



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 11:09 AM UTC

PDB ID : 4BY7 / pdb_00004by7
Title : elongating RNA Polymerase II-Bye1 TLD complex
Authors : Kinkelin, K.; Wozniak, G.G.; Rothbart, S.B.; Lidschreiber, M.; Strahl, B.D.; Cramer, P.
Deposited on : 2013-07-18
Resolution : 3.15 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

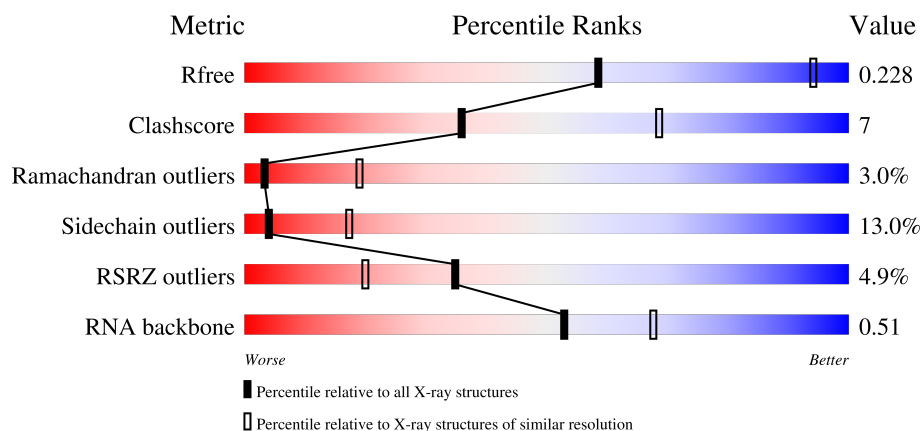
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)
RNA backbone	3983	1113 (3.42-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	1733	2% 58% 19% 5% 18%
2	B	1224	5% 65% 21% • 9%
3	C	318	57% 22% 5% 16%
4	D	221	5% 58% 19% • 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	11	
15	T	26	
16	X	146	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 33261 atoms, of which 34 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	1426	Total	C	N	O	S	0	0	0
			11223	7068	1959	2134	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
			1387	860	246	279	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	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- 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	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called 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 , 5'-D(*DAP*AP*AP*GP*TP*AP*CP*TP*TP*GP*A

P*GP*CP*DTP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	13	Total	C	N	O	P	0	0	0
			269	128	52	76	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	10	Total	C	N	O	P	0	0	0
			215	96	41	68	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	25	Total	Br	C	N	O	P	0	0
			504	1	240	83	155	25		

- Molecule 16 is a protein called TRANSCRIPTION FACTOR BYE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	X	119	Total	C	N	O	S	0	0	0
			977	628	162	184	3			

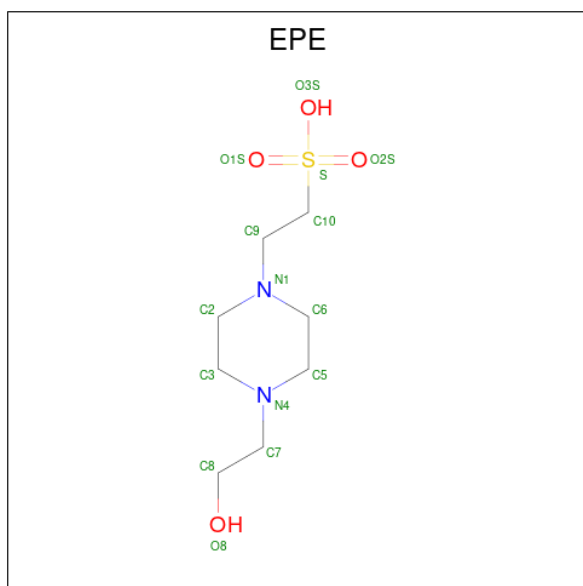
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 19 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).

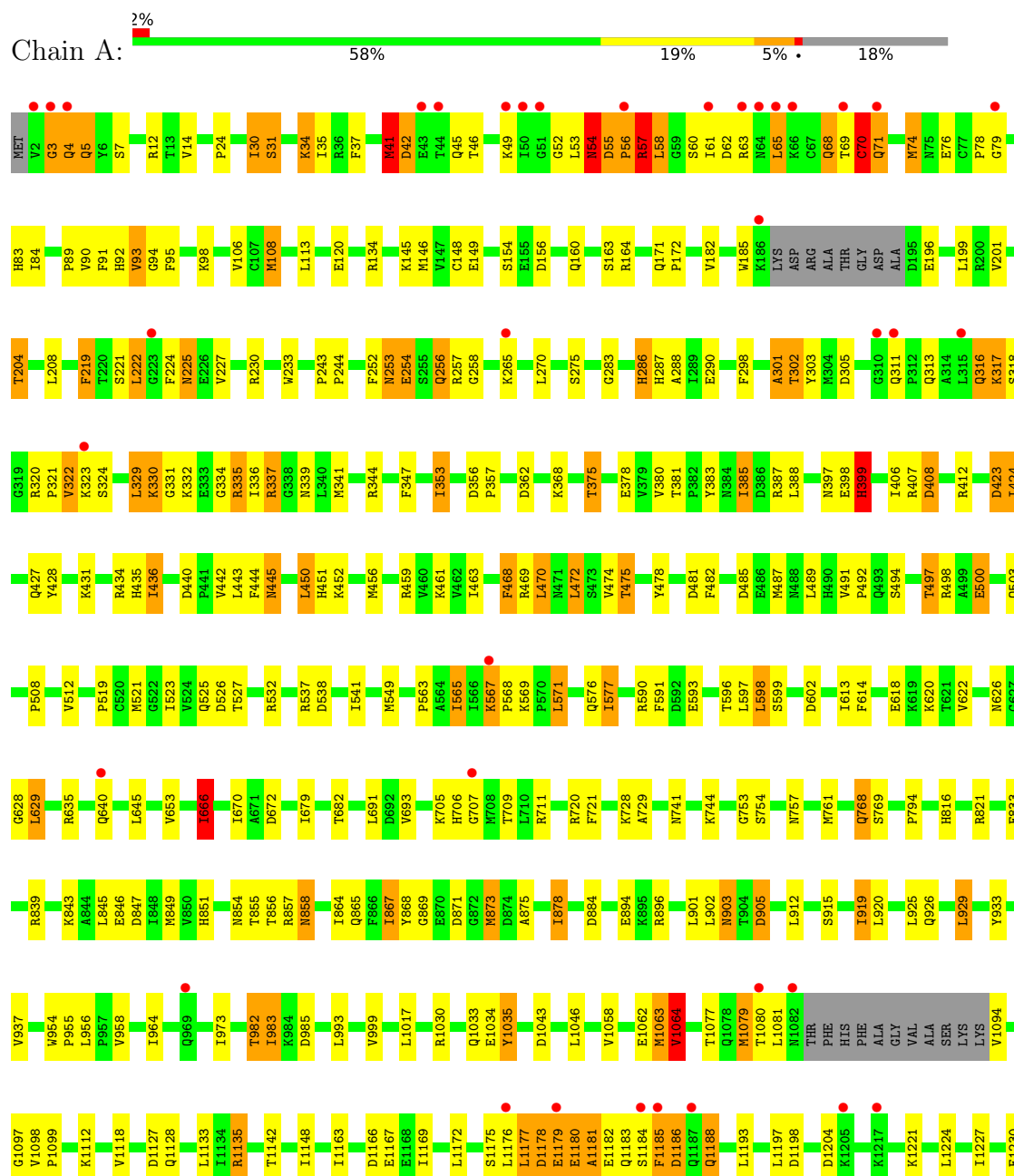


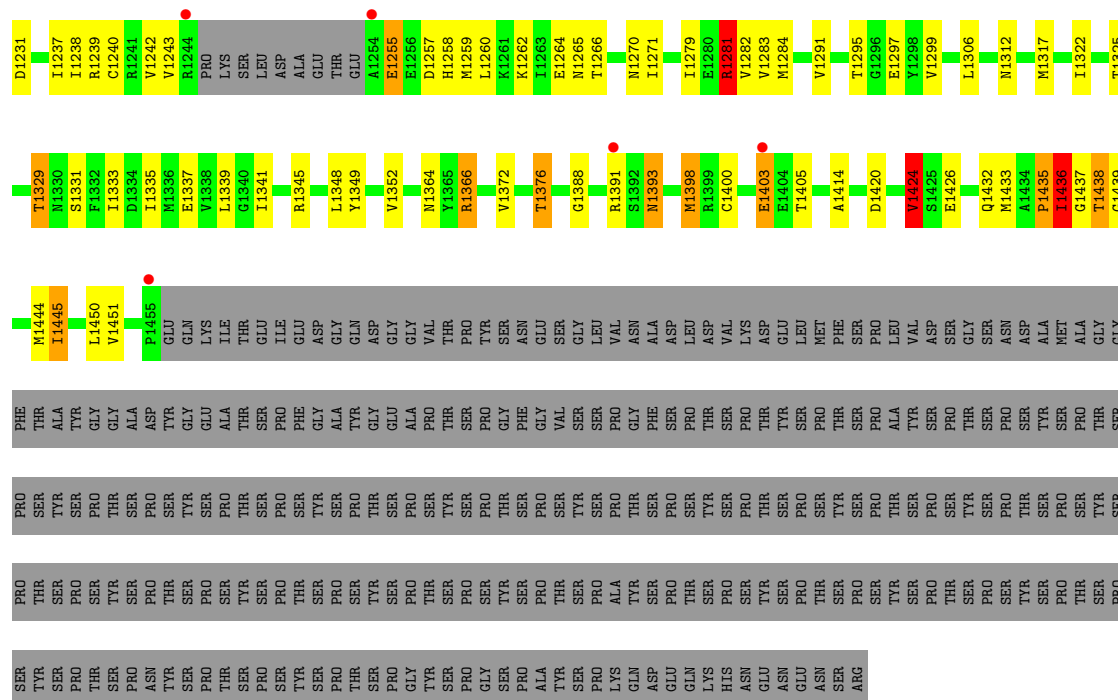
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
19	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
19	G	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

3 Residue-property plots

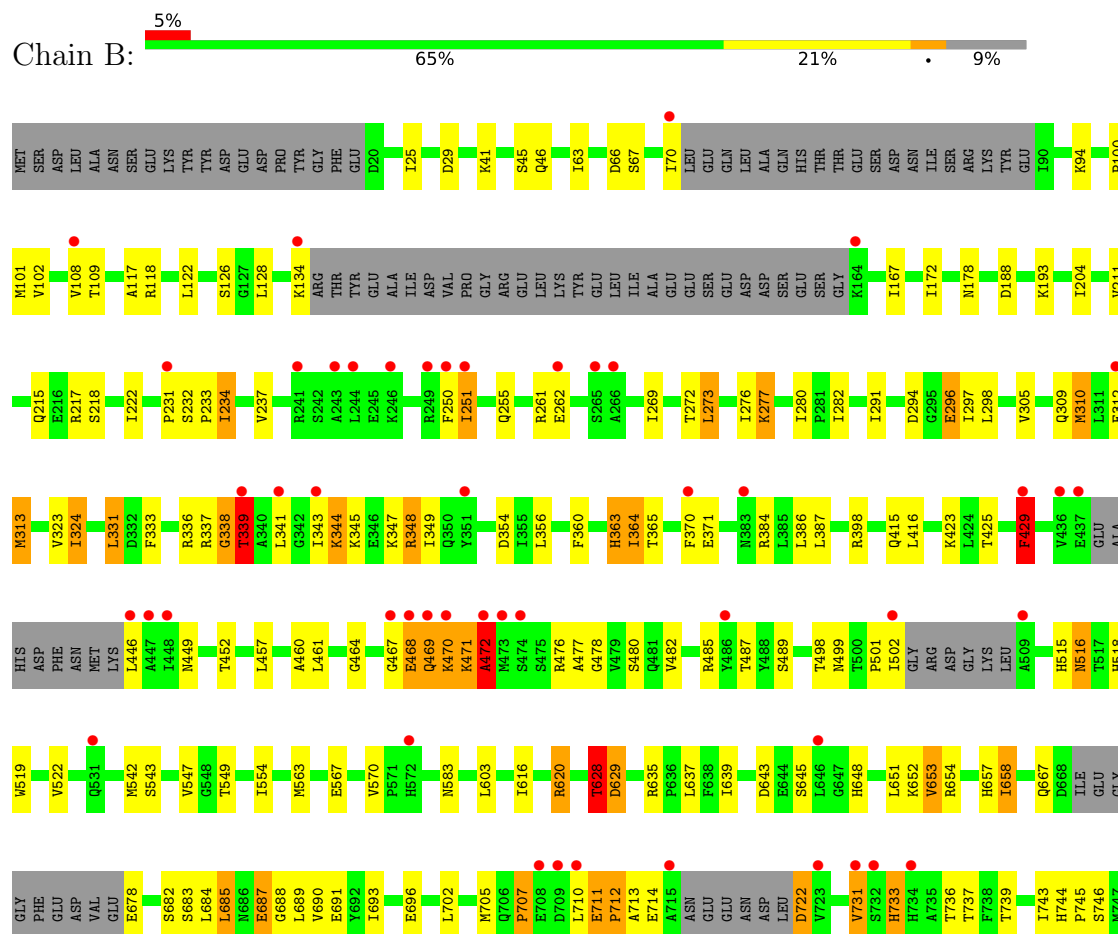
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

