.46	118.04	110.93
9	K	63	VAL	CB-CA-C	6.45	119.08	111.59
1	A	1123	GLY	CA-C-N	6.37	133.16	121.70
1	A	1123	GLY	C-N-CA	6.37	133.16	121.70
2	B	1028	GLU	CB-CG-CD	6.33	123.37	112.60
1	A	351	THR	CA-C-N	6.33	129.22	120.49
1	A	351	THR	C-N-CA	6.33	129.22	120.49
2	B	345	LYS	CA-C-N	6.31	133.06	121.70
2	B	345	LYS	C-N-CA	6.31	133.06	121.70
1	A	794	PRO	CA-C-N	6.29	128.71	120.28
1	A	794	PRO	C-N-CA	6.29	128.71	120.28
2	B	415	GLN	CA-C-N	6.29	128.62	120.44
2	B	415	GLN	C-N-CA	6.29	128.62	120.44
4	E	150	VAL	N-CA-C	6.28	113.28	107.56
2	B	886	LYS	CA-C-N	6.25	132.96	121.70
2	B	886	LYS	C-N-CA	6.25	132.96	121.70
1	A	716	ASP	CA-CB-CG	6.23	118.83	112.60
8	J	19	GLU	CA-C-N	6.14	128.42	120.44
8	J	19	GLU	C-N-CA	6.14	128.42	120.44
1	A	612	ILE	N-CA-CB	6.13	118.02	111.46
4	E	21	GLU	CA-C-N	6.13	128.74	120.65
4	E	21	GLU	C-N-CA	6.13	128.74	120.65
1	A	946	VAL	N-CA-C	-6.12	105.17	110.74
9	K	63	VAL	N-CA-CB	6.11	119.55	112.40
2	B	618	ASP	CA-C-N	6.10	128.76	120.77
2	B	618	ASP	C-N-CA	6.10	128.76	120.77
1	A	116	ASP	CA-C-N	6.09	132.66	121.70
1	A	116	ASP	C-N-CA	6.09	132.66	121.70
2	B	1121	GLY	CA-C-N	6.08	128.43	120.28
2	B	1121	GLY	C-N-CA	6.08	128.43	120.28
2	B	1113	VAL	N-CA-C	6.07	116.19	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	PRO	N-CA-C	6.04	118.07	110.70
2	B	825	VAL	N-CA-C	6.04	116.56	108.11
7	I	78	CYS	N-CA-C	-6.03	101.85	110.59
2	B	366	GLN	N-CA-C	-6.01	105.91	113.72
3	C	172	PRO	CA-C-N	6.00	132.99	121.54
3	C	172	PRO	C-N-CA	6.00	132.99	121.54
2	B	397	ASP	CA-CB-CG	5.95	118.55	112.60
6	H	128	ASN	CA-C-N	5.93	129.72	120.82
6	H	128	ASN	C-N-CA	5.93	129.72	120.82
1	A	825	ILE	N-CA-CB	5.91	116.82	110.62
2	B	1009	ASP	N-CA-C	-5.88	106.11	113.28
2	B	834	ASN	CA-CB-CG	5.83	118.43	112.60
6	H	84	ALA	CA-C-N	5.83	126.56	120.03
6	H	84	ALA	C-N-CA	5.83	126.56	120.03
9	K	82	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	468	PHE	CA-CB-CG	5.81	119.61	113.80
5	F	154	ASP	CA-CB-CG	5.79	118.39	112.60
8	J	60	PHE	CA-CB-CG	5.79	119.59	113.80
3	C	82	TYR	N-CA-C	-5.78	100.58	109.76
4	E	58	MET	N-CA-C	5.77	117.37	111.14
2	B	280	ILE	N-CA-C	5.76	114.22	107.77
2	B	1011	ILE	N-CA-CB	5.72	119.10	111.90
2	B	427	ASP	CA-CB-CG	5.71	118.31	112.60
3	C	40	GLU	N-CA-C	5.70	120.94	113.30
6	H	16	ASP	CA-CB-CG	5.70	118.30	112.60
2	B	609	ILE	N-CA-C	-5.69	100.29	108.48
2	B	709	ASP	CA-CB-CG	5.68	118.28	112.60
4	E	46	TYR	N-CA-C	5.68	119.91	112.92
6	H	139	ASN	CA-CB-CG	5.65	118.25	112.60
2	B	1065	GLN	CB-CA-C	5.65	118.30	110.16
3	C	60	ASP	CA-CB-CG	5.64	118.24	112.60
4	E	203	GLU	CA-C-N	5.64	131.16	122.42
4	E	203	GLU	C-N-CA	5.64	131.16	122.42
1	A	237	THR	N-CA-C	-5.63	106.76	113.97
3	C	150	GLY	CA-C-N	5.63	128.76	120.82
3	C	150	GLY	C-N-CA	5.63	128.76	120.82
1	A	758	ILE	CA-C-N	5.62	128.60	120.79
1	A	758	ILE	C-N-CA	5.62	128.60	120.79
10	L	40	LEU	CA-C-N	5.62	128.74	120.82
10	L	40	LEU	C-N-CA	5.62	128.74	120.82
1	A	622	VAL	N-CA-CB	-5.61	105.07	112.36
7	I	52	ILE	N-CA-C	5.60	116.80	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	ASP	N-CA-C	-5.60	103.72	111.28
2	B	581	PHE	CA-CB-CG	5.60	119.40	113.80
2	B	838	SER	N-CA-C	-5.59	101.93	110.14
4	E	48	ASP	CA-CB-CG	5.57	118.17	112.60
2	B	890	TYR	CA-C-N	5.54	129.46	120.60
2	B	890	TYR	C-N-CA	5.54	129.46	120.60
7	I	97	MET	CA-C-N	5.51	128.10	120.49
7	I	97	MET	C-N-CA	5.51	128.10	120.49
1	A	983	ILE	N-CA-C	-5.50	105.00	110.62
1	A	1269	GLU	N-CA-C	5.49	118.45	111.69
1	A	1335	ILE	CA-C-N	5.49	127.58	120.44
1	A	1335	ILE	C-N-CA	5.49	127.58	120.44
4	E	113	GLN	N-CA-C	5.48	118.09	111.40
2	B	136	THR	CB-CA-C	5.47	118.46	111.40
2	B	629	ASP	CA-CB-CG	5.47	118.07	112.60
2	B	711	GLU	N-CA-C	5.47	121.90	109.81
2	B	476	ARG	CA-C-N	5.47	131.99	121.54
2	B	476	ARG	C-N-CA	5.47	131.99	121.54
1	A	544	ASP	CA-C-N	5.46	127.87	120.44
1	A	544	ASP	C-N-CA	5.46	127.87	120.44
1	A	708	MET	N-CA-C	5.45	117.47	109.24
1	A	622	VAL	N-CA-C	5.44	118.38	113.10
9	K	27	ALA	N-CA-C	5.41	116.98	108.55
3	C	241	ASP	CA-CB-CG	5.40	118.00	112.60
10	L	65	VAL	N-CA-C	5.39	115.66	108.11
6	H	16	ASP	N-CA-C	5.37	118.11	109.15
1	A	777	PHE	CA-CB-CG	5.36	119.16	113.80
2	B	469	GLN	CA-C-N	5.33	127.95	120.28
2	B	469	GLN	C-N-CA	5.33	127.95	120.28
2	B	1152	MET	CA-C-N	5.32	127.72	120.54
2	B	1152	MET	C-N-CA	5.32	127.72	120.54
2	B	1154	ALA	N-CA-C	-5.29	100.67	109.46
2	B	1122	ARG	CA-C-N	5.29	127.89	120.28
2	B	1122	ARG	C-N-CA	5.29	127.89	120.28
1	A	436	ILE	CB-CA-C	5.28	118.41	111.33
2	B	694	ASP	CA-CB-CG	5.28	117.88	112.60
7	I	53	GLY	CA-C-N	5.28	127.62	120.65
7	I	53	GLY	C-N-CA	5.28	127.62	120.65
2	B	1144	ALA	N-CA-C	5.27	116.71	111.07
1	A	985	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	612	ILE	CB-CA-C	5.26	117.08	111.35
1	A	1424	VAL	CA-C-N	5.25	128.04	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1424	VAL	C-N-CA	5.25	128.04	120.38
5	F	87	LYS	CA-C-N	5.24	127.73	120.29
5	F	87	LYS	C-N-CA	5.24	127.73	120.29
1	A	249	SER	N-CA-C	5.22	116.42	108.12
1	A	1233	ASP	CA-C-N	5.22	127.59	120.54
1	A	1233	ASP	C-N-CA	5.22	127.59	120.54
2	B	790	ASP	N-CA-C	5.22	117.91	109.40
2	B	276	ILE	CA-C-N	5.22	127.22	120.44
2	B	276	ILE	C-N-CA	5.22	127.22	120.44
3	C	173	ALA	CA-C-N	5.21	131.48	121.54
3	C	173	ALA	C-N-CA	5.21	131.48	121.54
8	J	9	SER	N-CA-C	5.19	116.75	111.14
3	C	258	ILE	CA-C-N	5.19	127.49	120.38
3	C	258	ILE	C-N-CA	5.19	127.49	120.38
10	L	59	ALA	CA-C-N	5.19	131.45	121.54
10	L	59	ALA	C-N-CA	5.19	131.45	121.54
5	F	148	VAL	CA-C-N	5.18	127.22	120.28
5	F	148	VAL	C-N-CA	5.18	127.22	120.28
1	A	134	ARG	CA-C-N	5.18	127.22	120.28
1	A	134	ARG	C-N-CA	5.18	127.22	120.28
1	A	1161	THR	CB-CA-C	5.18	118.28	109.53
2	B	486	TYR	N-CA-C	5.17	117.00	111.36
3	C	56	THR	CA-C-N	5.16	128.62	120.47
3	C	56	THR	C-N-CA	5.16	128.62	120.47
2	B	976	ILE	N-CA-C	5.15	115.76	110.36
7	I	116	ASN	CA-CB-CG	5.14	117.75	112.60
1	A	874	ASP	CA-C-N	5.14	127.42	120.38
1	A	874	ASP	C-N-CA	5.14	127.42	120.38
1	A	229	SER	N-CA-C	5.13	116.68	107.80
2	B	24	PRO	CA-C-N	5.13	128.04	120.91
2	B	24	PRO	C-N-CA	5.13	128.04	120.91
2	B	964	VAL	N-CA-C	5.13	116.11	108.46
3	C	241	ASP	CA-C-N	5.12	127.66	120.28
3	C	241	ASP	C-N-CA	5.12	127.66	120.28
2	B	743	ILE	N-CA-CB	5.12	117.51	110.54
1	A	1419	ASP	CA-C-N	5.12	127.14	120.28
1	A	1419	ASP	C-N-CA	5.12	127.14	120.28
10	L	62	LYS	CA-C-N	5.12	128.79	120.60
10	L	62	LYS	C-N-CA	5.12	128.79	120.60
1	A	537	ARG	CA-C-N	5.11	128.07	120.31
1	A	537	ARG	C-N-CA	5.11	128.07	120.31
1	A	1005	GLU	N-CA-C	5.09	116.83	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1076	ALA	CA-C-N	5.09	127.10	120.28
1	A	1076	ALA	C-N-CA	5.09	127.10	120.28
2	B	680	THR	CA-C-N	5.08	128.04	120.31
2	B	680	THR	C-N-CA	5.08	128.04	120.31
1	A	399	HIS	CA-C-O	-5.07	113.21	120.16
2	B	257	LYS	N-CA-C	5.05	116.62	108.34
2	B	648	HIS	CA-CB-CG	-5.04	108.76	113.80
2	B	186	GLU	CA-C-N	5.03	126.98	120.44
2	B	186	GLU	C-N-CA	5.03	126.98	120.44
1	A	1344	GLY	CA-C-N	5.03	127.32	120.54
1	A	1344	GLY	C-N-CA	5.03	127.32	120.54
2	B	308	TRP	CA-C-N	5.02	127.32	120.54
2	B	308	TRP	C-N-CA	5.02	127.32	120.54
4	E	65	THR	CA-C-N	5.01	127.25	120.38
4	E	65	THR	C-N-CA	5.01	127.25	120.38
2	B	628	THR	CA-C-N	5.01	128.31	120.75
2	B	628	THR	C-N-CA	5.01	128.31	120.75
3	C	96	SER	N-CA-C	5.01	116.68	109.07
3	C	18	VAL	N-CA-CB	5.01	118.15	111.64
2	B	689	LEU	CA-C-N	5.00	130.82	122.57
2	B	689	LEU	C-N-CA	5.00	130.82	122.57

