



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:52 AM UTC

PDB ID : 4BY1 / pdb_00004by1
Title : elongating RNA Polymerase II-Bye1 TLD complex soaked with AMPCPP
Authors : Kinkelin, K.; Wozniak, G.G.; Rothbart, S.B.; Lidschreiber, M.; Strahl, B.D.; Cramer, P.
Deposited on : 2013-07-17
Resolution : 3.60 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

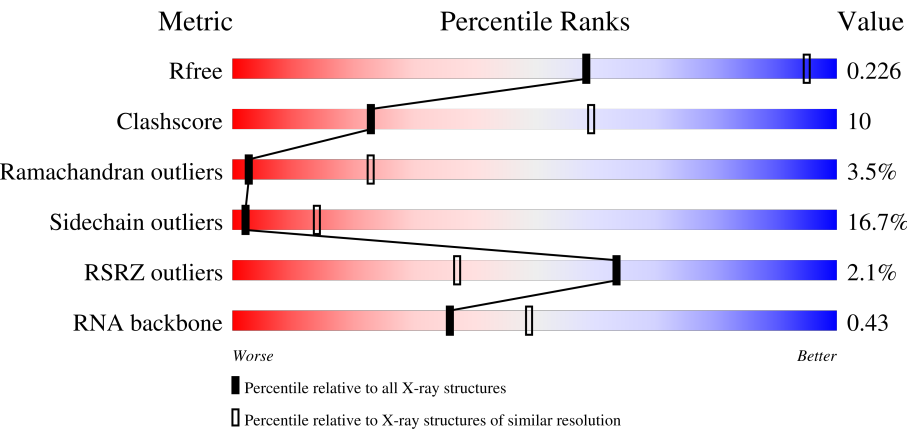
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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	0% 49% 26% 6% 18%
2	B	1224	2% 57% 27% 6% 10%
3	C	318	52% 27% 16%
4	D	221	4% 53% 24% 20%

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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 33026 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	1427	Total	C	N	O	S	0	0	0
			11230	7072	1960	2136	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8793	5569	1538	1631	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	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	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	85	Total	C	N	O	S	0	0	0
			688	439	116	130	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(*AP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*G

P*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	11	Total	C	N	O	P	0	0	0
			229	109	44	65	11			

- 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(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*TP*TP*CP*CP*BRUP*GP*GP*TP*CP*AP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	24	Total	Br	C	N	O	P	0	0
			481	1	230	75	151	24		

- Molecule 16 is a protein called TRANSCRIPTION FACTOR BYE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	X	116	Total	C	N	O	S	0	0	0
			953	611	158	181	3			

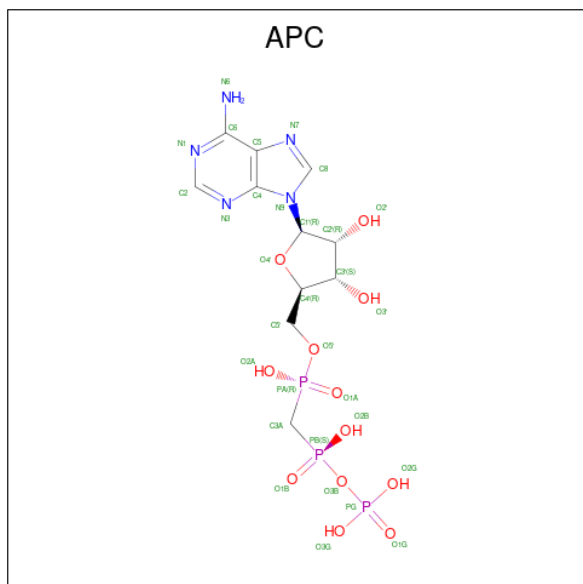
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

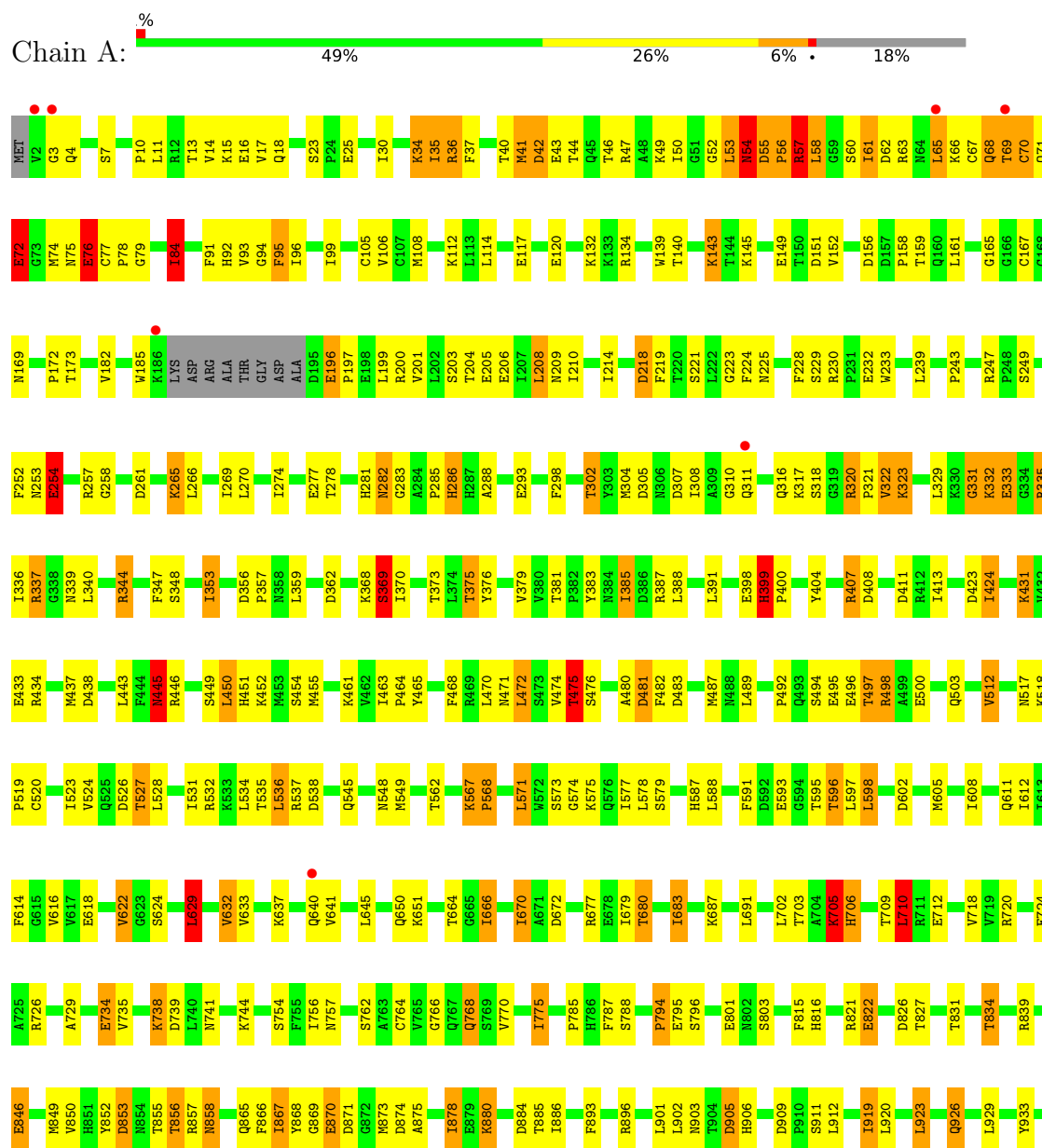


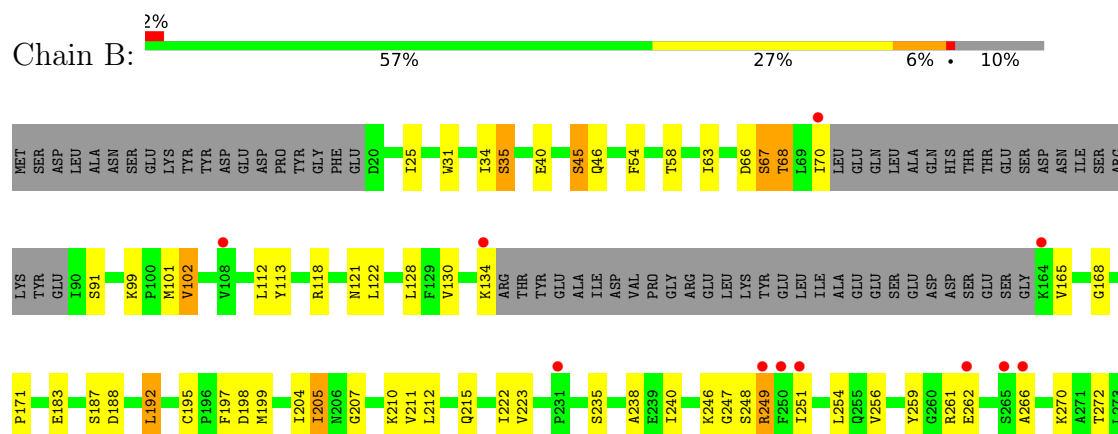
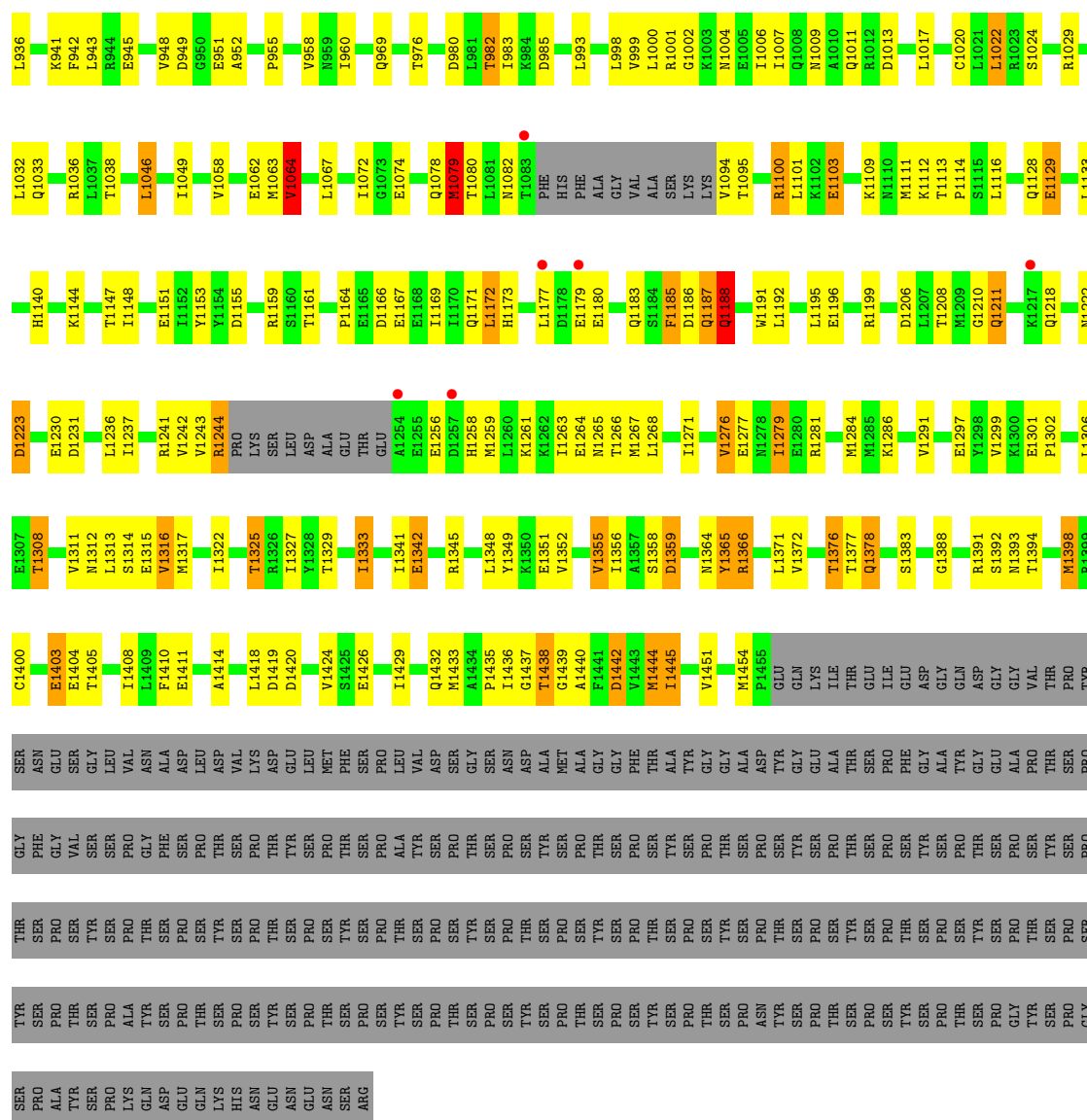
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	P	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