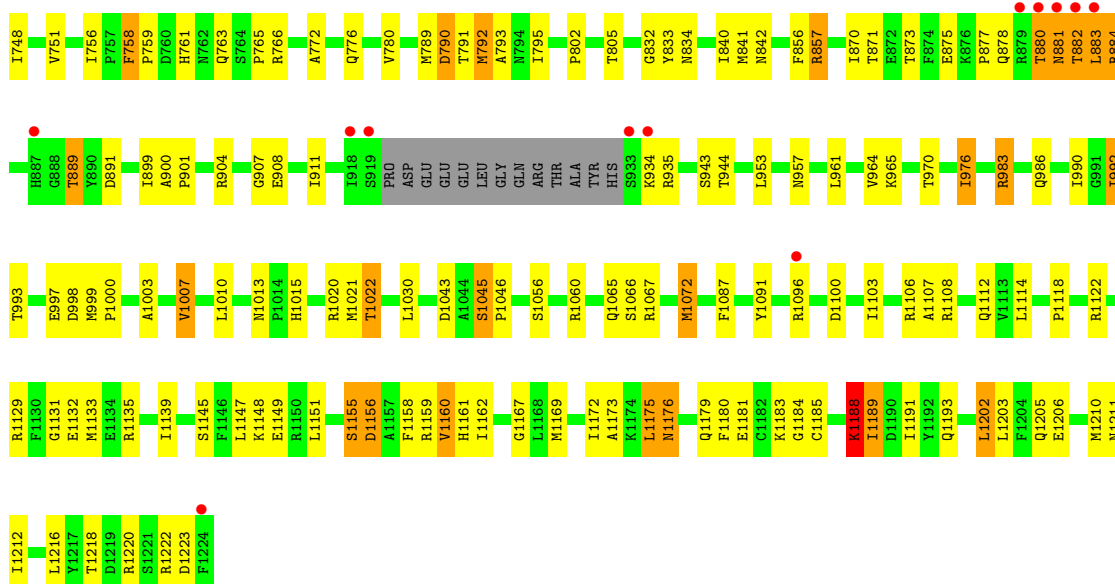
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1





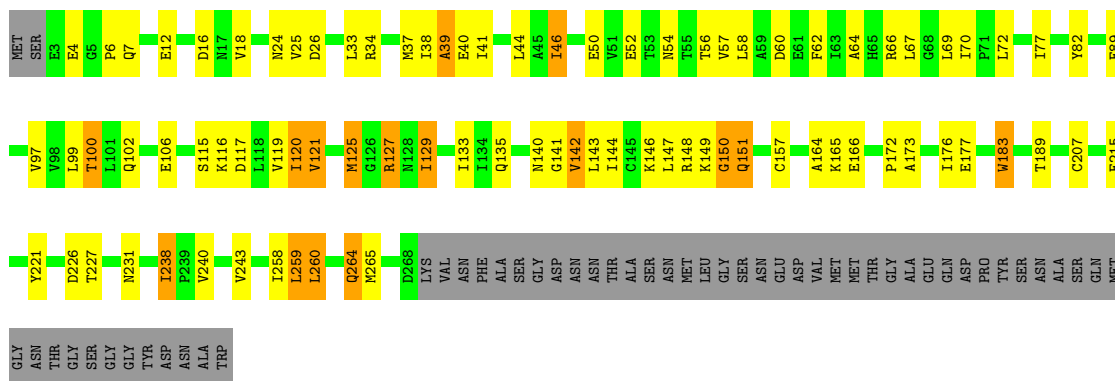
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2





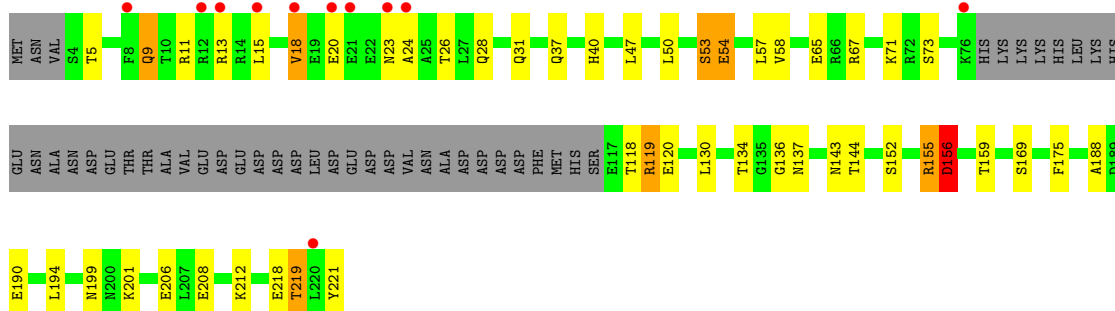
● Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C:

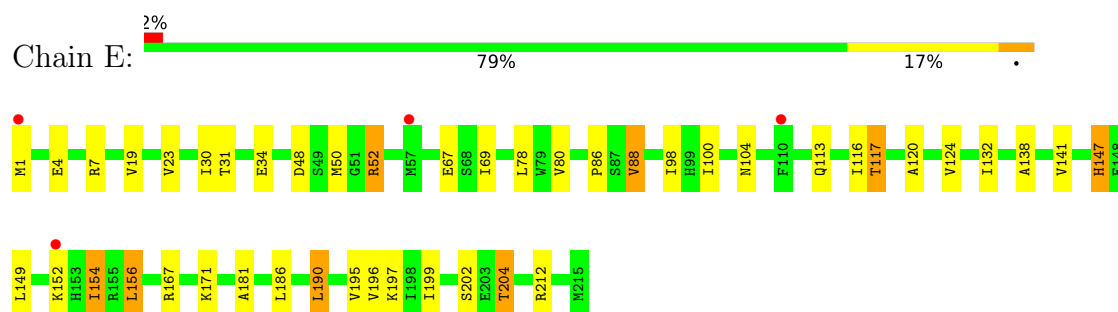


- Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

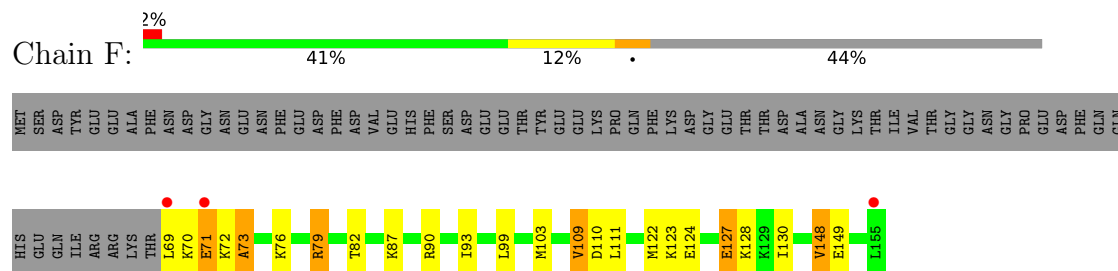
Chain D:



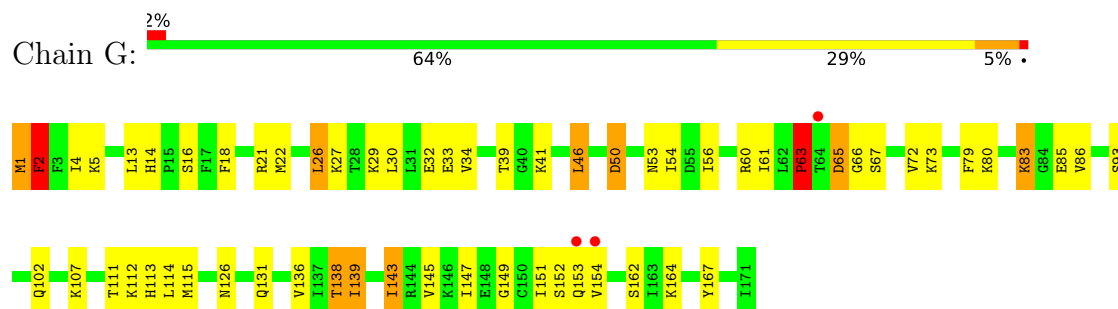
● Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



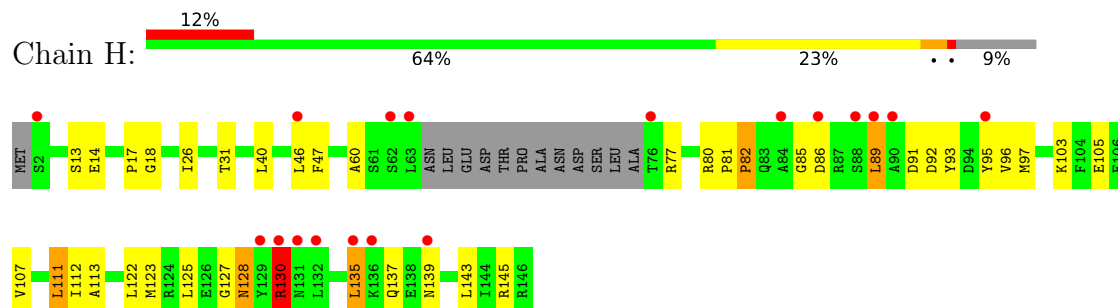
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



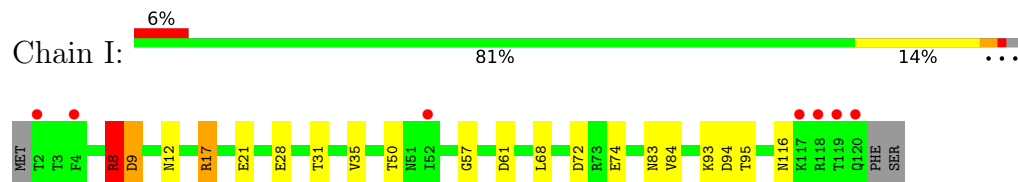
- Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7



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



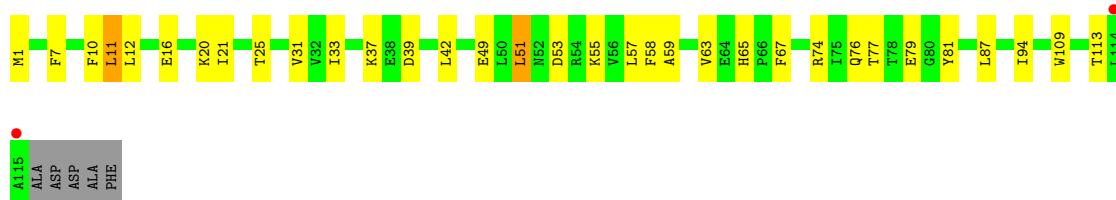
- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



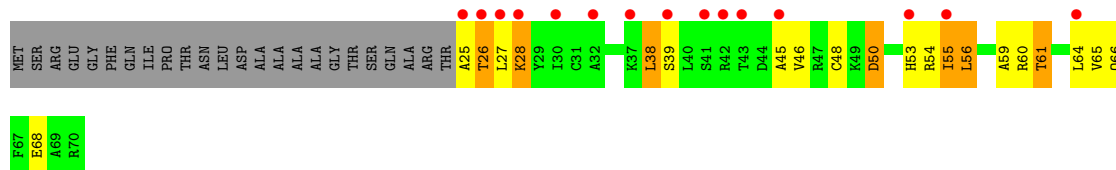
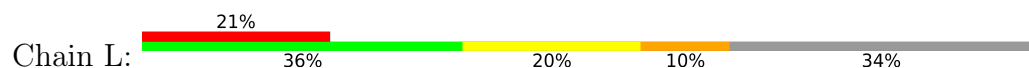
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



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



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



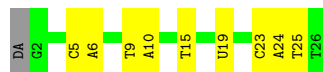
- Molecule 13: , 5'-D(*DAP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*DTP)-3'



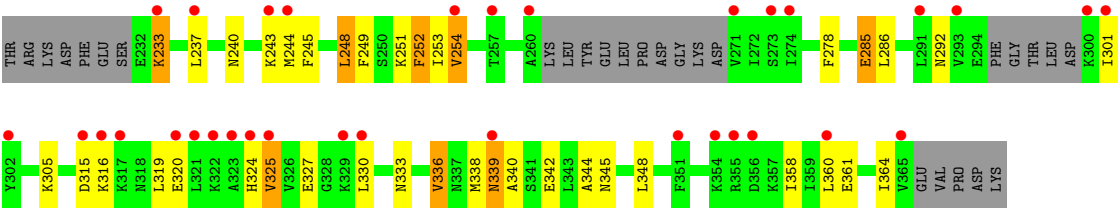
- Molecule 14: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'



- Molecule 15: 5'-D(*DAP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*DAP *TP*TP*CP*CP*BP*GP*GP*TP*CP*AP*TP*T)-3'



