



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:59 PM UTC

PDB ID : 3S1N / pdb_00003s1n
Title : RNA Polymerase II Initiation Complex with a 5-nt RNA (variant 2)
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-15
Resolution : 3.10 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

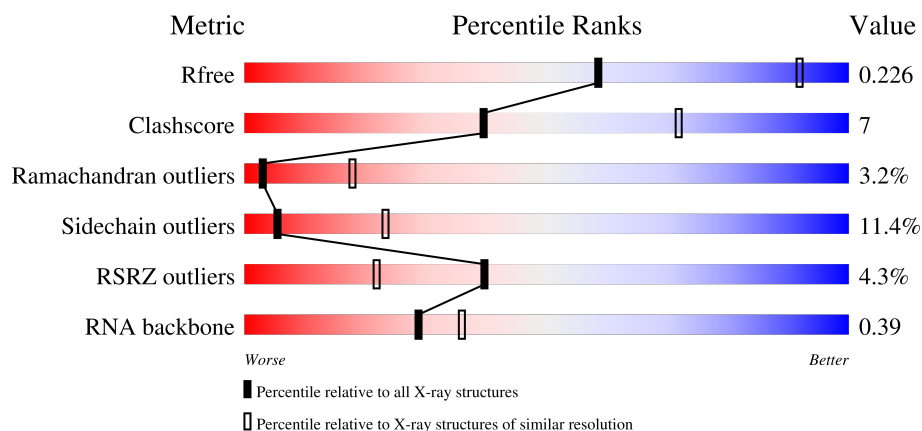
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	4% 58% 19% . 19%
2	B	1224	4% 67% 21% . 9%
3	C	318	61% 19% . 16%
4	E	215	3% 79% 18% .

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Mol	Chain	Length	Quality of chain
5	F	155	48%7%45%
6	H	146	9% 61%24%6%9%
7	I	122	2% 75%18%5%
8	J	70	% 63%19%10%7%
9	K	120	% 70%21%5%
10	L	70	10% 41%17%6%34%
11	R	5	80%20%
12	T	29	7% 28%72%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 28570 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1405	Total	C	N	O	S	0	0	0
			11043	6965	1936	2081	61			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

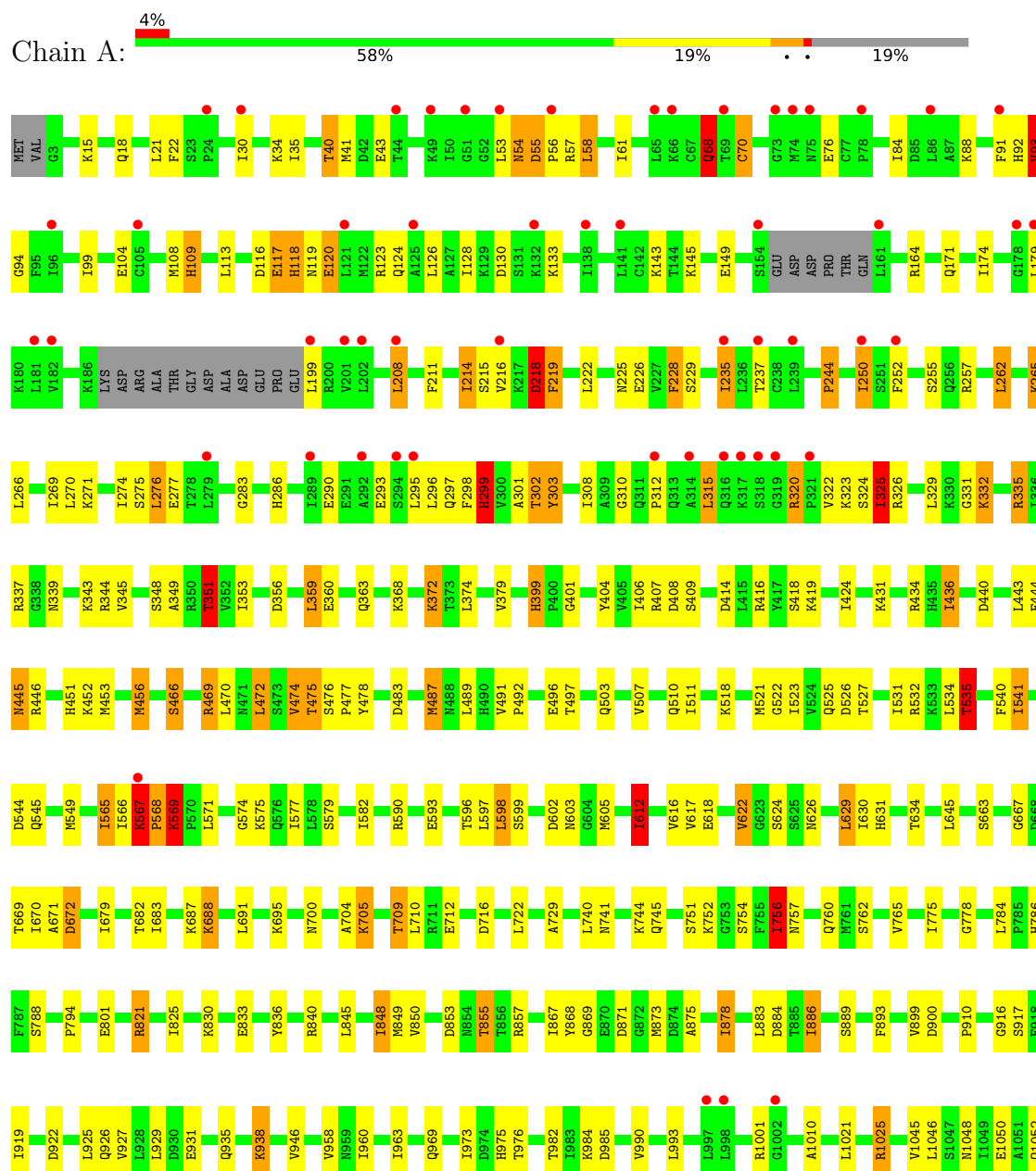
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

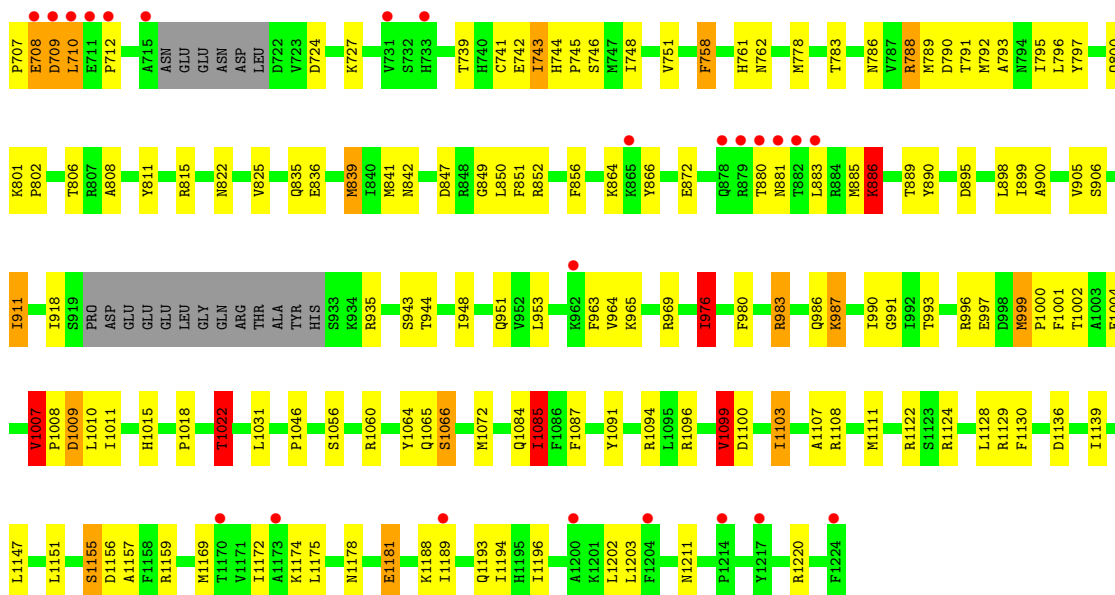
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

3 Residue-property plots

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

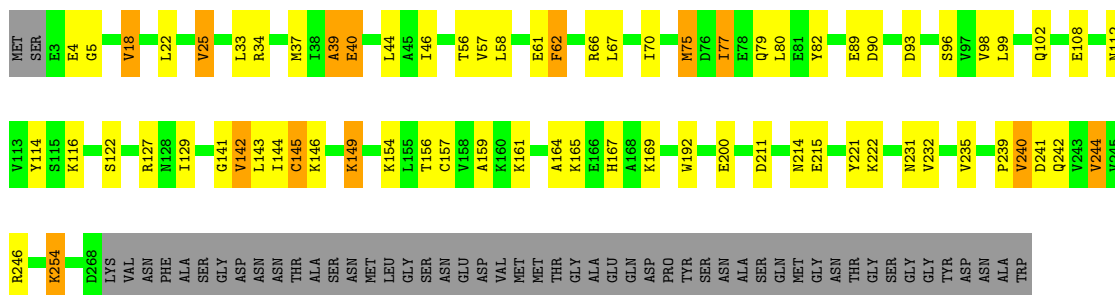
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