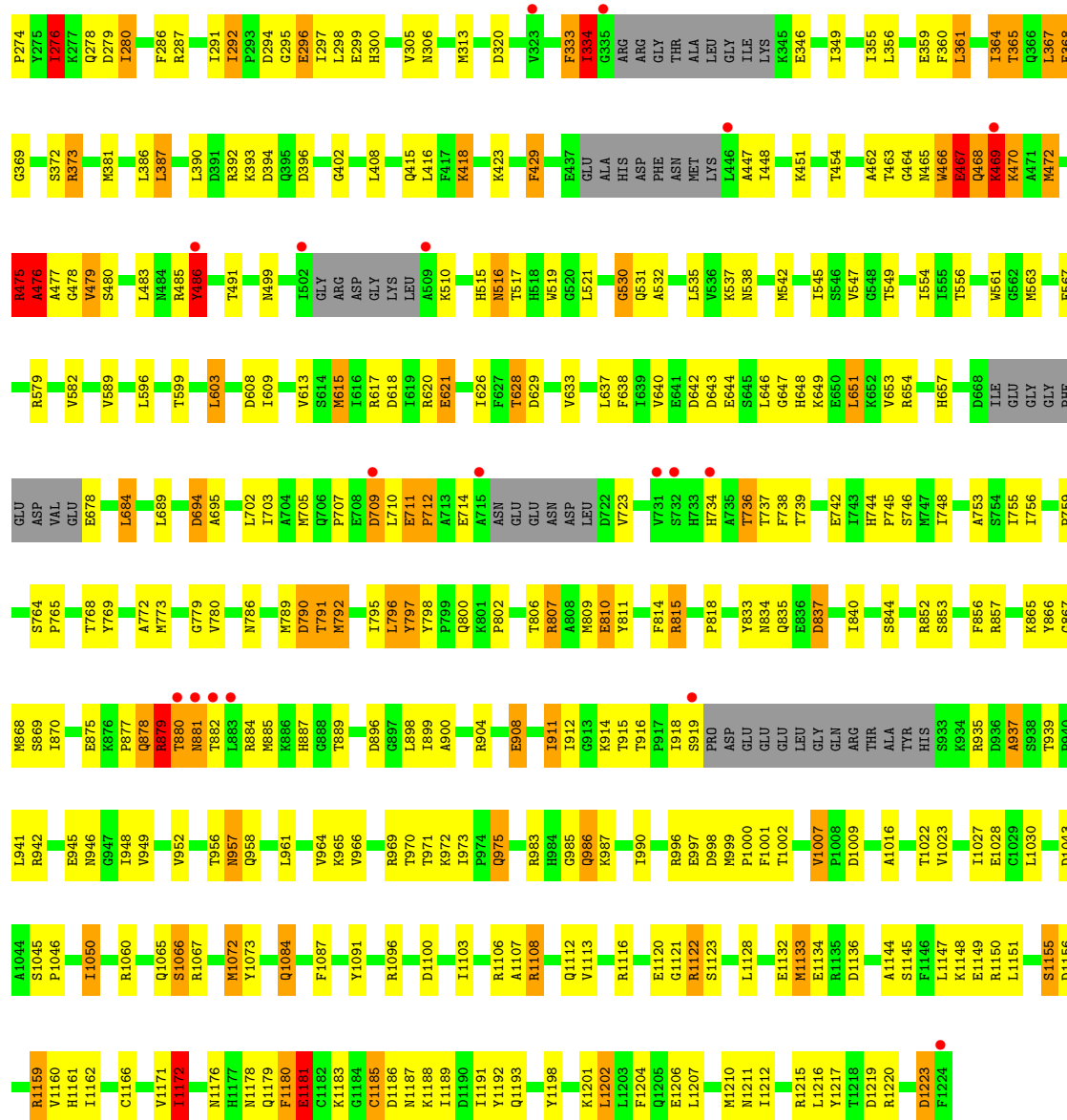
3 Residue-property plots

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

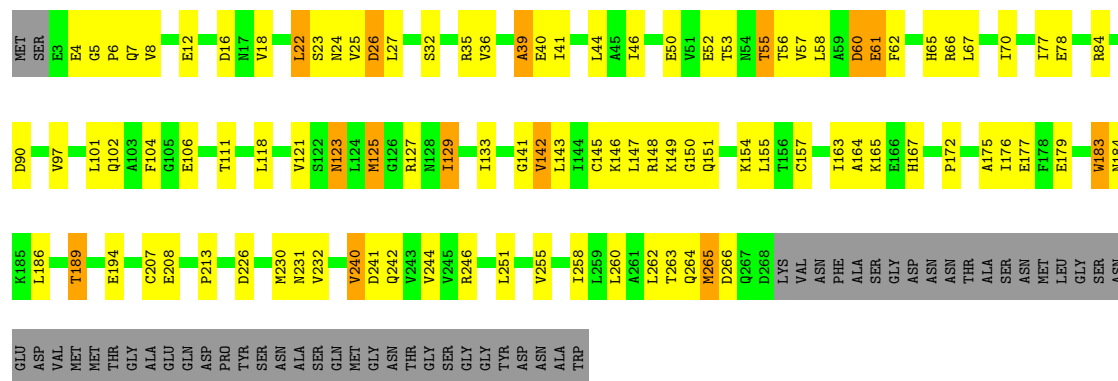




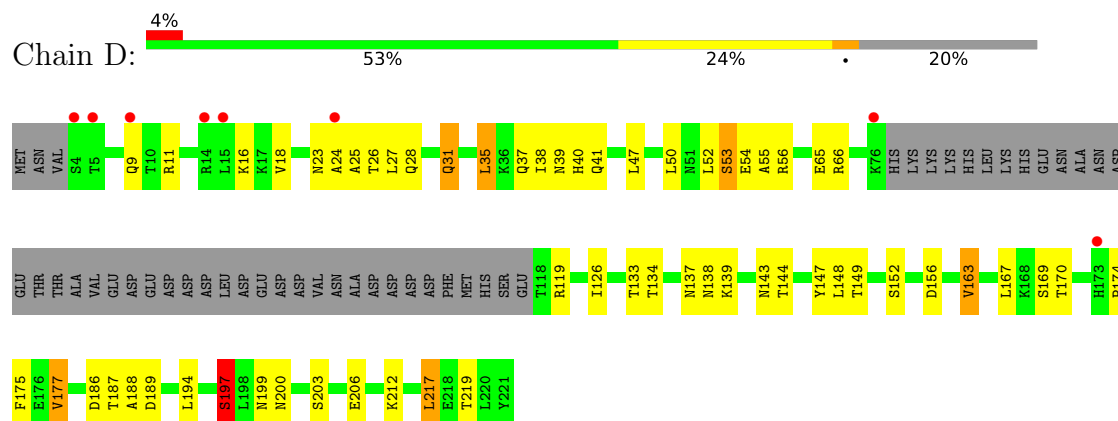


- Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

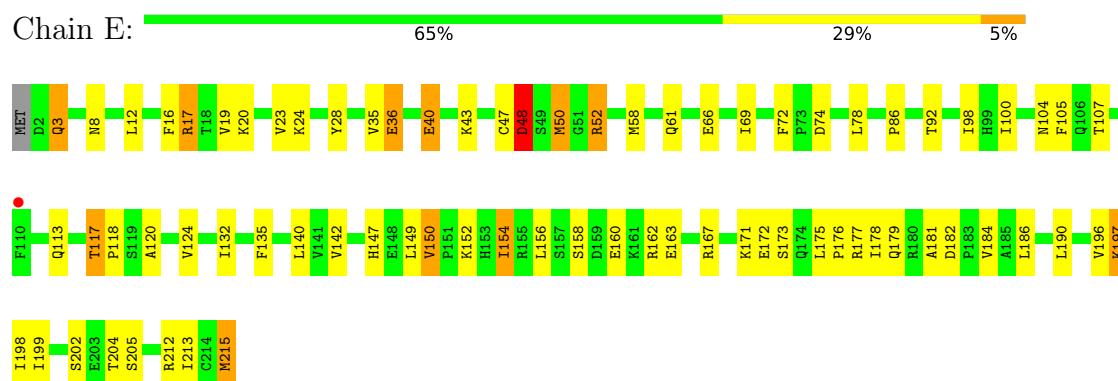
Chain C: 52% 27% . 16%



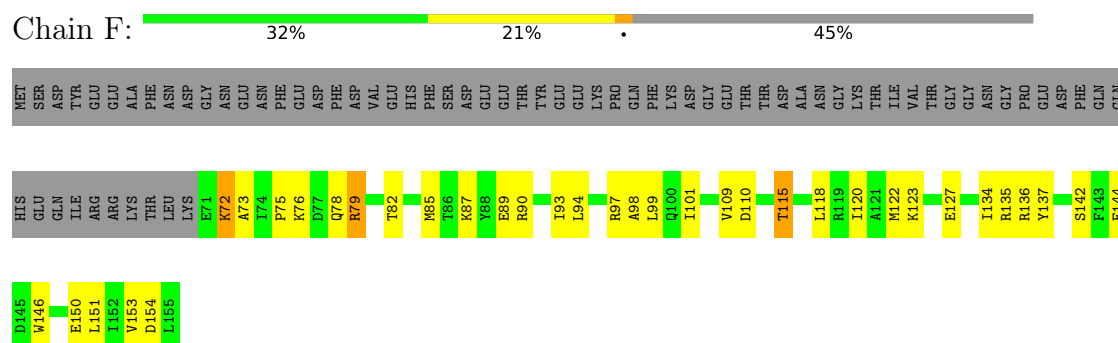
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4



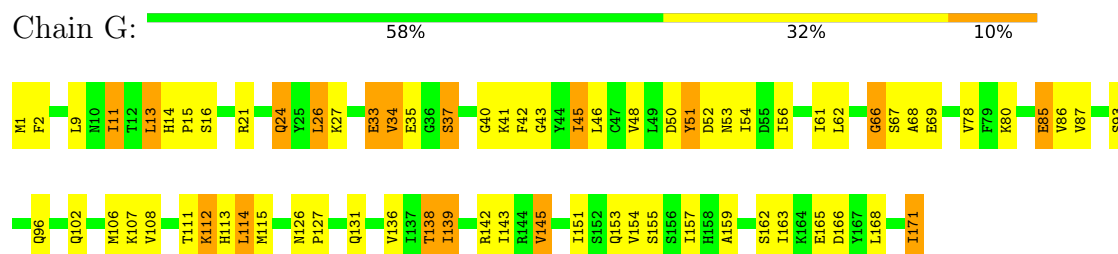
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



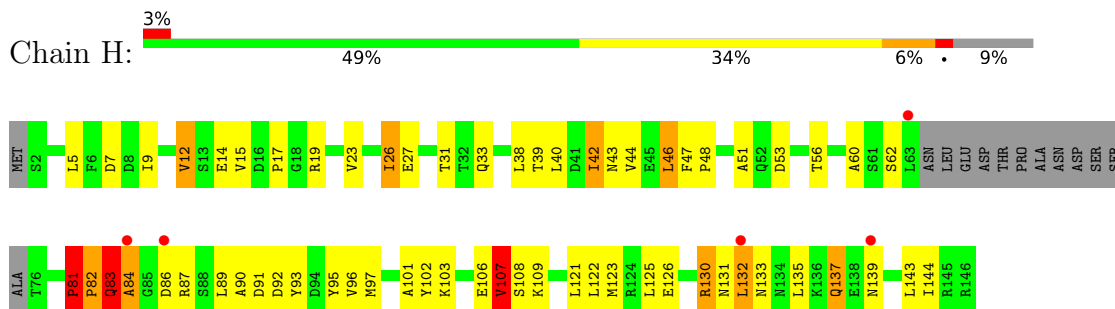
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



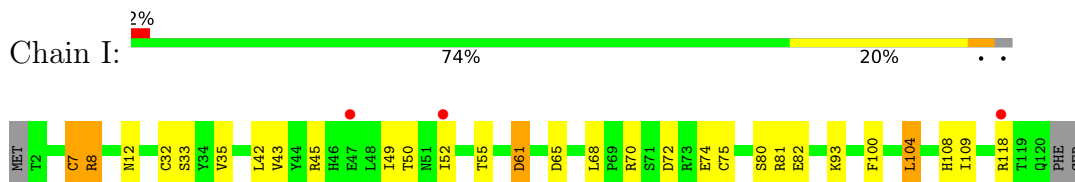
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7



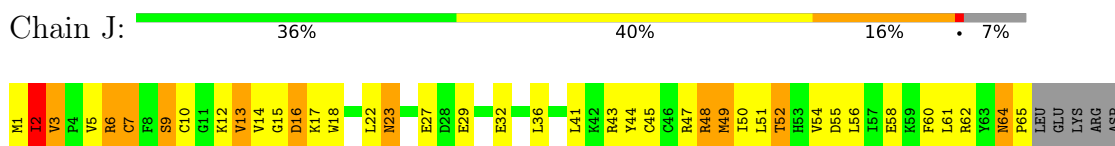
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



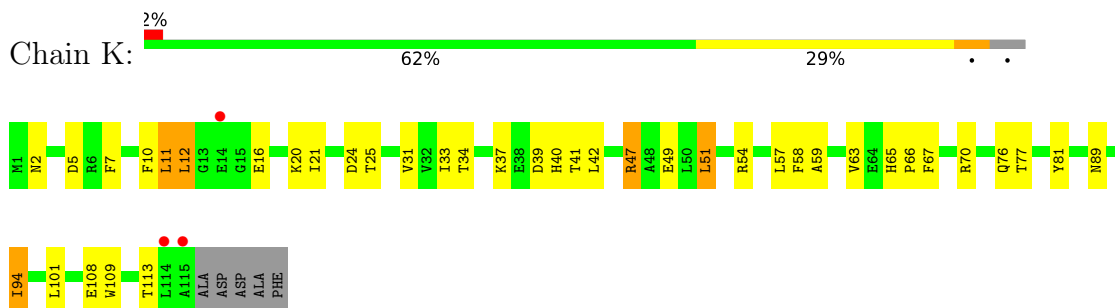
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



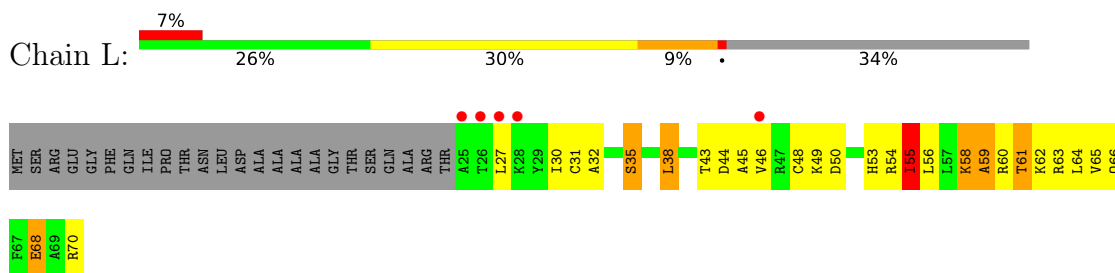
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



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

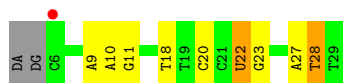




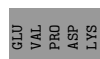
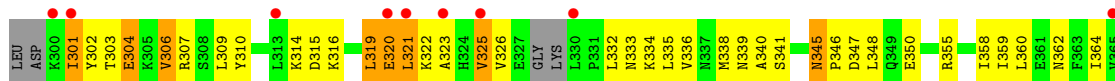
- Molecule 14: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'