- Molecule 16: TRANSCRIPTION FACTOR BYE1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.50Å 390.68Å 281.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.84 – 3.15 48.84 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.84-3.15) 99.9 (48.84-3.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.189 , 0.212 0.206 , 0.228	Depositor DCC
R_{free} test set	4003 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å ²)	99.4	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 115.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.003 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 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	33261	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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, EPE, 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	0.89	9/11424 (0.1%)	1.48	103/15452 (0.7%)
2	B	0.85	1/9030 (0.0%)	1.40	71/12174 (0.6%)
3	C	0.83	0/2133	1.36	17/2891 (0.6%)
4	D	0.85	1/1397 (0.1%)	1.51	9/1878 (0.5%)
5	E	0.78	0/1796	1.32	6/2416 (0.2%)
6	F	0.93	0/717	1.38	5/967 (0.5%)
7	G	0.85	1/1368 (0.1%)	1.35	7/1844 (0.4%)
8	H	0.82	0/1085	1.24	3/1467 (0.2%)
9	I	0.82	0/989	1.26	3/1331 (0.2%)
10	J	0.84	0/541	1.51	9/727 (1.2%)
11	K	0.73	0/938	1.26	5/1267 (0.4%)
12	L	0.95	0/364	1.45	2/482 (0.4%)
13	N	0.45	0/302	0.59	0/464
14	P	0.81	1/240 (0.4%)	0.77	0/372
15	T	0.53	0/539	0.67	0/825
16	X	0.84	1/990 (0.1%)	1.59	8/1325 (0.6%)
All	All	0.85	14/33853 (0.0%)	1.40	248/45882 (0.5%)

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
15	T	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	PRO	C-N	9.31	1.46	1.33
1	A	55	ASP	CA-C	-8.63	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	ARG	CA-C	7.12	1.62	1.52
4	D	24	ALA	CA-C	6.69	1.61	1.52
1	A	1403	GLU	CA-C	5.78	1.60	1.52
14	P	3	C	C1'-N1	5.69	1.56	1.48
1	A	30	ILE	CG1-CD1	5.50	1.73	1.51
2	B	1172	ILE	CG1-CD1	5.38	1.72	1.51
7	G	1	MET	C-N	5.37	1.41	1.33
16	X	254	VAL	CA-C	5.35	1.57	1.52
1	A	487	MET	SD-CE	-5.18	1.66	1.79
1	A	54	ASN	CA-C	5.12	1.59	1.52
1	A	61	ILE	CA-C	5.08	1.58	1.52
1	A	69	THR	C-N	5.04	1.40	1.33

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ASN	CA-C-N	12.87	136.73	122.83
1	A	54	ASN	C-N-CA	12.87	136.73	122.83
1	A	54	ASN	CA-CB-CG	10.10	122.69	112.60
8	H	92	ASP	N-CA-C	-9.06	101.19	112.88
1	A	1177	LEU	CA-C-N	9.05	137.99	121.70
1	A	1177	LEU	C-N-CA	9.05	137.99	121.70
10	J	5	VAL	N-CA-C	-8.78	98.33	109.30
7	G	1	MET	CA-C-N	8.25	137.31	121.54
7	G	1	MET	C-N-CA	8.25	137.31	121.54
2	B	628	THR	CA-C-N	8.23	133.57	121.31
2	B	628	THR	C-N-CA	8.23	133.57	121.31
1	A	56	PRO	CA-C-N	8.01	136.83	121.54
1	A	56	PRO	C-N-CA	8.01	136.83	121.54
5	E	171	LYS	N-CA-C	-7.93	98.13	110.42
1	A	219	PHE	CA-CB-CG	7.89	121.69	113.80
6	F	70	LYS	CA-C-N	7.68	136.22	121.54
6	F	70	LYS	C-N-CA	7.68	136.22	121.54
1	A	666	ILE	N-CA-CB	7.66	120.04	110.47
4	D	26	THR	N-CA-C	-7.56	103.62	112.92
3	C	39	ALA	N-CA-C	7.52	122.75	113.50
7	G	2	PHE	N-CA-C	-7.34	95.17	110.80
2	B	1184	GLY	CA-C-N	7.22	135.34	121.54
2	B	1184	GLY	C-N-CA	7.22	135.34	121.54
4	D	24	ALA	CA-C-N	7.21	134.19	122.65
4	D	24	ALA	C-N-CA	7.21	134.19	122.65
1	A	445	ASN	CA-CB-CG	7.19	119.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1403	GLU	CA-C-N	-7.12	111.14	122.95
1	A	1403	GLU	C-N-CA	-7.12	111.14	122.95
1	A	1435	PRO	CA-C-N	7.04	132.77	123.06
1	A	1435	PRO	C-N-CA	7.04	132.77	123.06
2	B	339	THR	CA-C-N	7.03	134.35	121.70
2	B	339	THR	C-N-CA	7.03	134.35	121.70
2	B	1155	SER	CA-C-N	6.96	134.96	121.18
2	B	1155	SER	C-N-CA	6.96	134.96	121.18
2	B	1169	MET	CA-C-N	6.90	130.79	120.31
2	B	1169	MET	C-N-CA	6.90	130.79	120.31
1	A	999	VAL	N-CA-C	-6.84	106.22	111.62
4	D	54	GLU	N-CA-C	-6.83	103.76	111.07
1	A	468	PHE	CA-CB-CG	6.81	120.61	113.80
1	A	55	ASP	N-CA-CB	6.76	121.17	111.51
2	B	1188	LYS	CA-C-N	6.74	129.58	122.97
2	B	1188	LYS	C-N-CA	6.74	129.58	122.97
2	B	791	THR	N-CA-C	-6.73	99.69	109.59
2	B	1156	ASP	N-CA-C	6.73	121.08	113.01
1	A	60	SER	CA-C-N	6.70	133.26	122.68
1	A	60	SER	C-N-CA	6.70	133.26	122.68
2	B	296	GLU	N-CA-C	-6.60	96.74	110.80
1	A	3	GLY	CA-C-N	6.55	134.05	121.54
1	A	3	GLY	C-N-CA	6.55	134.05	121.54
1	A	1230	GLU	CA-C-N	6.42	129.76	120.38
1	A	1230	GLU	C-N-CA	6.42	129.76	120.38
1	A	252	PHE	CA-CB-CG	6.40	120.20	113.80
7	G	18	PHE	CA-CB-CG	6.38	120.18	113.80
2	B	501	PRO	CA-C-N	6.38	133.19	121.70
2	B	501	PRO	C-N-CA	6.38	133.19	121.70
1	A	399	HIS	N-CA-CB	6.37	121.72	110.37
1	A	62	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	794	PRO	CA-C-N	6.36	128.71	120.44
1	A	794	PRO	C-N-CA	6.36	128.71	120.44
1	A	1063	MET	CA-C-N	6.32	133.34	121.97
1	A	1063	MET	C-N-CA	6.32	133.34	121.97
1	A	224	PHE	CA-CB-CG	-6.30	107.50	113.80
1	A	399	HIS	CA-C-O	-6.30	111.53	120.16
2	B	736	THR	N-CA-C	-6.29	105.26	113.12
5	E	48	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	1445	ILE	N-CA-CB	6.27	119.22	110.56
2	B	790	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	1043	ASP	CA-C-N	6.26	128.68	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1043	ASP	C-N-CA	6.26	128.68	120.28
3	C	183	TRP	N-CA-C	-6.24	99.83	109.76
9	I	93	LYS	CA-C-N	6.24	128.93	120.38
9	I	93	LYS	C-N-CA	6.24	128.93	120.38
1	A	91	PHE	CA-CB-CG	6.20	120.00	113.80
16	X	233	LYS	CA-C-N	6.20	128.87	120.38
16	X	233	LYS	C-N-CA	6.20	128.87	120.38
2	B	998	ASP	CA-CB-CG	6.19	118.79	112.60
2	B	363	HIS	N-CA-C	-6.17	102.39	110.53
1	A	398	GLU	CA-C-O	-6.16	113.96	121.36
11	K	77	THR	CA-C-N	6.15	129.50	120.82
11	K	77	THR	C-N-CA	6.15	129.50	120.82
1	A	58	LEU	N-CA-C	6.10	120.79	113.23
1	A	884	ASP	CA-C-N	6.05	128.99	120.28
1	A	884	ASP	C-N-CA	6.05	128.99	120.28
1	A	845	LEU	CA-C-N	6.04	133.07	121.54
1	A	845	LEU	C-N-CA	6.04	133.07	121.54
5	E	88	VAL	CA-C-N	6.01	126.05	120.34
5	E	88	VAL	C-N-CA	6.01	126.05	120.34
2	B	66	ASP	CA-C-N	6.01	133.02	121.54
2	B	66	ASP	C-N-CA	6.01	133.02	121.54
2	B	884	ARG	CA-C-N	6.01	129.65	120.82
2	B	884	ARG	C-N-CA	6.01	129.65	120.82
2	B	707	PRO	CA-C-N	6.00	129.82	120.82
2	B	707	PRO	C-N-CA	6.00	129.82	120.82
2	B	297	ILE	N-CA-C	-5.99	104.90	110.53
10	J	9	SER	N-CA-C	5.98	117.67	111.03
1	A	602	ASP	N-CA-C	-5.98	103.01	111.56
3	C	135	GLN	CA-C-N	5.93	129.26	120.90
3	C	135	GLN	C-N-CA	5.93	129.26	120.90
1	A	705	LYS	CA-C-N	5.92	132.84	121.54
1	A	705	LYS	C-N-CA	5.92	132.84	121.54
1	A	24	PRO	CA-C-N	5.91	128.48	120.38
1	A	24	PRO	C-N-CA	5.91	128.48	120.38
1	A	1185	PHE	CA-CB-CG	5.86	119.66	113.80
3	C	82	TYR	N-CA-C	-5.86	100.45	109.76
2	B	733	HIS	CA-C-N	5.85	129.59	120.82
2	B	733	HIS	C-N-CA	5.85	129.59	120.82
4	D	156	ASP	CA-CB-CG	5.83	118.44	112.60
2	B	1189	ILE	N-CA-C	5.82	116.95	111.48
1	A	622	VAL	N-CA-CB	-5.77	104.61	112.28
1	A	317	LYS	CA-C-N	5.76	132.54	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	LYS	C-N-CA	5.76	132.54	121.54
2	B	722	ASP	CA-C-N	5.73	129.06	120.69
2	B	722	ASP	C-N-CA	5.73	129.06	120.69
1	A	408	ASP	CA-C-N	5.73	128.53	120.28
1	A	408	ASP	C-N-CA	5.73	128.53	120.28
1	A	256	GLN	CA-C-N	5.72	132.47	121.54
1	A	256	GLN	C-N-CA	5.72	132.47	121.54
2	B	343	ILE	CA-C-N	5.71	132.44	121.54
2	B	343	ILE	C-N-CA	5.71	132.44	121.54
4	D	31	GLN	N-CA-C	-5.66	105.10	112.23
1	A	1388	GLY	N-CA-C	5.65	115.35	110.21
4	D	143	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	1335	ILE	CA-C-N	5.62	127.81	120.28
1	A	1335	ILE	C-N-CA	5.62	127.81	120.28
16	X	253	ILE	CA-C-N	5.62	124.83	120.33
16	X	253	ILE	C-N-CA	5.62	124.83	120.33
1	A	252	PHE	CA-C-N	5.60	132.24	121.54
1	A	252	PHE	C-N-CA	5.60	132.24	121.54
1	A	301	ALA	CA-C-N	5.59	128.34	120.28
1	A	301	ALA	C-N-CA	5.59	128.34	120.28
16	X	301	ILE	CA-C-N	5.59	128.57	120.79
16	X	301	ILE	C-N-CA	5.59	128.57	120.79
1	A	1064	VAL	N-CA-CB	-5.59	102.01	111.23
1	A	222	LEU	N-CA-C	-5.58	103.34	110.53
1	A	78	PRO	CA-C-N	-5.56	112.49	121.05
1	A	78	PRO	C-N-CA	-5.56	112.49	121.05
1	A	1424	VAL	N-CA-CB	5.53	116.65	110.62
2	B	470	LYS	CA-C-N	5.52	131.64	121.70
2	B	470	LYS	C-N-CA	5.52	131.64	121.70
1	A	1097	GLY	CA-C-N	5.51	125.72	120.43
1	A	1097	GLY	C-N-CA	5.51	125.72	120.43
2	B	1131	GLY	CA-C-N	5.50	127.65	120.28
2	B	1131	GLY	C-N-CA	5.50	127.65	120.28
11	K	63	VAL	N-CA-CB	5.49	118.19	111.60
2	B	880	THR	CA-C-N	5.48	132.01	121.54
2	B	880	THR	C-N-CA	5.48	132.01	121.54
10	J	6	ARG	CA-C-N	5.48	128.55	120.82
10	J	6	ARG	C-N-CA	5.48	128.55	120.82
2	B	472	ALA	CA-C-N	5.47	127.87	120.38
2	B	472	ALA	C-N-CA	5.47	127.87	120.38
1	A	288	ALA	N-CA-C	-5.46	106.99	113.97
9	I	8	ARG	N-CA-C	-5.46	102.21	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	59	LYS	CA-C-N	5.44	127.57	120.28
10	J	59	LYS	C-N-CA	5.44	127.57	120.28
3	C	120	ILE	N-CA-CB	5.44	116.86	110.82
2	B	232	SER	N-CA-C	5.43	115.85	109.60
2	B	371	GLU	CA-C-N	5.43	127.83	120.38
2	B	371	GLU	C-N-CA	5.43	127.83	120.38
2	B	429	PHE	CA-CB-CG	5.40	119.20	113.80
1	A	498	ARG	N-CA-C	-5.40	105.31	111.14
3	C	264	GLN	CA-C-N	5.39	127.50	120.28
3	C	264	GLN	C-N-CA	5.39	127.50	120.28
3	C	238	ILE	N-CA-CB	-5.39	103.67	111.21
2	B	1003	ALA	CA-C-N	5.38	129.22	120.60
2	B	1003	ALA	C-N-CA	5.38	129.22	120.60
2	B	415	GLN	CA-C-N	5.37	127.91	120.29
2	B	415	GLN	C-N-CA	5.37	127.91	120.29
2	B	881	ASN	CA-CB-CG	5.36	117.96	112.60
7	G	65	ASP	CA-CB-CG	5.36	117.96	112.60
7	G	50	ASP	CA-CB-CG	5.35	117.95	112.60
10	J	1	MET	CA-C-N	5.34	131.59	121.97
10	J	1	MET	C-N-CA	5.34	131.59	121.97
3	C	60	ASP	CA-CB-CG	5.34	117.94	112.60
3	C	89	GLU	N-CA-C	-5.33	100.04	108.73
2	B	231	PRO	CA-C-N	5.32	128.22	120.51
2	B	231	PRO	C-N-CA	5.32	128.22	120.51
11	K	39	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	1181	ALA	CA-C-N	5.30	131.25	121.70
1	A	1181	ALA	C-N-CA	5.30	131.25	121.70
1	A	35	ILE	CB-CA-C	5.30	117.28	111.08
1	A	78	PRO	N-CA-C	-5.29	101.88	110.40
8	H	130	ARG	CA-C-N	5.29	127.36	120.28
8	H	130	ARG	C-N-CA	5.29	127.36	120.28
1	A	1436	ILE	N-CA-CB	-5.27	102.22	111.39
2	B	1122	ARG	CA-C-N	5.25	127.58	120.38
2	B	1122	ARG	C-N-CA	5.25	127.58	120.38
2	B	643	ASP	CA-C-N	5.24	131.56	121.54
2	B	643	ASP	C-N-CA	5.24	131.56	121.54
1	A	672	ASP	CA-CB-CG	5.24	117.84	112.60
2	B	1007	VAL	N-CA-CB	-5.24	103.88	111.21
1	A	1127	ASP	CA-CB-CG	5.23	117.83	112.60
6	F	110	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	440	ASP	CA-CB-CG	5.22	117.82	112.60
2	B	1180	PHE	CA-CB-CG	-5.21	108.59	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ASP	CA-CB-CG	5.20	117.80	112.60
16	X	338	MET	CA-C-N	5.20	131.46	121.54
16	X	338	MET	C-N-CA	5.20	131.46	121.54
2	B	629	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	305	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	628	GLY	CA-C-N	5.18	127.48	120.38
1	A	628	GLY	C-N-CA	5.18	127.48	120.38
1	A	1198	ASP	CA-C-N	5.17	127.46	120.38
1	A	1198	ASP	C-N-CA	5.17	127.46	120.38
1	A	244	PRO	N-CA-C	5.17	117.00	110.70
1	A	1182	GLU	CA-C-N	5.16	131.40	121.54
1	A	1182	GLU	C-N-CA	5.16	131.40	121.54
1	A	721	PHE	CA-CB-CG	5.16	118.96	113.80
1	A	1179	GLU	CA-C-N	5.16	131.39	121.54
1	A	1179	GLU	C-N-CA	5.16	131.39	121.54
4	D	9	GLN	CA-C-N	5.16	127.70	120.28
4	D	9	GLN	C-N-CA	5.16	127.70	120.28
5	E	147	HIS	CA-C-N	5.16	127.96	120.79
5	E	147	HIS	C-N-CA	5.16	127.96	120.79
1	A	31	SER	N-CA-C	5.14	117.68	109.96
1	A	537	ARG	CA-C-N	5.14	128.82	120.60
1	A	537	ARG	C-N-CA	5.14	128.82	120.60
1	A	468	PHE	N-CA-C	-5.13	101.60	109.76
3	C	26	ASP	CA-CB-CG	5.12	117.72	112.60
7	G	46	LEU	N-CA-C	5.12	116.67	111.14
3	C	150	GLY	CA-C-N	5.12	128.60	121.02
3	C	150	GLY	C-N-CA	5.12	128.60	121.02
1	A	1204	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	154	SER	CA-C-N	5.08	127.41	120.54
1	A	154	SER	C-N-CA	5.08	127.41	120.54
3	C	62	PHE	N-CA-C	-5.08	105.65	111.14
12	L	25	ALA	CA-C-N	5.08	131.24	121.54
12	L	25	ALA	C-N-CA	5.08	131.24	121.54
1	A	41	MET	CA-C-N	5.08	131.24	121.54
1	A	41	MET	C-N-CA	5.08	131.24	121.54
2	B	478	GLY	CA-C-N	5.07	127.05	120.56
2	B	478	GLY	C-N-CA	5.07	127.05	120.56
3	C	117	ASP	CA-CB-CG	5.07	117.67	112.60
10	J	14	VAL	CB-CA-C	5.06	116.40	110.88
2	B	188	ASP	CA-CB-CG	5.06	117.66	112.60
2	B	758	PHE	CA-C-O	-5.05	116.98	120.47
1	A	148	CYS	N-CA-C	-5.05	102.17	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	53	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	1393	ASN	CA-CB-CG	5.05	117.65	112.60
3	C	121	VAL	CB-CA-C	5.04	116.38	110.88
1	A	452	LYS	N-CA-C	-5.04	105.97	111.82
2	B	425	THR	CA-C-N	5.04	127.04	120.28
2	B	425	THR	C-N-CA	5.04	127.04	120.28
2	B	648	HIS	CA-C-N	5.03	127.99	120.95
2	B	648	HIS	C-N-CA	5.03	127.99	120.95
2	B	881	ASN	CA-C-N	5.03	131.15	121.54
2	B	881	ASN	C-N-CA	5.03	131.15	121.54
6	F	127	GLU	CA-C-N	5.02	129.27	122.19
6	F	127	GLU	C-N-CA	5.02	129.27	122.19

