



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:10 PM UTC

PDB ID : 4A3B / pdb_00004a3b
Title : RNA Polymerase II initial transcribing complex with a 4nt 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

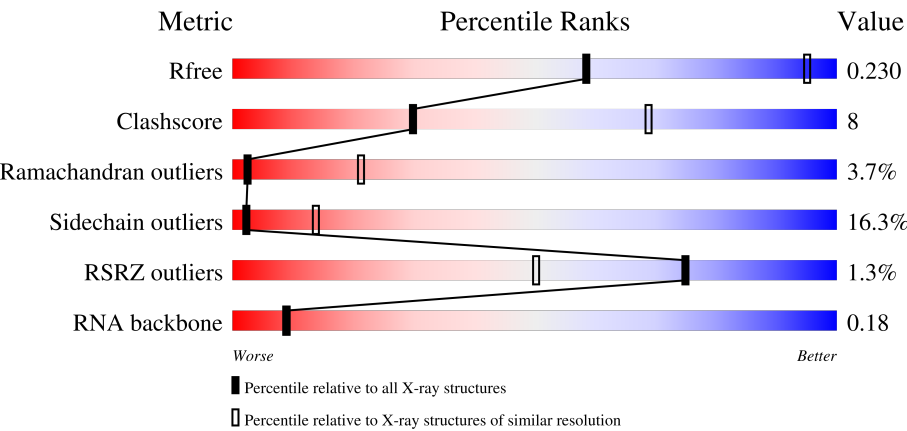
1 Overall quality at a glance i

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% 54%22%5%18%
2	B	1224	2% 56%29%6%9%
3	C	318	52%26%5%16%
4	D	221	2% 49%26%.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	4	
15	T	26	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31612 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(*TP*AP*AP*GP*TP*A P*CP*TP*TP*GP*AP*GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	4	Total	C	N	O	P	0	0	0
			84	40	17	23	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	4	Total	C	N	O	P	0	0	0
			90	40	20	26	4			

- Molecule 15 is a DNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	12	Total	Br	C	N	O	P	0	0
			242	1	116	36	77	12		

- 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		

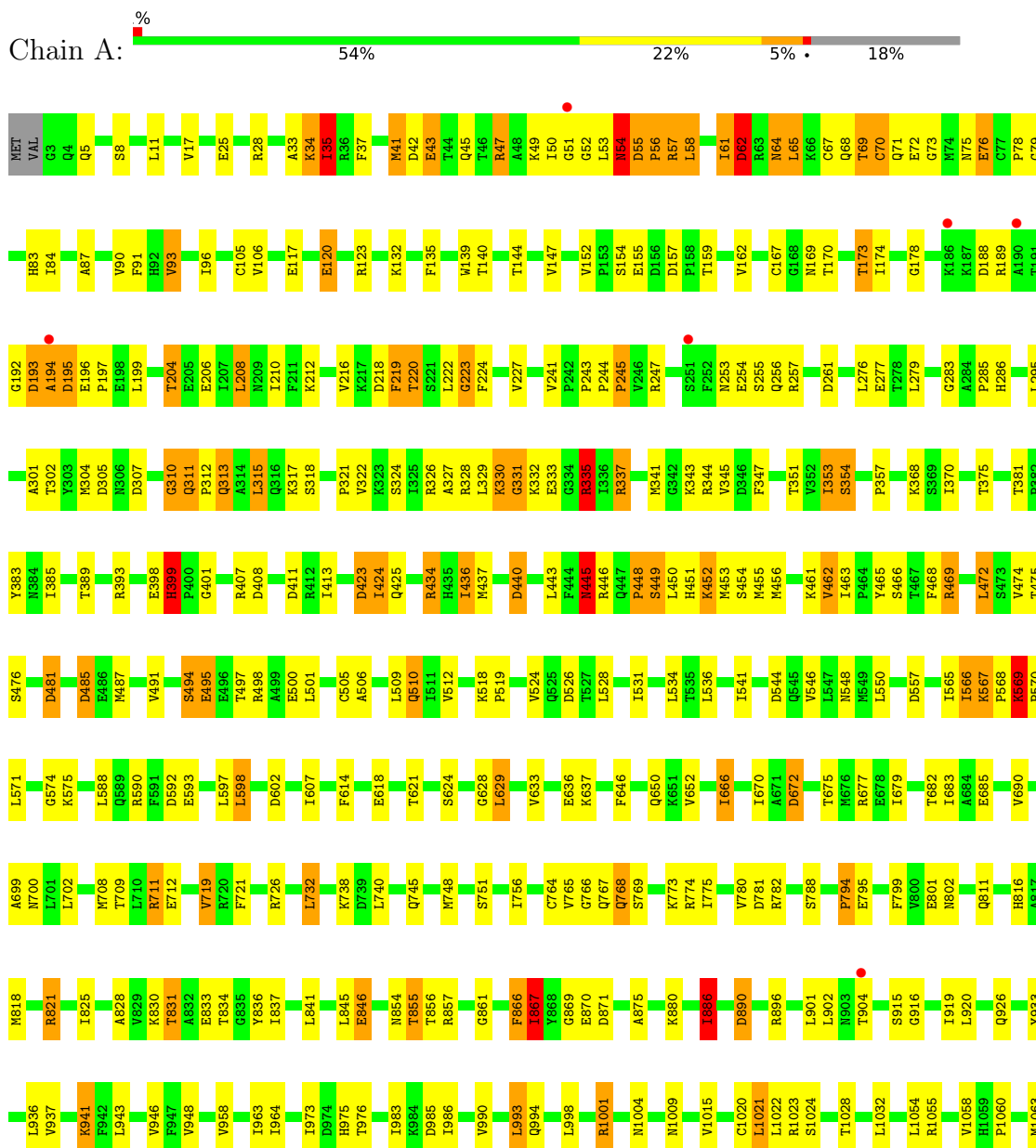
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

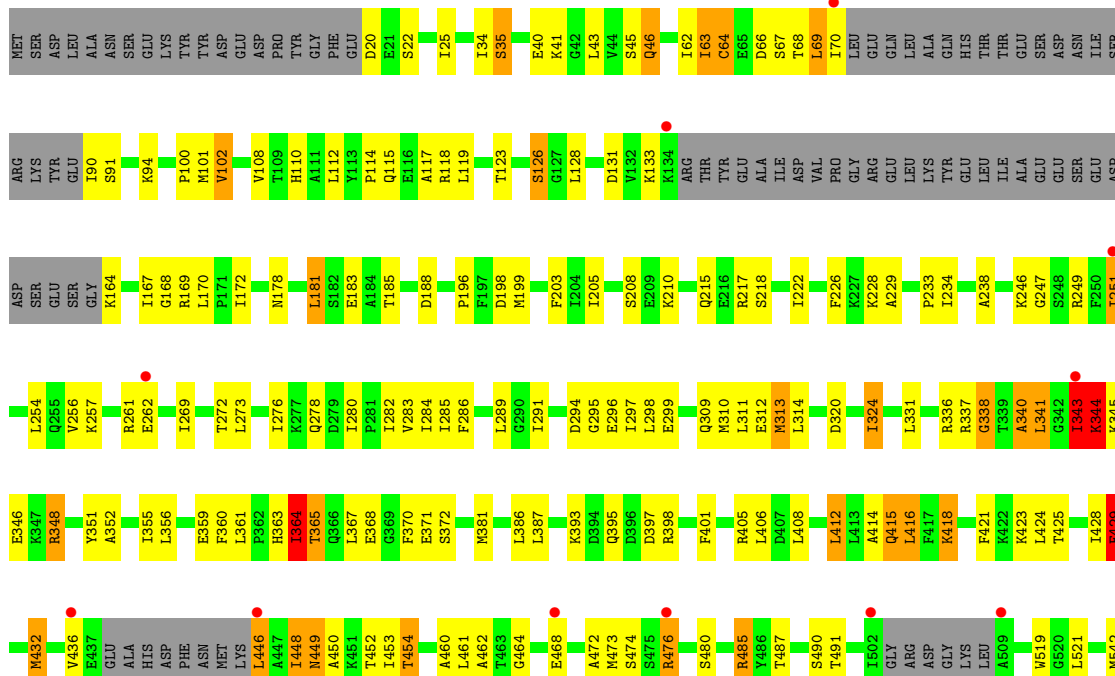
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

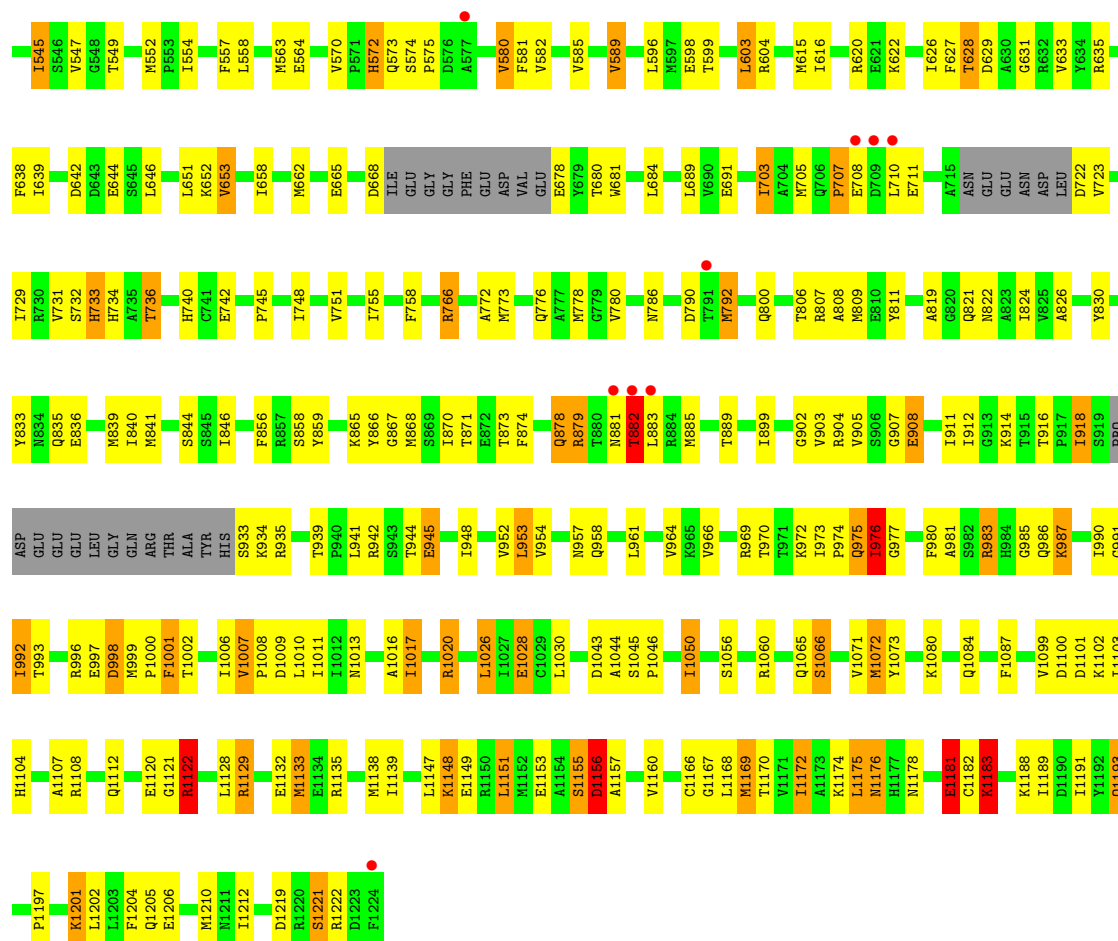
3 Residue-property plots

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

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

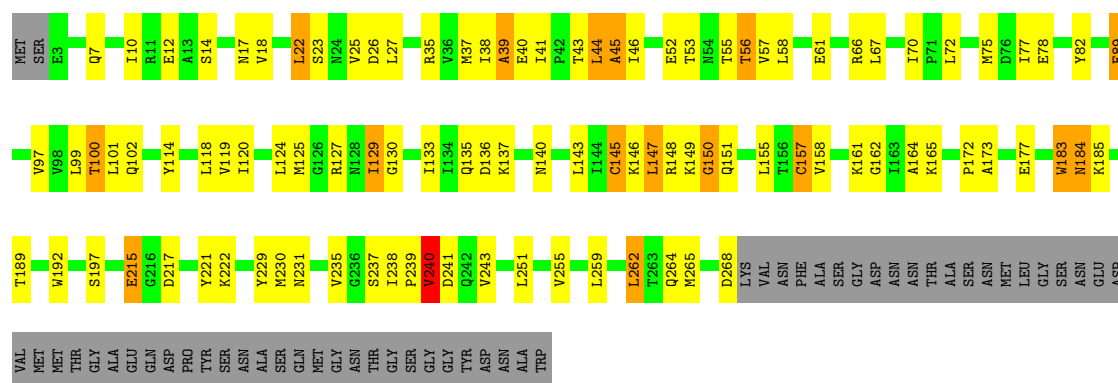






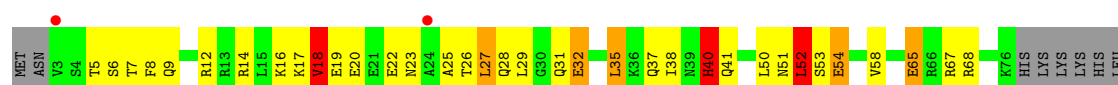
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

