



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:41 PM UTC

PDB ID : 3S17 / pdb_00003s17
Title : RNA Polymerase II Initiation Complex with a 9-nt RNA
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-14
Resolution : 3.20 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

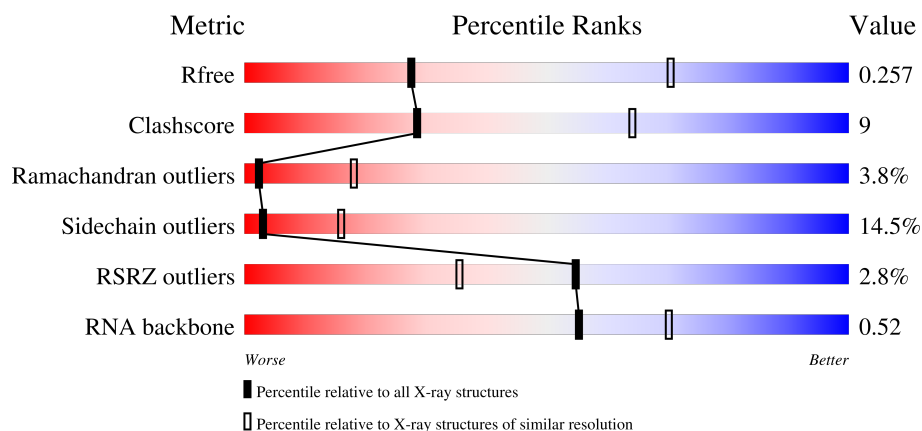
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	2% 54% 21% 5% 19%
2	B	1224	3% 59% 25% 6% 9%
3	C	318	54% 25% 5% 16%
4	E	215	% 73% 24%

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	9	
12	T	29	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 28757 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*UP*CP*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	9	Total	C	N	O	P	0	0	0
			195	88	40	59	8			

- 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

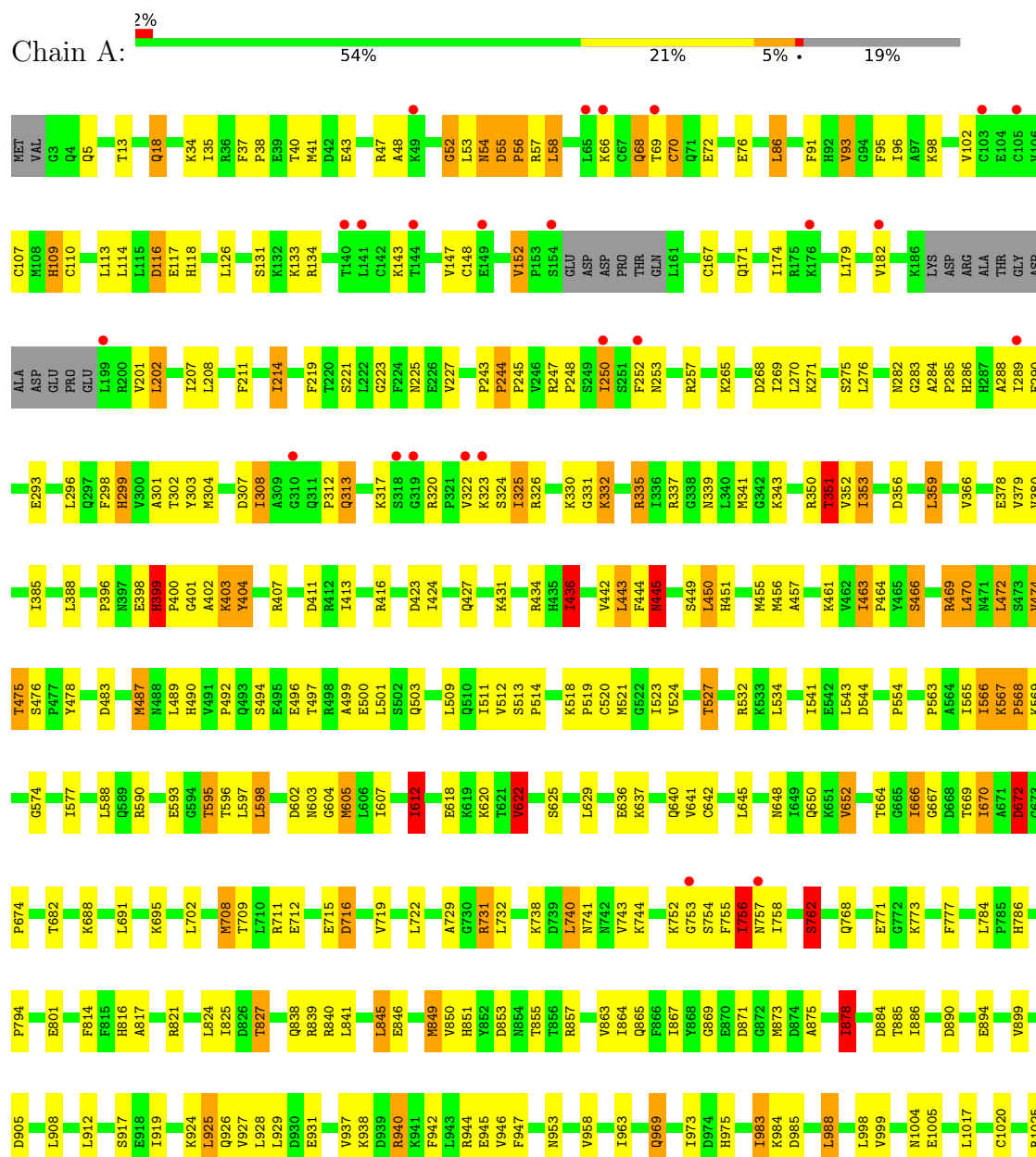
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

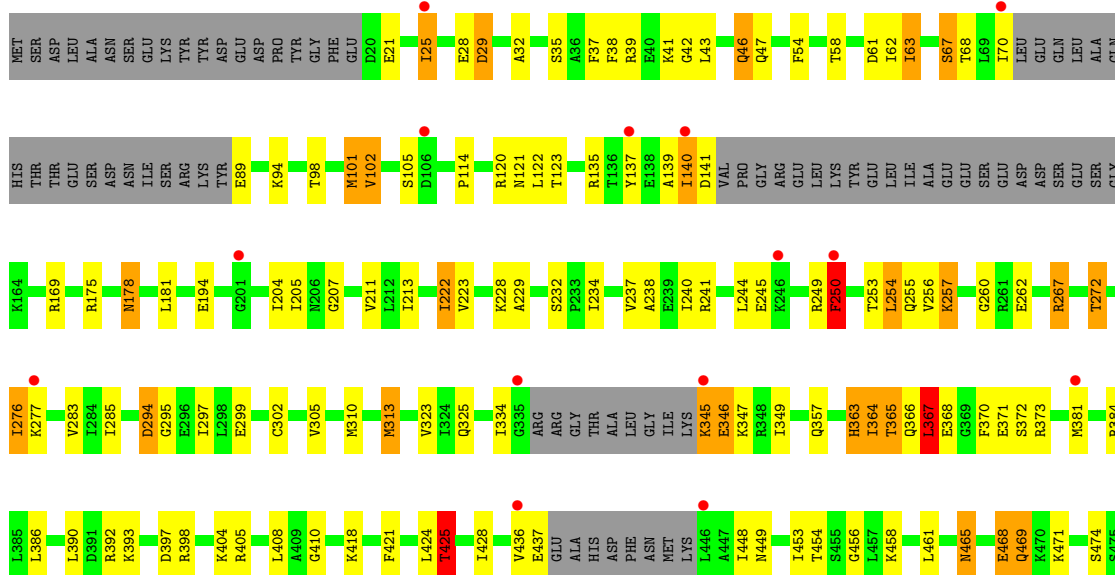
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