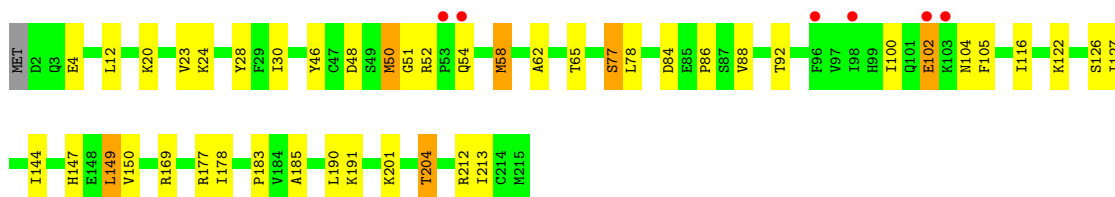
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 61% 19% 16%



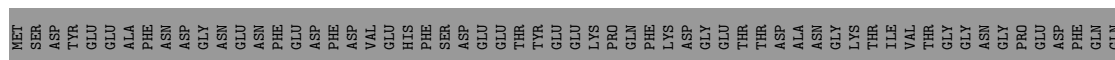
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 3% 79% 18%



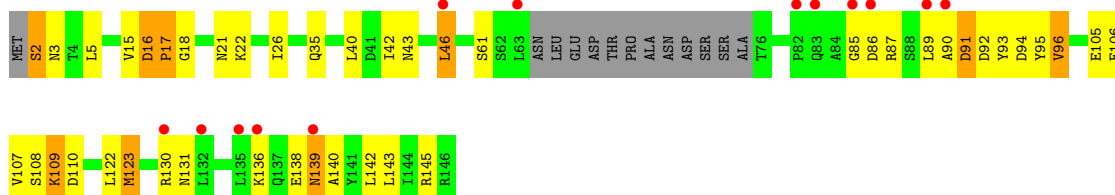
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 48% 7% 45%

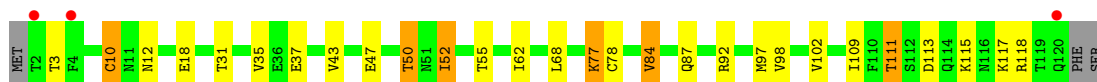
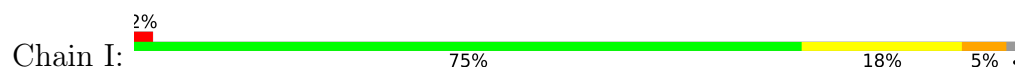




- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



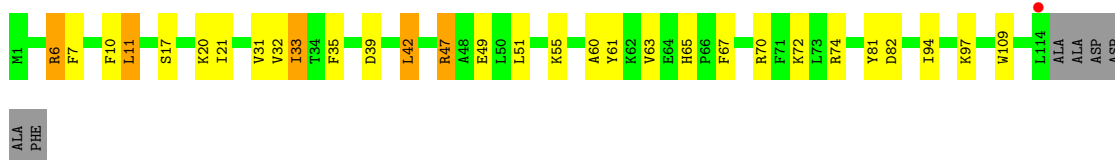
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



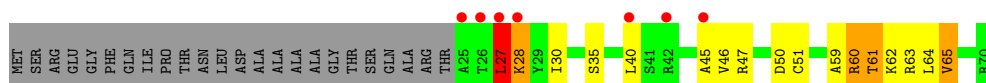
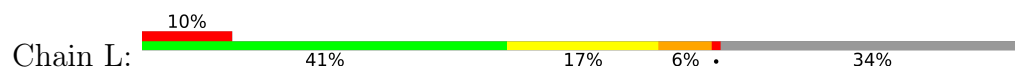
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



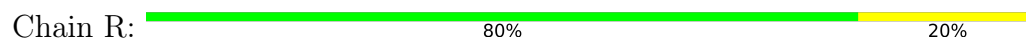
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



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

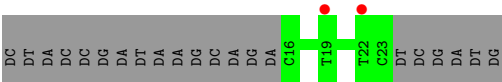


- Molecule 11: RNA (5'-R(*AP*GP*AP*GP*C)-3')





● Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*GP*CP*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	157.30Å 221.13Å 191.94Å 90.00° 97.52° 90.00°	Depositor
Resolution (Å)	47.80 – 3.10 47.80 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.80-3.10) 99.8 (47.80-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.07Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.191 , 0.232 (Not available) , 0.226	Depositor DCC
R_{free} test set	5960 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28570	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: MG, 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	0.79	4/11241 (0.0%)	1.43	59/15199 (0.4%)
2	B	0.77	1/9033 (0.0%)	1.36	38/12181 (0.3%)
3	C	0.73	0/2133	1.35	7/2891 (0.2%)
4	E	0.75	0/1788	1.37	10/2406 (0.4%)
5	F	0.75	0/700	1.31	1/945 (0.1%)
6	H	0.73	0/1086	1.26	11/1470 (0.7%)
7	I	0.73	0/989	1.33	4/1331 (0.3%)
8	J	0.80	0/541	1.52	5/727 (0.7%)
9	K	0.67	0/937	1.29	2/1265 (0.2%)
10	L	0.85	0/365	1.42	6/485 (1.2%)
11	R	0.56	0/120	0.95	0/186
12	T	0.44	0/180	1.12	0/275
All	All	0.77	5/29113 (0.0%)	1.38	143/39361 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	487	MET	SD-CE	-6.92	1.62	1.79
1	A	456	MET	SD-CE	-6.28	1.63	1.79
1	A	756	ILE	CG1-CD1	5.78	1.74	1.51
1	A	605	MET	SD-CE	-5.38	1.66	1.79
2	B	839	MET	SD-CE	-5.34	1.66	1.79