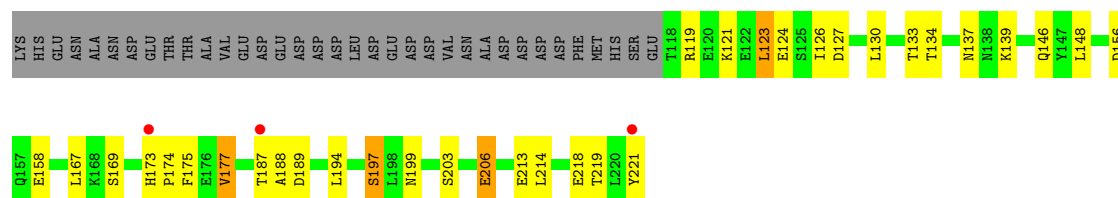
Chain C: 52% 26% 5% 16%



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

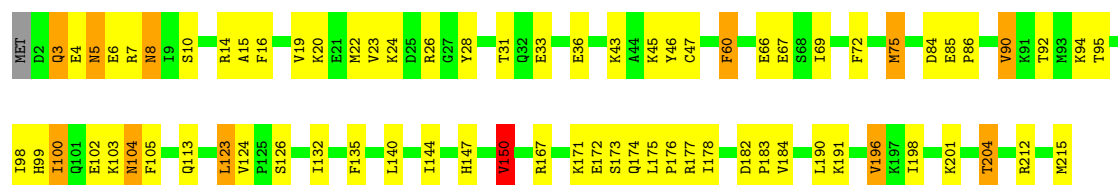
Chain D: 2% 49% 26% 19%





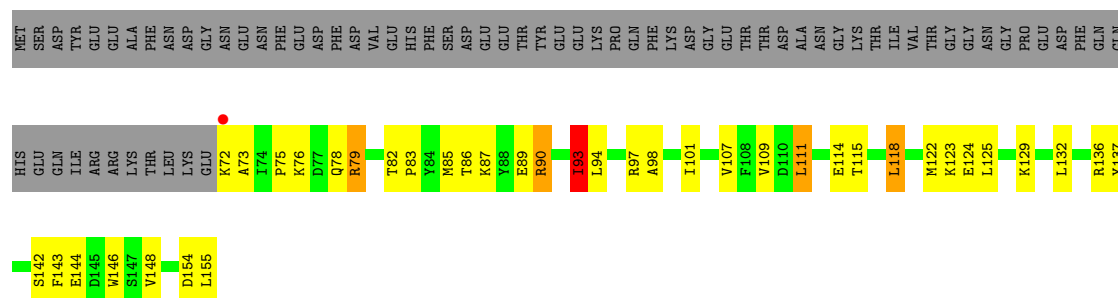
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E: 65% 29% 5%



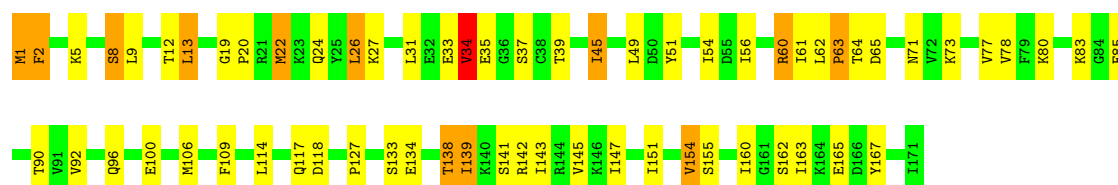
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F: 29% 22% 46%



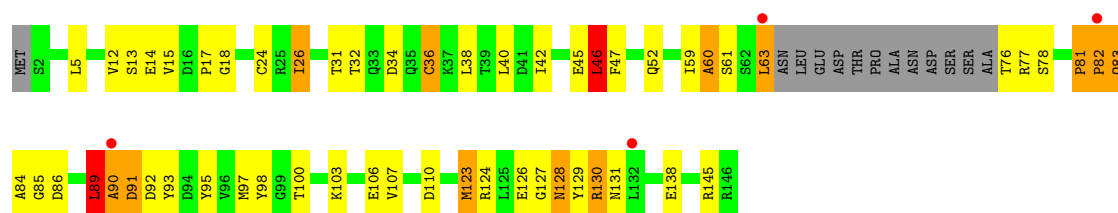
• Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G: 63% 30% 7%

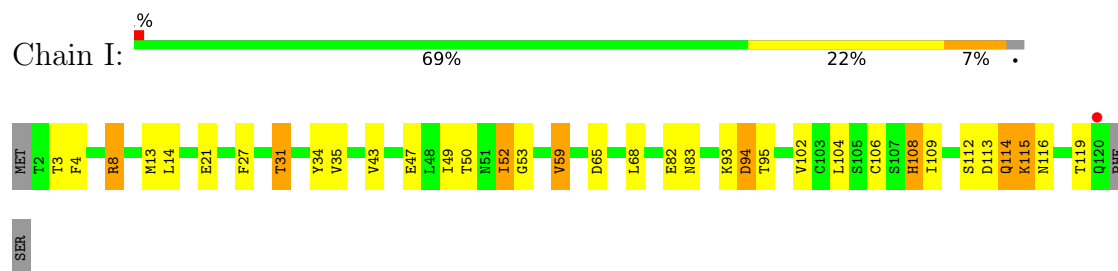


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

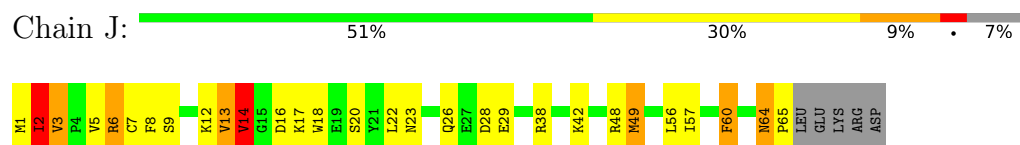
Chain H: 3% 53% 29% 8% 9%



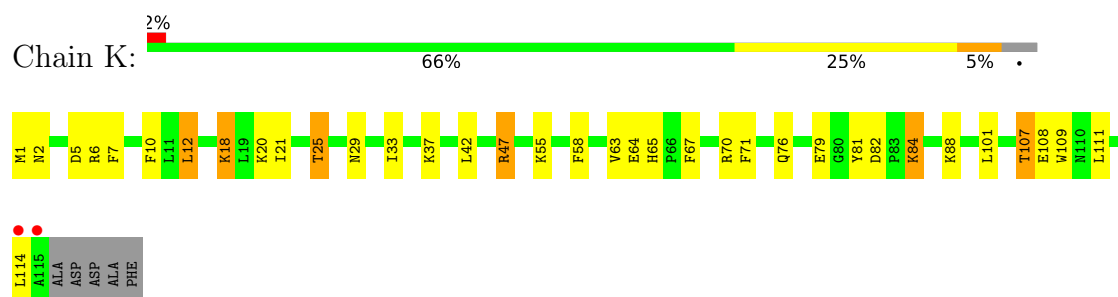
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



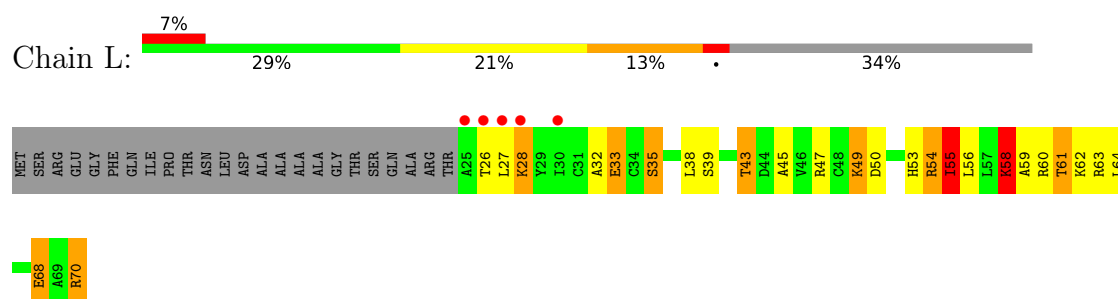
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



• 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(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*TP)-3'

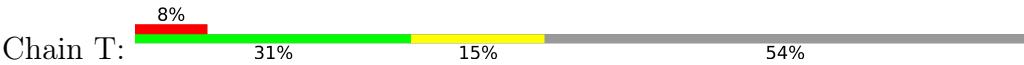


• Molecule 14: TRANSCRIPT RNA 5'-R(*AP*GP*GP*A)-3'





● Molecule 15: TEMPLATE DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.09Å 392.97Å 281.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.89 – 3.50 48.89 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.89-3.50) 95.8 (48.89-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.166 , 0.197 (Not available) , 0.230	Depositor DCC
R_{free} test set	3021 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	112.6	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 114.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.025 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.023 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31612	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: BRU, ZN, MG

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	7/11374 (0.1%)	1.56	137/15383 (0.9%)
2	B	0.89	1/9029 (0.0%)	1.51	113/12171 (0.9%)
3	C	0.85	0/2133	1.45	14/2891 (0.5%)
4	D	0.87	1/1444 (0.1%)	1.65	21/1935 (1.1%)
5	E	0.83	0/1788	1.48	20/2406 (0.8%)
6	F	1.00	1/691 (0.1%)	1.42	6/933 (0.6%)
7	G	0.86	1/1368 (0.1%)	1.39	11/1844 (0.6%)
8	H	0.90	0/1086	1.46	15/1470 (1.0%)
9	I	0.81	1/989 (0.1%)	1.34	11/1331 (0.8%)
10	J	0.90	1/541 (0.2%)	1.56	10/727 (1.4%)
11	K	0.81	0/938	1.37	6/1267 (0.5%)
12	L	0.99	0/365	1.73	11/485 (2.3%)
13	N	0.53	0/94	0.58	0/143
14	P	0.75	0/101	0.69	0/156
15	T	0.60	0/245	0.69	0/373
All	All	0.89	13/32186 (0.0%)	1.50	375/43515 (0.9%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	PRO	C-N	6.11	1.42	1.33
1	A	867	ILE	CG1-CD1	6.08	1.75	1.51
2	B	881	ASN	C-N	5.99	1.41	1.33
7	G	1	MET	C-N	5.96	1.42	1.33
1	A	57	ARG	CA-C	5.76	1.60	1.52
1	A	57	ARG	C-N	5.72	1.41	1.33
1	A	54	ASN	CA-C	5.71	1.60	1.52
10	J	49	MET	SD-CE	-5.67	1.65	1.79
6	F	93	ILE	CG1-CD1	-5.28	1.31	1.51
9	I	119	THR	CA-C	5.27	1.58	1.52
4	D	18	VAL	CA-C	5.20	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	MET	SD-CE	5.07	1.92	1.79
1	A	1398	MET	SD-CE	5.04	1.92	1.79

