



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:45 PM EDT

PDB ID : 4A3G / pdb_00004a3g
Title : RNA Polymerase II initial transcribing complex with a 2nt DNA-RNA hybrid
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on : 2011-09-30
Resolution : 3.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

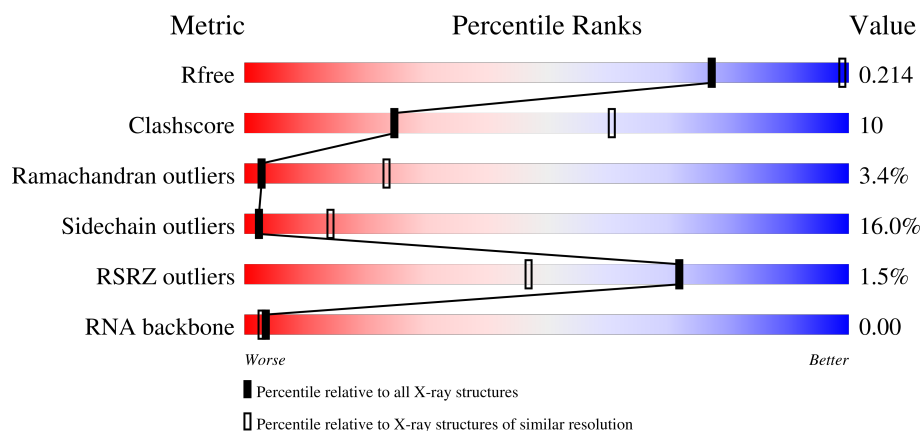
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



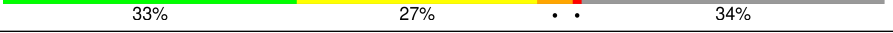
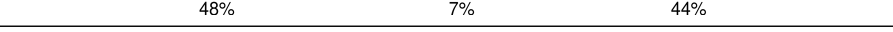
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	1732	2% 51% 24% 6% 18%
2	B	1224	2% 56% 28% 7% 9%
3	C	318	51% 27% 6% 16%
4	D	221	3% 52% 22% 7% 19%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	2	
15	T	27	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31728 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	1422	Total	C	N	O	S	0	0	0
			11174	7037	1954	2121	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8859	5609	1554	1641	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 POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

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

- Molecule 13 is a DNA chain called NON TEMPLATE DNA 5'-D(*GP*GP*CP*AP*CP*AP*AP*CP*TP*GP*CP *GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	9	Total	C	N	O	P	0	0	0
			181	87	36	50	8			

- Molecule 14 is a RNA chain called TRANSCRIPT RNA 5'-R(*CP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	2	Total	C	N	O	P	0	0	0
			42	19	8	13	2			

- Molecule 15 is a DNA chain called TEMPLATE DNA 5'-D(*AP*GP*CP*GP*CP*AP*GP*TP*TP*GP*TP*GP *CP*TP*AP*TP*GP*AP*BRUP*AP*TP*TP*TP*TP*TP*AP*D T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	15	Total	Br	C	N	O	P	0	0	0
			309	1	147	53	93	15			

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total	Zn	0	0
			2	2		
16	B	1	Total	Zn	0	0
			1	1		
16	C	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	J	1	Total	Zn	0	0
			1	1		
16	L	1	Total	Zn	0	0
			1	1		

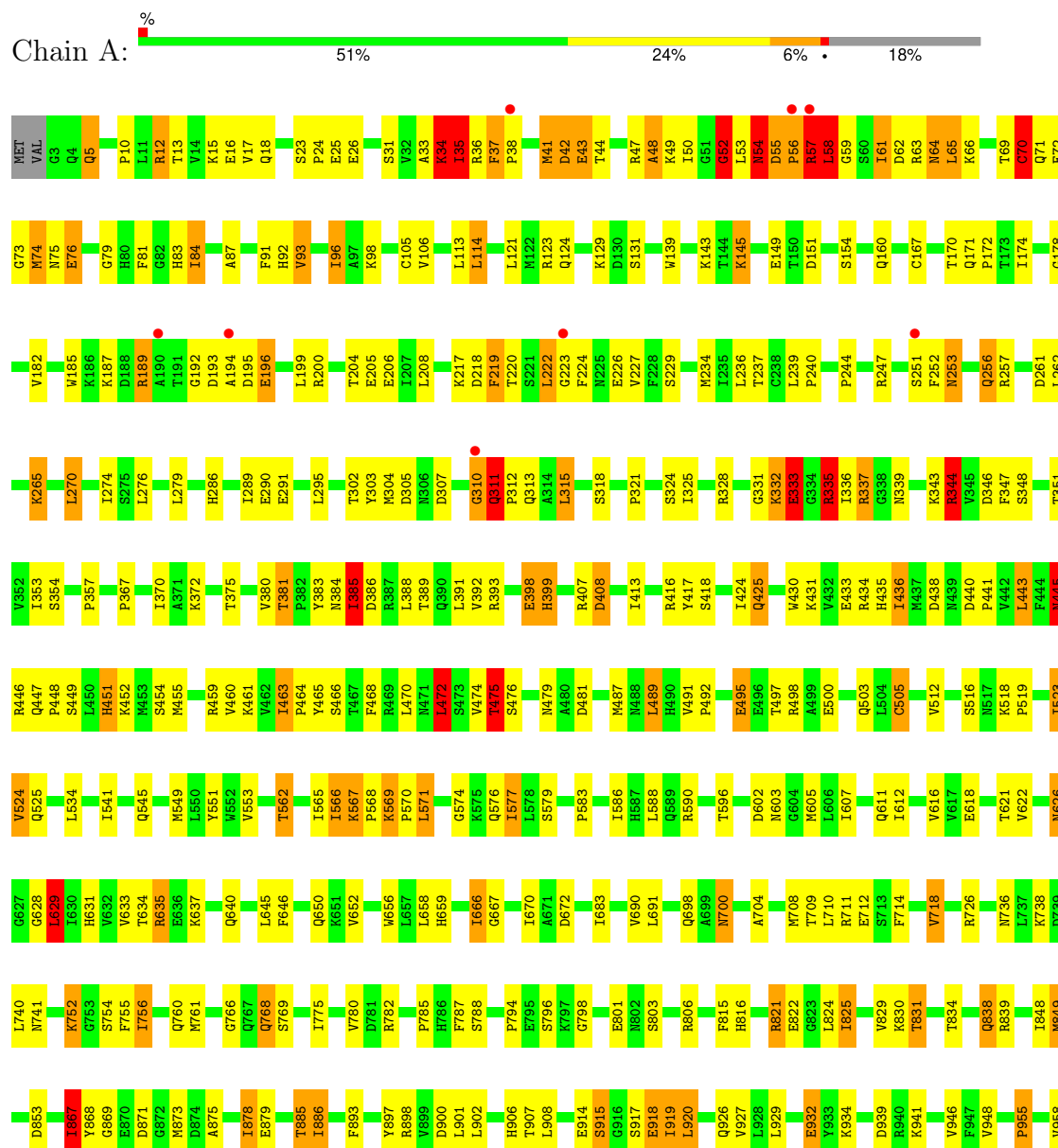
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

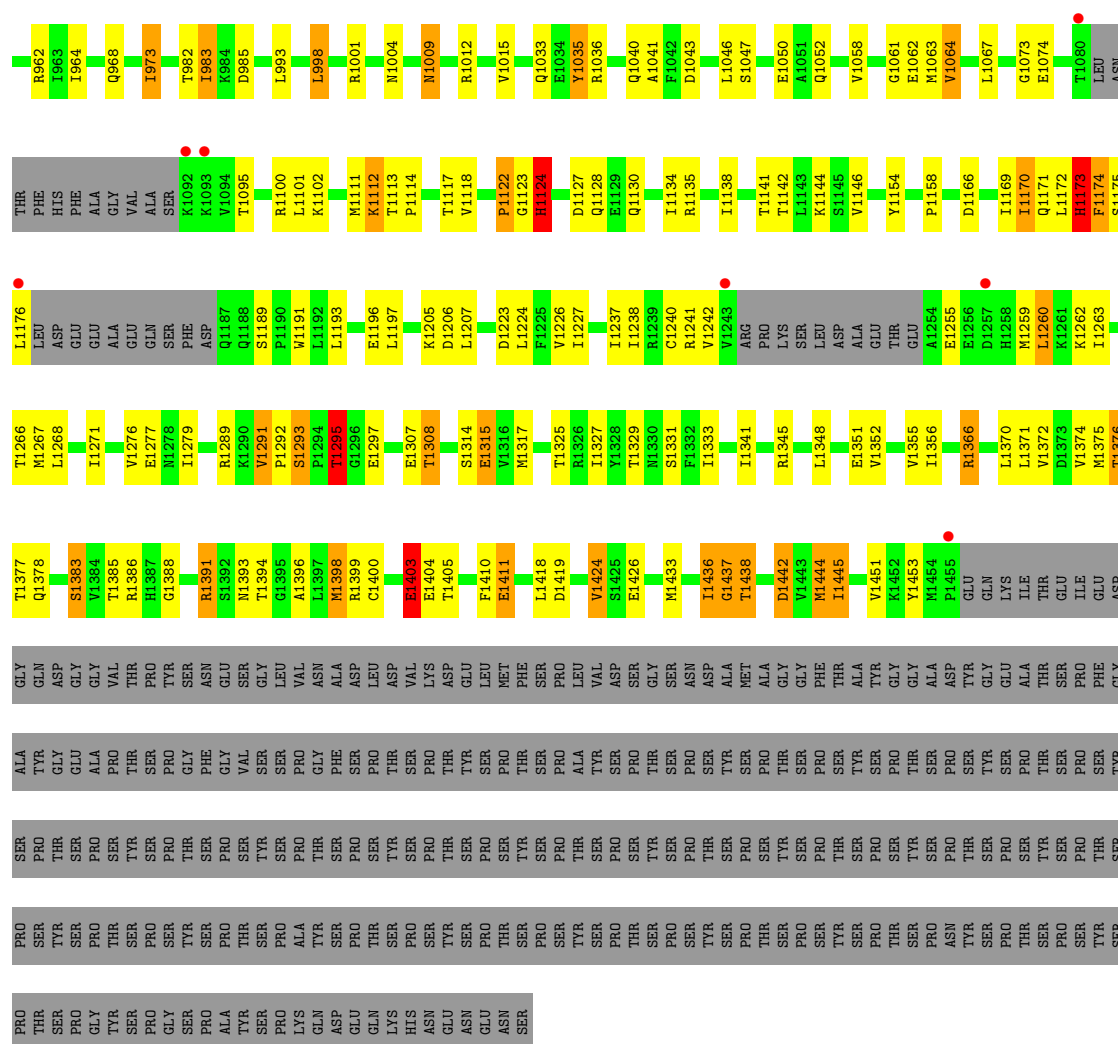
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots [i](#)

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

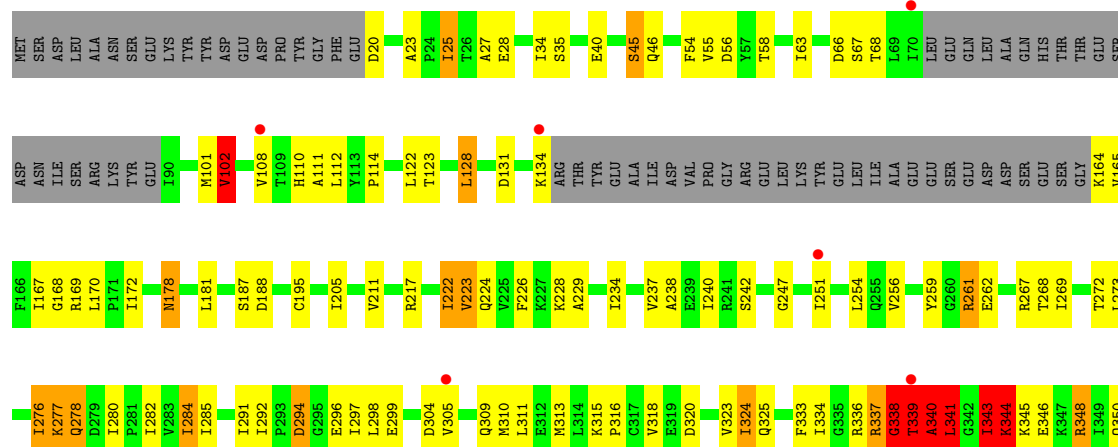
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