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	647	GLY	CA-C-N	11.31	142.07	121.70
2	B	647	GLY	C-N-CA	11.31	142.07	121.70
3	C	39	ALA	N-CA-C	9.80	125.37	113.41
1	A	218	ASP	CA-C-N	9.79	139.32	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	ASP	C-N-CA	9.79	139.32	121.70
1	A	1123	GLY	CA-C-N	8.32	136.68	121.70
1	A	1123	GLY	C-N-CA	8.32	136.68	121.70
1	A	117	GLU	CA-C-N	7.69	135.55	121.70
1	A	117	GLU	C-N-CA	7.69	135.55	121.70
1	A	445	ASN	CA-CB-CG	7.41	120.01	112.60
2	B	140	ILE	CA-C-N	7.30	134.85	121.70
2	B	140	ILE	C-N-CA	7.30	134.85	121.70
8	J	5	VAL	N-CA-C	-7.24	100.25	109.30
10	L	62	LYS	N-CA-C	-7.07	104.26	113.17
1	A	1097	GLY	CA-C-N	7.02	124.66	120.24
1	A	1097	GLY	C-N-CA	7.02	124.66	120.24
2	B	1009	ASP	N-CA-C	-7.01	104.53	113.23
6	H	2	SER	CA-C-N	6.83	133.99	121.70
6	H	2	SER	C-N-CA	6.83	133.99	121.70
1	A	1207	LEU	N-CA-C	6.78	119.98	109.07
1	A	296	LEU	N-CA-C	-6.70	105.64	113.88
1	A	298	PHE	CA-C-N	6.63	133.63	121.70
1	A	298	PHE	C-N-CA	6.63	133.63	121.70
1	A	351	THR	CA-C-N	6.56	129.29	120.50
1	A	351	THR	C-N-CA	6.56	129.29	120.50
4	E	48	ASP	CA-CB-CG	6.47	119.07	112.60
7	I	31	THR	N-CA-C	-6.43	105.44	113.55
9	K	82	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	603	ASN	CA-CB-CG	6.41	119.01	112.60
1	A	886	ILE	N-CA-C	6.38	117.13	110.62
1	A	466	SER	N-CA-C	6.34	121.02	113.16
2	B	345	LYS	CA-C-N	6.28	133.01	121.70
2	B	345	LYS	C-N-CA	6.28	133.01	121.70
4	E	102	GLU	N-CA-C	6.27	118.11	111.28
2	B	886	LYS	CA-C-N	6.25	132.94	121.70
2	B	886	LYS	C-N-CA	6.25	132.94	121.70
6	H	92	ASP	N-CA-C	-6.23	103.73	113.02
2	B	648	HIS	N-CA-CB	6.20	121.05	110.50
1	A	900	ASP	CA-CB-CG	6.20	118.80	112.60
2	B	847	ASP	CA-CB-CG	6.10	118.70	112.60
2	B	1022	THR	CB-CA-C	6.09	122.55	110.42
6	H	122	LEU	N-CA-C	5.98	119.33	110.48
3	C	40	GLU	N-CA-C	5.98	120.59	112.88
5	F	154	ASP	CA-CB-CG	5.97	118.57	112.60
7	I	118	ARG	N-CA-C	5.97	118.00	110.24
1	A	612	ILE	N-CA-CB	5.96	117.83	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	139	ASN	CA-C-N	5.92	132.84	121.54
6	H	139	ASN	C-N-CA	5.92	132.84	121.54
4	E	58	MET	N-CA-C	5.91	117.39	111.07
2	B	363	HIS	N-CA-C	-5.87	103.19	110.41
2	B	890	TYR	CA-C-N	5.86	128.94	120.38
2	B	890	TYR	C-N-CA	5.86	128.94	120.38
6	H	138	GLU	N-CA-C	-5.84	105.41	112.54
2	B	581	PHE	CA-CB-CG	5.83	119.63	113.80
1	A	848	ILE	N-CA-CB	5.82	117.63	111.00
4	E	150	VAL	N-CA-C	5.81	112.85	107.56
1	A	244	PRO	N-CA-C	5.79	117.77	110.70
4	E	4	GLU	N-CA-C	-5.78	106.18	113.18
8	J	18	TRP	N-CA-C	5.69	117.28	111.14
6	H	130	ARG	CA-C-N	5.68	132.38	121.54
6	H	130	ARG	C-N-CA	5.68	132.38	121.54
1	A	1233	ASP	CA-C-N	5.67	129.33	120.82
1	A	1233	ASP	C-N-CA	5.67	129.33	120.82
1	A	893	PHE	CA-C-N	5.66	127.80	120.44
1	A	893	PHE	C-N-CA	5.66	127.80	120.44
3	C	145	CYS	N-CA-C	5.66	116.02	108.38
1	A	535	THR	CB-CA-C	5.63	120.14	110.01
1	A	602	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	452	LYS	N-CA-C	-5.60	105.95	112.89
1	A	228	PHE	N-CA-C	5.58	120.08	112.04
1	A	672	ASP	CA-CB-CG	5.58	118.18	112.60
2	B	1099	VAL	N-CA-CB	5.58	116.47	110.62
1	A	1311	VAL	N-CA-C	5.55	116.12	108.12
1	A	917	SER	CA-C-N	5.55	128.27	120.28
1	A	917	SER	C-N-CA	5.55	128.27	120.28
1	A	1098	VAL	N-CA-CB	5.54	113.99	110.50
3	C	62	PHE	N-CA-C	-5.52	105.16	111.07
10	L	62	LYS	CA-C-N	5.51	128.22	120.28
10	L	62	LYS	C-N-CA	5.51	128.22	120.28
2	B	1007	VAL	CB-CA-C	5.50	114.72	109.33
8	J	1	MET	CA-C-N	5.47	131.82	121.97
8	J	1	MET	C-N-CA	5.47	131.82	121.97
10	L	27	LEU	CA-C-N	5.47	131.99	121.54
10	L	27	LEU	C-N-CA	5.47	131.99	121.54
2	B	476	ARG	CA-C-N	5.43	131.91	121.54
2	B	476	ARG	C-N-CA	5.43	131.91	121.54
3	C	200	GLU	N-CA-C	5.43	118.11	111.82
1	A	884	ASP	N-CA-C	5.42	119.37	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	GLU	CA-C-N	5.40	127.78	120.44
4	E	4	GLU	C-N-CA	5.40	127.78	120.44
1	A	1072	ILE	CA-C-N	5.40	126.08	120.03
1	A	1072	ILE	C-N-CA	5.40	126.08	120.03
1	A	985	ASP	CA-CB-CG	5.35	117.95	112.60
2	B	842	ASN	CA-CB-CG	5.35	117.95	112.60
1	A	1138	ILE	N-CA-C	5.34	116.22	111.90
9	K	39	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	794	PRO	CA-C-N	5.32	127.35	120.44
1	A	794	PRO	C-N-CA	5.32	127.35	120.44
2	B	739	THR	N-CA-C	-5.31	107.35	113.88
2	B	66	ASP	CA-C-N	5.30	127.33	120.44
2	B	66	ASP	C-N-CA	5.30	127.33	120.44
2	B	1130	PHE	N-CA-C	-5.29	102.25	109.71
2	B	294	ASP	CA-CB-CG	5.29	117.89	112.60
6	H	91	ASP	CA-C-N	5.25	130.43	122.08
6	H	91	ASP	C-N-CA	5.25	130.43	122.08
1	A	237	THR	N-CA-C	-5.24	106.95	113.55
2	B	758	PHE	CA-CB-CG	5.24	119.04	113.80
3	C	82	TYR	N-CA-C	-5.23	101.44	109.76
4	E	46	TYR	N-CA-C	5.22	119.34	112.92
2	B	1085	ILE	N-CA-C	5.18	116.05	108.53
1	A	1001	ARG	N-CA-C	5.17	119.23	113.02
3	C	96	SER	N-CA-C	5.16	116.64	108.96
2	B	370	PHE	CA-C-N	5.16	127.50	120.54
2	B	370	PHE	C-N-CA	5.16	127.50	120.54
7	I	10	CYS	N-CA-C	5.16	116.59	111.07
1	A	1010	ALA	CA-C-N	5.15	127.14	120.44
1	A	1010	ALA	C-N-CA	5.15	127.14	120.44
2	B	436	VAL	N-CA-C	-5.14	105.53	110.72
1	A	1366	ARG	N-CA-C	5.14	118.33	111.75
10	L	65	VAL	N-CA-C	5.13	115.98	108.53
2	B	1001	PHE	N-CA-C	5.13	117.19	109.23
1	A	474	VAL	CA-C-N	5.13	127.11	120.44
1	A	474	VAL	C-N-CA	5.13	127.11	120.44
1	A	93	VAL	N-CA-C	5.12	115.74	110.36
1	A	1269	GLU	N-CA-C	5.10	118.66	112.23
2	B	99	LYS	N-CA-C	-5.08	103.28	110.29
7	I	78	CYS	N-CA-C	-5.07	102.97	110.48
1	A	612	ILE	CB-CA-C	5.07	116.87	111.35
1	A	716	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	276	LEU	N-CA-C	-5.06	105.85	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	64	ASN	N-CA-C	5.06	120.99	109.81
2	B	638	PHE	CA-CB-CG	5.05	118.85	113.80
2	B	743	ILE	N-CA-CB	5.05	116.46	110.55
1	A	116	ASP	CA-C-N	5.03	130.76	121.70
1	A	116	ASP	C-N-CA	5.03	130.76	121.70
1	A	671	ALA	CA-C-N	5.03	127.99	120.90
1	A	671	ALA	C-N-CA	5.03	127.99	120.90
4	E	48	ASP	CA-C-N	5.03	127.27	120.38
4	E	48	ASP	C-N-CA	5.03	127.27	120.38
2	B	397	ASP	CA-CB-CG	5.01	117.61	112.60
2	B	294	ASP	CA-C-N	5.01	125.54	119.98
2	B	294	ASP	C-N-CA	5.01	125.54	119.98
1	A	526	ASP	CA-CB-CG	5.00	117.60	112.60

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	182	0
2	B	8861	0	8884	132	0
3	C	2095	0	2051	35	0
4	E	1752	0	1776	18	0
5	F	688	0	707	4	0
6	H	1068	0	1040	15	0
7	I	971	0	927	13	0
8	J	532	0	542	15	0
9	K	919	0	929	18	0
10	L	363	0	386	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	383	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 7.