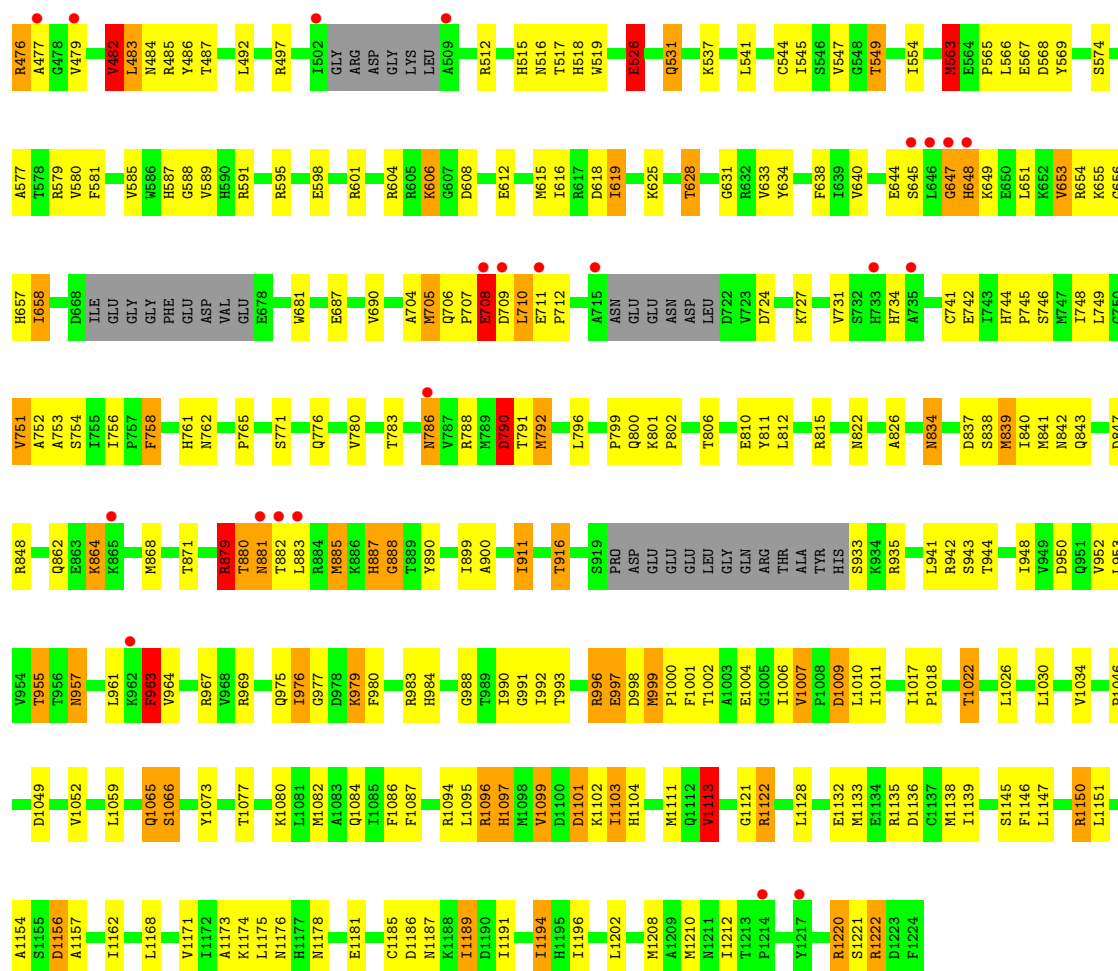
3 Residue-property plots

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

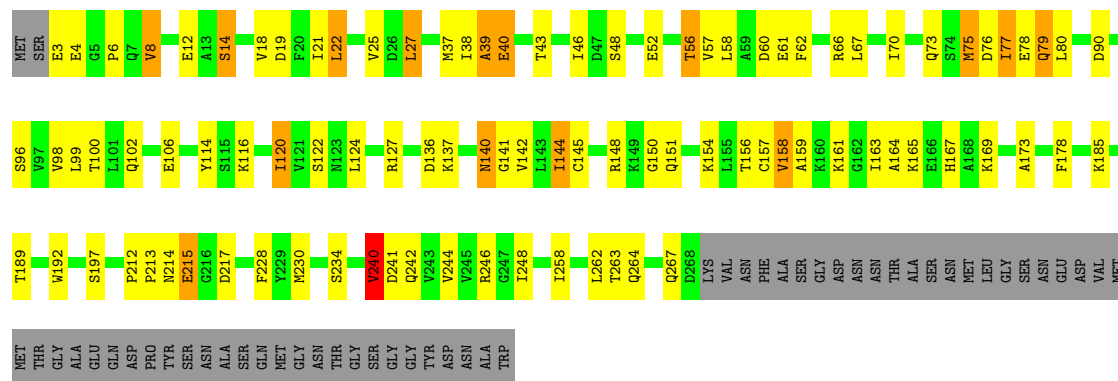






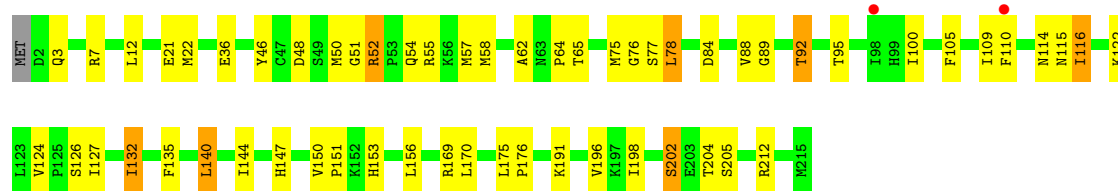
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 54% 25% 5% 16%

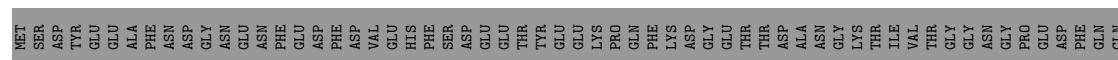
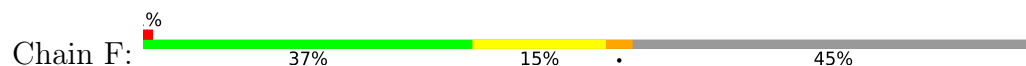


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 73% 24% 3%



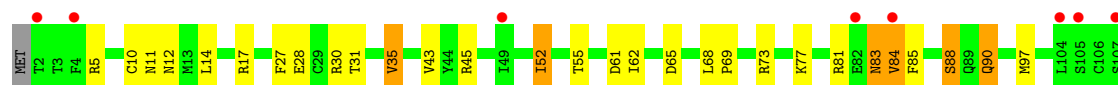
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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



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

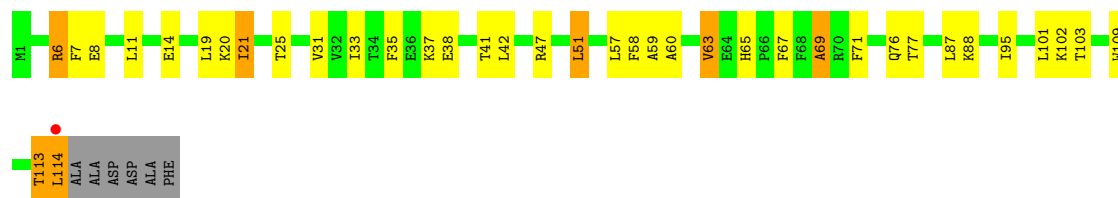


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

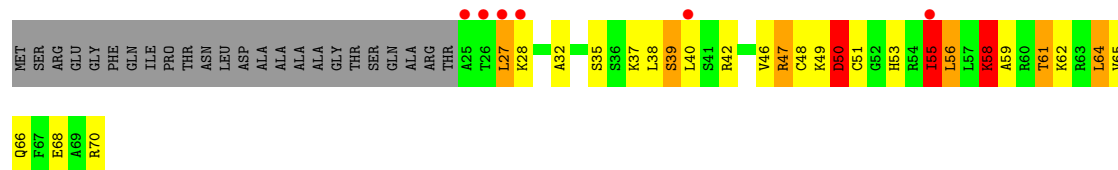
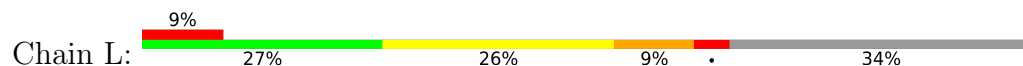


- Molecule 9: DNA-directed RNA polymerase II subunit RPB11





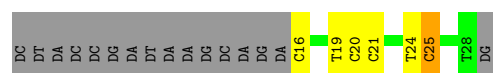
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



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



- Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*C
P*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	159.97Å 220.90Å 192.03Å 90.00° 98.16° 90.00°	Depositor
Resolution (Å)	43.65 – 3.20 43.65 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.65-3.20) 99.9 (43.65-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.19Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.188 , 0.236 0.208 , 0.257	Depositor DCC
R_{free} test set	5511 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.836	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 88.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28757	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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	0.82	3/11241 (0.0%)	1.47	79/15199 (0.5%)
2	B	0.85	3/9033 (0.0%)	1.45	69/12181 (0.6%)
3	C	0.80	1/2133 (0.0%)	1.43	18/2891 (0.6%)
4	E	0.78	0/1788	1.42	12/2406 (0.5%)
5	F	0.80	0/700	1.37	8/945 (0.8%)
6	H	0.80	0/1086	1.36	15/1470 (1.0%)
7	I	0.82	0/989	1.38	5/1331 (0.4%)
8	J	0.83	0/541	1.57	10/727 (1.4%)
9	K	0.75	0/937	1.40	6/1265 (0.5%)
10	L	0.87	0/365	1.59	7/485 (1.4%)
11	R	0.61	0/219	1.17	2/341 (0.6%)
12	T	0.42	0/290	1.32	3/444 (0.7%)
All	All	0.82	7/29322 (0.0%)	1.45	234/39685 (0.6%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	758	PHE	CA-C	6.28	1.57	1.53
2	B	705	MET	SD-CE	-6.10	1.64	1.79
2	B	563	MET	SD-CE	-5.60	1.65	1.79
3	C	212	PRO	CA-C	5.58	1.54	1.51
1	A	605	MET	SD-CE	-5.50	1.65	1.79
1	A	487	MET	SD-CE	-5.50	1.65	1.79
1	A	756	ILE	CG1-CD1	5.20	1.72	1.51