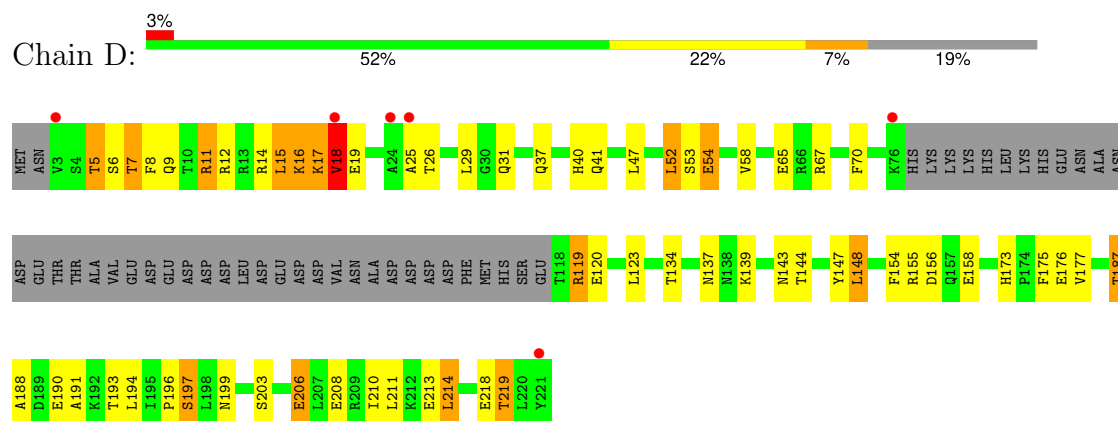


• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

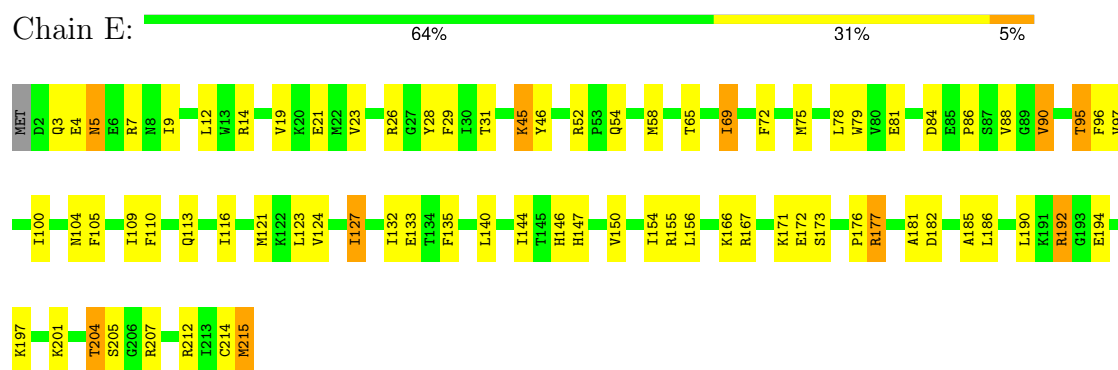
Chain B: 2% 56% 28% 7% 9%



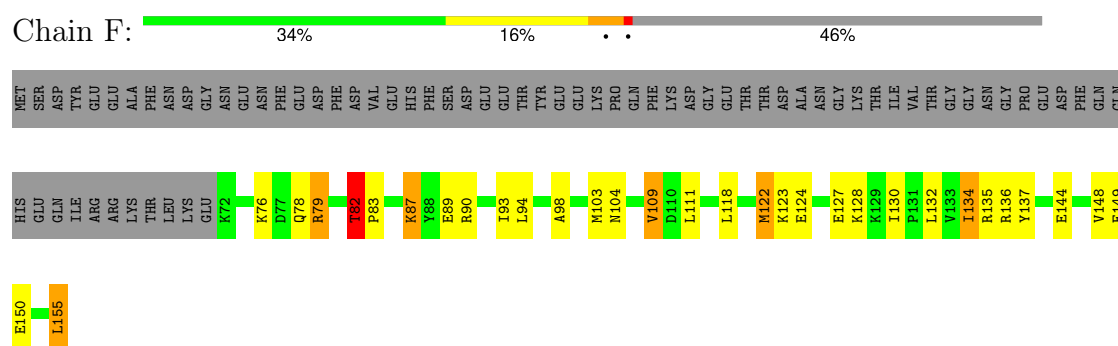
- Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4



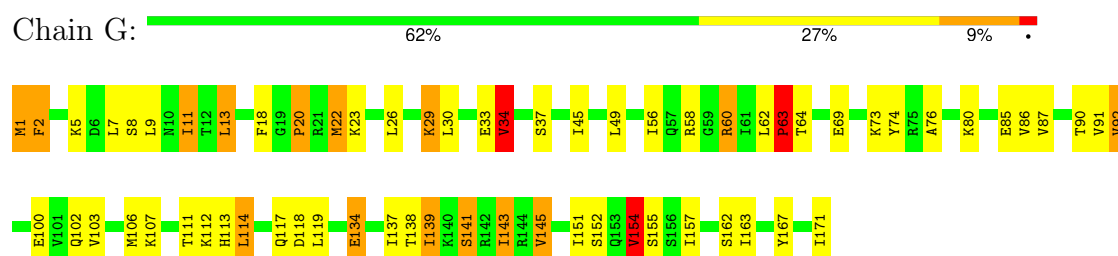
● Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



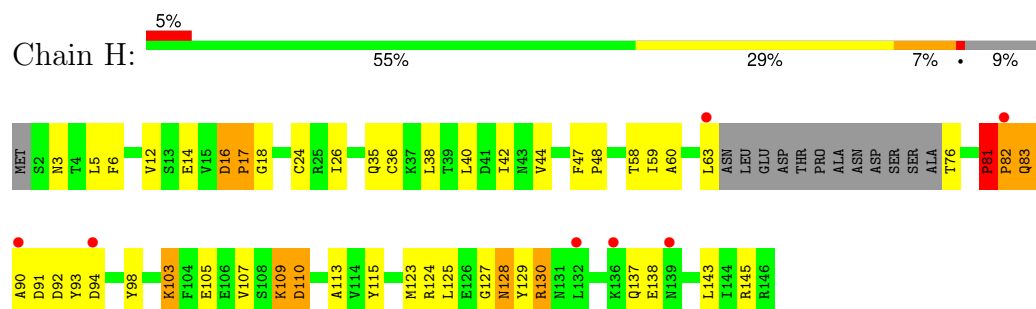
● Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



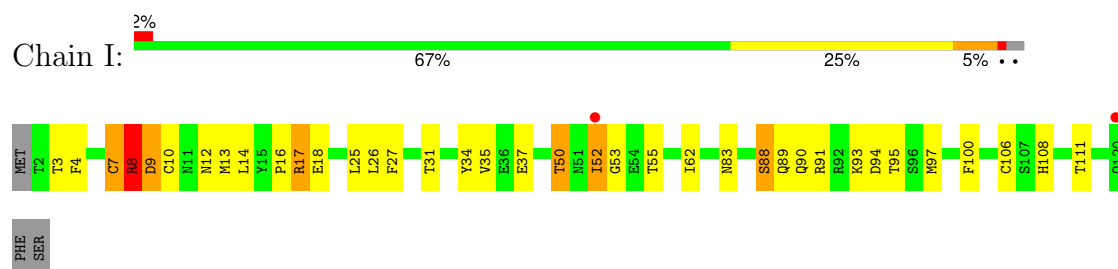
- Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7



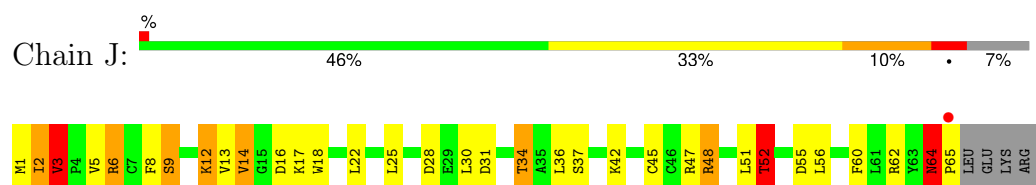
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



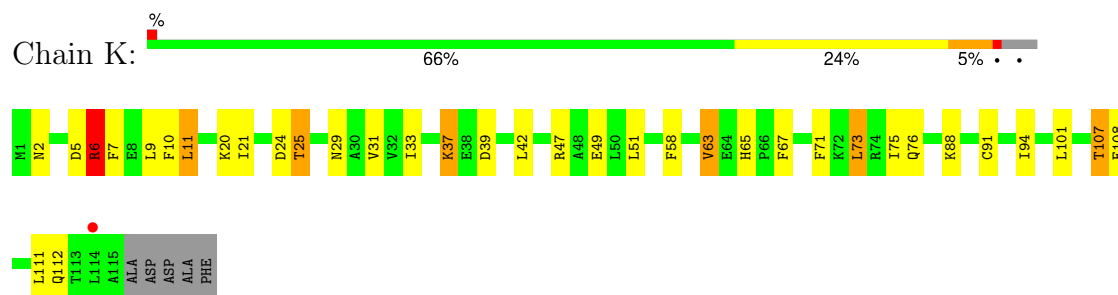
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



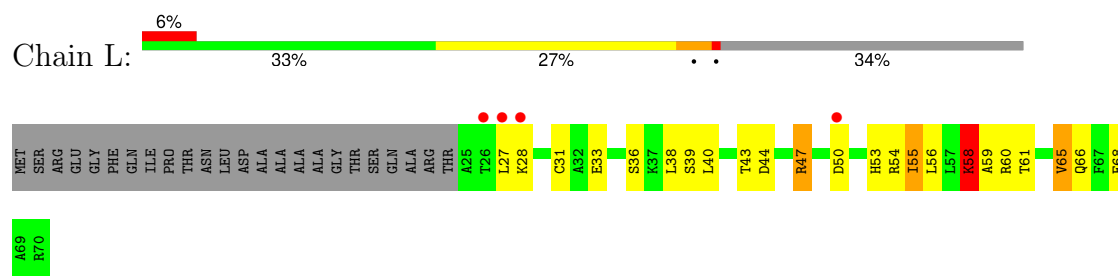
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



• Molecule 13: NON TEMPLATE DNA 5'-D(*GP*GP*CP*AP*CP*AP*AP*CP*TP*GP*CP*GP*CP*TP)-3'



- Molecule 14: TRANSCRIPT RNA 5'-R(*CP*AP)-3'



- Molecule 15: TEMPLATE DNA 5'-D(*AP*GP*CP*GP*CP*AP*GP*TP*TP*GP*TP*GP *C
P*TP*AP*TP*GP*AP*BRUP*AP*TP*TP*TP*TP*TP*AP*DT)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.67Å 394.13Å 282.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 3.50 49.27 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.27-3.50) 99.9 (49.27-3.50)	Depositor EDS
R_{merge}	0.96	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.166 , 0.194 0.187 , 0.214	Depositor DCC
R_{free} test set	3045 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	103.7	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 113.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.036 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.043 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31728	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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, BRU

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	0.91	4/11374 (0.0%)	1.56	145/15383 (0.9%)
2	B	0.89	3/9029 (0.0%)	1.49	88/12171 (0.7%)
3	C	0.86	2/2133 (0.1%)	1.47	25/2891 (0.9%)
4	D	0.87	2/1444 (0.1%)	1.62	17/1935 (0.9%)
5	E	0.82	0/1788	1.49	18/2406 (0.7%)
6	F	0.97	0/691	1.46	8/933 (0.9%)
7	G	0.87	1/1368 (0.1%)	1.42	10/1844 (0.5%)
8	H	0.86	0/1086	1.42	15/1470 (1.0%)
9	I	0.80	0/989	1.36	7/1331 (0.5%)
10	J	0.99	0/541	1.74	8/727 (1.1%)
11	K	0.80	0/938	1.39	9/1267 (0.7%)
12	L	0.96	0/365	1.69	6/485 (1.2%)
13	N	0.56	0/203	0.69	0/311
14	P	1.22	1/46 (2.2%)	0.73	0/69
15	T	0.50	0/323	0.61	0/497
All	All	0.88	13/32318 (0.0%)	1.50	356/43720 (0.8%)

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
1	A	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	25	ALA	CA-C	7.98	1.62	1.53
1	A	54	ASN	CA-C	7.52	1.62	1.52
7	G	1	MET	C-N	6.68	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	9	C	C1'-N1	6.37	1.58	1.48
1	A	867	ILE	CG1-CD1	6.08	1.75	1.51
2	B	817	LEU	CA-C	5.63	1.59	1.52
2	B	1107	ALA	CA-C	-5.53	1.47	1.53
3	C	148	ARG	CA-C	5.51	1.56	1.52
2	B	990	ILE	CA-C	5.38	1.58	1.53
1	A	56	PRO	CA-C	5.32	1.59	1.52
4	D	18	VAL	CA-C	5.31	1.59	1.52
1	A	1398	MET	SD-CE	5.28	1.92	1.79
3	C	115	SER	CA-C	5.07	1.59	1.52