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	T	15	DT	Sidechain
15	T	25	DT	Sidechain

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	11223	0	11273	195	0
2	B	8859	0	8902	127	0
3	C	2095	0	2051	37	0
4	D	1387	0	1366	21	0
5	E	1760	0	1788	24	0
6	F	705	0	731	15	0
7	G	1340	0	1357	35	0
8	H	1068	0	1039	29	0
9	I	971	0	927	6	0
10	J	532	0	542	12	0
11	K	920	0	929	15	0
12	L	363	0	385	7	0
13	N	269	0	147	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	P	215	0	109	1	0
15	T	504	0	274	4	0
16	X	977	0	996	13	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
19	A	15	17	17	1	0
19	G	15	17	17	0	0
All	All	33227	34	32850	481	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 7.

All (481) 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:53:LEU:HD23	1:A:54:ASN:H	1.23	1.02
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.45	0.94
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.49	0.94
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.83	0.93
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.52	0.92
1:A:567:LYS:HB3	8:H:96:VAL:H	1.34	0.91
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.37	0.90
4:D:53:SER:HB3	4:D:152:SER:HB2	1.54	0.89
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.19	0.88
1:A:1177:LEU:HB3	1:A:1179:GLU:H	1.37	0.87
3:C:56:THR:HG22	3:C:58:LEU:H	1.38	0.87
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.58	0.86
1:A:869:GLY:O	5:E:204:THR:HG21	1.77	0.85
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.39	0.85
2:B:654:ARG:H	2:B:657:HIS:HD2	1.28	0.82
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.63	0.80
16:X:316:LYS:HG2	16:X:320:GLU:HB3	1.62	0.80
11:K:65:HIS:HD2	11:K:67:PHE:H	1.29	0.80
1:A:68:GLN:OE1	1:A:70:CYS:HB3	1.82	0.78
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.65	0.78
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.13	0.77
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.67	0.76
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.67	0.75
2:B:277:LYS:H	2:B:338:GLY:HA3	1.51	0.75
2:B:345:LYS:HA	2:B:348:ARG:HD3	1.69	0.75
11:K:65:HIS:CD2	11:K:67:PHE:H	2.05	0.74
1:A:53:LEU:HD23	1:A:54:ASN:N	2.00	0.73
8:H:95:TYR:HE1	8:H:97:MET:HG3	1.54	0.73
6:F:99:LEU:HG	6:F:103:MET:HE2	1.69	0.73
1:A:567:LYS:HB3	8:H:96:VAL:N	2.03	0.72
3:C:100:THR:HG22	3:C:119:VAL:HB	1.69	0.71
6:F:103:MET:HE1	7:G:66:GLY:H	1.56	0.71
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.20	0.70
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.21	0.70
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.20	0.69
1:A:494:SER:HB3	1:A:497:THR:HB	1.73	0.69
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.75	0.69
1:A:503:GLN:NE2	6:F:90:ARG:HH21	1.90	0.68
1:A:903:ASN:HD22	1:A:905:ASP:H	1.42	0.66
2:B:273:LEU:H	2:B:276:ILE:HD11	1.60	0.66
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.79	0.66
1:A:741:ASN:HD22	1:A:744:LYS:H	1.42	0.66
2:B:744:HIS:HD2	2:B:746:SER:H	1.43	0.66
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.78	0.66
1:A:1364:ASN:HD22	1:A:1366:ARG:HD2	1.60	0.66
4:D:23:ASN:HA	4:D:28:GLN:O	1.96	0.66
4:D:155:ARG:HB2	4:D:219:THR:HG21	1.78	0.66
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.76	0.66
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.76	0.65
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.61	0.65
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.78	0.65
2:B:705:MET:H	2:B:710:LEU:HD12	1.62	0.65
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.79	0.65
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.80	0.64
2:B:882:THR:HG1	2:B:935:ARG:N	1.95	0.64
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.79	0.64
4:D:119:ARG:HH21	4:D:120:GLU:HB2	1.63	0.64
1:A:57:ARG:O	1:A:68:GLN:HG2	1.98	0.64
2:B:363:HIS:O	2:B:364:ILE:HB	1.98	0.63
1:A:298:PHE:O	1:A:302:THR:HB	1.98	0.62
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:26:LEU:HD13	7:G:56:ILE:HD11	1.81	0.62
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.82	0.62
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.81	0.61
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.47	0.61
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.82	0.61
7:G:1:MET:HE1	7:G:79:PHE:HA	1.81	0.61
1:A:65:LEU:HD23	1:A:71:GLN:HB2	1.83	0.61
3:C:46:ILE:HG12	3:C:157:CYS:HB3	1.83	0.60
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.84	0.60
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.15	0.60
2:B:711:GLU:H	2:B:712:PRO:HD3	1.66	0.60
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.67	0.60
1:A:225:ASN:HD22	1:A:227:VAL:H	1.49	0.60
1:A:565:ILE:HG23	1:A:567:LYS:HG3	1.83	0.60
7:G:14:HIS:CD2	7:G:16:SER:H	2.20	0.60
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.83	0.60
2:B:333:PHE:O	2:B:337:ARG:HG2	2.02	0.59
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.85	0.59
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.30	0.59
1:A:1424:VAL:HG13	1:A:1436:ILE:HG12	1.83	0.59
5:E:31:THR:HG23	5:E:34:GLU:H	1.67	0.59
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.33	0.59
1:A:55:ASP:N	1:A:56:PRO:HD3	2.18	0.58
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.51	0.58
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.97	0.58
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.84	0.58
1:A:1177:LEU:HB3	1:A:1179:GLU:N	2.13	0.58
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.39	0.58
7:G:1:MET:HE2	7:G:2:PHE:H	1.69	0.57
2:B:1013:ASN:OD1	2:B:1015:HIS:HD2	1.87	0.57
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.85	0.57
7:G:1:MET:CE	7:G:80:LYS:H	2.17	0.57
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.68	0.57
3:C:142:VAL:H	10:J:16:ASP:HB3	1.70	0.57
1:A:1176:LEU:HB3	16:X:240:ASN:HB3	1.87	0.57
7:G:111:THR:HG22	7:G:113:HIS:H	1.70	0.57
1:A:4:GLN:O	1:A:5:GLN:HB3	2.04	0.56
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.88	0.56
8:H:95:TYR:CE1	8:H:97:MET:HG3	2.37	0.56
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.89	0.56
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:VAL:HG13	6:F:123:LYS:HE3	1.88	0.56
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.36	0.56
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.88	0.56
8:H:130:ARG:H	8:H:130:ARG:HD2	1.71	0.56
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.89	0.55
5:E:1:MET:HE3	5:E:4:GLU:HG2	1.86	0.55
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.22	0.55
1:A:321:PRO:O	1:A:322:VAL:HB	2.07	0.55
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.41	0.55
1:A:761:MET:HG3	2:B:1021:MET:HG2	1.88	0.55
1:A:353:ILE:HD12	1:A:482:PHE:HD1	1.72	0.55
1:A:563:PRO:HA	1:A:576:GLN:HE22	1.71	0.55
1:A:754:SER:H	1:A:757:ASN:HD22	1.55	0.55
1:A:1178:ASP:C	1:A:1180:GLU:H	2.15	0.55
2:B:1013:ASN:OD1	2:B:1015:HIS:CD2	2.60	0.55
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.88	0.54
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.87	0.54
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.88	0.54
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.43	0.54
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.89	0.54
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.89	0.54
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.90	0.54
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.90	0.54
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.90	0.54
1:A:472:LEU:O	1:A:475:THR:HB	2.08	0.53
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.89	0.53
2:B:515:HIS:H	2:B:518:HIS:CD2	2.26	0.53
1:A:709:THR:HG22	1:A:711:ARG:H	1.72	0.53
1:A:92:HIS:HD2	1:A:94:GLY:H	1.56	0.53
2:B:685:LEU:HD12	2:B:690:VAL:HG13	1.91	0.53
2:B:792:MET:HA	2:B:856:PHE:O	2.09	0.53
2:B:344:LYS:O	2:B:347:LYS:HG2	2.07	0.53
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.74	0.53
3:C:148:ARG:HD3	3:C:149:LYS:HE3	1.90	0.53
1:A:933:TYR:O	1:A:937:VAL:HG23	2.10	0.52
2:B:1096:ARG:HH11	2:B:1096:ARG:HB2	1.73	0.52
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.91	0.52
2:B:449:ASN:HD22	2:B:452:THR:HG23	1.75	0.52
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.90	0.52
1:A:567:LYS:CB	1:A:568:PRO:CD	2.83	0.52
3:C:143:LEU:HD21	3:C:146:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:HE1	2:B:1210:MET:O	1.93	0.52
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.92	0.52
4:D:73:SER:HB2	7:G:21:ARG:HH12	1.74	0.52