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11043	0	11133	202	0
2	B	8861	0	8884	168	0
3	C	2095	0	2051	47	0
4	E	1752	0	1776	26	0
5	F	688	0	707	6	0
6	H	1068	0	1040	20	0
7	I	971	0	927	14	0
8	J	532	0	542	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	919	0	929	20	0
10	L	363	0	386	11	0
11	R	107	0	56	0	0
12	T	162	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
14	A	1	0	0	0	0
All	All	28570	0	28522	473	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 (473) 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	1.74	1.57
2:B:801:LYS:O	8:J:52:THR:HG23	1.74	0.87
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.58	0.86
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.41	0.85
1:A:567:LYS:HB3	6:H:96:VAL:H	1.44	0.82
1:A:218:ASP:H	1:A:219:PHE:HB3	1.44	0.81
2:B:1002:THR:HG22	2:B:1004:GLU:H	1.45	0.81
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.62	0.80
2:B:345:LYS:HA	2:B:347:LYS:H	1.47	0.78
1:A:855:THR:HG21	1:A:857:ARG:HE	1.46	0.77
3:C:167:HIS:HD2	3:C:169:LYS:H	1.33	0.77
2:B:515:HIS:HD2	2:B:517:THR:H	1.29	0.77
2:B:864:LYS:HB3	2:B:872:GLU:H	1.48	0.77
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.68	0.76
2:B:706:GLN:O	2:B:710:LEU:HB2	1.86	0.75
2:B:1072:MET:HG3	2:B:1085:ILE:HB	1.67	0.75
2:B:1175:LEU:HD23	2:B:1176:ASN:H	1.52	0.75
9:K:65:HIS:HD2	9:K:67:PHE:H	1.33	0.75
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.53	0.74
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.70	0.74
1:A:869:GLY:O	4:E:204:THR:HG21	1.88	0.73
1:A:756:ILE:HD13	1:A:756:ILE:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.70	0.72
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.70	0.72
2:B:486:TYR:OH	2:B:1096:ARG:HB3	1.91	0.71
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.74	0.70
1:A:754:SER:H	1:A:757:ASN:HD22	1.40	0.70
1:A:511:ILE:HA	1:A:521:MET:HE3	1.74	0.69
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.73	0.69
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.76	0.69
2:B:744:HIS:HD2	2:B:746:SER:H	1.39	0.69
6:H:123:MET:HE2	6:H:142:LEU:HD12	1.76	0.68
1:A:596:THR:O	1:A:598:LEU:N	2.27	0.68
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.75	0.68
1:A:567:LYS:O	1:A:569:LYS:N	2.24	0.68
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.58	0.67
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.77	0.67
1:A:567:LYS:HE3	6:H:46:LEU:HD12	1.76	0.66
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.78	0.65
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.28	0.65
1:A:456:MET:HE3	1:A:510:GLN:HB2	1.78	0.65
2:B:486:TYR:CE2	2:B:1096:ARG:HD2	2.32	0.65
1:A:399:HIS:O	1:A:401:GLY:N	2.30	0.65
1:A:299:HIS:HA	1:A:302:THR:HG22	1.78	0.65
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.79	0.64
2:B:604:ARG:HD3	2:B:611:PRO:HA	1.78	0.64
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.80	0.64
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.79	0.64
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.13	0.64
2:B:654:ARG:H	2:B:657:HIS:HD2	1.44	0.64
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.78	0.64
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.44	0.64
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.80	0.64
1:A:472:LEU:O	1:A:475:THR:HB	1.98	0.64
2:B:241:ARG:HA	2:B:253:THR:HG22	1.80	0.63
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.80	0.63
3:C:98:VAL:H	3:C:122:SER:HB2	1.64	0.63
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.80	0.63
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.81	0.63
2:B:1034:VAL:HG22	2:B:1059:LEU:HB2	1.80	0.62
3:C:221:TYR:HB3	6:H:46:LEU:HD22	1.81	0.62
1:A:441:PRO:HG2	1:A:498:ARG:HB2	1.82	0.62
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:HA	1:A:907:THR:HG23	1.83	0.61
1:A:907:THR:HG22	1:A:908:LEU:H	1.66	0.61
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.34	0.61
2:B:835:GLN:O	2:B:838:SER:HB2	2.00	0.61
1:A:503:GLN:NE2	5:F:90:ARG:HH22	1.99	0.60
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.84	0.60
2:B:651:LEU:HD21	2:B:741:CYS:HB3	1.82	0.60
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.84	0.60
4:E:22:MET:HE2	4:E:187:TYR:HA	1.84	0.60
3:C:235:VAL:HG22	8:J:13:VAL:HG23	1.84	0.59
1:A:863:VAL:HG23	4:E:170:LEU:HD21	1.83	0.59
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.82	0.59
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.83	0.59
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.84	0.59
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.84	0.58
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.85	0.58
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.31	0.58
2:B:363:HIS:O	2:B:364:ILE:HB	2.03	0.58
2:B:542:MET:HE3	2:B:747:MET:HG3	1.85	0.58
1:A:91:PHE:HE1	1:A:99:ILE:HG21	1.67	0.58
2:B:563:MET:HE1	2:B:587:HIS:HB2	1.85	0.58
9:K:32:VAL:HG22	9:K:74:ARG:HG3	1.85	0.58
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.86	0.58
7:I:111:THR:HG23	7:I:113:ASP:H	1.68	0.58
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	1.86	0.57
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.34	0.57
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.86	0.57
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.86	0.57
2:B:705:MET:H	2:B:710:LEU:HG	1.69	0.57
3:C:46:ILE:HA	3:C:159:ALA:HA	1.87	0.57
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.86	0.57
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.04	0.57
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.87	0.57
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.86	0.57
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.87	0.57
1:A:1377:THR:HG22	4:E:176:PRO:HB3	1.87	0.57
9:K:7:PHE:O	9:K:11:LEU:HB2	2.05	0.57
6:H:2:SER:HB3	6:H:3:ASN:HB2	1.87	0.56
1:A:667:GLY:HA2	1:A:670:ILE:HG12	1.86	0.56
3:C:75:MET:HE2	3:C:239:PRO:HG2	1.87	0.56
10:L:27:LEU:HD23	10:L:37:LYS:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:SER:HB3	1:A:520:CYS:HB3	1.88	0.56
1:A:1086:PHE:HB3	1:A:1092:LYS:HB3	1.86	0.56
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.88	0.56
2:B:223:VAL:HG13	2:B:384:ARG:HH21	1.71	0.56
1:A:527:THR:HG21	1:A:650:GLN:HA	1.88	0.56
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.88	0.56
6:H:44:VAL:HG12	6:H:48:PRO:HA	1.87	0.56
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.39	0.56
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.88	0.55
1:A:848:ILE:HD12	1:A:864:ILE:HG13	1.87	0.55
1:A:541:ILE:HD11	1:A:577:ILE:HG12	1.88	0.55
3:C:165:LYS:O	9:K:6:ARG:NH1	2.39	0.55
1:A:741:ASN:HB3	1:A:744:LYS:HB2	1.88	0.55
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.89	0.55
2:B:277:LYS:NZ	2:B:335:GLY:H	2.04	0.55
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.70	0.55
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.89	0.55
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.07	0.55
2:B:1082:MET:HA	3:C:189:THR:HA	1.88	0.55
1:A:535:THR:HG21	1:A:617:VAL:H	1.70	0.55
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.41	0.55
1:A:315:LEU:HA	1:A:320:ARG:HB3	1.89	0.55
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.42	0.55
1:A:273:ASN:HA	1:A:296:LEU:HD11	1.88	0.55
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.22	0.54
2:B:38:PHE:H	2:B:41:LYS:HB2	1.72	0.54
2:B:346:GLU:HA	2:B:349:ILE:HD12	1.89	0.54
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.89	0.54
2:B:492:LEU:O	2:B:496:ARG:HG3	2.08	0.54
2:B:916:THR:HG23	2:B:935:ARG:HB3	1.88	0.54
2:B:979:LYS:HE3	2:B:987:LYS:HB2	1.88	0.54
10:L:47:ARG:HG3	10:L:52:GLY:HA2	1.90	0.54
1:A:756:ILE:CD1	1:A:756:ILE:H	2.21	0.54
2:B:983:ARG:HH11	2:B:983:ARG:HB2	1.73	0.54
1:A:225:ASN:HD22	1:A:227:VAL:H	1.56	0.54
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.42	0.54
3:C:37:MET:HE2	3:C:244:VAL:HA	1.90	0.54
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.90	0.53
8:J:1:MET:H2	8:J:57:ILE:H	1.56	0.53
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.90	0.53
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.91	0.53
9:K:57:LEU:HB2	9:K:76:GLN:HG2	1.90	0.53
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.43	0.53
2:B:515:HIS:CD2	2:B:517:THR:H	2.19	0.53