All (375) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	THR	N-CA-C	-12.13	96.64	112.41
2	B	1016	ALA	CA-C-N	10.39	128.64	120.33
2	B	1016	ALA	C-N-CA	10.39	128.64	120.33
1	A	34	LYS	CA-C-N	10.29	140.22	121.70
1	A	34	LYS	C-N-CA	10.29	140.22	121.70
4	D	54	GLU	N-CA-C	-9.68	100.69	111.14
1	A	341	MET	CA-C-N	9.48	128.91	121.61
1	A	341	MET	C-N-CA	9.48	128.91	121.61
1	A	42	ASP	CA-CB-CG	9.08	121.68	112.60
3	C	39	ALA	N-CA-C	9.04	124.61	111.87
5	E	150	VAL	N-CA-C	8.90	116.37	107.55
8	H	81	PRO	N-CA-C	8.73	121.35	110.70
1	A	72	GLU	N-CA-C	8.62	121.45	111.11
7	G	34	VAL	N-CA-C	7.88	117.99	110.42
1	A	194	ALA	CA-C-N	7.87	135.87	121.70
1	A	194	ALA	C-N-CA	7.87	135.87	121.70
2	B	1155	SER	CA-C-N	7.84	132.58	120.82
2	B	1155	SER	C-N-CA	7.84	132.58	120.82
1	A	56	PRO	CA-C-N	7.77	136.38	121.54
1	A	56	PRO	C-N-CA	7.77	136.38	121.54
2	B	338	GLY	CA-C-N	7.70	135.56	121.70
2	B	338	GLY	C-N-CA	7.70	135.56	121.70
2	B	296	GLU	N-CA-C	-7.61	102.33	111.69
10	J	5	VAL	N-CA-C	-7.60	99.77	109.58
12	L	32	ALA	N-CA-C	7.50	120.34	111.71
4	D	25	ALA	CA-C-N	7.49	134.25	122.49
4	D	25	ALA	C-N-CA	7.49	134.25	122.49
2	B	1017	ILE	N-CA-C	7.42	121.25	112.35
1	A	445	ASN	CA-CB-CG	7.25	119.85	112.60
1	A	311	GLN	N-CA-C	7.22	125.77	109.81
1	A	672	ASP	CA-CB-CG	7.14	119.74	112.60
4	D	188	ALA	N-CA-C	-7.13	103.55	111.82
2	B	198	ASP	CA-C-N	7.12	131.14	120.31
2	B	198	ASP	C-N-CA	7.12	131.14	120.31
8	H	92	ASP	N-CA-C	-7.11	102.94	113.61
1	A	794	PRO	CA-C-N	7.04	129.59	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	794	PRO	C-N-CA	7.04	129.59	120.44
8	H	36	CYS	N-CA-C	7.04	120.15	108.96
2	B	1009	ASP	N-CA-C	-7.03	103.69	112.90
2	B	1156	ASP	N-CA-C	7.00	122.92	111.37
2	B	188	ASP	CA-CB-CG	6.98	119.58	112.60
2	B	43	LEU	N-CA-C	6.97	121.23	112.87
1	A	54	ASN	CA-CB-CG	6.96	119.56	112.60
8	H	129	TYR	N-CA-C	6.94	120.22	111.69
2	B	1169	MET	CA-C-N	6.88	129.81	120.38
2	B	1169	MET	C-N-CA	6.88	129.81	120.38
2	B	320	ASP	CA-CB-CG	6.86	119.46	112.60
5	E	95	THR	CA-C-N	6.86	129.77	120.38
5	E	95	THR	C-N-CA	6.86	129.77	120.38
2	B	359	GLU	N-CA-C	6.85	118.82	111.36
5	E	60	PHE	CA-CB-CG	6.85	120.65	113.80
1	A	399	HIS	CA-CB-CG	-6.79	107.01	113.80
12	L	55	ILE	N-CA-CB	6.78	118.02	110.62
1	A	219	PHE	CA-CB-CG	6.77	120.57	113.80
8	H	83	GLN	CA-C-N	6.75	131.50	120.63
8	H	83	GLN	C-N-CA	6.75	131.50	120.63
10	J	9	SER	N-CA-C	6.75	118.52	111.03
12	L	49	LYS	CA-C-N	6.75	134.43	121.54
12	L	49	LYS	C-N-CA	6.75	134.43	121.54
3	C	135	GLN	CA-C-N	6.73	131.34	121.31
3	C	135	GLN	C-N-CA	6.73	131.34	121.31
1	A	399	HIS	N-CA-CB	6.72	122.34	110.37
2	B	998	ASP	CA-CB-CG	6.70	119.30	112.60
2	B	1102	LYS	CA-C-N	6.70	129.74	120.49
2	B	1102	LYS	C-N-CA	6.70	129.74	120.49
1	A	218	ASP	CA-CB-CG	6.67	119.28	112.60
1	A	34	LYS	N-CA-C	-6.66	96.16	108.02
1	A	68	GLN	CA-C-N	6.66	134.26	121.54
1	A	68	GLN	C-N-CA	6.66	134.26	121.54
4	D	189	ASP	CA-CB-CG	6.60	119.20	112.60
10	J	13	VAL	CA-C-N	-6.59	114.83	122.14
10	J	13	VAL	C-N-CA	-6.59	114.83	122.14
1	A	495	GLU	N-CA-C	-6.56	105.24	113.18
2	B	732	SER	N-CA-C	6.55	118.73	108.96
2	B	1013	ASN	N-CA-C	6.55	117.90	109.65
2	B	1122	ARG	CA-C-N	6.55	129.38	120.54
2	B	1122	ARG	C-N-CA	6.55	129.38	120.54
1	A	71	GLN	CA-C-N	6.54	129.37	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	GLN	C-N-CA	6.54	129.37	120.54
2	B	628	THR	CA-C-N	6.47	133.90	121.54
2	B	628	THR	C-N-CA	6.47	133.90	121.54
1	A	35	ILE	N-CA-CB	6.46	122.47	111.50
4	D	31	GLN	N-CA-C	-6.45	104.18	111.14
11	K	2	ASN	N-CA-C	-6.45	103.94	113.61
4	D	133	THR	N-CA-C	6.43	118.17	111.03
10	J	14	VAL	CB-CA-C	6.33	117.46	110.62
7	G	12	THR	CA-C-N	6.33	130.55	121.50
7	G	12	THR	C-N-CA	6.33	130.55	121.50
3	C	145	CYS	N-CA-C	6.32	116.42	108.45
2	B	707	PRO	CA-C-N	6.30	130.28	120.82
2	B	707	PRO	C-N-CA	6.30	130.28	120.82
1	A	557	ASP	CA-CB-CG	6.29	118.89	112.60
2	B	703	ILE	N-CA-C	6.29	118.08	108.71
12	L	55	ILE	N-CA-C	6.29	116.40	110.30
1	A	223	GLY	CA-C-N	6.25	133.48	121.54
1	A	223	GLY	C-N-CA	6.25	133.48	121.54
1	A	5	GLN	N-CA-C	6.24	118.98	110.55
2	B	581	PHE	CA-CB-CG	6.22	120.02	113.80
1	A	510	GLN	N-CA-C	6.21	120.33	112.87
1	A	614	PHE	CA-CB-CG	6.20	120.00	113.80
1	A	1403	GLU	N-CA-C	6.20	124.01	110.80
1	A	602	ASP	CA-CB-CG	6.19	118.79	112.60
12	L	60	ARG	N-CA-C	6.19	118.28	110.24
2	B	902	GLY	CA-C-N	6.17	129.71	120.69
2	B	902	GLY	C-N-CA	6.17	129.71	120.69
4	D	197	SER	N-CA-C	-6.17	105.89	113.41
1	A	1072	ILE	N-CA-C	-6.14	106.28	111.56
2	B	294	ASP	N-CA-C	-6.12	102.45	110.53
2	B	66	ASP	CA-C-N	6.11	128.39	120.44
2	B	66	ASP	C-N-CA	6.11	128.39	120.44
6	F	87	LYS	CA-C-N	6.11	128.97	120.29
6	F	87	LYS	C-N-CA	6.11	128.97	120.29
10	J	16	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	452	LYS	N-CA-C	-6.09	104.75	111.82
12	L	64	LEU	N-CA-C	6.07	119.79	110.20
5	E	171	LYS	N-CA-C	-6.06	100.41	110.17
1	A	424	ILE	CA-C-N	-6.06	114.36	122.42
1	A	424	ILE	C-N-CA	-6.06	114.36	122.42
2	B	1028	GLU	CA-C-N	6.06	128.65	120.65
2	B	1028	GLU	C-N-CA	6.06	128.65	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	53	GLY	CA-C-N	6.06	128.39	120.28
9	I	53	GLY	C-N-CA	6.06	128.39	120.28
1	A	71	GLN	N-CA-C	6.04	120.19	112.34
1	A	886	ILE	N-CA-C	6.03	116.50	110.23
1	A	1266	THR	N-CA-C	-6.03	104.62	111.07
4	D	51	ASN	CA-CB-CG	6.00	118.60	112.60
2	B	903	VAL	N-CA-C	5.98	117.14	109.30
1	A	677	ARG	CA-C-N	5.98	128.57	120.38
1	A	677	ARG	C-N-CA	5.98	128.57	120.38
2	B	881	ASN	CA-C-N	5.97	128.53	120.65
2	B	881	ASN	C-N-CA	5.97	128.53	120.65
2	B	1183	LYS	N-CA-C	-5.97	101.57	110.23
1	A	998	LEU	N-CA-C	5.97	119.25	109.76
7	G	117	GLN	CA-C-N	5.96	128.54	120.38
7	G	117	GLN	C-N-CA	5.96	128.54	120.38
1	A	78	PRO	CA-C-N	-5.96	113.13	120.64
1	A	78	PRO	C-N-CA	-5.96	113.13	120.64
1	A	637	LYS	N-CA-C	5.95	120.61	113.23
1	A	1001	ARG	N-CA-C	5.94	121.19	113.88
2	B	208	SER	N-CA-C	5.92	119.25	110.48
8	H	34	ASP	CA-C-N	5.91	129.00	120.38
8	H	34	ASP	C-N-CA	5.91	129.00	120.38
2	B	976	ILE	N-CA-C	5.87	119.31	111.44
2	B	215	GLN	CA-C-N	5.86	129.08	120.82
2	B	215	GLN	C-N-CA	5.86	129.08	120.82
1	A	1361	SER	N-CA-C	5.85	117.84	110.24
2	B	472	ALA	CA-C-N	5.85	132.71	121.54
2	B	472	ALA	C-N-CA	5.85	132.71	121.54
12	L	62	LYS	N-CA-C	-5.84	105.65	112.89
2	B	45	SER	CA-C-N	5.84	128.42	120.54
2	B	45	SER	C-N-CA	5.84	128.42	120.54
2	B	733	HIS	CA-C-N	5.83	129.57	120.82
2	B	733	HIS	C-N-CA	5.83	129.57	120.82
2	B	228	LYS	CA-C-N	5.81	132.63	121.54
2	B	228	LYS	C-N-CA	5.81	132.63	121.54
8	H	110	ASP	CA-CB-CG	5.80	118.41	112.60
1	A	636	GLU	N-CA-C	5.80	118.07	111.11
11	K	25	THR	CA-C-N	5.79	128.31	120.38
11	K	25	THR	C-N-CA	5.79	128.31	120.38
2	B	397	ASP	CA-CB-CG	5.79	118.39	112.60
8	H	12	VAL	N-CA-C	5.79	115.88	108.12
7	G	163	ILE	N-CA-C	-5.78	105.76	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1222	ARG	N-CA-C	5.77	118.34	111.71
5	E	172	GLU	CA-C-N	5.76	128.32	120.54
5	E	172	GLU	C-N-CA	5.76	128.32	120.54
1	A	1054	LEU	CA-C-N	5.74	128.25	120.38
1	A	1054	LEU	C-N-CA	5.74	128.25	120.38
1	A	495	GLU	CB-CG-CD	5.73	122.34	112.60
3	C	183	TRP	N-CA-C	-5.73	98.41	108.20
2	B	882	THR	N-CA-C	5.73	117.21	110.97
1	A	526	ASP	CA-CB-CG	5.72	118.33	112.60
2	B	958	GLN	CA-C-N	5.72	127.94	120.28
2	B	958	GLN	C-N-CA	5.72	127.94	120.28
3	C	17	ASN	N-CA-C	5.70	118.78	108.69
2	B	836	GLU	CB-CG-CD	5.70	122.29	112.60
2	B	454	THR	CA-C-N	5.67	128.15	120.38
2	B	454	THR	C-N-CA	5.67	128.15	120.38
3	C	221	TYR	CA-C-N	5.65	128.41	120.28
3	C	221	TYR	C-N-CA	5.65	128.41	120.28
2	B	418	LYS	CA-C-N	5.65	128.16	120.54
2	B	418	LYS	C-N-CA	5.65	128.16	120.54
11	K	84	LYS	CA-C-N	5.64	127.78	120.44
11	K	84	LYS	C-N-CA	5.64	127.78	120.44
1	A	245	PRO	CA-C-N	5.63	130.47	121.34
1	A	245	PRO	C-N-CA	5.63	130.47	121.34
1	A	462	VAL	N-CA-CB	5.63	117.07	110.82
1	A	331	GLY	CA-C-N	5.62	132.28	121.54
1	A	331	GLY	C-N-CA	5.62	132.28	121.54
1	A	1435	PRO	CA-C-N	5.62	130.82	123.06
1	A	1435	PRO	C-N-CA	5.62	130.82	123.06
7	G	33	GLU	CA-C-N	5.61	127.63	120.56
7	G	33	GLU	C-N-CA	5.61	127.63	120.56
9	I	113	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	818	MET	CA-C-N	5.60	126.16	119.94
