



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:44 AM UTC

PDB ID : 3S16 / pdb_00003s16
Title : RNA Polymerase II Initiation Complex with an 8-nt RNA
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-14
Resolution : 3.24 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

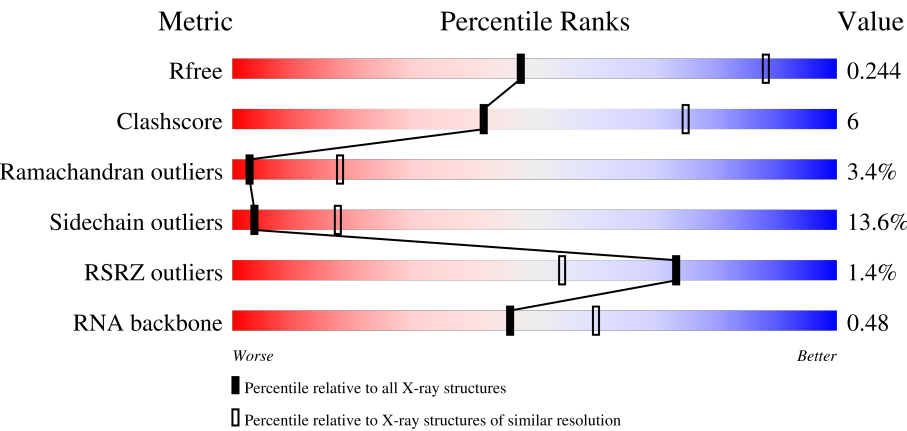
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)
RNA backbone	3983	1047 (3.52-2.96)

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% 58% 19% • 19%
2	B	1224	% 63% 24% • 9%
3	C	318	55% 23% 5% 16%
4	E	215	77% 21% •

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Mol	Chain	Length	Quality of chain
5	F	155	47%7%•45%
6	H	146	3% 60%27%•9%
7	I	122	74%20%••
8	J	70	49%37%7%7%
9	K	120	70%19%6%5%
10	L	70	6% 40%19%••34%
11	R	8	88%12%
12	T	29	28%17%55%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 28735 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(*UP*CP*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	8	Total	C	N	O	P	0	0	0
			173	78	35	53	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	13	Total	C	N	O	P	0	0	0
			261	125	43	80	13			

- 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

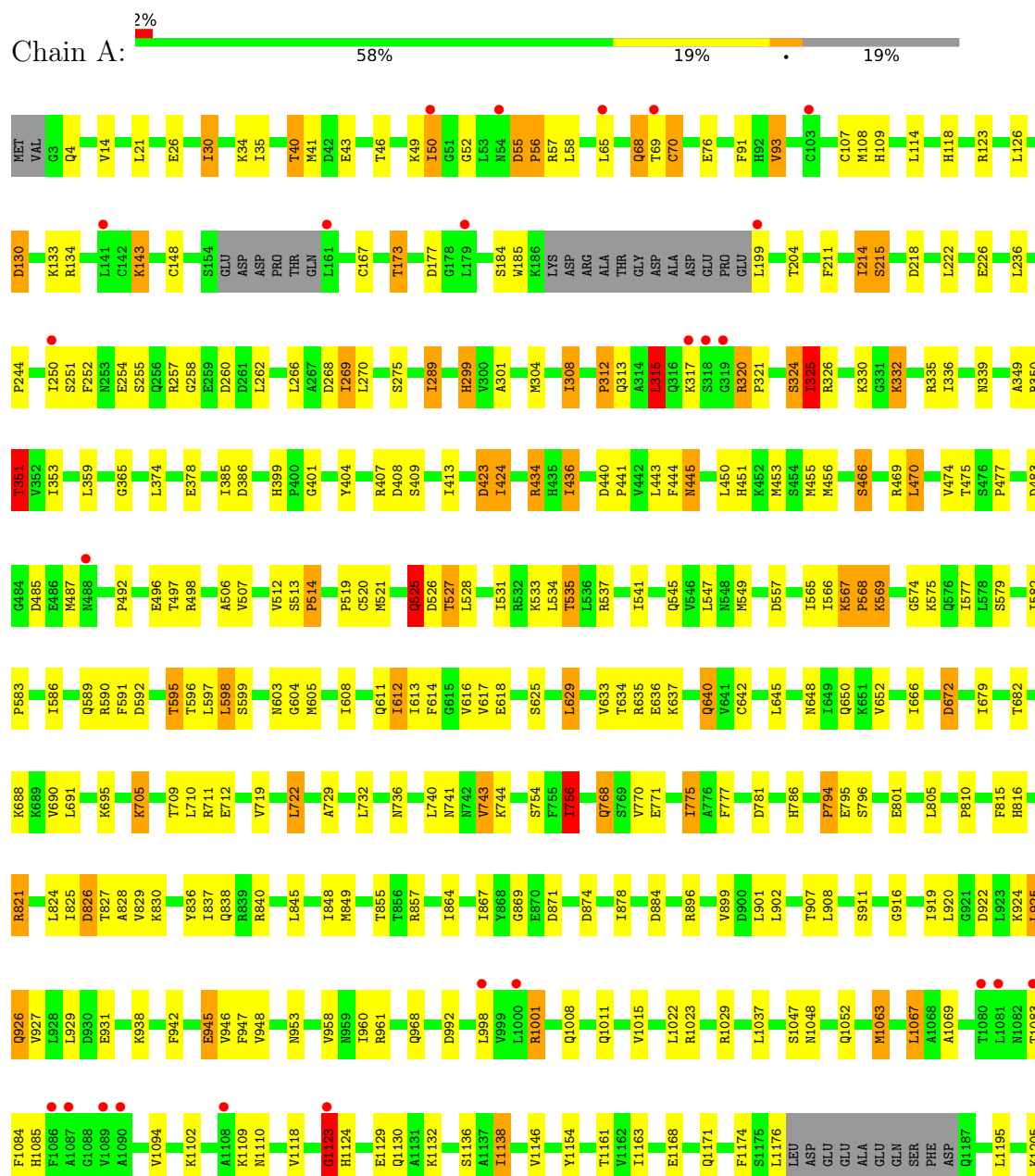
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

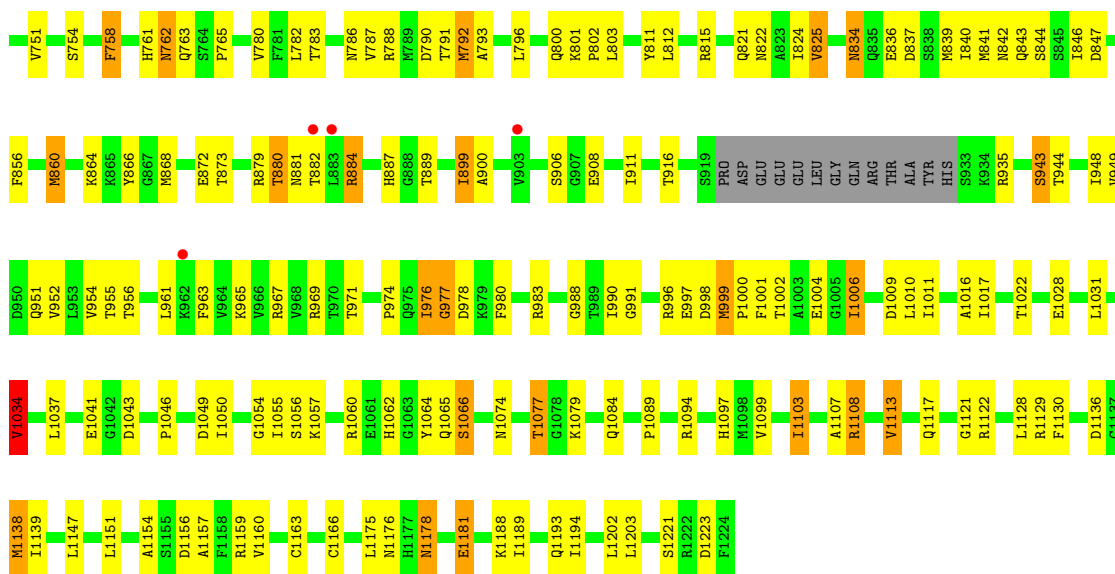
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