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.73	0.53
2:B:864:LYS:H	2:B:872:GLU:HB2	1.73	0.53
3:C:142:VAL:H	8:J:16:ASP:HB3	1.74	0.53
1:A:6:TYR:O	2:B:1175:LEU:HD21	2.08	0.53
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.72	0.53
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.91	0.53
3:C:37:MET:HG2	3:C:243:VAL:HG12	1.91	0.53
1:A:629:LEU:O	1:A:633:VAL:HG23	2.09	0.52
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.90	0.52
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.89	0.52
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.90	0.52
3:C:148:ARG:HB3	3:C:151:GLN:HG3	1.91	0.52
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.92	0.52
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.43	0.52
1:A:982:THR:HB	1:A:985:ASP:H	1.74	0.52
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.74	0.52
2:B:516:ASN:H	2:B:516:ASN:HD22	1.57	0.52
4:E:190:LEU:HD23	4:E:214:CYS:HB2	1.91	0.52
1:A:265:LYS:HD3	1:A:322:VAL:HG21	1.92	0.52
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.75	0.52
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.56	0.52
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.92	0.52
2:B:1048:THR:OG1	2:B:1050:ILE:HD12	2.10	0.52
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.91	0.52
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.91	0.52
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.50	0.52
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.92	0.52
2:B:578:THR:HB	2:B:593:PRO:HG3	1.91	0.52
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.08	0.52
1:A:1342:GLU:HG3	4:E:198:ILE:HG21	1.92	0.51
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.40	0.51
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.91	0.51
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.92	0.51
2:B:915:THR:HG21	2:B:934:LYS:HD2	1.93	0.51
2:B:999:MET:HE3	2:B:999:MET:HA	1.92	0.51
7:I:50:THR:HG22	7:I:52:ILE:H	1.76	0.51
10:L:61:THR:HB	10:L:63:ARG:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:834:ASN:HA	2:B:838:SER:HB3	1.92	0.51
6:H:2:SER:CB	6:H:3:ASN:HB2	2.41	0.51
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.92	0.51
1:A:925:LEU:HD23	1:A:983:ILE:HB	1.92	0.51
1:A:648:ASN:O	1:A:652:VAL:HG23	2.11	0.51
2:B:882:THR:HB	2:B:934:LYS:O	2.10	0.51
9:K:58:PHE:HE2	9:K:74:ARG:HB3	1.76	0.51
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.91	0.51
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.93	0.51
2:B:424:LEU:O	2:B:428:ILE:HG12	2.10	0.50
1:A:469:ARG:NH2	2:B:991:GLY:O	2.37	0.50
1:A:571:LEU:HD22	6:H:46:LEU:HD11	1.94	0.50
2:B:36:ALA:HB2	2:B:661:LEU:HD22	1.92	0.50
1:A:709:THR:HB	1:A:712:GLU:HB2	1.94	0.50
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.93	0.50
3:C:66:ARG:NH2	8:J:3:VAL:O	2.35	0.50
4:E:78:LEU:HD12	4:E:107:THR:HB	1.93	0.50
1:A:541:ILE:HG12	1:A:546:VAL:HG22	1.93	0.50
2:B:953:LEU:O	2:B:964:VAL:HG23	2.12	0.50
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.93	0.50
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.93	0.50
6:H:40:LEU:HD13	6:H:123:MET:HG3	1.94	0.50
1:A:324:SER:O	1:A:326:ARG:N	2.45	0.50
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.93	0.50
7:I:75:CYS:O	7:I:78:CYS:O	2.30	0.50
1:A:626:ASN:O	1:A:631:HIS:CD2	2.65	0.50
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.92	0.50
2:B:489:SER:HA	2:B:492:LEU:HD12	1.94	0.50
10:L:42:ARG:NH1	10:L:43:THR:OG1	2.44	0.50
2:B:35:SER:O	2:B:39:ARG:HB2	2.12	0.49
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.93	0.49
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.44	0.49
8:J:1:MET:H2	8:J:57:ILE:HG22	1.77	0.49
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.78	0.49
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.44	0.49
1:A:1336:MET:HE2	1:A:1381:LEU:HD12	1.94	0.49
2:B:345:LYS:HA	2:B:347:LYS:N	2.22	0.49
1:A:826:ASP:HB2	1:A:830:LYS:HZ3	1.74	0.49
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.95	0.49
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.45	0.49
1:A:218:ASP:N	1:A:219:PHE:HB3	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:HIS:HB3	1:A:454:SER:H	1.76	0.49
6:H:137:GLN:HB3	6:H:139:ASN:HB2	1.94	0.49
8:J:48:ARG:O	8:J:52:THR:HB	2.13	0.49
1:A:95:PHE:HE2	1:A:1414:ALA:HB2	1.78	0.49
1:A:374:LEU:HA	2:B:1107:ALA:HB2	1.94	0.49
1:A:30:ILE:HG13	2:B:1170:THR:HG23	1.95	0.48
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.94	0.48
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.43	0.48
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.95	0.48
2:B:976:ILE:O	2:B:990:ILE:O	2.31	0.48
2:B:1172:ILE:HG22	2:B:1174:LYS:HG3	1.95	0.48
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.59	0.48
2:B:234:ILE:HD13	2:B:257:LYS:HD2	1.95	0.48
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.28	0.48
2:B:797:TYR:O	8:J:1:MET:HG2	2.12	0.48
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.48	0.48
6:H:89:LEU:C	6:H:91:ASP:H	2.22	0.48
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.95	0.48
4:E:147:HIS:CD2	4:E:149:LEU:HB2	2.49	0.48
7:I:102:VAL:HG22	7:I:109:ILE:HG12	1.95	0.48
1:A:285:PRO:HD2	1:A:289:ILE:HB	1.96	0.48
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.96	0.48
1:A:709:THR:HG22	1:A:711:ARG:H	1.78	0.48
2:B:977:GLY:HA3	2:B:1099:VAL:HG13	1.95	0.47
3:C:10:ILE:HD13	3:C:20:PHE:HB3	1.96	0.47
1:A:503:GLN:HE21	5:F:90:ARG:NH1	2.12	0.47
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.95	0.47
1:A:857:ARG:HD3	1:A:861:GLY:O	2.13	0.47
2:B:647:GLY:HA2	2:B:648:HIS:C	2.39	0.47
1:A:512:VAL:HA	1:A:519:PRO:HA	1.96	0.47
6:H:83:GLN:C	6:H:85:GLY:H	2.22	0.47
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.96	0.47
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.95	0.47
10:L:55:ILE:H	10:L:55:ILE:HG12	1.55	0.47
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.96	0.47
3:C:108:GLU:HA	3:C:149:LYS:HD3	1.97	0.47
1:A:135:PHE:HD1	1:A:222:LEU:HB2	1.80	0.47
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.29	0.47
1:A:119:ASN:HB3	1:A:122:MET:HB3	1.97	0.47
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.96	0.47
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.50	0.47
1:A:378:GLU:OE2	1:A:434:ARG:HD3	2.15	0.46
6:H:95:TYR:HB3	6:H:144:ILE:HB	1.96	0.46
1:A:276:LEU:HD13	1:A:296:LEU:HD12	1.97	0.46
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.80	0.46
1:A:535:THR:HG22	1:A:616:VAL:HA	1.97	0.46
1:A:596:THR:O	1:A:599:SER:N	2.49	0.46
2:B:745:PRO:O	2:B:748:ILE:HG12	2.16	0.46
4:E:79:TRP:HB3	4:E:100:ILE:HD11	1.96	0.46
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.96	0.46
1:A:456:MET:HE2	1:A:507:VAL:HA	1.98	0.46
3:C:134:ILE:HG23	3:C:141:GLY:H	1.81	0.46
4:E:147:HIS:CD2	4:E:149:LEU:H	2.33	0.46
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.48	0.46
6:H:126:GLU:C	6:H:130:ARG:HH22	2.24	0.46
2:B:126:SER:HB2	2:B:172:ILE:HD11	1.98	0.46
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.96	0.46
3:C:20:PHE:HE1	3:C:22:LEU:HD13	1.80	0.46
7:I:101:PHE:O	7:I:109:ILE:HA	2.16	0.46
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.39	0.46
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.96	0.46
3:C:241:ASP:HB3	9:K:109:TRP:CD2	2.50	0.46
1:A:1080:THR:HG22	1:A:1081:LEU:HD12	1.97	0.46
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.49	0.46
2:B:982:SER:OG	2:B:986:GLN:HB2	2.16	0.46
1:A:225:ASN:HB3	1:A:229:SER:H	1.80	0.46
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.97	0.46
2:B:884:ARG:HE	2:B:935:ARG:HH21	1.64	0.46
3:C:18:VAL:HG22	3:C:240:VAL:HB	1.98	0.46
1:A:55:ASP:O	1:A:57:ARG:N	2.49	0.45
1:A:219:PHE:H	1:A:222:LEU:HG	1.81	0.45
1:A:855:THR:CG2	1:A:857:ARG:HE	2.22	0.45
2:B:999:MET:HE2	2:B:1011:ILE:CD1	2.45	0.45
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.98	0.45
2:B:1034:VAL:CG2	2:B:1059:LEU:HB2	2.46	0.45
3:C:70:ILE:HG21	3:C:115:SER:HB2	1.98	0.45
1:A:53:LEU:HG	1:A:54:ASN:HD22	1.81	0.45
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.46	0.45
1:A:456:MET:HG2	1:A:510:GLN:HG3	1.98	0.45
1:A:738:LYS:HD2	1:A:740:LEU:HD21	1.99	0.45
2:B:658:ILE:HG23	2:B:662:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:1:MET:N	8:J:57:ILE:H	2.14	0.45
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.98	0.45