1	A	818	MET	C-N-CA	5.60	126.16	119.94
1	A	375	THR	N-CA-C	5.59	117.51	108.34
1	A	575	LYS	CA-C-N	5.58	128.07	120.54
1	A	575	LYS	C-N-CA	5.58	128.07	120.54
1	A	54	ASN	CA-C-N	5.57	135.39	121.80
1	A	54	ASN	C-N-CA	5.57	135.39	121.80
9	I	93	LYS	CA-C-N	5.56	130.03	121.19
9	I	93	LYS	C-N-CA	5.56	130.03	121.19
1	A	244	PRO	N-CA-C	5.56	117.48	110.70
1	A	481	ASP	CA-CB-CG	5.55	118.15	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1032	LEU	N-CA-C	5.55	118.52	111.69
1	A	485	ASP	CA-CB-CG	5.55	118.15	112.60
5	E	5	ASN	N-CA-C	-5.54	105.64	112.90
2	B	905	VAL	CA-C-O	-5.54	117.31	121.68
1	A	854	ASN	CA-C-N	5.54	128.73	120.87
1	A	854	ASN	C-N-CA	5.54	128.73	120.87
4	D	40	HIS	CA-C-N	5.52	128.44	120.38
4	D	40	HIS	C-N-CA	5.52	128.44	120.38
1	A	69	THR	N-CA-CB	5.51	119.80	110.49
2	B	340	ALA	CA-C-N	5.51	132.07	121.54
2	B	340	ALA	C-N-CA	5.51	132.07	121.54
1	A	310	GLY	CA-C-N	5.50	135.21	121.80
1	A	310	GLY	C-N-CA	5.50	135.21	121.80
1	A	1168	GLU	CA-C-N	5.50	128.28	120.53
1	A	1168	GLU	C-N-CA	5.50	128.28	120.53
9	I	94	ASP	CA-C-N	5.49	132.03	121.54
9	I	94	ASP	C-N-CA	5.49	132.03	121.54
1	A	963	ILE	N-CA-CB	5.49	116.97	110.55
1	A	1311	VAL	CA-C-N	5.49	129.44	121.26
1	A	1311	VAL	C-N-CA	5.49	129.44	121.26
1	A	1404	GLU	N-CA-C	5.48	119.66	112.92
7	G	45	ILE	N-CA-C	-5.48	99.84	108.23
9	I	112	SER	CA-C-N	5.47	128.88	121.05
9	I	112	SER	C-N-CA	5.47	128.88	121.05
6	F	114	GLU	N-CA-C	5.47	118.16	109.96
1	A	890	ASP	CA-C-N	5.46	127.87	120.44
1	A	890	ASP	C-N-CA	5.46	127.87	120.44
1	A	1117	THR	CB-CA-C	5.46	120.61	111.22
2	B	1101	ASP	N-CA-C	-5.44	106.81	113.50
2	B	1201	LYS	N-CA-C	-5.43	105.36	111.28
2	B	203	PHE	CA-CB-CG	5.43	119.23	113.80
8	H	59	ILE	CB-CA-C	5.43	120.20	111.29
10	J	8	PHE	CA-CB-CG	5.43	119.23	113.80
5	E	182	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	398	GLU	CA-C-O	-5.43	115.04	121.66
6	F	83	PRO	N-CA-C	-5.42	106.95	114.27
1	A	440	ASP	CA-CB-CG	5.42	118.02	112.60
4	D	7	THR	CA-C-N	5.41	128.08	120.28
4	D	7	THR	C-N-CA	5.41	128.08	120.28
3	C	82	TYR	N-CA-C	-5.41	101.16	109.76
5	E	66	GLU	CA-C-N	5.40	127.52	120.28
5	E	66	GLU	C-N-CA	5.40	127.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ASN	N-CA-C	-5.38	103.43	110.53
1	A	91	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	472	LEU	N-CA-C	5.38	119.10	112.54
1	A	866	PHE	CA-CB-CG	-5.37	108.43	113.80
2	B	401	PHE	N-CA-C	5.37	117.21	111.36
1	A	55	ASP	N-CA-CB	5.37	119.92	110.37
4	D	20	GLU	CA-C-N	5.36	129.29	121.31
4	D	20	GLU	C-N-CA	5.36	129.29	121.31
1	A	317	LYS	CA-C-N	5.35	131.77	121.54
1	A	317	LYS	C-N-CA	5.35	131.77	121.54
2	B	414	ALA	CA-C-N	5.35	127.45	120.28
2	B	414	ALA	C-N-CA	5.35	127.45	120.28
5	E	5	ASN	CA-C-N	5.35	127.98	120.28
5	E	5	ASN	C-N-CA	5.35	127.98	120.28
7	G	141	SER	N-CA-C	5.30	117.91	110.23
1	A	592	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	544	ASP	CA-C-N	5.29	127.63	120.44
1	A	544	ASP	C-N-CA	5.29	127.63	120.44
2	B	1129	ARG	N-CA-C	5.28	117.85	109.24
5	E	8	ASN	CA-C-N	5.28	127.32	120.88
5	E	8	ASN	C-N-CA	5.28	127.32	120.88
10	J	60	PHE	CA-CB-CG	5.28	119.08	113.80
5	E	196	VAL	N-CA-CB	5.27	119.29	110.86
5	E	24	LYS	CA-C-N	5.27	127.34	120.28
5	E	24	LYS	C-N-CA	5.27	127.34	120.28
11	K	71	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	1419	ASP	CA-C-N	5.26	128.31	120.31
1	A	1419	ASP	C-N-CA	5.26	128.31	120.31
3	C	45	ALA	CA-C-N	5.26	128.37	120.69
3	C	45	ALA	C-N-CA	5.26	128.37	120.69
8	H	85	GLY	N-CA-C	-5.26	106.42	112.73
4	D	31	GLN	CA-C-N	5.25	127.59	120.65
4	D	31	GLN	C-N-CA	5.25	127.59	120.65
1	A	466	SER	N-CA-C	5.25	121.99	110.80
2	B	945	GLU	CA-C-N	5.25	131.57	121.54
2	B	945	GLU	C-N-CA	5.25	131.57	121.54
6	F	143	PHE	N-CA-C	5.25	117.05	109.07
1	A	1118	VAL	N-CA-C	5.25	115.18	107.15
2	B	908	GLU	N-CA-C	-5.25	103.73	111.81
2	B	415	GLN	CA-C-N	5.24	127.57	120.44
2	B	415	GLN	C-N-CA	5.24	127.57	120.44
2	B	945	GLU	N-CA-C	5.24	116.69	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1072	ILE	CA-C-N	5.24	125.91	119.99
1	A	1072	ILE	C-N-CA	5.24	125.91	119.99
2	B	464	GLY	N-CA-C	-5.24	107.31	114.64
2	B	874	PHE	CA-CB-CG	5.23	119.03	113.80
1	A	1403	GLU	CA-C-N	-5.22	114.29	122.65
1	A	1403	GLU	C-N-CA	-5.22	114.29	122.65
1	A	423	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	375	THR	CB-CA-C	5.22	118.49	110.14
1	A	985	ASP	CA-CB-CG	5.22	117.82	112.60
2	B	1001	PHE	N-CA-C	5.22	118.24	109.95
3	C	136	ASP	CA-CB-CG	5.22	117.82	112.60
10	J	26	GLN	CA-C-N	5.21	127.22	120.44
10	J	26	GLN	C-N-CA	5.21	127.22	120.44
7	G	13	LEU	N-CA-C	5.21	118.04	109.76
8	H	38	LEU	N-CA-C	5.21	117.08	108.13
2	B	1133	MET	N-CA-C	5.21	116.95	111.28
2	B	69	LEU	CA-C-N	5.18	131.03	121.70
2	B	69	LEU	C-N-CA	5.18	131.03	121.70
1	A	33	ALA	CA-C-N	5.18	130.22	122.86
1	A	33	ALA	C-N-CA	5.18	130.22	122.86
5	E	123	LEU	CA-C-N	5.18	124.47	120.33
5	E	123	LEU	C-N-CA	5.18	124.47	120.33
2	B	957	ASN	CA-CB-CG	5.18	117.78	112.60
2	B	429	PHE	CA-CB-CG	5.17	118.97	113.80
2	B	736	THR	N-CA-C	-5.17	105.64	112.94
9	I	31	THR	N-CA-C	-5.17	105.80	112.68
6	F	154	ASP	N-CA-C	-5.17	104.57	111.24
1	A	1167	GLU	CA-C-N	5.17	127.48	120.65
1	A	1167	GLU	C-N-CA	5.17	127.48	120.65
1	A	285	PRO	CA-C-N	5.17	131.41	121.54
1	A	285	PRO	C-N-CA	5.17	131.41	121.54
2	B	722	ASP	CA-C-N	5.17	127.43	120.50
2	B	722	ASP	C-N-CA	5.17	127.43	120.50
1	A	253	ASN	CA-CB-CG	5.16	117.76	112.60
8	H	45	GLU	N-CA-C	-5.16	105.57	111.14
1	A	25	GLU	CA-C-N	5.15	127.61	120.29
1	A	25	GLU	C-N-CA	5.15	127.61	120.29
1	A	204	THR	CA-C-N	5.15	127.19	120.28
1	A	204	THR	C-N-CA	5.15	127.19	120.28
4	D	7	THR	N-CA-C	5.13	116.09	108.86
2	B	181	LEU	N-CA-C	5.11	117.59	111.71
1	A	173	THR	CB-CA-C	5.11	119.98	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	116	ASN	N-CA-C	5.10	117.43	109.52
12	L	58	LYS	N-CA-C	5.10	121.26	113.61
1	A	1376	THR	CB-CA-C	5.10	119.35	110.79
2	B	41	LYS	N-CA-C	5.10	116.69	111.03
1	A	1402	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	333	GLU	CB-CG-CD	5.09	121.26	112.60
2	B	628	THR	N-CA-C	-5.09	107.23	113.50
1	A	193	ASP	CA-C-N	5.09	130.86	121.70
1	A	193	ASP	C-N-CA	5.09	130.86	121.70
2	B	331	LEU	CA-C-N	5.08	127.09	120.28
2	B	331	LEU	C-N-CA	5.08	127.09	120.28
2	B	432	MET	CA-C-N	5.08	127.36	120.65
2	B	432	MET	C-N-CA	5.08	127.36	120.65
3	C	222	LYS	CA-C-N	5.06	127.89	120.71
3	C	222	LYS	C-N-CA	5.06	127.89	120.71
8	H	60	ALA	N-CA-C	5.06	121.57	110.80
1	A	1165	GLU	CA-C-N	5.05	127.31	120.38
1	A	1165	GLU	C-N-CA	5.05	127.31	120.38
2	B	991	GLY	CA-C-N	5.05	127.02	121.97
2	B	991	GLY	C-N-CA	5.05	127.02	121.97
2	B	196	PRO	CA-C-N	5.05	127.04	120.28
2	B	196	PRO	C-N-CA	5.05	127.04	120.28
1	A	1325	THR	N-CA-C	-5.04	107.81	114.31
1	A	17	VAL	N-CA-CB	5.04	118.25	111.90
2	B	199	MET	N-CA-C	5.04	117.66	111.82
4	D	188	ALA	CA-C-N	5.04	127.34	120.54
4	D	188	ALA	C-N-CA	5.04	127.34	120.54
2	B	1181	GLU	N-CA-C	5.04	121.53	110.80
2	B	627	PHE	N-CA-C	5.03	116.59	108.34
1	A	1021	LEU	CA-C-N	5.03	127.33	120.54
1	A	1021	LEU	C-N-CA	5.03	127.33	120.54
2	B	732	SER	CA-C-N	5.03	131.00	122.65
2	B	732	SER	C-N-CA	5.03	131.00	122.65
2	B	918	ILE	N-CA-C	5.03	115.61	108.42
2	B	1221	SER	CA-C-N	5.03	127.52	120.28
2	B	1221	SER	C-N-CA	5.03	127.52	120.28
1	A	329	LEU	CA-C-N	5.02	127.90	120.82
1	A	329	LEU	C-N-CA	5.02	127.90	120.82
1	A	721	PHE	CA-CB-CG	5.02	118.82	113.80
1	A	781	ASP	CA-CB-CG	5.01	117.61	112.60
2	B	276	ILE	CA-C-N	5.00	127.75	120.79
2	B	276	ILE	C-N-CA	5.00	127.75	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	43	THR	CA-C-N	5.00	127.88	120.17
12	L	43	THR	C-N-CA	5.00	127.88	120.17
2	B	1071	VAL	N-CA-CB	5.00	116.55	110.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11174	0	11233	193	0
2	B	8859	0	8901	183	0
3	C	2095	0	2051	48	0
4	D	1434	0	1460	22	0
5	E	1752	0	1776	30	0
6	F	679	0	701	23	0
7	G	1340	0	1357	27	0
8	H	1068	0	1040	20	0
9	I	971	0	927	13	0
10	J	532	0	542	16	0
11	K	920	0	929	14	0
12	L	363	0	386	9	0
13	N	84	0	46	3	0
14	P	90	0	45	1	0
15	T	242	0	136	3	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	31612	0	31530	535	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 8.