3 Residue-property plots [i](#)

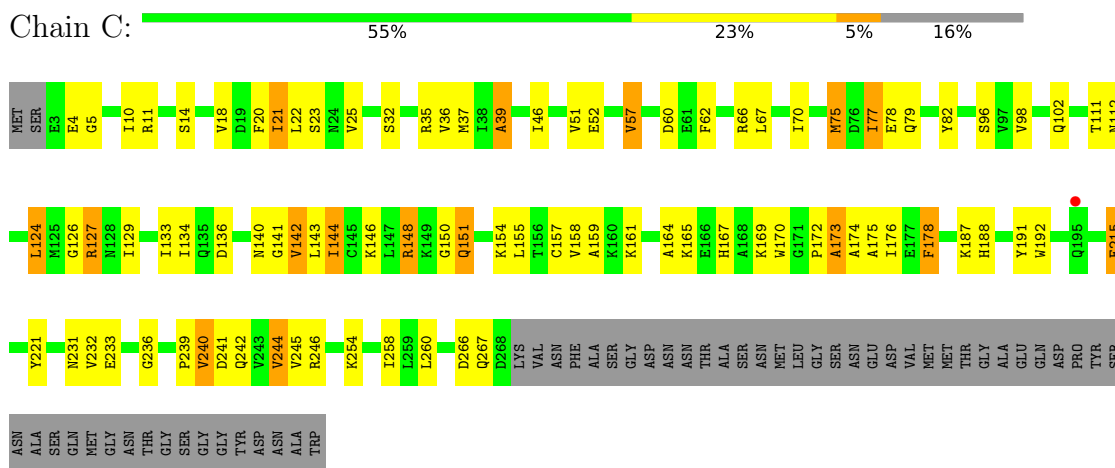
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

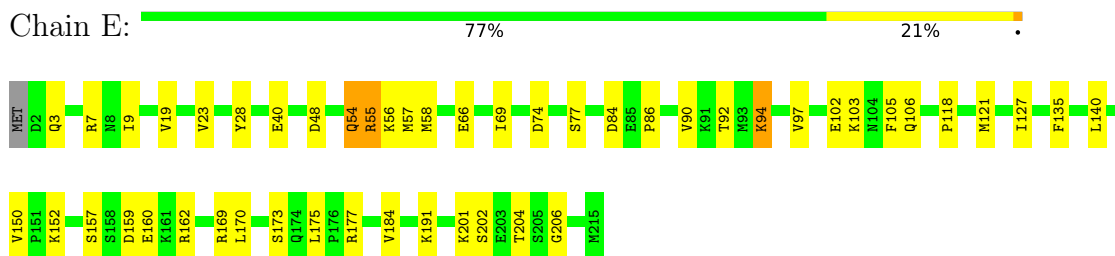




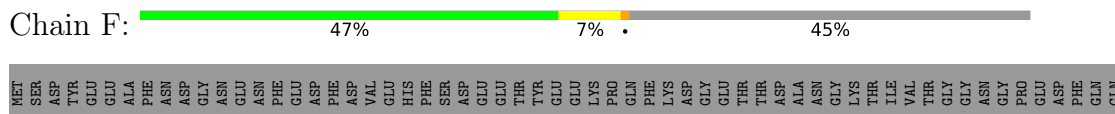
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



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

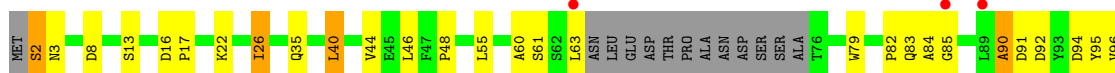


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2





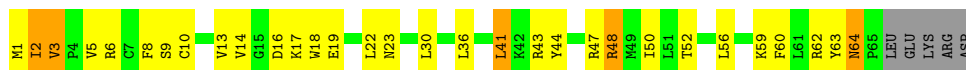
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



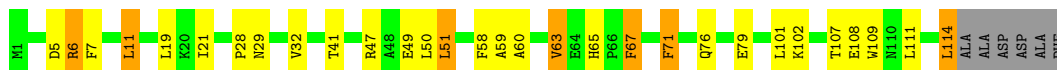
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



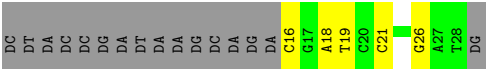
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.84Å 221.12Å 192.75Å 90.00° 97.61° 90.00°	Depositor
Resolution (Å)	29.86 – 3.24 29.86 – 3.24	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.86-3.24) 99.3 (29.86-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.24Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.183 , 0.227 0.201 , 0.244	Depositor DCC
R_{free} test set	5152 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 113.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28735	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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	2/11241 (0.0%)	1.42	59/15199 (0.4%)
2	B	0.80	2/9033 (0.0%)	1.42	56/12181 (0.5%)
3	C	0.75	0/2133	1.37	14/2891 (0.5%)
4	E	0.74	0/1788	1.36	11/2406 (0.5%)
5	F	0.77	0/700	1.33	0/945
6	H	0.71	0/1086	1.24	7/1470 (0.5%)
7	I	0.75	0/989	1.35	3/1331 (0.2%)
8	J	0.79	0/541	1.53	6/727 (0.8%)
9	K	0.72	0/937	1.40	9/1265 (0.7%)
10	L	0.81	0/365	1.38	5/485 (1.0%)
11	R	0.59	0/194	0.93	0/302
12	T	0.44	0/290	1.28	2/444 (0.5%)
All	All	0.78	4/29297 (0.0%)	1.40	172/39646 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	758	PHE	CA-C	6.96	1.58	1.53
2	B	1017	ILE	CA-CB	5.66	1.56	1.54
1	A	605	MET	SD-CE	-5.23	1.66	1.79
1	A	487	MET	SD-CE	-5.19	1.66	1.79