All (356) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	THR	N-CA-C	-12.50	95.31	112.30
4	D	25	ALA	CA-C-N	10.87	140.28	122.14
4	D	25	ALA	C-N-CA	10.87	140.28	122.14
3	C	39	ALA	N-CA-C	10.45	123.65	111.11
1	A	34	LYS	CA-C-N	10.34	140.58	121.97
1	A	34	LYS	C-N-CA	10.34	140.58	121.97
7	G	34	VAL	N-CA-C	10.18	121.00	110.62
8	H	92	ASP	N-CA-C	-9.91	98.42	111.71
4	D	54	GLU	N-CA-C	-9.79	100.60	111.07
12	L	55	ILE	N-CA-CB	9.45	121.98	110.64
1	A	42	ASP	CA-CB-CG	9.14	121.74	112.60
1	A	56	PRO	CA-C-N	8.96	138.65	121.54
1	A	56	PRO	C-N-CA	8.96	138.65	121.54
2	B	296	GLU	N-CA-C	-8.93	100.03	112.45
10	J	5	VAL	N-CA-C	-8.90	97.10	109.21
1	A	64	ASN	N-CA-C	-8.86	97.75	110.59
2	B	976	ILE	N-CA-C	8.78	118.85	110.42
10	J	14	VAL	CB-CA-C	8.36	118.97	110.70
1	A	886	ILE	N-CA-C	8.29	119.06	110.36
1	A	218	ASP	CA-CB-CG	8.21	120.81	112.60
5	E	9	ILE	N-CA-C	-8.19	103.28	110.74
3	C	38	ILE	CA-C-N	8.04	131.40	120.54
3	C	38	ILE	C-N-CA	8.04	131.40	120.54
8	H	81	PRO	N-CA-C	8.03	120.50	110.70
10	J	55	ASP	CA-CB-CG	8.03	120.63	112.60
1	A	223	GLY	CA-C-N	7.96	134.32	120.87
1	A	223	GLY	C-N-CA	7.96	134.32	120.87
4	D	31	GLN	N-CA-C	-7.93	101.94	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	PHE	N-CA-C	7.88	120.75	110.43
1	A	1419	ASP	CA-C-N	7.75	131.00	120.38
1	A	1419	ASP	C-N-CA	7.75	131.00	120.38
1	A	54	ASN	CA-CB-CG	7.72	120.32	112.60
2	B	1013	ASN	N-CA-C	7.65	119.29	109.65
8	H	138	GLU	N-CA-C	-7.64	103.21	112.54
2	B	1121	GLY	CA-C-N	7.49	130.65	120.54
2	B	1121	GLY	C-N-CA	7.49	130.65	120.54
2	B	628	THR	CA-C-N	7.46	135.78	121.54
2	B	628	THR	C-N-CA	7.46	135.78	121.54
1	A	57	ARG	CA-C-N	7.45	135.77	121.54
1	A	57	ARG	C-N-CA	7.45	135.77	121.54
2	B	1122	ARG	CA-C-N	7.39	130.52	120.54
2	B	1122	ARG	C-N-CA	7.39	130.52	120.54
2	B	882	THR	N-CA-C	7.38	119.40	111.36
12	L	53	HIS	N-CA-C	7.30	119.73	110.24
2	B	339	THR	CA-C-N	7.29	135.47	121.54
2	B	339	THR	C-N-CA	7.29	135.47	121.54
4	D	7	THR	CA-C-N	7.26	130.59	120.29
4	D	7	THR	C-N-CA	7.26	130.59	120.29
1	A	1333	ILE	N-CA-C	-7.23	103.25	110.62
1	A	629	LEU	N-CA-C	-7.22	103.41	111.28
1	A	35	ILE	CB-CA-C	7.21	123.12	111.29
1	A	1112	LYS	N-CA-C	7.18	118.80	110.97
12	L	58	LYS	N-CA-C	7.14	121.44	112.87
1	A	399	HIS	N-CA-CB	7.11	123.03	110.37
1	A	194	ALA	CA-C-N	7.09	134.47	121.70
1	A	194	ALA	C-N-CA	7.09	134.47	121.70
4	D	26	THR	CA-C-N	7.07	132.47	122.08
4	D	26	THR	C-N-CA	7.07	132.47	122.08
1	A	47	ARG	CA-C-N	7.04	134.99	121.54
1	A	47	ARG	C-N-CA	7.04	134.99	121.54
9	I	93	LYS	CA-C-N	6.97	129.93	120.38
9	I	93	LYS	C-N-CA	6.97	129.93	120.38
1	A	69	THR	CA-C-N	6.96	134.84	121.54
1	A	69	THR	C-N-CA	6.96	134.84	121.54
2	B	294	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	998	LEU	N-CA-C	6.88	119.78	109.25
1	A	219	PHE	CA-CB-CG	6.84	120.64	113.80
12	L	55	ILE	N-CA-C	6.83	116.96	110.74
2	B	1177	HIS	N-CA-C	-6.80	104.72	113.16
4	D	188	ALA	N-CA-C	-6.79	103.94	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	128	ASN	CA-CB-CG	6.78	119.38	112.60
4	D	37	GLN	N-CA-C	6.71	118.33	108.86
6	F	82	THR	CB-CA-C	-6.71	98.92	109.52
5	E	5	ASN	N-CA-C	-6.69	103.15	112.45
1	A	35	ILE	N-CA-CB	6.68	122.26	111.23
10	J	9	SER	N-CA-C	6.67	118.24	110.97
3	C	62	PHE	CA-C-N	6.63	128.92	120.56
3	C	62	PHE	C-N-CA	6.63	128.92	120.56
1	A	1403	GLU	N-CA-C	6.59	124.84	110.80
1	A	1207	LEU	N-CA-C	6.56	119.86	109.50
1	A	23	SER	N-CA-C	-6.51	101.58	109.72
2	B	188	ASP	CA-CB-CG	6.47	119.07	112.60
5	E	95	THR	CA-C-N	6.45	128.83	120.44
5	E	95	THR	C-N-CA	6.45	128.83	120.44
10	J	52	THR	CB-CA-C	6.45	121.86	110.37
1	A	311	GLN	N-CA-C	6.45	124.05	109.81
1	A	1138	ILE	N-CA-C	6.44	117.35	111.81
5	E	171	LYS	N-CA-C	-6.44	99.72	109.95
2	B	818	PRO	N-CA-C	6.40	120.17	111.22
2	B	530	GLY	CA-C-N	6.37	130.89	120.63
2	B	530	GLY	C-N-CA	6.37	130.89	120.63
1	A	425	GLN	CA-C-N	6.36	129.74	120.71
1	A	425	GLN	C-N-CA	6.36	129.74	120.71
5	E	96	PHE	CA-CB-CG	6.34	120.14	113.80
1	A	1404	GLU	N-CA-C	6.34	121.82	113.20
8	H	129	TYR	N-CA-C	6.32	119.15	111.82
2	B	1181	GLU	N-CA-C	6.27	124.15	110.80
5	E	172	GLU	CA-C-N	6.24	128.55	120.44
5	E	172	GLU	C-N-CA	6.24	128.55	120.44
1	A	505	CYS	N-CA-C	6.24	120.49	112.26
1	A	1403	GLU	CA-C-N	-6.21	111.06	122.31
1	A	1403	GLU	C-N-CA	-6.21	111.06	122.31
3	C	85	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	70	CYS	CA-C-N	-6.20	111.70	122.36
1	A	70	CYS	C-N-CA	-6.20	111.70	122.36
1	A	91	PHE	CA-CB-CG	6.19	119.99	113.80
1	A	551	TYR	CA-C-N	6.17	129.17	120.28
1	A	551	TYR	C-N-CA	6.17	129.17	120.28
1	A	472	LEU	N-CA-C	6.16	118.79	111.71
2	B	45	SER	CA-C-N	6.15	128.84	120.54
2	B	45	SER	C-N-CA	6.15	128.84	120.54
1	A	914	GLU	CA-C-N	6.14	129.12	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	914	GLU	C-N-CA	6.14	129.12	120.28
4	D	173	HIS	CB-CA-C	6.13	118.27	109.26
2	B	890	TYR	N-CA-C	-6.11	105.83	113.28
1	A	885	THR	CA-C-N	6.10	128.46	120.60
1	A	885	THR	C-N-CA	6.10	128.46	120.60
2	B	1155	SER	CA-C-N	6.07	133.13	121.54
2	B	1155	SER	C-N-CA	6.07	133.13	121.54
2	B	359	GLU	N-CA-C	6.05	120.39	112.89
1	A	900	ASP	CA-CB-CG	6.04	118.64	112.60
8	H	16	ASP	N-CA-C	6.03	120.27	107.91
1	A	310	GLY	CA-C-N	6.01	136.46	121.80
1	A	310	GLY	C-N-CA	6.01	136.46	121.80
2	B	964	VAL	N-CA-C	6.01	117.34	108.45
2	B	998	ASP	CA-CB-CG	5.99	118.59	112.60
2	B	454	THR	CA-C-N	5.95	128.17	120.44
2	B	454	THR	C-N-CA	5.95	128.17	120.44
1	A	344	ARG	N-CA-C	-5.94	99.59	109.46
1	A	17	VAL	N-CA-CB	5.93	119.32	112.15
1	A	1043	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	1061	GLY	N-CA-C	-5.91	107.25	113.58
1	A	123	ARG	CA-C-N	5.91	128.48	120.44
1	A	123	ARG	C-N-CA	5.91	128.48	120.44
1	A	346	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	70	CYS	N-CA-C	-5.89	98.25	110.80
2	B	343	ILE	CA-C-N	5.89	132.78	121.54
2	B	343	ILE	C-N-CA	5.89	132.78	121.54
3	C	194	GLU	N-CA-C	-5.88	106.75	114.04
2	B	561	TRP	N-CA-C	5.87	120.57	113.17
1	A	853	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	897	TYR	N-CA-C	5.86	120.47	112.68
2	B	647	GLY	N-CA-C	5.85	118.65	111.45
2	B	1018	PRO	N-CA-C	5.85	121.84	113.47
11	K	25	THR	CA-C-N	5.84	128.91	120.38
11	K	25	THR	C-N-CA	5.84	128.91	120.38
1	A	1436	ILE	N-CA-CB	-5.84	103.31	111.25
5	E	182	ASP	CA-CB-CG	5.84	118.44	112.60
2	B	883	LEU	CA-C-N	5.83	130.17	122.06
2	B	883	LEU	C-N-CA	5.83	130.17	122.06
7	G	141	SER	N-CA-C	5.83	118.52	110.35
8	H	110	ASP	N-CA-C	-5.83	106.16	113.28
1	A	52	GLY	CA-C-N	5.83	131.91	122.29
1	A	52	GLY	C-N-CA	5.83	131.91	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	128	ASN	CA-C-N	5.82	129.16	120.31
8	H	128	ASN	C-N-CA	5.82	129.16	120.31
2	B	366	GLN	N-CA-C	-5.82	106.16	113.72
1	A	463	ILE	N-CA-C	5.82	114.29	107.84
1	A	825	ILE	N-CA-CB	5.81	117.61	110.64
2	B	338	GLY	CA-C-N	5.81	132.15	121.70
2	B	338	GLY	C-N-CA	5.81	132.15	121.70
3	C	40	GLU	N-CA-C	5.80	121.07	113.30
3	C	257	SER	CA-C-N	5.78	128.63	120.42
3	C	257	SER	C-N-CA	5.78	128.63	120.42
2	B	1166	CYS	N-CA-C	-5.77	101.08	110.20
2	B	68	THR	CB-CA-C	5.77	116.90	109.80
2	B	880	THR	CA-C-N	5.77	132.56	121.54
2	B	880	THR	C-N-CA	5.77	132.56	121.54
3	C	108	GLU	N-CA-C	-5.76	105.08	111.36
10	J	14	VAL	CA-C-N	5.76	126.33	119.94
10	J	14	VAL	C-N-CA	5.76	126.33	119.94
1	A	794	PRO	CA-C-N	5.71	127.87	120.44
1	A	794	PRO	C-N-CA	5.71	127.87	120.44
2	B	340	ALA	N-CA-C	-5.71	98.64	110.80
7	G	117	GLN	CA-C-N	5.71	128.50	120.28
7	G	117	GLN	C-N-CA	5.71	128.50	120.28
5	E	96	PHE	CA-C-N	5.71	127.75	120.56
5	E	96	PHE	C-N-CA	5.71	127.75	120.56
2	B	1028	GLU	CB-CG-CD	5.70	122.29	112.60
1	A	398	GLU	CA-C-O	-5.70	115.35	121.56
2	B	681	TRP	N-CA-C	-5.69	104.46	111.40
2	B	340	ALA	CA-C-N	5.67	132.38	121.54
2	B	340	ALA	C-N-CA	5.67	132.38	121.54
7	G	154	VAL	CA-C-N	5.67	132.06	122.65
7	G	154	VAL	C-N-CA	5.67	132.06	122.65
1	A	408	ASP	N-CA-C	-5.67	105.25	111.82
1	A	331	GLY	CA-C-N	5.66	132.36	121.54
1	A	331	GLY	C-N-CA	5.66	132.36	121.54
2	B	581	PHE	CA-CB-CG	5.65	119.45	113.80
1	A	466	SER	N-CA-C	5.65	119.87	113.15
6	F	104	ASN	CA-CB-CG	5.64	118.25	112.60
1	A	143	LYS	CA-C-N	5.62	128.08	120.44
1	A	143	LYS	C-N-CA	5.62	128.08	120.44
2	B	1222	ARG	N-CA-C	5.61	119.88	111.96
10	J	64	ASN	N-CA-C	5.61	122.20	109.81
1	A	445	ASN	CA-CB-CG	5.61	118.20	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	GLU	CA-C-N	5.60	127.72	120.44
1	A	495	GLU	C-N-CA	5.60	127.72	120.44
2	B	1180	PHE	CA-CB-CG	-5.60	108.20	113.80
8	H	138	GLU	CB-CG-CD	5.59	122.11	112.60
2	B	1129	ARG	N-CA-C	5.59	117.81	109.59
1	A	154	SER	N-CA-C	5.58	117.49	110.24
1	A	451	HIS	CA-C-N	5.57	129.18	120.82
1	A	451	HIS	C-N-CA	5.57	129.18	120.82
2	B	320	ASP	CA-CB-CG	5.57	118.17	112.60
2	B	736	THR	N-CA-C	-5.56	106.16	113.17
7	G	18	PHE	CA-CB-CG	5.55	119.36	113.80
3	C	60	ASP	CA-CB-CG	5.54	118.14	112.60
9	I	8	ARG	N-CA-C	-5.54	101.65	109.96
1	A	244	PRO	N-CA-C	5.54	117.45	110.70
1	A	898	ARG	N-CA-C	5.53	118.37	110.24
2	B	242	SER	N-CA-C	5.52	117.23	108.67
2	B	807	ARG	N-CA-C	-5.52	105.42	111.82
11	K	6	ARG	N-CA-C	5.50	119.10	112.38
1	A	637	LYS	N-CA-C	5.50	119.16	112.23
2	B	1146	PHE	CA-C-N	5.50	127.65	120.28
2	B	1146	PHE	C-N-CA	5.50	127.65	120.28
1	A	256	GLN	N-CA-C	5.50	118.05	108.76
1	A	5	GLN	N-CA-C	5.48	117.95	110.55
5	E	177	ARG	N-CA-C	5.48	118.63	110.14
1	A	26	GLU	CA-C-N	5.47	127.65	120.60
1	A	26	GLU	C-N-CA	5.47	127.65	120.60
2	B	102	VAL	N-CA-C	5.46	115.72	107.80
2	B	1144	ALA	N-CA-C	5.46	117.66	111.11
4	D	120	GLU	N-CA-C	-5.46	104.97	111.69
2	B	943	SER	CA-C-N	5.46	128.61	120.31
2	B	943	SER	C-N-CA	5.46	128.61	120.31
8	H	83	GLN	CA-C-N	5.46	131.96	121.54
8	H	83	GLN	C-N-CA	5.46	131.96	121.54
1	A	35	ILE	CA-C-N	5.45	131.96	121.54
1	A	35	ILE	C-N-CA	5.45	131.96	121.54
3	C	214	ASN	CA-C-N	5.45	128.99	120.82
3	C	214	ASN	C-N-CA	5.45	128.99	120.82
1	A	718	VAL	CA-C-N	5.44	127.62	120.60
1	A	718	VAL	C-N-CA	5.44	127.62	120.60
11	K	63	VAL	N-CA-CB	5.44	118.12	111.60
1	A	955	PRO	CB-CA-C	5.42	116.33	111.40
1	A	1189	SER	N-CA-C	5.42	115.83	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	SER	N-CA-C	5.42	118.17	107.98
1	A	983	ILE	N-CA-C	-5.42	105.10	110.62
1	A	1266	THR	N-CA-C	-5.41	105.02	111.03
3	C	135	GLN	CA-C-N	5.41	129.37	121.31
3	C	135	GLN	C-N-CA	5.41	129.37	121.31
1	A	741	ASN	CA-C-N	5.41	127.52	120.28
1	A	741	ASN	C-N-CA	5.41	127.52	120.28
1	A	523	ILE	CB-CA-C	5.40	119.00	111.34
1	A	425	GLN	N-CA-C	5.40	117.46	108.02
2	B	709	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	24	PRO	CA-C-N	5.38	127.75	120.38
1	A	24	PRO	C-N-CA	5.38	127.75	120.38
1	A	1127	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	399	HIS	CA-CB-CG	-5.36	108.44	113.80
3	C	135	GLN	N-CA-C	-5.36	107.11	113.97
9	I	53	GLY	CA-C-N	5.36	127.72	120.38
9	I	53	GLY	C-N-CA	5.36	127.72	120.38
1	A	475	THR	CB-CA-C	5.35	119.20	110.96
1	A	1375	MET	CA-C-N	5.35	127.72	120.44
1	A	1375	MET	C-N-CA	5.35	127.72	120.44
8	H	110	ASP	CA-C-N	5.35	128.44	120.95
8	H	110	ASP	C-N-CA	5.35	128.44	120.95
1	A	939	ASP	CA-CB-CG	5.34	117.94	112.60
6	F	122	MET	CA-C-N	5.33	127.42	120.28
6	F	122	MET	C-N-CA	5.33	127.42	120.28
6	F	87	LYS	CA-C-N	5.32	127.68	120.44
6	F	87	LYS	C-N-CA	5.32	127.68	120.44
5	E	5	ASN	CA-C-N	5.32	127.94	120.28
5	E	5	ASN	C-N-CA	5.32	127.94	120.28
1	A	222	LEU	N-CA-C	-5.32	103.87	110.41
2	B	752	ALA	N-CA-C	5.32	116.76	110.97
3	C	35	ARG	CA-C-N	5.31	127.45	120.60
3	C	35	ARG	C-N-CA	5.31	127.45	120.60
1	A	54	ASN	CB-CA-C	5.30	120.97	110.42
2	B	1156	ASP	N-CA-C	5.30	122.08	110.80
1	A	700	ASN	CA-CB-CG	5.29	117.89	112.60
2	B	56	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	229	SER	N-CA-C	5.29	118.81	108.18
3	C	213	PRO	N-CA-C	5.29	120.79	113.65
7	G	33	GLU	CA-C-N	5.28	127.70	120.46
7	G	33	GLU	C-N-CA	5.28	127.70	120.46
2	B	1182	CYS	N-CA-C	-5.28	98.61	107.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	GLY	N-CA-C	5.27	125.67	113.18
1	A	1424	VAL	CA-C-N	5.26	127.65	120.54
1	A	1424	VAL	C-N-CA	5.26	127.65	120.54
4	D	143	ASN	CA-CB-CG	5.25	117.85	112.60
4	D	196	PRO	CA-C-N	5.25	127.84	120.28
4	D	196	PRO	C-N-CA	5.25	127.84	120.28
2	B	707	PRO	CA-C-N	5.25	128.69	120.82
2	B	707	PRO	C-N-CA	5.25	128.69	120.82
5	E	54	GLN	CA-C-N	5.25	128.04	120.38
5	E	54	GLN	C-N-CA	5.25	128.04	120.38
2	B	642	ASP	N-CA-C	-5.24	105.69	111.71
1	A	79	GLY	N-CA-C	-5.23	104.86	111.72
1	A	1445	ILE	N-CA-CB	5.23	117.78	110.56
11	K	39	ASP	CA-CB-CG	5.23	117.83	112.60
2	B	425	THR	CB-CA-C	5.23	119.18	110.81
3	C	215	GLU	N-CA-C	5.23	120.00	111.37
1	A	1295	THR	CB-CA-C	5.22	120.03	110.11
2	B	449	ASN	N-CA-C	5.22	116.98	108.63
4	D	70	PHE	CA-CB-CG	5.22	119.02	113.80
2	B	397	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	562	THR	CB-CA-C	5.21	118.42	109.82
1	A	73	GLY	CA-C-N	5.21	131.49	121.54
1	A	73	GLY	C-N-CA	5.21	131.49	121.54
2	B	1180	PHE	N-CA-C	5.21	119.86	112.93
9	I	52	ILE	N-CA-CB	5.21	117.85	111.60
9	I	9	ASP	CA-CB-CG	5.19	117.79	112.60
3	C	207	CYS	CA-C-N	5.18	127.99	120.79
3	C	207	CYS	C-N-CA	5.18	127.99	120.79
11	K	2	ASN	CA-C-N	5.18	130.31	121.35
11	K	2	ASN	C-N-CA	5.18	130.31	121.35
1	A	333	GLU	N-CA-CB	5.18	119.24	110.49
2	B	627	PHE	N-CA-C	5.18	116.83	108.34
2	B	1139	ILE	CA-C-N	5.17	127.21	120.28
2	B	1139	ILE	C-N-CA	5.17	127.21	120.28
1	A	932	GLU	CB-CG-CD	5.16	121.38	112.60
2	B	475	SER	CA-C-N	5.16	131.40	121.54
2	B	475	SER	C-N-CA	5.16	131.40	121.54
1	A	1411	GLU	CB-CG-CD	5.16	121.37	112.60
8	H	36	CYS	N-CA-C	5.16	117.16	108.96
1	A	1122	PRO	N-CA-C	5.16	123.09	112.47
1	A	893	PHE	N-CA-C	-5.16	105.55	111.07
1	A	1043	ASP	CA-C-N	5.16	127.14	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1043	ASP	C-N-CA	5.16	127.14	120.44
1	A	690	VAL	CA-C-N	5.15	127.44	120.38
1	A	690	VAL	C-N-CA	5.15	127.44	120.38
2	B	66	ASP	CA-C-N	5.15	131.37	121.54
2	B	66	ASP	C-N-CA	5.15	131.37	121.54
1	A	54	ASN	CA-C-N	5.14	134.34	121.80
1	A	54	ASN	C-N-CA	5.14	134.34	121.80
1	A	1371	LEU	CA-C-N	5.13	127.22	120.60
1	A	1371	LEU	C-N-CA	5.13	127.22	120.60
1	A	1226	VAL	CA-C-N	5.12	129.97	122.69
1	A	1226	VAL	C-N-CA	5.12	129.97	122.69
12	L	44	ASP	CA-C-N	5.10	131.28	121.54
12	L	44	ASP	C-N-CA	5.10	131.28	121.54
2	B	368	GLU	N-CA-C	5.10	116.64	111.14
3	C	87	PHE	N-CA-C	5.09	119.49	113.28
11	K	24	ASP	CA-C-N	5.08	127.04	120.44
11	K	24	ASP	C-N-CA	5.08	127.04	120.44
6	F	150	GLU	N-CA-C	5.07	119.18	112.89
1	A	424	ILE	CA-C-N	-5.07	115.67	123.07
1	A	424	ILE	C-N-CA	-5.07	115.67	123.07
7	G	63	PRO	N-CA-C	5.07	122.91	112.47
2	B	694	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	234	MET	N-CA-C	-5.06	106.62	112.89
2	B	608	ASP	CA-C-N	5.05	130.08	122.75
2	B	608	ASP	C-N-CA	5.05	130.08	122.75
1	A	1102	LYS	N-CA-C	-5.05	105.47	110.97
5	E	21	GLU	CA-C-N	5.04	127.35	120.54
5	E	21	GLU	C-N-CA	5.04	127.35	120.54
6	F	132	LEU	N-CA-C	5.04	117.96	109.95
1	A	602	ASP	N-CA-C	-5.02	105.19	111.92
2	B	1159	ARG	N-CA-C	5.02	116.71	108.52
3	C	136	ASP	CA-CB-CG	5.02	117.62	112.60
2	B	55	VAL	CA-C-N	5.00	127.30	120.54
2	B	55	VAL	C-N-CA	5.00	127.30	120.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain,Peptide

