



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:56 AM UTC

PDB ID : 3S14 / pdb_00003s14
Title : RNA Polymerase II Initiation Complex with a 6-nt RNA
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-14
Resolution : 2.85 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

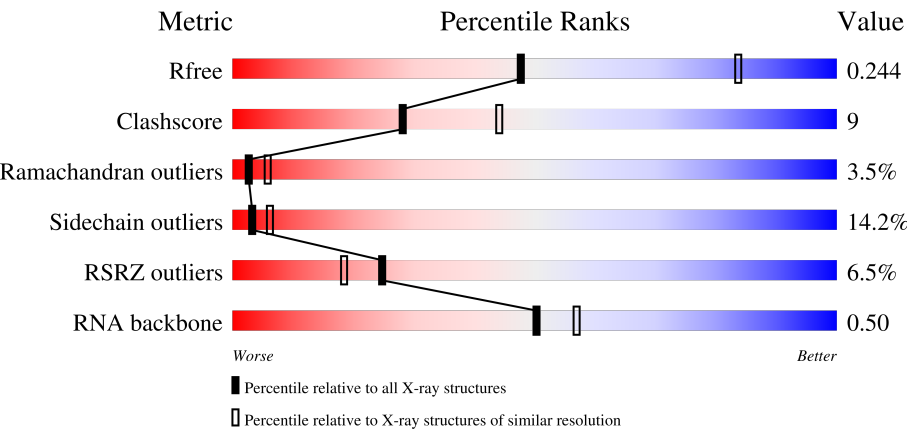
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)
RNA backbone	3983	1009 (3.06-2.66)

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	B	1224	
3	C	318	
4	E	215	

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Mol	Chain	Length	Quality of chain
5	F	155	% 42%11%45% .
6	H	146	13% 61%25%9% . .
7	I	122	6% 66%25%5% . .
8	J	70	3% 59%21%10%7% .
9	K	120	2% 69%19%6%5% .
10	L	70	19% 30%23%11%34% .
11	R	6	67%33%
12	T	29	7% 21%24%55%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 28695 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a RNA chain called RNA (5'-R(*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	6	Total	C	N	O	P	0	0	0
			133	60	30	38	5			

- 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

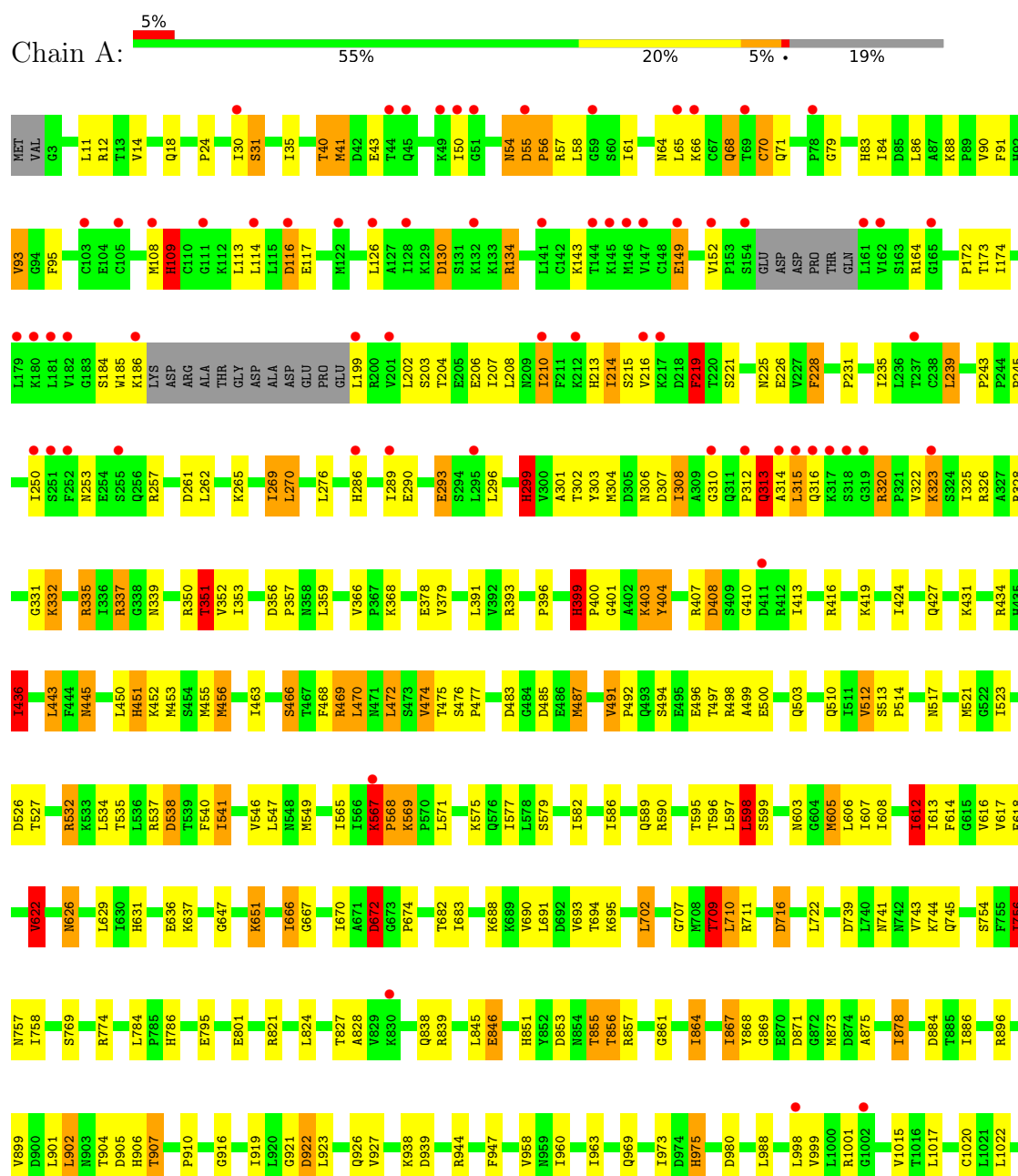
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

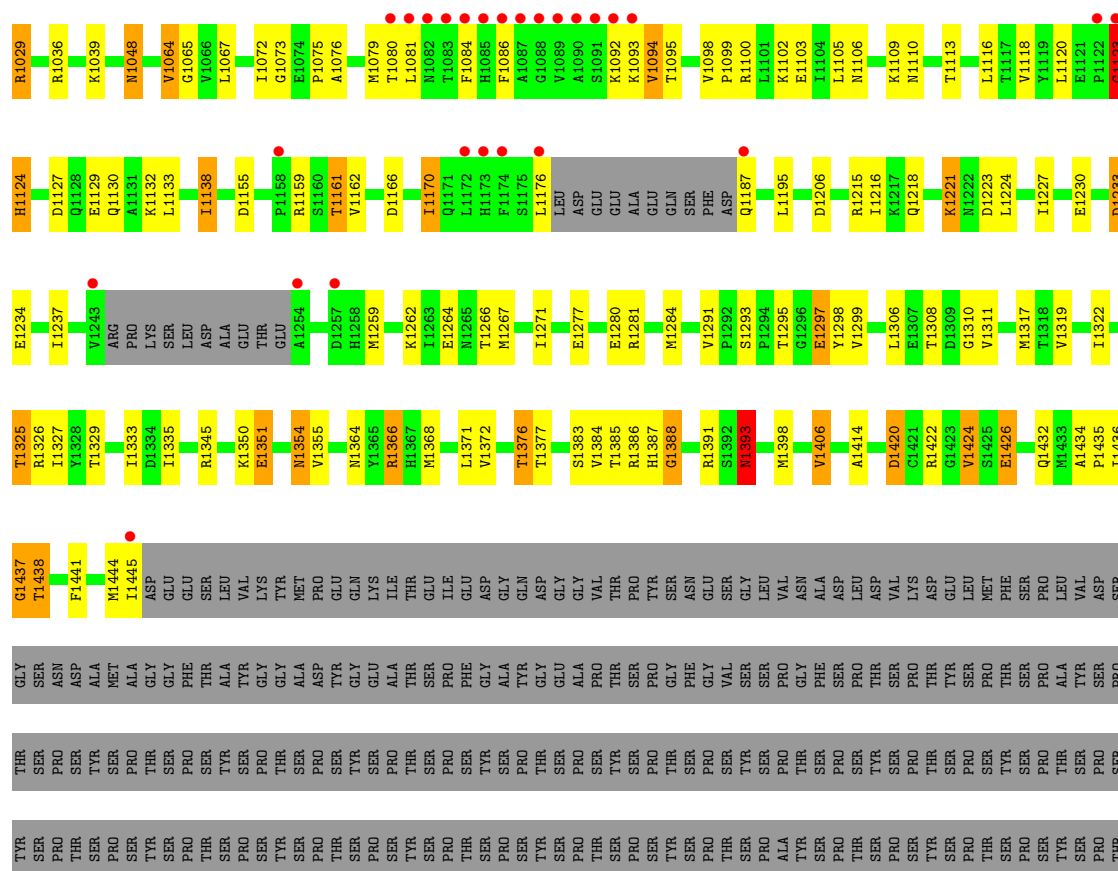
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

3 Residue-property plots

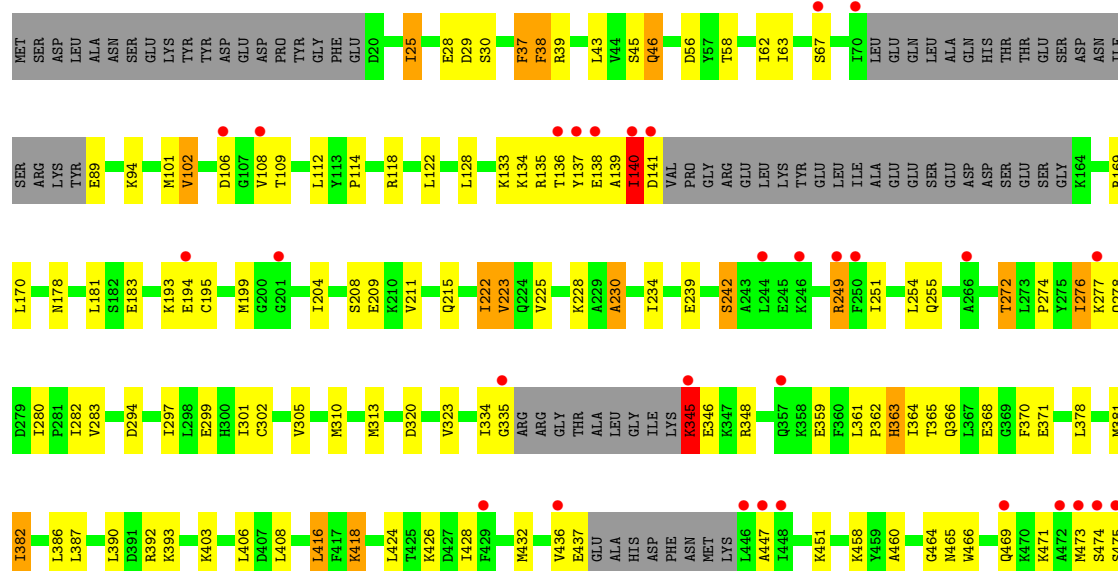
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

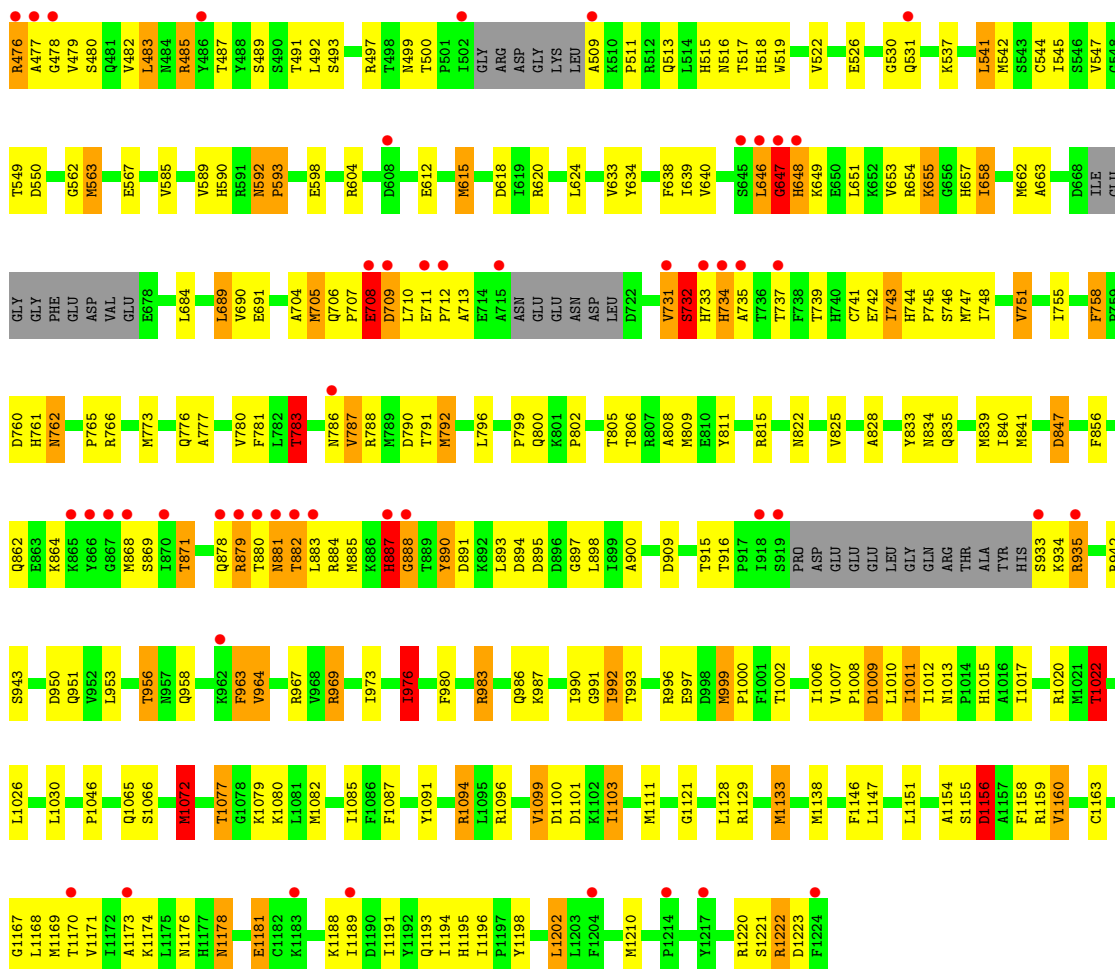
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