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	647	GLY	CA-C-N	9.99	139.69	121.70
2	B	647	GLY	C-N-CA	9.99	139.69	121.70
2	B	1016	ALA	CA-C-N	9.91	129.95	120.43
2	B	1016	ALA	C-N-CA	9.91	129.95	120.43
1	A	506	ALA	CA-C-N	7.61	127.74	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	506	ALA	C-N-CA	7.61	127.74	120.43
12	T	26	DG	P-O3'-C3'	7.59	131.58	120.20
3	C	240	VAL	N-CA-C	7.54	118.28	110.36
12	T	16	DC	P-O3'-C3'	7.53	131.49	120.20
10	L	58	LYS	N-CA-C	7.52	121.29	112.72
8	J	41	LEU	CA-C-N	7.51	131.22	120.79
8	J	41	LEU	C-N-CA	7.51	131.22	120.79
2	B	24	PRO	CA-C-N	7.36	130.37	120.50
2	B	24	PRO	C-N-CA	7.36	130.37	120.50
1	A	466	SER	N-CA-C	7.35	121.83	113.01
3	C	172	PRO	CA-C-N	7.25	135.40	121.54
3	C	172	PRO	C-N-CA	7.25	135.40	121.54
2	B	140	ILE	CA-C-N	7.25	134.75	121.70
2	B	140	ILE	C-N-CA	7.25	134.75	121.70
2	B	37	PHE	N-CA-C	-7.24	101.51	110.41
6	H	92	ASP	N-CA-C	-7.12	102.94	113.61
2	B	167	ILE	N-CA-C	-7.08	99.61	109.45
4	E	102	GLU	N-CA-C	7.08	118.89	111.03
6	H	2	SER	CA-C-N	6.95	134.22	121.70
6	H	2	SER	C-N-CA	6.95	134.22	121.70
2	B	276	ILE	CA-C-N	6.94	129.89	120.38
2	B	276	ILE	C-N-CA	6.94	129.89	120.38
7	I	107	SER	N-CA-C	-6.94	104.12	112.58
1	A	445	ASN	CA-CB-CG	6.86	119.46	112.60
1	A	827	THR	N-CA-C	-6.84	103.05	111.40
2	B	345	LYS	CA-C-N	6.80	133.94	121.70
2	B	345	LYS	C-N-CA	6.80	133.94	121.70
1	A	244	PRO	N-CA-C	6.77	118.96	110.70
1	A	947	PHE	CA-C-N	6.71	129.25	120.60
1	A	947	PHE	C-N-CA	6.71	129.25	120.60
2	B	628	THR	CA-C-N	6.70	134.34	121.54
2	B	628	THR	C-N-CA	6.70	134.34	121.54
2	B	629	ASP	CA-CB-CG	6.64	119.24	112.60
2	B	1113	VAL	N-CA-C	6.64	116.79	110.42
8	J	18	TRP	N-CA-C	6.56	118.09	111.07
9	K	32	VAL	N-CA-C	6.50	115.70	106.53
2	B	758	PHE	CA-CB-CG	6.46	120.26	113.80
9	K	63	VAL	CA-C-N	6.34	129.63	120.38
9	K	63	VAL	C-N-CA	6.34	129.63	120.38
8	J	5	VAL	N-CA-C	-6.30	100.57	108.89
2	B	1122	ARG	CA-C-N	6.28	129.01	120.54
2	B	1122	ARG	C-N-CA	6.28	129.01	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	91	ASP	N-CA-C	6.27	119.79	108.69
8	J	8	PHE	CA-CB-CG	6.26	120.06	113.80
4	E	55	ARG	N-CA-C	6.25	117.75	111.07
6	H	60	ALA	N-CA-C	6.22	120.69	112.72
3	C	178	PHE	CA-CB-CG	6.20	120.00	113.80
2	B	1121	GLY	CA-C-N	6.10	128.45	120.28
2	B	1121	GLY	C-N-CA	6.10	128.45	120.28
1	A	794	PRO	CA-C-N	6.08	128.71	120.38
1	A	794	PRO	C-N-CA	6.08	128.71	120.38
1	A	1375	MET	CA-C-N	6.05	128.66	120.44
1	A	1375	MET	C-N-CA	6.05	128.66	120.44
2	B	825	VAL	N-CA-C	6.02	116.78	108.12
4	E	150	VAL	N-CA-C	6.00	113.02	107.56
2	B	482	VAL	N-CA-C	5.95	121.71	109.34
7	I	31	THR	N-CA-C	-5.94	106.37	113.97
3	C	39	ALA	N-CA-C	5.93	121.43	113.72
1	A	445	ASN	N-CA-C	5.90	118.03	109.07
3	C	150	GLY	CA-C-N	5.88	129.19	120.90
3	C	150	GLY	C-N-CA	5.88	129.19	120.90
1	A	143	LYS	N-CA-C	5.83	117.64	111.28
1	A	483	ASP	CA-CB-CG	5.81	118.41	112.60
2	B	1017	ILE	N-CA-C	5.79	119.91	112.67
8	J	64	ASN	N-CA-C	5.78	122.59	109.81
3	C	82	TYR	N-CA-C	-5.75	100.62	109.76
1	A	485	ASP	CA-CB-CG	5.71	118.31	112.60
10	L	59	ALA	N-CA-C	5.69	122.92	110.80
1	A	864	ILE	N-CA-C	-5.69	106.27	111.67
1	A	1228	TRP	N-CA-C	5.68	117.90	108.99
3	C	172	PRO	N-CA-C	-5.67	106.61	114.27
2	B	265	SER	CA-C-N	5.64	132.31	121.54
2	B	265	SER	C-N-CA	5.64	132.31	121.54
7	I	10	CYS	N-CA-C	5.63	117.42	111.28
2	B	842	ASN	CA-CB-CG	5.63	118.23	112.60
9	K	63	VAL	N-CA-CB	5.61	117.72	111.89
1	A	1123	GLY	CA-C-N	5.60	131.79	121.70
1	A	1123	GLY	C-N-CA	5.60	131.79	121.70
2	B	38	PHE	CA-CB-CG	5.58	119.38	113.80
2	B	582	VAL	CB-CA-C	5.57	117.36	110.73
2	B	834	ASN	CA-CB-CG	5.57	118.17	112.60
1	A	574	GLY	CA-C-N	5.56	128.04	120.54
1	A	574	GLY	C-N-CA	5.56	128.04	120.54
2	B	280	ILE	N-CA-C	5.55	113.37	107.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	62	LYS	CA-C-N	5.55	128.27	120.28
10	L	62	LYS	C-N-CA	5.55	128.27	120.28
2	B	709	ASP	CA-CB-CG	5.54	118.14	112.60
2	B	1054	GLY	CA-C-N	5.52	127.51	120.56
2	B	1054	GLY	C-N-CA	5.52	127.51	120.56
1	A	526	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	514	PRO	CA-C-N	5.50	127.91	120.65
1	A	514	PRO	C-N-CA	5.50	127.91	120.65
2	B	481	GLN	CA-C-N	5.50	131.87	121.97
2	B	481	GLN	C-N-CA	5.50	131.87	121.97
2	B	542	MET	CA-C-N	5.46	128.46	120.71
2	B	542	MET	C-N-CA	5.46	128.46	120.71
4	E	177	ARG	N-CA-C	5.44	118.60	109.95
2	B	1034	VAL	CA-C-N	5.43	127.83	120.44
2	B	1034	VAL	C-N-CA	5.43	127.83	120.44
1	A	557	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	1118	VAL	N-CA-C	5.37	116.32	108.53
2	B	1154	ALA	N-CA-C	-5.37	102.54	110.48
2	B	847	ASP	CA-CB-CG	5.36	117.96	112.60
2	B	1055	ILE	CA-C-N	5.35	127.71	120.38
2	B	1055	ILE	C-N-CA	5.35	127.71	120.38
1	A	743	VAL	N-CA-CB	5.33	118.20	110.52
4	E	170	LEU	N-CA-C	5.31	117.95	110.14
1	A	884	ASP	N-CA-C	5.31	119.39	113.01
2	B	1006	ILE	N-CA-CB	5.30	117.52	110.26
9	K	50	LEU	CA-C-N	5.29	127.89	120.28
9	K	50	LEU	C-N-CA	5.29	127.89	120.28
4	E	160	GLU	CA-C-N	5.27	127.61	120.44
4	E	160	GLU	C-N-CA	5.27	127.61	120.44
1	A	1280	GLU	N-CA-C	5.25	117.08	111.36
4	E	58	MET	N-CA-C	5.25	116.68	111.07
1	A	1437	GLY	CA-C-N	5.24	127.56	120.38
1	A	1437	GLY	C-N-CA	5.24	127.56	120.38
10	L	62	LYS	N-CA-C	-5.22	106.75	113.02
9	K	63	VAL	CB-CA-C	5.20	118.89	112.45
2	B	45	SER	CA-C-N	5.19	128.61	120.82
2	B	45	SER	C-N-CA	5.19	128.61	120.82
1	A	408	ASP	CA-C-N	5.19	131.45	121.54
1	A	408	ASP	C-N-CA	5.19	131.45	121.54
3	C	60	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	91	PHE	CA-CB-CG	5.18	118.98	113.80
1	A	436	ILE	CB-CA-C	5.17	118.26	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	140	ILE	N-CA-C	5.17	115.32	110.30
3	C	191	TYR	N-CA-C	5.17	117.80	110.10
1	A	1424	VAL	CA-C-N	5.17	127.51	120.54
1	A	1424	VAL	C-N-CA	5.17	127.51	120.54
3	C	78	GLU	CB-CG-CD	5.17	121.38	112.60
1	A	1371	LEU	CA-C-N	5.16	127.06	120.56
1	A	1371	LEU	C-N-CA	5.16	127.06	120.56
2	B	680	THR	CA-C-N	5.14	127.17	120.28
2	B	680	THR	C-N-CA	5.14	127.17	120.28
1	A	1023	ARG	CA-C-N	5.14	127.17	120.28
1	A	1023	ARG	C-N-CA	5.14	127.17	120.28
1	A	690	VAL	CA-C-N	5.12	127.45	120.54
1	A	690	VAL	C-N-CA	5.12	127.45	120.54
3	C	96	SER	N-CA-C	5.12	116.85	109.07
2	B	762	ASN	CA-CB-CG	5.12	117.72	112.60
9	K	67	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	1063	MET	CA-C-N	5.11	128.99	120.62
1	A	1063	MET	C-N-CA	5.11	128.99	120.62
3	C	266	ASP	CA-CB-CG	5.10	117.70	112.60
6	H	92	ASP	CA-C-N	5.09	130.24	120.97
6	H	92	ASP	C-N-CA	5.09	130.24	120.97
9	K	71	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	351	THR	CA-C-N	5.06	127.28	120.50
1	A	351	THR	C-N-CA	5.06	127.28	120.50
1	A	948	VAL	N-CA-C	5.06	115.67	110.36
1	A	173	THR	CA-C-N	5.04	127.34	120.63
1	A	173	THR	C-N-CA	5.04	127.34	120.63
2	B	550	ASP	CA-CB-CG	5.04	117.64	112.60
2	B	479	VAL	N-CA-C	-5.04	103.08	109.58
1	A	743	VAL	CA-C-N	5.03	127.27	120.38
1	A	743	VAL	C-N-CA	5.03	127.27	120.38
1	A	756	ILE	CA-C-N	5.02	126.97	120.44
1	A	756	ILE	C-N-CA	5.02	126.97	120.44
1	A	1271	ILE	N-CA-C	5.02	115.26	107.28
2	B	1077	THR	N-CA-C	5.02	119.54	113.41
1	A	1299	VAL	N-CA-C	5.02	117.04	108.86
4	E	48	ASP	CA-CB-CG	5.02	117.62	112.60
4	E	157	SER	CA-C-N	5.02	127.00	120.28
4	E	157	SER	C-N-CA	5.02	127.00	120.28
1	A	874	ASP	CA-C-N	5.00	127.23	120.38
1	A	874	ASP	C-N-CA	5.00	127.23	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11043	0	11133	150	0
2	B	8861	0	8884	140	0
3	C	2095	0	2051	49	0
4	E	1752	0	1776	12	0
5	F	688	0	707	4	0
6	H	1068	0	1040	20	0
7	I	971	0	927	9	0
8	J	532	0	542	17	0
9	K	919	0	929	14	0
10	L	363	0	386	7	0
11	R	173	0	88	0	0
12	T	261	0	148	2	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	28735	0	28611	366	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (366) 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)
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.38	1.01
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.23	1.00
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.85	0.92
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.61	0.82
2:B:996:ARG:HH22	3:C:173:ALA:HB1	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:HIS:HD2	3:C:169:LYS:H	1.31	0.78
6:H:40:LEU:HD21	6:H:142:LEU:HD21	1.65	0.78
2:B:345:LYS:HA	2:B:347:LYS:H	1.48	0.76
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.52	0.75
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.70	0.73
2:B:54:PHE:HA	2:B:58:THR:HB	1.69	0.72
1:A:351:THR:HG21	1:A:466:SER:O	1.90	0.72
2:B:801:LYS:O	8:J:52:THR:HG23	1.90	0.72
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.72	0.71
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.72	0.71
1:A:441:PRO:HG2	1:A:498:ARG:HB2	1.72	0.71
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.76	0.69
1:A:469:ARG:NH2	2:B:991:GLY:O	2.27	0.67
1:A:869:GLY:O	4:E:204:THR:HG21	1.94	0.67
1:A:567:LYS:HE2	6:H:46:LEU:CB	2.25	0.67
2:B:604:ARG:HD3	2:B:611:PRO:HA	1.77	0.67
2:B:345:LYS:HA	2:B:347:LYS:N	2.11	0.66
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.78	0.66
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.77	0.65
1:A:567:LYS:HE2	6:H:46:LEU:HB2	1.77	0.65
1:A:55:ASP:H	1:A:56:PRO:HD2	1.61	0.65
2:B:955:THR:HG22	2:B:956:THR:H	1.62	0.65
2:B:1163:CYS:HB3	2:B:1166:CYS:HB2	1.77	0.65
1:A:535:THR:HG21	1:A:617:VAL:H	1.62	0.64
1:A:596:THR:C	1:A:598:LEU:H	2.05	0.64
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.64	0.63
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.81	0.63
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.63	0.63
2:B:365:THR:HG23	2:B:367:LEU:H	1.64	0.63
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.81	0.62
3:C:11:ARG:HD2	3:C:21:ILE:HD11	1.82	0.61
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.48	0.61
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.65	0.60
2:B:1002:THR:HG22	2:B:1004:GLU:H	1.66	0.60
2:B:1181:GLU:HG2	2:B:1188:LYS:HG2	1.84	0.60
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.83	0.60
1:A:57:ARG:HB3	1:A:68:GLN:HB3	1.82	0.60
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.83	0.59
3:C:242:GLN:HA	3:C:245:VAL:HG22	1.83	0.59
1:A:741:ASN:HD22	1:A:744:LYS:H	1.49	0.59
1:A:567:LYS:HB3	6:H:96:VAL:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG21	1:A:857:ARG:HE	1.68	0.58
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.84	0.58
1:A:709:THR:HB	1:A:712:GLU:HB2	1.85	0.58
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.39	0.58
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.85	0.58
3:C:66:ARG:NH2	8:J:3:VAL:O	2.37	0.58
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.84	0.58
3:C:62:PHE:O	3:C:66:ARG:HG3	2.03	0.58
2:B:976:ILE:O	2:B:990:ILE:HB	2.03	0.58
1:A:512:VAL:HA	1:A:519:PRO:HA	1.86	0.57
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.85	0.57
1:A:899:VAL:HG22	1:A:1029:ARG:HD3	1.85	0.57
1:A:592:ASP:HB2	1:A:603:ASN:HD22	1.70	0.57
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.86	0.56
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.86	0.56
3:C:167:HIS:CD2	3:C:169:LYS:H	2.18	0.56
1:A:4:GLN:HE22	2:B:1159:ARG:H	1.54	0.56
1:A:535:THR:HG21	1:A:617:VAL:N	2.21	0.56
2:B:549:THR:HB	2:B:628:THR:HG22	1.88	0.56
2:B:640:VAL:HG12	2:B:649:LYS:HB3	1.88	0.55
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.87	0.55
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.87	0.55
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.87	0.55
1:A:795:GLU:HG3	2:B:731:VAL:HG11	1.89	0.55
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.70	0.55
2:B:864:LYS:H	2:B:872:GLU:HB2	1.72	0.55
1:A:49:LYS:HB3	1:A:55:ASP:HB3	1.88	0.55
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.53	0.55
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.89	0.55
1:A:531:ILE:O	1:A:535:THR:HB	2.07	0.55
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.05	0.55
8:J:36:LEU:HD13	8:J:47:ARG:HG2	1.89	0.55
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.89	0.55
1:A:871:ASP:HB3	4:E:204:THR:HG22	1.89	0.55
8:J:1:MET:H1	8:J:56:LEU:H	1.54	0.54
1:A:640:GLN:CD	1:A:640:GLN:H	2.15	0.54
2:B:497:ARG:HE	2:B:538:ASN:HD21	1.55	0.54
2:B:745:PRO:O	2:B:748:ILE:HG12	2.08	0.54
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.72	0.54
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.89	0.54
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.89	0.54