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	11174	0	11233	232	0
2	B	8859	0	8901	192	0
3	C	2095	0	2051	57	0
4	D	1434	0	1460	30	0
5	E	1752	0	1776	38	0
6	F	679	0	701	23	0
7	G	1340	0	1357	40	0
8	H	1068	0	1040	22	0
9	I	971	0	927	18	0
10	J	532	0	542	17	0
11	K	920	0	929	21	0
12	L	363	0	386	8	0
13	N	181	0	102	1	0
14	P	42	0	22	1	0
15	T	309	0	169	1	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31728	0	31596	618	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 10.

All (618) 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	1.75	1.54
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.90	1.05
7:G:1:MET:HE1	7:G:80:LYS:O	1.58	1.03
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.47	0.95
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:766:ARG:HE	2:B:1020:ARG:HG2	1.39	0.85
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.38	0.85
5:E:185:ALA:HA	5:E:190:LEU:HD12	1.61	0.83
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.59	0.83
3:C:148:ARG:H	3:C:151:GLN:HG3	1.45	0.82
1:A:869:GLY:O	5:E:204:THR:HG21	1.78	0.82
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.60	0.82
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.63	0.80
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.62	0.80
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.64	0.80
4:D:155:ARG:H	4:D:219:THR:HG21	1.47	0.79
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.62	0.78
1:A:61:ILE:HG22	1:A:62:ASP:H	1.51	0.75
4:D:40:HIS:HB3	7:G:73:LYS:NZ	2.02	0.75
2:B:429:PHE:HA	2:B:432:MET:HE3	1.69	0.74
1:A:332:LYS:O	1:A:333:GLU:HG2	1.88	0.74
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.18	0.74
1:A:53:LEU:HD23	1:A:54:ASN:HB3	1.70	0.73
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.70	0.73
2:B:1084:GLN:OE1	3:C:189:THR:HG22	1.88	0.73
1:A:1388:GLY:O	1:A:1391:ARG:HG3	1.89	0.73
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.71	0.72
2:B:510:LYS:H	2:B:511:PRO:HD3	1.54	0.72
1:A:63:ARG:HA	1:A:74:MET:HG3	1.72	0.72
8:H:82:PRO:C	8:H:84:ALA:H	1.96	0.71
1:A:1329:THR:HG22	1:A:1331:SER:H	1.55	0.71
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.20	0.71
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.55	0.71
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.73	0.71
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.56	0.71
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.73	0.70
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.71	0.70
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.26	0.70
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.39	0.70
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.74	0.69
2:B:880:THR:O	2:B:934:LYS:HG3	1.92	0.69
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.75	0.69
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.32	0.69
1:A:114:LEU:HD21	1:A:171:GLN:HG3	1.74	0.69
4:D:154:PHE:HA	4:D:219:THR:HB	1.76	0.68
1:A:1386:ARG:HB3	1:A:1403:GLU:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:H	2:B:934:LYS:C	2.02	0.68
4:D:187:THR:HB	4:D:190:GLU:H	1.59	0.67
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.76	0.67
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.58	0.67
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.78	0.66
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.28	0.66
1:A:55:ASP:H	1:A:56:PRO:HD3	1.61	0.66
5:E:23:VAL:HG13	5:E:78:LEU:HD23	1.78	0.66
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.76	0.66
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.79	0.65
1:A:41:MET:HB2	1:A:49:LYS:HA	1.79	0.65
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.77	0.65
1:A:41:MET:CB	1:A:49:LYS:HA	2.27	0.65
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.62	0.65
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.79	0.65
5:E:19:VAL:O	5:E:23:VAL:HG23	1.97	0.64
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.77	0.64
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.79	0.64
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.79	0.64
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.78	0.64
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.79	0.63
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.79	0.63
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.82	0.62
7:G:91:VAL:HB	7:G:139:ILE:O	1.98	0.62
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.34	0.62
4:D:5:THR:HG21	7:G:74:TYR:OH	2.00	0.62
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.80	0.62
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.65	0.62
7:G:34:VAL:O	7:G:37:SER:HB3	1.99	0.61
1:A:629:LEU:O	1:A:633:VAL:HG23	2.00	0.61
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.81	0.61
11:K:107:THR:O	11:K:111:LEU:HG	2.00	0.61
7:G:143:ILE:HG22	7:G:145:VAL:HG22	1.82	0.61
2:B:510:LYS:N	2:B:511:PRO:HD3	2.15	0.61
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.16	0.61
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.82	0.61
5:E:5:ASN:HD21	5:E:52:ARG:HE	1.47	0.61
2:B:933:SER:O	2:B:935:ARG:N	2.34	0.60
2:B:881:ASN:HB3	2:B:934:LYS:H	1.66	0.60
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.83	0.60
1:A:512:VAL:HA	1:A:519:PRO:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:LYS:HG2	1:A:571:LEU:HD13	1.84	0.60
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.84	0.60
1:A:982:THR:HB	1:A:985:ASP:H	1.67	0.60
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.36	0.60
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.67	0.59
1:A:464:PRO:HD2	11:K:67:PHE:HD2	1.67	0.59
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.35	0.59
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.84	0.59
7:G:111:THR:HG22	7:G:113:HIS:H	1.67	0.59
2:B:975:GLN:O	2:B:990:ILE:HD12	2.03	0.59
1:A:42:ASP:O	1:A:44:THR:N	2.35	0.59
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.85	0.59
2:B:311:LEU:HB3	9:I:4:PHE:HE1	1.68	0.59
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.85	0.59
8:H:5:LEU:HB2	8:H:59:ILE:HG22	1.83	0.59
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.38	0.58
2:B:997:GLU:HG2	3:C:39:ALA:HB2	1.86	0.58
5:E:90:VAL:HG23	5:E:123:LEU:HD11	1.85	0.58
7:G:1:MET:SD	7:G:2:PHE:N	2.69	0.58
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.67	0.58
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.86	0.58
1:A:472:LEU:O	1:A:475:THR:HB	2.03	0.58
2:B:284:ILE:HG12	2:B:324:ILE:HD13	1.86	0.58
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.84	0.58
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.44	0.57
1:A:756:ILE:HD13	1:A:760:GLN:HG3	1.86	0.57
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.68	0.57
14:P:10:A:H61	15:T:19:DT:H3	1.52	0.57
1:A:41:MET:HA	1:A:50:ILE:H	1.69	0.57
6:F:128:LYS:HD3	6:F:149:GLU:O	2.04	0.57
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.86	0.57
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.68	0.57
11:K:6:ARG:O	11:K:9:LEU:HG	2.04	0.57
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.87	0.57
2:B:999:MET:HB3	2:B:1007:VAL:HG22	1.87	0.57
2:B:309:GLN:HB2	9:I:52:ILE:HD11	1.86	0.56
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.85	0.56
6:F:89:GLU:O	6:F:93:ILE:HD12	2.05	0.56
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.40	0.56
2:B:472:ALA:HB1	2:B:475:SER:HB2	1.88	0.56
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.88	0.56
1:A:1173:HIS:HB3	1:A:1227:ILE:HG23	1.87	0.56
5:E:97:VAL:HG13	5:E:127:ILE:HG12	1.87	0.56
3:C:149:LYS:HG3	3:C:150:GLY:H	1.71	0.56
1:A:1352:VAL:O	1:A:1356:ILE:HD12	2.06	0.56
6:F:109:VAL:CG1	6:F:123:LYS:HG2	2.33	0.56
3:C:255:VAL:HG21	11:K:94:ILE:HG21	1.88	0.56
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.39	0.56
1:A:915:SER:HB2	1:A:919:ILE:HD13	1.88	0.56
1:A:646:PHE:O	1:A:650:GLN:HG2	2.06	0.55
1:A:709:THR:HB	1:A:712:GLU:H	1.71	0.55
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.88	0.55
7:G:92:VAL:CG2	7:G:102:GLN:HB2	2.36	0.55
6:F:90:ARG:HD3	6:F:155:LEU:HD13	1.87	0.55
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.88	0.55
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.89	0.55
1:A:105:CYS:SG	1:A:139:TRP:HA	2.47	0.55
1:A:93:VAL:HA	1:A:96:ILE:HD12	1.87	0.55
2:B:882:THR:C	2:B:884:ARG:H	2.15	0.55
1:A:12:ARG:HB3	2:B:1218:THR:HG22	1.89	0.55
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.87	0.55
9:I:8:ARG:HG3	9:I:34:TYR:CE2	2.42	0.55
3:C:115:SER:HB2	3:C:142:VAL:H	1.72	0.54
3:C:161:LYS:O	3:C:170:TRP:NE1	2.40	0.54
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.41	0.54
1:A:567:LYS:HA	1:A:568:PRO:C	2.32	0.54
2:B:336:ARG:HH21	2:B:337:ARG:HH21	1.54	0.54
2:B:428:ILE:HG22	2:B:432:MET:HE2	1.89	0.54
1:A:43:GLU:CD	1:A:48:ALA:HB3	2.32	0.54
1:A:901:LEU:HA	1:A:907:THR:HG23	1.88	0.54
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.89	0.54
12:L:31:CYS:HB3	12:L:36:SER:H	1.72	0.54
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.89	0.54
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.90	0.54
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.88	0.54
7:G:106:MET:HG3	7:G:157:ILE:O	2.07	0.54
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.40	0.54
1:A:907:THR:HG22	1:A:908:LEU:H	1.71	0.54
1:A:66:LYS:HB3	1:A:71:GLN:O	2.08	0.54
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.90	0.54
4:D:8:PHE:CZ	7:G:5:LYS:NZ	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:HB3	2:B:1218:THR:CG2	2.38	0.54
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.90	0.54
4:D:54:GLU:O	4:D:58:VAL:HG23	2.08	0.54
1:A:31:SER:OG	1:A:33:ALA:O	2.26	0.54
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.08	0.54
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.39	0.54
6:F:111:LEU:HD12	6:F:111:LEU:H	1.73	0.54
1:A:332:LYS:H	1:A:337:ARG:CB	2.20	0.53
6:F:82:THR:HG22	6:F:83:PRO:HD2	1.90	0.53
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.89	0.53
2:B:420:LEU:HD21	2:B:456:GLY:HA3	1.90	0.53
1:A:75:ASN:O	1:A:76:GLU:HB2	2.09	0.53
4:D:190:GLU:HA	7:G:167:TYR:CE2	2.44	0.53
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.90	0.53
1:A:313:GLN:O	1:A:315:LEU:HG	2.09	0.53
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.90	0.53
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.90	0.53
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.34	0.53
2:B:822:ASN:O	10:J:48:ARG:NH1	2.39	0.53
3:C:149:LYS:C	3:C:151:GLN:H	2.15	0.53
5:E:176:PRO:O	5:E:212:ARG:HA	2.09	0.53
9:I:50:THR:HG22	9:I:52:ILE:H	1.72	0.53
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.92	0.52