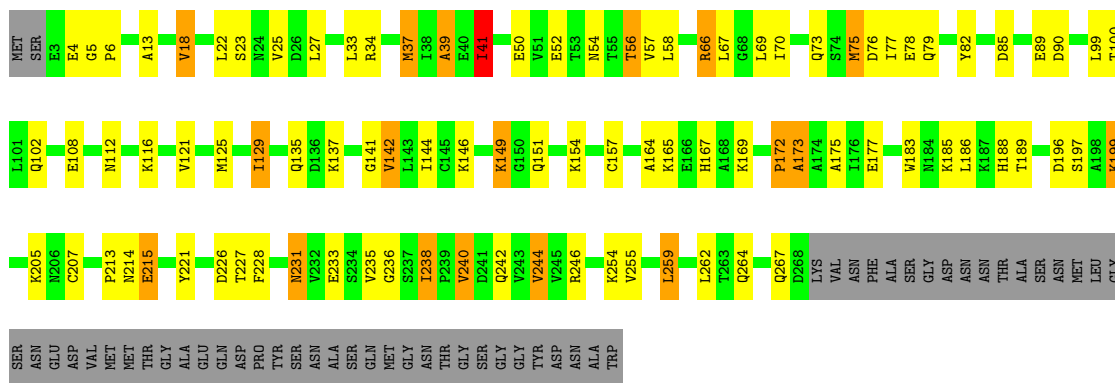
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2





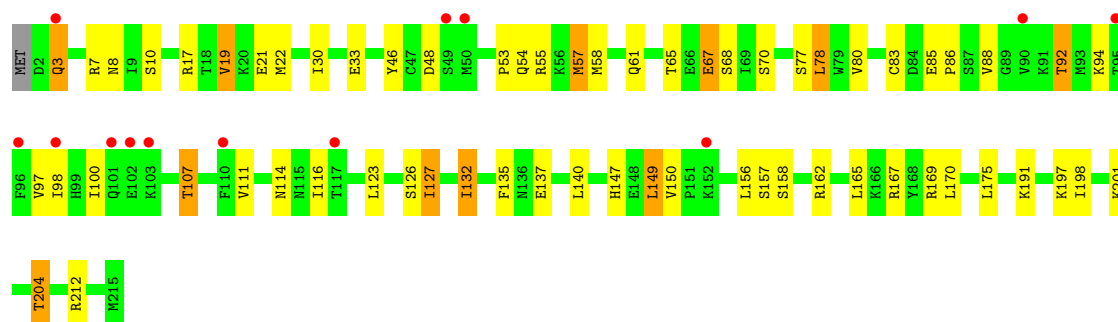
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 54% 23% 6% 16%

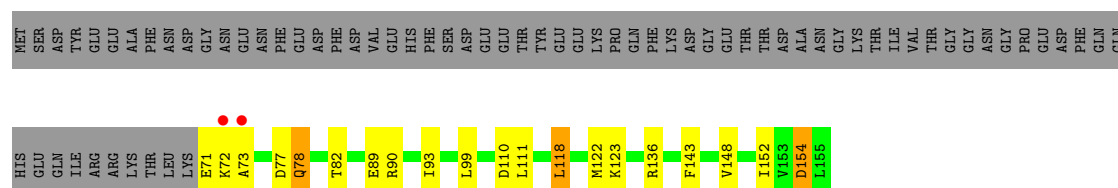


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

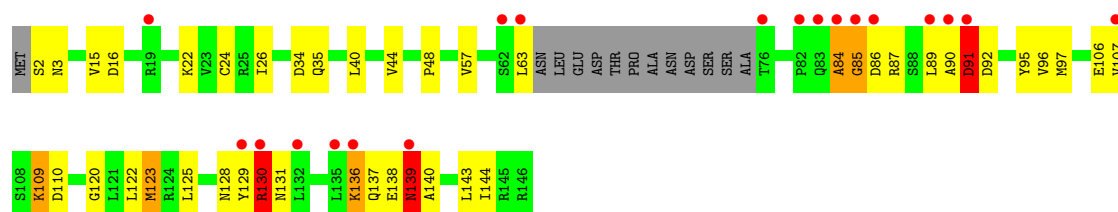
Chain E: 6% 70% 24% 5%



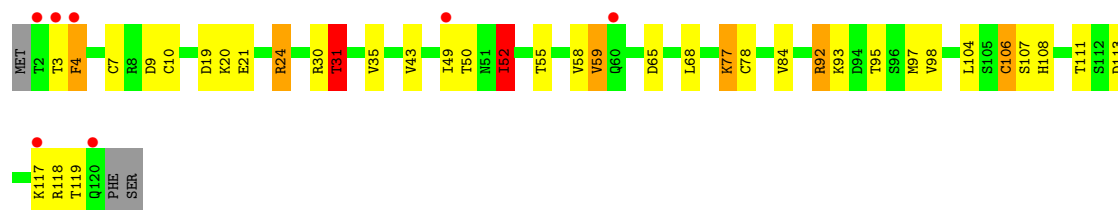
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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



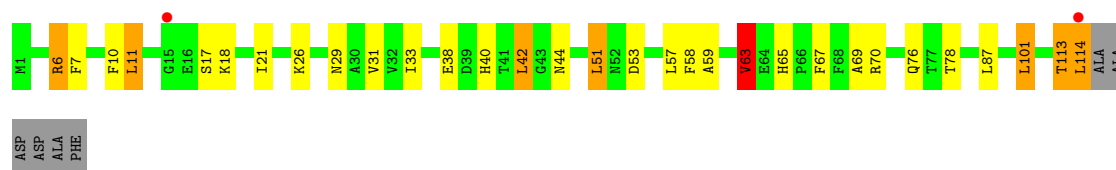
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



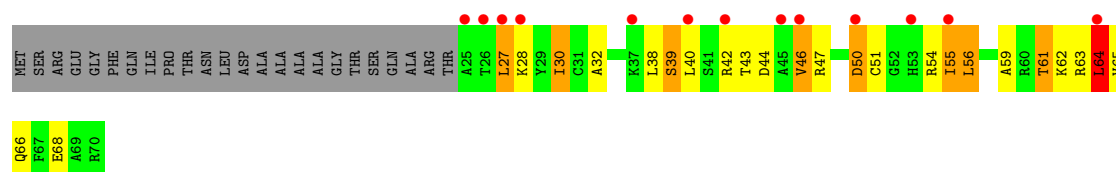
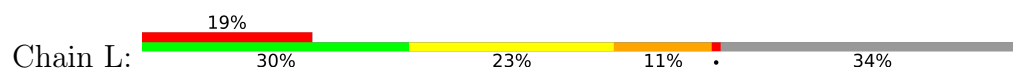
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



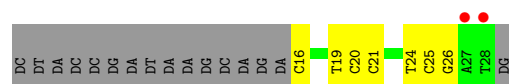
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: RNA (5'-R(*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*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	159.34Å 221.34Å 192.37Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	39.46 – 2.85 39.46 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.46-2.85) 99.9 (39.46-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.86Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.189 , 0.227 0.205 , 0.244	Depositor DCC
R_{free} test set	7772 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28695	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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	0.88	5/11241 (0.0%)	1.49	97/15199 (0.6%)
2	B	0.89	5/9033 (0.1%)	1.45	85/12181 (0.7%)
3	C	0.86	1/2133 (0.0%)	1.47	22/2891 (0.8%)
4	E	0.80	1/1788 (0.1%)	1.45	21/2406 (0.9%)
5	F	0.81	0/700	1.36	3/945 (0.3%)
6	H	0.84	0/1086	1.40	17/1470 (1.2%)
7	I	0.90	1/989 (0.1%)	1.47	13/1331 (1.0%)
8	J	0.96	2/541 (0.4%)	1.59	6/727 (0.8%)
9	K	0.76	0/937	1.42	6/1265 (0.5%)
10	L	0.95	0/365	1.50	10/485 (2.1%)
11	R	0.62	0/150	1.18	0/234
12	T	0.49	0/290	1.39	2/444 (0.5%)
All	All	0.87	15/29253 (0.1%)	1.46	282/39578 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	756	ILE	CG1-CD1	8.08	1.83	1.51
1	A	456	MET	SD-CE	-7.92	1.59	1.79
1	A	605	MET	SD-CE	-7.88	1.59	1.79
2	B	1072	MET	SD-CE	-7.34	1.61	1.79
8	J	49	MET	SD-CE	-7.28	1.61	1.79
1	A	487	MET	SD-CE	-7.28	1.61	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1	MET	SD-CE	7.09	1.97	1.79
2	B	705	MET	SD-CE	-6.87	1.62	1.79
2	B	973	ILE	CA-C	6.83	1.58	1.52
1	A	867	ILE	CG1-CD1	6.62	1.77	1.51
2	B	758	PHE	CA-C	6.58	1.57	1.53
3	C	37	MET	SD-CE	-5.35	1.66	1.79
2	B	662	MET	SD-CE	5.26	1.92	1.79
4	E	127	ILE	CA-C	5.07	1.58	1.52
7	I	106	CYS	CA-C	-5.03	1.47	1.52