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	647	GLY	CA-C-N	11.15	141.78	121.70
2	B	647	GLY	C-N-CA	11.15	141.78	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	39	ALA	N-CA-C	9.80	123.74	111.69
10	L	55	ILE	N-CA-C	9.78	120.55	111.45
1	A	116	ASP	CA-C-N	9.66	139.09	121.70
1	A	116	ASP	C-N-CA	9.66	139.09	121.70
1	A	1097	GLY	CA-C-N	8.69	125.72	120.24
1	A	1097	GLY	C-N-CA	8.69	125.72	120.24
6	H	92	ASP	N-CA-C	-8.53	101.87	112.88
1	A	445	ASN	CA-CB-CG	8.09	120.69	112.60
2	B	479	VAL	N-CA-C	-7.92	98.39	108.84
2	B	363	HIS	N-CA-C	-7.74	100.10	110.55
2	B	37	PHE	N-CA-C	-7.68	100.96	110.41
2	B	1009	ASP	N-CA-C	-7.65	104.09	113.50
10	L	58	LYS	N-CA-C	7.56	121.60	112.38
3	C	40	GLU	N-CA-C	7.48	123.32	113.30
12	T	16	DC	P-O3'-C3'	7.32	131.18	120.20
8	J	1	MET	CA-C-N	7.18	134.89	121.97
8	J	1	MET	C-N-CA	7.18	134.89	121.97
1	A	947	PHE	CA-C-N	7.14	130.60	120.53
1	A	947	PHE	C-N-CA	7.14	130.60	120.53
2	B	842	ASN	CA-CB-CG	7.10	119.70	112.60
2	B	140	ILE	CA-C-N	6.98	134.27	121.70
2	B	140	ILE	C-N-CA	6.98	134.27	121.70
6	H	2	SER	CA-C-N	6.97	134.25	121.70
6	H	2	SER	C-N-CA	6.97	134.25	121.70
2	B	963	PHE	CA-CB-CG	6.91	120.71	113.80
8	J	5	VAL	N-CA-C	-6.90	100.68	109.58
1	A	1123	GLY	CA-C-N	6.86	134.04	121.70
1	A	1123	GLY	C-N-CA	6.86	134.04	121.70
2	B	345	LYS	CA-C-N	6.79	133.92	121.70
2	B	345	LYS	C-N-CA	6.79	133.92	121.70
1	A	1375	MET	CA-C-N	6.71	129.57	120.44
1	A	1375	MET	C-N-CA	6.71	129.57	120.44
2	B	648	HIS	N-CA-CB	6.63	121.77	110.50
2	B	916	THR	CB-CA-C	6.58	117.72	110.15
2	B	1154	ALA	N-CA-C	-6.53	98.99	109.96
6	H	91	ASP	N-CA-C	6.47	118.96	108.41
1	A	827	THR	N-CA-C	-6.43	104.20	111.14
1	A	366	VAL	N-CA-C	6.42	114.25	107.76
1	A	622	VAL	N-CA-C	6.34	118.25	112.29
1	A	1437	GLY	CA-C-N	6.34	128.78	120.28
1	A	1437	GLY	C-N-CA	6.34	128.78	120.28
2	B	1122	ARG	CA-C-N	6.30	129.57	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1122	ARG	C-N-CA	6.30	129.57	120.38
1	A	794	PRO	CA-C-N	6.28	128.98	120.38
1	A	794	PRO	C-N-CA	6.28	128.98	120.38
2	B	786	ASN	CA-C-N	6.26	129.08	122.14
2	B	786	ASN	C-N-CA	6.26	129.08	122.14
10	L	40	LEU	CA-C-N	6.24	129.72	120.87
10	L	40	LEU	C-N-CA	6.24	129.72	120.87
1	A	1424	VAL	CA-C-N	6.21	128.51	120.44
1	A	1424	VAL	C-N-CA	6.21	128.51	120.44
2	B	32	ALA	CA-C-N	6.17	128.46	120.56
2	B	32	ALA	C-N-CA	6.17	128.46	120.56
2	B	474	SER	CA-C-N	6.16	128.82	120.38
2	B	474	SER	C-N-CA	6.16	128.82	120.38
2	B	1007	VAL	CB-CA-C	6.15	115.36	109.33
3	C	214	ASN	CA-C-N	6.13	128.78	120.38
3	C	214	ASN	C-N-CA	6.13	128.78	120.38
2	B	1086	PHE	N-CA-C	-6.12	100.33	109.15
8	J	18	TRP	N-CA-C	6.11	117.61	111.07
1	A	474	VAL	CA-C-N	6.09	128.36	120.44
1	A	474	VAL	C-N-CA	6.09	128.36	120.44
1	A	436	ILE	CB-CA-C	6.05	119.44	111.33
3	C	240	VAL	N-CA-CB	6.03	117.20	110.51
2	B	711	GLU	N-CA-C	5.99	123.06	109.81
3	C	240	VAL	N-CA-C	5.98	116.64	110.36
1	A	351	THR	CA-C-N	5.97	129.41	120.69
1	A	351	THR	C-N-CA	5.97	129.41	120.69
2	B	47	GLN	CA-C-N	5.97	128.20	120.44
2	B	47	GLN	C-N-CA	5.97	128.20	120.44
4	E	150	VAL	N-CA-C	5.97	112.99	107.56
1	A	1004	ASN	CA-C-N	5.94	129.73	120.82
1	A	1004	ASN	C-N-CA	5.94	129.73	120.82
1	A	1086	PHE	CA-CB-CG	5.92	119.72	113.80
2	B	541	LEU	N-CA-C	5.92	117.40	111.07
1	A	602	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	463	ILE	N-CA-C	5.90	115.53	108.45
8	J	60	PHE	CA-CB-CG	5.89	119.69	113.80
6	H	139	ASN	CA-C-N	5.87	132.74	121.54
6	H	139	ASN	C-N-CA	5.87	132.74	121.54
1	A	313	GLN	N-CA-C	5.85	118.30	109.23
7	I	116	ASN	N-CA-C	5.84	118.47	110.24
1	A	777	PHE	CA-CB-CG	5.83	119.63	113.80
1	A	758	ILE	CA-C-N	5.78	128.34	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	758	ILE	C-N-CA	5.78	128.34	120.54
10	L	40	LEU	N-CA-C	5.77	118.95	109.72
5	F	87	LYS	CA-C-N	5.76	128.47	120.29
5	F	87	LYS	C-N-CA	5.76	128.47	120.29
1	A	864	ILE	N-CA-C	-5.76	107.23	111.90
7	I	31	THR	N-CA-C	-5.75	106.39	113.41
1	A	762	SER	N-CA-C	5.72	121.16	113.72
8	J	8	PHE	CA-CB-CG	5.72	119.52	113.80
3	C	56	THR	CA-C-N	5.71	129.66	120.30
3	C	56	THR	C-N-CA	5.71	129.66	120.30
8	J	2	ILE	N-CA-C	5.69	121.18	109.34
1	A	152	VAL	N-CA-C	5.67	114.14	107.84
2	B	482	VAL	N-CA-C	5.67	121.14	109.34
1	A	483	ASP	CA-CB-CG	5.67	118.27	112.60
2	B	397	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	985	ASP	CA-CB-CG	5.66	118.26	112.60
7	I	11	ASN	N-CA-C	-5.65	106.33	113.23
4	E	115	ASN	N-CA-C	5.65	117.38	108.96
2	B	392	ARG	N-CA-C	-5.61	107.08	114.31
1	A	969	GLN	CA-C-N	5.60	128.11	120.54
1	A	969	GLN	C-N-CA	5.60	128.11	120.54
3	C	78	GLU	CB-CG-CD	5.60	122.12	112.60
4	E	48	ASP	CA-CB-CG	5.60	118.20	112.60
3	C	60	ASP	CA-CB-CG	5.60	118.20	112.60
4	E	48	ASP	CA-C-N	5.59	129.21	120.82
4	E	48	ASP	C-N-CA	5.59	129.21	120.82
2	B	1189	ILE	N-CA-C	5.59	116.37	111.56
2	B	890	TYR	CA-C-N	5.56	129.58	120.63
2	B	890	TYR	C-N-CA	5.56	129.58	120.63
1	A	884	ASP	N-CA-C	5.54	119.88	113.18
2	B	1065	GLN	CB-CA-C	5.54	118.13	110.16
4	E	48	ASP	N-CA-C	5.54	117.05	110.19
1	A	1162	VAL	N-CA-C	-5.53	104.92	113.16
3	C	120	ILE	CA-C-N	5.51	128.85	122.35
3	C	120	ILE	C-N-CA	5.51	128.85	122.35
1	A	1271	ILE	N-CA-C	5.51	116.03	107.99
2	B	790	ASP	N-CA-C	5.51	118.71	109.95
5	F	100	GLN	CA-C-N	5.50	127.70	120.60
5	F	100	GLN	C-N-CA	5.50	127.70	120.60
1	A	109	HIS	CA-C-N	5.50	127.91	120.38
1	A	109	HIS	C-N-CA	5.50	127.91	120.38
1	A	708	MET	N-CA-C	5.49	118.40	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	197	SER	CA-C-N	5.48	127.57	120.44
3	C	197	SER	C-N-CA	5.48	127.57	120.44
1	A	983	ILE	N-CA-C	-5.48	105.16	110.42
1	A	716	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	1138	ILE	N-CA-C	5.45	116.31	111.90
1	A	445	ASN	N-CA-C	5.43	117.32	109.07
2	B	606	LYS	N-CA-C	-5.40	105.83	112.90
6	H	122	LEU	N-CA-C	5.39	117.83	110.55
1	A	466	SER	N-CA-C	5.39	119.86	113.28
1	A	411	ASP	N-CA-C	5.39	118.04	110.23
9	K	113	THR	CA-C-N	5.38	131.39	121.70
9	K	113	THR	C-N-CA	5.38	131.39	121.70
2	B	881	ASN	CA-C-N	5.36	129.72	121.19
2	B	881	ASN	C-N-CA	5.36	129.72	121.19
2	B	366	GLN	N-CA-C	-5.36	105.38	112.94
2	B	834	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	753	GLY	N-CA-C	5.34	118.94	112.48
1	A	1354	ASN	N-CA-C	5.33	117.84	111.71
2	B	294	ASP	CA-CB-CG	5.33	117.93	112.60
2	B	628	THR	CA-C-N	5.32	128.79	120.75
2	B	628	THR	C-N-CA	5.32	128.79	120.75
1	A	351	THR	CB-CA-C	-5.32	101.38	110.95
6	H	130	ARG	CA-C-N	5.31	131.68	121.54
6	H	130	ARG	C-N-CA	5.31	131.68	121.54
9	K	69	ALA	N-CA-C	5.31	117.06	111.28
1	A	1404	GLU	CA-C-N	5.30	129.62	121.19
1	A	1404	GLU	C-N-CA	5.30	129.62	121.19
2	B	250	PHE	CA-CB-CG	5.29	119.09	113.80
2	B	1186	ASP	CA-C-N	5.27	128.25	120.82
2	B	1186	ASP	C-N-CA	5.27	128.25	120.82
1	A	890	ASP	CA-C-N	5.27	127.60	120.44
1	A	890	ASP	C-N-CA	5.27	127.60	120.44
5	F	123	LYS	CA-C-N	5.27	128.07	120.38
5	F	123	LYS	C-N-CA	5.27	128.07	120.38
6	H	91	ASP	CA-C-N	5.26	130.80	122.60
6	H	91	ASP	C-N-CA	5.26	130.80	122.60
4	E	21	GLU	CA-C-N	5.25	127.59	120.65
4	E	21	GLU	C-N-CA	5.25	127.59	120.65
2	B	1121	GLY	CA-C-N	5.24	127.26	120.44
2	B	1121	GLY	C-N-CA	5.24	127.26	120.44
11	R	9	G	C4'-C3'-O3'	-5.24	105.14	113.00
1	A	244	PRO	N-CA-C	5.23	117.08	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	25	DC	P-O5'-C5'	5.22	127.84	120.00
1	A	917	SER	CA-C-N	5.22	128.95	120.60
1	A	917	SER	C-N-CA	5.22	128.95	120.60
2	B	456	GLY	CA-C-N	5.21	127.22	120.44
2	B	456	GLY	C-N-CA	5.21	127.22	120.44
2	B	222	ILE	CB-CA-C	5.21	117.92	110.84
10	L	62	LYS	N-CA-C	-5.20	107.11	112.93
5	F	148	VAL	CA-C-N	5.18	127.54	120.54
5	F	148	VAL	C-N-CA	5.18	127.54	120.54
1	A	1376	THR	N-CA-C	5.18	116.73	111.14
1	A	114	LEU	N-CA-C	5.17	117.32	111.11
2	B	618	ASP	CA-CB-CG	5.17	117.78	112.60
9	K	63	VAL	N-CA-CB	5.17	119.76	111.23
7	I	10	CYS	N-CA-C	5.17	117.00	111.36
2	B	1222	ARG	CA-C-N	5.16	131.40	121.54
2	B	1222	ARG	C-N-CA	5.16	131.40	121.54
6	H	129	TYR	CA-C-N	5.16	127.19	120.28
6	H	129	TYR	C-N-CA	5.16	127.19	120.28
1	A	1408	ILE	N-CA-C	-5.16	105.47	110.42
2	B	425	THR	CB-CA-C	5.15	119.43	110.68
1	A	878	ILE	N-CA-CB	-5.14	103.84	112.47
1	A	946	VAL	N-CA-C	-5.14	106.06	110.74
2	B	102	VAL	N-CA-C	5.13	115.25	107.75
9	K	35	PHE	CA-CB-CG	5.13	118.93	113.80
7	I	5	ARG	N-CA-C	5.13	117.33	109.95
2	B	1101	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	91	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	937	VAL	CA-C-N	5.12	127.14	120.28
1	A	937	VAL	C-N-CA	5.12	127.14	120.28
1	A	574	GLY	CA-C-N	5.11	127.44	120.54
1	A	574	GLY	C-N-CA	5.11	127.44	120.54
1	A	622	VAL	CB-CA-C	5.11	118.88	111.88
1	A	612	ILE	N-CA-CB	5.09	116.47	110.82
4	E	22	MET	CA-C-N	5.09	127.17	120.60
4	E	22	MET	C-N-CA	5.09	127.17	120.60
12	T	24	DT	O4'-C1'-N1	5.09	116.04	108.40
1	A	399	HIS	N-CA-CB	5.08	119.41	110.37
2	B	957	ASN	CA-C-N	5.08	127.79	120.38
2	B	957	ASN	C-N-CA	5.08	127.79	120.38
6	H	138	GLU	N-CA-C	-5.07	106.92	113.01
2	B	1113	VAL	N-CA-C	5.06	115.17	110.42
1	A	1228	TRP	N-CA-C	5.05	115.98	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	7	ARG	CA-C-N	5.05	127.05	120.28
4	E	7	ARG	C-N-CA	5.05	127.05	120.28
2	B	1009	ASP	CA-CB-CG	5.04	117.64	112.60
3	C	150	GLY	CA-C-N	5.04	127.86	120.71
3	C	150	GLY	C-N-CA	5.04	127.86	120.71
2	B	29	ASP	CA-C-N	5.03	127.02	120.28
2	B	29	ASP	C-N-CA	5.03	127.02	120.28
8	J	2	ILE	CA-C-N	5.03	131.44	122.13
8	J	2	ILE	C-N-CA	5.03	131.44	122.13
2	B	228	LYS	CA-C-N	5.03	131.14	121.54
2	B	228	LYS	C-N-CA	5.03	131.14	121.54
3	C	96	SER	N-CA-C	5.02	116.83	109.24
11	R	8	A	O4'-C4'-C3'	-5.02	98.98	104.00
2	B	681	TRP	N-CA-C	-5.02	105.89	111.36
8	J	64	ASN	N-CA-C	5.02	120.90	109.81
10	L	56	LEU	N-CA-C	5.01	121.48	110.80
3	C	8	VAL	N-CA-C	5.01	115.34	108.12
1	A	1344	GLY	CA-C-N	5.01	126.95	120.44
1	A	1344	GLY	C-N-CA	5.01	126.95	120.44
9	K	71	PHE	CA-CB-CG	5.01	118.81	113.80
2	B	1156	ASP	N-CA-C	5.01	121.47	110.80
6	H	16	ASP	N-CA-C	5.01	117.51	109.15

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	202	0
2	B	8861	0	8884	201	0
3	C	2095	0	2051	47	0
4	E	1752	0	1776	21	0
5	F	688	0	707	11	0
6	H	1068	0	1040	18	0
7	I	971	0	927	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	532	0	542	18	0
9	K	919	0	929	23	0
10	L	363	0	386	10	0
11	R	195	0	99	1	0
12	T	261	0	148	3	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	28757	0	28622	506	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 9.