All (383) 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:535:THR:HG21	1:A:617:VAL:H	1.29	0.96
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.48	0.94
2:B:801:LYS:O	8:J:52:THR:HG23	1.76	0.86
2:B:345:LYS:HA	2:B:347:LYS:H	1.44	0.83
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.61	0.81
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.63	0.80
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.47	0.80
1:A:565:ILE:HG23	1:A:567:LYS:HG3	1.63	0.78
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.66	0.77
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.50	0.77
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.67	0.76
1:A:754:SER:H	1:A:757:ASN:HD22	1.34	0.75
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.00	0.75
2:B:515:HIS:HD2	2:B:517:THR:H	1.31	0.75
2:B:744:HIS:HD2	2:B:746:SER:H	1.33	0.75
1:A:218:ASP:H	1:A:219:PHE:HB3	1.52	0.74
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.52	0.74
1:A:535:THR:CG2	1:A:617:VAL:H	1.99	0.74
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.70	0.74
1:A:869:GLY:O	4:E:204:THR:HG21	1.88	0.72
1:A:315:LEU:HA	1:A:320:ARG:HB3	1.72	0.72
1:A:756:ILE:HD13	1:A:756:ILE:H	1.53	0.72
1:A:511:ILE:HA	1:A:521:MET:HE3	1.72	0.71
1:A:469:ARG:NH2	2:B:991:GLY:O	2.24	0.70
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.27	0.70
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.20	0.70
2:B:654:ARG:H	2:B:657:HIS:HD2	1.39	0.69
1:A:531:ILE:O	1:A:535:THR:HB	1.93	0.69
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.75	0.68
1:A:219:PHE:H	1:A:222:LEU:HG	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.59	0.67
1:A:368:LYS:HD3	1:A:372:LYS:HE3	1.76	0.66
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.76	0.66
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.78	0.65
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.77	0.65
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.79	0.65
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.30	0.64
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.79	0.64
1:A:1123:GLY:CA	1:A:1124:HIS:HB2	2.27	0.64
1:A:855:THR:HG21	1:A:857:ARG:HE	1.63	0.63
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.80	0.63
1:A:741:ASN:HD22	1:A:744:LYS:H	1.45	0.63
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.80	0.63
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.82	0.62
2:B:515:HIS:H	2:B:518:HIS:CD2	2.17	0.62
3:C:167:HIS:HD2	3:C:169:LYS:H	1.44	0.62
2:B:864:LYS:H	2:B:872:GLU:HB2	1.64	0.62
2:B:1072:MET:HG3	2:B:1085:ILE:HB	1.80	0.62
2:B:43:LEU:HD11	2:B:811:TYR:O	2.00	0.62
1:A:545:GLN:HG2	1:A:549:MET:HE2	1.82	0.62
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.82	0.61
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.82	0.61
3:C:66:ARG:NH2	8:J:3:VAL:O	2.31	0.61
3:C:37:MET:HE2	3:C:244:VAL:HA	1.81	0.61
1:A:1329:THR:HG22	1:A:1331:SER:H	1.66	0.61
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.48	0.61
1:A:40:THR:HG23	1:A:54:ASN:HD21	1.67	0.60
2:B:1002:THR:HG22	2:B:1004:GLU:H	1.65	0.60
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.33	0.60
1:A:53:LEU:HG	1:A:54:ASN:HD22	1.66	0.60
1:A:596:THR:C	1:A:598:LEU:H	2.10	0.60
1:A:399:HIS:O	1:A:401:GLY:N	2.32	0.60
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.84	0.59
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.84	0.59
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.85	0.59
2:B:346:GLU:HA	2:B:349:ILE:HD12	1.84	0.59
1:A:535:THR:HG21	1:A:617:VAL:N	2.10	0.58
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.51	0.58
1:A:1105:LEU:HB3	1:A:1384:VAL:HG22	1.86	0.58
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.36	0.58
1:A:567:LYS:HB3	6:H:95:TYR:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.86	0.58
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.86	0.58
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.84	0.57
1:A:567:LYS:HZ3	6:H:95:TYR:HE1	1.53	0.57
1:A:709:THR:HB	1:A:712:GLU:H	1.70	0.57
3:C:56:THR:HG22	3:C:58:LEU:H	1.70	0.57
9:K:65:HIS:HD2	9:K:67:PHE:H	1.51	0.57
3:C:93:ASP:O	3:C:127:ARG:NH2	2.36	0.57
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.87	0.57
1:A:1086:PHE:HB3	1:A:1092:LYS:HB3	1.87	0.57
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.87	0.56
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.87	0.56
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.87	0.56
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.87	0.56
7:I:111:THR:HG23	7:I:113:ASP:H	1.71	0.56
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.87	0.55
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.88	0.55
2:B:839:MET:CE	2:B:980:PHE:HB2	2.35	0.55
3:C:165:LYS:O	9:K:6:ARG:NH1	2.40	0.55
1:A:91:PHE:HE1	1:A:99:ILE:HG21	1.71	0.55
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.88	0.55
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.87	0.55
2:B:486:TYR:OH	2:B:1096:ARG:HB3	2.07	0.55
2:B:424:LEU:O	2:B:428:ILE:HG12	2.06	0.55
3:C:221:TYR:HB3	6:H:46:LEU:HD22	1.89	0.54
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.90	0.54
1:A:120:GLU:HA	1:A:123:ARG:HB2	1.90	0.54
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.54	0.54
2:B:275:TYR:HB2	2:B:355:ILE:HD11	1.89	0.54
1:A:208:LEU:HD23	1:A:235:ILE:HD11	1.88	0.54
2:B:651:LEU:HD21	2:B:741:CYS:HB3	1.88	0.54
3:C:75:MET:HE2	3:C:239:PRO:HG2	1.89	0.54
1:A:456:MET:HE3	1:A:510:GLN:HB2	1.89	0.54
1:A:567:LYS:HB3	6:H:96:VAL:H	1.73	0.54
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.73	0.54
2:B:516:ASN:H	2:B:516:ASN:HD22	1.56	0.54
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.89	0.54
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.88	0.54
8:J:28:ASP:HB3	8:J:30:LEU:HD12	1.89	0.53
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.72	0.53
6:H:2:SER:HB3	6:H:3:ASN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:THR:O	1:A:762:SER:HB3	2.09	0.53
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.90	0.53
1:A:700:ASN:HD22	7:I:115:LYS:HB2	1.73	0.53
1:A:756:ILE:H	1:A:756:ILE:CD1	2.22	0.53
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.91	0.52
1:A:935:GLN:HE22	1:A:938:LYS:HD3	1.73	0.52
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.74	0.52
2:B:640:VAL:CG1	2:B:649:LYS:HB3	2.40	0.52
3:C:108:GLU:HA	3:C:149:LYS:HG2	1.91	0.52
2:B:778:MET:HE3	2:B:1094:ARG:HG3	1.92	0.52
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.43	0.52
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.90	0.52
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.38	0.52
8:J:1:MET:N	8:J:57:ILE:H	2.08	0.52
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.92	0.52
2:B:515:HIS:CD2	2:B:517:THR:H	2.20	0.52
10:L:59:ALA:O	10:L:60:ARG:HB3	2.10	0.52
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.91	0.52
4:E:88:VAL:HB	4:E:116:ILE:HD13	1.92	0.52
1:A:351:THR:HG21	1:A:466:SER:O	2.11	0.51
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.92	0.51
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.93	0.51
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.76	0.51
1:A:57:ARG:HA	1:A:68:GLN:HB3	1.91	0.51
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.74	0.51
1:A:626:ASN:O	1:A:631:HIS:CD2	2.63	0.51
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.92	0.51
1:A:269:ILE:HG22	1:A:299:HIS:HB2	1.93	0.51
1:A:541:ILE:HD11	1:A:577:ILE:HG12	1.93	0.51
2:B:302:CYS:HA	2:B:310:MET:HE3	1.92	0.51
7:I:50:THR:HG22	7:I:52:ILE:H	1.76	0.51
7:I:87:GLN:HE22	7:I:97:MET:HE2	1.76	0.51
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.94	0.50
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.93	0.50
7:I:10:CYS:HB3	7:I:12:ASN:HD22	1.76	0.50
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.44	0.50
2:B:241:ARG:HA	2:B:253:THR:HG22	1.93	0.50
2:B:839:MET:HE1	2:B:980:PHE:CB	2.40	0.50
1:A:567:LYS:O	1:A:569:LYS:N	2.45	0.50
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.92	0.50
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD11	1:A:325:ILE:HG12	1.94	0.50
4:E:50:MET:HG2	4:E:52:ARG:HH11	1.76	0.50
1:A:218:ASP:N	1:A:219:PHE:HB3	2.22	0.49
1:A:472:LEU:O	1:A:475:THR:HB	2.12	0.49
1:A:503:GLN:NE2	5:F:90:ARG:HH22	2.11	0.49
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.94	0.49
1:A:1081:LEU:HD23	1:A:1083:THR:HB	1.93	0.49
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.93	0.49
2:B:797:TYR:O	8:J:1:MET:HG2	2.13	0.49
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.93	0.49
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.47	0.49
7:I:50:THR:H	7:I:92:ARG:HH22	1.60	0.49
1:A:117:GLU:H	1:A:118:HIS:HB2	1.77	0.49
2:B:999:MET:HE2	2:B:1011:ILE:CD1	2.43	0.49
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.94	0.49
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.28	0.49
1:A:225:ASN:HD22	1:A:228:PHE:H	1.60	0.49
1:A:1191:TRP:HZ3	7:I:43:VAL:HG21	1.77	0.49
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.77	0.49
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.94	0.49
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.13	0.49
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.77	0.49
2:B:345:LYS:HA	2:B:347:LYS:N	2.22	0.48
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.95	0.48
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.48	0.48
4:E:147:HIS:CD2	4:E:149:LEU:H	2.31	0.48
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.28	0.48
1:A:299:HIS:HA	1:A:302:THR:HG22	1.96	0.48
3:C:98:VAL:H	3:C:122:SER:HB2	1.78	0.48
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.94	0.48
6:H:2:SER:N	6:H:61:SER:HG	2.11	0.48
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.96	0.48
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.96	0.48
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.95	0.48
1:A:626:ASN:O	1:A:631:HIS:HD2	1.97	0.48
7:I:62:ILE:HG12	7:I:84:VAL:HG11	1.95	0.48
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.95	0.48