- Molecule 15: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP *TP*TP*CP*CP*BRUP*GP*GP*TP*CP*AP*AP*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	222.24Å 391.58Å 281.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.95 – 3.60 48.95 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.95-3.60) 99.9 (48.95-3.60)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.57Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.175 , 0.206 0.195 , 0.226	Depositor DCC
R_{free} test set	2784 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	106.1	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 141.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.019 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.027 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33026	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BRU, APC, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.91	11/11431 (0.1%)	1.53	122/15462 (0.8%)
2	B	0.88	3/8963 (0.0%)	1.44	88/12085 (0.7%)
3	C	0.85	0/2133	1.39	16/2891 (0.6%)
4	D	0.90	0/1365	1.62	20/1837 (1.1%)
5	E	0.85	0/1788	1.44	12/2406 (0.5%)
6	F	0.94	0/700	1.43	5/945 (0.5%)
7	G	0.88	0/1368	1.40	11/1844 (0.6%)
8	H	0.83	0/1086	1.39	15/1470 (1.0%)
9	I	0.83	0/989	1.31	4/1331 (0.3%)
10	J	0.89	1/541 (0.2%)	1.53	5/727 (0.7%)
11	K	0.75	0/938	1.36	7/1267 (0.6%)
12	L	1.07	0/365	1.67	6/485 (1.2%)
13	N	0.46	0/257	0.66	0/395
14	P	1.02	2/240 (0.8%)	0.85	0/372
15	T	0.58	0/512	0.68	0/783
16	X	0.96	1/963 (0.1%)	1.61	17/1287 (1.3%)
All	All	0.88	18/33639 (0.1%)	1.46	328/45587 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	P	0	1
15	T	0	3
All	All	0	4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1172	ILE	CG1-CD1	6.45	1.76	1.51
16	X	254	VAL	CA-C	6.20	1.59	1.52
1	A	84	ILE	CG1-CD1	6.14	1.75	1.51
2	B	467	GLU	CA-C	6.01	1.60	1.52
1	A	56	PRO	C-N	5.92	1.42	1.33
1	A	54	ASN	CA-C	5.88	1.60	1.52
1	A	1398	MET	SD-CE	5.81	1.94	1.79
1	A	69	THR	C-N	5.60	1.41	1.33
14	P	2	U	C1'-N1	5.46	1.55	1.47
10	J	49	MET	SD-CE	-5.41	1.66	1.79
1	A	69	THR	CA-C	5.38	1.59	1.52
14	P	2	U	C3'-O3'	5.35	1.51	1.43
1	A	1403	GLU	CA-C	5.26	1.59	1.52
1	A	53	LEU	N-CA	5.25	1.52	1.45
1	A	520	CYS	CA-C	5.19	1.60	1.52
1	A	1454	MET	CA-C	5.14	1.58	1.52
2	B	292	ILE	CA-C	5.09	1.58	1.52
1	A	61	ILE	CA-C	5.01	1.58	1.53

All (328) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	THR	N-CA-C	-12.57	96.66	112.88
2	B	296	GLU	N-CA-C	-11.08	99.28	113.12
1	A	223	GLY	CA-C-N	9.88	135.35	120.82
1	A	223	GLY	C-N-CA	9.88	135.35	120.82
2	B	1016	ALA	CA-C-N	9.16	129.23	120.43
2	B	1016	ALA	C-N-CA	9.16	129.23	120.43
1	A	56	PRO	CA-C-N	8.84	138.42	121.54
1	A	56	PRO	C-N-CA	8.84	138.42	121.54
4	D	25	ALA	CA-C-N	8.66	136.11	122.60
4	D	25	ALA	C-N-CA	8.66	136.11	122.60
4	D	31	GLN	N-CA-C	-8.10	101.72	111.69
8	H	92	ASP	N-CA-C	-8.10	100.45	111.87
2	B	1122	ARG	CA-C-N	8.07	130.94	120.44
2	B	1122	ARG	C-N-CA	8.07	130.94	120.44
1	A	56	PRO	N-CA-C	-7.97	106.39	114.68
10	J	5	VAL	N-CA-C	-7.84	98.55	109.21
2	B	628	THR	CA-C-N	7.70	132.78	121.31
2	B	628	THR	C-N-CA	7.70	132.78	121.31
2	B	1133	MET	CA-C-N	7.58	130.44	120.28
2	B	1133	MET	C-N-CA	7.58	130.44	120.28
1	A	219	PHE	CA-CB-CG	7.48	121.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	294	ASP	CA-CB-CG	7.48	120.08	112.60
5	E	48	ASP	CA-CB-CG	7.46	120.06	112.60
1	A	3	GLY	CA-C-N	7.40	135.67	121.54
1	A	3	GLY	C-N-CA	7.40	135.67	121.54
1	A	1186	ASP	N-CA-C	-7.39	98.62	109.11
1	A	399	HIS	N-CA-CB	7.37	123.48	110.37
1	A	718	VAL	CA-C-N	7.26	129.96	120.60
1	A	718	VAL	C-N-CA	7.26	129.96	120.60
6	F	87	LYS	CA-C-N	7.26	130.00	120.28
6	F	87	LYS	C-N-CA	7.26	130.00	120.28
8	H	131	ASN	CA-CB-CG	7.26	119.86	112.60
3	C	226	ASP	N-CA-C	-7.20	98.80	109.81
1	A	65	LEU	N-CA-C	-7.17	102.65	111.33
1	A	452	LYS	N-CA-C	-7.12	103.52	111.28
1	A	254	GLU	CA-C-N	6.99	130.59	120.38
1	A	254	GLU	C-N-CA	6.99	130.59	120.38
3	C	60	ASP	CA-CB-CG	6.92	119.53	112.60
1	A	224	PHE	CA-CB-CG	-6.89	106.91	113.80
1	A	1063	MET	CA-C-N	6.88	134.35	121.97
1	A	1063	MET	C-N-CA	6.88	134.35	121.97
1	A	54	ASN	CA-CB-CG	6.87	119.47	112.60
3	C	62	PHE	CA-C-N	6.81	129.28	120.56
3	C	62	PHE	C-N-CA	6.81	129.28	120.56
1	A	734	GLU	CA-C-N	6.81	129.79	120.46
1	A	734	GLU	C-N-CA	6.81	129.79	120.46
1	A	57	ARG	CA-C-N	6.81	134.54	121.54
1	A	57	ARG	C-N-CA	6.81	134.54	121.54
1	A	874	ASP	CA-CB-CG	6.79	119.39	112.60
1	A	408	ASP	CA-CB-CG	6.78	119.38	112.60
1	A	252	PHE	CA-C-N	6.73	134.40	121.54
1	A	252	PHE	C-N-CA	6.73	134.40	121.54
1	A	517	ASN	CA-CB-CG	6.73	119.33	112.60
2	B	880	THR	CA-C-N	6.73	134.39	121.54
2	B	880	THR	C-N-CA	6.73	134.39	121.54
4	D	54	GLU	N-CA-C	-6.73	104.03	111.36
2	B	709	ASP	CA-CB-CG	6.72	119.32	112.60
8	H	131	ASN	CA-C-N	6.66	129.52	120.54
8	H	131	ASN	C-N-CA	6.66	129.52	120.54
4	D	26	THR	CA-C-N	6.64	131.56	122.07
4	D	26	THR	C-N-CA	6.64	131.56	122.07
1	A	288	ALA	N-CA-C	-6.63	105.48	113.97
2	B	1185	CYS	N-CA-C	-6.60	105.38	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	83	GLN	CA-C-N	6.59	131.24	120.63
8	H	83	GLN	C-N-CA	6.59	131.24	120.63
4	D	143	ASN	CA-CB-CG	6.56	119.16	112.60
2	B	478	GLY	CA-C-N	6.55	128.81	120.56
2	B	478	GLY	C-N-CA	6.55	128.81	120.56
3	C	26	ASP	CA-CB-CG	6.54	119.14	112.60
2	B	469	LYS	CA-C-N	6.54	134.02	121.54
2	B	469	LYS	C-N-CA	6.54	134.02	121.54
1	A	218	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	362	ASP	CA-CB-CG	6.51	119.11	112.60
2	B	807	ARG	N-CA-C	-6.46	104.33	111.82
1	A	481	ASP	CA-CB-CG	6.45	119.05	112.60
12	L	49	LYS	CA-C-N	6.43	133.82	121.54
12	L	49	LYS	C-N-CA	6.43	133.82	121.54
2	B	1180	PHE	CA-CB-CG	-6.40	107.40	113.80
2	B	45	SER	CA-C-N	6.38	129.15	120.54
2	B	45	SER	C-N-CA	6.38	129.15	120.54
9	I	93	LYS	CA-C-N	6.34	129.41	120.28
9	I	93	LYS	C-N-CA	6.34	129.41	120.28
4	D	37	GLN	CA-C-N	6.33	130.68	121.18
4	D	37	GLN	C-N-CA	6.33	130.68	121.18
1	A	1064	VAL	N-CA-CB	-6.31	100.81	111.23
2	B	638	PHE	CA-CB-CG	6.31	120.11	113.80
12	L	59	ALA	CA-C-N	6.29	133.56	121.54
12	L	59	ALA	C-N-CA	6.29	133.56	121.54
2	B	837	ASP	CA-CB-CG	6.28	118.88	112.60
2	B	791	THR	CB-CA-C	-6.27	100.01	110.29
8	H	92	ASP	CA-C-N	6.26	132.38	122.62
8	H	92	ASP	C-N-CA	6.26	132.38	122.62
1	A	308	ILE	CA-C-N	6.24	130.19	120.82
1	A	308	ILE	C-N-CA	6.24	130.19	120.82
1	A	846	GLU	CA-C-N	6.24	132.59	120.99
1	A	846	GLU	C-N-CA	6.24	132.59	120.99
1	A	1223	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	602	ASP	N-CA-C	-6.21	103.35	111.74
1	A	143	LYS	CA-C-N	6.21	128.52	120.44
1	A	143	LYS	C-N-CA	6.21	128.52	120.44
2	B	467	GLU	CA-C-N	6.18	132.83	121.70
2	B	467	GLU	C-N-CA	6.18	132.83	121.70
2	B	1155	SER	CA-C-N	6.18	133.34	121.54
2	B	1155	SER	C-N-CA	6.18	133.34	121.54
5	E	160	GLU	CA-C-N	6.16	128.79	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	160	GLU	C-N-CA	6.16	128.79	120.65
5	E	171	LYS	N-CA-C	-6.15	100.54	110.32
1	A	452	LYS	CA-C-N	6.13	130.96	120.72
1	A	452	LYS	C-N-CA	6.13	130.96	120.72
2	B	1028	GLU	CB-CG-CD	6.13	123.02	112.60
16	X	233	LYS	CA-C-N	6.11	128.46	120.28
16	X	233	LYS	C-N-CA	6.11	128.46	120.28
2	B	67	SER	CA-C-N	6.10	133.19	121.54
2	B	67	SER	C-N-CA	6.10	133.19	121.54
1	A	398	GLU	CA-C-O	-6.10	114.80	121.87
2	B	647	GLY	N-CA-C	6.09	117.54	111.21
11	K	39	ASP	CA-CB-CG	6.08	118.69	112.60
1	A	381	THR	CB-CA-C	6.08	118.01	108.84
3	C	244	VAL	CA-C-N	6.08	128.44	120.60
3	C	244	VAL	C-N-CA	6.08	128.44	120.60
3	C	183	TRP	N-CA-C	-6.05	99.99	109.25
7	G	33	GLU	CA-C-N	6.03	128.08	120.72
7	G	33	GLU	C-N-CA	6.03	128.08	120.72
2	B	188	ASP	CA-CB-CG	6.03	118.63	112.60
2	B	736	THR	N-CA-C	-6.01	104.09	112.45
7	G	48	VAL	N-CA-CB	6.00	117.67	110.95
1	A	72	GLU	CB-CG-CD	5.94	122.69	112.60
16	X	301	ILE	CA-C-N	5.90	132.80	121.54
16	X	301	ILE	C-N-CA	5.90	132.80	121.54
2	B	476	ALA	CA-C-N	5.89	132.79	121.54
2	B	476	ALA	C-N-CA	5.89	132.79	121.54
2	B	694	ASP	CA-CB-CG	5.88	118.48	112.60
4	D	189	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	438	ASP	CA-CB-CG	5.86	118.46	112.60
2	B	99	LYS	N-CA-C	-5.83	102.81	110.39
1	A	710	LEU	CA-C-N	5.83	128.02	120.44
1	A	710	LEU	C-N-CA	5.83	128.02	120.44
1	A	399	HIS	CA-CB-CG	-5.83	107.97	113.80
2	B	937	ALA	CA-C-N	5.83	129.14	120.87
2	B	937	ALA	C-N-CA	5.83	129.14	120.87
1	A	285	PRO	CA-C-N	5.82	132.65	121.54
1	A	285	PRO	C-N-CA	5.82	132.65	121.54
2	B	809	MET	CA-C-N	5.81	128.87	120.79
2	B	809	MET	C-N-CA	5.81	128.87	120.79
1	A	1049	ILE	N-CA-C	-5.80	105.19	110.82
8	H	81	PRO	N-CA-C	5.80	117.77	110.70
2	B	320	ASP	CA-CB-CG	5.79	118.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	276	ILE	CA-C-N	5.79	129.50	120.82
2	B	276	ILE	C-N-CA	5.79	129.50	120.82
1	A	710	LEU	N-CA-C	-5.78	104.98	111.28
2	B	467	GLU	CB-CG-CD	5.78	122.42	112.60
10	J	16	ASP	CA-CB-CG	5.78	118.38	112.60
2	B	790	ASP	CA-CB-CG	5.77	118.37	112.60
2	B	530	GLY	CA-C-N	5.76	132.53	121.54
2	B	530	GLY	C-N-CA	5.76	132.53	121.54
2	B	642	ASP	N-CA-C	-5.75	105.10	111.71
16	X	252	PHE	CA-C-N	5.73	130.30	121.19
16	X	252	PHE	C-N-CA	5.73	130.30	121.19
2	B	818	PRO	N-CA-C	5.73	119.24	111.22
1	A	252	PHE	CA-CB-CG	5.70	119.50	113.80
2	B	1186	ASP	CA-C-N	5.69	130.30	121.26
2	B	1186	ASP	C-N-CA	5.69	130.30	121.26
1	A	677	ARG	CA-C-N	5.68	127.89	120.28
1	A	677	ARG	C-N-CA	5.68	127.89	120.28
2	B	896	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	526	ASP	CA-CB-CG	5.66	118.26	112.60
2	B	1136	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	331	GLY	N-CA-C	5.63	126.53	113.18
16	X	334	LYS	CA-C-N	5.60	128.55	120.38
16	X	334	LYS	C-N-CA	5.60	128.55	120.38
1	A	158	PRO	CA-C-N	5.58	128.22	120.29
1	A	158	PRO	C-N-CA	5.58	128.22	120.29
4	D	197	SER	N-CA-C	-5.58	104.83	111.69
3	C	213	PRO	N-CA-C	5.57	121.07	113.84
1	A	1187	GLN	CA-C-N	5.56	131.71	121.70
1	A	1187	GLN	C-N-CA	5.56	131.71	121.70
2	B	1001	PHE	N-CA-C	5.55	118.78	109.95
16	X	314	LYS	CA-C-N	5.54	132.12	121.54
16	X	314	LYS	C-N-CA	5.54	132.12	121.54
1	A	794	PRO	CA-C-N	5.54	127.64	120.44
1	A	794	PRO	C-N-CA	5.54	127.64	120.44
1	A	408	ASP	CA-C-N	5.52	128.23	120.28
1	A	408	ASP	C-N-CA	5.52	128.23	120.28
11	K	25	THR	CA-C-N	5.52	128.00	120.54
11	K	25	THR	C-N-CA	5.52	128.00	120.54
1	A	445	ASN	CA-CB-CG	5.52	118.12	112.60
1	A	1231	ASP	CA-C-N	5.50	127.65	120.28
1	A	1231	ASP	C-N-CA	5.50	127.65	120.28
1	A	1185	PHE	CA-CB-CG	5.48	119.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	535	LEU	N-CA-C	-5.48	106.27	113.12
2	B	415	GLN	CA-C-N	5.48	127.56	120.44
2	B	415	GLN	C-N-CA	5.48	127.56	120.44
2	B	66	ASP	CA-CB-CG	5.48	118.08	112.60
2	B	306	ASN	N-CA-C	-5.47	105.91	112.59
16	X	320	GLU	CA-C-N	5.47	128.05	120.29
16	X	320	GLU	C-N-CA	5.47	128.05	120.29
1	A	1420	ASP	CA-CB-CG	5.46	118.06	112.60
2	B	486	TYR	N-CA-C	-5.46	104.17	112.04
1	A	853	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	293	GLU	CB-CG-CD	5.45	121.87	112.60
6	F	154	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	1103	GLU	CA-C-N	5.45	127.51	120.70
1	A	1103	GLU	C-N-CA	5.45	127.51	120.70
8	H	90	ALA	CA-C-N	5.44	130.41	122.85
8	H	90	ALA	C-N-CA	5.44	130.41	122.85
1	A	1317	MET	CA-C-N	5.43	128.56	120.31
1	A	1317	MET	C-N-CA	5.43	128.56	120.31
6	F	154	ASP	CA-C-N	5.42	131.47	121.70
6	F	154	ASP	C-N-CA	5.42	131.47	121.70
1	A	870	GLU	CB-CG-CD	5.42	121.82	112.60
9	I	100	PHE	CA-CB-CG	5.42	119.22	113.80
2	B	810	GLU	CA-C-N	5.41	128.53	120.31
2	B	810	GLU	C-N-CA	5.41	128.53	120.31
1	A	1419	ASP	CA-C-N	5.40	128.26	120.38
1	A	1419	ASP	C-N-CA	5.40	128.26	120.38
8	H	101	ALA	N-CA-C	-5.39	101.00	109.25
12	L	63	ARG	CA-C-N	5.38	128.74	121.05
12	L	63	ARG	C-N-CA	5.38	128.74	121.05
4	D	24	ALA	N-CA-C	5.38	114.68	108.49
7	G	139	ILE	CA-C-N	-5.37	113.91	122.29
7	G	139	ILE	C-N-CA	-5.37	113.91	122.29
1	A	1072	ILE	N-CA-C	-5.36	105.90	111.58
5	E	118	PRO	CA-C-N	5.36	127.73	120.44
5	E	118	PRO	C-N-CA	5.36	127.73	120.44
16	X	350	GLU	N-CA-C	-5.36	105.55	112.68
1	A	705	LYS	CA-C-N	5.35	131.75	121.54
1	A	705	LYS	C-N-CA	5.35	131.75	121.54
4	D	200	ASN	CA-C-N	5.35	127.98	120.28
4	D	200	ASN	C-N-CA	5.35	127.98	120.28
8	H	132	LEU	CA-C-N	5.33	127.74	120.54
8	H	132	LEU	C-N-CA	5.33	127.74	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1410	PHE	CA-CB-CG	5.30	119.10	113.80
10	J	16	ASP	CA-C-N	5.29	127.64	120.38
10	J	16	ASP	C-N-CA	5.29	127.64	120.38
2	B	1087	PHE	CA-CB-CG	5.28	119.08	113.80
5	E	173	SER	CA-C-N	5.28	129.04	120.60
5	E	173	SER	C-N-CA	5.28	129.04	120.60
7	G	2	PHE	N-CA-C	-5.27	101.18	109.25
2	B	768	THR	CA-C-N	5.27	127.60	120.65
2	B	768	THR	C-N-CA	5.27	127.60	120.65
3	C	65	HIS	CA-C-N	5.27	127.60	120.38
3	C	65	HIS	C-N-CA	5.27	127.60	120.38
1	A	99	ILE	N-CA-C	-5.27	105.58	110.53
2	B	198	ASP	CA-C-N	5.27	129.63	120.68
2	B	198	ASP	C-N-CA	5.27	129.63	120.68
1	A	229	SER	N-CA-C	5.26	116.00	107.32
2	B	643	ASP	CA-C-N	5.26	129.10	121.26
2	B	643	ASP	C-N-CA	5.26	129.10	121.26
1	A	205	GLU	CA-C-N	5.26	127.59	120.65
1	A	205	GLU	C-N-CA	5.26	127.59	120.65
1	A	475	THR	CA-C-N	5.25	127.30	120.26
1	A	475	THR	C-N-CA	5.25	127.30	120.26
3	C	265	MET	CA-C-N	5.25	127.75	120.29
3	C	265	MET	C-N-CA	5.25	127.75	120.29
1	A	317	LYS	CA-C-N	5.25	131.56	121.54
1	A	317	LYS	C-N-CA	5.25	131.56	121.54
1	A	596	THR	N-CA-C	5.25	116.73	110.44
3	C	266	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	1403	GLU	CA-C-N	-5.23	114.86	122.86
1	A	1403	GLU	C-N-CA	-5.23	114.86	122.86
2	B	1113	VAL	CA-C-N	5.21	127.72	120.63
2	B	1113	VAL	C-N-CA	5.21	127.72	120.63
16	X	234	GLU	CA-C-N	5.21	127.78	120.28
16	X	234	GLU	C-N-CA	5.21	127.78	120.28
5	E	172	GLU	CA-C-N	5.20	127.20	120.44
5	E	172	GLU	C-N-CA	5.20	127.20	120.44
7	G	34	VAL	N-CA-C	5.20	115.31	110.42
2	B	908	GLU	N-CA-C	-5.20	107.46	112.97
8	H	7	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	724	GLU	N-CA-C	-5.17	105.53	111.07
1	A	214	ILE	N-CA-CB	5.17	116.56	110.82
1	A	1211	GLN	CA-C-N	5.16	127.15	120.70
1	A	1211	GLN	C-N-CA	5.16	127.15	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	GLU	CA-C-N	5.15	127.44	120.44
1	A	25	GLU	C-N-CA	5.15	127.44	120.44
1	A	310	GLY	CA-C-N	5.15	134.36	121.80
1	A	310	GLY	C-N-CA	5.15	134.36	121.80
2	B	1134	GLU	CB-CG-CD	5.14	121.35	112.60
4	D	188	ALA	N-CA-C	-5.14	106.26	112.54
4	D	197	SER	CA-C-N	5.14	127.42	120.38
4	D	197	SER	C-N-CA	5.14	127.42	120.38
2	B	333	PHE	CA-C-N	5.13	131.21	121.97
2	B	333	PHE	C-N-CA	5.13	131.21	121.97
1	A	1404	GLU	CA-C-N	5.13	131.34	121.54
1	A	1404	GLU	C-N-CA	5.13	131.34	121.54
1	A	672	ASP	CA-CB-CG	5.12	117.72	112.60
2	B	1219	ASP	CA-CB-CG	5.12	117.72	112.60
11	K	24	ASP	CA-C-N	5.12	127.56	120.29
11	K	24	ASP	C-N-CA	5.12	127.56	120.29
4	D	170	THR	N-CA-C	-5.11	107.18	113.41
16	X	325	VAL	CA-C-N	5.11	127.10	120.56
16	X	325	VAL	C-N-CA	5.11	127.10	120.56
2	B	418	LYS	CA-C-N	5.10	127.07	120.44
2	B	418	LYS	C-N-CA	5.10	127.07	120.44
1	A	1011	GLN	CA-C-N	5.10	127.37	120.38
1	A	1011	GLN	C-N-CA	5.10	127.37	120.38
1	A	331	GLY	CA-C-N	5.09	131.27	121.54
1	A	331	GLY	C-N-CA	5.09	131.27	121.54
1	A	224	PHE	N-CA-C	5.09	116.86	110.24
2	B	1009	ASP	N-CA-C	-5.09	106.23	112.90
10	J	9	SER	N-CA-C	5.09	117.22	111.02
2	B	429	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	95	PHE	CA-CB-CG	-5.08	108.72	113.80
2	B	369	GLY	N-CA-C	5.08	120.04	114.40
1	A	369	SER	CA-C-N	5.08	127.63	120.42
1	A	369	SER	C-N-CA	5.08	127.63	120.42
9	I	61	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	1313	LEU	CA-C-N	5.07	131.23	121.54
1	A	1313	LEU	C-N-CA	5.07	131.23	121.54
1	A	91	PHE	CA-CB-CG	5.07	118.87	113.80
2	B	1028	GLU	CA-C-N	5.06	127.02	120.44
2	B	1028	GLU	C-N-CA	5.06	127.02	120.44
1	A	532	ARG	CA-C-N	5.05	127.01	120.44
1	A	532	ARG	C-N-CA	5.05	127.01	120.44
7	G	51	TYR	CA-C-N	5.05	127.00	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	51	TYR	C-N-CA	5.05	127.00	120.44
3	C	194	GLU	N-CA-C	-5.04	107.20	113.55
2	B	66	ASP	CA-C-N	5.03	131.15	121.54
2	B	66	ASP	C-N-CA	5.03	131.15	121.54
5	E	8	ASN	CA-C-N	5.03	126.90	120.56
5	E	8	ASN	C-N-CA	5.03	126.90	120.56
1	A	55	ASP	N-CA-CB	5.03	119.32	110.37
4	D	37	GLN	CB-CG-CD	-5.03	104.06	112.60
7	G	40	GLY	CA-C-N	5.01	127.31	120.54
7	G	40	GLY	C-N-CA	5.01	127.31	120.54
3	C	39	ALA	N-CA-C	5.01	119.02	111.96
11	K	94	ILE	CA-C-N	5.01	126.87	120.56
11	K	94	ILE	C-N-CA	5.01	126.87	120.56