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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	0.54
2:B:1107:ALA:O	2:B:1108:ARG:HB2	2.07	0.53
1:A:474:VAL:HG23	1:A:521:MET:HE3	1.90	0.53
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.90	0.53
1:A:545:GLN:HG2	1:A:549:MET:HE2	1.91	0.53
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.42	0.53
8:J:1:MET:H1	8:J:56:LEU:HB2	1.73	0.53
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.73	0.53
2:B:1074:ASN:HD22	2:B:1077:THR:H	1.56	0.53
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.90	0.53
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.44	0.53
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.91	0.53
2:B:976:ILE:HG23	2:B:977:GLY:H	1.74	0.53
9:K:65:HIS:CD2	9:K:67:PHE:H	2.27	0.53
1:A:705:LYS:HE3	1:A:705:LYS:H	1.73	0.52
1:A:55:ASP:O	1:A:57:ARG:N	2.42	0.52
3:C:164:ALA:HA	3:C:167:HIS:O	2.10	0.52
2:B:955:THR:HG22	2:B:956:THR:N	2.23	0.52
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.92	0.52
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.92	0.52
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.90	0.52
2:B:996:ARG:NH2	3:C:174:ALA:O	2.43	0.52
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.40	0.52
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.91	0.52
2:B:980:PHE:CE2	2:B:1094:ARG:HD2	2.45	0.52
1:A:1292:PRO:HA	1:A:1298:TYR:HA	1.92	0.52
2:B:1129:ARG:HB3	12:T:21:DC:H5"	1.92	0.52
2:B:313:MET:HE2	2:B:390:LEU:HG	1.92	0.51
1:A:315:LEU:HG	1:A:320:ARG:HH21	1.76	0.51
1:A:399:HIS:O	1:A:401:GLY:N	2.37	0.51
1:A:777:PHE:HD1	1:A:781:ASP:C	2.18	0.51
2:B:95:ILE:HD11	2:B:128:LEU:HB3	1.92	0.51
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.43	0.51
2:B:935:ARG:CZ	2:B:935:ARG:HA	2.40	0.51
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.93	0.51
1:A:456:MET:HE2	1:A:507:VAL:HG22	1.92	0.51
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.91	0.51
2:B:803:LEU:H	2:B:822:ASN:HD21	1.55	0.51
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.93	0.51
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.75	0.51
2:B:908:GLU:HG2	2:B:943:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.93	0.51
2:B:126:SER:HB2	2:B:172:ILE:HD11	1.93	0.51
2:B:860:MET:HG3	2:B:965:LYS:HG2	1.93	0.51
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.92	0.51
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.60	0.51
1:A:466:SER:HB3	2:B:1103:ILE:CD1	2.41	0.50
1:A:1279:ILE:HD12	1:A:1308:THR:HG21	1.94	0.50
2:B:39:ARG:HH12	2:B:665:GLU:HG3	1.75	0.50
1:A:629:LEU:O	1:A:633:VAL:HG23	2.11	0.50
2:B:515:HIS:CD2	2:B:517:THR:H	2.30	0.50
1:A:423:ASP:CG	1:A:424:ILE:H	2.20	0.50
2:B:55:VAL:HA	2:B:59:LEU:HD23	1.93	0.50
1:A:899:VAL:HB	1:A:929:LEU:HD22	1.94	0.49
1:A:916:GLY:O	1:A:919:ILE:HG22	2.12	0.49
1:A:185:TRP:HB2	1:A:199:LEU:HD12	1.94	0.49
5:F:77:ASP:O	5:F:78:GLN:HB2	2.13	0.49
2:B:846:ILE:HG23	2:B:974:PRO:HD2	1.93	0.49
3:C:20:PHE:HE1	3:C:22:LEU:HD13	1.78	0.49
1:A:595:THR:HG21	1:A:604:GLY:HA3	1.95	0.49
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.95	0.49
2:B:654:ARG:H	2:B:657:HIS:HD2	1.61	0.49
3:C:170:TRP:HH2	10:L:70:ARG:HH21	1.60	0.49
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.95	0.49
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.93	0.49
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.95	0.49
1:A:434:ARG:NH2	1:A:440:ASP:OD1	2.45	0.48
8:J:1:MET:N	8:J:56:LEU:H	2.10	0.48
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.94	0.48
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.78	0.48
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.96	0.48
2:B:43:LEU:HD11	2:B:811:TYR:O	2.13	0.48
3:C:14:SER:HA	9:K:114:LEU:HD22	1.94	0.48
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.46	0.48
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.96	0.48
6:H:2:SER:HB3	6:H:3:ASN:HB2	1.95	0.48
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.93	0.48
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.94	0.48
7:I:111:THR:HG23	7:I:113:ASP:H	1.79	0.48
2:B:706:GLN:H	2:B:710:LEU:HG	1.78	0.48
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.95	0.48
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HA	3:C:159:ALA:HA	1.94	0.48
6:H:135:LEU:C	6:H:137:GLN:H	2.22	0.48
1:A:567:LYS:HE2	6:H:46:LEU:HB3	1.95	0.48
1:A:786:HIS:CE1	2:B:705:MET:HE1	2.48	0.48
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.96	0.48
2:B:955:THR:HG23	10:L:54:ARG:O	2.13	0.48
3:C:10:ILE:HD12	9:K:108:GLU:HB3	1.96	0.48
3:C:124:LEU:O	3:C:127:ARG:HG2	2.13	0.48
1:A:924:LYS:O	1:A:927:VAL:HG12	2.14	0.47
3:C:165:LYS:O	9:K:6:ARG:NH1	2.47	0.47
1:A:68:GLN:HE21	1:A:70:CYS:HB3	1.79	0.47
2:B:640:VAL:CG1	2:B:649:LYS:HB3	2.43	0.47
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.49	0.47
1:A:596:THR:C	1:A:598:LEU:N	2.72	0.47
3:C:174:ALA:HB3	3:C:233:GLU:O	2.14	0.47
1:A:826:ASP:HA	1:A:829:VAL:HB	1.96	0.47
2:B:36:ALA:HB2	2:B:661:LEU:HD22	1.96	0.47
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.61	0.47
1:A:336:ILE:HD11	2:B:1203:LEU:HD13	1.97	0.47
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.79	0.47
6:H:63:LEU:HB2	6:H:90:ALA:HB2	1.95	0.47
9:K:65:HIS:HD2	9:K:67:PHE:H	1.62	0.47
1:A:579:SER:HB3	1:A:611:GLN:HA	1.96	0.47
1:A:919:ILE:HD11	1:A:925:LEU:HG	1.97	0.47
2:B:35:SER:O	2:B:39:ARG:HB2	2.15	0.46
2:B:241:ARG:HA	2:B:253:THR:HG22	1.96	0.46
2:B:916:THR:HG23	2:B:935:ARG:HB3	1.96	0.46
2:B:705:MET:H	2:B:710:LEU:HD12	1.80	0.46
1:A:107:CYS:HB3	1:A:114:LEU:HD21	1.97	0.46
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.96	0.46
1:A:50:ILE:HG23	1:A:52:GLY:H	1.80	0.46
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.97	0.46
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.97	0.46
2:B:731:VAL:O	2:B:732:SER:HB2	2.16	0.46
1:A:648:ASN:O	1:A:652:VAL:HG23	2.15	0.46
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.89	0.46
1:A:315:LEU:HD23	1:A:317:LYS:H	1.81	0.46
1:A:770:VAL:HG12	1:A:771:GLU:HG2	1.97	0.46
2:B:58:THR:O	2:B:62:ILE:HG12	2.15	0.46
2:B:199:MET:SD	2:B:199:MET:N	2.88	0.46
2:B:837:ASP:O	2:B:988:GLY:HA2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:118:PRO:HA	4:E:121:MET:HB2	1.97	0.46
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.97	0.46
1:A:614:PHE:HB3	6:H:122:LEU:HD21	1.98	0.46
1:A:1129:GLU:HA	1:A:1132:LYS:HE3	1.98	0.46
7:I:97:MET:HE3	7:I:97:MET:HB2	1.84	0.46
1:A:374:LEU:HD23	2:B:1107:ALA:HB2	1.98	0.45
1:A:525:GLN:NE2	2:B:836:GLU:H	2.14	0.45
1:A:709:THR:HB	1:A:712:GLU:H	1.81	0.45
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.97	0.45
9:K:7:PHE:O	9:K:11:LEU:HB2	2.17	0.45
7:I:92:ARG:HD2	7:I:94:ASP:OD2	2.16	0.45
1:A:26:GLU:HG2	1:A:30:ILE:HD13	1.97	0.45
1:A:514:PRO:HG2	1:A:1067:LEU:HD21	1.97	0.45
1:A:810:PRO:HG2	2:B:705:MET:HG2	1.98	0.45
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.82	0.45
2:B:291:ILE:HG12	2:B:300:HIS:NE2	2.32	0.45
3:C:37:MET:HE2	3:C:244:VAL:HA	1.98	0.45
2:B:618:ASP:OD2	2:B:621:GLU:HB2	2.15	0.45
4:E:19:VAL:O	4:E:23:VAL:HG23	2.16	0.45
1:A:535:THR:CG2	1:A:617:VAL:H	2.28	0.45