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.96	0.48
1:A:117:GLU:N	1:A:118:HIS:HB2	2.29	0.47
1:A:567:LYS:HE3	6:H:46:LEU:HD12	1.95	0.47
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:109:LYS:HG3	6:H:110:ASP:H	1.78	0.47
1:A:705:LYS:HE3	1:A:705:LYS:H	1.78	0.47
1:A:855:THR:CG2	1:A:857:ARG:HE	2.26	0.47
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.98	0.47
2:B:101:MET:HE3	2:B:169:ARG:HH11	1.80	0.47
2:B:953:LEU:O	2:B:964:VAL:HG23	2.15	0.47
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.79	0.47
7:I:102:VAL:HG22	7:I:109:ILE:HG12	1.95	0.47
1:A:821:ARG:O	1:A:825:ILE:HG12	2.15	0.47
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.48	0.47
2:B:849:GLY:O	2:B:852:ARG:HB2	2.15	0.47
1:A:15:LYS:HB3	2:B:1220:ARG:HG3	1.96	0.47
1:A:266:LEU:HA	1:A:269:ILE:HG12	1.95	0.47
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.96	0.47
1:A:451:HIS:HB3	1:A:453:MET:H	1.80	0.47
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.50	0.47
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.97	0.47
1:A:219:PHE:HZ	1:A:226:GLU:HA	1.80	0.46
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.96	0.46
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.98	0.46
2:B:516:ASN:H	2:B:516:ASN:ND2	2.12	0.46
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.96	0.46
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.98	0.46
3:C:221:TYR:HD1	3:C:222:LYS:HG2	1.81	0.46
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.97	0.46
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.47	0.46
2:B:1100:ASP:HA	2:B:1103:ILE:CD1	2.46	0.46
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.98	0.46
2:B:1100:ASP:HA	2:B:1103:ILE:HD11	1.98	0.46
1:A:663:SER:HB2	2:B:1085:ILE:HG13	1.98	0.46
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.98	0.46
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.98	0.46
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.40	0.46
4:E:185:ALA:HA	4:E:190:LEU:HD12	1.98	0.46
6:H:89:LEU:C	6:H:91:ASP:H	2.23	0.46
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.97	0.46
2:B:806:THR:HG22	2:B:808:ALA:H	1.81	0.46
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.48	0.46
3:C:46:ILE:HA	3:C:159:ALA:HA	1.98	0.46
9:K:7:PHE:O	9:K:11:LEU:HB2	2.16	0.46
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.98	0.46
1:A:211:PHE:HA	1:A:214:ILE:HD11	1.99	0.45
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.16	0.45
2:B:620:ARG:HD2	7:I:68:LEU:HD11	1.99	0.45
4:E:147:HIS:HD2	4:E:149:LEU:H	1.64	0.45
1:A:752:LYS:HB3	2:B:1018:PRO:HG2	1.99	0.45
2:B:1060:ARG:HA	2:B:1064:TYR:O	2.16	0.45
2:B:1099:VAL:O	2:B:1103:ILE:HG13	2.16	0.45
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.82	0.45
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.50	0.45
4:E:24:LYS:HB3	4:E:30:ILE:HB	1.98	0.45
1:A:575:LYS:HB3	1:A:612:ILE:HG13	1.97	0.45
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.98	0.45
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.98	0.45
3:C:33:LEU:HG	3:C:37:MET:HE3	1.99	0.45
3:C:142:VAL:H	8:J:16:ASP:HB3	1.81	0.45
1:A:120:GLU:HG2	1:A:124:GLN:HE21	1.80	0.45
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.97	0.45
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.98	0.45
2:B:466:TRP:HB3	2:B:475:SER:HB2	1.98	0.45
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.47	0.45
1:A:374:LEU:HA	2:B:1107:ALA:HB2	1.99	0.45
1:A:935:GLN:NE2	1:A:938:LYS:HD3	2.31	0.45
4:E:77:SER:HB2	4:E:105:PHE:CD2	2.52	0.45
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.98	0.45
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.98	0.45
1:A:1021:LEU:HD11	1:A:1025:ARG:HH11	1.81	0.45
2:B:128:LEU:HD11	2:B:170:LEU:HB2	1.99	0.45
10:L:61:THR:HB	10:L:63:ARG:H	1.82	0.45
1:A:540:PHE:HB3	1:A:571:LEU:HG	1.98	0.45
2:B:745:PRO:O	2:B:748:ILE:HG12	2.17	0.45
2:B:724:ASP:HB3	2:B:727:LYS:HD2	1.98	0.44
2:B:864:LYS:HB3	2:B:872:GLU:H	1.81	0.44
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.52	0.44
4:E:147:HIS:CD2	4:E:149:LEU:HB2	2.52	0.44
1:A:544:ASP:HB2	9:K:47:ARG:NH2	2.32	0.44
1:A:70:CYS:HB2	2:B:1172:ILE:HG23	1.99	0.44
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.82	0.44
7:I:47:GLU:OE1	7:I:50:THR:HG23	2.17	0.44
1:A:58:LEU:HD23	1:A:244:PRO:HD3	1.98	0.44
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:VAL:O	2:B:480:SER:HA	2.17	0.44
2:B:706:GLN:O	2:B:710:LEU:HB2	2.16	0.44
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.83	0.44
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.83	0.44
3:C:143:LEU:HD21	3:C:146:LYS:HE3	2.00	0.44
8:J:48:ARG:O	8:J:52:THR:HB	2.17	0.44
1:A:596:THR:O	1:A:598:LEU:N	2.51	0.44
1:A:92:HIS:HD2	1:A:94:GLY:H	1.66	0.44
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.99	0.44
1:A:456:MET:HE2	1:A:507:VAL:HA	2.00	0.44
3:C:18:VAL:HG22	3:C:240:VAL:HB	2.00	0.44
1:A:55:ASP:O	1:A:57:ARG:N	2.51	0.44
1:A:899:VAL:HB	1:A:929:LEU:HD22	2.00	0.44
1:A:1128:GLN:HG2	1:A:1132:LYS:HE3	2.00	0.44
3:C:18:VAL:HG23	3:C:232:VAL:HB	2.00	0.44
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.13	0.44
4:E:12:LEU:HD11	4:E:58:MET:HE1	2.00	0.44
8:J:17:LYS:HD3	8:J:41:LEU:HD21	1.99	0.44
2:B:898:LEU:HD21	2:B:964:VAL:HG11	2.00	0.43
9:K:32:VAL:HG22	9:K:74:ARG:HG3	2.00	0.43
1:A:21:LEU:HD12	1:A:229:SER:HB2	2.00	0.43
3:C:62:PHE:O	3:C:66:ARG:HG3	2.19	0.43
1:A:324:SER:O	1:A:326:ARG:N	2.43	0.43
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.99	0.43
2:B:476:ARG:O	2:B:478:GLY:N	2.51	0.43
2:B:486:TYR:OH	2:B:778:MET:HE2	2.18	0.43
1:A:704:ALA:HB2	1:A:710:LEU:HA	2.00	0.43
1:A:108:MET:O	1:A:109:HIS:HB2	2.19	0.43
1:A:534:LEU:O	1:A:574:GLY:HA3	2.18	0.43
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.32	0.43
1:A:1154:TYR:CE1	7:I:18:GLU:HG3	2.53	0.43
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.88	0.43
1:A:525:GLN:HB3	2:B:835:GLN:HG2	2.01	0.43
2:B:219:ALA:HB2	2:B:405:ARG:HG2	2.00	0.43
3:C:67:LEU:HA	3:C:70:ILE:HD12	2.00	0.43
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	2.00	0.43
1:A:483:ASP:O	2:B:987:LYS:HE2	2.18	0.43
2:B:640:VAL:HG12	2:B:649:LYS:HB3	2.00	0.43
4:E:77:SER:HB2	4:E:105:PHE:HD2	1.83	0.42
1:A:535:THR:HG23	1:A:616:VAL:HA	2.01	0.42
6:H:93:TYR:HA	6:H:145:ARG:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:7:PHE:HA	9:K:10:PHE:CZ	2.54	0.42
1:A:265:LYS:HD3	1:A:322:VAL:HG21	2.01	0.42
1:A:1388:GLY:O	1:A:1391:ARG:HG3	2.20	0.42
2:B:918:ILE:HG13	2:B:935:ARG:HD2	2.00	0.42
9:K:61:TYR:HA	9:K:72:LYS:O	2.19	0.42
1:A:751:SER:HB2	2:B:1015:HIS:CE1	2.55	0.42
1:A:830:LYS:HE2	1:A:1082:ASN:HD22	1.85	0.42
9:K:55:LYS:HB2	9:K:81:TYR:CD1	2.54	0.42
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.52	0.42
1:A:778:GLY:HA3	2:B:516:ASN:ND2	2.35	0.42
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.54	0.42
2:B:706:GLN:H	2:B:710:LEU:HG	1.84	0.42
6:H:40:LEU:HD13	6:H:123:MET:HG3	2.01	0.42
1:A:688:LYS:HD3	1:A:688:LYS:HA	1.96	0.42
1:A:1266:THR:HA	1:A:1270:ASN:HD22	1.85	0.42
1:A:629:LEU:HD13	1:A:645:LEU:HD21	2.02	0.42
1:A:963:ILE:HG22	1:A:1045:VAL:HG22	2.00	0.42
1:A:518:LYS:HE2	1:A:624:SER:O	2.19	0.41
1:A:579:SER:HA	1:A:582:ILE:HD12	2.01	0.41
1:A:1089:VAL:HB	1:A:1092:LYS:HD3	2.01	0.41
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	2.01	0.41
2:B:566:LEU:HD11	2:B:586:TRP:CE2	2.54	0.41
1:A:446:ARG:HD3	1:A:478:TYR:O	2.20	0.41
2:B:69:LEU:HD12	2:B:90:ILE:HB	2.01	0.41
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.56	0.41
2:B:758:PHE:CZ	2:B:1031:LEU:HD22	2.55	0.41
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.35	0.41
2:B:140:ILE:HB	2:B:141:ASP:HB2	2.03	0.41
1:A:348:SER:HA	1:A:489:LEU:O	2.20	0.41
1:A:1156:PRO:HA	1:A:1190:PRO:HB3	2.03	0.41
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	2.02	0.41
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.17	0.41
1:A:982:THR:HG22	1:A:984:LYS:H	1.86	0.41
2:B:634:TYR:CD1	2:B:692:TYR:HB3	2.56	0.41
2:B:983:ARG:HH11	2:B:983:ARG:HB2	1.86	0.41
1:A:683:ILE:HG21	1:A:801:GLU:HG3	2.03	0.41
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.20	0.41
1:A:1138:ILE:HG13	1:A:1282:VAL:HG21	2.03	0.41
3:C:254:LYS:HD3	9:K:42:LEU:HD13	2.02	0.41
2:B:181:LEU:HD22	2:B:189:LEU:HD23	2.03	0.41
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HA	1:A:277:GLU:HB2	2.03	0.41
1:A:290:GLU:HA	1:A:293:GLU:HB2	2.03	0.41
2:B:1103:ILE:HG13	2:B:1103:ILE:H	1.66	0.41
3:C:39:ALA:HA	3:C:164:ALA:HB3	2.01	0.41
5:F:111:LEU:HD23	5:F:114:GLU:O	2.20	0.41
2:B:619:ILE:H	2:B:619:ILE:HG12	1.78	0.41
2:B:841:MET:O	2:B:993:THR:HA	2.21	0.40
2:B:1172:ILE:HG22	2:B:1174:LYS:HG3	2.03	0.40
1:A:883:LEU:O	1:A:886:ILE:HG22	2.21	0.40
2:B:408:LEU:HD11	2:B:545:ILE:HD12	2.02	0.40
3:C:44:LEU:HD22	3:C:129:ILE:HG13	2.03	0.40
1:A:567:LYS:HZ3	6:H:43:ASN:HB3	1.87	0.40
1:A:993:LEU:HD22	1:A:1046:LEU:HG	2.04	0.40
2:B:789:MET:HE3	2:B:953:LEU:HB2	2.03	0.40
2:B:976:ILE:O	2:B:990:ILE:HB	2.20	0.40
1:A:522:GLY:HA2	1:A:630:ILE:HD13	2.03	0.40
1:A:871:ASP:HB3	4:E:204:THR:HG23	2.03	0.40
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.62	0.40
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.02	0.40
2:B:356:LEU:HA	2:B:360:PHE:HB3	2.04	0.40
6:H:96:VAL:HG13	6:H:143:LEU:HG	2.03	0.40
1:A:145:LYS:HB3	1:A:171:GLN:HE22	1.86	0.40
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	2.04	0.40
5:F:107:VAL:HG12	5:F:109:VAL:H	1.86	0.40
9:K:35:PHE:O	9:K:70:ARG:HA	2.21	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%)	1237 (89%)	112 (8%)	46 (3%)	3 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1096/1224 (90%)	966 (88%)	94 (9%)	36 (3%)	3	17
3	C	264/318 (83%)	247 (94%)	11 (4%)	6 (2%)	5	23
4	E	212/215 (99%)	201 (95%)	7 (3%)	4 (2%)	6	27
5	F	83/155 (54%)	74 (89%)	8 (10%)	1 (1%)	10	37
6	H	129/146 (88%)	99 (77%)	22 (17%)	8 (6%)	1	7
7	I	117/122 (96%)	101 (86%)	14 (12%)	2 (2%)	7	30
8	J	63/70 (90%)	59 (94%)	2 (3%)	2 (3%)	3	18
9	K	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
10	L	44/70 (63%)	31 (70%)	6 (14%)	7 (16%)	0	0
All	All	3515/4173 (84%)	3124 (89%)	279 (8%)	112 (3%)	3	18