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	P	3	C	Sidechain
15	T	18	DT	Sidechain
15	T	23	DG	Sidechain
15	T	28	DT	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11230	0	11280	298	0
2	B	8793	0	8824	178	0
3	C	2095	0	2051	50	0
4	D	1356	0	1319	19	0
5	E	1752	0	1776	42	0
6	F	688	0	707	21	0
7	G	1340	0	1357	37	0
8	H	1068	0	1040	39	0
9	I	971	0	927	8	0
10	J	532	0	542	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	920	0	929	24	0
12	L	363	0	386	9	0
13	N	229	0	125	3	0
14	P	215	0	109	5	0
15	T	481	0	264	7	0
16	X	953	0	969	24	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	P	31	0	14	0	0
All	All	33026	0	32619	685	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (685) 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)
2:B:1172:ILE:CD1	2:B:1172:ILE:CG1	1.76	1.58
1:A:84:ILE:CG1	1:A:84:ILE:CD1	1.75	1.56
1:A:853:ASP:OD1	1:A:855:THR:HG22	1.55	1.04
1:A:1187:GLN:HA	1:A:1188:GLN:HB2	1.42	0.98
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.17	0.93
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.52	0.91
1:A:53:LEU:HD23	1:A:54:ASN:H	1.36	0.90
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.53	0.89
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.38	0.88
2:B:654:ARG:H	2:B:657:HIS:HD2	1.21	0.88
1:A:1187:GLN:HA	1:A:1188:GLN:CB	2.04	0.87
1:A:254:GLU:HB2	2:B:935:ARG:HH22	1.40	0.86
1:A:225:ASN:HD22	1:A:228:PHE:H	1.23	0.86
1:A:855:THR:HG21	1:A:857:ARG:HE	1.41	0.86
9:I:82:GLU:HB3	9:I:104:LEU:HB2	1.58	0.85
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.57	0.85
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.10	0.82
1:A:1079:MET:HE3	1:A:1359:ASP:HB2	1.60	0.82
8:H:95:TYR:HE1	8:H:97:MET:HG3	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.62	0.81
2:B:516:ASN:H	2:B:516:ASN:HD22	1.30	0.79
2:B:1215:ARG:HB3	2:B:1217:TYR:HE1	1.48	0.79
1:A:41:MET:CB	1:A:49:LYS:HA	2.13	0.79
1:A:41:MET:HA	1:A:50:ILE:H	1.48	0.79
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.65	0.79
1:A:492:PRO:HB2	1:A:497:THR:HG23	1.65	0.79
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.18	0.79
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.63	0.79
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.48	0.79
1:A:1187:GLN:CA	1:A:1188:GLN:HB2	2.13	0.78
2:B:798:TYR:HE2	3:C:66:ARG:HH21	1.30	0.78
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.14	0.78
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.66	0.77
1:A:450:LEU:HD12	1:A:1074:GLU:HG2	1.66	0.77
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.32	0.77
7:G:127:PRO:HB2	7:G:139:ILE:HD13	1.68	0.75
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.68	0.74
2:B:654:ARG:H	2:B:657:HIS:CD2	2.05	0.74
1:A:41:MET:HB3	1:A:49:LYS:HA	1.69	0.74
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.68	0.73
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.70	0.73
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.71	0.73
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.69	0.72
1:A:855:THR:CG2	1:A:857:ARG:HE	2.03	0.72
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.73	0.71
1:A:1148:ILE:HA	9:I:49:ILE:HD12	1.71	0.71
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.72	0.71
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.72	0.71
1:A:53:LEU:HD23	1:A:54:ASN:N	2.06	0.71
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.71	0.71
1:A:567:LYS:HB3	8:H:96:VAL:H	1.57	0.70
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.38	0.70
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.74	0.70
7:G:21:ARG:HD3	7:G:24:GLN:HB2	1.73	0.70
1:A:347:PHE:H	2:B:1107:ALA:HA	1.57	0.70
7:G:1:MET:HE1	7:G:80:LYS:O	1.91	0.69
2:B:711:GLU:H	2:B:712:PRO:HD3	1.57	0.68
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.29	0.68
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.75	0.68
2:B:113:TYR:CD2	2:B:192:LEU:HD21	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1215:ARG:HB3	2:B:1217:TYR:CE1	2.28	0.68
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.75	0.68
7:G:9:LEU:HD23	7:G:11:ILE:HG12	1.74	0.68
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.76	0.67
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.76	0.67
1:A:320:ARG:HE	1:A:323:LYS:HE3	1.59	0.67
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.76	0.67
10:J:48:ARG:HE	10:J:49:MET:HE2	1.59	0.67
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.77	0.67
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.58	0.66
1:A:254:GLU:HB2	2:B:935:ARG:NH2	2.10	0.66
1:A:56:PRO:CD	1:A:58:LEU:HG	2.26	0.66
8:H:95:TYR:CE1	8:H:97:MET:HG3	2.28	0.66
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.77	0.66
1:A:34:LYS:HB2	1:A:36:ARG:HE	1.59	0.65
4:D:27:LEU:HD11	4:D:197:SER:HB3	1.78	0.65
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.27	0.65
3:C:4:GLU:H	3:C:7:GLN:HE22	1.45	0.65
4:D:53:SER:HB3	4:D:152:SER:HB2	1.79	0.65
7:G:34:VAL:O	7:G:37:SER:HB3	1.96	0.65
16:X:321:LEU:O	16:X:325:VAL:HG23	1.97	0.64
3:C:50:GLU:HG2	12:L:66:GLN:HG3	1.79	0.64
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.80	0.64
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.80	0.64
5:E:20:LYS:HD3	5:E:35:VAL:HA	1.79	0.64
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.62	0.64
2:B:853:SER:HB3	2:B:972:LYS:HB2	1.79	0.64
1:A:1378:GLN:HE21	5:E:177:ARG:HH12	1.45	0.63
16:X:233:LYS:HA	16:X:236:LYS:HD2	1.79	0.63
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.92	0.63
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.79	0.63
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.81	0.63
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.80	0.63
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.80	0.63
3:C:46:ILE:HD12	3:C:46:ILE:H	1.64	0.62
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.81	0.62
1:A:754:SER:H	1:A:757:ASN:HD22	1.47	0.62
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.82	0.62
1:A:1444:MET:HE3	6:F:135:ARG:HB2	1.79	0.62
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.95	0.62
1:A:492:PRO:CB	1:A:497:THR:HG23	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HD13	3:C:67:LEU:O	2.00	0.62
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.63	0.62
2:B:599:THR:O	2:B:603:LEU:HB2	2.00	0.62
2:B:235:SER:HA	2:B:261:ARG:HH21	1.64	0.61
7:G:26:LEU:HD13	7:G:56:ILE:HD11	1.81	0.61
2:B:515:HIS:HD2	2:B:517:THR:H	1.47	0.61
1:A:827:THR:O	1:A:831:THR:HB	2.00	0.61
1:A:497:THR:HG21	2:B:1149:GLU:OE2	2.00	0.61
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.83	0.61
14:P:3:C:H42	15:T:27:DA:N6	1.98	0.61
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.83	0.60
2:B:957:ASN:HD22	2:B:961:LEU:H	1.47	0.60
1:A:43:GLU:HG3	1:A:46:THR:HB	1.83	0.60
3:C:52:GLU:HA	12:L:64:LEU:HD22	1.83	0.60
7:G:111:THR:HG22	7:G:113:HIS:H	1.67	0.60
11:K:65:HIS:HD2	11:K:67:PHE:H	1.49	0.60
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.84	0.60
8:H:125:LEU:HG	8:H:130:ARG:NH2	2.17	0.60
6:F:118:LEU:O	6:F:122:MET:HG3	2.01	0.60
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.84	0.60
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.49	0.60
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.42	0.59
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.84	0.59
4:D:186:ASP:O	4:D:212:LYS:HE3	2.02	0.59
1:A:866:PHE:O	1:A:867:ILE:HD12	2.02	0.59
1:A:867:ILE:HD11	1:A:1000:LEU:HD21	1.85	0.59
11:K:65:HIS:CD2	11:K:67:PHE:H	2.21	0.59
1:A:567:LYS:HB3	8:H:96:VAL:N	2.17	0.59
6:F:72:LYS:HB2	6:F:142:SER:HA	1.85	0.59
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.85	0.58
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.85	0.58
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.68	0.58
2:B:171:PRO:HB3	2:B:205:ILE:HD11	1.84	0.58
1:A:703:THR:HG22	16:X:362:ASN:HD21	1.68	0.58
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.85	0.58
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.84	0.58
1:A:278:THR:O	1:A:282:ASN:HB2	2.04	0.58
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.85	0.58
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.85	0.58
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.84	0.58
1:A:34:LYS:HG3	1:A:36:ARG:HH21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.85	0.57
2:B:792:MET:HA	2:B:856:PHE:O	2.04	0.57
2:B:744:HIS:HD2	2:B:746:SER:H	1.51	0.57
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.70	0.57
1:A:770:VAL:HG13	1:A:822:GLU:HG3	1.86	0.57
3:C:143:LEU:HD21	3:C:146:LYS:HE2	1.85	0.57
1:A:61:ILE:HG22	1:A:62:ASP:H	1.70	0.57
2:B:276:ILE:HD11	2:B:355:ILE:HG21	1.87	0.57
1:A:92:HIS:HE1	2:B:1210:MET:O	1.87	0.57
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.87	0.57
7:G:131:GLN:HG3	7:G:136:VAL:HG22	1.86	0.57
8:H:5:LEU:O	8:H:133:ASN:HB3	2.05	0.57
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.87	0.56
3:C:22:LEU:HD22	3:C:230:MET:HE1	1.87	0.56
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.39	0.56
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.05	0.56
1:A:472:LEU:O	1:A:475:THR:HB	2.06	0.56
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.86	0.56
1:A:1442:ASP:HB3	1:A:1444:MET:HE1	1.87	0.56
2:B:515:HIS:CD2	2:B:517:THR:H	2.23	0.56
2:B:914:LYS:HE3	2:B:937:ALA:HB1	1.86	0.56
1:A:982:THR:H	1:A:985:ASP:HB2	1.71	0.56
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.87	0.56
1:A:1388:GLY:O	1:A:1391:ARG:HG3	2.06	0.56
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.88	0.56
1:A:933:TYR:HA	1:A:936:LEU:HD12	1.87	0.56
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.71	0.56
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.88	0.56
7:G:50:ASP:OD2	7:G:53:ASN:HB2	2.06	0.56
7:G:106:MET:HG3	7:G:157:ILE:O	2.06	0.56
6:F:99:LEU:CD2	7:G:66:GLY:H	2.19	0.55
16:X:285:GLU:HB3	16:X:336:VAL:HG21	1.88	0.55
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.88	0.55
3:C:142:VAL:H	10:J:16:ASP:HB3	1.71	0.55
2:B:1181:GLU:HA	2:B:1188:LYS:HA	1.87	0.55
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.36	0.55
1:A:816:HIS:HE2	2:B:764:SER:H	1.53	0.55
5:E:176:PRO:O	5:E:212:ARG:HA	2.07	0.55
1:A:492:PRO:HB2	1:A:497:THR:CG2	2.36	0.55
1:A:67:CYS:C	1:A:68:GLN:HG3	2.30	0.55
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:VAL:CG2	2:B:483:LEU:HD13	2.37	0.55
1:A:203:SER:OG	1:A:206:GLU:HB2	2.07	0.55
2:B:1185:CYS:C	2:B:1187:ASN:H	2.14	0.55
3:C:143:LEU:HG	10:J:2:ILE:HD11	1.88	0.55
5:E:50:MET:HE2	16:X:294:GLU:HB3	1.88	0.54
1:A:35:ILE:HG13	1:A:56:PRO:HG2	1.90	0.54
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.90	0.54
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.90	0.54
1:A:1442:ASP:HB2	6:F:137:TYR:CE2	2.37	0.54
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.90	0.54
2:B:465:ASN:HA	2:B:476:ALA:HB1	1.90	0.54
1:A:903:ASN:HD22	1:A:906:HIS:H	1.56	0.54
11:K:12:LEU:HD23	11:K:16:GLU:O	2.08	0.54
3:C:251:LEU:O	3:C:255:VAL:HG23	2.08	0.53
1:A:567:LYS:CB	8:H:95:TYR:HA	2.38	0.53
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.90	0.53
1:A:1004:ASN:HD21	1:A:1007:ILE:HG12	1.73	0.53
1:A:1155:ASP:HB3	1:A:1241:ARG:NH2	2.22	0.53
2:B:187:SER:HB3	10:J:62:ARG:HH22	1.74	0.53
6:F:89:GLU:O	6:F:93:ILE:HD12	2.08	0.53
5:E:19:VAL:O	5:E:23:VAL:HG23	2.08	0.53
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.91	0.53
1:A:942:PHE:O	1:A:945:GLU:HB2	2.09	0.53
1:A:41:MET:HB2	1:A:49:LYS:HA	1.91	0.53
2:B:463:THR:C	2:B:465:ASN:H	2.17	0.53
8:H:23:VAL:HG12	8:H:43:ASN:HA	1.91	0.53
1:A:225:ASN:ND2	1:A:228:PHE:H	2.00	0.52
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.90	0.52
2:B:1100:ASP:HA	2:B:1103:ILE:HG22	1.90	0.52
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.67	0.52