1:A:1229:SER:HB3	1:A:1237:ILE:H	1.82	0.45
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.99	0.45
2:B:872:GLU:HG2	2:B:916:THR:HB	1.98	0.45
3:C:11:ARG:HD2	3:C:21:ILE:CD1	2.47	0.45
3:C:148:ARG:H	3:C:151:GLN:HG3	1.80	0.45
1:A:4:GLN:HE22	2:B:1159:ARG:N	2.15	0.45
1:A:901:LEU:HD23	1:A:907:THR:HG23	1.99	0.45
2:B:579:ARG:HA	2:B:589:VAL:HG12	1.99	0.45
6:H:136:LYS:H	6:H:136:LYS:HD3	1.81	0.45
12:T:18:DA:H5''	12:T:19:DT:H5'	1.98	0.45
1:A:378:GLU:OE2	1:A:434:ARG:HD3	2.17	0.45
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.99	0.44
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.41	0.44
1:A:591:PHE:HD2	1:A:595:THR:HB	1.82	0.44
2:B:498:THR:HB	2:B:537:LYS:HB2	2.00	0.44
8:J:14:VAL:HA	8:J:17:LYS:HD2	1.99	0.44
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.99	0.44
1:A:586:ILE:HD11	1:A:637:LYS:HG3	1.99	0.44
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.99	0.44
3:C:66:ARG:NH1	3:C:144:ILE:O	2.51	0.44
1:A:575:LYS:HD2	6:H:120:GLY:HA3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	1.99	0.44
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.98	0.44
3:C:258:ILE:HD12	9:K:19:LEU:HD21	1.99	0.44
2:B:102:VAL:HG23	2:B:112:LEU:HD22	2.00	0.44
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.32	0.44
1:A:211:PHE:HA	1:A:214:ILE:HD11	1.98	0.44
1:A:567:LYS:HD3	6:H:95:TYR:CG	2.52	0.44
2:B:647:GLY:HA3	2:B:648:HIS:HB2	1.99	0.44
2:B:1031:LEU:O	2:B:1034:VAL:HG12	2.18	0.44
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	2.00	0.44
3:C:133:ILE:HG21	3:C:236:GLY:HA3	1.99	0.44
2:B:744:HIS:CD2	2:B:746:SER:OG	2.70	0.44
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.82	0.44
2:B:424:LEU:O	2:B:428:ILE:HG12	2.18	0.43
2:B:880:THR:C	2:B:882:THR:H	2.26	0.43
2:B:1037:LEU:HD13	2:B:1062:HIS:HB3	2.00	0.43
2:B:882:THR:HA	2:B:935:ARG:HH12	1.83	0.43
3:C:75:MET:HE2	3:C:239:PRO:HG3	2.00	0.43
4:E:77:SER:HB2	4:E:105:PHE:HA	1.99	0.43
2:B:128:LEU:HB2	2:B:167:ILE:HB	2.00	0.43
4:E:202:SER:HB3	4:E:206:GLY:H	1.82	0.43
1:A:642:CYS:O	1:A:645:LEU:HB3	2.19	0.43
1:A:824:LEU:HD21	2:B:765:PRO:HB3	2.01	0.43
2:B:293:PRO:HG2	2:B:296:GLU:HB2	2.00	0.43
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.00	0.43
2:B:956:THR:HB	10:L:46:VAL:HG21	1.99	0.43
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.19	0.43
3:C:175:ALA:HB2	8:J:10:CYS:HB2	2.01	0.43
5:F:72:LYS:HG2	5:F:142:SER:HA	2.00	0.43
1:A:527:THR:HG21	1:A:650:GLN:HG2	2.01	0.43
1:A:1353:TYR:C	1:A:1353:TYR:CD2	2.96	0.43
2:B:615:MET:HE3	2:B:615:MET:HB2	1.93	0.43
1:A:567:LYS:O	1:A:569:LYS:N	2.52	0.43
1:A:251:SER:HB3	1:A:258:GLY:HA3	2.01	0.43
1:A:528:LEU:O	1:A:531:ILE:HG22	2.19	0.42
1:A:946:VAL:HG22	4:E:201:LYS:HD2	2.01	0.42
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.19	0.42
3:C:70:ILE:HD11	3:C:144:ILE:HD12	2.02	0.42
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.55	0.42
3:C:142:VAL:H	8:J:16:ASP:HB3	1.84	0.42
8:J:14:VAL:HB	8:J:50:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:O	1:A:56:PRO:C	2.61	0.42
1:A:148:CYS:HB3	1:A:167:CYS:O	2.19	0.42
2:B:1060:ARG:HA	2:B:1064:TYR:O	2.20	0.42
1:A:173:THR:HB	1:A:184:SER:HB3	2.01	0.42
1:A:304:MET:HG2	1:A:325:ILE:HD12	2.01	0.42
1:A:729:ALA:HA	1:A:732:LEU:HD12	2.01	0.42
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.83	0.42
1:A:579:SER:HA	1:A:582:ILE:HD12	2.01	0.42
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.01	0.42
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.60	0.42
1:A:1352:VAL:O	1:A:1355:VAL:HG12	2.19	0.42
4:E:54:GLN:HE21	4:E:57:MET:HE3	1.84	0.42
1:A:324:SER:O	1:A:326:ARG:N	2.53	0.42
2:B:900:ALA:HB3	10:L:61:THR:HG23	2.02	0.42
3:C:18:VAL:O	3:C:231:ASN:HA	2.20	0.42
1:A:775:ILE:HG21	1:A:815:PHE:CE2	2.55	0.42
2:B:515:HIS:H	2:B:518:HIS:CD2	2.38	0.42
3:C:143:LEU:HD21	3:C:146:LYS:HE3	2.01	0.42
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.55	0.42
1:A:466:SER:HB3	2:B:1103:ILE:HD11	2.01	0.42
3:C:46:ILE:HG23	3:C:157:CYS:HB2	2.02	0.42
2:B:824:ILE:HD13	2:B:1089:PRO:HB3	2.01	0.41
2:B:1079:LYS:HE2	3:C:188:HIS:CE1	2.54	0.41
1:A:289:ILE:H	1:A:289:ILE:HG13	1.59	0.41
1:A:756:ILE:H	1:A:756:ILE:HG13	1.55	0.41
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.20	0.41
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.55	0.41
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.03	0.41
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.02	0.41
3:C:241:ASP:HB3	9:K:109:TRP:CD2	2.56	0.41
6:H:79:TRP:CZ2	6:H:82:PRO:HD3	2.55	0.41
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.03	0.41
2:B:976:ILE:O	2:B:978:ASP:N	2.45	0.41
4:E:94:LYS:HA	4:E:97:VAL:HB	2.01	0.41
1:A:1154:TYR:CD2	7:I:25:LEU:HB2	2.55	0.41
2:B:899:ILE:HD12	2:B:949:VAL:HG21	2.03	0.41
3:C:52:GLU:HA	10:L:64:LEU:HD22	2.03	0.41
6:H:83:GLN:HE21	6:H:85:GLY:H	1.68	0.41
7:I:26:LEU:HD23	7:I:37:GLU:HA	2.01	0.41
1:A:312:PRO:HB2	1:A:313:GLN:H	1.76	0.41
6:H:26:ILE:HG22	6:H:40:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:61:THR:HB	10:L:63:ARG:H	1.86	0.41
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.21	0.41
2:B:581:PHE:HB2	2:B:625:LYS:HG2	2.02	0.41
5:F:89:GLU:O	5:F:93:ILE:HG12	2.21	0.41
1:A:453:MET:HB3	1:A:477:PRO:HB2	2.03	0.41
1:A:942:PHE:O	1:A:945:GLU:HG2	2.21	0.41
3:C:134:ILE:HG12	3:C:141:GLY:H	1.86	0.41
4:E:66:GLU:HA	4:E:69:ILE:HD12	2.02	0.41
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.52	0.41
2:B:277:LYS:H	2:B:277:LYS:HG3	1.65	0.41
1:A:466:SER:HB3	2:B:1103:ILE:HD12	2.02	0.40
2:B:282:ILE:HD13	2:B:382:ILE:HD13	2.03	0.40
3:C:51:VAL:HG12	3:C:155:LEU:HB3	2.03	0.40
6:H:61:SER:HA	6:H:141:TYR:HD1	1.86	0.40
1:A:547:LEU:HD22	9:K:58:PHE:HD1	1.87	0.40
8:J:17:LYS:HD3	8:J:41:LEU:HD21	2.03	0.40
1:A:586:ILE:HD11	1:A:637:LYS:CG	2.52	0.40
1:A:775:ILE:HG21	1:A:815:PHE:CD2	2.56	0.40
1:A:1205:LYS:HB2	1:A:1207:LEU:HD12	2.03	0.40
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.22	0.40
2:B:803:LEU:N	2:B:822:ASN:HD21	2.18	0.40
7:I:65:ASP:HB3	7:I:68:LEU:HD12	2.04	0.40
1:A:589:GLN:HB3	1:A:961:ARG:HH22	1.86	0.40
1:A:591:PHE:HA	1:A:595:THR:HG21	2.03	0.40
2:B:213:ILE:HD12	2:B:497:ARG:HB3	2.03	0.40
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.57	0.40
3:C:176:ILE:HG12	3:C:232:VAL:HG12	2.03	0.40
7:I:84:VAL:HG23	7:I:104:LEU:HD11	2.04	0.40
1:A:492:PRO:HB3	1:A:497:THR:HG22	2.04	0.40
1:A:711:ARG:HA	7:I:97:MET:HE1	2.03	0.40
1:A:821:ARG:HG3	1:A:825:ILE:HD11	2.03	0.40
6:H:123:MET:HE2	6:H:142:LEU:HD13	2.03	0.40
9:K:7:PHE:HB2	9:K:11:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1395/1733 (80%)	1212 (87%)	137 (10%)	46 (3%)	3	18
2	B	1096/1224 (90%)	960 (88%)	91 (8%)	45 (4%)	2	14
3	C	264/318 (83%)	234 (89%)	24 (9%)	6 (2%)	5	25
4	E	212/215 (99%)	191 (90%)	18 (8%)	3 (1%)	9	35
5	F	83/155 (54%)	73 (88%)	9 (11%)	1 (1%)	10	38
6	H	129/146 (88%)	100 (78%)	23 (18%)	6 (5%)	2	12
7	I	117/122 (96%)	100 (86%)	14 (12%)	3 (3%)	4	23
8	J	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	3	19
9	K	112/120 (93%)	102 (91%)	8 (7%)	2 (2%)	6	31
10	L	44/70 (63%)	27 (61%)	11 (25%)	6 (14%)	0	1
All	All	3515/4173 (84%)	3056 (87%)	339 (10%)	120 (3%)	3	18