All (535) 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	1.56
1:A:53:LEU:HD23	1:A:54:ASN:H	1.27	0.98
7:G:1:MET:HE1	7:G:80:LYS:O	1.60	0.98
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.46	0.97
6:F:90:ARG:HH11	6:F:90:ARG:HG3	1.31	0.94
1:A:855:THR:HG21	1:A:857:ARG:HE	1.32	0.94
1:A:35:ILE:HG21	1:A:241:VAL:HG21	1.46	0.92
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.55	0.88
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.40	0.85
12:L:28:LYS:HB2	12:L:39:SER:HA	1.58	0.83
3:C:56:THR:HG21	3:C:145:CYS:SG	2.19	0.82
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.61	0.82
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.61	0.82
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.61	0.81
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.65	0.79
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.48	0.79
2:B:126:SER:HB2	2:B:172:ILE:HD11	1.63	0.79
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.63	0.79
8:H:47:PHE:HB3	8:H:95:TYR:HD2	1.49	0.78
3:C:46:ILE:HD12	3:C:46:ILE:H	1.47	0.78
2:B:1172:ILE:HD11	2:B:1183:LYS:HE2	1.65	0.77
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.67	0.76
8:H:47:PHE:HB3	8:H:95:TYR:CD2	2.22	0.75
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.67	0.75
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.68	0.75
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.69	0.74
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.70	0.74
2:B:428:ILE:HG22	2:B:432:MET:HE2	1.71	0.73
1:A:53:LEU:HD23	1:A:54:ASN:N	2.04	0.73
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.72	0.71
1:A:855:THR:CG2	1:A:857:ARG:HE	2.04	0.71
3:C:46:ILE:HD13	3:C:67:LEU:O	1.91	0.71
1:A:216:VAL:O	1:A:220:THR:HB	1.91	0.70
2:B:705:MET:H	2:B:710:LEU:HD12	1.56	0.70
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.73	0.70
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.74	0.70
2:B:168:GLY:H	2:B:450:ALA:HB1	1.57	0.70
10:J:48:ARG:HE	10:J:49:MET:HE2	1.56	0.69
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.32	0.69
3:C:66:ARG:NH2	10:J:3:VAL:O	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.76	0.68
2:B:247:GLY:H	2:B:418:LYS:HZ1	1.41	0.68
8:H:82:PRO:C	8:H:84:ALA:H	2.02	0.67
2:B:882:THR:HG1	2:B:935:ARG:N	1.92	0.67
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.74	0.67
3:C:43:THR:HG22	3:C:44:LEU:H	1.60	0.67
1:A:64:ASN:O	1:A:65:LEU:HB3	1.93	0.67
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.75	0.66
2:B:809:MET:HE1	2:B:983:ARG:HH21	1.60	0.66
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.75	0.66
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.78	0.66
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.78	0.65
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.78	0.65
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.77	0.65
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.97	0.65
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.80	0.64
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.79	0.64
4:D:40:HIS:HA	7:G:73:LYS:HE3	1.80	0.64
3:C:56:THR:HG23	3:C:147:LEU:HD23	1.78	0.64
1:A:646:PHE:O	1:A:650:GLN:HG2	1.97	0.64
2:B:126:SER:CB	2:B:172:ILE:HD11	2.28	0.64
2:B:558:LEU:HB3	2:B:563:MET:HE3	1.80	0.64
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.78	0.64
1:A:49:LYS:HD3	1:A:61:ILE:HG13	1.80	0.64
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.79	0.63
9:I:50:THR:HG22	9:I:52:ILE:H	1.63	0.63
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.29	0.63
1:A:857:ARG:HD3	1:A:861:GLY:O	1.99	0.62
2:B:70:ILE:HD13	2:B:429:PHE:HZ	1.64	0.62
1:A:1387:HIS:CE1	13:N:4:DG:H4'	2.34	0.62
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.80	0.62
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.33	0.62
7:G:1:MET:SD	7:G:2:PHE:N	2.68	0.62
2:B:878:GLN:HA	2:B:885:MET:HE1	1.82	0.62
1:A:53:LEU:CD2	1:A:54:ASN:H	2.09	0.61
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.64	0.61
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.31	0.61
2:B:918:ILE:HD13	2:B:935:ARG:HH12	1.65	0.61
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.82	0.61
1:A:869:GLY:O	5:E:204:THR:HG21	2.02	0.60
2:B:247:GLY:H	2:B:418:LYS:NZ	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.83	0.60
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.83	0.60
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.84	0.60
2:B:826:ALA:HB2	2:B:1087:PHE:CD1	2.37	0.60
6:F:94:LEU:HD21	6:F:125:LEU:HD22	1.84	0.60
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.82	0.60
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.84	0.59
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.83	0.59
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.84	0.59
4:D:32:GLU:HG3	7:G:5:LYS:NZ	2.18	0.59
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.68	0.59
5:E:100:ILE:HA	5:E:105:PHE:HD2	1.67	0.59
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.36	0.59
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.84	0.59
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.84	0.59
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.83	0.59
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.02	0.58
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.67	0.58
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.86	0.58
11:K:82:ASP:OD2	11:K:84:LYS:HB2	2.04	0.58
1:A:565:ILE:O	1:A:570:PRO:HA	2.04	0.58
2:B:1168:LEU:HB2	2:B:1170:THR:OG1	2.04	0.58
8:H:127:GLY:N	8:H:130:ARG:HH21	2.01	0.58
1:A:310:GLY:O	1:A:312:PRO:HD2	2.04	0.57
1:A:446:ARG:HB2	1:A:487:MET:SD	2.44	0.57
1:A:11:LEU:HB2	2:B:1193:GLN:HG2	1.87	0.57
1:A:548:ASN:HD21	11:K:47:ARG:HH21	1.51	0.57
1:A:75:ASN:O	1:A:76:GLU:HB2	2.05	0.57
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.85	0.57
6:F:90:ARG:HH11	6:F:90:ARG:CG	2.07	0.57
1:A:567:LYS:HA	1:A:569:LYS:N	2.20	0.57
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.87	0.57
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.05	0.57
1:A:709:THR:HB	1:A:712:GLU:H	1.70	0.56
8:H:63:LEU:C	8:H:90:ALA:HB3	2.30	0.56
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.41	0.56
3:C:22:LEU:HD22	3:C:230:MET:HE1	1.87	0.56
8:H:15:VAL:HG22	8:H:26:ILE:HD11	1.88	0.56
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.87	0.56
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.88	0.56
8:H:89:LEU:C	8:H:91:ASP:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:TYR:HA	1:A:936:LEU:HD12	1.88	0.56
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.88	0.56
1:A:120:GLU:HA	1:A:123:ARG:HG2	1.88	0.55
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.88	0.55
9:I:4:PHE:HE2	9:I:13:MET:HB2	1.71	0.55
1:A:61:ILE:HG22	1:A:62:ASP:H	1.70	0.55
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.87	0.55
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.88	0.55
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.88	0.55
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.89	0.55
2:B:425:THR:HA	2:B:428:ILE:HD12	1.88	0.55
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.71	0.55
8:H:95:TYR:HE1	8:H:97:MET:HG3	1.72	0.55
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.88	0.55
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.72	0.54
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.89	0.54
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.88	0.54
2:B:662:MET:HA	2:B:665:GLU:HB2	1.89	0.54
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.89	0.54
3:C:149:LYS:HG3	3:C:150:GLY:H	1.72	0.54
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.89	0.54
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.05	0.54
6:F:90:ARG:HG3	6:F:90:ARG:NH1	2.09	0.54
10:J:1:MET:HG3	10:J:60:PHE:CE2	2.37	0.54
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.90	0.54
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.89	0.54
2:B:1166:CYS:O	2:B:1168:LEU:N	2.41	0.54
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.90	0.54
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.89	0.54
14:P:8:G:H1	15:T:21:DC:H42	1.56	0.54
6:F:90:ARG:CG	6:F:90:ARG:NH1	2.69	0.53
1:A:34:LYS:HB2	1:A:83:HIS:CE1	2.43	0.53
3:C:100:THR:HG22	3:C:119:VAL:HG13	1.89	0.53
1:A:494:SER:HB3	1:A:497:THR:H	1.74	0.53
3:C:75:MET:HE1	3:C:239:PRO:HG3	1.91	0.53
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.74	0.53
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.90	0.53
1:A:933:TYR:O	1:A:937:VAL:HG23	2.09	0.53
3:C:66:ARG:NH2	10:J:2:ILE:HG23	2.23	0.53
1:A:495:GLU:HG3	6:F:98:ALA:HB1	1.89	0.53
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:846:ILE:HG23	2:B:974:PRO:HD2	1.90	0.53
7:G:34:VAL:O	7:G:37:SER:HB3	2.08	0.53
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.91	0.53
3:C:114:TYR:CD1	3:C:140:ASN:HB3	2.44	0.53
1:A:1451:VAL:HG23	7:G:20:PRO:HB3	1.92	0.52
2:B:34:ILE:HG12	2:B:542:MET:CE	2.40	0.52
5:E:176:PRO:O	5:E:212:ARG:HA	2.09	0.52
1:A:55:ASP:N	1:A:56:PRO:HD3	2.23	0.52
1:A:1445:ILE:HG23	6:F:132:LEU:HD23	1.91	0.52
10:J:48:ARG:HE	10:J:49:MET:CE	2.22	0.52
1:A:568:PRO:HG2	8:H:46:LEU:HD12	1.91	0.52
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.92	0.52
10:J:65:PRO:HB3	12:L:35:SER:OG	2.10	0.52
1:A:1148:ILE:HA	9:I:49:ILE:HD12	1.91	0.52
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.92	0.52
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.92	0.52
2:B:599:THR:O	2:B:603:LEU:HD12	2.10	0.52
1:A:567:LYS:HA	1:A:568:PRO:C	2.35	0.52
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.90	0.51
1:A:315:LEU:HA	1:A:321:PRO:HA	1.93	0.51
1:A:528:LEU:HD23	1:A:751:SER:HA	1.91	0.51
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.92	0.51
3:C:173:ALA:HB2	3:C:243:VAL:HG11	1.91	0.51
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.92	0.51
2:B:68:THR:HG23	2:B:91:SER:HB3	1.91	0.51
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.91	0.51
8:H:95:TYR:CE1	8:H:97:MET:HG3	2.45	0.51
1:A:629:LEU:O	1:A:633:VAL:HG23	2.10	0.51
2:B:246:LYS:HG2	2:B:249:ARG:HH21	1.76	0.51
2:B:841:MET:O	2:B:993:THR:HA	2.10	0.51
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.93	0.51
1:A:254:GLU:HB3	2:B:935:ARG:HH21	1.76	0.51
1:A:135:PHE:HD2	1:A:223:GLY:H	1.58	0.51
1:A:208:LEU:HD22	1:A:212:LYS:HE3	1.93	0.51
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	1.91	0.51
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.93	0.51
3:C:46:ILE:H	3:C:46:ILE:CD1	2.16	0.51
1:A:867:ILE:CD1	1:A:867:ILE:CB	2.80	0.50
12:L:68:GLU:HB2	12:L:70:ARG:HD2	1.93	0.50
3:C:37:MET:HA	3:C:41:ILE:HD12	1.94	0.50
1:A:1172:LEU:C	1:A:1174:PHE:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:MET:HG2	2:B:386:LEU:HD22	1.92	0.50
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.46	0.50
4:D:123:LEU:HD21	4:D:146:GLN:HG2	1.92	0.50
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.94	0.50
3:C:14:SER:O	3:C:240:VAL:HG21	2.11	0.50
1:A:353:ILE:HG12	1:A:487:MET:HG3	1.92	0.50
2:B:976:ILE:HG13	2:B:990:ILE:HG22	1.93	0.50
1:A:370:ILE:HD11	2:B:1103:ILE:HG13	1.94	0.50
2:B:792:MET:HA	2:B:856:PHE:O	2.12	0.50
1:A:506:ALA:H	1:A:509:LEU:HD12	1.77	0.50
5:E:72:PHE:HB2	5:E:75:MET:HB2	1.93	0.50
1:A:1421:CYS:HA	1:A:1426:GLU:HG3	1.94	0.49
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.47	0.49
2:B:210:LYS:NZ	2:B:462:ALA:O	2.46	0.49
2:B:911:ILE:HG23	2:B:966:VAL:HG11	1.93	0.49
8:H:36:CYS:HA	8:H:126:GLU:O	2.12	0.49
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.12	0.49
1:A:846:GLU:HA	1:A:1066:VAL:HG22	1.95	0.49
2:B:487:THR:HG23	2:B:490:SER:H	1.78	0.49
1:A:327:ALA:HA	1:A:330:LYS:HE3	1.95	0.49
2:B:128:LEU:HB2	2:B:167:ILE:O	2.12	0.49
2:B:1104:HIS:HB2	2:B:1122:ARG:HG3	1.95	0.49
5:E:10:SER:O	5:E:14:ARG:HG3	2.13	0.49
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.94	0.49
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.95	0.49
3:C:99:LEU:HB3	3:C:118:LEU:HD22	1.94	0.49
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.94	0.49
2:B:824:ILE:HG22	2:B:1008:PRO:HA	1.94	0.49
5:E:15:ALA:O	5:E:19:VAL:HG23	2.12	0.49
1:A:448:PRO:O	1:A:449:SER:HB2	2.13	0.49
1:A:765:VAL:HG23	1:A:802:ASN:O	2.13	0.49
8:H:100:THR:HG23	8:H:138:GLU:HA	1.94	0.49
2:B:416:LEU:HD11	2:B:460:ALA:HB1	1.93	0.49
1:A:51:GLY:C	1:A:56:PRO:HB3	2.38	0.48
1:A:1325:THR:HA	5:E:147:HIS:HA	1.94	0.48
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.94	0.48
3:C:165:LYS:O	11:K:6:ARG:NH1	2.46	0.48
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.95	0.48
1:A:855:THR:HG21	1:A:857:ARG:NE	2.15	0.48
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.94	0.48
2:B:311:LEU:HA	2:B:314:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.95	0.48
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.79	0.48
7:G:90:THR:HG22	7:G:142:ARG:HG2	1.94	0.48
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.95	0.48
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.48	0.48
1:A:56:PRO:CD	1:A:58:LEU:HG	2.44	0.48
1:A:518:LYS:HE2	1:A:624:SER:O	2.13	0.48
1:A:337:ARG:HD2	2:B:1132:GLU:OE1	2.14	0.48
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.60	0.48
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.49	0.48
2:B:975:GLN:NE2	2:B:1100:ASP:OD2	2.47	0.48
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.44	0.48
1:A:194:ALA:HA	1:A:195:ASP:C	2.39	0.48
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.96	0.48
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.95	0.48
6:F:72:LYS:HE3	6:F:142:SER:OG	2.14	0.48
1:A:866:PHE:O	1:A:867:ILE:HD12	2.14	0.47
5:E:43:LYS:O	5:E:47:CYS:HB2	2.14	0.47
1:A:310:GLY:C	1:A:312:PRO:HD2	2.38	0.47
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.96	0.47
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.95	0.47