1:A:362:ASP:OD2	1:A:459:ARG:HD3	2.10	0.52
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.92	0.52
10:J:48:ARG:CZ	10:J:49:MET:HE1	2.39	0.52
1:A:982:THR:H	1:A:985:ASP:HB2	1.75	0.52
3:C:56:THR:HG22	3:C:57:VAL:N	2.25	0.52
8:H:89:LEU:C	8:H:91:ASP:H	2.18	0.52
16:X:248:LEU:O	16:X:252:PHE:HB3	2.10	0.52
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.75	0.52
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.92	0.52
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.92	0.52
1:A:1081:LEU:HD12	1:A:1099:PRO:HD3	1.92	0.51
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.10	0.51
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.92	0.51
3:C:54:ASN:OD1	3:C:56:THR:HB	2.10	0.51
6:F:99:LEU:HG	6:F:103:MET:CE	2.40	0.51
7:G:1:MET:HE3	7:G:80:LYS:H	1.75	0.51
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.92	0.51
6:F:128:LYS:HE2	6:F:148:VAL:O	2.10	0.51
1:A:41:MET:HB3	1:A:49:LYS:HA	1.92	0.51
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.93	0.51
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.92	0.51
8:H:47:PHE:HB3	8:H:95:TYR:CD2	2.46	0.51
1:A:549:MET:SD	1:A:577:ILE:HD11	2.50	0.51
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.92	0.51
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.92	0.51
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.93	0.51
6:F:103:MET:HE1	7:G:66:GLY:N	2.26	0.51
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.92	0.50
2:B:323:VAL:HG23	2:B:324:ILE:HD12	1.93	0.50
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.93	0.50
8:H:111:LEU:HA	8:H:127:GLY:O	2.10	0.50
1:A:929:LEU:HD21	1:A:983:ILE:HG12	1.94	0.50
1:A:42:ASP:HA	1:A:46:THR:O	2.11	0.50
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.17	0.50
3:C:66:ARG:HH21	10:J:2:ILE:HG23	1.77	0.50
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.94	0.50
7:G:102:GLN:HE22	7:G:107:LYS:HE2	1.76	0.50
2:B:789:MET:HE3	2:B:965:LYS:HB3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:19:VAL:HG11	5:E:80:VAL:HG11	1.93	0.50
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.93	0.50
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.47	0.50
1:A:903:ASN:ND2	1:A:905:ASP:H	2.09	0.50
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.94	0.50
3:C:4:GLU:H	3:C:7:GLN:HE22	1.60	0.50
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.94	0.50
1:A:55:ASP:C	1:A:57:ARG:H	2.19	0.49
7:G:112:LYS:HA	7:G:115:MET:HE3	1.93	0.49
2:B:1100:ASP:HA	2:B:1103:ILE:HG22	1.94	0.49
1:A:590:ARG:O	1:A:591:PHE:HB2	2.12	0.49
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.94	0.49
3:C:66:ARG:NH2	10:J:2:ILE:HG23	2.27	0.49
7:G:14:HIS:HD2	7:G:16:SER:H	1.59	0.49
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.76	0.49
5:E:147:HIS:CD2	5:E:149:LEU:H	2.30	0.49
1:A:55:ASP:CG	1:A:55:ASP:O	2.55	0.49
1:A:856:THR:HB	1:A:865:GLN:HB2	1.95	0.49
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.94	0.49
2:B:654:ARG:H	2:B:657:HIS:CD2	2.19	0.49
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.94	0.49
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.60	0.49
5:E:23:VAL:HG23	5:E:30:ILE:HD13	1.94	0.49
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.13	0.49
1:A:567:LYS:CB	8:H:96:VAL:H	2.13	0.49
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.47	0.49
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.48	0.48
1:A:709:THR:HG23	9:I:94:ASP:HA	1.95	0.48
9:I:8:ARG:O	9:I:9:ASP:HB2	2.13	0.48
1:A:149:GLU:HB3	1:A:164:ARG:HD3	1.95	0.48
1:A:225:ASN:ND2	1:A:227:VAL:H	2.12	0.48
6:F:69:LEU:C	6:F:71:GLU:H	2.21	0.48
2:B:193:LYS:HE3	10:J:65:PRO:HD2	1.95	0.48
2:B:653:VAL:HG13	2:B:689:LEU:HB3	1.95	0.48
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.95	0.48
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.95	0.48
1:A:134:ARG:HD2	1:A:221:SER:O	2.13	0.48
15:T:9:DT:H2'	15:T:10:DA:C8	2.48	0.48
5:E:147:HIS:HD2	5:E:149:LEU:H	1.59	0.48
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.96	0.48
1:A:925:LEU:HD23	1:A:983:ILE:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:542:MET:HE1	2:B:743:ILE:HB	1.96	0.48
3:C:50:GLU:HG3	12:L:66:GLN:HG3	1.96	0.48
2:B:310:MET:O	2:B:313:MET:HB2	2.13	0.48
2:B:792:MET:H	2:B:857:ARG:HA	1.79	0.48
2:B:841:MET:O	2:B:993:THR:HA	2.13	0.47
2:B:901:PRO:HD2	12:L:59:ALA:C	2.39	0.47
4:D:134:THR:HG23	4:D:136:GLY:H	1.79	0.47
10:J:6:ARG:HA	10:J:12:LYS:O	2.14	0.47
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.97	0.47
4:D:37:GLN:HE22	7:G:5:LYS:HE3	1.79	0.47
16:X:305:LYS:HE2	16:X:339:ASN:HD22	1.79	0.47
12:L:28:LYS:H	12:L:39:SER:HA	1.79	0.47
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.97	0.47
1:A:497:THR:HG21	2:B:1149:GLU:OE2	2.15	0.47
2:B:1022:THR:HG23	2:B:1022:THR:O	2.15	0.47
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.79	0.47
1:A:868:TYR:CZ	1:A:1064:VAL:HG22	2.50	0.47
2:B:1107:ALA:O	2:B:1108:ARG:HB2	2.14	0.47
5:E:50:MET:HB2	5:E:52:ARG:HD2	1.96	0.47
7:G:1:MET:HE2	7:G:2:PHE:N	2.29	0.47
7:G:83:LYS:HD2	7:G:149:GLY:HA2	1.96	0.47
11:K:10:PHE:HD1	11:K:11:LEU:HD13	1.80	0.47
1:A:3:GLY:HA3	2:B:1159:ARG:HB3	1.96	0.47
1:A:31:SER:OG	1:A:83:HIS:HD2	1.98	0.47
1:A:512:VAL:HA	1:A:519:PRO:HA	1.97	0.47
1:A:567:LYS:CB	8:H:95:TYR:HA	2.44	0.47
1:A:847:ASP:HB3	1:A:1398:MET:HE1	1.97	0.47
1:A:851:HIS:CD2	1:A:857:ARG:HB2	2.49	0.47
1:A:230:ARG:HD2	1:A:233:TRP:CZ2	2.49	0.47
1:A:1227:ILE:HG13	1:A:1239:ARG:HB2	1.97	0.47
1:A:63:ARG:HG3	1:A:74:MET:HE3	1.96	0.46
1:A:182:VAL:HG22	1:A:201:VAL:HG22	1.96	0.46
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.30	0.46
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.97	0.46
3:C:99:LEU:HD13	3:C:120:ILE:HG13	1.96	0.46
1:A:399:HIS:O	1:A:435:HIS:CD2	2.68	0.46
2:B:702:LEU:H	2:B:739:THR:HG1	1.64	0.46
6:F:128:LYS:HG3	6:F:149:GLU:HA	1.97	0.46
1:A:337:ARG:HD2	2:B:1132:GLU:OE2	2.15	0.46
2:B:705:MET:HE3	2:B:705:MET:HA	1.98	0.46
2:B:744:HIS:CD2	2:B:746:SER:H	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:48:ARG:O	10:J:52:THR:HG22	2.16	0.46
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.99	0.46
1:A:7:SER:OG	2:B:1161:HIS:CE1	2.65	0.46
1:A:92:HIS:HD2	1:A:94:GLY:N	2.14	0.46
2:B:1188:LYS:H	2:B:1189:ILE:HD12	1.80	0.46
11:K:12:LEU:HD22	11:K:16:GLU:HB3	1.97	0.46
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.98	0.46
5:E:156:LEU:HD13	5:E:195:VAL:HG12	1.98	0.46
8:H:95:TYR:HE1	8:H:97:MET:CG	2.26	0.46
1:A:707:GLY:HA3	1:A:1281:ARG:HD2	1.98	0.46
16:X:245:PHE:HA	16:X:248:LEU:HD23	1.97	0.46
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.98	0.46
3:C:6:PRO:HA	3:C:24:ASN:HB3	1.97	0.46
10:J:1:MET:HG3	10:J:60:PHE:CE2	2.51	0.46
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.96	0.45
1:A:89:PRO:HG2	1:A:204:THR:HB	1.98	0.45
1:A:915:SER:O	1:A:919:ILE:HB	2.15	0.45
2:B:516:ASN:H	2:B:516:ASN:HD22	1.64	0.45
16:X:325:VAL:HB	16:X:330:LEU:HD22	1.98	0.45
1:A:565:ILE:HG12	1:A:567:LYS:HE2	1.98	0.45
1:A:1177:LEU:HD11	16:X:237:LEU:HB3	1.98	0.45
8:H:135:LEU:C	8:H:137:GLN:H	2.22	0.45
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.98	0.45
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.57	0.45
1:A:1329:THR:HG22	1:A:1331:SER:H	1.80	0.45
3:C:64:ALA:HA	3:C:67:LEU:HD12	1.98	0.45
12:L:38:LEU:HD13	12:L:56:LEU:HD21	1.98	0.45
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.97	0.45
8:H:47:PHE:CD2	8:H:95:TYR:HD2	2.34	0.45
13:N:5:DA:H2''	13:N:6:DG:H8	1.80	0.45
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.98	0.45
8:H:47:PHE:HB3	8:H:95:TYR:HD2	1.82	0.45
9:I:68:LEU:HB3	9:I:84:VAL:HG22	1.98	0.45
1:A:855:THR:HG22	1:A:857:ARG:HG3	1.99	0.45
3:C:173:ALA:HB2	3:C:243:VAL:HG11	1.99	0.45
1:A:596:THR:C	1:A:598:LEU:H	2.25	0.45
6:F:76:LYS:HA	6:F:79:ARG:CD	2.47	0.45
13:N:6:DG:H2'	13:N:7:DT:C6	2.52	0.45
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.52	0.45
1:A:456:MET:HB2	1:A:478:TYR:OH	2.17	0.45
2:B:766:ARG:CZ	2:B:1020:ARG:HD3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.98	0.44
1:A:1266:THR:HG23	1:A:1270:ASN:HD22	1.82	0.44
2:B:620:ARG:HG3	9:I:57:GLY:HA3	1.99	0.44
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.17	0.44
2:B:745:PRO:O	2:B:748:ILE:HG12	2.17	0.44
3:C:33:LEU:HG	3:C:37:MET:HE2	1.97	0.44
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.99	0.44
3:C:147:LEU:HB3	3:C:151:GLN:HB3	1.99	0.44
1:A:56:PRO:CD	1:A:58:LEU:HG	2.41	0.44