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	50	ILE
1	A	56	PRO
1	A	257	ARG
1	A	315	LEU
1	A	324	SER
1	A	325	ILE
1	A	404	TYR
1	A	409	SER
1	A	1001	ARG
2	B	67	SER
2	B	168	GLY
2	B	250	PHE
2	B	264	SER

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Mol	Chain	Res	Type
2	B	266	ALA
2	B	477	ALA
2	B	482	VAL
2	B	531	GLN
2	B	648	HIS
2	B	712	PRO
2	B	731	VAL
2	B	732	SER
2	B	751	VAL
2	B	880	THR
2	B	944	THR
2	B	1046	PRO
2	B	1097	HIS
2	B	1156	ASP
3	C	173	ALA
6	H	109	LYS
8	J	2	ILE
9	K	28	PRO
1	A	55	ASP
1	A	76	GLU
1	A	214	ILE
1	A	332	LYS
1	A	385	ILE
1	A	423	ASP
1	A	1083	THR
1	A	1084	PHE
1	A	1123	GLY
1	A	1437	GLY
2	B	137	TYR
2	B	139	ALA
2	B	465	ASN
2	B	629	ASP
2	B	646	LEU
2	B	792	MET
2	B	884	ARG
2	B	943	SER
2	B	1066	SER
2	B	1108	ARG
2	B	1178	ASN
2	B	1223	ASP
3	C	5	GLY
3	C	142	VAL