All (506) 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:567:LYS:HB2	1:A:568:PRO:HD2	1.44	1.00
4:E:77:SER:HB3	4:E:105:PHE:HA	1.53	0.89
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.52	0.89
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.39	0.88
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.39	0.87
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.56	0.87
1:A:567:LYS:HB3	6:H:96:VAL:H	1.41	0.85
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.47	0.78
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.65	0.78
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.66	0.77
2:B:706:GLN:O	2:B:710:LEU:HB2	1.85	0.77
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.67	0.76
1:A:511:ILE:HA	1:A:521:MET:HE3	1.67	0.76
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.68	0.76
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.14	0.75
1:A:741:ASN:HD22	1:A:744:LYS:H	1.35	0.74
2:B:363:HIS:O	2:B:364:ILE:HB	1.85	0.74
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.21	0.74
3:C:56:THR:HG21	3:C:145:CYS:SG	2.28	0.73
2:B:862:GLN:HG2	2:B:963:PHE:HB2	1.69	0.73
2:B:801:LYS:O	8:J:52:THR:HG23	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:MET:HE3	2:B:580:VAL:HB	1.69	0.73
8:J:48:ARG:O	8:J:52:THR:HB	1.88	0.73
1:A:399:HIS:O	1:A:401:GLY:N	2.23	0.72
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.71	0.71
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.06	0.70
1:A:37:PHE:HD1	1:A:52:GLY:HA3	1.56	0.70
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.25	0.69
1:A:855:THR:HG21	1:A:857:ARG:HE	1.58	0.69
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.74	0.69
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.74	0.68
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.75	0.68
1:A:1323:ASP:OD1	1:A:1325:THR:HG23	1.93	0.68
2:B:975:GLN:HG2	2:B:976:ILE:H	1.57	0.68
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.75	0.68
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.20	0.67
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.76	0.67
2:B:654:ARG:H	2:B:657:HIS:HD2	1.42	0.67
2:B:1002:THR:HG22	2:B:1004:GLU:H	1.59	0.67
1:A:885:THR:O	1:A:940:ARG:HD3	1.95	0.67
1:A:669:THR:O	1:A:762:SER:HB3	1.96	0.66
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.78	0.66
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.78	0.65
2:B:879:ARG:O	2:B:882:THR:HG22	1.96	0.65
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.27	0.65
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.77	0.65
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.78	0.65
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.77	0.64
2:B:211:VAL:CG2	2:B:483:LEU:HD13	2.27	0.64
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.79	0.64
2:B:465:ASN:HA	2:B:476:ARG:HA	1.80	0.64
2:B:515:HIS:HD2	2:B:517:THR:H	1.45	0.64
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.33	0.64
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.79	0.64
2:B:638:PHE:CD2	2:B:653:VAL:HG21	2.33	0.63
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.80	0.63
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.64	0.63
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.97	0.63
2:B:744:HIS:HD2	2:B:746:SER:H	1.46	0.63
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.46	0.62
1:A:756:ILE:HD13	1:A:756:ILE:H	1.63	0.62
1:A:1325:THR:HA	4:E:147:HIS:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:THR:C	1:A:598:LEU:H	2.07	0.62
2:B:38:PHE:H	2:B:41:LYS:HB2	1.64	0.62
2:B:563:MET:HE1	2:B:587:HIS:HB2	1.81	0.61
6:H:137:GLN:HB3	6:H:139:ASN:HB2	1.82	0.61
2:B:313:MET:HE2	2:B:390:LEU:HG	1.82	0.61
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.81	0.61
1:A:326:ARG:HG2	1:A:1406:VAL:HG11	1.83	0.61
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.82	0.60
1:A:456:MET:HB2	1:A:478:TYR:OH	2.01	0.60
1:A:869:GLY:O	4:E:204:THR:HG21	2.02	0.60
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.82	0.60
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.83	0.60
2:B:1104:HIS:HB2	2:B:1122:ARG:HG3	1.84	0.60
1:A:56:PRO:HB2	1:A:57:ARG:HH21	1.66	0.60
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.85	0.60
1:A:378:GLU:OE2	1:A:434:ARG:HD3	2.01	0.59
2:B:283:VAL:HG12	2:B:297:ILE:HG21	1.83	0.59
3:C:73:GLN:HE21	3:C:75:MET:H	1.50	0.59
1:A:68:GLN:NE2	1:A:70:CYS:HB3	2.17	0.59
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.37	0.59
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.66	0.59
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.85	0.59
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.84	0.59
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.66	0.59
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.84	0.59
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.84	0.59
1:A:899:VAL:HB	1:A:929:LEU:HD22	1.85	0.58
7:I:116:ASN:HD22	7:I:118:ARG:HH12	1.49	0.58
2:B:43:LEU:HD11	2:B:811:TYR:O	2.03	0.58
3:C:46:ILE:HA	3:C:159:ALA:HA	1.84	0.58
1:A:754:SER:H	1:A:757:ASN:HD22	1.51	0.58
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.04	0.58
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.86	0.58
1:A:554:PRO:HD2	1:A:648:ASN:ND2	2.18	0.58
1:A:1161:THR:OG1	1:A:1170:ILE:HG13	2.03	0.58
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.69	0.58
2:B:515:HIS:H	2:B:518:HIS:HD2	1.52	0.58
2:B:753:ALA:HA	2:B:756:ILE:HD12	1.85	0.58
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.34	0.57
7:I:111:THR:HG23	7:I:113:ASP:H	1.68	0.57
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.86	0.57
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.86	0.57
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.86	0.57
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.38	0.57
1:A:72:GLU:HB3	1:A:76:GLU:HG3	1.86	0.57
1:A:466:SER:HB3	2:B:1103:ILE:CD1	2.35	0.57
3:C:76:ASP:HB3	3:C:79:GLN:HG3	1.85	0.57
7:I:28:GLU:HB3	7:I:35:VAL:HG13	1.87	0.57
3:C:167:HIS:HD2	3:C:169:LYS:H	1.51	0.57
7:I:88:SER:C	7:I:90:GLN:H	2.13	0.57
2:B:843:GLN:HB2	2:B:993:THR:HB	1.87	0.57
2:B:887:HIS:HA	2:B:888:GLY:C	2.29	0.57
2:B:405:ARG:HB3	2:B:631:GLY:HA3	1.87	0.56
2:B:651:LEU:HD21	2:B:741:CYS:HB3	1.88	0.56
1:A:95:PHE:CE2	1:A:1414:ALA:HB2	2.41	0.56
1:A:404:TYR:HA	1:A:413:ILE:O	2.05	0.56
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	1.87	0.56
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.87	0.56
1:A:34:LYS:HE2	1:A:57:ARG:HH12	1.71	0.56
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.53	0.56
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.87	0.56
1:A:58:LEU:HD23	1:A:244:PRO:HD3	1.87	0.56
2:B:984:HIS:HB3	2:B:1022:THR:OG1	2.06	0.56
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.88	0.56
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.86	0.56
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.54	0.56
12:T:19:DT:H2'	12:T:20:DC:C6	2.41	0.56
2:B:792:MET:HE1	12:T:25:DC:H5''	1.87	0.56
2:B:916:THR:HG23	2:B:935:ARG:HB3	1.87	0.56
3:C:262:LEU:HD11	9:K:87:LEU:HD23	1.88	0.56
2:B:241:ARG:HA	2:B:253:THR:HG22	1.87	0.55
2:B:834:ASN:HA	2:B:838:SER:HB2	1.88	0.55
2:B:408:LEU:HD11	2:B:545:ILE:HD13	1.89	0.55
2:B:976:ILE:O	2:B:990:ILE:HB	2.06	0.55
3:C:6:PRO:HB3	3:C:25:VAL:HG22	1.89	0.55
9:K:21:ILE:HG13	9:K:33:ILE:HG12	1.87	0.55
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.89	0.55
2:B:260:GLY:O	2:B:267:ARG:HD3	2.06	0.55
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.88	0.55
2:B:516:ASN:H	2:B:516:ASN:HD22	1.55	0.55
1:A:709:THR:HG22	1:A:711:ARG:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.72	0.55
1:A:709:THR:HB	1:A:712:GLU:HB2	1.89	0.55
1:A:1084:PHE:HZ	1:A:1093:LYS:HA	1.72	0.55
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.42	0.55
2:B:975:GLN:O	2:B:990:ILE:HD12	2.07	0.54
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.90	0.54
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	1.89	0.54
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.39	0.54
1:A:554:PRO:HD2	1:A:648:ASN:HD22	1.72	0.54
3:C:22:LEU:HD22	3:C:230:MET:HE1	1.90	0.54
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.87	0.54
10:L:38:LEU:HD21	10:L:48:CYS:HA	1.90	0.54
3:C:14:SER:HA	9:K:114:LEU:HD22	1.88	0.54
1:A:55:ASP:O	1:A:57:ARG:N	2.40	0.54
2:B:486:TYR:CZ	2:B:1096:ARG:HG3	2.43	0.53
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.90	0.53
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.31	0.53
2:B:953:LEU:O	2:B:964:VAL:HG23	2.08	0.53
1:A:472:LEU:O	1:A:475:THR:HB	2.09	0.53
2:B:370:PHE:O	2:B:372:SER:N	2.36	0.53
8:J:3:VAL:CG1	8:J:18:TRP:HB2	2.36	0.53
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.74	0.53
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.91	0.53
2:B:724:ASP:HB3	2:B:727:LYS:HD2	1.91	0.53
4:E:64:PRO:HD3	4:E:76:GLY:HA2	1.91	0.53
2:B:35:SER:O	2:B:39:ARG:HB2	2.09	0.53
5:F:128:LYS:HG2	5:F:149:GLU:HA	1.91	0.53
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.44	0.52
1:A:666:ILE:HG12	2:B:1026:LEU:HB2	1.91	0.52
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.90	0.52
2:B:762:ASN:HD21	2:B:984:HIS:HD2	1.56	0.52
4:E:202:SER:HB3	4:E:205:SER:H	1.75	0.52
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.91	0.52
2:B:255:GLN:H	2:B:272:THR:HB	1.73	0.52
2:B:483:LEU:HG	2:B:484:ASN:H	1.74	0.52
2:B:950:ASP:HB3	2:B:967:ARG:HG2	1.90	0.52
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.89	0.52
1:A:68:GLN:NE2	1:A:68:GLN:O	2.42	0.52
1:A:116:ASP:HB3	1:A:117:GLU:HB2	1.90	0.52
1:A:494:SER:HB3	1:A:497:THR:OG1	2.09	0.52
2:B:428:ILE:HD12	2:B:448:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:H	2:B:518:HIS:CD2	2.26	0.52
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.44	0.52
5:F:93:ILE:HD13	5:F:134:ILE:HD11	1.91	0.52
1:A:863:VAL:HG23	4:E:170:LEU:HD21	1.90	0.52
2:B:839:MET:HE3	2:B:1010:LEU:CD1	2.34	0.52
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.91	0.52
1:A:731:ARG:HD3	1:A:755:PHE:CZ	2.45	0.52
1:A:18:GLN:HE21	1:A:1418:LEU:HB2	1.74	0.52
1:A:672:ASP:HB3	1:A:674:PRO:HD2	1.92	0.52
2:B:1168:LEU:HD22	2:B:1208:MET:HE2	1.91	0.52
2:B:976:ILE:HG23	2:B:977:GLY:H	1.75	0.52
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.91	0.52
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.92	0.52
9:K:65:HIS:HD2	9:K:67:PHE:H	1.58	0.52
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.92	0.51
1:A:984:LYS:O	1:A:988:LEU:HB2	2.10	0.51
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.91	0.51
2:B:640:VAL:CG1	2:B:649:LYS:HB3	2.40	0.51
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.92	0.51
4:E:50:MET:HB3	4:E:52:ARG:HH12	1.75	0.51
1:A:899:VAL:HG22	1:A:1029:ARG:HG3	1.92	0.51
1:A:1130:GLN:HE21	1:A:1134:ILE:HD11	1.75	0.51
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.46	0.51
4:E:198:ILE:HD13	4:E:212:ARG:HG3	1.92	0.51
9:K:38:GLU:O	9:K:69:ALA:O	2.28	0.51
1:A:37:PHE:CD1	1:A:52:GLY:HA3	2.42	0.51
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.92	0.51
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.92	0.51
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.58	0.51
3:C:98:VAL:HG22	3:C:158:VAL:HG13	1.92	0.51
2:B:1082:MET:HA	3:C:189:THR:HA	1.93	0.51
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.93	0.51
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.92	0.50
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.46	0.50
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.36	0.50
6:H:125:LEU:HG	6:H:130:ARG:NH1	2.25	0.50
2:B:276:ILE:HG13	2:B:334:ILE:HG23	1.93	0.50
2:B:997:GLU:CD	2:B:997:GLU:H	2.19	0.50
6:H:10:PHE:HB3	6:H:28:ALA:HB1	1.94	0.50
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.93	0.50
1:A:290:GLU:HA	1:A:293:GLU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:LEU:O	1:A:1020:CYS:HB2	2.12	0.50
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.91	0.50
1:A:899:VAL:CG2	1:A:1029:ARG:HG3	2.41	0.50
1:A:1259:MET:HA	1:A:1262:LYS:HE2	1.93	0.50
2:B:516:ASN:H	2:B:516:ASN:ND2	2.09	0.50
4:E:88:VAL:HG13	4:E:92:THR:HB	1.93	0.50
1:A:499:ALA:HB2	5:F:118:LEU:HD11	1.94	0.50
1:A:265:LYS:HD3	1:A:322:VAL:HG21	1.93	0.50
1:A:513:SER:HB3	1:A:520:CYS:HB3	1.93	0.50
6:H:113:ALA:HB2	6:H:126:GLU:HG3	1.92	0.50
1:A:211:PHE:HA	1:A:214:ILE:HD11	1.94	0.49
2:B:58:THR:O	2:B:62:ILE:HG12	2.12	0.49
2:B:63:ILE:O	2:B:67:SER:HB3	2.11	0.49
9:K:65:HIS:CD2	9:K:67:PHE:H	2.30	0.49
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.92	0.49
2:B:706:GLN:H	2:B:710:LEU:HG	1.78	0.49
2:B:744:HIS:CD2	2:B:746:SER:OG	2.65	0.49
2:B:549:THR:HB	2:B:628:THR:HB	1.95	0.49
1:A:86:LEU:HD11	1:A:296:LEU:HD21	1.94	0.49
1:A:492:PRO:HG3	1:A:501:LEU:HD12	1.95	0.49
1:A:512:VAL:HA	1:A:519:PRO:HA	1.94	0.49
2:B:140:ILE:HB	2:B:141:ASP:HB2	1.93	0.49
1:A:642:CYS:O	1:A:645:LEU:HB3	2.12	0.49