2:B:219:ALA:HB3	2:B:222:ILE:HD11	1.97	0.45
1:A:40:THR:HG23	1:A:54:ASN:HD21	1.82	0.45
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.98	0.45
2:B:1139:ILE:HG13	2:B:1147:LEU:HD11	1.99	0.45
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.52	0.45
3:C:164:ALA:HA	3:C:167:HIS:O	2.17	0.45
3:C:235:VAL:HG11	8:J:6:ARG:NH2	2.32	0.45
7:I:10:CYS:SG	7:I:31:THR:HB	2.58	0.45
7:I:62:ILE:HG12	7:I:84:VAL:HG11	1.98	0.45
1:A:306:ASN:HD21	1:A:313:GLN:HB2	1.82	0.44
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.99	0.44
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.17	0.44
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.99	0.44
4:E:19:VAL:O	4:E:23:VAL:HG23	2.17	0.44
1:A:899:VAL:HG22	1:A:1029:ARG:HH11	1.82	0.44
2:B:225:VAL:HG11	2:B:385:LEU:HA	1.97	0.44
3:C:148:ARG:H	3:C:151:GLN:HG3	1.82	0.44
1:A:1129:GLU:HA	1:A:1132:LYS:HE3	1.98	0.44
3:C:93:ASP:O	3:C:127:ARG:NH2	2.48	0.44
10:L:61:THR:HB	10:L:63:ARG:HB2	1.98	0.44
1:A:663:SER:HB2	2:B:1085:ILE:HG13	1.97	0.44
2:B:654:ARG:H	2:B:657:HIS:CD2	2.31	0.44
6:H:36:CYS:HB2	6:H:129:TYR:OH	2.18	0.44
1:A:271:LYS:O	1:A:275:SER:HB2	2.18	0.44
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.51	0.44
3:C:57:VAL:HG12	3:C:58:LEU:HD23	1.99	0.44
3:C:234:SER:HB2	3:C:240:VAL:HG13	2.00	0.44
7:I:63:GLY:O	7:I:70:ARG:NH2	2.50	0.44
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.99	0.44
2:B:1097:HIS:HB3	2:B:1102:LYS:HE3	2.00	0.44
3:C:70:ILE:CD1	3:C:144:ILE:HD12	2.48	0.44
9:K:65:HIS:CD2	9:K:67:PHE:H	2.23	0.44
1:A:567:LYS:HD2	1:A:568:PRO:HD2	2.00	0.44
2:B:277:LYS:HZ2	2:B:335:GLY:H	1.65	0.44
8:J:52:THR:HG22	8:J:52:THR:O	2.18	0.44
1:A:304:MET:HG2	1:A:325:ILE:HD12	1.99	0.43
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.52	0.43
1:A:982:THR:H	1:A:985:ASP:HB2	1.83	0.43
2:B:63:ILE:O	2:B:67:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:HG11	2:B:122:LEU:HD13	2.00	0.43
1:A:595:THR:HG21	1:A:604:GLY:HA3	2.00	0.43
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.48	0.43
2:B:302:CYS:HA	2:B:310:MET:HE3	2.00	0.43
2:B:420:LEU:HB3	2:B:453:ILE:HG13	2.00	0.43
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.99	0.43
1:A:828:ALA:HB2	2:B:530:GLY:HA2	2.00	0.43
1:A:837:ILE:HD11	1:A:1102:LYS:HG3	2.00	0.43
1:A:848:ILE:HD13	1:A:858:ASN:HB3	2.00	0.43
2:B:123:THR:HA	2:B:204:ILE:O	2.18	0.43
4:E:55:ARG:HA	4:E:58:MET:HE2	2.00	0.43
4:E:88:VAL:HB	4:E:116:ILE:HD13	2.00	0.43
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.53	0.43
1:A:492:PRO:HB3	1:A:497:THR:HG22	2.00	0.43
1:A:901:LEU:H	1:A:926:GLN:NE2	2.17	0.43
2:B:211:VAL:HG13	2:B:495:LEU:HD23	2.00	0.43
2:B:592:ASN:H	2:B:593:PRO:HD3	1.84	0.43
7:I:45:ARG:HE	7:I:47:GLU:HG3	1.84	0.43
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	2.00	0.43
1:A:362:ASP:HB3	1:A:508:PRO:HD3	2.00	0.43
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	2.00	0.43
2:B:898:LEU:HD21	2:B:964:VAL:HG11	2.00	0.43
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.54	0.43
1:A:614:PHE:HB3	6:H:122:LEU:HD21	2.01	0.43
2:B:485:ARG:HG3	2:B:781:PHE:CD1	2.54	0.43
2:B:1013:ASN:OD1	2:B:1015:HIS:HD2	1.99	0.43
2:B:1056:SER:HB3	2:B:1066:SER:HB2	2.00	0.43
3:C:177:GLU:HB2	3:C:231:ASN:HB3	2.01	0.43
1:A:348:SER:HA	1:A:489:LEU:O	2.19	0.43
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.54	0.43
6:H:109:LYS:HG3	6:H:110:ASP:H	1.83	0.43
9:K:23:PRO:HA	9:K:31:VAL:HG23	2.01	0.43
1:A:672:ASP:HB3	1:A:675:THR:H	1.83	0.43
1:A:993:LEU:HD22	1:A:1046:LEU:HG	2.01	0.43
10:L:32:ALA:HB3	10:L:55:ILE:HG13	2.01	0.43
1:A:456:MET:HE3	1:A:510:GLN:CB	2.48	0.42
3:C:18:VAL:O	3:C:231:ASN:HA	2.19	0.42
5:F:72:LYS:HE2	5:F:142:SER:HB3	2.01	0.42
7:I:47:GLU:OE1	7:I:50:THR:HG23	2.19	0.42
1:A:38:PRO:HA	1:A:270:LEU:HD13	2.00	0.42
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HA	1:A:269:ILE:HG12	2.01	0.42
1:A:356:ASP:OD2	9:K:65:HIS:HE1	2.02	0.42
1:A:935:GLN:HE22	1:A:938:LYS:HD2	1.84	0.42
2:B:792:MET:HA	2:B:856:PHE:O	2.19	0.42
4:E:100:ILE:HG13	4:E:105:PHE:HB2	2.02	0.42
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.85	0.42
2:B:360:PHE:HE2	2:B:374:LYS:HB3	1.83	0.42
2:B:841:MET:O	2:B:993:THR:HA	2.19	0.42
1:A:1062:GLU:C	1:A:1064:VAL:H	2.28	0.42
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	2.00	0.42
8:J:14:VAL:HA	8:J:17:LYS:HD2	2.00	0.42
1:A:88:LYS:HE2	1:A:205:GLU:HB2	2.00	0.42
1:A:1116:LEU:HB3	1:A:1308:THR:HB	2.02	0.42
2:B:1006:ILE:CD1	8:J:43:ARG:HB2	2.49	0.42
4:E:94:LYS:O	4:E:98:ILE:HG12	2.19	0.42
1:A:760:GLN:HG2	1:A:765:VAL:HA	2.01	0.42
2:B:378:LEU:HG	2:B:382:ILE:HD11	2.02	0.42
2:B:1210:MET:HB3	2:B:1212:ILE:HD12	2.02	0.42
4:E:135:PHE:HB3	4:E:140:LEU:HD11	2.01	0.42
1:A:1266:THR:HG23	1:A:1270:ASN:HD22	1.84	0.42
4:E:147:HIS:HD2	4:E:149:LEU:HB2	1.85	0.42
10:L:38:LEU:HD21	10:L:49:LYS:H	1.85	0.42
1:A:92:HIS:HD2	1:A:94:GLY:H	1.67	0.42
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.68	0.42
2:B:516:ASN:H	2:B:516:ASN:ND2	2.16	0.42
2:B:800:GLN:CB	8:J:52:THR:HG22	2.45	0.42
2:B:1000:PRO:HB2	2:B:1072:MET:HE3	2.02	0.42
1:A:325:ILE:O	1:A:328:ARG:HB2	2.20	0.42
1:A:445:ASN:HB2	1:A:455:MET:HG3	2.02	0.42
2:B:515:HIS:H	2:B:518:HIS:CD2	2.38	0.42
8:J:14:VAL:HB	8:J:50:ILE:HD11	2.01	0.42
1:A:565:ILE:HG22	1:A:569:LYS:O	2.20	0.41
3:C:114:TYR:CG	3:C:140:ASN:HB2	2.55	0.41
5:F:82:THR:HG22	5:F:84:TYR:H	1.85	0.41
1:A:152:VAL:HG23	1:A:162:VAL:HB	2.02	0.41
1:A:117:GLU:N	1:A:118:HIS:HB2	2.36	0.41
2:B:95:ILE:HD11	2:B:128:LEU:HB3	2.02	0.41
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.84	0.41
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.52	0.41
1:A:265:LYS:HG2	1:A:303:TYR:HB2	2.03	0.41
1:A:333:GLU:HA	1:A:338:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:ASN:O	1:A:907:THR:OG1	2.39	0.41
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	2.21	0.41
2:B:545:ILE:HG12	2:B:633:VAL:HG22	2.03	0.41
1:A:265:LYS:HE3	1:A:299:HIS:HB3	2.03	0.41
2:B:282:ILE:HG21	2:B:382:ILE:HD12	2.02	0.41
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.34	0.41
2:B:1099:VAL:O	2:B:1103:ILE:HG13	2.20	0.41
3:C:98:VAL:H	3:C:122:SER:CB	2.32	0.41
1:A:541:ILE:CD1	1:A:577:ILE:HG12	2.50	0.41
1:A:1174:PHE:HD1	1:A:1175:SER:H	1.69	0.41
2:B:618:ASP:OD2	2:B:621:GLU:HB2	2.20	0.41
7:I:55:THR:HG23	7:I:58:VAL:HG21	2.02	0.41
1:A:70:CYS:HA	2:B:1174:LYS:HG2	2.03	0.41
1:A:523:ILE:HG23	1:A:527:THR:HB	2.03	0.41
1:A:597:LEU:HD12	1:A:597:LEU:H	1.86	0.41
2:B:69:LEU:HD12	2:B:90:ILE:HB	2.01	0.41
2:B:219:ALA:HB2	2:B:405:ARG:HG2	2.02	0.41
2:B:333:PHE:O	2:B:334:ILE:HG13	2.21	0.41
2:B:420:LEU:HD21	2:B:456:GLY:HA3	2.03	0.41
2:B:610:ASN:HB3	2:B:613:VAL:HG23	2.03	0.41
2:B:1168:LEU:C	2:B:1170:THR:H	2.28	0.41
1:A:351:THR:HG22	1:A:352:VAL:H	1.85	0.41
10:L:46:VAL:HG23	10:L:47:ARG:H	1.86	0.41
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.86	0.40
1:A:568:PRO:O	1:A:569:LYS:HB2	2.21	0.40
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	2.03	0.40
2:B:555:ILE:H	2:B:555:ILE:HG12	1.58	0.40
1:A:567:LYS:HB3	6:H:95:TYR:HA	2.02	0.40
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.57	0.40
1:A:946:VAL:HG13	4:E:201:LYS:HB3	2.04	0.40
7:I:84:VAL:HB	7:I:104:LEU:HD21	2.04	0.40
1:A:456:MET:HE2	1:A:507:VAL:HG22	2.03	0.40
1:A:741:ASN:HD22	1:A:744:LYS:H	1.69	0.40
1:A:889:SER:HB3	1:A:1297:GLU:HG3	2.04	0.40
2:B:798:TYR:HE2	3:C:66:ARG:HH21	1.69	0.40
2:B:844:SER:HG	2:B:996:ARG:H	1.67	0.40
3:C:22:LEU:HG	3:C:25:VAL:HG21	2.02	0.40
7:I:58:VAL:HG11	7:I:109:ILE:HD11	2.04	0.40
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.03	0.40
2:B:601:ARG:HA	2:B:615:MET:HE1	2.04	0.40
2:B:900:ALA:HB3	10:L:61:THR:HG23	2.02	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%)	1242 (89%)	110 (8%)	43 (3%)	3	16
2	B	1096/1224 (90%)	949 (87%)	112 (10%)	35 (3%)	3	15
3	C	264/318 (83%)	239 (90%)	18 (7%)	7 (3%)	4	18
4	E	212/215 (99%)	202 (95%)	8 (4%)	2 (1%)	14	41
5	F	83/155 (54%)	74 (89%)	6 (7%)	3 (4%)	2	13
6	H	129/146 (88%)	107 (83%)	14 (11%)	8 (6%)	1	6
7	I	117/122 (96%)	101 (86%)	15 (13%)	1 (1%)	14	41
8	J	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	3	15
9	K	112/120 (93%)	105 (94%)	6 (5%)	1 (1%)	14	41
10	L	44/70 (63%)	26 (59%)	10 (23%)	8 (18%)	0	0
All	All	3515/4173 (84%)	3102 (88%)	303 (9%)	110 (3%)	3	16