2:B:446:LEU:HD12	2:B:448:ILE:HD11	1.96	0.47
6:F:93:ILE:HG12	6:F:148:VAL:HG11	1.95	0.47
7:G:138:THR:HG22	7:G:139:ILE:H	1.78	0.47
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.96	0.47
2:B:563:MET:HG3	2:B:580:VAL:HG21	1.96	0.47
4:D:65:GLU:HA	4:D:68:ARG:HG3	1.96	0.47
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.96	0.47
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.96	0.47
1:A:1189:SER:HB3	1:A:1242:VAL:H	1.79	0.47
2:B:953:LEU:HD11	12:L:55:ILE:HG22	1.97	0.47
4:D:27:LEU:HD23	4:D:197:SER:CB	2.45	0.47
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.95	0.47
2:B:310:MET:O	2:B:313:MET:HB3	2.15	0.47
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.62	0.47
1:A:679:ILE:HG13	1:A:732:LEU:HD13	1.95	0.47
2:B:20:ASP:C	2:B:22:SER:H	2.23	0.47
2:B:766:ARG:HH21	2:B:1020:ARG:HG2	1.78	0.47
1:A:70:CYS:O	1:A:70:CYS:SG	2.72	0.47
1:A:206:GLU:O	1:A:210:ILE:HG12	2.14	0.47
1:A:41:MET:CB	1:A:49:LYS:HA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:MET:HA	1:A:50:ILE:H	1.80	0.46
2:B:283:VAL:HG13	2:B:297:ILE:HD13	1.96	0.46
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.80	0.46
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.96	0.46
1:A:719:VAL:HG23	1:A:774:ARG:HD2	1.97	0.46
1:A:886:ILE:HG12	1:A:943:LEU:HB3	1.97	0.46
2:B:778:MET:O	2:B:819:ALA:HA	2.15	0.46
2:B:839:MET:CE	2:B:980:PHE:HB2	2.44	0.46
6:F:85:MET:HE2	6:F:148:VAL:HG12	1.97	0.46
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.97	0.46
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.97	0.46
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.51	0.46
3:C:66:ARG:HH21	10:J:2:ILE:HG23	1.80	0.46
1:A:709:THR:HG22	1:A:711:ARG:H	1.80	0.46
1:A:344:ARG:CZ	2:B:1120:GLU:HG3	2.45	0.46
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.49	0.46
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.15	0.46
2:B:64:CYS:HA	2:B:67:SER:HB3	1.96	0.46
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.98	0.46
1:A:534:LEU:O	1:A:574:GLY:HA3	2.15	0.46
2:B:70:ILE:HD13	2:B:429:PHE:CZ	2.47	0.46
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.97	0.46
2:B:916:THR:O	2:B:935:ARG:N	2.48	0.46
1:A:453:MET:O	1:A:456:MET:HE2	2.15	0.46
5:E:23:VAL:HG12	5:E:28:TYR:HB2	1.98	0.46
1:A:313:GLN:O	1:A:315:LEU:HG	2.16	0.46
1:A:1387:HIS:HE1	13:N:4:DG:H4'	1.78	0.46
2:B:485:ARG:NH1	2:B:491:THR:HG21	2.30	0.46
2:B:1169:MET:HE3	2:B:1169:MET:HB2	1.85	0.46
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.97	0.46
4:D:8:PHE:HB2	4:D:38:ILE:HB	1.98	0.46
11:K:65:HIS:HE1	11:K:67:PHE:CD1	2.34	0.46
1:A:833:GLU:O	1:A:837:ILE:HD13	2.15	0.45
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.98	0.45
2:B:622:LYS:HE3	9:I:59:VAL:HG22	1.97	0.45
11:K:107:THR:O	11:K:111:LEU:HG	2.16	0.45
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.49	0.45
3:C:251:LEU:O	3:C:255:VAL:HG23	2.16	0.45
6:F:101:ILE:HG12	6:F:107:VAL:HG22	1.99	0.45
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.52	0.45
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:LEU:HD11	4:D:174:PRO:HD2	1.98	0.45
1:A:1436:ILE:O	1:A:1437:GLY:C	2.60	0.45
1:A:1444:MET:HE2	1:A:1444:MET:HB2	1.64	0.45
3:C:58:LEU:HD21	10:J:57:ILE:HD12	1.97	0.45
3:C:149:LYS:C	3:C:151:GLN:H	2.25	0.45
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.16	0.45
2:B:343:ILE:HD13	2:B:344:LYS:H	1.81	0.45
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.52	0.45
2:B:62:ILE:HG23	2:B:418:LYS:HG3	1.99	0.45
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.65	0.45
2:B:1221:SER:HB3	4:D:12:ARG:HD2	1.98	0.45
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.99	0.45
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.98	0.45
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.99	0.44
2:B:338:GLY:HA3	2:B:340:ALA:H	1.82	0.44
2:B:361:LEU:HD11	2:B:381:MET:HE1	1.99	0.44
3:C:148:ARG:HG3	3:C:149:LYS:H	1.82	0.44
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	1.98	0.44
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.48	0.44
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.99	0.44
3:C:184:ASN:HD21	3:C:189:THR:H	1.64	0.44
1:A:836:TYR:HB2	15:T:18:DT:H4'	2.00	0.44
1:A:1400:CYS:HB2	1:A:1405:THR:HA	1.99	0.44
2:B:233:PRO:HG2	2:B:234:ILE:HD12	2.00	0.44
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.81	0.44
3:C:89:GLU:O	3:C:89:GLU:HG2	2.18	0.44
7:G:27:LYS:HD3	7:G:51:TYR:CE1	2.52	0.44
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.57	0.44
1:A:588:LEU:HD23	1:A:607:ILE:HD12	2.00	0.44
3:C:148:ARG:HH11	3:C:149:LYS:HE2	1.82	0.44
1:A:343:LYS:HD3	2:B:1156:ASP:HB2	2.00	0.44
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.98	0.44
1:A:828:ALA:O	1:A:831:THR:HG22	2.18	0.44
2:B:1174:LYS:O	2:B:1176:ASN:N	2.50	0.44
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.00	0.44
6:F:111:LEU:HD12	6:F:111:LEU:H	1.81	0.44
6:F:118:LEU:O	6:F:122:MET:HG3	2.18	0.44
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.53	0.44
12:L:33:GLU:OE1	12:L:55:ILE:HD11	2.18	0.44
1:A:399:HIS:O	1:A:401:GLY:N	2.50	0.44
2:B:564:GLU:HB2	2:B:589:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:755:ILE:HA	2:B:809:MET:HE2	2.00	0.44
2:B:865:LYS:HB2	2:B:961:LEU:HD21	1.98	0.44
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.52	0.44
7:G:31:LEU:HD11	7:G:51:TYR:CE2	2.53	0.44
1:A:443:LEU:HD23	1:A:501:LEU:HD22	1.99	0.44
4:D:32:GLU:HG3	7:G:5:LYS:HZ1	1.80	0.44
5:E:90:VAL:HG23	5:E:123:LEU:HD11	2.00	0.44
10:J:6:ARG:H	10:J:14:VAL:H	1.64	0.44
1:A:50:ILE:HG22	1:A:52:GLY:N	2.33	0.44
1:A:986:ILE:O	1:A:990:VAL:HG23	2.17	0.44
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.99	0.44
2:B:405:ARG:HB3	2:B:631:GLY:HA3	1.99	0.44
1:A:351:THR:HG22	1:A:468:PHE:CD2	2.53	0.44
1:A:354:SER:O	1:A:469:ARG:HA	2.17	0.44
2:B:343:ILE:O	2:B:344:LYS:HB2	2.18	0.44
4:D:52:LEU:HB2	4:D:148:LEU:HD23	1.99	0.44
5:E:16:PHE:CE2	5:E:20:LYS:HE2	2.53	0.44
1:A:866:PHE:C	1:A:867:ILE:HD12	2.43	0.43
13:N:2:DA:H61	15:T:16:DT:H3	1.65	0.43
2:B:351:TYR:O	2:B:352:ALA:HA	2.18	0.43
2:B:429:PHE:HA	2:B:432:MET:HE3	1.99	0.43
2:B:952:VAL:HB	12:L:58:LYS:HB2	2.00	0.43
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.00	0.43
2:B:981:ALA:HB2	2:B:987:LYS:HA	2.00	0.43
3:C:147:LEU:HB3	3:C:151:GLN:HB2	2.00	0.43
1:A:528:LEU:O	1:A:531:ILE:HG22	2.18	0.43
1:A:780:VAL:O	1:A:782:ARG:HD3	2.18	0.43
2:B:234:ILE:HG12	2:B:257:LYS:HB3	2.00	0.43
2:B:364:ILE:HA	2:B:585:VAL:HG13	2.00	0.43
5:E:86:PRO:HA	5:E:113:GLN:HB2	2.00	0.43
11:K:7:PHE:HA	11:K:10:PHE:CZ	2.54	0.43
1:A:50:ILE:C	1:A:52:GLY:H	2.26	0.43
2:B:449:ASN:HD22	2:B:452:THR:HG23	1.84	0.43
2:B:822:ASN:O	10:J:48:ARG:NH1	2.52	0.43
4:D:121:LYS:HA	4:D:124:GLU:HG2	2.00	0.43
9:I:102:VAL:HG22	9:I:109:ILE:HG13	2.00	0.43
2:B:70:ILE:HD12	2:B:70:ILE:H	1.84	0.43
2:B:114:PRO:HG3	2:B:181:LEU:HD11	2.00	0.43
7:G:26:LEU:HD13	7:G:56:ILE:HD11	2.00	0.43
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	2.18	0.43
3:C:183:TRP:O	3:C:185:LYS:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASP:HB3	1:A:64:ASN:O	2.18	0.43
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.66	0.43
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.18	0.43
2:B:999:MET:HG3	2:B:1000:PRO:HD2	2.00	0.43
2:B:1120:GLU:HG2	2:B:1121:GLY:N	2.34	0.43
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.82	0.43
7:G:19:GLY:O	7:G:22:MET:HB2	2.19	0.43
1:A:745:GLN:HA	1:A:748:MET:HE3	2.01	0.43
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.50	0.43
1:A:50:ILE:HG22	1:A:52:GLY:H	1.84	0.43
1:A:154:SER:HB3	1:A:162:VAL:HG23	2.01	0.42
1:A:841:LEU:O	1:A:845:LEU:HG	2.19	0.42
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	2.00	0.42
2:B:1181:GLU:HG2	2:B:1182:CYS:N	2.34	0.42
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.43	0.42
2:B:46:GLN:H	2:B:46:GLN:HG3	1.50	0.42
2:B:745:PRO:O	2:B:748:ILE:HG12	2.18	0.42
2:B:780:VAL:HG21	10:J:56:LEU:HD22	2.01	0.42
4:D:167:LEU:HB3	4:D:177:VAL:HG22	2.01	0.42
1:A:708:MET:HG2	1:A:712:GLU:HB3	2.02	0.42
2:B:69:LEU:HD11	2:B:425:THR:HG23	2.00	0.42
2:B:766:ARG:NH2	2:B:1020:ARG:HG2	2.33	0.42
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.19	0.42
2:B:710:LEU:HA	2:B:733:HIS:HB3	2.02	0.42
11:K:12:LEU:HD11	11:K:18:LYS:HG2	2.00	0.42
1:A:1323:ASP:C	1:A:1325:THR:H	2.28	0.42
5:E:3:GLN:HE21	5:E:5:ASN:HB2	1.84	0.42
7:G:127:PRO:HB2	7:G:139:ILE:HD13	2.02	0.42
2:B:1169:MET:HE1	2:B:1204:PHE:HB2	2.02	0.42
3:C:56:THR:HG22	3:C:57:VAL:HG22	2.01	0.42
3:C:215:GLU:C	3:C:217:ASP:H	2.28	0.42
7:G:62:LEU:HA	7:G:63:PRO:HD2	1.81	0.42
1:A:304:MET:HG2	2:B:1210:MET:HG2	2.02	0.42
2:B:638:PHE:CD1	2:B:653:VAL:HG21	2.55	0.42
2:B:806:THR:HG22	2:B:808:ALA:H	1.84	0.42
2:B:1002:THR:HG22	2:B:1072:MET:HE2	2.02	0.42
4:D:17:LYS:H	4:D:17:LYS:HG3	1.68	0.42
1:A:700:ASN:HB3	9:I:115:LYS:HB2	2.02	0.42
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	2.02	0.42
2:B:284:ILE:HG12	2:B:324:ILE:HD13	2.01	0.42
2:B:365:THR:HG21	2:B:370:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1219:ASP:OD1	4:D:14:ARG:NH2	2.53	0.42
3:C:262:LEU:HD22	11:K:88:LYS:HE3	2.01	0.42
6:F:79:ARG:HB2	6:F:79:ARG:HH11	1.83	0.42
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.50	0.42
1:A:56:PRO:HD3	1:A:58:LEU:HG	2.01	0.42
1:A:546:VAL:O	1:A:550:LEU:HG	2.20	0.42
2:B:558:LEU:HD23	2:B:596:LEU:HD11	2.01	0.42
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.02	0.42
4:D:54:GLU:O	4:D:58:VAL:HG23	2.19	0.42
5:E:102:GLU:C	5:E:104:ASN:H	2.28	0.42
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.54	0.42
1:A:64:ASN:O	1:A:65:LEU:CB	2.64	0.41
1:A:512:VAL:HA	1:A:519:PRO:HA	2.02	0.41
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.20	0.41
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.53	0.41
1:A:456:MET:HG2	1:A:510:GLN:HG3	2.02	0.41
1:A:690:VAL:HG11	1:A:794:PRO:HD3	2.02	0.41
1:A:768:GLN:CG	1:A:816:HIS:HA	2.42	0.41
2:B:424:LEU:O	2:B:428:ILE:HG13	2.20	0.41
2:B:705:MET:N	2:B:710:LEU:HD12	2.30	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.55	0.41
7:G:100:GLU:HG3	7:G:109:PHE:HB2	2.02	0.41
8:H:82:PRO:O	8:H:84:ALA:N	2.49	0.41
1:A:946:VAL:HG22	5:E:201:LYS:HD2	2.01	0.41
2:B:90:ILE:HA	2:B:133:LYS:O	2.20	0.41
7:G:9:LEU:HD22	7:G:34:VAL:HG23	2.02	0.41
1:A:598:LEU:HG	8:H:124:ARG:HB2	2.03	0.41
1:A:675:THR:HG23	1:A:732:LEU:HD22	2.02	0.41
1:A:767:GLN:HA	1:A:799:PHE:HA	2.01	0.41
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.62	0.41
2:B:406:LEU:HD12	2:B:545:ILE:HD11	2.01	0.41
2:B:557:PHE:CZ	2:B:603:LEU:HD11	2.56	0.41
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.53	0.41
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.79	0.41
7:G:8:SER:HB2	7:G:71:ASN:HD21	1.86	0.41
1:A:1105:LEU:HB3	1:A:1384:VAL:HB	2.02	0.41
2:B:112:LEU:HD21	2:B:117:ALA:HB2	2.03	0.41
2:B:115:GLN:O	2:B:119:LEU:HD12	2.20	0.41
4:D:23:ASN:HA	4:D:28:GLN:O	2.19	0.41
4:D:127:ASP:HA	4:D:130:LEU:HD12	2.03	0.41
5:E:3:GLN:NE2	5:E:5:ASN:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PRO:HD2	1:A:58:LEU:HG	2.02	0.41
1:A:105:CYS:SG	1:A:139:TRP:HA	2.61	0.41
2:B:295:GLY:H	2:B:298:LEU:CD1	2.34	0.41
7:G:34:VAL:HG13	7:G:45:ILE:HG21	2.02	0.41
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	2.02	0.41
1:A:699:ALA:HB1	9:I:114:GLN:HG3	2.03	0.41
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.35	0.41
2:B:873:THR:O	2:B:914:LYS:HA	2.21	0.41
1:A:37:PHE:HD2	1:A:52:GLY:CA	2.34	0.41
1:A:937:VAL:O	1:A:941:LYS:HG2	2.20	0.41
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.21	0.41
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	2.01	0.41
2:B:703:ILE:HA	2:B:740:HIS:O	2.21	0.41
2:B:1056:SER:HB3	2:B:1066:SER:HB2	2.03	0.41
2:B:1148:LYS:HE2	2:B:1153:GLU:OE1	2.20	0.41
1:A:347:PHE:H	2:B:1107:ALA:HA	1.86	0.41
1:A:830:LYS:HE3	1:A:1098:VAL:HB	2.03	0.41
2:B:286:PHE:HD1	2:B:291:ILE:HD13	1.86	0.41
2:B:295:GLY:O	2:B:299:GLU:HB2	2.21	0.41
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.56	0.41
4:D:194:LEU:HD21	7:G:167:TYR:HB2	2.03	0.41
1:A:302:THR:HA	1:A:305:ASP:O	2.21	0.40
1:A:1149:ALA:HB2	9:I:47:GLU:HA	2.03	0.40
4:D:27:LEU:HD11	4:D:173:HIS:HB2	2.03	0.40
5:E:124:VAL:HG13	5:E:132:ILE:HB	2.03	0.40
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.61	0.40
8:H:82:PRO:C	8:H:84:ALA:N	2.77	0.40
2:B:101:MET:HE3	2:B:101:MET:HB2	2.01	0.40
2:B:128:LEU:HD21	2:B:170:LEU:CB	2.51	0.40
2:B:299:GLU:HG3	2:B:572:HIS:NE2	2.37	0.40
2:B:766:ARG:HH21	2:B:1020:ARG:HH11	1.68	0.40
1:A:383:TYR:HB3	6:F:115:THR:HG22	2.04	0.40
2:B:123:THR:HG23	2:B:205:ILE:HA	2.02	0.40
2:B:412:LEU:HD13	2:B:412:LEU:HA	1.96	0.40
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.88	0.40
6:F:109:VAL:HG12	6:F:124:GLU:HG2	2.02	0.40
7:G:60:ARG:O	7:G:60:ARG:HG3	2.20	0.40
8:H:5:LEU:HD11	8:H:61:SER:HB3	2.04	0.40
2:B:249:ARG:HH12	2:B:415:GLN:HA	1.87	0.40
2:B:809:MET:HE1	2:B:983:ARG:NH2	2.30	0.40
2:B:1156:ASP:HB3	2:B:1197:PRO:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PHE:HA	1:A:222:LEU:HD12	2.03	0.40
2:B:35:SER:HA	2:B:811:TYR:CE1	2.57	0.40
5:E:100:ILE:HG23	5:E:105:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	1211 (86%)	145 (10%)	58 (4%)	2	19
2	B	1095/1224 (90%)	951 (87%)	114 (10%)	30 (3%)	4	27
3	C	264/318 (83%)	231 (88%)	26 (10%)	7 (3%)	4	27
4	D	174/221 (79%)	147 (84%)	19 (11%)	8 (5%)	2	17
5	E	212/215 (99%)	194 (92%)	11 (5%)	7 (3%)	3	23
6	F	82/155 (53%)	75 (92%)	6 (7%)	1 (1%)	10	41
7	G	169/171 (99%)	158 (94%)	7 (4%)	4 (2%)	4	29
8	H	129/146 (88%)	100 (78%)	15 (12%)	14 (11%)	0	5
9	I	117/122 (96%)	99 (85%)	16 (14%)	2 (2%)	7	35
10	J	63/70 (90%)	54 (86%)	5 (8%)	4 (6%)	1	12
11	K	113/120 (94%)	104 (92%)	8 (7%)	1 (1%)	14	47
12	L	44/70 (63%)	30 (68%)	6 (14%)	8 (18%)	0	1
All	All	3876/4564 (85%)	3354 (86%)	378 (10%)	144 (4%)	2	21