2:B:837:ASP:O	2:B:988:GLY:HA2	2.12	0.49
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.60	0.49
1:A:490:HIS:HB3	2:B:1150:ARG:HH21	1.78	0.49
1:A:667:GLY:HA2	1:A:670:ILE:HG12	1.95	0.49
2:B:864:LYS:HG2	2:B:871:THR:HA	1.94	0.49
2:B:999:MET:HE2	2:B:1011:ILE:CD1	2.41	0.48
3:C:58:LEU:HD21	8:J:57:ILE:HD12	1.95	0.48
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.94	0.48
1:A:444:PHE:CE2	1:A:470:LEU:HD22	2.49	0.48
2:B:140:ILE:H	2:B:141:ASP:C	2.22	0.48
2:B:839:MET:CE	2:B:1010:LEU:HD11	2.35	0.48
5:F:110:ASP:O	5:F:123:LYS:HE2	2.14	0.48
10:L:28:LYS:HB2	10:L:39:SER:HA	1.95	0.48
2:B:123:THR:HA	2:B:204:ILE:O	2.14	0.48
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.96	0.48
2:B:237:VAL:HG22	2:B:257:LYS:HB3	1.94	0.48
2:B:705:MET:HG3	2:B:745:PRO:HG3	1.95	0.48
1:A:469:ARG:NH2	2:B:991:GLY:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ILE:HD13	2:B:653:VAL:HB	1.95	0.48
3:C:262:LEU:HD13	9:K:88:LYS:HG3	1.96	0.48
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.96	0.48
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.95	0.48
2:B:887:HIS:HA	2:B:888:GLY:O	2.13	0.48
1:A:1105:LEU:HB3	1:A:1384:VAL:CG2	2.44	0.47
3:C:165:LYS:O	9:K:6:ARG:NH1	2.47	0.47
10:L:49:LYS:O	10:L:50:ASP:HB2	2.14	0.47
2:B:999:MET:HE3	2:B:999:MET:HA	1.96	0.47
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.43	0.47
1:A:839:ARG:NH2	1:A:1402:PHE:HA	2.29	0.47
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.96	0.47
1:A:341:MET:HB2	2:B:1132:GLU:HG2	1.96	0.47
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.96	0.47
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.14	0.47
2:B:302:CYS:HA	2:B:310:MET:HE3	1.96	0.47
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.96	0.47
2:B:515:HIS:N	2:B:518:HIS:HD2	2.13	0.47
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.79	0.47
3:C:248:ILE:HD13	9:K:102:LYS:HA	1.94	0.47
1:A:975:HIS:CG	1:A:1036:ARG:HD3	2.50	0.47
1:A:1166:ASP:O	1:A:1168:GLU:N	2.48	0.47
3:C:234:SER:HB3	3:C:240:VAL:HG13	1.97	0.47
1:A:325:ILE:HB	2:B:1210:MET:SD	2.55	0.47
1:A:511:ILE:HA	1:A:521:MET:CE	2.43	0.47
2:B:565:PRO:HD2	2:B:568:ASP:HB2	1.96	0.47
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.14	0.47
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.68	0.47
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.50	0.47
4:E:78:LEU:HD21	4:E:109:ILE:HG12	1.97	0.47
1:A:1422:ARG:HG3	2:B:1220:ARG:HH12	1.80	0.46
2:B:745:PRO:O	2:B:748:ILE:HG12	2.16	0.46
1:A:53:LEU:HG	1:A:54:ASN:HD22	1.80	0.46
1:A:886:ILE:HG13	1:A:944:ARG:HG3	1.96	0.46
1:A:942:PHE:O	1:A:945:GLU:HG2	2.15	0.46
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.80	0.46
1:A:225:ASN:HD22	1:A:227:VAL:H	1.63	0.46
2:B:563:MET:HA	2:B:589:VAL:O	2.15	0.46
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.97	0.46
2:B:822:ASN:HD22	8:J:52:THR:CG2	2.27	0.46
10:L:68:GLU:C	10:L:70:ARG:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:63:LEU:HB2	6:H:90:ALA:H	1.80	0.46
8:J:1:MET:HB2	8:J:56:LEU:HD12	1.97	0.46
1:A:396:PRO:HG2	1:A:416:ARG:HB3	1.98	0.46
1:A:523:ILE:HG23	1:A:527:THR:HB	1.98	0.46
2:B:492:LEU:HB3	2:B:751:VAL:HG21	1.98	0.46
2:B:727:LYS:HE2	2:B:1049:ASP:HB3	1.98	0.46
4:E:55:ARG:HG2	4:E:58:MET:HE2	1.98	0.46
1:A:738:LYS:HD2	1:A:740:LEU:HD21	1.97	0.46
1:A:752:LYS:HB3	2:B:1018:PRO:HG2	1.98	0.46
1:A:497:THR:HG23	2:B:1146:PHE:HA	1.96	0.46
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.97	0.46
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.98	0.46
2:B:38:PHE:HA	2:B:42:GLY:H	1.81	0.46
2:B:1034:VAL:HG22	2:B:1059:LEU:HB2	1.98	0.46
1:A:756:ILE:H	1:A:756:ILE:CD1	2.29	0.45
3:C:173:ALA:HA	3:C:234:SER:HA	1.97	0.45
3:C:258:ILE:HG23	9:K:19:LEU:HD11	1.97	0.45
1:A:68:GLN:HE22	1:A:70:CYS:HB3	1.82	0.45
1:A:343:LYS:HE3	2:B:1151:LEU:HG	1.99	0.45
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.98	0.45
2:B:1185:CYS:C	2:B:1187:ASN:H	2.25	0.45
1:A:5:GLN:HB3	2:B:1175:LEU:HD22	1.97	0.45
2:B:839:MET:CE	2:B:980:PHE:HB2	2.47	0.45
1:A:1404:GLU:O	1:A:1408:ILE:HG12	2.16	0.45
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.80	0.45
1:A:743:VAL:HG13	2:B:1018:PRO:HB3	1.98	0.45
3:C:98:VAL:H	3:C:122:SER:CB	2.30	0.45
2:B:367:LEU:HB3	2:B:368:GLU:H	1.68	0.45
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.98	0.45
1:A:919:ILE:HD11	1:A:925:LEU:HG	1.98	0.45
1:A:116:ASP:CB	1:A:117:GLU:HB2	2.46	0.45
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.52	0.45
1:A:57:ARG:O	1:A:68:GLN:HG2	2.16	0.45
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.98	0.45
1:A:567:LYS:O	1:A:569:LYS:N	2.50	0.44
1:A:851:HIS:HB2	1:A:855:THR:HG22	2.00	0.44
1:A:924:LYS:O	1:A:927:VAL:HG12	2.16	0.44
2:B:882:THR:HG21	2:B:885:MET:HE3	1.98	0.44
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.99	0.44
1:A:814:PHE:O	1:A:817:ALA:HB3	2.18	0.44
5:F:72:LYS:HG2	5:F:142:SER:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:57:LEU:HB2	9:K:76:GLN:HG2	1.99	0.44
1:A:98:LYS:O	1:A:102:VAL:HG23	2.17	0.44
1:A:595:THR:HG21	1:A:604:GLY:HA3	1.99	0.44
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.99	0.44
12:T:20:DC:H2'	12:T:21:DC:O4'	2.17	0.44
3:C:99:LEU:HD13	3:C:120:ILE:HG12	2.00	0.44
1:A:351:THR:HG21	1:A:466:SER:O	2.18	0.44
1:A:449:SER:O	2:B:1133:MET:HG2	2.18	0.44
2:B:577:ALA:HB1	2:B:589:VAL:HB	1.99	0.44
7:I:65:ASP:HB3	7:I:68:LEU:HD12	1.99	0.44
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.99	0.44
6:H:135:LEU:C	6:H:137:GLN:H	2.26	0.44
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.52	0.44
3:C:12:GLU:HB2	3:C:19:ASP:HB3	1.99	0.44
3:C:98:VAL:H	3:C:122:SER:HB2	1.83	0.44
5:F:133:VAL:HG22	5:F:147:SER:HA	2.00	0.44
10:L:32:ALA:HB3	10:L:55:ILE:HB	1.98	0.44
4:E:176:PRO:O	4:E:212:ARG:HA	2.17	0.43
1:A:57:ARG:HA	1:A:68:GLN:HB3	2.00	0.43
2:B:54:PHE:HB2	2:B:410:GLY:HA2	2.00	0.43
1:A:1308:THR:HG22	1:A:1310:GLY:O	2.18	0.43
2:B:295:GLY:O	2:B:299:GLU:HB2	2.18	0.43
2:B:515:HIS:CD2	2:B:517:THR:H	2.29	0.43
1:A:738:LYS:HA	6:H:19:ARG:HH22	1.83	0.43
1:A:304:MET:O	1:A:326:ARG:HB2	2.18	0.43
1:A:637:LYS:HB3	1:A:641:VAL:HG11	2.01	0.43
1:A:824:LEU:HD21	2:B:765:PRO:HB3	2.00	0.43
1:A:1084:PHE:HE2	1:A:1094:VAL:H	1.66	0.43
1:A:1411:GLU:HA	1:A:1414:ALA:HB3	2.01	0.43
2:B:841:MET:O	2:B:993:THR:HA	2.19	0.43
4:E:46:TYR:HD2	4:E:57:MET:HB3	1.83	0.43
4:E:124:VAL:HG22	4:E:132:ILE:HD11	2.01	0.43
7:I:73:ARG:O	7:I:81:ARG:HA	2.18	0.43
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.00	0.43
1:A:983:ILE:HD12	1:A:1028:THR:HG21	2.01	0.43
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	2.00	0.43
1:A:182:VAL:HG22	1:A:201:VAL:HG12	2.01	0.43
1:A:250:ILE:HD11	2:B:1113:VAL:HG21	2.01	0.43
2:B:421:PHE:O	2:B:425:THR:HB	2.18	0.43
3:C:22:LEU:HG	3:C:25:VAL:HG21	2.01	0.43
3:C:241:ASP:HB3	9:K:109:TRP:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.48	0.43
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.99	0.43
1:A:1428:VAL:HG21	2:B:1135:ARG:HD2	2.01	0.43
2:B:62:ILE:HG23	2:B:418:LYS:HG3	2.01	0.43
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.16	0.43
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.83	0.43
3:C:77:ILE:HD12	3:C:161:LYS:HG3	2.00	0.42
4:E:151:PRO:HD2	4:E:153:HIS:HE1	1.84	0.42
9:K:113:THR:O	9:K:114:LEU:HB2	2.19	0.42
3:C:70:ILE:CD1	3:C:144:ILE:HD12	2.48	0.42
4:E:62:ALA:HB3	4:E:78:LEU:HB3	2.01	0.42
4:E:110:PHE:HE2	4:E:116:ILE:HD11	1.84	0.42
7:I:69:PRO:HD2	7:I:85:PHE:O	2.19	0.42
1:A:855:THR:HG21	1:A:857:ARG:NE	2.29	0.42
1:A:849:MET:HB3	1:A:1063:MET:SD	2.59	0.42
1:A:1151:GLU:HG2	7:I:45:ARG:HG3	2.02	0.42
2:B:21:GLU:HB2	2:B:656:GLY:HA3	2.00	0.42
2:B:581:PHE:HB2	2:B:625:LYS:HG2	2.01	0.42
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.54	0.42
7:I:62:ILE:HG12	7:I:84:VAL:HG11	2.00	0.42
11:R:9:G:H2'	11:R:10:G:C8	2.55	0.42
1:A:107:CYS:HA	1:A:171:GLN:HE21	1.83	0.42
1:A:514:PRO:HG2	1:A:1067:LEU:HD21	2.01	0.42
1:A:563:PRO:HG2	1:A:566:ILE:HG12	2.00	0.42
1:A:841:LEU:O	1:A:845:LEU:HG	2.20	0.42
2:B:800:GLN:CB	8:J:52:THR:HG22	2.48	0.42
3:C:148:ARG:HB3	3:C:151:GLN:HG3	2.01	0.42
9:K:8:GLU:O	9:K:37:LYS:HD2	2.19	0.42
1:A:284:ALA:HB1	1:A:289:ILE:HD11	2.01	0.42
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.90	0.42
2:B:254:LEU:HD23	2:B:381:MET:HE1	2.02	0.42
2:B:519:TRP:CD1	2:B:519:TRP:C	2.97	0.42
3:C:40:GLU:HG2	3:C:163:ILE:HD12	2.01	0.42
1:A:715:GLU:O	1:A:719:VAL:HG23	2.19	0.42
1:A:729:ALA:HA	1:A:732:LEU:HD12	2.01	0.42
1:A:839:ARG:HH21	1:A:1402:PHE:HA	1.85	0.42
1:A:928:LEU:HA	1:A:931:GLU:HG2	2.01	0.42
2:B:654:ARG:H	2:B:657:HIS:CD2	2.29	0.42
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.20	0.42
2:B:754:SER:HB2	2:B:812:LEU:CD1	2.48	0.42
2:B:840:ILE:HG12	2:B:992:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.55	0.42
5:F:109:VAL:HG22	5:F:123:LYS:HE3	2.01	0.42
7:I:14:LEU:HB3	7:I:27:PHE:HB3	2.02	0.42
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	2.01	0.42
1:A:1293:SER:HB3	1:A:1299:VAL:HG23	2.01	0.42
2:B:563:MET:CE	2:B:587:HIS:HB2	2.47	0.42
3:C:114:TYR:CG	3:C:140:ASN:HB2	2.54	0.42
1:A:605:MET:HE2	1:A:607:ILE:HG13	2.02	0.42
1:A:648:ASN:O	1:A:652:VAL:HG23	2.19	0.42
3:C:99:LEU:HB2	3:C:157:CYS:HB2	2.02	0.42
1:A:298:PHE:O	1:A:298:PHE:CD1	2.73	0.41
1:A:356:ASP:HB3	1:A:359:LEU:HB2	2.01	0.41
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.49	0.41
2:B:1162:ILE:HG12	2:B:1194:ILE:HD12	2.01	0.41
6:H:80:ARG:HG2	9:K:57:LEU:HD22	2.01	0.41
2:B:424:LEU:O	2:B:428:ILE:HG12	2.20	0.41
2:B:563:MET:HE2	2:B:588:GLY:N	2.35	0.41
2:B:708:GLU:H	2:B:708:GLU:HG3	1.57	0.41
3:C:215:GLU:C	3:C:217:ASP:H	2.29	0.41
1:A:403:LYS:H	1:A:403:LYS:HG2	1.78	0.41
1:A:436:ILE:HD12	1:A:436:ILE:HA	1.87	0.41
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.95	0.41
1:A:605:MET:HE1	1:A:612:ILE:HD13	2.01	0.41
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.56	0.41
1:A:963:ILE:HG22	1:A:1045:VAL:HG22	2.01	0.41
3:C:62:PHE:O	3:C:66:ARG:HG3	2.20	0.41
9:K:7:PHE:O	9:K:11:LEU:HB2	2.20	0.41
1:A:332:LYS:HD2	1:A:332:LYS:HA	1.89	0.41
1:A:527:THR:HG21	1:A:650:GLN:HA	2.02	0.41
2:B:796:LEU:HD23	2:B:799:PRO:HA	2.03	0.41
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.55	0.41
6:H:81:PRO:O	6:H:82:PRO:C	2.63	0.41
1:A:351:THR:HG22	1:A:352:VAL:H	1.85	0.41
2:B:46:GLN:H	2:B:46:GLN:HG3	1.73	0.41
2:B:244:LEU:HD12	2:B:250:PHE:HB2	2.02	0.41
2:B:483:LEU:CG	2:B:484:ASN:H	2.33	0.41
2:B:704:ALA:HB1	2:B:710:LEU:HB3	2.02	0.41
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.85	0.41
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	2.03	0.41
1:A:1084:PHE:CZ	1:A:1093:LYS:HA	2.54	0.41
6:H:40:LEU:HD13	6:H:123:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:CYS:HB3	1:A:167:CYS:O	2.20	0.41
4:E:196:VAL:HG13	4:E:198:ILE:HD11	2.03	0.41
6:H:109:LYS:HD2	6:H:110:ASP:H	1.86	0.41
10:L:27:LEU:HB3	10:L:37:LYS:HD2	2.02	0.41
1:A:118:HIS:CD2	1:A:152:VAL:HG21	2.55	0.41
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.86	0.41
2:B:98:THR:O	2:B:178:ASN:ND2	2.53	0.41
2:B:101:MET:HE1	2:B:169:ARG:HH11	1.86	0.41
2:B:640:VAL:CG2	2:B:651:LEU:HD23	2.50	0.41
2:B:749:LEU:HD22	2:B:753:ALA:HB1	2.01	0.41
1:A:37:PHE:HA	1:A:38:PRO:HD3	2.00	0.41
2:B:294:ASP:H	7:I:12:ASN:ND2	2.19	0.41
2:B:900:ALA:HA	10:L:58:LYS:HD3	2.03	0.41
3:C:185:LYS:HG2	3:C:213:PRO:HG3	2.03	0.41
2:B:313:MET:HE3	2:B:386:LEU:HD13	2.03	0.40
8:J:43:ARG:HG3	8:J:46:CYS:SG	2.61	0.40
9:K:47:ARG:HD2	9:K:60:ALA:HA	2.03	0.40
1:A:565:ILE:HG22	1:A:569:LYS:O	2.22	0.40
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	2.03	0.40
2:B:880:THR:HG22	2:B:933:SER:HB2	2.03	0.40
2:B:957:ASN:HB3	2:B:961:LEU:HB2	2.03	0.40
7:I:83:ASN:HD22	7:I:83:ASN:C	2.28	0.40
1:A:134:ARG:HD2	1:A:221:SER:O	2.21	0.40
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.54	0.40
2:B:345:LYS:HA	2:B:347:LYS:H	1.87	0.40
1:A:1359:ASP:C	1:A:1361:SER:H	2.29	0.40
2:B:569:TYR:HE1	2:B:574:SER:HB2	1.87	0.40
2:B:601:ARG:HA	2:B:615:MET:HE1	2.03	0.40
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.54	0.40
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.54	0.40
4:E:88:VAL:HB	4:E:116:ILE:HG13	2.04	0.40
6:H:136:LYS:HD3	6:H:136:LYS:H	1.86	0.40
1:A:442:VAL:O	1:A:457:ALA:HA	2.22	0.40
2:B:346:GLU:HA	2:B:349:ILE:HD12	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%)	1221 (88%)	131 (9%)	43 (3%)	3	22
2	B	1096/1224 (90%)	952 (87%)	91 (8%)	53 (5%)	2	14
3	C	264/318 (83%)	238 (90%)	22 (8%)	4 (2%)	8	37
4	E	212/215 (99%)	199 (94%)	8 (4%)	5 (2%)	4	28
5	F	83/155 (54%)	73 (88%)	7 (8%)	3 (4%)	2	19
6	H	129/146 (88%)	100 (78%)	16 (12%)	13 (10%)	0	2
7	I	117/122 (96%)	101 (86%)	14 (12%)	2 (2%)	7	35
8	J	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	3	21
9	K	112/120 (93%)	106 (95%)	6 (5%)	0	100	100
10	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0	0
All	All	3515/4173 (84%)	3075 (88%)	307 (9%)	133 (4%)	2	18