1:A:1135:ARG:HD3	1:A:1282:VAL:HB	2.00	0.44
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.17	0.44
2:B:652:LYS:HD2	2:B:688:GLY:O	2.17	0.44
1:A:329:LEU:HA	1:A:335:ARG:H	1.82	0.44
1:A:492:PRO:CB	1:A:497:THR:HG23	2.47	0.44
1:A:846:GLU:OE1	1:A:1398:MET:HE2	2.18	0.44
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.18	0.44
11:K:51:LEU:HD13	11:K:59:ALA:HB3	2.00	0.44
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.83	0.44
2:B:464:GLY:HA2	2:B:480:SER:HB3	2.00	0.44
4:D:144:THR:HG21	7:G:46:LEU:HD13	2.00	0.44
9:I:8:ARG:O	9:I:9:ASP:CB	2.64	0.44
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	2.00	0.44
2:B:470:LYS:HB2	2:B:471:LYS:C	2.42	0.44
6:F:109:VAL:HB	6:F:124:GLU:HG2	2.00	0.44
16:X:285:GLU:HB3	16:X:336:VAL:HG21	1.99	0.44
1:A:55:ASP:O	1:A:55:ASP:OD2	2.36	0.43
2:B:126:SER:OG	2:B:172:ILE:HD11	2.18	0.43
3:C:44:LEU:HB2	3:C:77:ILE:HD13	2.00	0.43
2:B:957:ASN:HB3	2:B:961:LEU:HB2	2.00	0.43
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.53	0.43
1:A:1135:ARG:HD2	1:A:1135:ARG:C	2.44	0.43
2:B:889:THR:HG22	2:B:891:ASP:H	1.83	0.43
3:C:70:ILE:HD11	3:C:144:ILE:HG12	2.00	0.43
2:B:884:ARG:HD2	2:B:935:ARG:HB2	1.99	0.43
4:D:54:GLU:O	4:D:58:VAL:HG23	2.19	0.43
1:A:629:LEU:HD13	1:A:645:LEU:HD21	2.01	0.43
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	2.00	0.43
2:B:470:LYS:HD2	2:B:472:ALA:HB2	2.00	0.43
7:G:50:ASP:OD2	7:G:53:ASN:HB2	2.18	0.43
1:A:1317:MET:HE1	1:A:1339:LEU:HD21	2.00	0.43
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:131:GLN:HG2	7:G:136:VAL:HG22	2.00	0.43
1:A:316:GLN:HB3	1:A:322:VAL:HG23	2.01	0.43
2:B:117:ALA:HA	2:B:122:LEU:HB2	2.00	0.43
5:E:156:LEU:HD11	5:E:197:LYS:HB2	2.01	0.43
1:A:901:LEU:H	1:A:926:GLN:NE2	2.16	0.43
2:B:460:ALA:HB2	2:B:468:GLU:HG3	2.00	0.43
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.84	0.43
2:B:877:PRO:HA	2:B:934:LYS:HE3	2.00	0.43
2:B:1158:PHE:CE2	2:B:1160:VAL:HG13	2.54	0.43
3:C:18:VAL:CG1	11:K:109:TRP:HZ3	2.32	0.43
7:G:138:THR:HG22	7:G:139:ILE:H	1.83	0.43
2:B:331:LEU:HB3	2:B:349:ILE:HG23	2.01	0.42
2:B:683:SER:O	2:B:687:GLU:HB2	2.19	0.42
16:X:286:LEU:HD12	16:X:336:VAL:HG13	2.01	0.42
1:A:55:ASP:N	1:A:56:PRO:CD	2.82	0.42
1:A:527:THR:HG23	1:A:653:VAL:HB	2.01	0.42
4:D:194:LEU:HD22	7:G:86:VAL:HG11	2.00	0.42
1:A:53:LEU:CD2	1:A:54:ASN:H	2.12	0.42
1:A:982:THR:HB	1:A:985:ASP:H	1.85	0.42
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.84	0.42
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	2.01	0.42
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.20	0.42
8:H:80:ARG:HG2	11:K:57:LEU:HD22	2.01	0.42
1:A:92:HIS:CD2	1:A:94:GLY:H	2.35	0.42
1:A:854:ASN:HB3	1:A:867:ILE:HD11	1.99	0.42
1:A:858:ASN:C	1:A:858:ASN:HD22	2.28	0.42
1:A:1035:TYR:CD1	1:A:1035:TYR:N	2.88	0.42
2:B:233:PRO:HG2	2:B:234:ILE:HD12	2.02	0.42
2:B:276:ILE:HD13	2:B:280:ILE:HD12	2.02	0.42
1:A:219:PHE:HA	1:A:222:LEU:HD12	2.01	0.42
1:A:378:GLU:CD	1:A:387:ARG:HH22	2.26	0.42
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.02	0.42
2:B:468:GLU:O	2:B:468:GLU:HG2	2.19	0.42
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.55	0.42
4:D:67:ARG:HH11	4:D:71:LYS:NZ	2.17	0.42
8:H:93:TYR:CG	8:H:143:LEU:HB3	2.53	0.42
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.34	0.42
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	2.01	0.42
2:B:41:LYS:O	2:B:45:SER:HB3	2.20	0.42
7:G:1:MET:HE1	7:G:80:LYS:H	1.85	0.42
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:17:ARG:HB2	9:I:28:GLU:HG2	2.00	0.42
10:J:35:ALA:O	10:J:39:LEU:HD22	2.20	0.42
4:D:156:ASP:HB2	4:D:159:THR:OG1	2.20	0.42
16:X:249:PHE:HA	16:X:252:PHE:CD1	2.55	0.42
1:A:380:VAL:HG13	1:A:385:ILE:HG12	2.02	0.42
1:A:1279:ILE:HD11	1:A:1312:ASN:HB3	2.01	0.42
3:C:125:MET:HG3	3:C:127:ARG:HH21	1.84	0.42
3:C:259:LEU:HD12	3:C:259:LEU:HA	1.89	0.42
4:D:18:VAL:C	4:D:20:GLU:H	2.27	0.42
5:E:202:SER:C	5:E:204:THR:H	2.28	0.42
2:B:882:THR:HG22	2:B:883:LEU:N	2.34	0.42
3:C:142:VAL:H	10:J:16:ASP:CB	2.32	0.42
4:D:130:LEU:O	4:D:134:THR:HG22	2.18	0.42
7:G:143:ILE:HG22	7:G:145:VAL:HG13	2.02	0.42
16:X:345:ASN:HD22	16:X:348:LEU:HD12	1.85	0.42
1:A:330:LYS:O	1:A:334:GLY:HA3	2.20	0.42
1:A:336:ILE:HD11	2:B:1203:LEU:HD13	2.01	0.42
1:A:442:VAL:CG2	1:A:489:LEU:HD11	2.50	0.42
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.20	0.42
2:B:467:GLY:HA3	2:B:471:LYS:HD3	2.02	0.42
16:X:233:LYS:O	16:X:237:LEU:HG	2.20	0.42
1:A:450:LEU:HD23	2:B:1133:MET:HE1	2.01	0.41
1:A:912:LEU:HD22	1:A:1033:GLN:HA	2.02	0.41
4:D:190:GLU:HG3	7:G:167:TYR:CD1	2.55	0.41
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.01	0.41
2:B:237:VAL:HG11	2:B:255:GLN:HE21	1.85	0.41
4:D:50:LEU:HD11	7:G:4:ILE:HG13	2.01	0.41
5:E:117:THR:HB	5:E:120:ALA:H	1.86	0.41
1:A:871:ASP:CB	5:E:204:THR:HG23	2.49	0.41
1:A:1062:GLU:HB3	1:A:1064:VAL:HG23	2.01	0.41
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.01	0.41
2:B:976:ILE:O	2:B:990:ILE:O	2.38	0.41
3:C:260:LEU:HD23	3:C:264:GLN:HE22	1.85	0.41
13:N:5:DA:H2"	13:N:6:DG:C8	2.55	0.41
1:A:442:VAL:HG21	1:A:489:LEU:HD11	2.03	0.41
1:A:1186:ASP:HA	1:A:1188:GLN:HE21	1.85	0.41
2:B:291:ILE:HD12	2:B:291:ILE:N	2.35	0.41
7:G:65:ASP:OD1	7:G:67:SER:HB2	2.19	0.41
8:H:135:LEU:HD13	8:H:137:GLN:HE21	1.86	0.41
1:A:93:VAL:HG13	1:A:301:ALA:HB1	2.03	0.41
1:A:526:ASP:OD2	2:B:832:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:ILE:H	2:B:251:ILE:HG13	1.66	0.41
2:B:899:ILE:HD12	2:B:911:ILE:HG22	2.03	0.41
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.19	0.41
5:E:190:LEU:HD11	5:E:196:VAL:HG13	2.02	0.41
7:G:14:HIS:HD2	7:G:16:SER:OG	2.04	0.41
11:K:7:PHE:HB2	11:K:11:LEU:HD22	2.02	0.41
1:A:399:HIS:O	1:A:435:HIS:HD2	2.02	0.41
1:A:492:PRO:HB2	1:A:497:THR:CG2	2.50	0.41
5:E:154:ILE:O	5:E:196:VAL:HA	2.20	0.41
8:H:125:LEU:HG	8:H:130:ARG:NH2	2.33	0.41
1:A:108:MET:H	1:A:171:GLN:NE2	2.18	0.41
1:A:1424:VAL:HG11	2:B:1139:ILE:HG12	2.02	0.41
2:B:756:ILE:O	2:B:759:PRO:HD3	2.21	0.41
1:A:34:LYS:HB3	19:A:2459:EPE:O2S	2.20	0.41
1:A:380:VAL:HG12	1:A:428:TYR:HA	2.02	0.41
1:A:406:ILE:HG13	1:A:412:ARG:HG2	2.01	0.41
1:A:1079:MET:HB3	1:A:1098:VAL:HG23	2.01	0.41
2:B:336:ARG:HH12	2:B:345:LYS:HE2	1.86	0.41
2:B:339:THR:HG22	2:B:341:LEU:HD11	2.02	0.41
3:C:40:GLU:HG2	3:C:165:LYS:HD2	2.02	0.41
5:E:152:LYS:HD2	5:E:199:ILE:HB	2.03	0.41
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.91	0.41
5:E:181:ALA:HA	5:E:186:LEU:HD21	2.03	0.41
15:T:23:DC:H2''	15:T:24:DA:O5'	2.20	0.41
1:A:954:TRP:HA	1:A:955:PRO:HD3	1.97	0.41
2:B:842:ASN:HB2	2:B:999:MET:HE2	2.03	0.41
2:B:1072:MET:HE1	2:B:1087:PHE:HB2	2.02	0.41
3:C:149:LYS:HD2	3:C:150:GLY:H	1.86	0.41
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.02	0.40
11:K:33:ILE:HD13	11:K:87:LEU:HD22	2.04	0.40
16:X:249:PHE:HA	16:X:252:PHE:HD1	1.86	0.40
1:A:353:ILE:HG22	1:A:468:PHE:HB2	2.01	0.40
1:A:635:ARG:HA	1:A:635:ARG:HH11	1.86	0.40
1:A:753:GLY:HA2	1:A:757:ASN:HD22	1.85	0.40
2:B:336:ARG:HG2	2:B:348:ARG:HH21	1.86	0.40
2:B:476:ARG:HH22	14:P:6:C:H5'	1.87	0.40
2:B:1106:ARG:CZ	2:B:1118:PRO:HB3	2.50	0.40
2:B:1167:GLY:HA3	2:B:1216:LEU:H	1.86	0.40
4:D:37:GLN:NE2	7:G:5:LYS:HE3	2.36	0.40
15:T:5:DC:H2''	15:T:6:DA:C8	2.56	0.40
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1043:ASP:OD1	2:B:1045:SER:HB2	2.21	0.40
6:F:69:LEU:HD23	6:F:73:ALA:H	1.86	0.40
8:H:105:GLU:HB3	8:H:113:ALA:HB3	2.04	0.40
1:A:1030:ARG:O	1:A:1034:GLU:HB2	2.21	0.40
3:C:77:ILE:HD12	3:C:77:ILE:HA	1.96	0.40
12:L:60:ARG:HH21	12:L:65:VAL:HG21	1.85	0.40
15:T:24:DA:N3	15:T:24:DA:H2'	2.36	0.40
2:B:70:ILE:HD12	2:B:429:PHE:HE1	1.87	0.40
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.55	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	1418/1733 (82%)	1274 (90%)	96 (7%)	48 (3%)	3	16
2	B	1097/1224 (90%)	981 (89%)	84 (8%)	32 (3%)	3	20
3	C	264/318 (83%)	246 (93%)	14 (5%)	4 (2%)	8	33
4	D	174/221 (79%)	156 (90%)	11 (6%)	7 (4%)	2	14
5	E	213/215 (99%)	209 (98%)	4 (2%)	0	100	100
6	F	85/155 (55%)	79 (93%)	4 (5%)	2 (2%)	4	23
7	G	169/171 (99%)	153 (90%)	12 (7%)	4 (2%)	4	23
8	H	128/146 (88%)	103 (80%)	15 (12%)	10 (8%)	1	4
9	I	117/122 (96%)	102 (87%)	13 (11%)	2 (2%)	7	30
10	J	63/70 (90%)	55 (87%)	5 (8%)	3 (5%)	2	11
11	K	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
12	L	42/70 (60%)	32 (76%)	5 (12%)	5 (12%)	0	1
16	X	113/146 (77%)	101 (89%)	8 (7%)	4 (4%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3996/4711 (85%)	3603 (90%)	272 (7%)	121 (3%)	3	19