2:B:339:THR:OG1	2:B:351:TYR:HE2	1.93	0.52
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.91	0.52
1:A:464:PRO:HD2	11:K:67:PHE:CD2	2.45	0.52
2:B:338:GLY:HA3	2:B:340:ALA:H	1.74	0.52
1:A:440:ASP:O	1:A:460:VAL:HG23	2.10	0.52
2:B:901:PRO:HA	2:B:949:VAL:HG12	1.91	0.52
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.92	0.52
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.75	0.52
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.92	0.52
2:B:34:ILE:HG12	2:B:542:MET:CE	2.39	0.52
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.90	0.52
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.92	0.52
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.25	0.52
10:J:30:LEU:HD22	10:J:34:THR:HB	1.92	0.52
2:B:165:VAL:O	2:B:167:ILE:HD12	2.09	0.52
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	1.92	0.52
3:C:251:LEU:O	3:C:255:VAL:HG23	2.10	0.52
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LYS:H	1:A:337:ARG:HB3	1.75	0.51
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.92	0.51
2:B:234:ILE:HG21	2:B:237:VAL:HG22	1.91	0.51
2:B:1185:CYS:HA	4:D:17:LYS:HD3	1.91	0.51
2:B:323:VAL:HG23	2:B:324:ILE:HD12	1.91	0.51
5:E:46:TYR:CD1	5:E:58:MET:HG3	2.45	0.51
9:I:17:ARG:HG2	9:I:26:LEU:HB2	1.91	0.51
10:J:9:SER:OG	10:J:48:ARG:NH2	2.44	0.51
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.92	0.51
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.92	0.51
1:A:1095:THR:HG21	1:A:1112:LYS:HB3	1.92	0.51
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.91	0.51
3:C:114:TYR:HB3	3:C:140:ASN:O	2.11	0.51
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.93	0.51
1:A:708:MET:HG2	1:A:712:GLU:HB3	1.93	0.51
1:A:902:LEU:HG	1:A:926:GLN:HG2	1.92	0.51
3:C:82:TYR:HB3	3:C:84:ARG:HG2	1.92	0.51
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.93	0.51
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.93	0.51
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.93	0.51
2:B:766:ARG:NE	2:B:1020:ARG:HG2	2.19	0.51
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.93	0.51
12:L:60:ARG:HH22	12:L:65:VAL:HG22	1.75	0.51
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.44	0.51
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.93	0.50
2:B:545:ILE:HG12	2:B:633:VAL:HG22	1.93	0.50
2:B:789:MET:HE3	2:B:965:LYS:HB3	1.92	0.50
3:C:46:ILE:HD12	3:C:46:ILE:H	1.76	0.50
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.93	0.50
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.91	0.50
10:J:64:ASN:HB2	10:J:65:PRO:HD3	1.92	0.50
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.47	0.50
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.93	0.50
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.92	0.50
3:C:66:ARG:NH2	10:J:3:VAL:O	2.44	0.50
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.46	0.50
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.46	0.50
7:G:20:PRO:C	7:G:22:MET:H	2.19	0.50
1:A:114:LEU:HD22	1:A:145:LYS:HB3	1.93	0.50
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.94	0.50
1:A:55:ASP:CG	1:A:55:ASP:O	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:HG13	1:A:239:LEU:HB3	1.94	0.49
2:B:552:MET:HA	2:B:555:ILE:HB	1.93	0.49
1:A:416:ARG:HD2	1:A:417:TYR:CZ	2.46	0.49
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.47	0.49
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.94	0.49
3:C:148:ARG:HG3	3:C:149:LYS:N	2.27	0.49
5:E:12:LEU:HG	5:E:58:MET:HE1	1.93	0.49
1:A:549:MET:SD	1:A:577:ILE:HD11	2.52	0.49
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.94	0.49
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.95	0.49
2:B:345:LYS:HA	2:B:348:ARG:CD	2.42	0.49
5:E:26:ARG:O	5:E:75:MET:HE1	2.13	0.49
1:A:265:LYS:HE2	1:A:302:THR:OG1	2.12	0.49
1:A:315:LEU:HA	1:A:321:PRO:HA	1.94	0.49
1:A:549:MET:CE	1:A:656:TRP:HD1	2.24	0.49
1:A:901:LEU:O	1:A:920:LEU:HD23	2.12	0.49
6:F:118:LEU:O	6:F:122:MET:HG3	2.12	0.49
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.95	0.49
3:C:11:ARG:HB2	3:C:19:ASP:HB3	1.95	0.49
12:L:28:LYS:HB2	12:L:39:SER:HA	1.94	0.49
13:N:3:DC:H4'	13:N:4:DA:OP1	2.13	0.49
8:H:105:GLU:HB3	8:H:113:ALA:HB3	1.95	0.49
1:A:81:PHE:HE1	2:B:1205:GLN:HG2	1.76	0.49
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.95	0.49
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.94	0.49
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.12	0.49
1:A:867:ILE:CD1	1:A:867:ILE:CB	2.81	0.49
2:B:338:GLY:HA3	2:B:339:THR:HB	1.94	0.49
2:B:902:GLY:O	12:L:65:VAL:HG11	2.12	0.49
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.94	0.49
1:A:200:ARG:NH2	1:A:206:GLU:OE1	2.44	0.49
4:D:8:PHE:HZ	7:G:5:LYS:HZ3	1.56	0.49
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.95	0.49
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.12	0.48
3:C:84:ARG:HD2	11:K:11:LEU:HD21	1.95	0.48
5:E:29:PHE:HD1	5:E:65:THR:HG22	1.78	0.48
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.78	0.48
1:A:503:GLN:OE1	6:F:90:ARG:NH2	2.46	0.48
1:A:1170:ILE:O	1:A:1174:PHE:HB2	2.13	0.48
2:B:284:ILE:HG21	2:B:333:PHE:CD2	2.48	0.48
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:92:VAL:HG21	7:G:102:GLN:HB2	1.95	0.48
8:H:63:LEU:HB3	8:H:90:ALA:HB2	1.95	0.48
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.94	0.48
2:B:343:ILE:O	2:B:344:LYS:HB2	2.13	0.48
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.78	0.48
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.96	0.48
1:A:878:ILE:CG2	1:A:955:PRO:HB2	2.43	0.48
1:A:1172:LEU:C	1:A:1174:PHE:H	2.21	0.48
1:A:1325:THR:HG23	5:E:146:HIS:O	2.14	0.48
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.95	0.48
1:A:49:LYS:HE2	1:A:61:ILE:H	1.79	0.48
1:A:388:LEU:O	1:A:392:VAL:HG23	2.14	0.48
2:B:449:ASN:HD22	2:B:452:THR:HG23	1.79	0.48
2:B:510:LYS:H	2:B:511:PRO:CD	2.25	0.48
2:B:776:GLN:HA	2:B:1096:ARG:HH11	1.78	0.48
2:B:842:ASN:HB3	2:B:845:SER:HB2	1.96	0.48
8:H:103:LYS:HB3	8:H:115:TYR:CD1	2.48	0.48
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.95	0.48
2:B:310:MET:O	2:B:313:MET:HB3	2.14	0.48
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.13	0.47
1:A:344:ARG:CZ	2:B:1120:GLU:HG2	2.43	0.47
2:B:273:LEU:HD12	2:B:280:ILE:HD13	1.95	0.47
2:B:642:ASP:HA	2:B:649:LYS:HA	1.96	0.47
5:E:204:THR:HG22	5:E:205:SER:N	2.28	0.47
2:B:957:ASN:ND2	2:B:961:LEU:HD12	2.30	0.47
4:D:14:ARG:C	4:D:16:LYS:H	2.22	0.47
1:A:1276:VAL:HG11	1:A:1315:GLU:HB3	1.97	0.47
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.94	0.47
2:B:101:MET:HG2	2:B:111:ALA:HA	1.97	0.47
1:A:325:ILE:O	1:A:328:ARG:HB2	2.15	0.47
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.96	0.47
2:B:944:THR:HB	2:B:1122:ARG:HH21	1.80	0.47
3:C:6:PRO:HA	3:C:24:ASN:HB3	1.96	0.47
4:D:52:LEU:HD22	4:D:147:TYR:HE2	1.79	0.47
1:A:34:LYS:HG3	1:A:36:ARG:HH21	1.80	0.47
1:A:1442:ASP:HB2	6:F:137:TYR:CE2	2.44	0.47
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.96	0.47
3:C:262:LEU:HD13	11:K:88:LYS:HG2	1.96	0.47
4:D:8:PHE:HZ	7:G:5:LYS:NZ	2.12	0.47
7:G:49:LEU:HG	7:G:76:ALA:HA	1.97	0.47
8:H:58:THR:HB	8:H:143:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.96	0.47
9:I:88:SER:C	9:I:90:GLN:H	2.23	0.47
1:A:446:ARG:HB2	1:A:487:MET:SD	2.55	0.47
1:A:55:ASP:N	1:A:56:PRO:HD3	2.26	0.47
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.96	0.47
2:B:758:PHE:CE2	2:B:1027:ILE:HG22	2.50	0.47
2:B:1181:GLU:H	2:B:1188:LYS:HE3	1.80	0.47
7:G:111:THR:HB	7:G:114:LEU:HD23	1.97	0.47
1:A:829:VAL:C	1:A:831:THR:H	2.22	0.47
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.96	0.47
7:G:62:LEU:HD21	7:G:69:GLU:HB2	1.97	0.47
8:H:6:PHE:HB3	8:H:59:ILE:HB	1.96	0.47
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.96	0.46
2:B:226:PHE:CZ	2:B:398:ARG:HG3	2.51	0.46
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.96	0.46
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.97	0.46
1:A:1035:TYR:N	1:A:1035:TYR:CD1	2.82	0.46
11:K:10:PHE:HD1	11:K:11:LEU:HD13	1.79	0.46
1:A:37:PHE:O	1:A:53:LEU:HB2	2.16	0.46
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.50	0.46
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.45	0.46
4:D:144:THR:HG22	4:D:148:LEU:HD12	1.96	0.46
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.97	0.46
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.81	0.46
1:A:25:GLU:CD	1:A:25:GLU:H	2.23	0.46
2:B:604:ARG:HD3	2:B:611:PRO:HA	1.98	0.46
2:B:649:LYS:HE2	2:B:738:PHE:O	2.15	0.46
2:B:853:SER:HB3	2:B:1094:ARG:HH11	1.80	0.46
7:G:9:LEU:HD23	7:G:30:LEU:HD12	1.96	0.46
1:A:35:ILE:HG22	1:A:84:ILE:HG22	1.97	0.46
3:C:46:ILE:HD13	3:C:67:LEU:O	2.15	0.46
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.98	0.46
1:A:62:ASP:C	1:A:64:ASN:H	2.22	0.46
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.80	0.46
7:G:11:ILE:HG21	7:G:29:LYS:HG2	1.98	0.46
1:A:1095:THR:HG23	1:A:1113:THR:HG23	1.98	0.46
2:B:339:THR:HG1	2:B:351:TYR:HE2	1.56	0.46
2:B:882:THR:HG23	2:B:884:ARG:H	1.80	0.46
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.98	0.46
1:A:344:ARG:HG2	2:B:1127:GLY:O	2.15	0.45
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:ILE:HG23	2:B:224:GLN:HG3	1.97	0.45
5:E:109:ILE:HG12	5:E:133:GLU:HB2	1.97	0.45
10:J:6:ARG:HA	10:J:12:LYS:O	2.16	0.45
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.81	0.45
1:A:58:LEU:HB3	1:A:59:GLY:H	1.31	0.45
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.98	0.45
2:B:277:LYS:HB3	2:B:278:GLN:HE21	1.82	0.45
2:B:918:ILE:HD13	2:B:935:ARG:HH12	1.81	0.45
3:C:16:ASP:O	3:C:233:GLU:HA	2.16	0.45
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.57	0.45
4:D:175:PHE:CZ	7:G:85:GLU:HG3	2.50	0.45
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.98	0.45
8:H:113:ALA:HB1	8:H:124:ARG:HE	1.81	0.45
1:A:1433:MET:HE2	2:B:1145:SER:HB3	1.97	0.45
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.97	0.45
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.98	0.45
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.50	0.45
1:A:1276:VAL:HB	1:A:1279:ILE:HD13	1.98	0.45
2:B:394:ASP:OD2	9:I:91:ARG:HD2	2.16	0.45
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.98	0.45
6:F:93:ILE:HG21	6:F:148:VAL:HG11	1.97	0.45
11:K:108:GLU:O	11:K:112:GLN:HG2	2.17	0.45
1:A:1436:ILE:O	1:A:1437:GLY:C	2.59	0.45
2:B:1148:LYS:HD3	2:B:1152:MET:HG3	1.98	0.45
2:B:765:PRO:O	2:B:769:TYR:HD1	1.99	0.45
6:F:109:VAL:HG22	6:F:127:GLU:OE1	2.16	0.45
1:A:524:VAL:HG12	1:A:525:GLN:HG2	1.98	0.45
1:A:49:LYS:HG2	1:A:61:ILE:HD12	1.99	0.45
1:A:55:ASP:O	1:A:55:ASP:OD2	2.34	0.45
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.99	0.45
1:A:302:THR:HA	1:A:305:ASP:O	2.17	0.45