All (133) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	55	ASP
1	A	66	LYS
1	A	250	ILE
1	A	283	GLY
1	A	399	HIS
1	A	567	LYS
1	A	1167	GLU
2	B	67	SER
2	B	137	TYR
2	B	250	PHE
2	B	371	GLU
2	B	449	ASN
2	B	469	GLN

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Mol	Chain	Res	Type
2	B	477	ALA
2	B	482	VAL
2	B	648	HIS
2	B	712	PRO
2	B	751	VAL
2	B	943	SER
2	B	976	ILE
2	B	1046	PRO
2	B	1156	ASP
3	C	141	GLY
3	C	267	GLN
6	H	131	ASN
8	J	2	ILE
8	J	6	ARG
10	L	50	ASP
10	L	56	LEU
10	L	64	LEU
1	A	56	PRO
1	A	312	PRO
1	A	331	GLY
1	A	404	TYR
1	A	423	ASP
1	A	1123	GLY
1	A	1234	GLU
1	A	1437	GLY
2	B	139	ALA
2	B	229	ALA
2	B	465	ASN
2	B	483	LEU
2	B	526	GLU
2	B	879	ARG
2	B	883	LEU
2	B	887	HIS
2	B	888	GLY
2	B	1096	ARG
2	B	1220	ARG
4	E	126	SER
5	F	111	LEU
6	H	18	GLY
6	H	90	ALA
6	H	109	LYS
6	H	140	ALA