All (282) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	647	GLY	CA-C-N	11.84	143.01	121.70
2	B	647	GLY	C-N-CA	11.84	143.01	121.70
2	B	1101	ASP	CA-CB-CG	9.64	122.24	112.60
12	T	16	DC	P-O3'-C3'	8.85	133.47	120.20
6	H	92	ASP	N-CA-C	-8.84	100.48	112.94
3	C	172	PRO	CA-C-N	8.65	138.06	121.54
3	C	172	PRO	C-N-CA	8.65	138.06	121.54
1	A	1123	GLY	CA-C-N	8.50	137.00	121.70
1	A	1123	GLY	C-N-CA	8.50	137.00	121.70
1	A	114	LEU	N-CA-C	8.36	120.47	111.36
3	C	39	ALA	N-CA-C	8.10	123.29	113.41
1	A	537	ARG	CA-C-N	8.04	132.53	120.31
1	A	537	ARG	C-N-CA	8.04	132.53	120.31
2	B	223	VAL	N-CA-CB	7.82	119.05	110.53
7	I	78	CYS	CA-C-N	-7.77	110.06	122.95
7	I	78	CYS	C-N-CA	-7.77	110.06	122.95
2	B	648	HIS	N-CA-CB	7.55	123.34	110.50
3	C	175	ALA	N-CA-C	7.51	120.82	110.24
8	J	5	VAL	N-CA-C	-7.38	99.17	109.21
1	A	1420	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	947	PHE	CA-C-N	7.36	130.09	120.60
1	A	947	PHE	C-N-CA	7.36	130.09	120.60
2	B	140	ILE	CA-C-N	7.31	134.85	121.70
2	B	140	ILE	C-N-CA	7.31	134.85	121.70
2	B	479	VAL	N-CA-C	-7.24	99.34	108.89
2	B	1154	ALA	N-CA-C	-7.23	98.82	110.32
2	B	37	PHE	N-CA-C	-7.14	100.64	110.35
3	C	78	GLU	CB-CG-CD	7.04	124.58	112.60
1	A	1393	ASN	CA-CB-CG	6.98	119.58	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	VAL	N-CA-C	6.87	115.47	107.84
2	B	39	ARG	N-CA-C	-6.86	103.86	111.82
1	A	622	VAL	CB-CA-C	6.83	119.67	111.20
1	A	622	VAL	N-CA-CB	-6.79	103.50	112.26
7	I	78	CYS	N-CA-C	-6.79	101.39	110.55
1	A	1437	GLY	CA-C-N	6.78	129.66	120.38
1	A	1437	GLY	C-N-CA	6.78	129.66	120.38
2	B	1022	THR	CA-C-N	6.75	130.04	120.53
2	B	1022	THR	C-N-CA	6.75	130.04	120.53
1	A	109	HIS	CA-C-N	6.72	129.62	120.54
1	A	109	HIS	C-N-CA	6.72	129.62	120.54
2	B	345	LYS	CA-C-N	6.72	133.79	121.70
2	B	345	LYS	C-N-CA	6.72	133.79	121.70
1	A	939	ASP	CA-CB-CG	6.70	119.30	112.60
4	E	48	ASP	CA-CB-CG	6.64	119.24	112.60
6	H	138	GLU	N-CA-C	-6.50	104.61	112.54
1	A	445	ASN	CA-CB-CG	6.49	119.09	112.60
1	A	1127	ASP	CA-CB-CG	6.47	119.07	112.60
2	B	38	PHE	CA-CB-CG	6.46	120.26	113.80
2	B	363	HIS	N-CA-C	-6.46	99.72	109.79
2	B	1077	THR	CB-CA-C	6.45	119.33	109.34
2	B	737	THR	CB-CA-C	6.44	122.53	111.45
3	C	135	GLN	CA-C-N	6.41	129.81	120.71
3	C	135	GLN	C-N-CA	6.41	129.81	120.71
2	B	1077	THR	N-CA-CB	-6.36	101.18	110.40
2	B	783	THR	CB-CA-C	6.35	122.38	110.63
1	A	1311	VAL	N-CA-C	6.35	117.44	108.17
8	J	9	SER	N-CA-C	6.32	117.96	111.14
1	A	1435	PRO	CA-C-N	6.25	131.69	123.06
1	A	1435	PRO	C-N-CA	6.25	131.69	123.06
6	H	139	ASN	CA-C-N	6.23	133.43	121.54
6	H	139	ASN	C-N-CA	6.23	133.43	121.54
2	B	1066	SER	N-CA-C	6.22	120.43	112.34
3	C	89	GLU	N-CA-C	-6.21	99.08	108.96
6	H	129	TYR	CA-C-N	6.17	129.17	120.28
6	H	129	TYR	C-N-CA	6.17	129.17	120.28
9	K	63	VAL	N-CA-CB	6.17	121.40	111.23
1	A	716	ASP	CA-CB-CG	6.14	118.74	112.60
2	B	447	ALA	CA-C-N	6.12	131.67	122.98
2	B	447	ALA	C-N-CA	6.12	131.67	122.98
1	A	366	VAL	N-CA-C	6.11	114.61	107.77
3	C	82	TYR	N-CA-C	-6.11	100.05	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	THR	CA-C-N	6.09	128.66	120.50
1	A	351	THR	C-N-CA	6.09	128.66	120.50
1	A	526	ASP	CA-CB-CG	6.07	118.67	112.60
3	C	214	ASN	CA-C-N	6.07	129.24	120.38
3	C	214	ASN	C-N-CA	6.07	129.24	120.38
2	B	976	ILE	N-CA-C	6.04	117.51	110.62
2	B	887	HIS	CA-C-N	6.00	132.50	121.70
2	B	887	HIS	C-N-CA	6.00	132.50	121.70
2	B	743	ILE	N-CA-CB	5.97	117.53	110.55
7	I	58	VAL	CA-C-N	5.95	132.67	122.67
7	I	58	VAL	C-N-CA	5.95	132.67	122.67
1	A	512	VAL	N-CA-CB	5.93	117.75	111.00
1	A	450	LEU	CA-C-N	5.88	131.82	122.59
1	A	450	LEU	C-N-CA	5.88	131.82	122.59
6	H	91	ASP	CA-C-N	5.88	131.43	122.37
6	H	91	ASP	C-N-CA	5.88	131.43	122.37
8	J	18	TRP	N-CA-C	5.88	117.36	111.07
1	A	491	VAL	N-CA-C	5.87	114.42	107.73
2	B	828	ALA	N-CA-C	5.85	118.00	108.76
1	A	1162	VAL	N-CA-C	-5.83	104.12	112.35
3	C	262	LEU	CA-C-N	5.81	127.99	120.44
3	C	262	LEU	C-N-CA	5.81	127.99	120.44
9	K	113	THR	CA-C-N	5.79	132.13	121.70
9	K	113	THR	C-N-CA	5.79	132.13	121.70
2	B	847	ASP	CA-CB-CG	5.78	118.38	112.60
2	B	648	HIS	CA-CB-CG	-5.77	108.03	113.80
9	K	53	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	538	ASP	CA-CB-CG	5.76	118.36	112.60
7	I	117	LYS	CA-C-N	5.76	132.54	121.54
7	I	117	LYS	C-N-CA	5.76	132.54	121.54
6	H	130	ARG	CA-C-N	5.76	132.54	121.54
6	H	130	ARG	C-N-CA	5.76	132.54	121.54
4	E	165	LEU	CA-C-N	5.74	127.90	120.44
4	E	165	LEU	C-N-CA	5.74	127.90	120.44
2	B	734	HIS	CA-C-N	5.72	131.36	121.64
2	B	734	HIS	C-N-CA	5.72	131.36	121.64
1	A	906	HIS	N-CA-C	5.71	119.55	112.59
2	B	230	ALA	N-CA-C	5.71	122.42	109.81
2	B	1156	ASP	CA-CB-CG	5.70	118.30	112.60
4	E	33	GLU	CA-C-N	5.70	127.92	120.28
4	E	33	GLU	C-N-CA	5.70	127.92	120.28
3	C	172	PRO	N-CA-C	-5.69	107.03	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	132	ILE	N-CA-CB	5.69	119.27	111.41
2	B	294	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	261	ASP	CA-C-N	5.68	127.89	120.28
1	A	261	ASP	C-N-CA	5.68	127.89	120.28
6	H	3	ASN	CA-C-N	5.68	129.54	121.42
6	H	3	ASN	C-N-CA	5.68	129.54	121.42
2	B	711	GLU	N-CA-C	5.67	122.35	109.81
9	K	44	ASN	CA-C-N	5.67	127.87	120.28
9	K	44	ASN	C-N-CA	5.67	127.87	120.28
2	B	593	PRO	CA-C-N	5.66	127.86	120.28
2	B	593	PRO	C-N-CA	5.66	127.86	120.28
8	J	55	ASP	CA-CB-CG	5.66	118.26	112.60
2	B	418	LYS	CA-C-N	5.65	128.11	120.65
2	B	418	LYS	C-N-CA	5.65	128.11	120.65
1	A	474	VAL	CA-C-N	5.64	127.84	120.28
1	A	474	VAL	C-N-CA	5.64	127.84	120.28
10	L	56	LEU	N-CA-C	5.64	122.81	110.80
1	A	603	ASN	CA-CB-CG	5.62	118.22	112.60
1	A	709	THR	CA-C-N	5.61	127.80	120.28
1	A	709	THR	C-N-CA	5.61	127.80	120.28
1	A	758	ILE	CA-C-N	5.60	127.79	120.28
1	A	758	ILE	C-N-CA	5.60	127.79	120.28
2	B	1121	GLY	CA-C-N	5.60	128.10	120.54
2	B	1121	GLY	C-N-CA	5.60	128.10	120.54
1	A	436	ILE	CA-CB-CG2	5.60	120.02	110.50
1	A	612	ILE	N-CA-CB	5.59	117.22	110.95
1	A	399	HIS	N-CA-CB	5.59	120.32	110.37
1	A	884	ASP	N-CA-C	5.58	118.90	111.75
2	B	881	ASN	CA-C-N	5.58	132.20	121.54
2	B	881	ASN	C-N-CA	5.58	132.20	121.54
1	A	886	ILE	N-CA-C	5.58	116.36	110.72
1	A	399	HIS	CA-C-O	-5.56	112.55	120.16
2	B	890	TYR	N-CA-C	-5.55	106.50	113.28
1	A	451	HIS	N-CA-CB	-5.54	101.91	111.55
2	B	320	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	91	PHE	CA-CB-CG	5.54	119.33	113.80
7	I	52	ILE	N-CA-CB	5.53	116.96	110.82
1	A	739	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	864	ILE	N-CA-C	-5.53	106.42	111.67
7	I	59	VAL	N-CA-CB	-5.52	100.48	111.91
3	C	85	ASP	CA-CB-CG	5.52	118.12	112.60
7	I	4	PHE	N-CA-C	5.51	118.69	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	150	VAL	N-CA-C	5.51	112.57	107.56
1	A	1039	LYS	CA-C-N	5.50	127.91	120.65
1	A	1039	LYS	C-N-CA	5.50	127.91	120.65
1	A	314	ALA	N-CA-C	5.49	117.16	110.41
2	B	541	LEU	N-CA-C	5.49	117.69	111.11
1	A	839	ARG	CA-C-N	5.48	127.57	120.44
1	A	839	ARG	C-N-CA	5.48	127.57	120.44
1	A	1354	ASN	N-CA-C	5.48	117.25	111.28
2	B	476	ARG	CA-C-N	5.47	132.00	121.54
2	B	476	ARG	C-N-CA	5.47	132.00	121.54
1	A	452	LYS	N-CA-C	-5.45	106.13	112.89
2	B	550	ASP	CA-CB-CG	5.45	118.05	112.60
10	L	64	LEU	CA-C-N	5.43	129.38	122.37
10	L	64	LEU	C-N-CA	5.43	129.38	122.37
3	C	215	GLU	N-CA-C	5.43	118.70	111.75
1	A	694	THR	CA-C-N	5.42	127.81	120.38
1	A	694	THR	C-N-CA	5.42	127.81	120.38
1	A	313	GLN	N-CA-C	5.42	117.92	109.52
1	A	451	HIS	CB-CA-C	-5.42	98.68	109.79
4	E	21	GLU	CA-C-N	5.41	127.79	120.65
4	E	21	GLU	C-N-CA	5.41	127.79	120.65
4	E	53	PRO	N-CA-C	5.41	118.96	110.80
1	A	436	ILE	CB-CA-C	5.40	120.12	111.69
1	A	598	LEU	N-CA-C	-5.39	105.92	112.88
3	C	151	GLN	N-CA-C	5.39	118.26	110.28
8	J	1	MET	CA-C-N	5.37	131.64	121.97
8	J	1	MET	C-N-CA	5.37	131.64	121.97
1	A	1120	LEU	CA-C-N	5.37	128.51	120.83
1	A	1120	LEU	C-N-CA	5.37	128.51	120.83
6	H	128	ASN	CA-CB-CG	5.37	117.97	112.60
2	B	464	GLY	CA-C-N	5.37	131.79	121.54
2	B	464	GLY	C-N-CA	5.37	131.79	121.54
2	B	739	THR	N-CA-C	-5.36	107.29	113.88
10	L	62	LYS	N-CA-C	-5.35	106.14	113.30
2	B	909	ASP	CA-CB-CG	5.34	117.94	112.60
6	H	2	SER	CA-C-N	5.33	131.30	121.70
6	H	2	SER	C-N-CA	5.33	131.30	121.70
2	B	1022	THR	CB-CA-C	5.32	121.01	110.42
5	F	148	VAL	CA-C-N	5.32	127.41	120.28
5	F	148	VAL	C-N-CA	5.32	127.41	120.28
2	B	760	ASP	CA-CB-CG	5.31	117.91	112.60
2	B	1011	ILE	N-CA-CB	5.29	118.52	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	41	ILE	N-CA-CB	5.28	118.60	111.21
6	H	91	ASP	N-CA-C	5.28	117.33	107.99
2	B	294	ASP	CA-C-N	5.26	125.82	119.98
2	B	294	ASP	C-N-CA	5.26	125.82	119.98
10	L	40	LEU	N-CA-C	5.25	116.50	108.52
2	B	392	ARG	N-CA-C	-5.25	107.26	113.97
2	B	663	ALA	N-CA-C	-5.23	105.47	111.07
1	A	351	THR	CB-CA-C	-5.23	101.43	111.78
4	E	7	ARG	N-CA-C	-5.23	105.50	111.14
2	B	432	MET	CA-C-N	5.22	127.28	120.28
2	B	432	MET	C-N-CA	5.22	127.28	120.28
2	B	1169	MET	CA-C-N	5.22	127.54	120.44
2	B	1169	MET	C-N-CA	5.22	127.54	120.44
4	E	92	THR	CA-C-N	5.22	127.28	120.28
4	E	92	THR	C-N-CA	5.22	127.28	120.28
1	A	1155	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	485	ASP	CA-CB-CG	5.22	117.82	112.60
4	E	22	MET	CA-C-N	5.21	127.12	120.56
4	E	22	MET	C-N-CA	5.21	127.12	120.56
4	E	157	SER	CA-C-N	5.20	127.50	120.38
4	E	157	SER	C-N-CA	5.20	127.50	120.38
1	A	31	SER	N-CA-C	5.19	116.99	110.24
2	B	1222	ARG	CA-C-N	5.19	131.45	121.54
2	B	1222	ARG	C-N-CA	5.19	131.45	121.54
3	C	108	GLU	N-CA-C	-5.19	105.71	111.36
1	A	307	ASP	CA-CB-CG	5.17	117.78	112.60
7	I	31	THR	N-CA-C	-5.17	107.35	113.97
2	B	1009	ASP	N-CA-C	-5.17	106.82	113.23
2	B	228	LYS	CA-C-N	5.17	128.19	120.90
2	B	228	LYS	C-N-CA	5.17	128.19	120.90
10	L	40	LEU	CA-C-N	5.17	128.04	120.71
10	L	40	LEU	C-N-CA	5.17	128.04	120.71
6	H	16	ASP	CA-CB-CG	5.16	117.76	112.60
7	I	113	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	1103	GLU	CA-C-N	5.14	126.99	120.72
1	A	1103	GLU	C-N-CA	5.14	126.99	120.72
1	A	622	VAL	N-CA-C	5.13	117.83	112.90
4	E	17	ARG	CA-C-N	5.13	127.15	120.28
4	E	17	ARG	C-N-CA	5.13	127.15	120.28
1	A	219	PHE	CA-CB-CG	5.12	118.92	113.80
3	C	255	VAL	N-CA-C	-5.12	105.41	111.00
10	L	50	ASP	CA-C-N	5.12	131.32	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	50	ASP	C-N-CA	5.12	131.32	121.54
12	T	24	DT	O4'-C1'-N1	5.12	116.08	108.40
2	B	136	THR	CA-C-N	5.11	131.31	121.54
2	B	136	THR	C-N-CA	5.11	131.31	121.54
1	A	980	ASP	CA-CB-CG	5.11	117.71	112.60
2	B	969	ARG	N-CA-C	5.11	116.74	108.41
1	A	134	ARG	CA-C-N	5.10	127.63	120.28
1	A	134	ARG	C-N-CA	5.10	127.63	120.28
1	A	228	PHE	N-CA-C	5.10	119.58	112.90
2	B	964	VAL	N-CA-C	5.07	116.66	108.85
3	C	236	GLY	CA-C-N	5.07	127.78	120.38
3	C	236	GLY	C-N-CA	5.07	127.78	120.38
2	B	56	ASP	N-CA-C	5.06	116.87	111.36
4	E	57	MET	CA-C-N	5.06	127.32	120.44
4	E	57	MET	C-N-CA	5.06	127.32	120.44
2	B	894	ASP	N-CA-C	-5.05	103.27	110.59
1	A	24	PRO	CA-C-N	5.05	127.46	120.29
1	A	24	PRO	C-N-CA	5.05	127.46	120.29
1	A	79	GLY	N-CA-C	-5.04	106.38	112.48
1	A	795	GLU	CB-CG-CD	5.04	121.16	112.60
2	B	689	LEU	CA-C-N	5.03	130.88	122.57
2	B	689	LEU	C-N-CA	5.03	130.88	122.57
2	B	933	SER	CA-C-N	5.03	128.22	120.82
2	B	933	SER	C-N-CA	5.03	128.22	120.82
1	A	672	ASP	CA-CB-CG	5.03	117.63	112.60
2	B	618	ASP	CA-C-N	5.03	127.09	120.60
2	B	618	ASP	C-N-CA	5.03	127.09	120.60
2	B	834	ASN	CA-CB-CG	5.03	117.63	112.60
10	L	68	GLU	N-CA-C	-5.03	101.12	109.46
1	A	1216	ILE	CA-C-N	5.02	127.01	120.28
1	A	1216	ILE	C-N-CA	5.02	127.01	120.28
1	A	210	ILE	CA-C-N	5.02	127.51	120.28
1	A	210	ILE	C-N-CA	5.02	127.51	120.28
2	B	891	ASP	N-CA-C	5.02	118.51	112.38
1	A	651	LYS	CA-C-N	5.02	126.97	120.70
1	A	651	LYS	C-N-CA	5.02	126.97	120.70
1	A	827	THR	N-CA-C	-5.02	105.70	111.07
1	A	466	SER	N-CA-C	5.01	119.09	112.92
1	A	612	ILE	CB-CA-C	5.01	116.95	111.08
7	I	4	PHE	CA-CB-CG	5.01	118.81	113.80
1	A	1371	LEU	CA-C-N	5.00	127.32	120.46
1	A	1371	LEU	C-N-CA	5.00	127.32	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	154	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	647	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11043	0	11133	231	0
2	B	8861	0	8884	189	0
3	C	2095	0	2051	41	0
4	E	1752	0	1776	23	0
5	F	688	0	707	8	0
6	H	1068	0	1040	21	0
7	I	971	0	927	10	0
8	J	532	0	542	18	0
9	K	919	0	929	18	0
10	L	363	0	386	9	0
11	R	133	0	67	1	0
12	T	261	0	148	4	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	28695	0	28590	510	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 (510) 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:867:ILE:CG1	1:A:867:ILE:CD1	1.77	1.57
1:A:756:ILE:CG1	1:A:756:ILE:CD1	1.83	1.55
2:B:1094:ARG:HH11	2:B:1094:ARG:HG2	1.04	1.14
1:A:565:ILE:HG23	1:A:567:LYS:HD2	1.20	1.11
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.95	1.01
1:A:565:ILE:HG12	1:A:567:LYS:HZ2	1.33	0.94