6:F:110:ASP:O	6:F:123:LYS:HE2	2.09	0.52
16:X:248:LEU:HA	16:X:252:PHE:HB3	1.90	0.52
1:A:519:PRO:O	1:A:624:SER:HB2	2.09	0.52
1:A:869:GLY:O	5:E:204:THR:HG21	2.09	0.52
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.90	0.52
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.91	0.52
1:A:850:VAL:CG2	1:A:1064:VAL:HG21	2.39	0.52
2:B:780:VAL:HG21	10:J:56:LEU:HD13	1.92	0.52
16:X:319:LEU:HD23	16:X:322:LYS:HB2	1.91	0.52
1:A:34:LYS:CG	1:A:36:ARG:HH21	2.21	0.52
1:A:10:PRO:HG2	2:B:1192:TYR:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:H	1:A:74:MET:HE2	1.74	0.52
2:B:744:HIS:CD2	2:B:746:SER:H	2.27	0.52
13:N:4:DA:H2"	13:N:5:DA:C8	2.44	0.52
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.92	0.52
2:B:705:MET:HE3	2:B:705:MET:HA	1.91	0.52
3:C:58:LEU:HD12	3:C:145:CYS:HB2	1.90	0.52
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.90	0.52
1:A:849:MET:HE1	1:A:1440:ALA:HB1	1.91	0.52
2:B:408:LEU:HD11	2:B:545:ILE:HD13	1.92	0.52
4:D:27:LEU:CD1	4:D:197:SER:HB3	2.38	0.52
5:E:179:GLN:HA	5:E:215:MET:HB2	1.91	0.52
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.75	0.51
1:A:1144:LYS:HG3	1:A:1268:LEU:HB3	1.92	0.51
8:H:82:PRO:C	8:H:84:ALA:H	2.19	0.51
1:A:42:ASP:HA	1:A:46:THR:O	2.10	0.51
1:A:68:GLN:OE1	1:A:70:CYS:HB3	2.10	0.51
1:A:182:VAL:HG22	1:A:201:VAL:HG22	1.91	0.51
1:A:687:LYS:HG2	1:A:794:PRO:HG2	1.92	0.51
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.75	0.51
1:A:84:ILE:HG12	1:A:270:LEU:HD13	1.91	0.51
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.41	0.51
2:B:1023:VAL:HG12	2:B:1027:ILE:HD11	1.91	0.51
3:C:123:ASN:HD22	3:C:125:MET:H	1.59	0.51
1:A:57:ARG:O	1:A:68:GLN:HG2	2.11	0.51
2:B:295:GLY:HA2	2:B:298:LEU:HB2	1.92	0.51
2:B:900:ALA:CB	12:L:61:THR:HG23	2.40	0.51
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.92	0.51
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.93	0.51
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.93	0.51
1:A:1243:VAL:O	1:A:1244:ARG:HB3	2.11	0.51
1:A:1286:LYS:HE3	1:A:1302:PRO:HB2	1.93	0.51
2:B:765:PRO:O	2:B:769:TYR:CD1	2.63	0.51
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.93	0.50
2:B:259:TYR:HE1	2:B:270:LYS:HB2	1.76	0.50
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.41	0.50
3:C:260:LEU:HD23	3:C:264:GLN:HE22	1.76	0.50
4:D:138:ASN:ND2	7:G:35:GLU:HG2	2.27	0.50
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.11	0.50
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.93	0.50
3:C:163:ILE:HD12	3:C:165:LYS:HB2	1.93	0.50
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1177:LEU:HD13	16:X:307:ARG:HH21	1.76	0.50
16:X:286:LEU:HD12	16:X:336:VAL:HG13	1.93	0.50
2:B:365:THR:HG23	2:B:367:LEU:H	1.76	0.50
2:B:756:ILE:O	2:B:759:PRO:HD3	2.12	0.50
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.92	0.50
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.41	0.50
3:C:66:ARG:NH2	10:J:2:ILE:HG23	2.26	0.50
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.92	0.50
3:C:104:PHE:CZ	3:C:150:GLY:HA2	2.47	0.50
14:P:2:U:H4'	14:P:3:C:C5'	2.41	0.50
1:A:710:LEU:HD12	1:A:710:LEU:H	1.77	0.50
2:B:286:PHE:HD1	2:B:291:ILE:HD13	1.77	0.50
1:A:1258:HIS:HA	1:A:1261:LYS:HD2	1.94	0.50
2:B:291:ILE:HD12	2:B:291:ILE:H	1.77	0.50
2:B:649:LYS:HE2	2:B:738:PHE:O	2.12	0.50
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.94	0.50
1:A:298:PHE:O	1:A:302:THR:HB	2.12	0.49
1:A:332:LYS:O	1:A:333:GLU:HB2	2.12	0.49
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.47	0.49
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.76	0.49
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.94	0.49
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.94	0.49
2:B:798:TYR:HE2	3:C:66:ARG:NH2	2.06	0.49
1:A:55:ASP:O	1:A:55:ASP:OD2	2.30	0.49
1:A:534:LEU:O	1:A:574:GLY:HA3	2.11	0.49
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.95	0.49
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.47	0.49
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.94	0.49
1:A:321:PRO:O	1:A:322:VAL:HB	2.12	0.49
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.95	0.49
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.48	0.49
2:B:168:GLY:HA2	2:B:454:THR:HG1	1.76	0.49
4:D:55:ALA:HB3	4:D:148:LEU:HD21	1.93	0.49
5:E:154:ILE:O	5:E:196:VAL:HA	2.11	0.49
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.95	0.49
1:A:348:SER:HB2	2:B:1128:LEU:HD12	1.95	0.49
1:A:738:LYS:HA	8:H:19:ARG:HH22	1.77	0.49
2:B:466:TRP:HB2	2:B:479:VAL:HG21	1.94	0.49
2:B:467:GLU:HG3	2:B:475:ARG:HB3	1.94	0.49
3:C:142:VAL:HG22	10:J:15:GLY:HA3	1.94	0.49
5:E:179:GLN:HE21	5:E:181:ALA:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG22	1:A:62:ASP:N	2.27	0.49
1:A:353:ILE:HD12	1:A:482:PHE:CD1	2.48	0.49
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.94	0.49
1:A:949:ASP:OD2	1:A:951:GLU:HB2	2.12	0.49
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.95	0.49
5:E:197:LYS:HD3	5:E:199:ILE:HD11	1.95	0.49
8:H:89:LEU:C	8:H:91:ASP:H	2.21	0.49
1:A:1129:GLU:O	1:A:1133:LEU:HG	2.13	0.49
1:A:1256:GLU:HA	1:A:1259:MET:HB2	1.94	0.49
3:C:84:ARG:HD3	11:K:11:LEU:HD21	1.95	0.49
4:D:40:HIS:CD2	4:D:41:GLN:HG3	2.47	0.49
7:G:41:LYS:HD2	7:G:42:PHE:CZ	2.48	0.49
1:A:304:MET:HG2	2:B:1210:MET:HG2	1.95	0.48
1:A:831:THR:O	1:A:834:THR:HG22	2.13	0.48
1:A:1172:LEU:HD12	16:X:310:TYR:HE2	1.78	0.48
2:B:615:MET:HG2	2:B:626:ILE:HG23	1.94	0.48
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.94	0.48
10:J:48:ARG:HE	10:J:49:MET:CE	2.23	0.48
1:A:741:ASN:HD22	1:A:744:LYS:H	1.61	0.48
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.94	0.48
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.96	0.48
1:A:7:SER:OG	2:B:1161:HIS:CE1	2.67	0.48
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.78	0.48
2:B:516:ASN:H	2:B:516:ASN:ND2	2.03	0.48
16:X:326:VAL:HG13	16:X:332:LEU:HD11	1.96	0.48
1:A:567:LYS:HG3	1:A:568:PRO:HD3	1.94	0.48
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.95	0.48
1:A:1032:LEU:O	1:A:1036:ARG:HD2	2.14	0.48
3:C:55:THR:HB	3:C:151:GLN:HA	1.95	0.48
3:C:148:ARG:HD3	3:C:149:LYS:HG3	1.96	0.48
8:H:38:LEU:HD12	8:H:39:THR:H	1.78	0.48
1:A:112:LYS:HD3	1:A:165:GLY:HA3	1.95	0.48
1:A:265:LYS:HD2	1:A:322:VAL:HG11	1.96	0.48
1:A:670:ILE:HD13	2:B:1067:ARG:HD2	1.96	0.48
2:B:68:THR:HG23	2:B:91:SER:HB3	1.95	0.48
2:B:969:ARG:HD3	3:C:61:GLU:OE2	2.14	0.48
2:B:1084:GLN:OE1	3:C:189:THR:HG22	2.14	0.48
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.94	0.47
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.96	0.47
12:L:68:GLU:HB2	12:L:70:ARG:HD2	1.96	0.47
1:A:266:LEU:HA	1:A:269:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:TYR:CE1	2:B:270:LYS:HB2	2.49	0.47
2:B:467:GLU:HG2	2:B:472:MET:HE2	1.94	0.47
3:C:32:SER:O	3:C:36:VAL:HG23	2.14	0.47
1:A:54:ASN:HD22	1:A:247:ARG:HH12	1.62	0.47
1:A:77:CYS:SG	1:A:78:PRO:O	2.73	0.47
1:A:579:SER:HB3	1:A:611:GLN:HA	1.96	0.47
1:A:588:LEU:HD12	1:A:632:VAL:HG21	1.97	0.47
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.29	0.47
3:C:101:LEU:HB2	3:C:118:LEU:HD23	1.95	0.47
4:D:23:ASN:HA	4:D:28:GLN:O	2.14	0.47
7:G:1:MET:HE3	7:G:85:GLU:OE1	2.14	0.47
7:G:115:MET:HG2	7:G:163:ILE:HD11	1.96	0.47
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.96	0.47
2:B:705:MET:H	2:B:710:LEU:HD12	1.79	0.47
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.96	0.47
5:E:23:VAL:HG12	5:E:28:TYR:HB2	1.96	0.47
7:G:145:VAL:HG13	7:G:163:ILE:HG23	1.95	0.47
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.45	0.47
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.97	0.47
16:X:238:ARG:NH1	16:X:287:TYR:HB2	2.29	0.47
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.96	0.47
1:A:768:GLN:HB3	1:A:775:ILE:HD11	1.96	0.47
1:A:1116:LEU:HB2	1:A:1311:VAL:HG22	1.95	0.47
1:A:1244:ARG:O	1:A:1244:ARG:HG3	2.14	0.47
2:B:898:LEU:HD22	2:B:964:VAL:HG11	1.97	0.47
8:H:107:VAL:HG21	8:H:126:GLU:HG3	1.96	0.47
2:B:797:TYR:HB2	2:B:852:ARG:O	2.15	0.47
15:T:20:DC:H5"	15:T:20:DC:H6	1.80	0.47
1:A:464:PRO:HD2	11:K:67:PHE:HD2	1.79	0.47
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.96	0.47
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.97	0.47
4:D:163:VAL:HG23	4:D:217:LEU:HD22	1.96	0.47
5:E:182:ASP:O	5:E:186:LEU:HG	2.14	0.47
1:A:335:ARG:HD3	2:B:1202:LEU:HD13	1.96	0.46
2:B:789:MET:HE3	2:B:965:LYS:HB3	1.96	0.46
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.96	0.46
7:G:114:LEU:HG	7:G:162:SER:HB3	1.97	0.46
8:H:135:LEU:C	8:H:137:GLN:H	2.22	0.46
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.51	0.46
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.13	0.46
2:B:792:MET:H	2:B:857:ARG:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.97	0.46
1:A:56:PRO:HD3	1:A:58:LEU:HG	1.96	0.46
1:A:323:LYS:N	1:A:323:LYS:HE2	2.30	0.46
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.98	0.46
8:H:130:ARG:HA	8:H:133:ASN:HD22	1.79	0.46
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.97	0.46
1:A:49:LYS:HZ3	1:A:61:ILE:N	2.13	0.46
2:B:579:ARG:HA	2:B:589:VAL:HG12	1.98	0.46
2:B:865:LYS:HE2	2:B:869:SER:HA	1.96	0.46
1:A:53:LEU:O	1:A:54:ASN:C	2.59	0.46
1:A:512:VAL:HA	1:A:519:PRO:HA	1.98	0.46
1:A:596:THR:C	1:A:598:LEU:H	2.22	0.46
2:B:486:TYR:HB3	2:B:1096:ARG:HD2	1.98	0.46
9:I:50:THR:HG22	9:I:52:ILE:H	1.79	0.46
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.85	0.46
2:B:1121:GLY:HA2	15:T:22:BRU:OP1	2.15	0.46
5:E:12:LEU:HG	5:E:58:MET:HE1	1.96	0.46
5:E:178:ILE:HB	5:E:212:ARG:HD3	1.98	0.46
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.99	0.46
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.80	0.46
5:E:117:THR:HB	5:E:120:ALA:H	1.80	0.46
11:K:10:PHE:CE1	11:K:11:LEU:HD13	2.50	0.46
1:A:379:VAL:HG22	1:A:431:LYS:HG3	1.97	0.46
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.97	0.46
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.15	0.46
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.97	0.46
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.51	0.46
1:A:787:PHE:CE2	1:A:796:SER:HA	2.51	0.46
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.97	0.46
2:B:467:GLU:CB	2:B:468:GLN:HA	2.46	0.46
13:N:5:DA:H2"	13:N:6:DG:C8	2.51	0.46
16:X:323:ALA:O	16:X:326:VAL:HB	2.16	0.46
1:A:503:GLN:NE2	6:F:90:ARG:HH21	2.14	0.45
1:A:587:HIS:CD2	1:A:608:ILE:HG12	2.51	0.45
2:B:346:GLU:H	2:B:349:ILE:HD13	1.82	0.45
2:B:986:GLN:HE22	2:B:1022:THR:HG21	1.81	0.45
5:E:17:ARG:HA	5:E:20:LYS:HD2	1.97	0.45
11:K:77:THR:HB	11:K:81:TYR:HB3	1.98	0.45
1:A:197:PRO:HG2	1:A:199:LEU:HD11	1.99	0.45
1:A:886:ILE:HD12	1:A:952:ALA:HA	1.97	0.45
2:B:802:PRO:HD3	2:B:814:PHE:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:884:ARG:HD2	2:B:935:ARG:HB2	1.99	0.45
9:I:7:CYS:SG	9:I:8:ARG:O	2.74	0.45
7:G:43:GLY:HA2	7:G:157:ILE:HD11	1.98	0.45
1:A:75:ASN:HD22	2:B:1116:ARG:NH1	2.15	0.45
1:A:92:HIS:HD2	1:A:94:GLY:H	1.65	0.45
1:A:527:THR:HG21	1:A:650:GLN:HA	1.97	0.45
2:B:603:LEU:HD12	2:B:609:ILE:HG13	1.98	0.45
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.99	0.45
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.16	0.45
5:E:66:GLU:HA	5:E:69:ILE:HD12	1.97	0.45
9:I:75:CYS:HB3	9:I:80:SER:H	1.82	0.45
11:K:20:LYS:HB3	11:K:34:THR:HB	1.99	0.45
4:D:9:GLN:HA	4:D:38:ILE:HD13	1.98	0.45
14:P:5:A:H2'	14:P:6:C:C6	2.52	0.45
1:A:886:ILE:HG12	1:A:943:LEU:HB3	1.98	0.45
1:A:999:VAL:HG12	1:A:1000:LEU:HG	1.98	0.45
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.32	0.45
7:G:138:THR:HG22	7:G:139:ILE:H	1.81	0.45
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.51	0.45
1:A:387:ARG:HH11	1:A:437:MET:HE1	1.81	0.45
1:A:709:THR:HB	1:A:712:GLU:H	1.81	0.45
1:A:1078:GLN:C	1:A:1080:THR:H	2.24	0.45