All (144) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG

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Mol	Chain	Res	Type
1	A	57	ARG
1	A	58	LEU
1	A	69	THR
1	A	193	ASP
1	A	257	ARG
1	A	286	HIS
1	A	311	GLN
1	A	318	SER
1	A	332	LYS
1	A	335	ARG
1	A	399	HIS
1	A	449	SER
1	A	775	ILE
1	A	1124	HIS
1	A	1405	THR
2	B	229	ALA
2	B	731	VAL
2	B	879	ARG
2	B	1167	GLY
2	B	1175	LEU
3	C	161	LYS
4	D	18	VAL
4	D	199	ASN
7	G	63	PRO
9	I	95	THR
10	J	6	ARG
12	L	43	THR
12	L	53	HIS
12	L	56	LEU
12	L	59	ALA
1	A	35	ILE
1	A	54	ASN
1	A	61	ILE
1	A	76	GLU
1	A	178	GLY
1	A	189	ARG
1	A	195	ASP
1	A	331	GLY
1	A	385	ILE
1	A	628	GLY
1	A	1175	SER
1	A	1403	GLU

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Mol	Chain	Res	Type
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	367	LEU
2	B	449	ASN
2	B	473	MET
2	B	476	ARG
2	B	772	ALA
2	B	867	GLY
2	B	1046	PRO
2	B	1066	SER
2	B	1157	ALA
2	B	1176	ASN
3	C	150	GLY
3	C	162	GLY
3	C	184	ASN
3	C	229	TYR
3	C	240	VAL
4	D	52	LEU
4	D	53	SER
4	D	119	ARG
5	E	104	ASN
5	E	126	SER
5	E	174	GLN
7	G	154	VAL
8	H	81	PRO
12	L	45	ALA
12	L	50	ASP
1	A	43	GLU
1	A	62	ASP
1	A	224	PHE
1	A	465	TYR
1	A	1064	VAL
1	A	1167	GLU
2	B	108	VAL
2	B	707	PRO
2	B	883	LEU
2	B	1181	GLU
5	E	36	GLU
7	G	2	PHE
8	H	46	LEU
8	H	82	PRO

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Mol	Chain	Res	Type
8	H	83	GLN
8	H	90	ALA
8	H	128	ASN
9	I	3	THR
10	J	2	ILE
10	J	17	LYS
11	K	64	GLU
12	L	26	THR
1	A	169	ASN
1	A	569	LYS
1	A	1242	VAL
1	A	1366	ARG
2	B	575	PRO
2	B	711	GLU
2	B	751	VAL
4	D	16	LYS
4	D	169	SER
5	E	45	LYS
8	H	89	LEU
1	A	155	GLU
1	A	167	CYS
1	A	196	GLU
1	A	846	GLU
1	A	958	VAL
1	A	975	HIS
1	A	1173	HIS
1	A	1255	GLU
1	A	1437	GLY
2	B	792	MET
3	C	237	SER
4	D	218	GLU
5	E	103	LYS
6	F	73	ALA
8	H	18	GLY
8	H	32	THR
8	H	52	GLN
8	H	60	ALA
8	H	131	ASN
1	A	65	LEU
1	A	1060	PRO
2	B	251	ILE
2	B	364	ILE

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Mol	Chain	Res	Type
2	B	1108	ARG
7	G	139	ILE
8	H	78	SER
12	L	28	LYS
1	A	73	GLY
1	A	192	GLY
1	A	567	LYS
1	A	283	GLY
1	A	1122	PRO
1	A	1123	GLY
5	E	90	VAL
8	H	107	VAL
1	A	197	PRO
1	A	916	GLY
2	B	907	GLY
10	J	64	ASN
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%)	1045 (84%)	195 (16%)	2	15
2	B	966/1061 (91%)	805 (83%)	161 (17%)	2	13
3	C	234/274 (85%)	193 (82%)	41 (18%)	2	11
4	D	160/200 (80%)	130 (81%)	30 (19%)	1	9
5	E	196/197 (100%)	169 (86%)	27 (14%)	3	19
6	F	74/137 (54%)	64 (86%)	10 (14%)	4	20
7	G	152/152 (100%)	123 (81%)	29 (19%)	1	8
8	H	117/128 (91%)	100 (86%)	17 (14%)	3	17
9	I	113/116 (97%)	101 (89%)	12 (11%)	6	27
10	J	60/65 (92%)	47 (78%)	13 (22%)	1	6
11	K	99/102 (97%)	84 (85%)	15 (15%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	40/57 (70%)	29 (72%)	11 (28%)	0	3
All	All	3451/4008 (86%)	2890 (84%)	561 (16%)	2	14

All (561) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	28	ARG
1	A	35	ILE
1	A	41	MET
1	A	43	GLU
1	A	45	GLN
1	A	47	ARG
1	A	62	ASP
1	A	67	CYS
1	A	70	CYS
1	A	84	ILE
1	A	90	VAL
1	A	93	VAL
1	A	96	ILE
1	A	106	VAL
1	A	117	GLU
1	A	120	GLU
1	A	132	LYS
1	A	140	THR
1	A	144	THR
1	A	147	VAL
1	A	152	VAL
1	A	157	ASP
1	A	159	THR
1	A	170	THR
1	A	173	THR
1	A	174	ILE
1	A	188	ASP
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	220	THR
1	A	227	VAL
1	A	255	SER
1	A	256	GLN
1	A	261	ASP

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Mol	Chain	Res	Type
1	A	277	GLU
1	A	279	LEU
1	A	295	LEU
1	A	307	ASP
1	A	313	GLN
1	A	315	LEU
1	A	322	VAL
1	A	324	SER
1	A	328	ARG
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	353	ILE
1	A	354	SER
1	A	381	THR
1	A	389	THR
1	A	393	ARG
1	A	408	ASP
1	A	411	ASP
1	A	423	ASP
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	454	SER
1	A	461	LYS
1	A	462	VAL
1	A	463	ILE
1	A	469	ARG
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	481	ASP
1	A	485	ASP
1	A	494	SER
1	A	498	ARG
1	A	500	GLU

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Mol	Chain	Res	Type
1	A	505	CYS
1	A	524	VAL
1	A	536	LEU
1	A	541	ILE
1	A	566	ILE
1	A	569	LYS
1	A	571	LEU
1	A	593	GLU
1	A	597	LEU
1	A	598	LEU
1	A	618	GLU
1	A	629	LEU
1	A	652	VAL
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	682	THR
1	A	685	GLU
1	A	702	LEU
1	A	711	ARG
1	A	719	VAL
1	A	732	LEU
1	A	738	LYS
1	A	740	LEU
1	A	756	ILE
1	A	764	CYS
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	788	SER
1	A	795	GLU
1	A	811	GLN
1	A	821	ARG
1	A	831	THR
1	A	834	THR
1	A	855	THR
1	A	856	THR
1	A	867	ILE
1	A	880	LYS
1	A	886	ILE
1	A	890	ASP
1	A	896	ARG

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Mol	Chain	Res	Type
1	A	904	THR
1	A	915	SER
1	A	919	ILE
1	A	920	LEU
1	A	941	LYS
1	A	948	VAL
1	A	964	ILE
1	A	973	ILE
1	A	976	THR
1	A	983	ILE
1	A	993	LEU
1	A	1001	ARG
1	A	1009	ASN
1	A	1015	VAL
1	A	1020	CYS
1	A	1021	LEU
1	A	1024	SER
1	A	1028	THR
1	A	1055	ARG
1	A	1058	VAL
1	A	1078	GLN
1	A	1096	SER
1	A	1105	LEU
1	A	1116	LEU
1	A	1118	VAL
1	A	1124	HIS
1	A	1134	ILE
1	A	1146	VAL
1	A	1159	ARG
1	A	1171	GLN
1	A	1172	LEU
1	A	1173	HIS
1	A	1176	LEU
1	A	1208	THR
1	A	1215	ARG
1	A	1218	GLN
1	A	1223	ASP
1	A	1226	VAL
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU

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Mol	Chain	Res	Type
1	A	1257	ASP
1	A	1260	LEU
1	A	1280	GLU
1	A	1288	ASP
1	A	1290	LYS
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1301	GLU
1	A	1308	THR
1	A	1322	ILE
1	A	1325	THR
1	A	1333	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1370	LEU
1	A	1376	THR
1	A	1386	ARG
1	A	1387	HIS
1	A	1391	ARG
1	A	1400	CYS
1	A	1403	GLU
1	A	1406	VAL
1	A	1420	ASP
1	A	1424	VAL
1	A	1426	GLU
1	A	1429	ILE
1	A	1433	MET
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
2	B	25	ILE
2	B	35	SER
2	B	40	GLU
2	B	46	GLN
2	B	63	ILE
2	B	64	CYS
2	B	94	LYS
2	B	102	VAL
2	B	110	HIS

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Mol	Chain	Res	Type
2	B	118	ARG
2	B	126	SER
2	B	178	ASN
2	B	183	GLU
2	B	185	THR
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	251	ILE
2	B	254	LEU
2	B	261	ARG
2	B	262	GLU
2	B	272	THR
2	B	273	LEU
2	B	278	GLN
2	B	280	ILE
2	B	289	LEU
2	B	309	GLN
2	B	312	GLU
2	B	313	MET
2	B	324	ILE
2	B	336	ARG
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	364	ILE
2	B	365	THR
2	B	368	GLU
2	B	371	GLU
2	B	372	SER
2	B	387	LEU
2	B	393	LYS
2	B	398	ARG
2	B	408	LEU
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	429	PHE
2	B	436	VAL