1:A:567:LYS:HB3	6:H:96:VAL:H	1.36	0.89
1:A:565:ILE:HG23	1:A:567:LYS:CD	2.03	0.88
2:B:1094:ARG:HG2	2:B:1094:ARG:NH1	1.86	0.88
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.21	0.87
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.88	0.87
1:A:869:GLY:O	4:E:204:THR:HG21	1.74	0.86
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.58	0.86
2:B:1094:ARG:HH11	2:B:1094:ARG:CG	1.89	0.85
2:B:542:MET:HE2	2:B:747:MET:HG3	1.57	0.84
8:J:48:ARG:O	8:J:52:THR:HB	1.77	0.84
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.59	0.84
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.59	0.84
1:A:741:ASN:HD22	1:A:744:LYS:H	1.26	0.83
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.62	0.82
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.62	0.80
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.46	0.79
1:A:756:ILE:HD13	1:A:756:ILE:H	1.46	0.79
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.46	0.79
9:K:65:HIS:HD2	9:K:67:PHE:H	1.32	0.78
1:A:68:GLN:NE2	1:A:70:CYS:HB3	1.97	0.78
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.65	0.78
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.14	0.77
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.32	0.77
2:B:744:HIS:HD2	2:B:746:SER:H	1.32	0.76
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.67	0.76
2:B:809:MET:HE1	2:B:983:ARG:HH21	1.51	0.75
2:B:884:ARG:HG3	2:B:935:ARG:HE	1.52	0.75
1:A:68:GLN:HE22	1:A:70:CYS:HB3	1.50	0.75
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.69	0.74
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.69	0.74
3:C:167:HIS:HD2	3:C:169:LYS:H	1.34	0.74
1:A:565:ILE:CG2	1:A:567:LYS:HD2	2.10	0.73
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.70	0.73
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.19	0.73
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.69	0.73
1:A:399:HIS:O	1:A:401:GLY:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:MET:HE2	2:B:390:LEU:HG	1.72	0.72
2:B:976:ILE:O	2:B:990:ILE:O	2.08	0.72
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.71	0.71
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.24	0.71
1:A:466:SER:HB3	2:B:1103:ILE:HD12	1.71	0.71
2:B:654:ARG:H	2:B:657:HIS:HD2	1.35	0.71
1:A:466:SER:HB3	2:B:1103:ILE:CD1	2.22	0.69
1:A:901:LEU:HA	1:A:907:THR:HG23	1.72	0.69
2:B:705:MET:HE3	2:B:742:GLU:HG3	1.74	0.69
3:C:56:THR:HG22	3:C:58:LEU:H	1.55	0.69
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.74	0.69
9:K:65:HIS:CD2	9:K:67:PHE:H	2.11	0.69
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.73	0.68
3:C:6:PRO:HB3	3:C:25:VAL:HG22	1.76	0.67
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.77	0.67
3:C:54:ASN:OD1	3:C:56:THR:HB	1.94	0.67
1:A:11:LEU:HD11	2:B:1195:HIS:HD2	1.60	0.66
1:A:535:THR:HG22	1:A:616:VAL:HA	1.77	0.66
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.77	0.66
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.76	0.66
4:E:55:ARG:HA	4:E:58:MET:HE3	1.77	0.66
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.76	0.66
1:A:754:SER:H	1:A:757:ASN:HD22	1.43	0.66
1:A:378:GLU:OE2	1:A:434:ARG:HD3	1.96	0.65
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.09	0.65
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.78	0.65
2:B:706:GLN:O	2:B:710:LEU:HB2	1.96	0.64
1:A:535:THR:HG21	1:A:617:VAL:H	1.61	0.64
3:C:41:ILE:HG12	3:C:172:PRO:HG3	1.79	0.64
1:A:605:MET:HE2	1:A:607:ILE:HG13	1.79	0.64
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.80	0.64
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.80	0.64
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.31	0.63
2:B:950:ASP:OD2	2:B:967:ARG:NH1	2.31	0.63
2:B:249:ARG:HG2	2:B:251:ILE:HD11	1.80	0.63
1:A:845:LEU:O	1:A:1065:GLY:HA3	1.99	0.63
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.65	0.62
5:F:110:ASP:O	5:F:123:LYS:HE2	2.00	0.62
8:J:1:MET:H1	8:J:56:LEU:HB2	1.63	0.62
1:A:404:TYR:HA	1:A:413:ILE:O	1.99	0.62
2:B:731:VAL:O	2:B:732:SER:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1156:ASP:HB2	2:B:1198:TYR:H	1.64	0.61
6:H:125:LEU:HG	6:H:130:ARG:NH1	2.15	0.61
1:A:55:ASP:O	1:A:57:ARG:N	2.33	0.61
1:A:315:LEU:HA	1:A:320:ARG:HB3	1.82	0.61
1:A:567:LYS:NZ	6:H:97:MET:HG2	2.15	0.61
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.31	0.61
2:B:800:GLN:HB3	8:J:52:THR:HG23	1.83	0.61
1:A:503:GLN:NE2	5:F:90:ARG:HH12	1.97	0.61
1:A:567:LYS:O	1:A:569:LYS:N	2.33	0.61
2:B:424:LEU:O	2:B:428:ILE:HG12	2.01	0.61
3:C:41:ILE:HD12	3:C:246:ARG:HB2	1.83	0.61
1:A:756:ILE:CD1	1:A:756:ILE:H	2.13	0.60
10:L:28:LYS:HB2	10:L:39:SER:HB2	1.83	0.60
1:A:596:THR:C	1:A:598:LEU:H	2.10	0.60
1:A:626:ASN:O	1:A:631:HIS:HD2	1.84	0.60
1:A:1105:LEU:HB3	1:A:1384:VAL:CG2	2.31	0.60
2:B:809:MET:HE1	2:B:983:ARG:NH2	2.15	0.60
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.84	0.60
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.66	0.60
3:C:37:MET:HE2	3:C:244:VAL:HA	1.84	0.60
1:A:855:THR:HG21	1:A:857:ARG:HE	1.66	0.60
2:B:25:ILE:CD1	2:B:658:ILE:HD13	2.31	0.60
2:B:864:LYS:HG2	2:B:871:THR:HA	1.83	0.60
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.84	0.59
1:A:290:GLU:HA	1:A:293:GLU:HB2	1.84	0.59
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.85	0.59
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.49	0.59
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.50	0.59
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.67	0.59
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.85	0.59
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.85	0.59
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.38	0.58
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.36	0.58
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.85	0.58
1:A:351:THR:HG21	1:A:466:SER:O	2.03	0.58
2:B:195:CYS:SG	2:B:783:THR:HB	2.43	0.58
2:B:365:THR:HG21	2:B:370:PHE:CG	2.39	0.58
1:A:567:LYS:HZ1	6:H:97:MET:HG2	1.69	0.58
3:C:66:ARG:NH2	8:J:3:VAL:O	2.26	0.58
10:L:30:ILE:HD11	10:L:59:ALA:HA	1.86	0.58
2:B:102:VAL:HG11	2:B:122:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:113:THR:O	9:K:114:LEU:HB2	2.03	0.58
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.86	0.57
2:B:515:HIS:CD2	2:B:517:THR:H	2.22	0.57
2:B:996:ARG:HH12	3:C:173:ALA:HB1	1.69	0.57
1:A:456:MET:HE2	1:A:510:GLN:CB	2.35	0.57
2:B:276:ILE:HD11	2:B:335:GLY:H	1.69	0.57
2:B:363:HIS:O	2:B:364:ILE:HB	2.03	0.57
1:A:11:LEU:HD11	2:B:1195:HIS:CD2	2.39	0.57
1:A:214:ILE:HG22	1:A:215:SER:H	1.70	0.57
3:C:33:LEU:HG	3:C:37:MET:HE3	1.85	0.57
4:E:78:LEU:HD12	4:E:107:THR:HB	1.87	0.57
6:H:125:LEU:HG	6:H:130:ARG:HH12	1.70	0.56
1:A:567:LYS:HG2	1:A:568:PRO:HD2	1.86	0.56
2:B:408:LEU:HD11	2:B:545:ILE:HD12	1.87	0.56
1:A:1086:PHE:HB3	1:A:1092:LYS:HD3	1.87	0.56
2:B:1013:ASN:OD1	2:B:1015:HIS:HD2	1.89	0.56
1:A:626:ASN:O	1:A:631:HIS:CD2	2.59	0.56
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.58	0.56
1:A:173:THR:HB	1:A:184:SER:HB3	1.88	0.56
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.88	0.55
1:A:456:MET:HE2	1:A:510:GLN:HB2	1.86	0.55
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.89	0.55
3:C:165:LYS:O	9:K:6:ARG:NH1	2.39	0.55
1:A:1123:GLY:CA	1:A:1124:HIS:HB2	2.37	0.55
2:B:887:HIS:HA	2:B:888:GLY:C	2.32	0.55
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.22	0.55
8:J:1:MET:N	8:J:56:LEU:H	2.05	0.55
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.70	0.55
6:H:137:GLN:HB3	6:H:139:ASN:HB2	1.88	0.55
1:A:567:LYS:HE3	6:H:96:VAL:O	2.06	0.55
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.42	0.55
5:F:77:ASP:O	5:F:78:GLN:HB2	2.07	0.55
6:H:40:LEU:HD13	6:H:123:MET:HG3	1.89	0.55
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.88	0.54
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.90	0.54
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.88	0.54
1:A:1327:ILE:O	4:E:147:HIS:HE1	1.90	0.54
2:B:542:MET:HE1	2:B:743:ILE:HB	1.88	0.54
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.87	0.54
1:A:711:ARG:NH1	7:I:95:THR:HG22	2.22	0.54
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:773:MET:HA	2:B:776:GLN:HG3	1.90	0.54
1:A:1372:VAL:O	1:A:1376:THR:HB	2.07	0.54
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.21	0.54
2:B:956:THR:HB	10:L:46:VAL:HG21	1.90	0.54
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.90	0.54
2:B:841:MET:O	2:B:993:THR:HA	2.07	0.54
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.90	0.54
2:B:211:VAL:CG2	2:B:483:LEU:HD13	2.38	0.54
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.89	0.54
3:C:56:THR:CG2	3:C:58:LEU:H	2.20	0.53
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.07	0.53
1:A:469:ARG:NH2	2:B:991:GLY:O	2.32	0.53
1:A:567:LYS:CB	6:H:95:TYR:HA	2.38	0.53
7:I:106:CYS:HB3	7:I:108:HIS:H	1.74	0.53
3:C:18:VAL:HG22	3:C:240:VAL:HB	1.91	0.53
3:C:142:VAL:H	8:J:16:ASP:HB3	1.74	0.53
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.19	0.52
6:H:136:LYS:H	6:H:136:LYS:HD3	1.75	0.52
1:A:57:ARG:HA	1:A:68:GLN:HB3	1.92	0.52
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.90	0.52
2:B:476:ARG:O	2:B:478:GLY:N	2.43	0.52
2:B:879:ARG:O	2:B:882:THR:HG22	2.09	0.52
1:A:56:PRO:HB2	1:A:57:ARG:HH21	1.73	0.52
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.90	0.52
1:A:672:ASP:HB3	1:A:674:PRO:HD2	1.92	0.52
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.58	0.52
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.44	0.52
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.44	0.52
4:E:147:HIS:CD2	4:E:149:LEU:HB2	2.45	0.52
1:A:463:ILE:HD13	1:A:469:ARG:HG3	1.90	0.52
2:B:1006:ILE:HD11	8:J:43:ARG:HB2	1.92	0.52
9:K:38:GLU:O	9:K:69:ALA:O	2.28	0.52
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.91	0.52
4:E:8:ASN:HD21	4:E:55:ARG:HH22	1.57	0.52
1:A:1076:ALA:HA	1:A:1079:MET:HG3	1.91	0.51
1:A:203:SER:HB3	1:A:206:GLU:HB2	1.92	0.51
1:A:856:THR:HG22	1:A:864:ILE:HB	1.92	0.51
1:A:902:LEU:HD23	1:A:921:GLY:O	2.10	0.51
2:B:708:GLU:O	2:B:710:LEU:N	2.43	0.51
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.93	0.51
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.45	0.51
8:J:6:ARG:HA	8:J:12:LYS:O	2.11	0.51
1:A:605:MET:HE1	1:A:612:ILE:HD13	1.92	0.51
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.45	0.51
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.92	0.51
4:E:147:HIS:HD2	4:E:149:LEU:H	1.56	0.51
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.92	0.51
4:E:88:VAL:HB	4:E:116:ILE:HD13	1.92	0.51
1:A:899:VAL:HG22	1:A:1029:ARG:HG3	1.93	0.51
1:A:1364:ASN:HD21	1:A:1366:ARG:HD2	1.73	0.51
2:B:893:LEU:HD22	2:B:897:GLY:O	2.10	0.51
1:A:306:ASN:HD21	1:A:313:GLN:HB2	1.76	0.50
1:A:868:TYR:OH	1:A:1366:ARG:HG3	2.11	0.50
7:I:50:THR:HG22	7:I:52:ILE:H	1.76	0.50
2:B:493:SER:HB3	2:B:497:ARG:NH2	2.27	0.50
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.42	0.50
2:B:640:VAL:CG1	2:B:649:LYS:HB3	2.41	0.50
2:B:254:LEU:CD2	2:B:381:MET:HE1	2.41	0.50
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.92	0.50
2:B:516:ASN:H	2:B:516:ASN:HD22	1.60	0.50
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.94	0.50
1:A:299:HIS:HA	1:A:302:THR:HG22	1.94	0.49
2:B:783:THR:HG22	8:J:63:TYR:OH	2.12	0.49
1:A:219:PHE:HZ	1:A:226:GLU:HA	1.76	0.49
3:C:13:ALA:O	9:K:114:LEU:HB3	2.12	0.49
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.28	0.49
2:B:345:LYS:HB3	2:B:348:ARG:HE	1.76	0.49
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.94	0.49
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.95	0.49
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.77	0.49
2:B:140:ILE:H	2:B:141:ASP:C	2.20	0.49
2:B:733:HIS:C	2:B:735:ALA:H	2.21	0.49
1:A:357:PRO:HG2	2:B:833:TYR:CE1	2.47	0.49
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.65	0.49
1:A:1105:LEU:HB3	1:A:1384:VAL:HG23	1.95	0.49
2:B:806:THR:HG22	2:B:808:ALA:H	1.78	0.49
6:H:57:VAL:HG22	6:H:144:ILE:HG12	1.95	0.49
2:B:879:ARG:NH1	2:B:879:ARG:HA	2.28	0.49
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.95	0.49
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	1.94	0.48
2:B:378:LEU:O	2:B:382:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:ALA:O	3:C:233:GLU:O	2.31	0.48
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.93	0.48
1:A:567:LYS:HG2	1:A:568:PRO:CD	2.43	0.48
2:B:704:ALA:HB1	2:B:710:LEU:HB3	1.95	0.48
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.96	0.48
2:B:1100:ASP:HA	2:B:1103:ILE:HD11	1.95	0.48
4:E:170:LEU:HD13	4:E:175:LEU:HD13	1.94	0.48