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	ASP
1	A	109	HIS
1	A	325	ILE
1	A	567	LYS
1	A	1223	ASP
2	B	139	ALA
2	B	367	LEU
2	B	469	GLN
2	B	477	ALA
2	B	648	HIS
2	B	712	PRO
2	B	751	VAL
2	B	880	THR
2	B	1046	PRO
2	B	1156	ASP
3	C	4	GLU
4	E	77	SER
6	H	85	GLY
6	H	109	LYS
6	H	131	ASN
6	H	140	ALA
8	J	2	ILE
10	L	28	LYS
10	L	46	VAL

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Mol	Chain	Res	Type
10	L	50	ASP
10	L	60	ARG
1	A	40	THR
1	A	219	PHE
1	A	286	HIS
1	A	299	HIS
1	A	409	SER
1	A	418	SER
1	A	569	LYS
1	A	597	LEU
1	A	1081	LEU
1	A	1123	GLY
1	A	1124	HIS
1	A	1437	GLY
2	B	137	TYR
2	B	707	PRO
2	B	709	ASP
2	B	850	LEU
2	B	881	ASN
2	B	883	LEU
2	B	1066	SER
3	C	5	GLY
3	C	141	GLY
4	E	86	PRO
6	H	90	ALA
10	L	64	LEU
1	A	68	GLN
1	A	76	GLU
1	A	118	HIS
1	A	250	ILE
1	A	312	PRO
1	A	332	LYS
1	A	922	ASP
1	A	1221	LYS
2	B	138	GLU
2	B	526	GLU
2	B	563	MET
2	B	792	MET
2	B	886	LYS
3	C	90	ASP
4	E	126	SER
6	H	108	SER

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Mol	Chain	Res	Type
8	J	6	ARG
1	A	214	ILE
1	A	255	SER
1	A	275	SER
1	A	424	ILE
1	A	775	ILE
1	A	1278	ASN
2	B	478	GLY
2	B	646	LEU
2	B	647	GLY
2	B	708	GLU
2	B	943	SER
2	B	1155	SER
2	B	1181	GLU
3	C	142	VAL
7	I	3	THR
7	I	77	LYS
1	A	257	ARG
1	A	593	GLU
1	A	958	VAL
1	A	975	HIS
2	B	364	ILE
2	B	447	ALA
2	B	592	ASN
2	B	1157	ALA
2	B	1169	MET
3	C	214	ASN
5	F	73	ALA
6	H	17	PRO
10	L	27	LEU
10	L	45	ALA
1	A	35	ILE
1	A	56	PRO
1	A	119	ASN
1	A	399	HIS
1	A	404	TYR
2	B	1108	ARG
1	A	283	GLY
1	A	310	GLY
6	H	18	GLY
1	A	331	GLY
1	A	568	PRO

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Mol	Chain	Res	Type
2	B	976	ILE
1	A	599	SER
4	E	51	GLY