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Mol	Chain	Res	Type
3	C	215	GLU
4	E	90	VAL
5	F	78	GLN
6	H	136	LYS
8	J	6	ARG
10	L	55	ILE
1	A	65	LEU
1	A	109	HIS
1	A	130	ASP
1	A	312	PRO
1	A	330	LYS
1	A	775	ILE
1	A	911	SER
2	B	105	SER
2	B	563	MET
2	B	707	PRO
2	B	881	ASN
2	B	976	ILE
2	B	1221	SER
3	C	267	GLN
4	E	86	PRO
6	H	128	ASN
7	I	3	THR
7	I	20	LYS
9	K	71	PHE
10	L	39	SER
1	A	215	SER
1	A	250	ILE
1	A	275	SER
1	A	525	GLN
1	A	567	LYS
1	A	569	LYS
1	A	583	PRO
1	A	958	VAL
1	A	1221	LYS
2	B	483	LEU
2	B	734	HIS
2	B	1157	ALA
2	B	1181	GLU
6	H	84	ALA
6	H	108	SER
1	A	308	ILE

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Mol	Chain	Res	Type
1	A	424	ILE
1	A	568	PRO
1	A	599	SER
1	A	672	ASP
1	A	922	ASP
1	A	1278	ASN
2	B	346	GLU
2	B	367	LEU
2	B	887	HIS
2	B	977	GLY
4	E	103	LYS
6	H	90	ALA
7	I	77	LYS
10	L	46	VAL
10	L	59	ALA
10	L	64	LEU
1	A	35	ILE
1	A	1405	THR
10	L	56	LEU
1	A	321	PRO
2	B	364	ILE
3	C	126	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%)	1048 (86%)	177 (14%)	3	15
2	B	967/1061 (91%)	838 (87%)	129 (13%)	4	18
3	C	234/274 (85%)	208 (89%)	26 (11%)	6	24
4	E	196/197 (100%)	175 (89%)	21 (11%)	6	25
5	F	75/137 (55%)	69 (92%)	6 (8%)	11	37
6	H	117/128 (91%)	102 (87%)	15 (13%)	4	19
7	I	113/116 (97%)	100 (88%)	13 (12%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	60/65 (92%)	47 (78%)	13 (22%)	1	5
9	K	99/102 (97%)	84 (85%)	15 (15%)	3	13
10	L	40/57 (70%)	31 (78%)	9 (22%)	1	4
All	All	3126/3657 (86%)	2702 (86%)	424 (14%)	3	17

All (424) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	30	ILE
1	A	34	LYS
1	A	40	THR
1	A	41	MET
1	A	43	GLU
1	A	46	THR
1	A	58	LEU
1	A	68	GLN
1	A	69	THR
1	A	70	CYS
1	A	93	VAL
1	A	108	MET
1	A	118	HIS
1	A	123	ARG
1	A	126	LEU
1	A	134	ARG
1	A	143	LYS
1	A	177	ASP
1	A	204	THR
1	A	222	LEU
1	A	226	GLU
1	A	236	LEU
1	A	252	PHE
1	A	254	GLU
1	A	255	SER
1	A	260	ASP
1	A	262	LEU
1	A	266	LEU
1	A	269	ILE
1	A	270	LEU
1	A	289	ILE
1	A	299	HIS

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Mol	Chain	Res	Type
1	A	308	ILE
1	A	315	LEU
1	A	320	ARG
1	A	325	ILE
1	A	332	LYS
1	A	335	ARG
1	A	351	THR
1	A	353	ILE
1	A	359	LEU
1	A	386	ASP
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	455	MET
1	A	470	LEU
1	A	475	THR
1	A	496	GLU
1	A	525	GLN
1	A	527	THR
1	A	533	LYS
1	A	535	THR
1	A	537	ARG
1	A	541	ILE
1	A	566	ILE
1	A	590	ARG
1	A	595	THR
1	A	597	LEU
1	A	598	LEU
1	A	612	ILE
1	A	616	VAL
1	A	618	GLU
1	A	625	SER
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	636	GLU
1	A	640	GLN
1	A	666	ILE
1	A	682	THR

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Mol	Chain	Res	Type
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	705	LYS
1	A	710	LEU
1	A	719	VAL
1	A	722	LEU
1	A	740	LEU
1	A	743	VAL
1	A	754	SER
1	A	756	ILE
1	A	768	GLN
1	A	796	SER
1	A	801	GLU
1	A	805	LEU
1	A	821	ARG
1	A	826	ASP
1	A	830	LYS
1	A	837	ILE
1	A	838	GLN
1	A	848	ILE
1	A	849	MET
1	A	867	ILE
1	A	878	ILE
1	A	896	ARG
1	A	908	LEU
1	A	920	LEU
1	A	925	LEU
1	A	926	GLN
1	A	931	GLU
1	A	938	LYS
1	A	945	GLU
1	A	953	ASN
1	A	960	ILE
1	A	968	GLN
1	A	992	ASP
1	A	998	LEU
1	A	1001	ARG
1	A	1008	GLN
1	A	1011	GLN
1	A	1015	VAL
1	A	1022	LEU

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Mol	Chain	Res	Type
1	A	1037	LEU
1	A	1047	SER
1	A	1048	ASN
1	A	1052	GLN
1	A	1067	LEU
1	A	1085	HIS
1	A	1094	VAL
1	A	1102	LYS
1	A	1109	LYS
1	A	1110	ASN
1	A	1130	GLN
1	A	1136	SER
1	A	1138	ILE
1	A	1146	VAL
1	A	1168	GLU
1	A	1171	GLN
1	A	1174	PHE
1	A	1176	LEU
1	A	1195	LEU
1	A	1229	SER
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1243	VAL
1	A	1261	LYS
1	A	1263	ILE
1	A	1264	GLU
1	A	1266	THR
1	A	1269	GLU
1	A	1271	ILE
1	A	1277	GLU
1	A	1280	GLU
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1303	GLU
1	A	1307	GLU
1	A	1319	VAL
1	A	1322	ILE
1	A	1325	THR
1	A	1333	ILE
1	A	1334	ASP

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Mol	Chain	Res	Type
1	A	1336	MET
1	A	1351	GLU
1	A	1354	ASN
1	A	1359	ASP
1	A	1371	LEU
1	A	1382	THR
1	A	1384	VAL
1	A	1385	THR
1	A	1387	HIS
1	A	1390	ASN
1	A	1391	ARG
1	A	1393	ASN
1	A	1403	GLU
1	A	1407	GLU
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1442	ASP
2	B	21	GLU
2	B	25	ILE
2	B	28	GLU
2	B	46	GLN
2	B	58	THR
2	B	59	LEU
2	B	63	ILE
2	B	70	ILE
2	B	89	GLU
2	B	95	ILE
2	B	101	MET
2	B	103	ASN
2	B	175	ARG
2	B	183	GLU
2	B	185	THR
2	B	189	LEU
2	B	194	GLU
2	B	217	ARG
2	B	218	SER
2	B	234	ILE
2	B	240	ILE
2	B	249	ARG
2	B	254	LEU
2	B	267	ARG

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Mol	Chain	Res	Type
2	B	277	LYS
2	B	278	GLN
2	B	282	ILE
2	B	289	LEU
2	B	313	MET
2	B	325	GLN
2	B	349	ILE
2	B	355	ILE
2	B	364	ILE
2	B	365	THR
2	B	387	LEU
2	B	393	LYS
2	B	404	LYS
2	B	408	LEU
2	B	413	LEU
2	B	416	LEU
2	B	437	GLU
2	B	449	ASN
2	B	458	LYS
2	B	461	LEU
2	B	471	LYS
2	B	479	VAL
2	B	482	VAL
2	B	485	ARG
2	B	493	SER
2	B	513	GLN
2	B	537	LYS
2	B	538	ASN
2	B	547	VAL
2	B	549	THR
2	B	566	LEU
2	B	567	GLU
2	B	591	ARG
2	B	602	THR
2	B	604	ARG
2	B	612	GLU
2	B	616	ILE
2	B	620	ARG
2	B	626	ILE
2	B	628	THR
2	B	645	SER
2	B	646	LEU

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Mol	Chain	Res	Type
2	B	653	VAL
2	B	655	LYS
2	B	658	ILE
2	B	703	ILE
2	B	705	MET
2	B	709	ASP
2	B	710	LEU
2	B	762	ASN
2	B	780	VAL
2	B	786	ASN
2	B	787	VAL
2	B	791	THR
2	B	792	MET
2	B	796	LEU
2	B	815	ARG
2	B	825	VAL
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	860	MET
2	B	866	TYR
2	B	868	MET
2	B	873	THR
2	B	879	ARG
2	B	884	ARG
2	B	889	THR
2	B	899	ILE
2	B	906	SER
2	B	911	ILE
2	B	948	ILE
2	B	951	GLN
2	B	954	VAL
2	B	961	LEU
2	B	963	PHE
2	B	967	ARG
2	B	969	ARG
2	B	971	THR
2	B	983	ARG
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1006	ILE