1:A:565:ILE:CG1	1:A:567:LYS:HZ2	2.16	0.48
1:A:1100:ARG:NH2	1:A:1351:GLU:HG3	2.27	0.48
2:B:37:PHE:O	2:B:38:PHE:HB2	2.12	0.48
2:B:302:CYS:HA	2:B:310:MET:HE2	1.95	0.48
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.48	0.48
2:B:796:LEU:HD23	2:B:799:PRO:HA	1.96	0.48
2:B:209:GLU:OE1	2:B:788:ARG:NH2	2.47	0.48
4:E:19:VAL:HG11	4:E:80:VAL:HG11	1.96	0.48
1:A:494:SER:O	1:A:498:ARG:HG3	2.13	0.48
1:A:754:SER:H	1:A:757:ASN:ND2	2.12	0.48
2:B:879:ARG:HH22	2:B:885:MET:HE2	1.79	0.48
1:A:575:LYS:HD2	6:H:120:GLY:HA3	1.96	0.47
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.96	0.47
2:B:887:HIS:H	2:B:890:TYR:HE1	1.62	0.47
1:A:216:VAL:HA	1:A:219:PHE:CD1	2.49	0.47
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.48	0.47
1:A:116:ASP:HB3	1:A:117:GLU:HG3	1.97	0.47
1:A:492:PRO:CB	1:A:497:THR:HG22	2.44	0.47
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.94	0.47
2:B:169:ARG:HH12	2:B:958:GLN:HE22	1.61	0.47
2:B:708:GLU:C	2:B:710:LEU:H	2.23	0.47
4:E:94:LYS:O	4:E:98:ILE:HG12	2.14	0.47
1:A:499:ALA:HB2	5:F:118:LEU:HD11	1.95	0.47
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.96	0.47
7:I:10:CYS:SG	7:I:31:THR:HB	2.55	0.47
8:J:63:TYR:C	8:J:65:PRO:HD2	2.40	0.47
1:A:535:THR:HG21	1:A:617:VAL:N	2.28	0.47
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.97	0.47
1:A:332:LYS:H	1:A:337:ARG:HB2	1.79	0.47
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.96	0.47
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.80	0.47
2:B:792:MET:HA	2:B:856:PHE:O	2.14	0.47
2:B:1129:ARG:HB3	12:T:21:DC:H5"	1.96	0.47
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.97	0.47
3:C:73:GLN:HE21	3:C:75:MET:H	1.62	0.47
8:J:1:MET:H1	8:J:56:LEU:H	1.62	0.47
2:B:102:VAL:O	2:B:109:THR:HA	2.15	0.47
6:H:89:LEU:C	6:H:91:ASP:H	2.23	0.47
8:J:6:ARG:HG2	8:J:11:GLY:O	2.15	0.47
1:A:134:ARG:HD2	1:A:221:SER:O	2.15	0.47
1:A:541:ILE:HG21	1:A:549:MET:CE	2.45	0.47
2:B:466:TRP:HB3	2:B:475:SER:HB2	1.96	0.47
2:B:509:ALA:O	2:B:511:PRO:HD3	2.16	0.46
3:C:56:THR:HG22	3:C:58:LEU:N	2.29	0.46
4:E:198:ILE:HD13	4:E:212:ARG:HG3	1.97	0.46
1:A:666:ILE:HG12	2:B:1026:LEU:HB2	1.96	0.46
1:A:851:HIS:HB2	1:A:855:THR:HG22	1.98	0.46
1:A:1259:MET:HA	1:A:1262:LYS:HE2	1.97	0.46
2:B:128:LEU:HD11	2:B:170:LEU:HB2	1.96	0.46
2:B:882:THR:O	2:B:884:ARG:N	2.45	0.46
7:I:49:ILE:HA	7:I:92:ARG:HH22	1.80	0.46
10:L:61:THR:HB	10:L:63:ARG:H	1.80	0.46
1:A:64:ASN:C	1:A:66:LYS:H	2.21	0.46
1:A:567:LYS:HB3	6:H:96:VAL:N	2.18	0.46
1:A:702:LEU:HD12	1:A:710:LEU:HD13	1.97	0.46
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.97	0.46
1:A:1161:THR:OG1	1:A:1170:ILE:HG13	2.15	0.46
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.96	0.46
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.46	0.46
1:A:614:PHE:HB3	6:H:122:LEU:HD21	1.98	0.46
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	1.97	0.46
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.46	0.46
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.98	0.46
1:A:1385:THR:HG22	1:A:1387:HIS:H	1.81	0.46
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.51	0.46
1:A:741:ASN:HB3	1:A:744:LYS:HB3	1.98	0.45
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.98	0.45
8:J:7:CYS:HA	8:J:49:MET:HG2	1.98	0.45
1:A:214:ILE:HG22	1:A:215:SER:N	2.32	0.45
1:A:1017:LEU:O	1:A:1020:CYS:HB2	2.15	0.45
1:A:1393:ASN:ND2	1:A:1393:ASN:H	2.13	0.45
2:B:487:THR:HB	2:B:777:ALA:O	2.16	0.45
2:B:745:PRO:O	2:B:748:ILE:HG12	2.16	0.45
1:A:95:PHE:CE2	1:A:1414:ALA:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HB	1:A:470:LEU:HD21	1.99	0.45
1:A:647:GLY:O	1:A:651:LYS:HG3	2.17	0.45
1:A:857:ARG:HD3	1:A:861:GLY:O	2.16	0.45
2:B:239:GLU:HG2	2:B:255:GLN:HG2	1.99	0.45
2:B:791:THR:O	2:B:792:MET:HB2	2.15	0.45
11:R:7:G:H2'	11:R:8:A:O4'	2.17	0.45
1:A:265:LYS:HD3	1:A:322:VAL:HG21	1.99	0.45
1:A:323:LYS:HE2	1:A:328:ARG:HE	1.80	0.45
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.98	0.45
1:A:596:THR:O	1:A:598:LEU:N	2.45	0.45
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.98	0.45
6:H:24:CYS:HB2	6:H:44:VAL:HG21	1.99	0.45
1:A:472:LEU:HD21	2:B:835:GLN:HB3	1.99	0.45
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.97	0.45
3:C:6:PRO:HB3	3:C:25:VAL:CG2	2.46	0.45
12:T:25:DC:H2'	12:T:26:DG:C8	2.50	0.45
1:A:707:GLY:O	1:A:1281:ARG:HD2	2.17	0.45
2:B:515:HIS:HD2	2:B:517:THR:H	1.63	0.45
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.98	0.45
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.99	0.45
2:B:1013:ASN:OD1	2:B:1015:HIS:CD2	2.69	0.45
7:I:65:ASP:HB3	7:I:68:LEU:HD12	1.98	0.45
8:J:1:MET:HE2	8:J:1:MET:HB2	1.82	0.45
2:B:708:GLU:H	2:B:708:GLU:HG3	1.49	0.45
2:B:942:ARG:HH22	12:T:25:DC:P	2.40	0.45
3:C:50:GLU:HG2	10:L:66:GLN:HG2	1.99	0.45
3:C:185:LYS:HG2	3:C:213:PRO:HB3	1.99	0.45
4:E:147:HIS:CD2	4:E:149:LEU:H	2.35	0.45
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.52	0.45
10:L:27:LEU:HD13	10:L:59:ALA:HB1	2.00	0.45
1:A:335:ARG:HD3	2:B:1202:LEU:HD13	2.00	0.44
2:B:755:ILE:HA	2:B:809:MET:HE2	2.00	0.44
2:B:1082:MET:HA	3:C:189:THR:HA	1.99	0.44
10:L:32:ALA:HB3	10:L:55:ILE:HB	1.98	0.44
2:B:620:ARG:CZ	7:I:68:LEU:HD21	2.48	0.44
3:C:22:LEU:HD11	9:K:101:LEU:HD21	2.00	0.44
3:C:231:ASN:HD22	3:C:231:ASN:C	2.26	0.44
1:A:225:ASN:HD22	1:A:228:PHE:H	1.65	0.44
1:A:396:PRO:HB3	1:A:403:LYS:HB3	1.99	0.44
2:B:766:ARG:CZ	2:B:1020:ARG:HD3	2.48	0.44
8:J:3:VAL:HG11	8:J:18:TRP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:HIS:H	1:A:210:ILE:HD12	1.81	0.44
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.17	0.44
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	1.98	0.44
2:B:1168:LEU:C	2:B:1170:THR:H	2.25	0.44
9:K:42:LEU:HD12	9:K:42:LEU:HA	1.83	0.44
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.98	0.44
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	2.00	0.44
1:A:567:LYS:CB	1:A:568:PRO:CD	2.96	0.44
2:B:282:ILE:HD13	2:B:382:ILE:HD12	1.99	0.44
2:B:406:LEU:HD12	2:B:633:VAL:HG21	1.99	0.44
2:B:862:GLN:HG2	2:B:963:PHE:HB2	2.00	0.44
2:B:1163:CYS:O	2:B:1167:GLY:HA2	2.17	0.44
1:A:219:PHE:CD2	1:A:231:PRO:HD3	2.53	0.44
1:A:315:LEU:HG	1:A:320:ARG:HH21	1.82	0.44
1:A:396:PRO:HG3	1:A:416:ARG:HB3	2.00	0.44
1:A:567:LYS:HE2	6:H:95:TYR:CG	2.52	0.44
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	2.00	0.44
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.18	0.44
2:B:492:LEU:HB2	2:B:751:VAL:HG11	1.99	0.44
2:B:709:ASP:O	2:B:710:LEU:HD22	2.17	0.44
7:I:7:CYS:HB3	7:I:10:CYS:HB2	2.00	0.44
1:A:690:VAL:HA	1:A:693:VAL:HG12	2.00	0.43
2:B:276:ILE:HD12	2:B:280:ILE:HD11	2.00	0.43
9:K:57:LEU:HB2	9:K:76:GLN:HG2	1.99	0.43
1:A:86:LEU:HD12	1:A:296:LEU:HD21	2.00	0.43
4:E:83:CYS:SG	4:E:85:GLU:HG2	2.58	0.43
1:A:535:THR:CG2	1:A:616:VAL:HA	2.46	0.43
1:A:579:SER:HA	1:A:582:ILE:HD12	2.00	0.43
3:C:27:LEU:HD13	3:C:228:PHE:HE2	1.83	0.43
1:A:219:PHE:HD2	1:A:231:PRO:HD3	1.82	0.43
1:A:456:MET:HE1	1:A:521:MET:HE2	1.99	0.43
6:H:84:ALA:O	6:H:85:GLY:C	2.61	0.43
6:H:96:VAL:HG13	6:H:143:LEU:HG	2.00	0.43
1:A:11:LEU:HD12	2:B:1193:GLN:O	2.18	0.43
1:A:517:ASN:ND2	1:A:1364:ASN:OD1	2.51	0.43
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.53	0.43
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	1.99	0.43
1:A:853:ASP:OD1	1:A:855:THR:HB	2.18	0.43
1:A:1385:THR:HG21	1:A:1387:HIS:CD2	2.53	0.43
4:E:156:LEU:HD23	4:E:197:LYS:HB2	2.01	0.43
1:A:84:ILE:HD11	1:A:270:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.67	0.43
2:B:301:ILE:HG22	2:B:310:MET:HE3	2.00	0.43
3:C:196:ASP:HB3	3:C:199:LYS:HB2	2.01	0.43
1:A:1215:ARG:HH21	1:A:1218:GLN:HG3	1.83	0.43
2:B:408:LEU:CD1	2:B:545:ILE:HD12	2.47	0.43
12:T:19:DT:H2'	12:T:20:DC:C6	2.54	0.43
1:A:84:ILE:CG2	1:A:239:LEU:HB3	2.48	0.43
2:B:406:LEU:HD12	2:B:633:VAL:CG2	2.48	0.43
2:B:509:ALA:C	2:B:511:PRO:HD3	2.43	0.43
2:B:592:ASN:H	2:B:593:PRO:HD3	1.82	0.43
1:A:443:LEU:HD13	1:A:455:MET:HE2	2.01	0.43
2:B:544:CYS:HB2	2:B:634:TYR:CZ	2.53	0.43
4:E:147:HIS:HD2	4:E:149:LEU:HB2	1.83	0.43
5:F:136:ARG:O	5:F:143:PHE:HA	2.19	0.43
1:A:408:ASP:C	1:A:410:GLY:H	2.27	0.43
1:A:1308:THR:HG22	1:A:1310:GLY:O	2.19	0.43
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.99	0.43
1:A:326:ARG:HG2	1:A:1406:VAL:HG11	1.99	0.42
1:A:871:ASP:HB3	4:E:204:THR:HG23	2.00	0.42
2:B:473:MET:C	2:B:475:SER:H	2.27	0.42
4:E:46:TYR:HD2	4:E:57:MET:HB3	1.83	0.42
2:B:1133:MET:HE3	2:B:1133:MET:HB2	1.94	0.42
4:E:111:VAL:HG12	4:E:137:GLU:HG2	2.01	0.42
1:A:540:PHE:HB3	1:A:571:LEU:HG	2.01	0.42
2:B:516:ASN:H	2:B:516:ASN:ND2	2.17	0.42
2:B:915:THR:HG21	2:B:934:LYS:HD3	2.00	0.42
1:A:31:SER:HB2	1:A:83:HIS:HB3	2.01	0.42
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.20	0.42
2:B:114:PRO:HG2	2:B:181:LEU:HD11	2.00	0.42
4:E:167:ARG:HA	4:E:167:ARG:HD3	1.75	0.42
1:A:535:THR:CG2	1:A:617:VAL:H	2.31	0.42
1:A:1422:ARG:HG3	2:B:1220:ARG:HH12	1.85	0.42
2:B:255:GLN:H	2:B:272:THR:HG22	1.84	0.42
2:B:615:MET:HE3	2:B:615:MET:HB2	1.88	0.42
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.54	0.42
2:B:283:VAL:HG13	2:B:297:ILE:HD13	2.01	0.42
2:B:485:ARG:HG3	2:B:781:PHE:CD1	2.54	0.42
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.53	0.42
1:A:919:ILE:O	1:A:922:ASP:HB2	2.20	0.42
2:B:43:LEU:HD11	2:B:811:TYR:O	2.19	0.42
2:B:483:LEU:HD11	2:B:491:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.34	0.42
2:B:882:THR:C	2:B:884:ARG:H	2.26	0.42
2:B:211:VAL:O	2:B:480:SER:HA	2.20	0.42
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.54	0.42
4:E:135:PHE:CB	4:E:140:LEU:HD11	2.49	0.42
1:A:41:MET:HA	1:A:50:ILE:H	1.84	0.41
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.35	0.41
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.34	0.41
2:B:242:SER:HB2	2:B:362:PRO:HD2	2.02	0.41
2:B:274:PRO:HG2	2:B:359:GLU:HB3	2.01	0.41
9:K:33:ILE:HD13	9:K:87:LEU:HD22	2.01	0.41
1:A:352:VAL:HB	2:B:1099:VAL:HG13	2.02	0.41
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	2.01	0.41
1:A:514:PRO:HB3	1:A:875:ALA:HB3	2.02	0.41
2:B:640:VAL:HG12	2:B:649:LYS:HB3	2.02	0.41
1:A:40:THR:HG22	1:A:41:MET:HG3	2.03	0.41
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.03	0.41
1:A:586:ILE:HD11	1:A:637:LYS:HG2	2.02	0.41
1:A:596:THR:C	1:A:598:LEU:N	2.77	0.41
1:A:944:ARG:HG2	1:A:1298:TYR:OH	2.20	0.41
2:B:29:ASP:OD2	2:B:655:LYS:HE2	2.21	0.41
2:B:639:ILE:HD11	2:B:691:GLU:HB2	2.02	0.41
9:K:7:PHE:HA	9:K:10:PHE:CZ	2.56	0.41
1:A:57:ARG:O	1:A:68:GLN:HG2	2.21	0.41
2:B:563:MET:HA	2:B:589:VAL:O	2.21	0.41
5:F:71:GLU:HA	5:F:72:LYS:HA	1.95	0.41
1:A:353:ILE:HD13	1:A:487:MET:CE	2.50	0.41
1:A:463:ILE:CD1	1:A:469:ARG:HG3	2.51	0.41
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.85	0.41
1:A:1271:ILE:HD13	1:A:1271:ILE:HA	2.01	0.41
2:B:222:ILE:HD13	2:B:403:LYS:HG3	2.03	0.41
2:B:515:HIS:H	2:B:518:HIS:CD2	2.38	0.41
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.85	0.41
2:B:1158:PHE:HD2	2:B:1160:VAL:HG22	1.85	0.41
1:A:304:MET:O	1:A:326:ARG:HB2	2.21	0.41
1:A:666:ILE:HG21	2:B:1030:LEU:HD22	2.03	0.41
1:A:709:THR:HG21	7:I:93:LYS:O	2.21	0.41
2:B:1079:LYS:HE3	3:C:188:HIS:CE1	2.56	0.41
1:A:567:LYS:HB2	6:H:95:TYR:HA	2.01	0.41
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.52	0.41
3:C:76:ASP:C	3:C:129:ILE:HD13	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.55	0.41
4:E:65:THR:HG22	4:E:67:GLU:H	1.86	0.41
2:B:46:GLN:H	2:B:46:GLN:HG3	1.64	0.41
2:B:276:ILE:HG13	2:B:334:ILE:HG23	2.03	0.41
2:B:651:LEU:HD21	2:B:741:CYS:HB3	2.02	0.41
1:A:589:GLN:HG3	1:A:606:LEU:HD13	2.02	0.40
1:A:975:HIS:ND1	1:A:1036:ARG:HD3	2.35	0.40
2:B:362:PRO:C	2:B:363:HIS:O	2.63	0.40
2:B:887:HIS:HA	2:B:888:GLY:O	2.21	0.40
1:A:353:ILE:HG22	1:A:468:PHE:HB2	2.03	0.40
1:A:1129:GLU:HA	1:A:1132:LYS:HE3	2.02	0.40
2:B:58:THR:O	2:B:62:ILE:HG12	2.21	0.40
3:C:259:LEU:HD12	3:C:259:LEU:HA	1.96	0.40
9:K:40:HIS:CE1	9:K:63:VAL:HG13	2.56	0.40
1:A:306:ASN:ND2	1:A:313:GLN:HB2	2.37	0.40
1:A:356:ASP:HA	1:A:357:PRO:HD2	1.98	0.40
7:I:19:ASP:HB2	7:I:24:ARG:HG2	2.03	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%)	1251 (90%)	100 (7%)	44 (3%)	3	7
2	B	1096/1224 (90%)	963 (88%)	86 (8%)	47 (4%)	2	4
3	C	264/318 (83%)	243 (92%)	13 (5%)	8 (3%)	3	8
4	E	212/215 (99%)	199 (94%)	10 (5%)	3 (1%)	9	19
5	F	83/155 (54%)	77 (93%)	3 (4%)	3 (4%)	2	5
6	H	129/146 (88%)	106 (82%)	17 (13%)	6 (5%)	2	3
7	I	117/122 (96%)	103 (88%)	9 (8%)	5 (4%)	2	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	63/70 (90%)	59 (94%)	2 (3%)	2 (3%)	3	7
9	K	112/120 (93%)	106 (95%)	5 (4%)	1 (1%)	14	28
10	L	44/70 (63%)	32 (73%)	7 (16%)	5 (11%)	0	0
All	All	3515/4173 (84%)	3139 (89%)	252 (7%)	124 (4%)	3	6