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%)	1076 (88%)	149 (12%)	5	20
2	B	967/1061 (91%)	862 (89%)	105 (11%)	6	24
3	C	234/274 (85%)	214 (92%)	20 (8%)	10	35
4	E	196/197 (100%)	178 (91%)	18 (9%)	8	31
5	F	75/137 (55%)	72 (96%)	3 (4%)	28	60
6	H	117/128 (91%)	97 (83%)	20 (17%)	2	10
7	I	113/116 (97%)	103 (91%)	10 (9%)	9	33
8	J	60/65 (92%)	48 (80%)	12 (20%)	1	6
9	K	99/102 (97%)	88 (89%)	11 (11%)	6	24
10	L	40/57 (70%)	31 (78%)	9 (22%)	1	4
All	All	3126/3657 (86%)	2769 (89%)	357 (11%)	5	23

All (357) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	22	PHE
1	A	30	ILE
1	A	34	LYS
1	A	41	MET
1	A	43	GLU
1	A	58	LEU
1	A	61	ILE
1	A	68	GLN
1	A	70	CYS

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Mol	Chain	Res	Type
1	A	84	ILE
1	A	88	LYS
1	A	93	VAL
1	A	104	GLU
1	A	113	LEU
1	A	120	GLU
1	A	126	LEU
1	A	128	ILE
1	A	143	LYS
1	A	149	GLU
1	A	164	ARG
1	A	174	ILE
1	A	179	LEU
1	A	199	LEU
1	A	208	LEU
1	A	216	VAL
1	A	218	ASP
1	A	235	ILE
1	A	250	ILE
1	A	252	PHE
1	A	262	LEU
1	A	265	LYS
1	A	270	LEU
1	A	271	LYS
1	A	276	LEU
1	A	295	LEU
1	A	299	HIS
1	A	302	THR
1	A	303	TYR
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	332	LYS
1	A	335	ARG
1	A	337	ARG
1	A	343	LYS
1	A	344	ARG
1	A	351	THR
1	A	359	LEU

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Mol	Chain	Res	Type
1	A	372	LYS
1	A	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	419	LYS
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	469	ARG
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	496	GLU
1	A	527	THR
1	A	535	THR
1	A	541	ILE
1	A	565	ILE
1	A	566	ILE
1	A	567	LYS
1	A	569	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	634	THR
1	A	672	ASP
1	A	682	THR
1	A	687	LYS
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	705	LYS
1	A	709	THR
1	A	722	LEU
1	A	740	LEU
1	A	756	ILE
1	A	788	SER
1	A	821	ARG
1	A	833	GLU

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Mol	Chain	Res	Type
1	A	848	ILE
1	A	849	MET
1	A	855	THR
1	A	867	ILE
1	A	878	ILE
1	A	919	ILE
1	A	925	LEU
1	A	926	GLN
1	A	927	VAL
1	A	931	GLU
1	A	938	LYS
1	A	960	ILE
1	A	969	GLN
1	A	973	ILE
1	A	976	THR
1	A	990	VAL
1	A	1025	ARG
1	A	1048	ASN
1	A	1050	GLU
1	A	1052	GLN
1	A	1067	LEU
1	A	1081	LEU
1	A	1094	VAL
1	A	1102	LYS
1	A	1109	LYS
1	A	1110	ASN
1	A	1116	LEU
1	A	1142	THR
1	A	1170	ILE
1	A	1176	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1221	LYS
1	A	1234	GLU
1	A	1237	ILE
1	A	1264	GLU
1	A	1267	MET
1	A	1280	GLU
1	A	1293	SER
1	A	1297	GLU
1	A	1299	VAL
1	A	1322	ILE

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Mol	Chain	Res	Type
1	A	1351	GLU
1	A	1354	ASN
1	A	1366	ARG
1	A	1376	THR
1	A	1385	THR
1	A	1390	ASN
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1403	GLU
1	A	1424	VAL
1	A	1426	GLU
1	A	1445	ILE
2	B	25	ILE
2	B	45	SER
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	89	GLU
2	B	102	VAL
2	B	134	LYS
2	B	135	ARG
2	B	175	ARG
2	B	194	GLU
2	B	223	VAL
2	B	225	VAL
2	B	234	ILE
2	B	262	GLU
2	B	272	THR
2	B	299	GLU
2	B	305	VAL
2	B	312	GLU
2	B	323	VAL
2	B	355	ILE
2	B	357	GLN
2	B	365	THR
2	B	366	GLN
2	B	384	ARG
2	B	387	LEU
2	B	393	LYS
2	B	396	ASP
2	B	426	LYS

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Mol	Chain	Res	Type
2	B	428	ILE
2	B	431	TYR
2	B	432	MET
2	B	437	GLU
2	B	451	LYS
2	B	471	LYS
2	B	479	VAL
2	B	485	ARG
2	B	516	ASN
2	B	531	GLN
2	B	547	VAL
2	B	555	ILE
2	B	566	LEU
2	B	578	THR
2	B	604	ARG
2	B	616	ILE
2	B	619	ILE
2	B	620	ARG
2	B	624	LEU
2	B	644	GLU
2	B	646	LEU
2	B	653	VAL
2	B	658	ILE
2	B	706	GLN
2	B	708	GLU
2	B	709	ASP
2	B	710	LEU
2	B	762	ASN
2	B	786	ASN
2	B	788	ARG
2	B	791	THR
2	B	795	ILE
2	B	796	LEU
2	B	815	ARG
2	B	825	VAL
2	B	836	GLU
2	B	866	TYR
2	B	885	MET
2	B	886	LYS
2	B	889	THR
2	B	895	ASP
2	B	905	VAL

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Mol	Chain	Res	Type
2	B	906	SER
2	B	911	ILE
2	B	948	ILE
2	B	951	GLN
2	B	963	PHE
2	B	965	LYS
2	B	976	ILE
2	B	983	ARG
2	B	987	LYS
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1022	THR
2	B	1065	GLN
2	B	1085	ILE
2	B	1099	VAL
2	B	1103	ILE
2	B	1111	MET
2	B	1124	ARG
2	B	1128	LEU
2	B	1129	ARG
2	B	1147	LEU
2	B	1151	LEU
2	B	1175	LEU
2	B	1178	ASN
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	1203	LEU
2	B	1211	ASN
3	C	18	VAL
3	C	25	VAL
3	C	34	ARG
3	C	40	GLU
3	C	57	VAL
3	C	75	MET
3	C	77	ILE
3	C	79	GLN

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Mol	Chain	Res	Type
3	C	80	LEU
3	C	89	GLU
3	C	145	CYS
3	C	149	LYS
3	C	156	THR
3	C	211	ASP
3	C	215	GLU
3	C	231	ASN
3	C	235	VAL
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
4	E	20	LYS
4	E	50	MET
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	104	ASN
4	E	122	LYS
4	E	127	ILE
4	E	144	ILE
4	E	149	LEU
4	E	169	ARG
4	E	177	ARG
4	E	191	LYS
4	E	204	THR
4	E	213	ILE
5	F	93	ILE
5	F	99	LEU
5	F	110	ASP
6	H	5	LEU
6	H	15	VAL
6	H	16	ASP
6	H	21	ASN
6	H	22	LYS
6	H	26	ILE
6	H	35	GLN
6	H	42	ILE
6	H	46	LEU

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Mol	Chain	Res	Type
6	H	86	ASP
6	H	87	ARG
6	H	94	ASP
6	H	96	VAL
6	H	105	GLU
6	H	106	GLU
6	H	107	VAL
6	H	123	MET
6	H	136	LYS
6	H	139	ASN
6	H	142	LEU
7	I	35	VAL
7	I	37	GLU
7	I	50	THR
7	I	52	ILE
7	I	55	THR
7	I	77	LYS
7	I	84	VAL
7	I	98	VAL
7	I	111	THR
7	I	117	LYS
8	J	1	MET
8	J	2	ILE
8	J	3	VAL
8	J	13	VAL
8	J	22	LEU
8	J	28	ASP
8	J	30	LEU
8	J	37	SER
8	J	48	ARG
8	J	57	ILE
8	J	59	LYS
8	J	62	ARG
9	K	6	ARG
9	K	11	LEU
9	K	17	SER
9	K	20	LYS
9	K	31	VAL
9	K	33	ILE
9	K	42	LEU
9	K	47	ARG
9	K	51	LEU

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Mol	Chain	Res	Type
9	K	63	VAL
9	K	97	LYS
10	L	27	LEU
10	L	28	LYS
10	L	30	ILE
10	L	35	SER
10	L	40	LEU
10	L	47	ARG
10	L	51	CYS
10	L	61	THR
10	L	65	VAL