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	57	ARG
1	A	76	GLU
1	A	253	ASN
1	A	257	ARG
1	A	311	GLN
1	A	322	VAL
1	A	332	LYS
1	A	525	GLN
1	A	567	LYS
1	A	706	HIS
1	A	1188	GLN
2	B	67	SER
2	B	344	LYS
2	B	469	GLN
2	B	477	ALA
2	B	712	PRO
2	B	731	VAL
2	B	880	THR
2	B	881	ASN
2	B	1046	PRO
2	B	1176	ASN
2	B	1181	GLU
2	B	1185	CYS
4	D	18	VAL
4	D	169	SER
7	G	2	PHE
9	I	9	ASP
10	J	2	ILE
16	X	315	ASP
16	X	339	ASN
1	A	254	GLU
1	A	318	SER
1	A	331	GLY
1	A	399	HIS
1	A	423	ASP
1	A	593	GLU

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Mol	Chain	Res	Type
1	A	1178	ASP
1	A	1184	SER
1	A	1221	LYS
1	A	1271	ILE
1	A	1281	ARG
2	B	262	GLU
2	B	339	THR
2	B	707	PRO
2	B	737	THR
2	B	772	ALA
2	B	907	GLY
3	C	141	GLY
3	C	215	GLU
3	C	227	THR
4	D	11	ARG
4	D	53	SER
4	D	199	ASN
6	F	71	GLU
6	F	73	ALA
8	H	82	PRO
8	H	139	ASN
10	J	6	ARG
12	L	45	ALA
12	L	55	ILE
12	L	56	LEU
16	X	340	ALA
1	A	4	GLN
1	A	42	ASP
1	A	1175	SER
1	A	1180	GLU
1	A	1181	ALA
1	A	1183	GLN
1	A	1255	GLU
1	A	1257	ASP
1	A	1403	GLU
1	A	1405	THR
2	B	250	PHE
2	B	472	ALA
2	B	645	SER
2	B	711	GLU
2	B	713	ALA
2	B	792	MET

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Mol	Chain	Res	Type
2	B	883	LEU
2	B	1155	SER
4	D	13	ARG
7	G	63	PRO
7	G	154	VAL
8	H	17	PRO
8	H	77	ARG
8	H	89	LEU
1	A	5	GLN
1	A	196	GLU
1	A	283	GLY
1	A	286	HIS
1	A	317	LYS
1	A	599	SER
2	B	282	ILE
2	B	338	GLY
2	B	364	ILE
2	B	1173	ALA
3	C	142	VAL
4	D	218	GLU
8	H	130	ARG
10	J	64	ASN
1	A	41	MET
1	A	108	MET
1	A	258	GLY
1	A	424	ILE
1	A	626	ASN
1	A	958	VAL
1	A	1185	PHE
1	A	1437	GLY
8	H	60	ALA
8	H	85	GLY
12	L	26	THR
12	L	50	ASP
1	A	70	CYS
8	H	18	GLY
8	H	128	ASN
9	I	95	THR
16	X	344	ALA
2	B	108	VAL
7	G	139	ILE
2	B	992	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1248/1520 (82%)	1080 (86%)	168 (14%)	4	16
2	B	966/1061 (91%)	839 (87%)	127 (13%)	4	17
3	C	234/274 (85%)	207 (88%)	27 (12%)	5	21
4	D	147/200 (74%)	131 (89%)	16 (11%)	6	23
5	E	197/197 (100%)	184 (93%)	13 (7%)	15	42
6	F	77/137 (56%)	67 (87%)	10 (13%)	4	17
7	G	152/152 (100%)	128 (84%)	24 (16%)	2	11
8	H	117/128 (91%)	106 (91%)	11 (9%)	8	29
9	I	113/116 (97%)	101 (89%)	12 (11%)	6	24
10	J	60/65 (92%)	49 (82%)	11 (18%)	2	8
11	K	99/102 (97%)	88 (89%)	11 (11%)	6	22
12	L	40/57 (70%)	28 (70%)	12 (30%)	0	1
16	X	109/136 (80%)	89 (82%)	20 (18%)	2	8
All	All	3559/4145 (86%)	3097 (87%)	462 (13%)	4	17

All (462) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	34	LYS
1	A	45	GLN
1	A	57	ARG
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS
1	A	71	GLN
1	A	74	MET
1	A	84	ILE
1	A	90	VAL
1	A	93	VAL

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Mol	Chain	Res	Type
1	A	98	LYS
1	A	106	VAL
1	A	113	LEU
1	A	120	GLU
1	A	145	LYS
1	A	146	MET
1	A	156	ASP
1	A	160	GLN
1	A	163	SER
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	225	ASN
1	A	253	ASN
1	A	254	GLU
1	A	256	GLN
1	A	265	LYS
1	A	270	LEU
1	A	275	SER
1	A	286	HIS
1	A	287	HIS
1	A	290	GLU
1	A	302	THR
1	A	303	TYR
1	A	313	GLN
1	A	316	GLN
1	A	320	ARG
1	A	323	LYS
1	A	324	SER
1	A	329	LEU
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	353	ILE
1	A	375	THR
1	A	381	THR
1	A	383	TYR
1	A	385	ILE
1	A	397	ASN
1	A	407	ARG
1	A	408	ASP
1	A	423	ASP

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Mol	Chain	Res	Type
1	A	424	ILE
1	A	427	GLN
1	A	431	LYS
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	461	LYS
1	A	463	ILE
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	481	ASP
1	A	497	THR
1	A	500	GLU
1	A	521	MET
1	A	523	ILE
1	A	532	ARG
1	A	538	ASP
1	A	565	ILE
1	A	571	LEU
1	A	577	ILE
1	A	597	LEU
1	A	598	LEU
1	A	613	ILE
1	A	618	GLU
1	A	620	LYS
1	A	629	LEU
1	A	640	GLN
1	A	666	ILE
1	A	670	ILE
1	A	691	LEU
1	A	693	VAL
1	A	720	ARG
1	A	768	GLN
1	A	769	SER
1	A	821	ARG
1	A	833	GLU

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Mol	Chain	Res	Type
1	A	849	MET
1	A	858	ASN
1	A	864	ILE
1	A	867	ILE
1	A	873	MET
1	A	878	ILE
1	A	894	GLU
1	A	896	ARG
1	A	903	ASN
1	A	905	ASP
1	A	919	ILE
1	A	920	LEU
1	A	929	LEU
1	A	964	ILE
1	A	973	ILE
1	A	982	THR
1	A	983	ILE
1	A	1035	TYR
1	A	1058	VAL
1	A	1064	VAL
1	A	1077	THR
1	A	1079	MET
1	A	1080	THR
1	A	1094	VAL
1	A	1112	LYS
1	A	1128	GLN
1	A	1133	LEU
1	A	1135	ARG
1	A	1142	THR
1	A	1148	ILE
1	A	1163	ILE
1	A	1167	GLU
1	A	1172	LEU
1	A	1186	ASP
1	A	1224	LEU
1	A	1231	ASP
1	A	1237	ILE
1	A	1242	VAL
1	A	1243	VAL
1	A	1255	GLU
1	A	1258	HIS
1	A	1260	LEU

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Mol	Chain	Res	Type
1	A	1264	GLU
1	A	1265	ASN
1	A	1281	ARG
1	A	1283	VAL
1	A	1284	MET
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1322	ILE
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1337	GLU
1	A	1341	ILE
1	A	1366	ARG
1	A	1376	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1400	CYS
1	A	1420	ASP
1	A	1424	VAL
1	A	1426	GLU
1	A	1436	ILE
1	A	1438	THR
1	A	1444	MET
1	A	1445	ILE
1	A	1450	LEU
1	A	1451	VAL
2	B	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	94	LYS
2	B	101	MET
2	B	102	VAL
2	B	109	THR
2	B	128	LEU
2	B	134	LYS
2	B	167	ILE
2	B	178	ASN
2	B	211	VAL

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Mol	Chain	Res	Type
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	234	ILE
2	B	251	ILE
2	B	261	ARG
2	B	272	THR
2	B	273	LEU
2	B	277	LYS
2	B	294	ASP
2	B	296	GLU
2	B	298	LEU
2	B	305	VAL
2	B	309	GLN
2	B	310	MET
2	B	312	GLU
2	B	313	MET
2	B	324	ILE
2	B	331	LEU
2	B	348	ARG
2	B	354	ASP
2	B	384	ARG
2	B	387	LEU
2	B	398	ARG
2	B	423	LYS
2	B	429	PHE
2	B	446	LEU
2	B	461	LEU
2	B	468	GLU
2	B	469	GLN
2	B	471	LYS
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	489	SER
2	B	498	THR
2	B	502	ILE
2	B	516	ASN
2	B	522	VAL
2	B	543	SER
2	B	547	VAL
2	B	549	THR

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Mol	Chain	Res	Type
2	B	554	ILE
2	B	563	MET
2	B	567	GLU
2	B	570	VAL
2	B	603	LEU
2	B	616	ILE
2	B	620	ARG
2	B	628	THR
2	B	629	ASP
2	B	635	ARG
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	685	LEU
2	B	687	GLU
2	B	696	GLU
2	B	714	GLU
2	B	722	ASP
2	B	731	VAL
2	B	751	VAL
2	B	776	GLN
2	B	780	VAL
2	B	790	ASP
2	B	795	ILE
2	B	857	ARG
2	B	870	ILE
2	B	871	THR
2	B	873	THR
2	B	875	GLU
2	B	878	GLN
2	B	882	THR
2	B	889	THR
2	B	904	ARG
2	B	908	GLU
2	B	943	SER
2	B	944	THR
2	B	953	LEU
2	B	964	VAL
2	B	970	THR

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Mol	Chain	Res	Type
2	B	976	ILE
2	B	983	ARG
2	B	997	GLU
2	B	1007	VAL
2	B	1010	LEU
2	B	1022	THR
2	B	1045	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1067	ARG
2	B	1072	MET
2	B	1112	GLN
2	B	1135	ARG
2	B	1145	SER
2	B	1147	LEU
2	B	1148	LYS
2	B	1151	LEU
2	B	1156	ASP
2	B	1160	VAL
2	B	1162	ILE
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1191	ILE
2	B	1202	LEU
2	B	1211	ASN
2	B	1212	ILE
2	B	1220	ARG
2	B	1222	ARG
2	B	1223	ASP
3	C	12	GLU
3	C	16	ASP
3	C	25	VAL
3	C	34	ARG
3	C	46	ILE
3	C	52	GLU
3	C	69	LEU
3	C	72	LEU
3	C	100	THR
3	C	102	GLN
3	C	106	GLU

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Mol	Chain	Res	Type
3	C	115	SER
3	C	121	VAL
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	151	GLN
3	C	166	GLU
3	C	189	THR
3	C	226	ASP
3	C	238	ILE
3	C	240	VAL
3	C	258	ILE
3	C	259	LEU
3	C	260	LEU
3	C	265	MET
4	D	5	THR
4	D	9	GLN
4	D	15	LEU
4	D	47	LEU
4	D	57	LEU
4	D	65	GLU
4	D	118	THR
4	D	119	ARG
4	D	137	ASN
4	D	155	ARG
4	D	156	ASP
4	D	201	LYS
4	D	206	GLU
4	D	212	LYS
4	D	219	THR
4	D	221	TYR
5	E	7	ARG
5	E	52	ARG
5	E	67	GLU
5	E	69	ILE
5	E	78	LEU
5	E	98	ILE
5	E	100	ILE
5	E	104	ASN
5	E	117	THR
5	E	154	ILE

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Mol	Chain	Res	Type
5	E	156	LEU
5	E	190	LEU
5	E	204	THR
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	87	LYS
6	F	93	ILE
6	F	109	VAL
6	F	111	LEU
6	F	122	MET
6	F	127	GLU
6	F	148	VAL
7	G	2	PHE
7	G	13	LEU
7	G	22	MET
7	G	26	LEU
7	G	29	LYS
7	G	32	GLU
7	G	33	GLU
7	G	34	VAL
7	G	39	THR
7	G	41	LYS
7	G	60	ARG
7	G	61	ILE
7	G	63	PRO
7	G	83	LYS
7	G	93	SER
7	G	114	LEU
7	G	126	ASN
7	G	138	THR
7	G	143	ILE
7	G	151	ILE
7	G	152	SER
7	G	153	GLN
7	G	162	SER
7	G	164	LYS
8	H	13	SER
8	H	14	GLU
8	H	26	ILE
8	H	31	THR
8	H	86	ASP

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Mol	Chain	Res	Type
8	H	103	LYS
8	H	107	VAL
8	H	111	LEU
8	H	112	ILE
8	H	128	ASN
8	H	135	LEU
9	I	8	ARG
9	I	12	ASN
9	I	17	ARG
9	I	21	GLU
9	I	31	THR
9	I	35	VAL
9	I	50	THR
9	I	61	ASP
9	I	72	ASP
9	I	74	GLU
9	I	83	ASN
9	I	116	ASN
10	J	3	VAL
10	J	6	ARG
10	J	12	LYS
10	J	14	VAL
10	J	22	LEU
10	J	23	ASN
10	J	27	GLU
10	J	28	ASP
10	J	37	SER
10	J	39	LEU
10	J	52	THR
11	K	1	MET
11	K	11	LEU
11	K	20	LYS
11	K	25	THR
11	K	31	VAL
11	K	37	LYS
11	K	42	LEU
11	K	51	LEU
11	K	74	ARG
11	K	79	GLU
11	K	113	THR
12	L	26	THR
12	L	27	LEU

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Mol	Chain	Res	Type
12	L	28	LYS
12	L	38	LEU
12	L	46	VAL
12	L	50	ASP
12	L	53	HIS
12	L	54	ARG
12	L	55	ILE
12	L	61	THR
12	L	64	LEU
12	L	68	GLU
16	X	243	LYS
16	X	244	MET
16	X	248	LEU
16	X	251	LYS
16	X	252	PHE
16	X	254	VAL
16	X	278	PHE
16	X	285	GLU
16	X	292	ASN
16	X	319	LEU
16	X	324	HIS
16	X	325	VAL
16	X	327	GLU
16	X	333	ASN
16	X	336	VAL
16	X	342	GLU
16	X	358	ILE
16	X	360	LEU
16	X	361	GLU
16	X	364	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	83	HIS
1	A	92	HIS
1	A	124	GLN
1	A	160	GLN
1	A	169	ASN
1	A	171	GLN
1	A	225	ASN