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.52	0.45
1:A:404:TYR:HE2	2:B:1108:ARG:HH22	1.64	0.45
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.99	0.45
7:G:1:MET:HE3	7:G:85:GLU:CD	2.41	0.45
8:H:9:ILE:HG13	8:H:56:THR:HG23	1.98	0.45
8:H:81:PRO:CB	8:H:82:PRO:HD3	2.44	0.45
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.82	0.45
1:A:483:ASP:HB3	2:B:837:ASP:HB3	1.97	0.45
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.97	0.45
5:E:61:GLN:HG3	5:E:105:PHE:HE1	1.82	0.45
7:G:21:ARG:HA	7:G:21:ARG:NE	2.32	0.45
1:A:49:LYS:HD3	1:A:61:ILE:HD12	1.99	0.44
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.16	0.44
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.99	0.44
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.97	0.44
1:A:277:GLU:HG2	1:A:281:HIS:CD2	2.52	0.44
1:A:739:ASP:H	8:H:19:ARG:NH1	2.14	0.44
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.99	0.44
2:B:1198:TYR:O	2:B:1201:LYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:TYR:HB3	6:F:115:THR:HG22	1.99	0.44
2:B:402:GLY:HA2	2:B:695:ALA:HB3	2.00	0.44
14:P:2:U:H4'	14:P:3:C:H5'	1.99	0.44
15:T:10:DA:H2''	15:T:11:DG:C8	2.53	0.44
1:A:834:THR:HG21	1:A:1080:THR:HG21	1.99	0.44
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.99	0.44
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.99	0.44
1:A:49:LYS:NZ	1:A:60:SER:HA	2.32	0.44
1:A:344:ARG:CZ	2:B:1120:GLU:HG3	2.48	0.44
1:A:754:SER:N	1:A:757:ASN:HD22	2.11	0.44
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.99	0.44
7:G:62:LEU:HD21	7:G:69:GLU:HB2	2.00	0.44
1:A:923:LEU:H	1:A:923:LEU:HG	1.52	0.44
2:B:882:THR:HG22	2:B:884:ARG:H	1.83	0.44
3:C:35:ARG:HB2	11:K:41:THR:HG23	2.00	0.44
7:G:14:HIS:CD2	7:G:16:SER:H	2.35	0.44
10:J:1:MET:HG3	10:J:60:PHE:CE2	2.47	0.44
10:J:48:ARG:O	10:J:52:THR:HG22	2.18	0.44
16:X:355:ARG:O	16:X:359:ILE:HG12	2.17	0.44
1:A:41:MET:HA	1:A:50:ILE:N	2.26	0.44
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.18	0.44
1:A:741:ASN:HB3	1:A:744:LYS:HB2	2.00	0.44
1:A:17:VAL:HG22	2:B:1216:LEU:HD23	2.00	0.44
1:A:332:LYS:H	1:A:337:ARG:CB	2.31	0.44
1:A:1391:ARG:HD2	1:A:1391:ARG:C	2.43	0.44
2:B:34:ILE:HG12	2:B:542:MET:CE	2.48	0.44
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.47	0.44
1:A:140:THR:HA	1:A:143:LYS:HE2	2.00	0.43
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.48	0.43
3:C:125:MET:HE3	3:C:125:MET:HA	1.99	0.43
3:C:164:ALA:HA	3:C:167:HIS:O	2.18	0.43
1:A:230:ARG:HD2	1:A:233:TRP:CZ2	2.53	0.43
1:A:494:SER:HB3	1:A:497:THR:HB	1.99	0.43
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.00	0.43
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.17	0.43
2:B:875:GLU:O	2:B:877:PRO:HD3	2.18	0.43
8:H:15:VAL:HG22	8:H:26:ILE:HG13	2.00	0.43
1:A:370:ILE:HD11	2:B:1103:ILE:HG13	1.99	0.43
2:B:390:LEU:HD13	2:B:392:ARG:CZ	2.48	0.43
2:B:975:GLN:O	2:B:990:ILE:HD12	2.17	0.43
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.99	0.43
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.99	0.43
8:H:93:TYR:CG	8:H:143:LEU:HB3	2.52	0.43
10:J:7:CYS:HA	10:J:49:MET:HG2	1.99	0.43
16:X:306:VAL:HA	16:X:309:LEU:HD12	2.01	0.43
1:A:856:THR:HB	1:A:865:GLN:HB2	2.01	0.43
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	1.99	0.43
2:B:210:LYS:HE2	2:B:462:ALA:HA	2.00	0.43
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.53	0.43
5:E:147:HIS:CD2	5:E:149:LEU:H	2.36	0.43
8:H:12:VAL:HG23	8:H:53:ASP:H	1.82	0.43
16:X:322:LYS:HD2	16:X:346:PRO:HD3	2.00	0.43
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.99	0.43
1:A:880:LYS:HA	1:A:955:PRO:HA	2.00	0.43
1:A:1116:LEU:HB3	1:A:1308:THR:OG1	2.18	0.43
2:B:54:PHE:HA	2:B:58:THR:HB	2.01	0.43
1:A:495:GLU:HG3	6:F:98:ALA:HB1	2.01	0.43
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	2.01	0.43
1:A:870:GLU:O	5:E:205:SER:HB3	2.19	0.43
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.81	0.43
16:X:278:PHE:HA	16:X:281:ASN:HB2	1.99	0.43
1:A:337:ARG:HD3	2:B:1132:GLU:CD	2.44	0.43
1:A:337:ARG:HD3	2:B:1132:GLU:OE2	2.19	0.43
1:A:1172:LEU:HD12	16:X:310:TYR:CE2	2.54	0.43
2:B:296:GLU:O	2:B:300:HIS:HD2	2.02	0.43
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.54	0.43
1:A:55:ASP:O	1:A:55:ASP:CG	2.59	0.43
1:A:483:ASP:OD2	2:B:987:LYS:HE2	2.19	0.43
1:A:535:THR:HG21	1:A:616:VAL:HA	2.01	0.43
1:A:858:ASN:H	1:A:858:ASN:HD22	1.67	0.43
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.99	0.43
1:A:1151:GLU:HG2	9:I:45:ARG:HG3	2.01	0.43
10:J:7:CYS:HA	10:J:49:MET:HE3	1.99	0.43
1:A:34:LYS:HG3	1:A:36:ARG:NH2	2.33	0.43
1:A:50:ILE:C	1:A:52:GLY:H	2.27	0.43
1:A:69:THR:C	1:A:71:GLN:H	2.27	0.43
5:E:17:ARG:HH12	5:E:36:GLU:HG2	1.84	0.43
8:H:23:VAL:HG11	8:H:121:LEU:HD21	1.99	0.43
13:N:11:DT:H3	15:T:9:DA:H61	1.65	0.43
5:E:40:GLU:HA	5:E:43:LYS:HD2	2.01	0.43
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:95:TYR:HB3	8:H:144:ILE:HB	2.00	0.43
1:A:637:LYS:HB3	1:A:641:VAL:HG11	2.00	0.42
2:B:246:LYS:HG3	2:B:249:ARG:HH21	1.83	0.42
2:B:952:VAL:HG22	2:B:966:VAL:HG13	2.01	0.42
1:A:71:GLN:HE22	2:B:1176:ASN:HB2	1.84	0.42
1:A:1400:CYS:HA	1:A:1408:ILE:HD12	2.01	0.42
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	2.01	0.42
2:B:35:SER:HA	2:B:811:TYR:CE1	2.53	0.42
16:X:304:GLU:HB3	16:X:307:ARG:NH1	2.34	0.42
1:A:75:ASN:O	1:A:76:GLU:HB2	2.19	0.42
1:A:680:THR:HA	1:A:683:ILE:HD12	2.01	0.42
2:B:248:SER:H	2:B:418:LYS:NZ	2.18	0.42
2:B:291:ILE:HG22	2:B:297:ILE:HG13	2.00	0.42
2:B:530:GLY:C	2:B:532:ALA:H	2.28	0.42
5:E:48:ASP:OD2	5:E:52:ARG:HB2	2.20	0.42
7:G:87:VAL:HG23	7:G:145:VAL:HG23	2.02	0.42
8:H:42:ILE:HG23	8:H:95:TYR:HE2	1.85	0.42
8:H:102:TYR:OH	8:H:122:LEU:HD22	2.18	0.42
1:A:302:THR:HA	1:A:305:ASP:O	2.20	0.42
4:D:35:LEU:HD11	4:D:174:PRO:HD2	2.01	0.42
4:D:167:LEU:HB3	4:D:177:VAL:HG22	2.00	0.42
7:G:142:ARG:HG2	7:G:171:ILE:HD12	2.01	0.42
1:A:332:LYS:H	1:A:337:ARG:HB3	1.85	0.42
1:A:375:THR:HG21	1:A:433:GLU:HB3	2.01	0.42
1:A:531:ILE:HG21	1:A:622:VAL:HG11	2.02	0.42
2:B:361:LEU:HD12	2:B:361:LEU:HA	1.92	0.42
2:B:912:ILE:HB	2:B:939:THR:OG1	2.18	0.42
2:B:1172:ILE:HD12	2:B:1172:ILE:N	2.35	0.42
2:B:1204:PHE:HA	2:B:1207:LEU:HD12	2.01	0.42
6:F:101:ILE:HD13	6:F:120:ILE:HG22	2.02	0.42
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.88	0.42
1:A:1325:THR:HA	5:E:147:HIS:HA	2.02	0.42
2:B:102:VAL:HG13	2:B:112:LEU:HD22	2.01	0.42
2:B:373:ARG:HE	2:B:567:GLU:HG2	1.83	0.42
2:B:702:LEU:H	2:B:739:THR:HG1	1.66	0.42
3:C:67:LEU:HD11	3:C:155:LEU:HD13	2.02	0.42
14:P:3:C:H42	15:T:27:DA:H62	1.66	0.42
1:A:105:CYS:SG	1:A:139:TRP:HA	2.60	0.42
1:A:683:ILE:HD13	1:A:801:GLU:HG3	2.00	0.42
1:A:705:LYS:HA	16:X:362:ASN:HA	2.02	0.42
2:B:165:VAL:HG11	2:B:448:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:MET:CE	2:B:390:LEU:HG	2.50	0.42
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.84	0.42
15:T:27:DA:H2''	15:T:28:DT:O5'	2.19	0.42
1:A:218:ASP:O	1:A:221:SER:HB2	2.19	0.42
1:A:901:LEU:HD22	1:A:919:ILE:HG23	2.02	0.42
2:B:810:GLU:HG3	2:B:815:ARG:HH12	1.85	0.42
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.01	0.42
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.50	0.42
2:B:878:GLN:HB2	2:B:879:ARG:H	1.76	0.42
7:G:27:LYS:HB3	7:G:51:TYR:CE1	2.55	0.42
7:G:112:LYS:HA	7:G:115:MET:HE3	2.01	0.42
8:H:12:VAL:HB	8:H:51:ALA:HA	2.01	0.42
16:X:285:GLU:HG3	16:X:288:LYS:HD2	2.02	0.42
1:A:55:ASP:C	1:A:57:ARG:H	2.28	0.41
1:A:567:LYS:CB	1:A:568:PRO:CD	2.97	0.41
1:A:775:ILE:HG21	1:A:815:PHE:CD1	2.55	0.41
3:C:97:VAL:HG21	3:C:129:ILE:HG23	2.02	0.41
2:B:640:VAL:HG22	2:B:651:LEU:HG	2.02	0.41
3:C:176:ILE:HG12	3:C:232:VAL:HG13	2.02	0.41
6:F:85:MET:HB2	6:F:151:LEU:HB3	2.02	0.41
1:A:471:ASN:O	1:A:474:VAL:HG12	2.20	0.41
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.50	0.41
2:B:31:TRP:HB3	2:B:807:ARG:HH21	1.85	0.41
5:E:152:LYS:HE3	5:E:199:ILE:HD13	2.03	0.41
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.54	0.41
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.84	0.41
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	2.03	0.41
4:D:66:ARG:HD2	4:D:133:THR:HB	2.02	0.41
7:G:15:PRO:HD3	7:G:67:SER:HA	2.02	0.41
1:A:497:THR:HG21	2:B:1149:GLU:CD	2.45	0.41
1:A:528:LEU:O	1:A:531:ILE:HG22	2.20	0.41
1:A:629:LEU:O	1:A:633:VAL:HG23	2.21	0.41
1:A:868:TYR:CE1	1:A:1064:VAL:HG22	2.55	0.41
2:B:753:ALA:HA	2:B:756:ILE:HD12	2.03	0.41
5:E:16:PHE:CD2	5:E:20:LYS:HE2	2.56	0.41
10:J:14:VAL:HG13	10:J:50:ILE:HG12	2.03	0.41
2:B:280:ILE:H	2:B:280:ILE:HG13	1.48	0.41
6:F:94:LEU:HD23	6:F:94:LEU:HA	1.89	0.41
7:G:13:LEU:HD23	7:G:13:LEU:HA	1.82	0.41
10:J:23:ASN:O	10:J:27:GLU:HB2	2.21	0.41
1:A:446:ARG:HB2	1:A:487:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:PHE:HA	1:A:595:THR:HB	2.03	0.41
1:A:1109:LYS:HD2	1:A:1333:ILE:HD13	2.03	0.41
2:B:918:ILE:HG13	2:B:919:SER:H	1.86	0.41
5:E:20:LYS:HB3	5:E:35:VAL:HG22	2.03	0.41
5:E:50:MET:HB3	5:E:52:ARG:HD2	2.01	0.41
1:A:387:ARG:NH1	1:A:437:MET:HE1	2.36	0.41
1:A:1017:LEU:O	1:A:1020:CYS:HB2	2.21	0.41
1:A:1327:ILE:O	5:E:147:HIS:HE1	2.02	0.41
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.21	0.41
2:B:1002:THR:HG22	2:B:1072:MET:HE2	2.03	0.41
3:C:6:PRO:HA	3:C:24:ASN:HB3	2.02	0.41
3:C:184:ASN:HD21	3:C:189:THR:H	1.67	0.41
4:D:56:ARG:HB2	4:D:148:LEU:HD22	2.01	0.41
10:J:36:LEU:HD23	10:J:41:LEU:HD13	2.02	0.41
1:A:596:THR:C	1:A:598:LEU:N	2.77	0.41
1:A:885:THR:HG23	1:A:893:PHE:HE1	1.86	0.41
1:A:903:ASN:ND2	1:A:905:ASP:H	2.19	0.41
1:A:912:LEU:HD22	1:A:1033:GLN:HA	2.03	0.41
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.61	0.41
2:B:618:ASP:OD1	2:B:621:GLU:HB2	2.21	0.41
2:B:705:MET:N	2:B:710:LEU:HD12	2.36	0.41
7:G:102:GLN:HE22	7:G:107:LYS:HE2	1.85	0.41
1:A:376:TYR:CE1	1:A:498:ARG:HD2	2.56	0.41
1:A:1196:GLU:HA	1:A:1236:LEU:O	2.20	0.41
11:K:65:HIS:HA	11:K:66:PRO:HD3	1.90	0.41
12:L:31:CYS:O	12:L:35:SER:HA	2.20	0.41
1:A:134:ARG:HD2	1:A:221:SER:O	2.21	0.40
1:A:605:MET:HE3	1:A:614:PHE:O	2.20	0.40
1:A:909:ASP:C	1:A:911:SER:H	2.29	0.40
1:A:1333:ILE:H	1:A:1333:ILE:HG13	1.62	0.40
1:A:1378:GLN:NE2	5:E:177:ARG:HH12	2.16	0.40
10:J:58:GLU:HA	10:J:61:LEU:HD12	2.02	0.40
1:A:1164:PRO:HA	1:A:1167:GLU:HG3	2.03	0.40
2:B:387:LEU:HD12	2:B:387:LEU:HA	1.91	0.40
5:E:17:ARG:O	5:E:20:LYS:HB2	2.22	0.40
5:E:135:PHE:HB3	5:E:140:LEU:CD1	2.48	0.40
16:X:316:LYS:HG2	16:X:320:GLU:HB3	2.04	0.40
2:B:31:TRP:HA	2:B:34:ILE:HD12	2.03	0.40
5:E:158:SER:O	5:E:162:ARG:HB2	2.22	0.40
8:H:47:PHE:CD2	8:H:95:TYR:HD2	2.38	0.40
11:K:40:HIS:CE1	11:K:63:VAL:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.91	0.40
1:A:943:LEU:HD11	1:A:1020:CYS:HB3	2.03	0.40
2:B:333:PHE:O	2:B:334:ILE:HG13	2.22	0.40
4:D:39:ASN:HD22	4:D:41:GLN:HB2	1.85	0.40
16:X:254:VAL:HG12	16:X:258:ILE:HD11	2.02	0.40
16:X:345:ASN:HB2	16:X:348:LEU:HB2	2.02	0.40
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	2.04	0.40
1:A:1279:ILE:CD1	1:A:1312:ASN:HB3	2.51	0.40
2:B:711:GLU:N	2:B:712:PRO:HD3	2.30	0.40
12:L:32:ALA:H	12:L:55:ILE:HD13	1.86	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	1419/1733 (82%)	1223 (86%)	142 (10%)	54 (4%)	2	21
2	B	1086/1224 (89%)	949 (87%)	99 (9%)	38 (4%)	3	23
3	C	264/318 (83%)	229 (87%)	31 (12%)	4 (2%)	8	37
4	D	173/221 (78%)	155 (90%)	11 (6%)	7 (4%)	2	20
5	E	212/215 (99%)	199 (94%)	11 (5%)	2 (1%)	14	46
6	F	83/155 (54%)	75 (90%)	7 (8%)	1 (1%)	10	41
7	G	169/171 (99%)	153 (90%)	14 (8%)	2 (1%)	10	41
8	H	129/146 (88%)	102 (79%)	18 (14%)	9 (7%)	1	10
9	I	117/122 (96%)	93 (80%)	23 (20%)	1 (1%)	14	46
10	J	63/70 (90%)	51 (81%)	6 (10%)	6 (10%)	0	6
11	K	113/120 (94%)	106 (94%)	6 (5%)	1 (1%)	14	46
12	L	44/70 (63%)	33 (75%)	3 (7%)	8 (18%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	X	106/146 (73%)	90 (85%)	9 (8%)	7 (7%)	1	12
All	All	3978/4711 (84%)	3458 (87%)	380 (10%)	140 (4%)	3	23