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	4	GLN
1	A	18	GLN
1	A	54	ASN
1	A	64	ASN
1	A	68	GLN
1	A	118	HIS
1	A	124	GLN
1	A	171	GLN
1	A	209	ASN
1	A	225	ASN
1	A	281	HIS
1	A	316	GLN
1	A	339	ASN
1	A	503	GLN
1	A	517	ASN
1	A	626	ASN
1	A	631	HIS
1	A	640	GLN
1	A	659	HIS
1	A	700	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	851	HIS
1	A	935	GLN

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Mol	Chain	Res	Type
1	A	965	GLN
1	A	972	HIS
1	A	1082	ASN
1	A	1188	GLN
1	A	1203	ASN
1	A	1222	ASN
1	A	1258	HIS
1	A	1270	ASN
1	A	1364	ASN
1	A	1427	ASN
2	B	47	GLN
2	B	53	GLN
2	B	103	ASN
2	B	115	GLN
2	B	121	ASN
2	B	215	GLN
2	B	325	GLN
2	B	363	HIS
2	B	366	GLN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	648	HIS
2	B	657	HIS
2	B	744	HIS
2	B	762	ASN
2	B	767	ASN
2	B	770	GLN
2	B	975	GLN
2	B	984	HIS
2	B	986	GLN
2	B	1015	HIS
2	B	1084	GLN
2	B	1093	GLN
2	B	1141	HIS
2	B	1161	HIS
2	B	1176	ASN
3	C	17	ASN
3	C	65	HIS
3	C	112	ASN
3	C	151	GLN

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Mol	Chain	Res	Type
3	C	214	ASN
3	C	231	ASN
3	C	242	GLN
4	E	147	HIS
6	H	131	ASN
7	I	12	ASN
7	I	46	HIS
7	I	87	GLN
8	J	53	HIS
9	K	65	HIS
9	K	89	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

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%)	0.24	75 (5%)	32	17	42, 82, 183, 220	0
2	B	1114/1224 (91%)	0.14	46 (4%)	41	23	39, 77, 146, 186	0
3	C	266/318 (83%)	-0.12	0	100	100	46, 72, 108, 145	0
4	E	214/215 (99%)	0.30	6 (2%)	55	34	52, 112, 155, 167	0
5	F	85/155 (54%)	-0.05	0	100	100	60, 90, 128, 150	0
6	H	133/146 (91%)	0.53	13 (9%)	13	7	72, 113, 146, 159	0
7	I	119/122 (97%)	0.21	3 (2%)	58	37	55, 84, 120, 131	0
8	J	65/70 (92%)	-0.19	1 (1%)	72	52	46, 66, 98, 109	0
9	K	114/120 (95%)	-0.19	1 (0%)	81	63	44, 74, 100, 118	0
10	L	46/70 (65%)	0.92	7 (15%)	5	3	53, 108, 135, 156	0
11	R	5/5 (100%)	1.35	0	100	100	170, 176, 182, 183	0
12	T	8/29 (27%)	1.71	2 (25%)	2	1	158, 164, 180, 181	0
All	All	3574/4207 (84%)	0.18	154 (4%)	40	22	39, 82, 167, 220	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	6.6
1	A	1087	ALA	5.9
2	B	715	ALA	5.7
6	H	85	GLY	5.7
1	A	65	LEU	5.0
1	A	250	ILE	4.8
2	B	882	THR	4.8
1	A	73	GLY	4.4
6	H	63	LEU	4.3
2	B	70	ILE	4.2
2	B	502	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	335	GLY	4.1
1	A	1090	ALA	4.0
1	A	1081	LEU	4.0
6	H	132	LEU	3.9
1	A	1091	SER	3.9
1	A	179	LEU	3.8
2	B	446	LEU	3.8
2	B	1170	THR	3.8
1	A	318	SER	3.7
2	B	1173	ALA	3.7
1	A	289	ILE	3.7
2	B	140	ILE	3.7
1	A	199	LEU	3.7
1	A	161	LEU	3.6
10	L	25	ALA	3.6
1	A	1176	LEU	3.5
6	H	46	LEU	3.5
2	B	709	ASP	3.5
10	L	28	LYS	3.5
1	A	252	PHE	3.4
1	A	30	ILE	3.4
2	B	448	ILE	3.4
1	A	1086	PHE	3.4
1	A	1089	VAL	3.4
1	A	201	VAL	3.3
10	L	45	ALA	3.3
2	B	648	HIS	3.3
2	B	250	PHE	3.2
4	E	98	ILE	3.2
10	L	26	THR	3.2
1	A	998	LEU	3.1
1	A	51	GLY	3.1
1	A	1088	GLY	3.0
1	A	567	LYS	3.0
2	B	1204	PHE	3.0
2	B	1189	ILE	3.0
1	A	319	GLY	3.0
1	A	86	LEU	3.0
10	L	27	LEU	2.9
2	B	345	LYS	2.8
2	B	486	TYR	2.8
12	T	19	DT	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	1200	ALA	2.8
9	K	114	LEU	2.8
2	B	474	SER	2.8
10	L	42	ARG	2.8
1	A	66	LYS	2.7
1	A	75	ASN	2.7
2	B	731	VAL	2.7
1	A	141	LEU	2.7
4	E	96	PHE	2.7
1	A	216	VAL	2.7
1	A	181	LEU	2.7
1	A	1445	ILE	2.7
6	H	135	LEU	2.7
2	B	881	ASN	2.7
1	A	96	ILE	2.6
2	B	865	LYS	2.6
2	B	712	PRO	2.6
2	B	708	GLU	2.6
2	B	880	THR	2.6
2	B	246	LYS	2.6
1	A	314	ALA	2.6
2	B	733	HIS	2.5
1	A	316	GLN	2.5
4	E	54	GLN	2.5
2	B	879	ARG	2.5
2	B	136	THR	2.5
1	A	317	LYS	2.5
1	A	69	THR	2.5
2	B	108	VAL	2.5
2	B	472	ALA	2.5
12	T	22	DT	2.5
2	B	436	VAL	2.5
1	A	125	ALA	2.5
1	A	292	ALA	2.5
7	I	4	PHE	2.5
1	A	1080	THR	2.5
4	E	53	PRO	2.4
1	A	1243	VAL	2.4
2	B	647	GLY	2.4
2	B	473	MET	2.4
1	A	294	SER	2.4
1	A	312	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1108	ALA	2.4
1	A	49	LYS	2.4
1	A	279	LEU	2.4
2	B	711	GLU	2.4
6	H	90	ALA	2.4
2	B	1224	PHE	2.4
1	A	178	GLY	2.3
7	I	2	THR	2.3
6	H	139	ASN	2.3
1	A	105	CYS	2.3
1	A	1254	ALA	2.3
4	E	103	LYS	2.3
6	H	136	LYS	2.3
2	B	139	ALA	2.3
6	H	83	GLN	2.3
1	A	237	THR	2.3
1	A	91	PHE	2.3
1	A	53	LEU	2.2
1	A	44	THR	2.2
2	B	878	GLN	2.2
6	H	86	ASP	2.2
1	A	1158	PRO	2.2
2	B	1214	PRO	2.2
1	A	182	VAL	2.2
1	A	74	MET	2.2
1	A	295	LEU	2.2
1	A	321	PRO	2.2
1	A	132	LYS	2.2
1	A	1084	PHE	2.2
2	B	251	ILE	2.2
1	A	24	PRO	2.2
1	A	78	PRO	2.2
1	A	1083	THR	2.2
2	B	1217	TYR	2.2
1	A	997	LEU	2.2
2	B	277	LYS	2.2
10	L	40	LEU	2.1
1	A	154	SER	2.1
1	A	1092	LYS	2.1
6	H	130	ARG	2.1
1	A	1085	HIS	2.1
1	A	138	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	208	LEU	2.1
1	A	235	ILE	2.1
2	B	710	LEU	2.1
7	I	120	GLN	2.1
1	A	1123	GLY	2.1
4	E	102	GLU	2.1
8	J	65	PRO	2.1
6	H	89	LEU	2.1
1	A	1187	GLN	2.1
6	H	82	PRO	2.1
2	B	477	ALA	2.1
1	A	1002	GLY	2.1
1	A	56	PRO	2.1
1	A	121	LEU	2.0
1	A	239	LEU	2.0
2	B	962	LYS	2.0
1	A	202	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	ZN	A	1734	1/1	0.76	0.09	300,300,300,300	0
13	ZN	B	1307	1/1	0.93	0.07	159,159,159,159	0
13	ZN	A	1735	1/1	0.95	0.07	146,146,146,146	0
13	ZN	I	203	1/1	0.99	0.03	94,94,94,94	0
13	ZN	L	105	1/1	0.99	0.02	102,102,102,102	0
14	MG	A	2001	1/1	0.99	0.03	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	ZN	J	101	1/1	1.00	0.02	57,57,57,57	0
13	ZN	C	319	1/1	1.00	0.01	66,66,66,66	0
13	ZN	I	204	1/1	1.00	0.02	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.