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.52	0.45
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.99	0.45
1:A:1410:PHE:CE1	2:B:1210:MET:HG2	2.52	0.45
2:B:848:ARG:HD2	10:J:8:PHE:O	2.17	0.45
3:C:148:ARG:N	3:C:151:GLN:HG3	2.24	0.45
1:A:946:VAL:HG22	5:E:201:LYS:HB3	1.99	0.44
2:B:228:LYS:O	2:B:261:ARG:NH2	2.50	0.44
1:A:18:GLN:O	2:B:1215:ARG:HB2	2.17	0.44
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.52	0.44
1:A:787:PHE:CZ	1:A:796:SER:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:VAL:HG21	2:B:380:TYR:HE2	1.82	0.44
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.52	0.44
2:B:758:PHE:HZ	2:B:1031:LEU:HD13	1.83	0.44
10:J:37:SER:OG	10:J:47:ARG:NH2	2.49	0.44
1:A:752:LYS:HA	1:A:752:LYS:HD3	1.72	0.44
1:A:1154:TYR:CE1	9:I:18:GLU:HG3	2.53	0.44
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.99	0.44
4:D:155:ARG:HB3	4:D:219:THR:HG21	1.98	0.44
5:E:69:ILE:H	5:E:69:ILE:HG13	1.66	0.44
2:B:510:LYS:N	2:B:511:PRO:CD	2.79	0.44
4:D:190:GLU:HA	7:G:167:TYR:CD2	2.51	0.44
1:A:562:THR:O	1:A:576:GLN:NE2	2.51	0.44
1:A:626:ASN:O	1:A:631:HIS:ND1	2.51	0.44
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.82	0.44
3:C:8:VAL:HG13	3:C:22:LEU:HD12	1.99	0.44
3:C:148:ARG:HG3	3:C:149:LYS:H	1.82	0.44
3:C:204:SER:O	3:C:207:CYS:HB2	2.18	0.44
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.99	0.44
11:K:73:LEU:HD21	11:K:75:ILE:HD11	1.99	0.44
1:A:381:THR:HG22	1:A:384:ASN:CG	2.43	0.44
2:B:20:ASP:HB2	2:B:23:ALA:HB2	2.00	0.44
2:B:54:PHE:HA	2:B:58:THR:HB	2.00	0.44
2:B:770:GLN:HG2	2:B:983:ARG:O	2.17	0.44
7:G:23:LYS:HG3	7:G:56:ILE:HD13	2.00	0.44
1:A:304:MET:O	1:A:324:SER:HB2	2.18	0.44
1:A:565:ILE:O	1:A:570:PRO:HA	2.18	0.44
1:A:1410:PHE:HE1	2:B:1210:MET:HG2	1.82	0.44
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.99	0.44
6:F:89:GLU:C	6:F:93:ILE:HD12	2.43	0.44
2:B:339:THR:OG1	2:B:351:TYR:CE2	2.67	0.44
8:H:127:GLY:N	8:H:130:ARG:HH21	2.16	0.44
1:A:38:PRO:HD3	1:A:270:LEU:HD12	2.00	0.43
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.48	0.43
1:A:658:LEU:HD23	1:A:659:HIS:NE2	2.33	0.43
1:A:667:GLY:HA2	1:A:670:ILE:HD12	2.00	0.43
2:B:315:LYS:N	2:B:316:PRO:HD2	2.33	0.43
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.32	0.43
3:C:116:LYS:HD3	3:C:140:ASN:HA	2.01	0.43
9:I:7:CYS:HB2	9:I:14:LEU:HD21	2.00	0.43
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.82	0.43
1:A:145:LYS:NZ	1:A:149:GLU:HB2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.87	0.43
1:A:1433:MET:CE	7:G:63:PRO:HB3	2.40	0.43
2:B:756:ILE:O	2:B:759:PRO:HD3	2.18	0.43
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.51	0.43
3:C:124:LEU:HD22	3:C:129:ILE:HG22	1.99	0.43
3:C:143:LEU:HD21	3:C:146:LYS:HE3	2.00	0.43
5:E:5:ASN:ND2	5:E:52:ARG:HE	2.15	0.43
5:E:155:ARG:HD2	5:E:194:GLU:OE2	2.19	0.43
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	2.00	0.43
3:C:36:VAL:HG21	3:C:251:LEU:HB2	2.00	0.43
1:A:247:ARG:HB3	1:A:262:LEU:HB2	2.00	0.43
1:A:388:LEU:HD23	1:A:391:LEU:HD12	2.01	0.43
1:A:1240:CYS:SG	1:A:1267:MET:HE1	2.58	0.43
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.59	0.43
1:A:873:MET:C	1:A:1058:VAL:HG13	2.43	0.43
2:B:1082:MET:HA	3:C:189:THR:HA	2.00	0.43
3:C:62:PHE:O	3:C:66:ARG:HG3	2.18	0.43
3:C:102:GLN:HA	3:C:153:LEU:O	2.19	0.43
1:A:698:GLN:HA	9:I:97:MET:O	2.19	0.43
2:B:123:THR:HG23	2:B:205:ILE:HA	2.01	0.43
3:C:125:MET:HB2	3:C:127:ARG:NE	2.33	0.43
4:D:52:LEU:H	4:D:52:LEU:HG	1.59	0.43
5:E:100:ILE:HG23	5:E:105:PHE:HB2	2.01	0.43
1:A:34:LYS:HA	1:A:83:HIS:O	2.19	0.43
2:B:35:SER:HA	2:B:811:TYR:CE1	2.54	0.43
2:B:361:LEU:HD12	2:B:361:LEU:HA	1.91	0.43
2:B:642:ASP:N	2:B:649:LYS:HE3	2.33	0.43
2:B:762:ASN:OD1	2:B:1022:THR:HA	2.19	0.43
3:C:161:LYS:O	3:C:170:TRP:CD1	2.72	0.43
1:A:348:SER:HA	1:A:489:LEU:O	2.19	0.43
1:A:579:SER:HB3	1:A:611:GLN:HA	2.00	0.43
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.99	0.43
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.99	0.43
4:D:208:GLU:HA	4:D:211:LEU:HD12	2.01	0.43
5:E:124:VAL:HG13	5:E:132:ILE:HB	2.01	0.43
1:A:1144:LYS:HG3	1:A:1268:LEU:HB3	2.00	0.43
2:B:338:GLY:CA	2:B:339:THR:HB	2.48	0.43
1:A:605:MET:HE2	1:A:607:ILE:HG13	2.01	0.42
5:E:88:VAL:HG21	5:E:110:PHE:HE2	1.85	0.42
11:K:7:PHE:C	11:K:9:LEU:H	2.27	0.42
4:D:176:GLU:OE2	4:D:197:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:194:LEU:HD22	7:G:86:VAL:HG11	2.01	0.42
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.19	0.42
2:B:491:THR:O	2:B:495:LEU:HD12	2.18	0.42
2:B:732:SER:HB2	2:B:734:HIS:CE1	2.54	0.42
1:A:472:LEU:HD21	2:B:835:GLN:HB3	2.00	0.42
2:B:102:VAL:HG11	2:B:122:LEU:HD13	2.01	0.42
3:C:77:ILE:HA	3:C:129:ILE:HD11	2.01	0.42
8:H:47:PHE:HE2	8:H:94:ASP:HB2	1.83	0.42
8:H:109:LYS:HB3	8:H:110:ASP:H	1.61	0.42
1:A:968:GLN:HG2	1:A:973:ILE:HG21	2.00	0.42
1:A:1158:PRO:HA	1:A:1241:ARG:CZ	2.50	0.42
2:B:986:GLN:HE22	2:B:1022:THR:HG21	1.82	0.42
1:A:253:ASN:HD21	1:A:256:GLN:HB2	1.83	0.42
1:A:714:PHE:O	1:A:718:VAL:HG23	2.20	0.42
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.19	0.42
5:E:4:GLU:O	5:E:7:ARG:HG2	2.19	0.42
6:F:134:ILE:HG22	6:F:136:ARG:HG3	2.02	0.42
8:H:81:PRO:HB2	8:H:82:PRO:HD3	2.00	0.42
9:I:16:PRO:HB3	9:I:25:LEU:HD11	2.01	0.42
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.55	0.42
1:A:441:PRO:HG2	1:A:498:ARG:HB3	2.01	0.42
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.52	0.42
2:B:338:GLY:CA	2:B:339:THR:CB	2.98	0.42
3:C:50:GLU:HG2	12:L:66:GLN:HG3	2.01	0.42
4:D:210:ILE:HG22	4:D:214:LEU:HD12	2.02	0.42
5:E:192:ARG:HB2	5:E:215:MET:O	2.20	0.42
11:K:10:PHE:CE1	11:K:11:LEU:HD13	2.54	0.42
1:A:518:LYS:HB2	1:A:519:PRO:HD2	2.01	0.42
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	2.01	0.42
2:B:539:LEU:HD21	2:B:545:ILE:HD11	2.00	0.42
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.01	0.42
3:C:102:GLN:HG2	3:C:154:LYS:HG3	2.01	0.42
7:G:119:LEU:HD21	7:G:137:ILE:HD12	2.02	0.42
1:A:189:ARG:HB2	1:A:193:ASP:HB3	2.01	0.42
1:A:347:PHE:H	2:B:1107:ALA:HA	1.84	0.42
1:A:1040:GLN:HG3	1:A:1041:ALA:N	2.34	0.42
2:B:318:VAL:HG11	9:I:13:MET:HG2	2.02	0.42
2:B:467:GLY:HA3	2:B:475:SER:HB3	2.00	0.42
8:H:16:ASP:HA	8:H:17:PRO:HD3	1.88	0.42
9:I:14:LEU:HB3	9:I:27:PHE:HB3	2.01	0.42
6:F:109:VAL:HG11	6:F:123:LYS:CG	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:100:PHE:HA	9:I:111:THR:HG22	2.02	0.41
1:A:227:VAL:HG12	4:D:15:LEU:HD23	2.01	0.41
1:A:1191:TRP:HH2	9:I:25:LEU:HD13	1.85	0.41
3:C:55:THR:HB	3:C:151:GLN:HA	2.02	0.41
5:E:23:VAL:O	5:E:28:TYR:HB2	2.19	0.41
1:A:871:ASP:CB	5:E:204:THR:HG23	2.49	0.41
1:A:1033:GLN:O	1:A:1036:ARG:NH1	2.53	0.41
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.03	0.41
2:B:603:LEU:HB3	2:B:609:ILE:HG13	2.01	0.41
3:C:201:TRP:HA	3:C:202:PRO:HD3	1.94	0.41
3:C:242:GLN:O	3:C:246:ARG:HB2	2.20	0.41
4:D:40:HIS:HB3	7:G:73:LYS:HZ1	1.82	0.41
1:A:92:HIS:HB2	1:A:236:LEU:HD21	2.03	0.41
1:A:709:THR:HG22	1:A:711:ARG:H	1.84	0.41
3:C:183:TRP:HB2	3:C:185:LYS:HE2	2.03	0.41
6:F:124:GLU:HB3	6:F:130:ILE:HG13	2.02	0.41
9:I:26:LEU:HD23	9:I:37:GLU:HA	2.02	0.41
1:A:495:GLU:HG3	6:F:98:ALA:HB1	2.03	0.41
1:A:1329:THR:HG22	1:A:1331:SER:N	2.30	0.41
9:I:10:CYS:C	9:I:12:ASN:H	2.27	0.41
1:A:34:LYS:HG3	1:A:34:LYS:O	2.21	0.41
1:A:1009:ASN:HA	1:A:1012:ARG:HD2	2.02	0.41
2:B:373:ARG:HA	2:B:566:LEU:HD23	2.02	0.41
2:B:862:GLN:HB3	2:B:963:PHE:CD1	2.55	0.41
2:B:901:PRO:HD3	12:L:58:LYS:HB3	2.03	0.41
1:A:534:LEU:O	1:A:574:GLY:HA3	2.19	0.41
2:B:102:VAL:HG23	2:B:110:HIS:HB3	2.03	0.41
5:E:156:LEU:HD11	5:E:197:LYS:HB2	2.03	0.41
1:A:567:LYS:HA	1:A:569:LYS:N	2.36	0.41
1:A:761:MET:O	1:A:803:SER:HB2	2.21	0.41
2:B:247:GLY:H	2:B:418:LYS:NZ	2.18	0.41
2:B:341:LEU:HD12	2:B:343:ILE:HB	2.03	0.41
10:J:1:MET:HB2	10:J:56:LEU:HD12	2.03	0.41
11:K:65:HIS:HE1	11:K:67:PHE:CD1	2.38	0.41
1:A:583:PRO:HG2	1:A:586:ILE:HG13	2.02	0.41
1:A:821:ARG:HG3	1:A:825:ILE:HD11	2.02	0.41
1:A:822:GLU:HA	1:A:825:ILE:HD12	2.02	0.41
1:A:849:MET:HB3	1:A:1063:MET:SD	2.60	0.41
1:A:918:GLU:H	1:A:918:GLU:HG3	1.59	0.41
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	2.02	0.41
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:542:MET:HG2	2:B:747:MET:HE3	2.03	0.41
7:G:13:LEU:HD23	7:G:13:LEU:HA	1.84	0.41
7:G:134:GLU:H	7:G:134:GLU:HG3	1.75	0.41
10:J:48:ARG:O	10:J:52:THR:HB	2.21	0.41
2:B:473:MET:HA	2:B:474:SER:HA	1.89	0.41
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.56	0.41
2:B:666:TYR:C	2:B:668:ASP:H	2.28	0.41
2:B:710:LEU:CA	2:B:733:HIS:HB3	2.45	0.41
7:G:106:MET:HG2	7:G:107:LYS:N	2.36	0.41
11:K:7:PHE:C	11:K:9:LEU:N	2.79	0.41
11:K:10:PHE:HA	11:K:37:LYS:HB3	2.03	0.41
1:A:62:ASP:HB3	1:A:64:ASN:O	2.20	0.40
1:A:785:PRO:HB2	2:B:703:ILE:HD12	2.03	0.40
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.21	0.40
1:A:1383:SER:HB2	1:A:1385:THR:HG23	2.01	0.40
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.19	0.40
2:B:909:ASP:O	2:B:940:PRO:HA	2.21	0.40
7:G:7:LEU:HB2	7:G:74:TYR:CZ	2.56	0.40
1:A:42:ASP:C	1:A:44:THR:N	2.79	0.40
5:E:147:HIS:HB3	5:E:150:VAL:HG23	2.02	0.40
8:H:82:PRO:C	8:H:84:ALA:N	2.70	0.40
1:A:56:PRO:O	1:A:57:ARG:HG3	2.21	0.40
1:A:121:LEU:O	1:A:124:GLN:HB3	2.21	0.40
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	2.03	0.40
1:A:1444:MET:HB2	1:A:1444:MET:HE2	1.57	0.40
2:B:291:ILE:N	2:B:291:ILE:HD12	2.35	0.40
2:B:1104:HIS:HB2	2:B:1122:ARG:HG3	2.03	0.40
2:B:1176:ASN:H	2:B:1178:ASN:H	1.69	0.40
3:C:173:ALA:HB2	3:C:243:VAL:HG11	2.02	0.40
7:G:154:VAL:HB	7:G:155:SER:H	1.62	0.40
1:A:367:PRO:HB3	1:A:465:TYR:O	2.21	0.40
1:A:1396:ALA:HA	1:A:1399:ARG:NH2	2.36	0.40
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.50	0.40
1:A:351:THR:HG22	1:A:468:PHE:CD2	2.56	0.40
2:B:291:ILE:HG22	2:B:297:ILE:HG13	2.03	0.40
2:B:510:LYS:HB2	2:B:513:GLN:OE1	2.22	0.40
2:B:1165:ILE:HG21	4:D:17:LYS:HB3	2.03	0.40
3:C:114:TYR:CD1	3:C:140:ASN:HB3	2.57	0.40
5:E:100:ILE:HA	5:E:105:PHE:HD2	1.87	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	1414/1732 (82%)	1224 (87%)	137 (10%)	53 (4%)	2	21
2	B	1095/1224 (90%)	956 (87%)	101 (9%)	38 (4%)	3	23
3	C	264/318 (83%)	232 (88%)	28 (11%)	4 (2%)	8	37
4	D	174/221 (79%)	155 (89%)	10 (6%)	9 (5%)	1	14
5	E	212/215 (99%)	192 (91%)	17 (8%)	3 (1%)	9	38
6	F	82/155 (53%)	75 (92%)	7 (8%)	0	100	100
7	G	169/171 (99%)	152 (90%)	12 (7%)	5 (3%)	3	25
8	H	129/146 (88%)	101 (78%)	20 (16%)	8 (6%)	1	12
9	I	117/122 (96%)	94 (80%)	18 (15%)	5 (4%)	2	18
10	J	63/70 (90%)	53 (84%)	4 (6%)	6 (10%)	0	6
11	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
12	L	44/70 (63%)	28 (64%)	14 (32%)	2 (4%)	2	17
All	All	3876/4564 (85%)	3370 (87%)	373 (10%)	133 (3%)	3	23