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	54	ASN
1	A	55	ASP
1	A	109	HIS
1	A	257	ARG
1	A	399	HIS
1	A	424	ILE
1	A	567	LYS
1	A	923	LEU
1	A	1234	GLU
2	B	67	SER
2	B	137	TYR
2	B	371	GLU
2	B	469	GLN
2	B	477	ALA
2	B	592	ASN
2	B	709	ASP
2	B	712	PRO
2	B	732	SER
2	B	734	HIS
2	B	883	LEU
2	B	887	HIS
2	B	1046	PRO
2	B	1156	ASP
2	B	1181	GLU
2	B	1223	ASP
3	C	173	ALA
3	C	227	THR
5	F	73	ALA
5	F	78	GLN
6	H	131	ASN
6	H	140	ALA
7	I	118	ARG

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Mol	Chain	Res	Type
8	J	2	ILE
1	A	56	PRO
1	A	214	ILE
1	A	250	ILE
1	A	1123	GLY
1	A	1124	HIS
1	A	1221	LYS
1	A	1437	GLY
2	B	138	GLU
2	B	368	GLU
2	B	465	ASN
2	B	483	LEU
2	B	526	GLU
2	B	531	GLN
2	B	648	HIS
2	B	888	GLY
2	B	1221	SER
3	C	141	GLY
3	C	142	VAL
6	H	90	ALA
6	H	109	LYS
8	J	6	ARG
10	L	46	VAL
10	L	51	CYS
1	A	310	GLY
1	A	312	PRO
1	A	331	GLY
1	A	332	LYS
1	A	597	LEU
1	A	672	ASP
1	A	1377	THR
2	B	139	ALA
2	B	249	ARG
2	B	474	SER
2	B	563	MET
2	B	646	LEU
2	B	882	THR
3	C	4	GLU
4	E	126	SER
10	L	42	ARG
10	L	56	LEU
10	L	64	LEU