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Mol	Chain	Res	Type
2	B	1010	LEU
2	B	1022	THR
2	B	1028	GLU
2	B	1034	VAL
2	B	1041	GLU
2	B	1049	ASP
2	B	1057	LYS
2	B	1065	GLN
2	B	1099	VAL
2	B	1103	ILE
2	B	1113	VAL
2	B	1138	MET
2	B	1147	LEU
2	B	1151	LEU
2	B	1160	VAL
2	B	1175	LEU
2	B	1176	ASN
2	B	1178	ASN
2	B	1189	ILE
2	B	1194	ILE
2	B	1202	LEU
3	C	4	GLU
3	C	21	ILE
3	C	23	SER
3	C	32	SER
3	C	35	ARG
3	C	36	VAL
3	C	57	VAL
3	C	75	MET
3	C	77	ILE
3	C	79	GLN
3	C	111	THR
3	C	124	LEU
3	C	127	ARG
3	C	129	ILE
3	C	136	ASP
3	C	140	ASN
3	C	144	ILE
3	C	148	ARG
3	C	151	GLN
3	C	187	LYS
3	C	215	GLU

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Mol	Chain	Res	Type
3	C	221	TYR
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	260	LEU
4	E	3	GLN
4	E	7	ARG
4	E	9	ILE
4	E	40	GLU
4	E	54	GLN
4	E	55	ARG
4	E	56	LYS
4	E	74	ASP
4	E	84	ASP
4	E	92	THR
4	E	94	LYS
4	E	106	GLN
4	E	127	ILE
4	E	152	LYS
4	E	159	ASP
4	E	162	ARG
4	E	169	ARG
4	E	173	SER
4	E	175	LEU
4	E	184	VAL
4	E	191	LYS
5	F	71	GLU
5	F	74	ILE
5	F	76	LYS
5	F	103	MET
5	F	133	VAL
5	F	152	ILE
6	H	8	ASP
6	H	13	SER
6	H	22	LYS
6	H	26	ILE
6	H	35	GLN
6	H	40	LEU
6	H	55	LEU
6	H	94	ASP
6	H	106	GLU
6	H	110	ASP

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Mol	Chain	Res	Type
6	H	130	ARG
6	H	133	ASN
6	H	135	LEU
6	H	139	ASN
6	H	145	ARG
7	I	4	PHE
7	I	9	ASP
7	I	21	GLU
7	I	52	ILE
7	I	62	ILE
7	I	70	ARG
7	I	73	ARG
7	I	84	VAL
7	I	97	MET
7	I	105	SER
7	I	107	SER
7	I	111	THR
7	I	116	ASN
8	J	2	ILE
8	J	3	VAL
8	J	9	SER
8	J	13	VAL
8	J	19	GLU
8	J	22	LEU
8	J	23	ASN
8	J	30	LEU
8	J	43	ARG
8	J	48	ARG
8	J	59	LYS
8	J	62	ARG
8	J	64	ASN
9	K	5	ASP
9	K	6	ARG
9	K	11	LEU
9	K	21	ILE
9	K	29	ASN
9	K	41	THR
9	K	49	GLU
9	K	51	LEU
9	K	63	VAL
9	K	79	GLU
9	K	101	LEU

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Mol	Chain	Res	Type
9	K	102	LYS
9	K	107	THR
9	K	111	LEU
9	K	114	LEU
10	L	27	LEU
10	L	42	ARG
10	L	43	THR
10	L	46	VAL
10	L	50	ASP
10	L	58	LYS
10	L	61	THR
10	L	65	VAL
10	L	66	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	18	GLN
1	A	68	GLN
1	A	75	ASN
1	A	119	ASN
1	A	209	ASN
1	A	299	HIS
1	A	427	GLN
1	A	447	GLN
1	A	503	GLN
1	A	510	GLN
1	A	517	ASN
1	A	525	GLN
1	A	603	ASN
1	A	626	ASN
1	A	631	HIS
1	A	640	GLN
1	A	660	ASN
1	A	741	ASN
1	A	757	ASN
1	A	768	GLN
1	A	1008	GLN
1	A	1110	ASN
1	A	1140	HIS
1	A	1171	GLN

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Mol	Chain	Res	Type
1	A	1203	ASN
1	A	1211	GLN
1	A	1218	GLN
1	A	1232	ASN
1	A	1354	ASN
1	A	1364	ASN
1	A	1432	GLN
2	B	103	ASN
2	B	215	GLN
2	B	325	GLN
2	B	363	HIS
2	B	383	ASN
2	B	433	GLN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	587	HIS
2	B	734	HIS
2	B	744	HIS
2	B	762	ASN
2	B	767	ASN
2	B	822	ASN
2	B	1015	HIS
2	B	1025	HIS
2	B	1074	ASN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1141	HIS
2	B	1161	HIS
2	B	1176	ASN
2	B	1205	GLN
2	B	1211	ASN
3	C	31	ASN
3	C	91	HIS
3	C	112	ASN
3	C	242	GLN
4	E	54	GLN
4	E	61	GLN
4	E	106	GLN

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Mol	Chain	Res	Type
4	E	114	ASN
4	E	115	ASN
6	H	52	GLN
6	H	83	GLN
6	H	133	ASN
6	H	134	ASN
6	H	137	GLN
7	I	12	ASN
7	I	60	GLN
7	I	83	ASN
7	I	89	GLN
7	I	120	GLN
8	J	23	ASN
9	K	65	HIS
9	K	112	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	7/8 (87%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	10	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	26 (1%) 66 46	46, 104, 194, 237	0
2	B	1114/1224 (91%)	-0.09	13 (1%) 76 58	45, 98, 166, 201	0
3	C	266/318 (83%)	-0.17	1 (0%) 88 79	67, 96, 146, 180	0
4	E	214/215 (99%)	-0.08	0 100 100	74, 135, 177, 193	0
5	F	85/155 (54%)	-0.26	0 100 100	77, 114, 151, 168	0
6	H	133/146 (91%)	0.13	5 (3%) 44 28	98, 141, 173, 183	0
7	I	119/122 (97%)	-0.01	0 100 100	72, 113, 145, 163	0
8	J	65/70 (92%)	-0.20	0 100 100	60, 88, 127, 138	0
9	K	114/120 (95%)	-0.31	0 100 100	64, 96, 127, 141	0
10	L	46/70 (65%)	0.57	4 (8%) 16 11	84, 137, 162, 175	0
11	R	8/8 (100%)	-0.13	0 100 100	100, 128, 162, 169	0
12	T	13/29 (44%)	0.72	0 100 100	109, 134, 191, 198	0
All	All	3582/4210 (85%)	-0.07	49 (1%) 73 54	45, 105, 180, 237	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	4.4
1	A	65	LEU	4.2
2	B	715	ALA	3.8
10	L	27	LEU	3.7
2	B	70	ILE	3.6
1	A	1089	VAL	3.5
2	B	335	GLY	3.4
6	H	85	GLY	3.4
10	L	28	LYS	3.3
1	A	1123	GLY	3.2
1	A	998	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
6	H	63	LEU	3.1
2	B	882	THR	3.0
1	A	69	THR	3.0
1	A	317	LYS	2.9
1	A	103	CYS	2.9
1	A	1108	ALA	2.8
1	A	50	ILE	2.8
1	A	1087	ALA	2.8
1	A	1389	PHE	2.7
2	B	446	LEU	2.7
1	A	1086	PHE	2.6
1	A	1081	LEU	2.6
1	A	250	ILE	2.6
2	B	477	ALA	2.6
6	H	132	LEU	2.5
2	B	140	ILE	2.4
1	A	54	ASN	2.4
2	B	709	ASP	2.4
1	A	141	LEU	2.4
1	A	1090	ALA	2.4
1	A	1000	LEU	2.4
2	B	708	GLU	2.4
1	A	1083	THR	2.4
1	A	319	GLY	2.3
1	A	179	LEU	2.3
6	H	139	ASN	2.2
3	C	195	GLN	2.2
1	A	1080	THR	2.1
2	B	962	LYS	2.1
6	H	89	LEU	2.1
1	A	488	ASN	2.1
2	B	648	HIS	2.1
10	L	55	ILE	2.1
10	L	26	THR	2.1
1	A	318	SER	2.0
1	A	161	LEU	2.0
1	A	199	LEU	2.0
2	B	903	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	ZN	A	1734	1/1	0.88	0.08	300,300,300,300	0
13	ZN	A	1735	1/1	0.98	0.04	133,133,133,133	0
13	ZN	B	1307	1/1	0.98	0.04	174,174,174,174	0
13	ZN	I	203	1/1	0.99	0.03	109,109,109,109	0
13	ZN	I	204	1/1	0.99	0.02	79,79,79,79	0
14	MG	A	2001	1/1	0.99	0.04	41,41,41,41	0
13	ZN	J	101	1/1	1.00	0.01	71,71,71,71	0
13	ZN	L	105	1/1	1.00	0.02	139,139,139,139	0
13	ZN	C	319	1/1	1.00	0.01	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.