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Mol	Chain	Res	Type
1	A	275	SER
1	A	286	HIS
1	A	332	LYS
1	A	543	LEU
1	A	846	GLU
1	A	1221	LYS
2	B	249	ARG
2	B	364	ILE
2	B	471	LYS
2	B	708	GLU
2	B	734	HIS
2	B	881	ASN
2	B	1066	SER
2	B	1157	ALA
2	B	1221	SER
3	C	4	GLU
4	E	114	ASN
6	H	35	GLN
6	H	132	LEU
10	L	39	SER
10	L	59	ALA
1	A	48	ALA
1	A	214	ILE
1	A	257	ARG
1	A	597	LEU
1	A	672	ASP
1	A	1084	PHE
2	B	367	LEU
2	B	619	ILE
2	B	709	ASP
2	B	792	MET
2	B	942	ARG
2	B	1099	VAL
2	B	1171	VAL
2	B	1173	ALA
2	B	1181	GLU
4	E	36	GLU
5	F	154	ASP
6	H	84	ALA
6	H	128	ASN
7	I	115	LYS
10	L	42	ARG

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Mol	Chain	Res	Type
10	L	47	ARG
1	A	35	ILE
1	A	54	ASN
1	A	109	HIS
1	A	324	SER
1	A	424	ILE
1	A	1081	LEU
1	A	1083	THR
1	A	1124	HIS
1	A	1377	THR
2	B	476	ARG
2	B	531	GLN
2	B	563	MET
2	B	707	PRO
2	B	1017	ILE
2	B	1097	HIS
3	C	90	ASP
6	H	86	ASP
6	H	136	LYS
10	L	46	VAL
1	A	248	PRO
1	A	400	PRO
1	A	958	VAL
2	B	346	GLU
2	B	468	GLU
2	B	647	GLY
5	F	73	ALA
1	A	568	PRO
4	E	51	GLY
1	A	52	GLY
6	H	82	PRO
6	H	107	VAL
4	E	89	GLY
7	I	52	ILE
1	A	308	ILE

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%)	1036 (85%)	189 (15%)	2	14
2	B	967/1061 (91%)	835 (86%)	132 (14%)	3	18
3	C	234/274 (85%)	203 (87%)	31 (13%)	4	19
4	E	196/197 (100%)	175 (89%)	21 (11%)	6	27
5	F	75/137 (55%)	66 (88%)	9 (12%)	5	23
6	H	117/128 (91%)	95 (81%)	22 (19%)	1	9
7	I	113/116 (97%)	97 (86%)	16 (14%)	3	17
8	J	60/65 (92%)	52 (87%)	8 (13%)	4	19
9	K	99/102 (97%)	84 (85%)	15 (15%)	3	14
10	L	40/57 (70%)	29 (72%)	11 (28%)	0	2
All	All	3126/3657 (86%)	2672 (86%)	454 (14%)	3	16

All (454) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	18	GLN
1	A	41	MET
1	A	43	GLU
1	A	47	ARG
1	A	58	LEU
1	A	68	GLN
1	A	69	THR
1	A	70	CYS
1	A	86	LEU
1	A	93	VAL
1	A	96	ILE
1	A	110	CYS
1	A	113	LEU
1	A	126	LEU
1	A	133	LYS
1	A	143	LYS
1	A	147	VAL
1	A	174	ILE
1	A	179	LEU
1	A	202	LEU
1	A	208	LEU
1	A	219	PHE

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Mol	Chain	Res	Type
1	A	247	ARG
1	A	252	PHE
1	A	253	ASN
1	A	270	LEU
1	A	271	LYS
1	A	276	LEU
1	A	282	ASN
1	A	299	HIS
1	A	302	THR
1	A	303	TYR
1	A	307	ASP
1	A	308	ILE
1	A	313	GLN
1	A	317	LYS
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	351	THR
1	A	353	ILE
1	A	359	LEU
1	A	380	VAL
1	A	385	ILE
1	A	398	GLU
1	A	403	LYS
1	A	407	ARG
1	A	427	GLN
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	461	LYS
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	489	LEU

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Mol	Chain	Res	Type
1	A	496	GLU
1	A	500	GLU
1	A	509	LEU
1	A	518	LYS
1	A	524	VAL
1	A	527	THR
1	A	532	ARG
1	A	541	ILE
1	A	544	ASP
1	A	566	ILE
1	A	588	LEU
1	A	590	ARG
1	A	593	GLU
1	A	595	THR
1	A	598	LEU
1	A	603	ASN
1	A	612	ILE
1	A	618	GLU
1	A	620	LYS
1	A	622	VAL
1	A	625	SER
1	A	629	LEU
1	A	636	GLU
1	A	640	GLN
1	A	652	VAL
1	A	664	THR
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	682	THR
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	702	LEU
1	A	708	MET
1	A	716	ASP
1	A	722	LEU
1	A	731	ARG
1	A	740	LEU
1	A	756	ILE
1	A	762	SER
1	A	771	GLU

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Mol	Chain	Res	Type
1	A	773	LYS
1	A	801	GLU
1	A	821	ARG
1	A	827	THR
1	A	838	GLN
1	A	845	LEU
1	A	849	MET
1	A	865	GLN
1	A	867	ILE
1	A	878	ILE
1	A	894	GLU
1	A	905	ASP
1	A	908	LEU
1	A	912	LEU
1	A	925	LEU
1	A	926	GLN
1	A	938	LYS
1	A	940	ARG
1	A	953	ASN
1	A	969	GLN
1	A	973	ILE
1	A	988	LEU
1	A	998	LEU
1	A	999	VAL
1	A	1005	GLU
1	A	1025	ARG
1	A	1029	ARG
1	A	1048	ASN
1	A	1050	GLU
1	A	1062	GLU
1	A	1067	LEU
1	A	1077	THR
1	A	1084	PHE
1	A	1109	LYS
1	A	1110	ASN
1	A	1121	GLU
1	A	1130	GLN
1	A	1132	LYS
1	A	1135	ARG
1	A	1138	ILE
1	A	1161	THR
1	A	1170	ILE

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Mol	Chain	Res	Type
1	A	1172	LEU
1	A	1195	LEU
1	A	1221	LYS
1	A	1223	ASP
1	A	1227	ILE
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1264	GLU
1	A	1266	THR
1	A	1267	MET
1	A	1269	GLU
1	A	1277	GLU
1	A	1280	GLU
1	A	1285	MET
1	A	1288	ASP
1	A	1293	SER
1	A	1297	GLU
1	A	1307	GLU
1	A	1322	ILE
1	A	1325	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1345	ARG
1	A	1350	LYS
1	A	1351	GLU
1	A	1361	SER
1	A	1366	ARG
1	A	1376	THR
1	A	1378	GLN
1	A	1385	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1403	GLU
1	A	1425	SER
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1444	MET
1	A	1445	ILE
2	B	25	ILE
2	B	28	GLU

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Mol	Chain	Res	Type
2	B	46	GLN
2	B	61	ASP
2	B	63	ILE
2	B	68	THR
2	B	70	ILE
2	B	89	GLU
2	B	94	LYS
2	B	101	MET
2	B	102	VAL
2	B	105	SER
2	B	122	LEU
2	B	135	ARG
2	B	175	ARG
2	B	178	ASN
2	B	194	GLU
2	B	222	ILE
2	B	223	VAL
2	B	232	SER
2	B	234	ILE
2	B	240	ILE
2	B	245	GLU
2	B	250	PHE
2	B	254	LEU
2	B	257	LYS
2	B	262	GLU
2	B	267	ARG
2	B	272	THR
2	B	276	ILE
2	B	277	LYS
2	B	285	ILE
2	B	305	VAL
2	B	313	MET
2	B	323	VAL
2	B	325	GLN
2	B	357	GLN
2	B	365	THR
2	B	367	LEU
2	B	384	ARG
2	B	393	LYS
2	B	398	ARG
2	B	404	LYS
2	B	425	THR

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Mol	Chain	Res	Type
2	B	436	VAL
2	B	437	GLU
2	B	453	ILE
2	B	458	LYS
2	B	468	GLU
2	B	469	GLN
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	526	GLU
2	B	531	GLN
2	B	537	LYS
2	B	547	VAL
2	B	549	THR
2	B	554	ILE
2	B	567	GLU
2	B	579	ARG
2	B	591	ARG
2	B	595	ARG
2	B	598	GLU
2	B	604	ARG
2	B	612	GLU
2	B	616	ILE
2	B	619	ILE
2	B	633	VAL
2	B	644	GLU
2	B	645	SER
2	B	653	VAL
2	B	655	LYS
2	B	658	ILE
2	B	687	GLU
2	B	690	VAL
2	B	708	GLU
2	B	710	LEU
2	B	731	VAL
2	B	776	GLN
2	B	780	VAL
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	806	THR
2	B	810	GLU