All (110) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	ASP
1	A	325	ILE
1	A	399	HIS
1	A	543	LEU
1	A	567	LYS
1	A	597	LEU
1	A	1123	GLY
2	B	139	ALA
2	B	248	SER
2	B	364	ILE
2	B	469	GLN

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Mol	Chain	Res	Type
2	B	477	ALA
2	B	531	GLN
2	B	646	LEU
2	B	712	PRO
2	B	731	VAL
2	B	1046	PRO
2	B	1156	ASP
2	B	1181	GLU
3	C	173	ALA
3	C	174	ALA
3	C	215	GLU
4	E	126	SER
6	H	109	LYS
6	H	140	ALA
8	J	6	ARG
10	L	46	VAL
10	L	60	ARG
10	L	64	LEU
1	A	219	PHE
1	A	672	ASP
1	A	775	ILE
1	A	1064	VAL
1	A	1221	LYS
1	A	1393	ASN
1	A	1437	GLY
2	B	137	TYR
2	B	465	ASN
2	B	592	ASN
2	B	647	GLY
2	B	709	ASP
2	B	886	LYS
2	B	1066	SER
3	C	142	VAL
3	C	227	THR
6	H	90	ALA
6	H	128	ASN
7	I	91	ARG
8	J	2	ILE
9	K	14	GLU
10	L	39	SER
10	L	45	ALA
10	L	51	CYS