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Mol	Chain	Res	Type
2	B	446	LEU
2	B	448	ILE
2	B	453	ILE
2	B	461	LEU
2	B	468	GLU
2	B	474	SER
2	B	476	ARG
2	B	480	SER
2	B	485	ARG
2	B	545	ILE
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	554	ILE
2	B	570	VAL
2	B	572	HIS
2	B	573	GLN
2	B	574	SER
2	B	580	VAL
2	B	589	VAL
2	B	598	GLU
2	B	603	LEU
2	B	604	ARG
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	628	THR
2	B	629	ASP
2	B	642	ASP
2	B	644	GLU
2	B	646	LEU
2	B	651	LEU
2	B	652	LYS
2	B	653	VAL
2	B	658	ILE
2	B	668	ASP
2	B	678	GLU
2	B	680	THR
2	B	689	LEU
2	B	708	GLU
2	B	723	VAL
2	B	729	ILE

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Mol	Chain	Res	Type
2	B	734	HIS
2	B	736	THR
2	B	766	ARG
2	B	776	GLN
2	B	786	ASN
2	B	790	ASP
2	B	830	TYR
2	B	835	GLN
2	B	844	SER
2	B	858	SER
2	B	868	MET
2	B	871	THR
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	889	THR
2	B	908	GLU
2	B	933	SER
2	B	934	LYS
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	945	GLU
2	B	953	LEU
2	B	954	VAL
2	B	964	VAL
2	B	970	THR
2	B	972	LYS
2	B	973	ILE
2	B	975	GLN
2	B	976	ILE
2	B	983	ARG
2	B	986	GLN
2	B	987	LYS
2	B	992	ILE
2	B	997	GLU
2	B	1006	ILE
2	B	1007	VAL
2	B	1017	ILE
2	B	1020	ARG
2	B	1026	LEU
2	B	1028	GLU

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Mol	Chain	Res	Type
2	B	1050	ILE
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1112	GLN
2	B	1122	ARG
2	B	1128	LEU
2	B	1129	ARG
2	B	1133	MET
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1149	GLU
2	B	1151	LEU
2	B	1156	ASP
2	B	1160	VAL
2	B	1172	ILE
2	B	1175	LEU
2	B	1178	ASN
2	B	1183	LYS
2	B	1188	LYS
2	B	1189	ILE
2	B	1191	ILE
2	B	1193	GLN
2	B	1202	LEU
2	B	1212	ILE
3	C	7	GLN
3	C	12	GLU
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	38	ILE
3	C	40	GLU
3	C	44	LEU
3	C	52	GLU
3	C	53	THR
3	C	55	THR
3	C	56	THR
3	C	70	ILE
3	C	78	GLU

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Mol	Chain	Res	Type
3	C	89	GLU
3	C	100	THR
3	C	101	LEU
3	C	102	GLN
3	C	120	ILE
3	C	124	LEU
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	137	LYS
3	C	147	LEU
3	C	155	LEU
3	C	157	CYS
3	C	158	VAL
3	C	197	SER
3	C	215	GLU
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	262	LEU
3	C	264	GLN
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	6	SER
4	D	9	GLN
4	D	18	VAL
4	D	22	GLU
4	D	27	LEU
4	D	29	LEU
4	D	32	GLU
4	D	35	LEU
4	D	37	GLN
4	D	40	HIS
4	D	41	GLN
4	D	50	LEU
4	D	52	LEU
4	D	65	GLU
4	D	67	ARG
4	D	123	LEU

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Mol	Chain	Res	Type
4	D	126	ILE
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	156	ASP
4	D	158	GLU
4	D	177	VAL
4	D	187	THR
4	D	206	GLU
4	D	213	GLU
4	D	214	LEU
4	D	219	THR
4	D	221	TYR
5	E	3	GLN
5	E	6	GLU
5	E	8	ASN
5	E	31	THR
5	E	33	GLU
5	E	46	TYR
5	E	60	PHE
5	E	67	GLU
5	E	69	ILE
5	E	75	MET
5	E	84	ASP
5	E	85	GLU
5	E	92	THR
5	E	99	HIS
5	E	100	ILE
5	E	144	ILE
5	E	150	VAL
5	E	173	SER
5	E	175	LEU
5	E	177	ARG
5	E	178	ILE
5	E	184	VAL
5	E	190	LEU
5	E	191	LYS
5	E	196	VAL
5	E	204	THR
5	E	215	MET
6	F	79	ARG
6	F	82	THR

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Mol	Chain	Res	Type
6	F	86	THR
6	F	90	ARG
6	F	93	ILE
6	F	111	LEU
6	F	118	LEU
6	F	123	LYS
6	F	129	LYS
6	F	155	LEU
7	G	8	SER
7	G	13	LEU
7	G	22	MET
7	G	24	GLN
7	G	26	LEU
7	G	34	VAL
7	G	35	GLU
7	G	39	THR
7	G	60	ARG
7	G	61	ILE
7	G	64	THR
7	G	65	ASP
7	G	83	LYS
7	G	92	VAL
7	G	96	GLN
7	G	106	MET
7	G	114	LEU
7	G	118	ASP
7	G	133	SER
7	G	134	GLU
7	G	138	THR
7	G	143	ILE
7	G	145	VAL
7	G	151	ILE
7	G	154	VAL
7	G	155	SER
7	G	160	ILE
7	G	162	SER
7	G	165	GLU
8	H	13	SER
8	H	14	GLU
8	H	26	ILE
8	H	31	THR
8	H	42	ILE

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Mol	Chain	Res	Type
8	H	46	LEU
8	H	63	LEU
8	H	76	THR
8	H	77	ARG
8	H	86	ASP
8	H	89	LEU
8	H	91	ASP
8	H	103	LYS
8	H	106	GLU
8	H	123	MET
8	H	128	ASN
8	H	130	ARG
9	I	8	ARG
9	I	21	GLU
9	I	31	THR
9	I	35	VAL
9	I	43	VAL
9	I	52	ILE
9	I	59	VAL
9	I	83	ASN
9	I	94	ASP
9	I	108	HIS
9	I	114	GLN
9	I	115	LYS
10	J	2	ILE
10	J	3	VAL
10	J	7	CYS
10	J	12	LYS
10	J	13	VAL
10	J	14	VAL
10	J	20	SER
10	J	22	LEU
10	J	23	ASN
10	J	28	ASP
10	J	29	GLU
10	J	38	ARG
10	J	42	LYS
11	K	1	MET
11	K	12	LEU
11	K	18	LYS
11	K	20	LYS
11	K	25	THR

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Mol	Chain	Res	Type
11	K	29	ASN
11	K	37	LYS
11	K	42	LEU
11	K	47	ARG
11	K	63	VAL
11	K	70	ARG
11	K	79	GLU
11	K	101	LEU
11	K	107	THR
11	K	114	LEU
12	L	27	LEU
12	L	33	GLU
12	L	35	SER
12	L	38	LEU
12	L	49	LYS
12	L	54	ARG
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	68	GLU
12	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	71	GLN
1	A	253	ASN
1	A	397	ASN
1	A	439	ASN
1	A	517	ASN
1	A	548	ASN
1	A	742	ASN
1	A	760	GLN
1	A	811	GLN
1	A	862	ASN
1	A	877	HIS
1	A	953	ASN
1	A	965	GLN
1	A	966	ASN
1	A	968	GLN
1	A	994	GLN

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Mol	Chain	Res	Type
1	A	1078	GLN
1	A	1106	ASN
1	A	1128	GLN
1	A	1140	HIS
1	A	1187	GLN
1	A	1387	HIS
1	A	1390	ASN
1	A	1393	ASN
2	B	103	ASN
2	B	325	GLN
2	B	357	GLN
2	B	363	HIS
2	B	415	GLN
2	B	449	ASN
2	B	499	ASN
2	B	590	HIS
2	B	667	GLN
2	B	706	GLN
2	B	776	GLN
2	B	786	ASN
2	B	835	GLN
2	B	878	GLN
2	B	957	ASN
2	B	975	GLN
2	B	986	GLN
2	B	1065	GLN
2	B	1084	GLN
2	B	1097	HIS
2	B	1176	ASN
2	B	1177	HIS
3	C	140	ASN
3	C	214	ASN
3	C	231	ASN
3	C	242	GLN
4	D	37	GLN
4	D	41	GLN
5	E	3	GLN
5	E	8	ASN
5	E	104	ASN
5	E	113	GLN
5	E	115	ASN
5	E	174	GLN

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Mol	Chain	Res	Type
6	F	78	GLN
7	G	71	ASN
8	H	52	GLN
8	H	131	ASN
8	H	134	ASN
9	I	46	HIS
9	I	51	ASN
9	I	60	GLN
9	I	89	GLN
9	I	90	GLN
9	I	120	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	3/4 (75%)	1 (33%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	9	G

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	15,14	18,21,22	0.80	0	25,30,33	2.75	11 (44%)

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	15,14	-	0/7/21/22	0/2/2/2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C5-C4-N3	5.65	119.83	113.34
15	T	22	BRU	C4-N3-C2	-5.17	120.56	127.34
15	T	22	BRU	C2'-C1'-N1	-4.94	101.46	113.81
15	T	22	BRU	O4-C4-C5	-4.72	119.78	125.80
15	T	22	BRU	O4'-C1'-N1	4.60	116.03	107.86
15	T	22	BRU	N3-C2-N1	4.32	120.51	114.89
15	T	22	BRU	BR-C5-C4	3.47	122.01	118.02
15	T	22	BRU	C1'-N1-C2	3.02	123.57	117.66
15	T	22	BRU	C6-N1-C2	-2.62	118.69	121.30
15	T	22	BRU	C6-C5-C4	-2.29	118.34	120.67
15	T	22	BRU	O2-C2-N3	-2.27	117.30	121.49

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	5.39
1	B	351:TYR	C	352:ALA	N	3.29

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%)	-0.18	11 (0%) 82 60	64, 115, 172, 239	0
2	B	1115/1224 (91%)	0.01	20 (1%) 67 42	71, 127, 187, 209	0
3	C	266/318 (83%)	-0.30	0 100 100	86, 115, 158, 185	0
4	D	178/221 (80%)	0.03	5 (2%) 55 32	96, 131, 179, 198	0
5	E	214/215 (99%)	-0.17	0 100 100	89, 146, 193, 206	0
6	F	84/155 (54%)	-0.45	1 (1%) 76 52	73, 97, 124, 137	0
7	G	171/171 (100%)	-0.17	0 100 100	85, 113, 154, 172	0
8	H	133/146 (91%)	0.27	4 (3%) 52 30	125, 157, 194, 214	0
9	I	119/122 (97%)	0.09	1 (0%) 82 60	120, 151, 192, 199	0
10	J	65/70 (92%)	-0.24	0 100 100	95, 115, 151, 161	0
11	K	115/120 (95%)	-0.36	2 (1%) 69 43	85, 114, 155, 174	0
12	L	46/70 (65%)	0.83	5 (10%) 10 7	103, 182, 199, 210	0
13	N	4/14 (28%)	1.49	2 (50%) 0 1	230, 230, 234, 239	0
14	P	4/4 (100%)	0.34	0 100 100	211, 220, 228, 240	0
15	T	11/26 (42%)	1.22	2 (18%) 3 4	188, 216, 258, 264	0
All	All	3947/4608 (85%)	-0.10	53 (1%) 75 50	64, 122, 185, 264	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	9.9
1	A	1243	VAL	5.6
12	L	28	LYS	4.7
12	L	25	ALA	4.7
2	B	446	LEU	4.7
4	D	3	VAL	4.1
4	D	24	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	70	ILE	4.0
2	B	502	ILE	3.9
2	B	1224	PHE	3.9
2	B	882	THR	3.9
2	B	708	GLU	3.8
12	L	26	THR	3.7
2	B	883	LEU	3.7
1	A	1080	THR	3.6
11	K	114	LEU	3.4
2	B	468	GLU	3.3
2	B	134	LYS	3.3
2	B	709	ASP	3.3
4	D	173	HIS	3.2
2	B	476	ARG	3.1
1	A	251	SER	3.1
2	B	881	ASN	3.1
2	B	710	LEU	3.1
2	B	509	ALA	3.1
11	K	115	ALA	3.0
6	F	72	LYS	3.0
8	H	63	LEU	2.9
2	B	251	ILE	2.8
8	H	82	PRO	2.8
8	H	90	ALA	2.5
2	B	577	ALA	2.5
4	D	221	TYR	2.5
4	D	187	THR	2.4
12	L	30	ILE	2.4
15	T	24	DG	2.3
2	B	262	GLU	2.3
9	I	120	GLN	2.3
1	A	51	GLY	2.2
1	A	186	LYS	2.2
1	A	904	THR	2.2
1	A	1176	LEU	2.2
13	N	5	DT	2.2
1	A	190	ALA	2.2
8	H	132	LEU	2.2
2	B	436	VAL	2.2
15	T	19	DT	2.1
2	B	343	ILE	2.1
13	N	2	DA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	791	THR	2.1
1	A	194	ALA	2.0
1	A	1093	LYS	2.0
1	A	1173	HIS	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	0.88	0.12	221,231,240,243	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	0.74	0.22	281,281,281,281	0
16	ZN	L	1071	1/1	0.97	0.05	201,201,201,201	0
16	ZN	I	1122	1/1	0.99	0.03	201,201,201,201	0
16	ZN	C	1269	1/1	1.00	0.03	96,96,96,96	0
16	ZN	I	1121	1/1	1.00	0.03	136,136,136,136	0
16	ZN	A	2456	1/1	1.00	0.02	155,155,155,155	0
16	ZN	J	1066	1/1	1.00	0.03	101,101,101,101	0
16	ZN	A	2457	1/1	1.00	0.01	81,81,81,81	0
16	ZN	B	2225	1/1	1.00	0.04	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.