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Mol	Chain	Res	Type
2	B	815	ARG
2	B	839	MET
2	B	864	LYS
2	B	868	MET
2	B	879	ARG
2	B	880	THR
2	B	885	MET
2	B	911	ILE
2	B	941	LEU
2	B	944	THR
2	B	948	ILE
2	B	955	THR
2	B	963	PHE
2	B	979	LYS
2	B	983	ARG
2	B	996	ARG
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1006	ILE
2	B	1007	VAL
2	B	1022	THR
2	B	1030	LEU
2	B	1052	VAL
2	B	1065	GLN
2	B	1066	SER
2	B	1077	THR
2	B	1097	HIS
2	B	1099	VAL
2	B	1101	ASP
2	B	1102	LYS
2	B	1103	ILE
2	B	1111	MET
2	B	1113	VAL
2	B	1145	SER
2	B	1147	LEU
2	B	1150	ARG
2	B	1176	ASN
2	B	1178	ASN
2	B	1189	ILE
2	B	1191	ILE
2	B	1194	ILE

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Mol	Chain	Res	Type
2	B	1196	ILE
2	B	1202	LEU
2	B	1212	ILE
2	B	1222	ARG
3	C	3	GLU
3	C	8	VAL
3	C	14	SER
3	C	21	ILE
3	C	22	LEU
3	C	27	LEU
3	C	37	MET
3	C	38	ILE
3	C	43	THR
3	C	48	SER
3	C	57	VAL
3	C	75	MET
3	C	77	ILE
3	C	79	GLN
3	C	80	LEU
3	C	100	THR
3	C	106	GLU
3	C	124	LEU
3	C	127	ARG
3	C	136	ASP
3	C	137	LYS
3	C	140	ASN
3	C	142	VAL
3	C	144	ILE
3	C	156	THR
3	C	158	VAL
3	C	215	GLU
3	C	240	VAL
3	C	244	VAL
3	C	263	THR
3	C	264	GLN
4	E	3	GLN
4	E	52	ARG
4	E	54	GLN
4	E	65	THR
4	E	75	MET
4	E	78	LEU
4	E	84	ASP

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Mol	Chain	Res	Type
4	E	92	THR
4	E	95	THR
4	E	100	ILE
4	E	116	ILE
4	E	122	LYS
4	E	127	ILE
4	E	132	ILE
4	E	140	LEU
4	E	144	ILE
4	E	156	LEU
4	E	169	ARG
4	E	175	LEU
4	E	191	LYS
4	E	202	SER
5	F	74	ILE
5	F	76	LYS
5	F	82	THR
5	F	93	ILE
5	F	99	LEU
5	F	111	LEU
5	F	118	LEU
5	F	124	GLU
5	F	128	LYS
6	H	2	SER
6	H	8	ASP
6	H	15	VAL
6	H	22	LYS
6	H	24	CYS
6	H	26	ILE
6	H	33	GLN
6	H	34	ASP
6	H	35	GLN
6	H	40	LEU
6	H	44	VAL
6	H	56	THR
6	H	63	LEU
6	H	83	GLN
6	H	86	ASP
6	H	100	THR
6	H	107	VAL
6	H	109	LYS
6	H	110	ASP

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Mol	Chain	Res	Type
6	H	111	LEU
6	H	130	ARG
6	H	136	LYS
7	I	17	ARG
7	I	30	ARG
7	I	35	VAL
7	I	43	VAL
7	I	52	ILE
7	I	55	THR
7	I	61	ASP
7	I	77	LYS
7	I	83	ASN
7	I	84	VAL
7	I	88	SER
7	I	90	GLN
7	I	97	MET
7	I	111	THR
7	I	116	ASN
7	I	119	THR
8	J	3	VAL
8	J	7	CYS
8	J	22	LEU
8	J	31	ASP
8	J	48	ARG
8	J	56	LEU
8	J	58	GLU
8	J	59	LYS
9	K	6	ARG
9	K	14	GLU
9	K	20	LYS
9	K	21	ILE
9	K	25	THR
9	K	31	VAL
9	K	41	THR
9	K	42	LEU
9	K	51	LEU
9	K	63	VAL
9	K	77	THR
9	K	95	ILE
9	K	101	LEU
9	K	103	THR
9	K	114	LEU

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Mol	Chain	Res	Type
10	L	27	LEU
10	L	35	SER
10	L	47	ARG
10	L	50	ASP
10	L	51	CYS
10	L	53	HIS
10	L	55	ILE
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 (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	54	ASN
1	A	64	ASN
1	A	68	GLN
1	A	92	HIS
1	A	118	HIS
1	A	169	ASN
1	A	171	GLN
1	A	209	ASN
1	A	225	ASN
1	A	256	GLN
1	A	273	ASN
1	A	299	HIS
1	A	339	ASN
1	A	390	GLN
1	A	394	ASN
1	A	427	GLN
1	A	503	GLN
1	A	517	ASN
1	A	611	GLN
1	A	626	ASN
1	A	631	HIS
1	A	648	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN

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Mol	Chain	Res	Type
1	A	786	HIS
1	A	926	GLN
1	A	935	GLN
1	A	953	ASN
1	A	1040	GLN
1	A	1052	GLN
1	A	1124	HIS
1	A	1130	GLN
1	A	1140	HIS
1	A	1188	GLN
1	A	1211	GLN
1	A	1265	ASN
1	A	1364	ASN
2	B	46	GLN
2	B	52	ASN
2	B	53	GLN
2	B	103	ASN
2	B	215	GLN
2	B	325	GLN
2	B	363	HIS
2	B	449	ASN
2	B	484	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	657	HIS
2	B	744	HIS
2	B	770	GLN
2	B	794	ASN
2	B	822	ASN
2	B	957	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1074	ASN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1161	HIS
2	B	1176	ASN
2	B	1177	HIS
2	B	1179	GLN

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Mol	Chain	Res	Type
3	C	73	GLN
3	C	91	HIS
3	C	112	ASN
3	C	123	ASN
3	C	131	HIS
3	C	151	GLN
3	C	167	HIS
3	C	242	GLN
4	E	5	ASN
4	E	32	GLN
4	E	54	GLN
4	E	106	GLN
4	E	115	ASN
4	E	146	HIS
4	E	174	GLN
6	H	11	GLN
7	I	12	ASN
7	I	60	GLN
7	I	83	ASN
7	I	87	GLN
7	I	120	GLN
9	K	65	HIS
9	K	89	ASN
9	K	110	ASN
10	L	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	8/9 (88%)	1 (12%)	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%)	0.20	39 (2%)	55	35	52, 98, 181, 233	0
2	B	1114/1224 (91%)	0.21	36 (3%)	50	31	53, 88, 148, 200	0
3	C	266/318 (83%)	0.03	0	100	100	62, 86, 123, 171	0
4	E	214/215 (99%)	0.21	2 (0%)	81	64	72, 128, 183, 201	0
5	F	85/155 (54%)	-0.04	1 (1%)	76	58	73, 100, 144, 162	0
6	H	133/146 (91%)	0.43	8 (6%)	27	17	94, 138, 168, 181	0
7	I	119/122 (97%)	0.27	8 (6%)	24	15	68, 101, 140, 152	0
8	J	65/70 (92%)	-0.04	0	100	100	57, 77, 111, 127	0
9	K	114/120 (95%)	-0.07	1 (0%)	81	64	61, 89, 116, 131	0
10	L	46/70 (65%)	0.82	6 (13%)	7	6	80, 124, 153, 164	0
11	R	9/9 (100%)	-0.12	0	100	100	79, 103, 145, 148	0
12	T	13/29 (44%)	0.49	0	100	100	85, 110, 168, 175	0
All	All	3583/4211 (85%)	0.19	101 (2%)	55	35	52, 96, 167, 233	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	708	GLU	5.7
2	B	715	ALA	5.4
2	B	335	GLY	4.9
10	L	27	LEU	4.8
2	B	883	LEU	4.8
1	A	141	LEU	4.7
1	A	252	PHE	4.7
2	B	882	THR	4.7
1	A	250	ILE	4.6
2	B	709	ASP	4.4
6	H	63	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	477	ALA	4.3
1	A	1390	ASN	4.1
1	A	1087	ALA	4.0
7	I	104	LEU	4.0
9	K	114	LEU	4.0
1	A	65	LEU	3.8
2	B	70	ILE	3.6
1	A	1081	LEU	3.6
1	A	1090	ALA	3.4
1	A	1445	ILE	3.4
1	A	199	LEU	3.3
7	I	105	SER	3.2
10	L	28	LYS	3.2
10	L	26	THR	3.2
2	B	502	ILE	3.2
2	B	509	ALA	3.2
1	A	323	LYS	3.2
6	H	85	GLY	3.1
1	A	182	VAL	3.1
1	A	1108	ALA	3.1
1	A	103	CYS	3.0
2	B	881	ASN	3.0
1	A	1085	HIS	3.0
1	A	289	ILE	2.9
1	A	1091	SER	2.8
10	L	40	LEU	2.8
1	A	1083	THR	2.8
2	B	446	LEU	2.8
10	L	25	ALA	2.7
1	A	753	GLY	2.7
1	A	322	VAL	2.7
1	A	318	SER	2.7
2	B	647	GLY	2.7
6	H	139	ASN	2.7
7	I	84	VAL	2.7
1	A	49	LYS	2.7
6	H	135	LEU	2.6
1	A	140	THR	2.6
1	A	310	GLY	2.6
2	B	1214	PRO	2.5
1	A	144	THR	2.5
4	E	110	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	645	SER	2.4
7	I	82	GLU	2.4
2	B	106	ASP	2.4
7	I	2	THR	2.4
7	I	49	ILE	2.4
1	A	154	SER	2.4
4	E	98	ILE	2.4
1	A	69	THR	2.3
2	B	201	GLY	2.3
1	A	1082	ASN	2.3
2	B	140	ILE	2.3
7	I	107	SER	2.3
2	B	786	ASN	2.3
1	A	319	GLY	2.3
2	B	648	HIS	2.3
2	B	250	PHE	2.3
2	B	137	TYR	2.3
2	B	711	GLU	2.2
2	B	25	ILE	2.2
10	L	55	ILE	2.2
2	B	381	MET	2.2
1	A	757	ASN	2.2
1	A	66	LYS	2.2
1	A	1084	PHE	2.2
1	A	1086	PHE	2.2
7	I	4	PHE	2.2
6	H	86	ASP	2.2
2	B	733	HIS	2.2
1	A	1176	LEU	2.1
2	B	345	LYS	2.1
2	B	735	ALA	2.1
1	A	1089	VAL	2.1
2	B	246	LYS	2.1
2	B	479	VAL	2.1
2	B	962	LYS	2.1
6	H	89	LEU	2.1
2	B	646	LEU	2.1
1	A	149	GLU	2.1
1	A	176	LYS	2.1
6	H	104	PHE	2.1
2	B	436	VAL	2.0
2	B	1217	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
5	F	83	PRO	2.0
6	H	136	LYS	2.0
1	A	105	CYS	2.0
1	A	1174	PHE	2.0
2	B	277	LYS	2.0
2	B	865	LYS	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(Å ²)	Q<0.9
13	ZN	A	1734	1/1	0.92	0.07	230,230,230,230	0
14	MG	A	2001	1/1	0.98	0.03	45,45,45,45	0
13	ZN	B	1307	1/1	0.99	0.04	144,144,144,144	0
13	ZN	C	319	1/1	0.99	0.03	88,88,88,88	0
13	ZN	I	203	1/1	0.99	0.03	104,104,104,104	0
13	ZN	A	1735	1/1	0.99	0.06	128,128,128,128	0
13	ZN	J	101	1/1	1.00	0.03	71,71,71,71	0
13	ZN	L	105	1/1	1.00	0.02	117,117,117,117	0
13	ZN	I	204	1/1	1.00	0.02	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.