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Mol	Chain	Res	Type
1	A	256	GLN
1	A	287	HIS
1	A	339	ASN
1	A	390	GLN
1	A	435	HIS
1	A	447	GLN
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	548	ASN
1	A	611	GLN
1	A	660	ASN
1	A	717	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	760	GLN
1	A	768	GLN
1	A	851	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	965	GLN
1	A	969	GLN
1	A	972	HIS
1	A	975	HIS
1	A	1078	GLN
1	A	1124	HIS
1	A	1130	GLN
1	A	1140	HIS
1	A	1188	GLN
1	A	1265	ASN
1	A	1270	ASN
1	A	1364	ASN
1	A	1387	HIS
1	A	1432	GLN
2	B	121	ASN
2	B	206	ASN
2	B	255	GLN
2	B	278	GLN
2	B	357	GLN
2	B	433	GLN

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Mol	Chain	Res	Type
2	B	449	ASN
2	B	499	ASN
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	590	HIS
2	B	592	ASN
2	B	706	GLN
2	B	744	HIS
2	B	776	GLN
2	B	786	ASN
2	B	862	GLN
2	B	975	GLN
2	B	986	GLN
2	B	1015	HIS
2	B	1040	ASN
2	B	1062	HIS
2	B	1112	GLN
2	B	1117	GLN
2	B	1161	HIS
2	B	1176	ASN
2	B	1179	GLN
2	B	1205	GLN
3	C	7	GLN
3	C	17	ASN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	184	ASN
3	C	203	GLN
3	C	231	ASN
3	C	264	GLN
4	D	9	GLN
4	D	31	GLN
4	D	37	GLN
4	D	132	GLN
4	D	150	ASN
4	D	179	GLN
5	E	8	ASN
5	E	115	ASN
5	E	146	HIS
5	E	147	HIS

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Mol	Chain	Res	Type
7	G	10	ASN
7	G	14	HIS
7	G	53	ASN
7	G	97	HIS
7	G	102	GLN
7	G	126	ASN
7	G	131	GLN
8	H	11	GLN
8	H	133	ASN
8	H	137	GLN
9	I	12	ASN
9	I	89	GLN
9	I	108	HIS
11	K	65	HIS
12	L	53	HIS
16	X	276	GLN
16	X	281	ASN
16	X	318	ASN
16	X	339	ASN
16	X	345	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/11 (81%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	3	C
14	P	5	A
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	19	15,14	18,21,22	1.34	3 (16%)	25,30,33	1.99	7 (28%)

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	19	15,14	-	0/7/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	19	BRU	C2-N1	2.71	1.42	1.38
15	T	19	BRU	C6-C5	2.63	1.39	1.34
15	T	19	BRU	C4-N3	-2.13	1.34	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	19	BRU	C5-C4-N3	4.38	118.38	113.34
15	T	19	BRU	O4-C4-C5	-4.09	120.59	125.80
15	T	19	BRU	N3-C2-N1	3.86	119.92	114.89
15	T	19	BRU	C4-N3-C2	-3.53	122.72	127.34
15	T	19	BRU	BR-C5-C4	3.23	121.74	118.02
15	T	19	BRU	C6-C5-C4	-2.99	117.64	120.67
15	T	19	BRU	O4'-C1'-N1	2.64	112.55	107.86

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 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
19	EPE	G	1172	-	15,15,15	1.24	1 (6%)	19,20,20	0.51	0
19	EPE	A	2459	-	15,15,15	1.02	1 (6%)	19,20,20	0.64	0

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
19	EPE	G	1172	-	-	3/9/19/19	0/1/1/1
19	EPE	A	2459	-	-	6/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	1172	EPE	C10-S	-4.73	1.71	1.77
19	A	2459	EPE	C10-S	-3.86	1.72	1.77

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	2459	EPE	C9-C10-S-O1S

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Mol	Chain	Res	Type	Atoms
19	A	2459	EPE	C9-C10-S-O2S
19	A	2459	EPE	C8-C7-N4-C3
19	A	2459	EPE	C9-C10-S-O3S
19	G	1172	EPE	N4-C7-C8-O8
19	A	2459	EPE	C10-C9-N1-C2
19	A	2459	EPE	C10-C9-N1-C6
19	G	1172	EPE	C10-C9-N1-C2
19	G	1172	EPE	C10-C9-N1-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	2459	EPE	1	0

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	1
8	H	1
12	L	1

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	4.90
1	H	62:SER	C	63:LEU	N	3.28
1	L	59:ALA	C	60:ARG	N	2.90

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	1426/1733 (82%)	0.04	42 (2%)	53	34	60, 98, 157, 213	0
2	B	1115/1224 (91%)	0.23	61 (5%)	30	17	61, 107, 165, 198	0
3	C	266/318 (83%)	-0.20	0	100	100	74, 96, 135, 164	0
4	D	178/221 (80%)	0.18	11 (6%)	26	15	79, 111, 156, 183	0
5	E	215/215 (100%)	0.08	4 (1%)	66	45	80, 134, 176, 192	0
6	F	87/155 (56%)	-0.26	3 (3%)	48	28	67, 81, 116, 141	0
7	G	171/171 (100%)	0.03	3 (1%)	67	47	77, 99, 135, 155	0
8	H	133/146 (91%)	0.71	18 (13%)	7	4	103, 140, 180, 198	0
9	I	119/122 (97%)	0.43	7 (5%)	28	16	108, 139, 175, 194	0
10	J	65/70 (92%)	-0.23	1 (1%)	72	52	82, 96, 138, 151	0
11	K	115/120 (95%)	-0.23	2 (1%)	69	48	68, 98, 135, 156	0
12	L	46/70 (65%)	1.65	15 (32%)	1	1	77, 172, 184, 191	0
13	N	13/14 (92%)	0.93	0	100	100	150, 182, 258, 261	0
14	P	10/11 (90%)	0.16	1 (10%)	12	7	85, 108, 157, 162	0
15	T	24/26 (92%)	0.67	0	100	100	98, 147, 265, 267	0
16	X	119/146 (81%)	1.41	33 (27%)	1	1	160, 190, 211, 222	0
All	All	4102/4762 (86%)	0.16	201 (4%)	35	20	60, 106, 177, 267	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	8.2
12	L	27	LEU	7.6
2	B	502	ILE	7.2
8	H	63	LEU	7.1
12	L	25	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	6.4
12	L	26	THR	6.2
2	B	70	ILE	6.1
11	K	115	ALA	5.8
2	B	882	THR	5.6
16	X	291	LEU	5.6
2	B	509	ALA	5.5
1	A	1176	LEU	5.4
2	B	1224	PHE	5.3
2	B	709	ASP	5.3
16	X	274	ILE	5.1
1	A	2	VAL	5.1
1	A	51	GLY	5.1
6	F	69	LEU	5.1
1	A	3	GLY	5.1
2	B	341	LEU	5.1
2	B	446	LEU	5.0
8	H	132	LEU	5.0
11	K	114	LEU	5.0
1	A	65	LEU	4.8
2	B	470	LYS	4.8
4	D	24	ALA	4.6
16	X	271	VAL	4.5
2	B	250	PHE	4.4
2	B	880	THR	4.4
2	B	881	ASN	4.4
4	D	220	LEU	4.2
2	B	251	ILE	4.2
2	B	468	GLU	4.2
4	D	76	LYS	4.2
2	B	879	ARG	4.2
2	B	486	TYR	4.1
2	B	710	LEU	4.1
8	H	136	LYS	4.1
12	L	28	LYS	4.1
2	B	339	THR	4.0
2	B	918	ILE	4.0
1	A	1082	ASN	3.9
12	L	42	ARG	3.9
2	B	467	GLY	3.9
8	H	90	ALA	3.9
2	B	249	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	186	LYS	3.8
12	L	64	LEU	3.8
8	H	46	LEU	3.7
16	X	339	ASN	3.7
9	I	120	GLN	3.7
2	B	887	HIS	3.6
1	A	1080	THR	3.6
2	B	469	GLN	3.5
1	A	265	LYS	3.5
16	X	320	GLU	3.5
2	B	734	HIS	3.5
16	X	300	LYS	3.5
16	X	365	VAL	3.5
9	I	119	THR	3.4
16	X	324	HIS	3.4
16	X	273	SER	3.4
14	P	2	U	3.4
2	B	108	VAL	3.4
16	X	325	VAL	3.4
2	B	343	ILE	3.3
1	A	56	PRO	3.3
4	D	12	ARG	3.3
2	B	708	GLU	3.3
2	B	934	LYS	3.3
8	H	139	ASN	3.3
2	B	919	SER	3.2
5	E	1	MET	3.2
2	B	447	ALA	3.2
8	H	130	ARG	3.1
16	X	316	LYS	3.1
1	A	1254	ALA	3.1
2	B	933	SER	3.1
2	B	134	LYS	3.1
4	D	15	LEU	3.0
1	A	61	ILE	3.0
2	B	266	ALA	3.0
16	X	321	LEU	3.0
8	H	84	ALA	3.0
9	I	4	PHE	3.0
16	X	355	ARG	3.0
2	B	646	LEU	2.9
12	L	37	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	715	ALA	2.9
9	I	52	ILE	2.9
12	L	45	ALA	2.9
2	B	351	TYR	2.9
16	X	293	VAL	2.9
1	A	323	LYS	2.9
1	A	310	GLY	2.9
1	A	1244	ARG	2.9
1	A	1179	GLU	2.9
16	X	237	LEU	2.9
7	G	153	GLN	2.8
2	B	262	GLU	2.8
2	B	436	VAL	2.8
6	F	155	LEU	2.8
8	H	62	SER	2.8
9	I	117	LYS	2.8
1	A	1185	PHE	2.8
12	L	55	ILE	2.8
2	B	429	PHE	2.7
16	X	351	PHE	2.7
8	H	129	TYR	2.7
2	B	164	LYS	2.7
1	A	50	ILE	2.7
2	B	1096	ARG	2.7
4	D	21	GLU	2.7
1	A	1391	ARG	2.7
16	X	233	LYS	2.7
8	H	2	SER	2.7
8	H	95	TYR	2.7
16	X	254	VAL	2.7
1	A	44	THR	2.6
1	A	66	LYS	2.6
4	D	23	ASN	2.6
16	X	360	LEU	2.6
12	L	30	ILE	2.6
1	A	1455	PRO	2.6
16	X	257	THR	2.6
2	B	244	LEU	2.6
12	L	41	SER	2.6
2	B	731	VAL	2.6
10	J	65	PRO	2.5
9	I	118	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
12	L	32	ALA	2.5
2	B	231	PRO	2.5
2	B	370	PHE	2.5
1	A	63	ARG	2.5
7	G	154	VAL	2.5
2	B	243	ALA	2.4
16	X	329	LYS	2.4
16	X	302	TYR	2.4
8	H	131	ASN	2.4
16	X	354	LYS	2.4
2	B	572	HIS	2.4
1	A	71	GLN	2.4
16	X	244	MET	2.4
1	A	315	LEU	2.4
1	A	79	GLY	2.4
2	B	265	SER	2.4
2	B	448	ILE	2.3
1	A	969	GLN	2.3
16	X	330	LEU	2.3
1	A	1403	GLU	2.3
16	X	301	ILE	2.3
5	E	152	LYS	2.3
2	B	472	ALA	2.3
8	H	135	LEU	2.3
5	E	110	PHE	2.3
1	A	1187	GLN	2.3
1	A	49	LYS	2.3
16	X	243	LYS	2.3
1	A	4	GLN	2.3
4	D	8	PHE	2.2
8	H	76	THR	2.2
12	L	43	THR	2.2
5	E	57	MET	2.2
1	A	567	LYS	2.2
12	L	53	HIS	2.2
8	H	88	SER	2.2
16	X	260	ALA	2.2
1	A	1217	LYS	2.2
1	A	640	GLN	2.2
1	A	223	GLY	2.2
2	B	723	VAL	2.2
9	I	2	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	732	SER	2.1
1	A	64	ASN	2.1
8	H	86	ASP	2.1
1	A	311	GLN	2.1
1	A	1184	SER	2.1
2	B	474	SER	2.1
6	F	71	GLU	2.1
2	B	312	GLU	2.1
4	D	13	ARG	2.1
1	A	43	GLU	2.1
4	D	18	VAL	2.1
1	A	1205	LYS	2.1
2	B	383	ASN	2.1
16	X	317	LYS	2.1
8	H	89	LEU	2.1
16	X	315	ASP	2.1
16	X	323	ALA	2.1
2	B	437	GLU	2.1
2	B	241	ARG	2.0
7	G	64	THR	2.0
1	A	707	GLY	2.0
2	B	531	GLN	2.0
12	L	39	SER	2.0
2	B	473	MET	2.0
16	X	356	ASP	2.0
2	B	246	LYS	2.0
16	X	322	LYS	2.0
4	D	20	GLU	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	19	20/21	0.96	0.08	91,98,105,114	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($\text{\AA}^2$)	Q<0.9
19	EPE	G	1172	15/15	0.62	0.35	217,230,230,231	0
19	EPE	A	2459	15/15	0.72	0.38	249,261,272,273	0
18	MG	A	2458	1/1	0.94	0.10	275,275,275,275	0
17	ZN	L	1071	1/1	0.98	0.05	193,193,193,193	0
17	ZN	I	1121	1/1	0.99	0.05	117,117,117,117	0
17	ZN	I	1122	1/1	0.99	0.06	191,191,191,191	0
17	ZN	J	1066	1/1	1.00	0.03	84,84,84,84	0
17	ZN	B	2225	1/1	1.00	0.05	87,87,87,87	0
17	ZN	C	1269	1/1	1.00	0.02	88,88,88,88	0
17	ZN	A	2456	1/1	1.00	0.02	124,124,124,124	0
17	ZN	A	2457	1/1	1.00	0.06	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.