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	35	ILE
1	A	57	ARG
1	A	58	LEU
1	A	76	GLU
1	A	169	ASN
1	A	253	ASN
1	A	311	GLN
1	A	567	LYS
1	A	629	LEU
1	A	706	HIS
1	A	1188	GLN
1	A	1403	GLU
1	A	1405	THR
2	B	367	LEU
2	B	470	LYS
2	B	477	ALA
2	B	531	GLN
2	B	879	ARG
2	B	881	ASN
2	B	1171	VAL
2	B	1181	GLU
4	D	53	SER
4	D	199	ASN
6	F	73	ALA
10	J	6	ARG
12	L	50	ASP
12	L	56	LEU
12	L	59	ALA
12	L	60	ARG
16	X	315	ASP
16	X	338	MET
1	A	167	CYS
1	A	258	GLY
1	A	283	GLY
1	A	318	SER

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Mol	Chain	Res	Type
1	A	322	VAL
1	A	331	GLY
1	A	423	ASP
1	A	536	LEU
1	A	537	ARG
1	A	593	GLU
1	A	846	GLU
1	A	1002	GLY
1	A	1281	ARG
1	A	1365	TYR
1	A	1437	GLY
2	B	247	GLY
2	B	266	ALA
2	B	334	ILE
2	B	364	ILE
2	B	466	TRP
2	B	469	LYS
2	B	475	ARG
2	B	476	ALA
2	B	712	PRO
2	B	792	MET
2	B	867	GLY
2	B	1046	PRO
2	B	1155	SER
3	C	141	GLY
4	D	18	VAL
4	D	169	SER
8	H	81	PRO
8	H	82	PRO
8	H	107	VAL
8	H	139	ASN
10	J	55	ASP
12	L	55	ILE
16	X	301	ILE
16	X	341	SER
1	A	44	THR
1	A	47	ARG
1	A	54	ASN
1	A	156	ASP
1	A	286	HIS
1	A	568	PRO
1	A	1079	MET