All (133) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	48	ALA
1	A	55	ASP
1	A	57	ARG
1	A	58	LEU
1	A	74	MET
1	A	76	GLU
1	A	195	ASP
1	A	257	ARG
1	A	286	HIS
1	A	318	SER
1	A	335	ARG

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Mol	Chain	Res	Type
1	A	449	SER
1	A	775	ILE
1	A	1124	HIS
2	B	340	ALA
2	B	343	ILE
2	B	344	LYS
2	B	510	LYS
2	B	731	VAL
2	B	751	VAL
2	B	881	ASN
2	B	1181	GLU
2	B	1223	ASP
3	C	161	LYS
4	D	18	VAL
4	D	119	ARG
4	D	199	ASN
8	H	81	PRO
9	I	9	ASP
10	J	6	ARG
1	A	70	CYS
1	A	72	GLU
1	A	178	GLY
1	A	189	ARG
1	A	311	GLN
1	A	628	GLY
1	A	1173	HIS
1	A	1206	ASP
1	A	1403	GLU
2	B	27	ALA
2	B	108	VAL
2	B	229	ALA
2	B	341	LEU
2	B	476	ARG
2	B	629	ASP
2	B	643	ASP
2	B	707	PRO
2	B	772	ALA
2	B	879	ARG
2	B	883	LEU
2	B	1046	PRO
2	B	1066	SER
2	B	1176	ASN

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Mol	Chain	Res	Type
3	C	90	ASP
4	D	11	ARG
4	D	53	SER
5	E	45	LYS
5	E	104	ASN
7	G	154	VAL
8	H	17	PRO
8	H	60	ALA
8	H	128	ASN
9	I	95	THR
10	J	17	LYS
10	J	62	ARG
10	J	64	ASN
12	L	56	LEU
12	L	59	ALA
1	A	332	LYS
1	A	830	LYS
1	A	1255	GLU
1	A	1314	SER
1	A	1378	GLN
1	A	1405	THR
2	B	28	GLU
2	B	67	SER
2	B	339	THR
2	B	526	GLU
2	B	711	GLU
2	B	869	SER
2	B	1157	ALA
4	D	15	LEU
7	G	63	PRO
8	H	84	ALA
9	I	3	THR
1	A	52	GLY
1	A	65	LEU
1	A	167	CYS
1	A	187	LYS
1	A	399	HIS
1	A	569	LYS
1	A	700	ASN
1	A	958	VAL
1	A	1122	PRO
1	A	1123	GLY

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Mol	Chain	Res	Type
2	B	338	GLY
2	B	868	MET
2	B	1108	ARG
2	B	1155	SER
4	D	16	LYS
4	D	218	GLU
7	G	2	PHE
8	H	18	GLY
8	H	82	PRO
8	H	83	GLN
9	I	89	GLN
1	A	336	ILE
1	A	385	ILE
1	A	418	SER
1	A	1437	GLY
2	B	648	HIS
2	B	886	LYS
3	C	214	ASN
4	D	191	ALA
5	E	3	GLN
10	J	2	ILE
1	A	310	GLY
1	A	780	VAL
3	C	38	ILE
7	G	20	PRO
9	I	88	SER
1	A	312	PRO
7	G	139	ILE
1	A	35	ILE
1	A	61	ILE
1	A	196	GLU
1	A	567	LYS
2	B	364	ILE
10	J	3	VAL
1	A	192	GLY
2	B	867	GLY
1	A	448	PRO

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1240/1519 (82%)	1027 (83%)	213 (17%)	2	12
2	B	966/1061 (91%)	810 (84%)	156 (16%)	2	14
3	C	234/274 (85%)	202 (86%)	32 (14%)	3	19
4	D	160/200 (80%)	130 (81%)	30 (19%)	1	9
5	E	196/197 (100%)	176 (90%)	20 (10%)	7	28
6	F	74/137 (54%)	66 (89%)	8 (11%)	6	26
7	G	152/152 (100%)	125 (82%)	27 (18%)	2	10
8	H	117/128 (91%)	103 (88%)	14 (12%)	5	23
9	I	113/116 (97%)	103 (91%)	10 (9%)	9	32
10	J	60/65 (92%)	46 (77%)	14 (23%)	1	5
11	K	99/102 (97%)	83 (84%)	16 (16%)	2	14
12	L	40/57 (70%)	28 (70%)	12 (30%)	0	2
All	All	3451/4008 (86%)	2899 (84%)	552 (16%)	2	14

All (552) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	THR
1	A	15	LYS
1	A	34	LYS
1	A	37	PHE
1	A	41	MET
1	A	54	ASN
1	A	58	LEU
1	A	65	LEU
1	A	70	CYS
1	A	84	ILE
1	A	93	VAL
1	A	96	ILE
1	A	98	LYS
1	A	106	VAL
1	A	113	LEU
1	A	114	LEU
1	A	129	LYS

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Mol	Chain	Res	Type
1	A	131	SER
1	A	145	LYS
1	A	151	ASP
1	A	160	GLN
1	A	170	THR
1	A	174	ILE
1	A	182	VAL
1	A	196	GLU
1	A	199	LEU
1	A	204	THR
1	A	205	GLU
1	A	208	LEU
1	A	217	LYS
1	A	219	PHE
1	A	220	THR
1	A	222	LEU
1	A	226	GLU
1	A	237	THR
1	A	252	PHE
1	A	253	ASN
1	A	261	ASP
1	A	265	LYS
1	A	270	LEU
1	A	274	ILE
1	A	279	LEU
1	A	289	ILE
1	A	290	GLU
1	A	291	GLU
1	A	295	LEU
1	A	307	ASP
1	A	311	GLN
1	A	315	LEU
1	A	333	GLU
1	A	335	ARG
1	A	337	ARG
1	A	343	LYS
1	A	344	ARG
1	A	354	SER
1	A	375	THR
1	A	381	THR
1	A	383	TYR
1	A	385	ILE

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Mol	Chain	Res	Type
1	A	386	ASP
1	A	389	THR
1	A	393	ARG
1	A	398	GLU
1	A	408	ASP
1	A	425	GLN
1	A	431	LYS
1	A	434	ARG
1	A	436	ILE
1	A	438	ASP
1	A	443	LEU
1	A	445	ASN
1	A	447	GLN
1	A	452	LYS
1	A	454	SER
1	A	459	ARG
1	A	461	LYS
1	A	463	ILE
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	479	ASN
1	A	481	ASP
1	A	489	LEU
1	A	500	GLU
1	A	505	CYS
1	A	516	SER
1	A	523	ILE
1	A	524	VAL
1	A	541	ILE
1	A	545	GLN
1	A	553	VAL
1	A	566	ILE
1	A	571	LEU
1	A	577	ILE
1	A	588	LEU
1	A	596	THR
1	A	603	ASN
1	A	616	VAL
1	A	618	GLU

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Mol	Chain	Res	Type
1	A	622	VAL
1	A	626	ASN
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	640	GLN
1	A	645	LEU
1	A	652	VAL
1	A	666	ILE
1	A	691	LEU
1	A	738	LYS
1	A	740	LEU
1	A	752	LYS
1	A	754	SER
1	A	755	PHE
1	A	756	ILE
1	A	768	GLN
1	A	769	SER
1	A	782	ARG
1	A	788	SER
1	A	806	ARG
1	A	821	ARG
1	A	824	LEU
1	A	831	THR
1	A	834	THR
1	A	838	GLN
1	A	839	ARG
1	A	848	ILE
1	A	849	MET
1	A	867	ILE
1	A	878	ILE
1	A	885	THR
1	A	886	ILE
1	A	906	HIS
1	A	915	SER
1	A	917	SER
1	A	918	GLU
1	A	919	ILE
1	A	920	LEU
1	A	927	VAL
1	A	929	LEU
1	A	932	GLU

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Mol	Chain	Res	Type
1	A	934	LYS
1	A	941	LYS
1	A	948	VAL
1	A	964	ILE
1	A	973	ILE
1	A	983	ILE
1	A	998	LEU
1	A	1001	ARG
1	A	1009	ASN
1	A	1015	VAL
1	A	1035	TYR
1	A	1047	SER
1	A	1050	GLU
1	A	1052	GLN
1	A	1062	GLU
1	A	1064	VAL
1	A	1067	LEU
1	A	1117	THR
1	A	1118	VAL
1	A	1124	HIS
1	A	1128	GLN
1	A	1134	ILE
1	A	1135	ARG
1	A	1142	THR
1	A	1146	VAL
1	A	1170	ILE
1	A	1171	GLN
1	A	1173	HIS
1	A	1174	PHE
1	A	1175	SER
1	A	1176	LEU
1	A	1196	GLU
1	A	1223	ASP
1	A	1237	ILE
1	A	1242	VAL
1	A	1260	LEU
1	A	1263	ILE
1	A	1277	GLU
1	A	1289	ARG
1	A	1291	VAL
1	A	1293	SER
1	A	1295	THR

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Mol	Chain	Res	Type
1	A	1297	GLU
1	A	1307	GLU
1	A	1308	THR
1	A	1315	GLU
1	A	1317	MET
1	A	1327	ILE
1	A	1341	ILE
1	A	1366	ARG
1	A	1370	LEU
1	A	1374	VAL
1	A	1376	THR
1	A	1383	SER
1	A	1391	ARG
1	A	1393	ASN
1	A	1394	THR
1	A	1398	MET
1	A	1400	CYS
1	A	1403	GLU
1	A	1411	GLU
1	A	1424	VAL
1	A	1426	GLU
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
1	A	1453	TYR
2	B	25	ILE
2	B	40	GLU
2	B	45	SER
2	B	46	GLN
2	B	63	ILE
2	B	102	VAL
2	B	128	LEU
2	B	134	LYS
2	B	169	ARG
2	B	178	ASN
2	B	187	SER
2	B	217	ARG
2	B	222	ILE
2	B	223	VAL
2	B	240	ILE