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Mol	Chain	Res	Type
10	L	56	LEU
1	A	40	THR
1	A	56	PRO
1	A	65	LEU
1	A	117	GLU
1	A	286	HIS
1	A	299	HIS
1	A	312	PRO
1	A	568	PRO
1	A	569	LYS
1	A	916	GLY
1	A	1223	ASP
1	A	1278	ASN
2	B	105	SER
2	B	367	LEU
2	B	471	LYS
2	B	478	GLY
2	B	792	MET
2	B	1155	SER
2	B	1157	ALA
6	H	86	ASP
1	A	130	ASP
1	A	214	ILE
1	A	250	ILE
1	A	310	GLY
1	A	332	LYS
2	B	138	GLU
2	B	447	ALA
2	B	881	ASN
4	E	86	PRO
5	F	154	ASP
6	H	34	ASP
6	H	108	SER
1	A	72	GLU
1	A	76	GLU
1	A	400	PRO
1	A	593	GLU
1	A	599	SER
1	A	922	ASP
1	A	958	VAL
1	A	1124	HIS
2	B	448	ILE

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Mol	Chain	Res	Type
2	B	707	PRO
2	B	751	VAL
2	B	943	SER
2	B	1169	MET
3	C	90	ASP
5	F	128	LYS
10	L	59	ALA
1	A	213	HIS
3	C	126	GLY
5	F	73	ALA
1	A	35	ILE
6	H	17	PRO
1	A	424	ILE
2	B	1018	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%)	1070 (87%)	155 (13%)	4	17
2	B	967/1061 (91%)	847 (88%)	120 (12%)	4	17
3	C	234/274 (85%)	208 (89%)	26 (11%)	6	21
4	E	196/197 (100%)	178 (91%)	18 (9%)	8	28
5	F	75/137 (55%)	70 (93%)	5 (7%)	15	39
6	H	117/128 (91%)	100 (86%)	17 (14%)	3	13
7	I	113/116 (97%)	100 (88%)	13 (12%)	5	20
8	J	60/65 (92%)	48 (80%)	12 (20%)	1	5
9	K	99/102 (97%)	86 (87%)	13 (13%)	4	16
10	L	40/57 (70%)	33 (82%)	7 (18%)	2	8
All	All	3126/3657 (86%)	2740 (88%)	386 (12%)	4	18