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Mol	Chain	Res	Type
1	A	130	ASP
1	A	568	PRO
1	A	569	LYS
1	A	958	VAL
1	A	1081	LEU
1	A	1233	ASP
2	B	346	GLU
3	C	5	GLY
7	I	3	THR
7	I	20	LYS
7	I	77	LYS
9	K	70	ARG
1	A	65	LEU
1	A	286	HIS
1	A	299	HIS
1	A	400	PRO
1	A	404	TYR
1	A	975	HIS
1	A	1093	LYS
2	B	230	ALA
2	B	482	VAL
2	B	707	PRO
2	B	708	GLU
2	B	713	ALA
2	B	943	SER
2	B	1178	ASN
3	C	90	ASP
3	C	149	LYS
4	E	3	GLN
5	F	154	ASP
6	H	84	ALA
7	I	107	SER
1	A	35	ILE
1	A	149	GLU
1	A	213	HIS
1	A	308	ILE
1	A	846	GLU
2	B	647	GLY
2	B	792	MET
2	B	1171	VAL
2	B	1173	ALA
2	B	1176	ASN

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Mol	Chain	Res	Type
4	E	86	PRO
1	A	599	SER
1	A	1388	GLY
6	H	85	GLY
2	B	731	VAL
2	B	751	VAL
2	B	1017	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%)	1047 (86%)	178 (14%)	3	6
2	B	967/1061 (91%)	839 (87%)	128 (13%)	4	7
3	C	234/274 (85%)	201 (86%)	33 (14%)	3	6
4	E	196/197 (100%)	170 (87%)	26 (13%)	4	7
5	F	75/137 (55%)	68 (91%)	7 (9%)	8	18
6	H	117/128 (91%)	100 (86%)	17 (14%)	3	6
7	I	113/116 (97%)	94 (83%)	19 (17%)	2	3
8	J	60/65 (92%)	48 (80%)	12 (20%)	1	2
9	K	99/102 (97%)	86 (87%)	13 (13%)	4	7
10	L	40/57 (70%)	28 (70%)	12 (30%)	0	0
All	All	3126/3657 (86%)	2681 (86%)	445 (14%)	3	6

All (445) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	18	GLN
1	A	30	ILE
1	A	41	MET
1	A	43	GLU
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	58	LEU
1	A	61	ILE
1	A	68	GLN
1	A	70	CYS
1	A	71	GLN
1	A	88	LYS
1	A	90	VAL
1	A	93	VAL
1	A	108	MET
1	A	113	LEU
1	A	116	ASP
1	A	126	LEU
1	A	130	ASP
1	A	143	LYS
1	A	149	GLU
1	A	164	ARG
1	A	174	ILE
1	A	186	LYS
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	219	PHE
1	A	235	ILE
1	A	239	LEU
1	A	253	ASN
1	A	262	LEU
1	A	269	ILE
1	A	270	LEU
1	A	276	LEU
1	A	289	ILE
1	A	293	GLU
1	A	299	HIS
1	A	303	TYR
1	A	308	ILE
1	A	313	GLN
1	A	315	LEU
1	A	316	GLN
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	335	ARG
1	A	337	ARG

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Mol	Chain	Res	Type
1	A	351	THR
1	A	368	LYS
1	A	391	LEU
1	A	393	ARG
1	A	403	LYS
1	A	407	ARG
1	A	408	ASP
1	A	419	LYS
1	A	427	GLN
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	451	HIS
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	496	GLU
1	A	512	VAL
1	A	513	SER
1	A	527	THR
1	A	532	ARG
1	A	538	ASP
1	A	541	ILE
1	A	546	VAL
1	A	567	LYS
1	A	590	ARG
1	A	595	THR
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	626	ASN
1	A	629	LEU
1	A	636	GLU
1	A	666	ILE
1	A	682	THR
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS

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Mol	Chain	Res	Type
1	A	702	LEU
1	A	709	THR
1	A	710	LEU
1	A	716	ASP
1	A	722	LEU
1	A	756	ILE
1	A	769	SER
1	A	774	ARG
1	A	821	ARG
1	A	846	GLU
1	A	855	THR
1	A	856	THR
1	A	878	ILE
1	A	896	ARG
1	A	902	LEU
1	A	904	THR
1	A	905	ASP
1	A	907	THR
1	A	922	ASP
1	A	926	GLN
1	A	927	VAL
1	A	938	LYS
1	A	960	ILE
1	A	969	GLN
1	A	973	ILE
1	A	988	LEU
1	A	998	LEU
1	A	999	VAL
1	A	1001	ARG
1	A	1015	VAL
1	A	1022	LEU
1	A	1029	ARG
1	A	1048	ASN
1	A	1064	VAL
1	A	1067	LEU
1	A	1080	THR
1	A	1084	PHE
1	A	1094	VAL
1	A	1095	THR
1	A	1109	LYS
1	A	1110	ASN
1	A	1116	LEU

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Mol	Chain	Res	Type
1	A	1138	ILE
1	A	1159	ARG
1	A	1161	THR
1	A	1170	ILE
1	A	1176	LEU
1	A	1187	GLN
1	A	1195	LEU
1	A	1206	ASP
1	A	1221	LYS
1	A	1223	ASP
1	A	1224	LEU
1	A	1227	ILE
1	A	1230	GLU
1	A	1233	ASP
1	A	1237	ILE
1	A	1264	GLU
1	A	1266	THR
1	A	1267	MET
1	A	1277	GLU
1	A	1280	GLU
1	A	1284	MET
1	A	1291	VAL
1	A	1293	SER
1	A	1297	GLU
1	A	1299	VAL
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1335	ILE
1	A	1350	LYS
1	A	1351	GLU
1	A	1354	ASN
1	A	1355	VAL
1	A	1366	ARG
1	A	1368	MET
1	A	1376	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1406	VAL
1	A	1420	ASP
1	A	1424	VAL

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Mol	Chain	Res	Type
1	A	1426	GLU
1	A	1438	THR
1	A	1444	MET
1	A	1445	ILE
2	B	25	ILE
2	B	28	GLU
2	B	30	SER
2	B	45	SER
2	B	46	GLN
2	B	63	ILE
2	B	89	GLU
2	B	94	LYS
2	B	101	MET
2	B	102	VAL
2	B	106	ASP
2	B	108	VAL
2	B	133	LYS
2	B	134	LYS
2	B	135	ARG
2	B	140	ILE
2	B	178	ASN
2	B	183	GLU
2	B	194	GLU
2	B	199	MET
2	B	208	SER
2	B	222	ILE
2	B	223	VAL
2	B	225	VAL
2	B	234	ILE
2	B	242	SER
2	B	272	THR
2	B	276	ILE
2	B	277	LYS
2	B	278	GLN
2	B	299	GLU
2	B	305	VAL
2	B	323	VAL
2	B	345	LYS
2	B	361	LEU
2	B	366	GLN
2	B	382	ILE
2	B	387	LEU

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Mol	Chain	Res	Type
2	B	393	LYS
2	B	416	LEU
2	B	418	LYS
2	B	426	LYS
2	B	436	VAL
2	B	437	GLU
2	B	451	LYS
2	B	458	LYS
2	B	471	LYS
2	B	485	ARG
2	B	489	SER
2	B	500	THR
2	B	513	GLN
2	B	522	VAL
2	B	537	LYS
2	B	541	LEU
2	B	547	VAL
2	B	549	THR
2	B	567	GLU
2	B	598	GLU
2	B	604	ARG
2	B	612	GLU
2	B	615	MET
2	B	624	LEU
2	B	646	LEU
2	B	653	VAL
2	B	655	LYS
2	B	658	ILE
2	B	690	VAL
2	B	708	GLU
2	B	732	SER
2	B	762	ASN
2	B	780	VAL
2	B	783	THR
2	B	786	ASN
2	B	787	VAL
2	B	815	ARG
2	B	825	VAL
2	B	839	MET
2	B	868	MET
2	B	869	SER
2	B	871	THR

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Mol	Chain	Res	Type
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	881	ASN
2	B	895	ASP
2	B	898	LEU
2	B	916	THR
2	B	935	ARG
2	B	951	GLN
2	B	953	LEU
2	B	956	THR
2	B	963	PHE
2	B	964	VAL
2	B	976	ILE
2	B	983	ARG
2	B	992	ILE
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1010	LEU
2	B	1012	ILE
2	B	1022	THR
2	B	1065	GLN
2	B	1072	MET
2	B	1077	THR
2	B	1080	LYS
2	B	1094	ARG
2	B	1096	ARG
2	B	1099	VAL
2	B	1103	ILE
2	B	1111	MET
2	B	1133	MET
2	B	1147	LEU
2	B	1151	LEU
2	B	1155	SER
2	B	1156	ASP
2	B	1160	VAL
2	B	1178	ASN
2	B	1181	GLU
2	B	1188	LYS
2	B	1189	ILE

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Mol	Chain	Res	Type
2	B	1191	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1210	MET
2	B	1222	ARG
3	C	18	VAL
3	C	23	SER
3	C	34	ARG
3	C	41	ILE
3	C	56	THR
3	C	57	VAL
3	C	66	ARG
3	C	69	LEU
3	C	75	MET
3	C	77	ILE
3	C	79	GLN
3	C	100	THR
3	C	116	LYS
3	C	121	VAL
3	C	125	MET
3	C	129	ILE
3	C	137	LYS
3	C	149	LYS
3	C	186	LEU
3	C	197	SER
3	C	199	LYS
3	C	205	LYS
3	C	215	GLU
3	C	226	ASP
3	C	231	ASN
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	259	LEU
3	C	264	GLN
3	C	267	GLN
4	E	3	GLN
4	E	10	SER
4	E	19	VAL

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Mol	Chain	Res	Type
4	E	30	ILE
4	E	54	GLN
4	E	61	GLN
4	E	67	GLU
4	E	68	SER
4	E	70	SER
4	E	77	SER
4	E	78	LEU
4	E	92	THR
4	E	97	VAL
4	E	100	ILE
4	E	107	THR
4	E	114	ASN
4	E	123	LEU
4	E	127	ILE
4	E	132	ILE
4	E	149	LEU
4	E	158	SER
4	E	162	ARG
4	E	169	ARG
4	E	191	LYS
4	E	201	LYS
4	E	204	THR
5	F	82	THR
5	F	93	ILE
5	F	99	LEU
5	F	111	LEU
5	F	118	LEU
5	F	122	MET
5	F	152	ILE
6	H	15	VAL
6	H	22	LYS
6	H	26	ILE
6	H	34	ASP
6	H	35	GLN
6	H	63	LEU
6	H	86	ASP
6	H	87	ARG
6	H	91	ASP
6	H	106	GLU
6	H	107	VAL
6	H	109	LYS