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Mol	Chain	Res	Type
2	B	251	ILE
2	B	261	ARG
2	B	262	GLU
2	B	267	ARG
2	B	272	THR
2	B	276	ILE
2	B	277	LYS
2	B	278	GLN
2	B	284	ILE
2	B	292	ILE
2	B	294	ASP
2	B	298	LEU
2	B	304	ASP
2	B	305	VAL
2	B	324	ILE
2	B	325	GLN
2	B	334	ILE
2	B	337	ARG
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	346	GLU
2	B	348	ARG
2	B	350	GLN
2	B	361	LEU
2	B	364	ILE
2	B	365	THR
2	B	367	LEU
2	B	370	PHE
2	B	371	GLU
2	B	393	LYS
2	B	396	ASP
2	B	398	ARG
2	B	408	LEU
2	B	412	LEU
2	B	415	GLN
2	B	416	LEU
2	B	423	LYS
2	B	425	THR
2	B	436	VAL
2	B	446	LEU
2	B	453	ILE

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Mol	Chain	Res	Type
2	B	466	TRP
2	B	468	GLU
2	B	474	SER
2	B	485	ARG
2	B	502	ILE
2	B	513	GLN
2	B	547	VAL
2	B	552	MET
2	B	563	MET
2	B	570	VAL
2	B	598	GLU
2	B	604	ARG
2	B	614	SER
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	624	LEU
2	B	628	THR
2	B	629	ASP
2	B	637	LEU
2	B	651	LEU
2	B	653	VAL
2	B	658	ILE
2	B	667	GLN
2	B	678	GLU
2	B	682	SER
2	B	689	LEU
2	B	690	VAL
2	B	693	ILE
2	B	708	GLU
2	B	709	ASP
2	B	734	HIS
2	B	737	THR
2	B	742	GLU
2	B	766	ARG
2	B	771	SER
2	B	790	ASP
2	B	795	ILE
2	B	835	GLN
2	B	841	MET
2	B	844	SER
2	B	853	SER

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Mol	Chain	Res	Type
2	B	878	GLN
2	B	882	THR
2	B	889	THR
2	B	904	ARG
2	B	906	SER
2	B	934	LYS
2	B	942	ARG
2	B	946	ASN
2	B	948	ILE
2	B	953	LEU
2	B	956	THR
2	B	964	VAL
2	B	965	LYS
2	B	969	ARG
2	B	970	THR
2	B	972	LYS
2	B	975	GLN
2	B	976	ILE
2	B	986	GLN
2	B	992	ILE
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1010	LEU
2	B	1020	ARG
2	B	1031	LEU
2	B	1041	GLU
2	B	1049	ASP
2	B	1065	GLN
2	B	1072	MET
2	B	1080	LYS
2	B	1084	GLN
2	B	1106	ARG
2	B	1112	GLN
2	B	1120	GLU
2	B	1123	SER
2	B	1129	ARG
2	B	1133	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1148	LYS

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Mol	Chain	Res	Type
2	B	1150	ARG
2	B	1151	LEU
2	B	1160	VAL
2	B	1165	ILE
2	B	1168	LEU
2	B	1169	MET
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1202	LEU
2	B	1210	MET
2	B	1212	ILE
2	B	1220	ARG
2	B	1222	ARG
3	C	4	GLU
3	C	7	GLN
3	C	8	VAL
3	C	22	LEU
3	C	25	VAL
3	C	44	LEU
3	C	55	THR
3	C	57	VAL
3	C	78	GLU
3	C	81	GLU
3	C	89	GLU
3	C	101	LEU
3	C	106	GLU
3	C	119	VAL
3	C	124	LEU
3	C	127	ARG
3	C	129	ILE
3	C	137	LYS
3	C	147	LEU
3	C	148	ARG
3	C	156	THR
3	C	158	VAL
3	C	195	GLN
3	C	215	GLU
3	C	238	ILE
3	C	240	VAL
3	C	254	LYS

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Mol	Chain	Res	Type
3	C	259	LEU
3	C	260	LEU
3	C	264	GLN
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	6	SER
4	D	7	THR
4	D	9	GLN
4	D	11	ARG
4	D	12	ARG
4	D	17	LYS
4	D	18	VAL
4	D	29	LEU
4	D	41	GLN
4	D	47	LEU
4	D	52	LEU
4	D	65	GLU
4	D	67	ARG
4	D	119	ARG
4	D	123	LEU
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	156	ASP
4	D	158	GLU
4	D	177	VAL
4	D	187	THR
4	D	193	THR
4	D	197	SER
4	D	206	GLU
4	D	213	GLU
4	D	214	LEU
4	D	219	THR
5	E	14	ARG
5	E	31	THR
5	E	45	LYS
5	E	69	ILE
5	E	72	PHE
5	E	84	ASP
5	E	90	VAL

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Mol	Chain	Res	Type
5	E	95	THR
5	E	121	MET
5	E	127	ILE
5	E	144	ILE
5	E	154	ILE
5	E	166	LYS
5	E	173	SER
5	E	177	ARG
5	E	192	ARG
5	E	204	THR
5	E	207	ARG
5	E	214	CYS
5	E	215	MET
6	F	78	GLN
6	F	79	ARG
6	F	82	THR
6	F	87	LYS
6	F	103	MET
6	F	109	VAL
6	F	134	ILE
6	F	155	LEU
7	G	8	SER
7	G	11	ILE
7	G	13	LEU
7	G	22	MET
7	G	26	LEU
7	G	29	LYS
7	G	34	VAL
7	G	58	ARG
7	G	60	ARG
7	G	64	THR
7	G	90	THR
7	G	92	VAL
7	G	100	GLU
7	G	112	LYS
7	G	114	LEU
7	G	118	ASP
7	G	134	GLU
7	G	138	THR
7	G	141	SER
7	G	143	ILE
7	G	145	VAL

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Mol	Chain	Res	Type
7	G	151	ILE
7	G	152	SER
7	G	154	VAL
7	G	162	SER
7	G	163	ILE
7	G	171	ILE
8	H	3	ASN
8	H	12	VAL
8	H	14	GLU
8	H	26	ILE
8	H	35	GLN
8	H	42	ILE
8	H	76	THR
8	H	86	ASP
8	H	91	ASP
8	H	103	LYS
8	H	107	VAL
8	H	109	LYS
8	H	130	ARG
8	H	137	GLN
9	I	7	CYS
9	I	8	ARG
9	I	17	ARG
9	I	31	THR
9	I	35	VAL
9	I	50	THR
9	I	55	THR
9	I	62	ILE
9	I	83	ASN
9	I	94	ASP
10	J	2	ILE
10	J	3	VAL
10	J	12	LYS
10	J	13	VAL
10	J	14	VAL
10	J	16	ASP
10	J	22	LEU
10	J	25	LEU
10	J	28	ASP
10	J	31	ASP
10	J	34	THR
10	J	42	LYS

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Mol	Chain	Res	Type
10	J	48	ARG
10	J	52	THR
11	K	6	ARG
11	K	11	LEU
11	K	20	LYS
11	K	21	ILE
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	33	ILE
11	K	37	LYS
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	73	LEU
11	K	91	CYS
11	K	101	LEU
11	K	107	THR
12	L	27	LEU
12	L	33	GLU
12	L	38	LEU
12	L	40	LEU
12	L	43	THR
12	L	47	ARG
12	L	50	ASP
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	65	VAL
12	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	253	ASN
1	A	358	ASN
1	A	363	GLN
1	A	399	HIS
1	A	451	HIS
1	A	490	HIS
1	A	493	GLN

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Mol	Chain	Res	Type
1	A	545	GLN
1	A	603	ASN
1	A	640	GLN
1	A	742	ASN
1	A	854	ASN
1	A	1106	ASN
1	A	1124	HIS
1	A	1140	HIS
1	A	1171	GLN
1	A	1393	ASN
2	B	46	GLN
2	B	53	GLN
2	B	121	ASN
2	B	224	GLN
2	B	278	GLN
2	B	325	GLN
2	B	350	GLN
2	B	357	GLN
2	B	395	GLN
2	B	415	GLN
2	B	433	GLN
2	B	449	ASN
2	B	686	ASN
2	B	734	HIS
2	B	957	ASN
2	B	975	GLN
2	B	1040	ASN
2	B	1062	HIS
2	B	1117	GLN
2	B	1195	HIS
3	C	7	GLN
3	C	17	ASN
3	C	79	GLN
3	C	91	HIS
3	C	131	HIS
3	C	135	GLN
3	C	140	ASN
3	C	151	GLN
3	C	203	GLN
3	C	214	ASN
3	C	231	ASN
3	C	264	GLN

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Mol	Chain	Res	Type
4	D	9	GLN
4	D	37	GLN
4	D	41	GLN
4	D	132	GLN
4	D	143	ASN
5	E	5	ASN
5	E	8	ASN
5	E	32	GLN
5	E	54	GLN
5	E	101	GLN
5	E	179	GLN
7	G	10	ASN
7	G	71	ASN
7	G	102	GLN
7	G	131	GLN
8	H	35	GLN
8	H	131	ASN
9	I	46	HIS
9	I	79	HIS
9	I	83	ASN
9	I	90	GLN
9	I	120	GLN
10	J	64	ASN
11	K	29	ASN
11	K	44	ASN
11	K	76	GLN
11	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	1/2 (50%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	10	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
15	BRU	T	22	15	18,21,22	2.01	4 (22%)	25,30,33	2.99	9 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BRU	T	22	15	-	0/7/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C6-C5	5.03	1.44	1.34
15	T	22	BRU	BR-C5	4.56	1.99	1.88
15	T	22	BRU	C6-N1	3.71	1.44	1.38
15	T	22	BRU	C1'-N1	2.55	1.54	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	O4'-C1'-N1	8.34	122.67	107.86
15	T	22	BRU	N3-C2-N1	5.32	121.82	114.89
15	T	22	BRU	C6-C5-C4	-5.11	115.49	120.67
15	T	22	BRU	C5-C4-N3	4.84	118.91	113.34
15	T	22	BRU	C6-N1-C2	-4.38	116.94	121.30
15	T	22	BRU	C2'-C1'-N1	3.63	122.89	113.81
15	T	22	BRU	BR-C5-C4	3.54	122.10	118.02
15	T	22	BRU	C4-N3-C2	-3.01	123.40	127.34
15	T	22	BRU	C1'-N1-C6	2.56	125.04	120.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	5.56
1	B	351:TYR	C	352:ALA	N	2.97

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	1422/1732 (82%)	-0.24	15 (1%) 78 54	57, 107, 167, 228	0
2	B	1115/1224 (91%)	-0.05	20 (1%) 67 42	62, 118, 181, 206	0
3	C	266/318 (83%)	-0.36	0 100 100	78, 111, 152, 186	0
4	D	178/221 (80%)	-0.05	6 (3%) 48 27	78, 118, 174, 194	0
5	E	214/215 (99%)	-0.13	0 100 100	81, 139, 190, 203	0
6	F	84/155 (54%)	-0.62	0 100 100	58, 83, 118, 131	0
7	G	171/171 (100%)	-0.24	0 100 100	81, 102, 144, 164	0
8	H	133/146 (91%)	0.39	8 (6%) 27 16	123, 155, 187, 211	0
9	I	119/122 (97%)	0.02	2 (1%) 69 43	111, 149, 190, 205	0
10	J	65/70 (92%)	-0.39	1 (1%) 72 47	88, 107, 144, 156	0
11	K	115/120 (95%)	-0.49	1 (0%) 81 58	72, 105, 141, 157	0
12	L	46/70 (65%)	0.42	4 (8%) 16 10	91, 138, 166, 184	0
13	N	9/14 (64%)	0.83	1 (11%) 10 7	216, 225, 263, 270	0
14	P	2/2 (100%)	1.12	0 100 100	185, 185, 185, 193	0
15	T	14/27 (51%)	0.52	0 100 100	141, 173, 267, 268	0
All	All	3953/4607 (85%)	-0.15	58 (1%) 72 47	57, 114, 180, 270	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	502	ILE	5.0
2	B	883	LEU	4.7
2	B	446	LEU	4.7
1	A	251	SER	4.5
2	B	882	THR	4.4
2	B	70	ILE	4.3
8	H	63	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1080	THR	4.1
12	L	26	THR	3.9
2	B	251	ILE	3.8
2	B	708	GLU	3.7
2	B	709	ASP	3.6
12	L	27	LEU	3.5
8	H	136	LYS	3.4
1	A	56	PRO	3.4
11	K	114	LEU	3.3
8	H	94	ASP	3.2
2	B	715	ALA	3.2
2	B	134	LYS	3.1
9	I	52	ILE	3.0
4	D	25	ALA	3.0
8	H	132	LEU	3.0
10	J	65	PRO	2.9
2	B	108	VAL	2.8
8	H	84	ALA	2.8
4	D	3	VAL	2.8
2	B	1224	PHE	2.8
2	B	934	LYS	2.7
1	A	1176	LEU	2.7
4	D	24	ALA	2.7
1	A	1092	LYS	2.7
8	H	82	PRO	2.6
4	D	221	TYR	2.6
1	A	1243	VAL	2.5
1	A	38	PRO	2.5
4	D	76	LYS	2.5
1	A	1257	ASP	2.4
13	N	2	DG	2.4
9	I	120	GLN	2.4
2	B	731	VAL	2.4
2	B	339	THR	2.4
1	A	1455	PRO	2.3
1	A	194	ALA	2.3
12	L	50	ASP	2.3
1	A	1093	LYS	2.3
4	D	18	VAL	2.3
2	B	509	ALA	2.3
12	L	28	LYS	2.3
1	A	57	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	643	ASP	2.2
8	H	90	ALA	2.2
2	B	305	VAL	2.1
1	A	190	ALA	2.1
1	A	223	GLY	2.1
8	H	139	ASN	2.1
2	B	473	MET	2.1
1	A	310	GLY	2.0
2	B	933	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
15	BRU	T	22	20/21	0.78	0.19	174,184,191,192	0

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
17	MG	A	2458	1/1	0.86	0.15	287,287,287,287	0
16	ZN	L	1071	1/1	0.99	0.02	144,144,144,144	0
16	ZN	I	1122	1/1	0.99	0.05	184,184,184,184	0
16	ZN	C	1269	1/1	1.00	0.02	84,84,84,84	0
16	ZN	I	1121	1/1	1.00	0.02	123,123,123,123	0
16	ZN	A	2456	1/1	1.00	0.02	137,137,137,137	0
16	ZN	J	1066	1/1	1.00	0.03	93,93,93,93	0
16	ZN	A	2457	1/1	1.00	0.01	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	ZN	B	2225	1/1	1.00	0.04	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.