All (386) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	18	GLN
1	A	34	LYS
1	A	41	MET
1	A	43	GLU
1	A	44	THR
1	A	58	LEU
1	A	61	ILE
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS
1	A	88	LYS
1	A	93	VAL
1	A	119	ASN
1	A	120	GLU
1	A	126	LEU
1	A	128	ILE
1	A	143	LYS
1	A	144	THR
1	A	146	MET
1	A	177	ASP
1	A	179	LEU
1	A	184	SER
1	A	208	LEU
1	A	222	LEU
1	A	225	ASN
1	A	250	ILE
1	A	262	LEU
1	A	265	LYS
1	A	270	LEU
1	A	271	LYS
1	A	296	LEU
1	A	299	HIS
1	A	302	THR
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	330	LYS
1	A	332	LYS
1	A	335	ARG

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Mol	Chain	Res	Type
1	A	336	ILE
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	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	447	GLN
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	461	LYS
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	496	GLU
1	A	518	LYS
1	A	527	THR
1	A	541	ILE
1	A	579	SER
1	A	590	ARG
1	A	595	THR
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	620	LYS
1	A	622	VAL
1	A	626	ASN
1	A	629	LEU
1	A	636	GLU
1	A	644	LYS
1	A	652	VAL

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Mol	Chain	Res	Type
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	702	LEU
1	A	710	LEU
1	A	722	LEU
1	A	740	LEU
1	A	741	ASN
1	A	756	ILE
1	A	821	ARG
1	A	825	ILE
1	A	826	ASP
1	A	830	LYS
1	A	845	LEU
1	A	855	THR
1	A	867	ILE
1	A	878	ILE
1	A	905	ASP
1	A	927	VAL
1	A	928	LEU
1	A	960	ILE
1	A	969	GLN
1	A	973	ILE
1	A	976	THR
1	A	999	VAL
1	A	1001	ARG
1	A	1015	VAL
1	A	1022	LEU
1	A	1047	SER
1	A	1048	ASN
1	A	1050	GLU
1	A	1064	VAL
1	A	1094	VAL
1	A	1102	LYS
1	A	1109	LYS
1	A	1110	ASN
1	A	1129	GLU
1	A	1136	SER
1	A	1168	GLU
1	A	1169	ILE
1	A	1174	PHE
1	A	1176	LEU

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Mol	Chain	Res	Type
1	A	1195	LEU
1	A	1221	LYS
1	A	1223	ASP
1	A	1230	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1256	GLU
1	A	1257	ASP
1	A	1267	MET
1	A	1269	GLU
1	A	1277	GLU
1	A	1280	GLU
1	A	1285	MET
1	A	1297	GLU
1	A	1300	LYS
1	A	1303	GLU
1	A	1322	ILE
1	A	1329	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1356	ILE
1	A	1376	THR
1	A	1378	GLN
1	A	1385	THR
1	A	1391	ARG
1	A	1398	MET
1	A	1426	GLU
1	A	1433	MET
2	B	25	ILE
2	B	26	THR
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	70	ILE
2	B	95	ILE
2	B	101	MET
2	B	102	VAL
2	B	105	SER
2	B	108	VAL
2	B	135	ARG
2	B	141	ASP
2	B	174	LEU

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Mol	Chain	Res	Type
2	B	175	ARG
2	B	187	SER
2	B	194	GLU
2	B	217	ARG
2	B	223	VAL
2	B	240	ILE
2	B	261	ARG
2	B	276	ILE
2	B	277	LYS
2	B	305	VAL
2	B	323	VAL
2	B	325	GLN
2	B	365	THR
2	B	367	LEU
2	B	382	ILE
2	B	393	LYS
2	B	416	LEU
2	B	426	LYS
2	B	435	THR
2	B	437	GLU
2	B	451	LYS
2	B	453	ILE
2	B	458	LYS
2	B	471	LYS
2	B	476	ARG
2	B	479	VAL
2	B	480	SER
2	B	485	ARG
2	B	487	THR
2	B	489	SER
2	B	516	ASN
2	B	522	VAL
2	B	537	LYS
2	B	547	VAL
2	B	554	ILE
2	B	555	ILE
2	B	556	THR
2	B	567	GLU
2	B	573	GLN
2	B	578	THR
2	B	604	ARG
2	B	616	ILE

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Mol	Chain	Res	Type
2	B	621	GLU
2	B	624	LEU
2	B	641	GLU
2	B	644	GLU
2	B	645	SER
2	B	646	LEU
2	B	653	VAL
2	B	655	LYS
2	B	658	ILE
2	B	690	VAL
2	B	708	GLU
2	B	710	LEU
2	B	737	THR
2	B	743	ILE
2	B	780	VAL
2	B	786	ASN
2	B	788	ARG
2	B	791	THR
2	B	796	LEU
2	B	815	ARG
2	B	838	SER
2	B	864	LYS
2	B	878	GLN
2	B	884	ARG
2	B	905	VAL
2	B	911	ILE
2	B	948	ILE
2	B	951	GLN
2	B	953	LEU
2	B	963	PHE
2	B	976	ILE
2	B	983	ARG
2	B	987	LYS
2	B	992	ILE
2	B	997	GLU
2	B	998	ASP
2	B	1006	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1012	ILE
2	B	1013	ASN
2	B	1033	LYS

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Mol	Chain	Res	Type
2	B	1065	GLN
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	1145	SER
2	B	1147	LEU
2	B	1159	ARG
2	B	1169	MET
2	B	1170	THR
2	B	1175	LEU
2	B	1181	GLU
2	B	1188	LYS
2	B	1189	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1210	MET
2	B	1211	ASN
2	B	1222	ARG
3	C	4	GLU
3	C	9	LYS
3	C	18	VAL
3	C	25	VAL
3	C	34	ARG
3	C	36	VAL
3	C	37	MET
3	C	57	VAL
3	C	69	LEU
3	C	75	MET
3	C	77	ILE
3	C	129	ILE
3	C	137	LYS
3	C	140	ASN
3	C	151	GLN
3	C	186	LEU
3	C	215	GLU
3	C	221	TYR
3	C	226	ASP
3	C	235	VAL

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Mol	Chain	Res	Type
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	259	LEU
3	C	260	LEU
3	C	264	GLN
4	E	4	GLU
4	E	7	ARG
4	E	52	ARG
4	E	54	GLN
4	E	65	THR
4	E	84	ASP
4	E	92	THR
4	E	100	ILE
4	E	102	GLU
4	E	107	THR
4	E	127	ILE
4	E	134	THR
4	E	156	LEU
4	E	169	ARG
4	E	190	LEU
4	E	200	ARG
4	E	204	THR
4	E	213	ILE
5	F	74	ILE
5	F	99	LEU
5	F	110	ASP
5	F	118	LEU
5	F	153	VAL
6	H	12	VAL
6	H	15	VAL
6	H	21	ASN
6	H	22	LYS
6	H	26	ILE
6	H	35	GLN
6	H	44	VAL
6	H	46	LEU
6	H	55	LEU
6	H	86	ASP
6	H	87	ARG
6	H	106	GLU
6	H	107	VAL