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Mol	Chain	Res	Type
6	H	110	ASP
6	H	123	MET
6	H	130	ARG
6	H	136	LYS
6	H	139	ASN
7	I	4	PHE
7	I	9	ASP
7	I	21	GLU
7	I	24	ARG
7	I	30	ARG
7	I	31	THR
7	I	35	VAL
7	I	43	VAL
7	I	52	ILE
7	I	55	THR
7	I	59	VAL
7	I	77	LYS
7	I	84	VAL
7	I	92	ARG
7	I	97	MET
7	I	98	VAL
7	I	104	LEU
7	I	111	THR
7	I	119	THR
8	J	1	MET
8	J	2	ILE
8	J	3	VAL
8	J	6	ARG
8	J	9	SER
8	J	13	VAL
8	J	22	LEU
8	J	26	GLN
8	J	31	ASP
8	J	48	ARG
8	J	52	THR
8	J	59	LYS
9	K	6	ARG
9	K	11	LEU
9	K	17	SER
9	K	18	LYS
9	K	26	LYS
9	K	29	ASN

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Mol	Chain	Res	Type
9	K	31	VAL
9	K	42	LEU
9	K	51	LEU
9	K	63	VAL
9	K	78	THR
9	K	101	LEU
9	K	114	LEU
10	L	27	LEU
10	L	30	ILE
10	L	38	LEU
10	L	39	SER
10	L	43	THR
10	L	44	ASP
10	L	47	ARG
10	L	50	ASP
10	L	54	ARG
10	L	55	ILE
10	L	61	THR
10	L	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN
1	A	18	GLN
1	A	68	GLN
1	A	92	HIS
1	A	209	ASN
1	A	225	ASN
1	A	299	HIS
1	A	306	ASN
1	A	339	ASN
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	589	GLN
1	A	631	HIS
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN

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Mol	Chain	Res	Type
1	A	760	GLN
1	A	768	GLN
1	A	786	HIS
1	A	865	GLN
1	A	906	HIS
1	A	926	GLN
1	A	1033	GLN
1	A	1052	GLN
1	A	1085	HIS
1	A	1124	HIS
1	A	1130	GLN
1	A	1140	HIS
1	A	1265	ASN
1	A	1270	ASN
1	A	1364	ASN
1	A	1387	HIS
1	A	1393	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	53	GLN
2	B	121	ASN
2	B	215	GLN
2	B	255	GLN
2	B	366	GLN
2	B	395	GLN
2	B	433	GLN
2	B	449	ASN
2	B	515	HIS
2	B	516	ASN
2	B	648	HIS
2	B	657	HIS
2	B	744	HIS
2	B	762	ASN
2	B	767	ASN
2	B	776	GLN
2	B	784	ASN
2	B	951	GLN
2	B	958	GLN
2	B	984	HIS
2	B	1015	HIS
2	B	1025	HIS
2	B	1074	ASN

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Mol	Chain	Res	Type
2	B	1141	HIS
2	B	1161	HIS
2	B	1176	ASN
2	B	1177	HIS
2	B	1195	HIS
3	C	17	ASN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	131	HIS
3	C	167	HIS
3	C	231	ASN
3	C	242	GLN
4	E	8	ASN
4	E	54	GLN
4	E	113	GLN
4	E	147	HIS
4	E	179	GLN
5	F	78	GLN
6	H	11	GLN
6	H	35	GLN
6	H	131	ASN
7	I	89	GLN
8	J	64	ASN
9	K	29	ASN
9	K	65	HIS
10	L	66	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [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%)	0.32	92 (6%) 25 18	37, 78, 167, 219	0
2	B	1114/1224 (91%)	0.21	79 (7%) 22 16	39, 70, 132, 181	0
3	C	266/318 (83%)	-0.10	0 100 100	46, 65, 106, 158	0
4	E	214/215 (99%)	0.51	13 (6%) 27 20	53, 107, 156, 168	0
5	F	85/155 (54%)	0.19	2 (2%) 59 51	57, 86, 127, 151	0
6	H	133/146 (91%)	0.72	19 (14%) 6 4	68, 112, 147, 158	0
7	I	119/122 (97%)	0.33	7 (5%) 28 21	53, 84, 122, 136	0
8	J	65/70 (92%)	-0.11	2 (3%) 51 43	44, 60, 95, 105	0
9	K	114/120 (95%)	-0.10	2 (1%) 67 61	42, 73, 96, 113	0
10	L	46/70 (65%)	1.40	13 (28%) 1 1	56, 101, 135, 144	0
11	R	6/6 (100%)	0.03	0 100 100	66, 78, 114, 130	0
12	T	13/29 (44%)	1.09	2 (15%) 5 4	84, 103, 163, 171	0
All	All	3580/4208 (85%)	0.27	231 (6%) 25 18	37, 77, 150, 219	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	8.8
1	A	250	ILE	6.8
2	B	715	ALA	6.7
1	A	65	LEU	6.5
2	B	882	THR	6.4
10	L	27	LEU	6.0
6	H	63	LEU	5.9
1	A	1091	SER	5.9
1	A	1087	ALA	5.5
1	A	1086	PHE	5.3
1	A	1081	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
2	B	446	LEU	5.1
1	A	1090	ALA	5.1
2	B	70	ILE	5.0
2	B	477	ALA	4.9
2	B	502	ILE	4.9
1	A	252	PHE	4.8
6	H	85	GLY	4.7
2	B	708	GLU	4.7
1	A	1083	THR	4.7
1	A	199	LEU	4.7
2	B	250	PHE	4.5
2	B	335	GLY	4.5
2	B	474	SER	4.5
1	A	154	SER	4.4
2	B	709	ASP	4.4
1	A	319	GLY	4.3
1	A	179	LEU	4.3
10	L	55	ILE	4.3
2	B	881	ASN	4.2
2	B	933	SER	4.1
1	A	161	LEU	4.1
10	L	28	LYS	4.0
1	A	103	CYS	4.0
2	B	447	ALA	3.9
2	B	1173	ALA	3.9
1	A	201	VAL	3.9
2	B	137	TYR	3.9
1	A	1176	LEU	3.8
2	B	712	PRO	3.8
10	L	25	ALA	3.8
6	H	132	LEU	3.8
1	A	1243	VAL	3.7
1	A	1085	HIS	3.7
1	A	141	LEU	3.7
1	A	567	LYS	3.7
1	A	69	THR	3.6
1	A	49	LYS	3.6
1	A	1088	GLY	3.6
2	B	887	HIS	3.6
1	A	1002	GLY	3.6
6	H	136	LYS	3.5
6	H	83	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	509	ALA	3.5
1	A	1089	VAL	3.5
10	L	26	THR	3.5
1	A	128	ILE	3.5
1	A	310	GLY	3.5
9	K	114	LEU	3.5
2	B	473	MET	3.4
10	L	40	LEU	3.4
2	B	1224	PHE	3.4
1	A	312	PRO	3.4
5	F	72	LYS	3.4
2	B	478	GLY	3.3
2	B	647	GLY	3.3
2	B	140	ILE	3.3
1	A	314	ALA	3.3
2	B	646	LEU	3.3
1	A	51	GLY	3.3
1	A	1082	ASN	3.3
6	H	89	LEU	3.3
6	H	139	ASN	3.3
2	B	865	LYS	3.3
4	E	103	LYS	3.3
6	H	130	ARG	3.3
2	B	246	LYS	3.2
2	B	866	TYR	3.2
1	A	144	THR	3.2
1	A	318	SER	3.1
1	A	147	VAL	3.1
10	L	50	ASP	3.1
2	B	879	ARG	3.1
10	L	42	ARG	3.1
2	B	962	LYS	3.1
7	I	117	LYS	3.1
2	B	645	SER	3.1
2	B	867	GLY	3.1
1	A	1445	ILE	3.1
4	E	95	THR	3.1
1	A	1173	HIS	3.0
1	A	316	GLN	3.0
7	I	60	GLN	3.0
1	A	66	LYS	3.0
2	B	880	THR	3.0

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Mol	Chain	Res	Type	RSRZ
10	L	45	ALA	3.0
1	A	1123	GLY	3.0
2	B	486	TYR	3.0
7	I	49	ILE	3.0
2	B	786	ASN	3.0
2	B	472	ALA	3.0
1	A	132	LYS	2.9
1	A	323	LYS	2.9
1	A	1092	LYS	2.9
6	H	135	LEU	2.9
2	B	734	HIS	2.9
6	H	86	ASP	2.9
12	T	27	DA	2.9
2	B	935	ARG	2.9
2	B	733	HIS	2.9
5	F	73	ALA	2.8
1	A	998	LEU	2.8
6	H	84	ALA	2.8
2	B	878	GLN	2.8
1	A	105	CYS	2.8
4	E	101	GLN	2.8
2	B	711	GLU	2.8
1	A	30	ILE	2.8
1	A	1187	GLN	2.7
2	B	648	HIS	2.7
8	J	1	MET	2.7
1	A	145	LYS	2.7
1	A	108	MET	2.7
1	A	317	LYS	2.6
2	B	870	ILE	2.6
9	K	15	GLY	2.6
1	A	44	THR	2.6
2	B	277	LYS	2.6
2	B	436	VAL	2.6
2	B	1214	PRO	2.6
1	A	50	ILE	2.6
2	B	475	SER	2.6
1	A	286	HIS	2.6
1	A	186	LYS	2.6
12	T	28	DT	2.6
10	L	64	LEU	2.6
1	A	1254	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1257	ASP	2.6
1	A	181	LEU	2.5
1	A	1084	PHE	2.5
1	A	126	LEU	2.5
1	A	180	LYS	2.5
1	A	289	ILE	2.5
2	B	731	VAL	2.5
4	E	3	GLN	2.5
7	I	4	PHE	2.5
8	J	65	PRO	2.5
1	A	182	VAL	2.4
1	A	1174	PHE	2.4
2	B	138	GLU	2.4
4	E	96	PHE	2.4
1	A	237	THR	2.4
2	B	448	ILE	2.4
6	H	90	ALA	2.4
10	L	53	HIS	2.4
2	B	244	LEU	2.4
2	B	608	ASP	2.4
1	A	251	SER	2.4
1	A	295	LEU	2.4
1	A	1172	LEU	2.4
2	B	476	ARG	2.3
2	B	531	GLN	2.3
2	B	868	MET	2.3
1	A	1080	THR	2.3
4	E	102	GLU	2.3
2	B	737	THR	2.3
1	A	830	LYS	2.3
2	B	888	GLY	2.3
1	A	114	LEU	2.3
2	B	67	SER	2.3
2	B	919	SER	2.3
4	E	98	ILE	2.3
1	A	162	VAL	2.3
7	I	120	GLN	2.3
10	L	37	LYS	2.3
2	B	136	THR	2.3
10	L	46	VAL	2.3
4	E	50	MET	2.2
1	A	315	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	210	ILE	2.2
2	B	918	ILE	2.2
2	B	249	ARG	2.2
6	H	82	PRO	2.2
7	I	2	THR	2.2
7	I	3	THR	2.2
2	B	266	ALA	2.2
1	A	78	PRO	2.2
6	H	62	SER	2.2
1	A	45	GLN	2.2
2	B	469	GLN	2.2
6	H	19	ARG	2.2
2	B	106	ASP	2.2
6	H	91	ASP	2.2
4	E	90	VAL	2.2
1	A	146	MET	2.2
4	E	49	SER	2.2
4	E	110	PHE	2.2
2	B	108	VAL	2.1
1	A	55	ASP	2.1
1	A	411	ASP	2.1
2	B	141	ASP	2.1
2	B	1170	THR	2.1
6	H	76	THR	2.1
2	B	1204	PHE	2.1
2	B	357	GLN	2.1
1	A	122	MET	2.1
2	B	345	LYS	2.1
1	A	116	ASP	2.1
1	A	59	GLY	2.1
2	B	429	PHE	2.1
6	H	107	VAL	2.1
1	A	111	GLY	2.1
2	B	735	ALA	2.1
2	B	1183	LYS	2.1
1	A	255	SER	2.0
1	A	216	VAL	2.0
1	A	1122	PRO	2.0
1	A	1158	PRO	2.0
1	A	165	GLY	2.0
2	B	201	GLY	2.0
1	A	149	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	194	GLU	2.0
4	E	152	LYS	2.0
1	A	152	VAL	2.0
2	B	1189	ILE	2.0
4	E	117	THR	2.0
1	A	212	LYS	2.0
1	A	217	LYS	2.0
1	A	1093	LYS	2.0
2	B	1217	TYR	2.0
6	H	129	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	ZN	A	1734	1/1	0.89	0.09	220,220,220,220	0
13	ZN	B	1307	1/1	0.97	0.05	123,123,123,123	0
13	ZN	A	1735	1/1	0.98	0.05	106,106,106,106	0
13	ZN	I	203	1/1	0.99	0.04	102,102,102,102	0
13	ZN	I	204	1/1	0.99	0.02	60,60,60,60	0
14	MG	A	2001	1/1	0.99	0.05	55,55,55,55	0
13	ZN	J	101	1/1	1.00	0.02	57,57,57,57	0
13	ZN	L	105	1/1	1.00	0.02	95,95,95,95	0
13	ZN	C	319	1/1	1.00	0.02	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.