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Mol	Chain	Res	Type
6	H	111	LEU
6	H	129	TYR
6	H	130	ARG
6	H	136	LYS
7	I	9	ASP
7	I	17	ARG
7	I	24	ARG
7	I	37	GLU
7	I	51	ASN
7	I	55	THR
7	I	60	GLN
7	I	62	ILE
7	I	77	LYS
7	I	84	VAL
7	I	87	GLN
7	I	97	MET
7	I	111	THR
8	J	2	ILE
8	J	3	VAL
8	J	6	ARG
8	J	7	CYS
8	J	22	LEU
8	J	26	GLN
8	J	37	SER
8	J	48	ARG
8	J	57	ILE
8	J	59	LYS
8	J	62	ARG
8	J	64	ASN
9	K	6	ARG
9	K	11	LEU
9	K	18	LYS
9	K	20	LYS
9	K	22	ASP
9	K	31	VAL
9	K	33	ILE
9	K	47	ARG
9	K	51	LEU
9	K	63	VAL
9	K	97	LYS
9	K	101	LEU
9	K	111	LEU

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Mol	Chain	Res	Type
10	L	30	ILE
10	L	35	SER
10	L	42	ARG
10	L	55	ILE
10	L	58	LYS
10	L	65	VAL
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN
1	A	18	GLN
1	A	54	ASN
1	A	68	GLN
1	A	171	GLN
1	A	209	ASN
1	A	225	ASN
1	A	306	ASN
1	A	339	ASN
1	A	390	GLN
1	A	394	ASN
1	A	503	GLN
1	A	584	ASN
1	A	603	ASN
1	A	626	ASN
1	A	631	HIS
1	A	640	GLN
1	A	659	HIS
1	A	660	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	851	HIS
1	A	865	GLN
1	A	926	GLN
1	A	935	GLN
1	A	965	GLN

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Mol	Chain	Res	Type
1	A	1082	ASN
1	A	1140	HIS
1	A	1232	ASN
1	A	1258	HIS
1	A	1270	ASN
1	A	1427	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	121	ASN
2	B	215	GLN
2	B	325	GLN
2	B	363	HIS
2	B	433	GLN
2	B	469	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	592	ASN
2	B	657	HIS
2	B	744	HIS
2	B	762	ASN
2	B	767	ASN
2	B	770	GLN
2	B	776	GLN
2	B	843	GLN
2	B	862	GLN
2	B	887	HIS
2	B	984	HIS
2	B	1015	HIS
2	B	1062	HIS
2	B	1076	HIS
2	B	1093	GLN
2	B	1097	HIS
2	B	1141	HIS
2	B	1161	HIS
2	B	1176	ASN
2	B	1177	HIS
2	B	1211	ASN
3	C	112	ASN
3	C	123	ASN
3	C	131	HIS

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Mol	Chain	Res	Type
3	C	151	GLN
3	C	167	HIS
3	C	242	GLN
3	C	267	GLN
4	E	54	GLN
4	E	101	GLN
4	E	106	GLN
4	E	147	HIS
4	E	179	GLN
7	I	46	HIS
7	I	83	ASN
7	I	120	GLN
8	J	23	ASN
9	K	65	HIS
9	K	110	ASN

5.3.3 RNA [i](#)

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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%)	0.06	28 (1%) 65 43	62, 106, 212, 241	0
2	B	1114/1224 (91%)	0.05	28 (2%) 58 36	60, 101, 178, 207	0
3	C	266/318 (83%)	-0.20	2 (0%) 82 65	72, 98, 138, 170	0
4	E	214/215 (99%)	0.05	2 (0%) 81 63	79, 137, 185, 197	0
5	F	85/155 (54%)	-0.29	0 100 100	87, 119, 155, 169	0
6	H	133/146 (91%)	0.18	7 (5%) 32 16	100, 141, 173, 184	0
7	I	119/122 (97%)	0.06	3 (2%) 58 36	77, 107, 146, 158	0
8	J	65/70 (92%)	-0.12	1 (1%) 72 51	64, 94, 131, 144	0
9	K	114/120 (95%)	-0.23	1 (0%) 81 63	64, 101, 127, 143	0
10	L	46/70 (65%)	0.78	6 (13%) 7 4	79, 135, 168, 176	0
11	R	5/5 (100%)	0.70	0 100 100	211, 213, 220, 220	0
12	T	8/29 (27%)	0.71	0 100 100	193, 198, 203, 205	0
All	All	3574/4207 (84%)	0.03	78 (2%) 62 41	60, 107, 200, 241	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1087	ALA	5.4
10	L	27	LEU	5.1
2	B	335	GLY	4.9
1	A	73	GLY	4.4
2	B	1204	PHE	4.2
2	B	715	ALA	4.2
2	B	1214	PRO	4.1
1	A	65	LEU	4.0
6	H	63	LEU	4.0
1	A	78	PRO	3.9
2	B	883	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1088	GLY	3.8
1	A	250	ILE	3.7
1	A	1081	LEU	3.7
6	H	85	GLY	3.5
2	B	1173	ALA	3.5
1	A	138	ILE	3.5
1	A	1108	ALA	3.4
2	B	1200	ALA	3.3
2	B	709	ASP	3.3
2	B	446	LEU	3.1
2	B	882	THR	3.1
4	E	98	ILE	3.1
1	A	75	ASN	3.1
9	K	114	LEU	3.0
1	A	179	LEU	3.0
6	H	46	LEU	3.0
2	B	1203	LEU	3.0
2	B	70	ILE	3.0
1	A	1086	PHE	2.9
10	L	28	LYS	2.9
10	L	66	GLN	2.8
2	B	502	ILE	2.8
2	B	1199	ALA	2.8
6	H	86	ASP	2.7
1	A	201	VAL	2.6
1	A	1123	GLY	2.6
1	A	289	ILE	2.6
1	A	1090	ALA	2.5
1	A	1091	SER	2.5
3	C	221	TYR	2.4
1	A	329	LEU	2.4
8	J	65	PRO	2.4
2	B	647	GLY	2.3
1	A	61	ILE	2.3
2	B	473	MET	2.3
2	B	711	GLU	2.3
2	B	140	ILE	2.3
2	B	1216	LEU	2.3
2	B	1162	ILE	2.3
1	A	252	PHE	2.3
10	L	50	ASP	2.3
1	A	96	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	467	GLY	2.3
10	L	55	ILE	2.3
3	C	251	LEU	2.3
2	B	708	GLU	2.2
1	A	74	MET	2.2
1	A	181	LEU	2.2
4	E	110	PHE	2.2
10	L	46	VAL	2.2
2	B	1169	MET	2.2
1	A	91	PHE	2.2
2	B	731	VAL	2.2
1	A	137	ALA	2.1
6	H	89	LEU	2.1
6	H	132	LEU	2.1
7	I	52	ILE	2.1
2	B	1170	THR	2.1
6	H	90	ALA	2.1
2	B	478	GLY	2.1
2	B	475	SER	2.0
1	A	1423	GLY	2.0
1	A	424	ILE	2.0
7	I	49	ILE	2.0
2	B	477	ALA	2.0
1	A	79	GLY	2.0
7	I	4	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	0.83	0.09	300,300,300,300	0
13	ZN	A	1735	1/1	0.94	0.07	190,190,190,190	0
13	ZN	B	1307	1/1	0.97	0.06	202,202,202,202	0
13	ZN	C	319	1/1	0.99	0.02	92,92,92,92	0
13	ZN	I	203	1/1	0.99	0.03	108,108,108,108	0
13	ZN	J	101	1/1	0.99	0.03	85,85,85,85	0
13	ZN	L	105	1/1	0.99	0.02	129,129,129,129	0
14	MG	A	2001	1/1	0.99	0.03	60,60,60,60	0
13	ZN	I	204	1/1	1.00	0.03	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.