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Mol	Chain	Res	Type
2	B	67	SER
2	B	68	THR
2	B	249	ARG
2	B	707	PRO
2	B	772	ALA
2	B	880	THR
3	C	90	ASP
3	C	142	VAL
4	D	11	ARG
4	D	119	ARG
5	E	3	GLN
9	I	32	CYS
10	J	2	ILE
12	L	35	SER
12	L	53	HIS
1	A	66	LYS
1	A	72	GLU
1	A	257	ARG
1	A	332	LYS
1	A	333	GLU
1	A	385	ILE
1	A	399	HIS
1	A	424	ILE
1	A	465	TYR
1	A	852	TYR
1	A	1206	ASP
2	B	45	SER
2	B	447	ALA
2	B	467	GLU
2	B	711	GLU
2	B	1223	ASP
4	D	16	LYS
5	E	36	GLU
7	G	154	VAL
8	H	60	ALA
8	H	83	GLN
8	H	84	ALA
10	J	13	VAL
11	K	70	ARG
12	L	45	ALA
16	X	302	TYR
16	X	340	ALA

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Mol	Chain	Res	Type
1	A	108	MET
1	A	958	VAL
1	A	1366	ARG
1	A	1392	SER
2	B	368	GLU
2	B	648	HIS
2	B	737	THR
2	B	1066	SER
2	B	1108	ARG
7	G	66	GLY
8	H	108	SER
16	X	339	ASN
1	A	775	ILE
8	H	17	PRO
10	J	29	GLU
10	J	64	ASN
1	A	196	GLU
1	A	1064	VAL
2	B	613	VAL
3	C	5	GLY

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	1249/1520 (82%)	1015 (81%)	234 (19%)	1	10
2	B	960/1061 (90%)	807 (84%)	153 (16%)	2	15
3	C	234/274 (85%)	201 (86%)	33 (14%)	3	19
4	D	140/200 (70%)	121 (86%)	19 (14%)	3	20
5	E	196/197 (100%)	168 (86%)	28 (14%)	3	19
6	F	75/137 (55%)	67 (89%)	8 (11%)	6	28
7	G	152/152 (100%)	128 (84%)	24 (16%)	2	15
8	H	117/128 (91%)	99 (85%)	18 (15%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	113/116 (97%)	97 (86%)	16 (14%)	3	19
10	J	60/65 (92%)	46 (77%)	14 (23%)	1	5
11	K	99/102 (97%)	87 (88%)	12 (12%)	5	23
12	L	40/57 (70%)	27 (68%)	13 (32%)	0	2
16	X	107/136 (79%)	87 (81%)	20 (19%)	1	10
All	All	3542/4145 (86%)	2950 (83%)	592 (17%)	2	14

All (592) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	13	THR
1	A	15	LYS
1	A	18	GLN
1	A	30	ILE
1	A	34	LYS
1	A	36	ARG
1	A	40	THR
1	A	41	MET
1	A	42	ASP
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS
1	A	76	GLU
1	A	84	ILE
1	A	93	VAL
1	A	96	ILE
1	A	106	VAL
1	A	114	LEU
1	A	117	GLU
1	A	120	GLU
1	A	132	LYS
1	A	145	LYS
1	A	149	GLU
1	A	151	ASP
1	A	152	VAL
1	A	159	THR
1	A	161	LEU
1	A	173	THR
1	A	196	GLU

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Mol	Chain	Res	Type
1	A	200	ARG
1	A	204	THR
1	A	208	LEU
1	A	209	ASN
1	A	210	ILE
1	A	232	GLU
1	A	239	LEU
1	A	249	SER
1	A	254	GLU
1	A	261	ASP
1	A	265	LYS
1	A	274	ILE
1	A	282	ASN
1	A	286	HIS
1	A	302	THR
1	A	307	ASP
1	A	316	GLN
1	A	320	ARG
1	A	323	LYS
1	A	329	LEU
1	A	335	ARG
1	A	336	ILE
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	369	SER
1	A	373	THR
1	A	375	THR
1	A	385	ILE
1	A	407	ARG
1	A	411	ASP
1	A	424	ILE
1	A	431	LYS
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	449	SER
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	461	LYS
1	A	463	ILE

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Mol	Chain	Res	Type
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	481	ASP
1	A	489	LEU
1	A	496	GLU
1	A	497	THR
1	A	498	ARG
1	A	500	GLU
1	A	512	VAL
1	A	518	LYS
1	A	523	ILE
1	A	524	VAL
1	A	527	THR
1	A	536	LEU
1	A	538	ASP
1	A	545	GLN
1	A	549	MET
1	A	562	THR
1	A	571	LEU
1	A	573	SER
1	A	577	ILE
1	A	597	LEU
1	A	598	LEU
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	632	VAL
1	A	640	GLN
1	A	645	LEU
1	A	651	LYS
1	A	664	THR
1	A	666	ILE
1	A	670	ILE
1	A	680	THR
1	A	683	ILE
1	A	691	LEU
1	A	702	LEU
1	A	705	LYS
1	A	706	HIS
1	A	710	LEU

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Mol	Chain	Res	Type
1	A	720	ARG
1	A	734	GLU
1	A	735	VAL
1	A	738	LYS
1	A	756	ILE
1	A	762	SER
1	A	764	CYS
1	A	768	GLN
1	A	788	SER
1	A	795	GLU
1	A	803	SER
1	A	821	ARG
1	A	822	GLU
1	A	826	ASP
1	A	834	THR
1	A	839	ARG
1	A	856	THR
1	A	858	ASN
1	A	867	ILE
1	A	878	ILE
1	A	880	LYS
1	A	884	ASP
1	A	896	ARG
1	A	905	ASP
1	A	919	ILE
1	A	920	LEU
1	A	923	LEU
1	A	926	GLN
1	A	929	LEU
1	A	941	LYS
1	A	948	VAL
1	A	960	ILE
1	A	969	GLN
1	A	976	THR
1	A	980	ASP
1	A	982	THR
1	A	983	ILE
1	A	998	LEU
1	A	1001	ARG
1	A	1009	ASN
1	A	1013	ASP
1	A	1022	LEU

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Mol	Chain	Res	Type
1	A	1024	SER
1	A	1029	ARG
1	A	1038	THR
1	A	1046	LEU
1	A	1062	GLU
1	A	1064	VAL
1	A	1067	LEU
1	A	1079	MET
1	A	1082	ASN
1	A	1100	ARG
1	A	1103	GLU
1	A	1128	GLN
1	A	1129	GLU
1	A	1147	THR
1	A	1159	ARG
1	A	1171	GLN
1	A	1172	LEU
1	A	1173	HIS
1	A	1179	GLU
1	A	1180	GLU
1	A	1183	GLN
1	A	1185	PHE
1	A	1188	GLN
1	A	1195	LEU
1	A	1199	ARG
1	A	1218	GLN
1	A	1222	ASN
1	A	1223	ASP
1	A	1230	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1244	ARG
1	A	1263	ILE
1	A	1264	GLU
1	A	1265	ASN
1	A	1266	THR
1	A	1267	MET
1	A	1271	ILE
1	A	1276	VAL
1	A	1277	GLU
1	A	1279	ILE
1	A	1284	MET

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Mol	Chain	Res	Type
1	A	1291	VAL
1	A	1297	GLU
1	A	1299	VAL
1	A	1301	GLU
1	A	1306	LEU
1	A	1308	THR
1	A	1314	SER
1	A	1315	GLU
1	A	1316	VAL
1	A	1322	ILE
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1341	ILE
1	A	1342	GLU
1	A	1355	VAL
1	A	1356	ILE
1	A	1358	SER
1	A	1359	ASP
1	A	1371	LEU
1	A	1376	THR
1	A	1378	GLN
1	A	1383	SER
1	A	1393	ASN
1	A	1394	THR
1	A	1398	MET
1	A	1411	GLU
1	A	1424	VAL
1	A	1426	GLU
1	A	1433	MET
1	A	1436	ILE
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	70	ILE

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Mol	Chain	Res	Type
2	B	101	MET
2	B	102	VAL
2	B	122	LEU
2	B	128	LEU
2	B	130	VAL
2	B	134	LYS
2	B	183	GLU
2	B	192	LEU
2	B	199	MET
2	B	205	ILE
2	B	222	ILE
2	B	223	VAL
2	B	240	ILE
2	B	251	ILE
2	B	262	GLU
2	B	272	THR
2	B	276	ILE
2	B	278	GLN
2	B	279	ASP
2	B	280	ILE
2	B	299	GLU
2	B	305	VAL
2	B	334	ILE
2	B	361	LEU
2	B	364	ILE
2	B	365	THR
2	B	368	GLU
2	B	372	SER
2	B	373	ARG
2	B	387	LEU
2	B	393	LYS
2	B	394	ASP
2	B	396	ASP
2	B	416	LEU
2	B	423	LYS
2	B	429	PHE
2	B	451	LYS
2	B	468	GLN
2	B	469	LYS
2	B	470	LYS
2	B	472	MET
2	B	475	ARG

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Mol	Chain	Res	Type
2	B	479	VAL
2	B	485	ARG
2	B	486	TYR
2	B	510	LYS
2	B	516	ASN
2	B	537	LYS
2	B	538	ASN
2	B	547	VAL
2	B	549	THR
2	B	554	ILE
2	B	556	THR
2	B	561	TRP
2	B	563	MET
2	B	582	VAL
2	B	596	LEU
2	B	603	LEU
2	B	615	MET
2	B	617	ARG
2	B	620	ARG
2	B	621	GLU
2	B	628	THR
2	B	629	ASP
2	B	637	LEU
2	B	644	GLU
2	B	646	LEU
2	B	651	LEU
2	B	653	VAL
2	B	678	GLU
2	B	684	LEU
2	B	694	ASP
2	B	709	ASP
2	B	714	GLU
2	B	723	VAL
2	B	734	HIS
2	B	736	THR
2	B	742	GLU
2	B	748	ILE
2	B	755	ILE
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	795	ILE

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Mol	Chain	Res	Type
2	B	796	LEU
2	B	797	TYR
2	B	806	THR
2	B	815	ARG
2	B	835	GLN
2	B	844	SER
2	B	868	MET
2	B	878	GLN
2	B	879	ARG
2	B	881	ASN
2	B	885	MET
2	B	887	HIS
2	B	889	THR
2	B	908	GLU
2	B	911	ILE
2	B	915	THR
2	B	916	THR
2	B	942	ARG
2	B	945	GLU
2	B	946	ASN
2	B	956	THR
2	B	957	ASN
2	B	958	GLN
2	B	970	THR
2	B	971	THR
2	B	973	ILE
2	B	975	GLN
2	B	986	GLN
2	B	997	GLU
2	B	998	ASP
2	B	1007	VAL
2	B	1045	SER
2	B	1050	ILE
2	B	1060	ARG
2	B	1065	GLN
2	B	1066	SER
2	B	1072	MET
2	B	1084	GLN
2	B	1106	ARG
2	B	1112	GLN
2	B	1122	ARG
2	B	1123	SER

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Mol	Chain	Res	Type
2	B	1133	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1162	ILE
2	B	1172	ILE
2	B	1178	ASN
2	B	1179	GLN
2	B	1181	GLU
2	B	1183	LYS
2	B	1189	ILE
2	B	1202	LEU
2	B	1211	ASN
2	B	1212	ILE
2	B	1220	ARG
2	B	1223	ASP
3	C	8	VAL
3	C	12	GLU
3	C	16	ASP
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	40	GLU
3	C	53	THR
3	C	55	THR
3	C	56	THR
3	C	57	VAL
3	C	60	ASP
3	C	61	GLU
3	C	78	GLU
3	C	102	GLN
3	C	106	GLU
3	C	111	THR
3	C	121	VAL
3	C	123	ASN

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Mol	Chain	Res	Type
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	186	LEU
3	C	189	THR
3	C	208	GLU
3	C	240	VAL
3	C	258	ILE
3	C	262	LEU
3	C	263	THR
3	C	265	MET
4	D	31	GLN
4	D	35	LEU
4	D	47	LEU
4	D	50	LEU
4	D	65	GLU
4	D	126	ILE
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	149	THR
4	D	156	ASP
4	D	163	VAL
4	D	177	VAL
4	D	187	THR
4	D	197	SER
4	D	203	SER
4	D	206	GLU
4	D	217	LEU
4	D	219	THR
5	E	3	GLN
5	E	17	ARG
5	E	24	LYS
5	E	40	GLU
5	E	47	CYS
5	E	48	ASP
5	E	50	MET
5	E	52	ARG
5	E	72	PHE
5	E	74	ASP
5	E	78	LEU

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Mol	Chain	Res	Type
5	E	92	THR
5	E	98	ILE
5	E	100	ILE
5	E	104	ASN
5	E	107	THR
5	E	117	THR
5	E	142	VAL
5	E	150	VAL
5	E	154	ILE
5	E	156	LEU
5	E	175	LEU
5	E	184	VAL
5	E	190	LEU
5	E	197	LYS
5	E	202	SER
5	E	213	ILE
5	E	215	MET
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	109	VAL
6	F	115	THR
6	F	127	GLU
6	F	150	GLU
6	F	153	VAL
7	G	11	ILE
7	G	13	LEU
7	G	24	GLN
7	G	26	LEU
7	G	33	GLU
7	G	37	SER
7	G	45	ILE
7	G	52	ASP
7	G	54	ILE
7	G	61	ILE
7	G	85	GLU
7	G	93	SER
7	G	96	GLN
7	G	112	LYS
7	G	114	LEU
7	G	126	ASN
7	G	138	THR

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Mol	Chain	Res	Type
7	G	143	ILE
7	G	145	VAL
7	G	151	ILE
7	G	153	GLN
7	G	155	SER
7	G	166	ASP
7	G	171	ILE
8	H	12	VAL
8	H	14	GLU
8	H	26	ILE
8	H	27	GLU
8	H	31	THR
8	H	33	GLN
8	H	42	ILE
8	H	46	LEU
8	H	62	SER
8	H	83	GLN
8	H	86	ASP
8	H	103	LYS
8	H	106	GLU
8	H	107	VAL
8	H	109	LYS
8	H	130	ARG
8	H	132	LEU
8	H	137	GLN
9	I	7	CYS
9	I	8	ARG
9	I	12	ASN
9	I	33	SER
9	I	35	VAL
9	I	42	LEU
9	I	55	THR
9	I	61	ASP
9	I	70	ARG
9	I	72	ASP
9	I	74	GLU
9	I	81	ARG
9	I	104	LEU
9	I	108	HIS
9	I	109	ILE
9	I	118	ARG
10	J	2	ILE

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Mol	Chain	Res	Type
10	J	3	VAL
10	J	6	ARG
10	J	7	CYS
10	J	12	LYS
10	J	13	VAL
10	J	17	LYS
10	J	22	LEU
10	J	23	ASN
10	J	32	GLU
10	J	43	ARG
10	J	48	ARG
10	J	52	THR
10	J	54	VAL
11	K	11	LEU
11	K	12	LEU
11	K	31	VAL
11	K	37	LYS
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	54	ARG
11	K	89	ASN
11	K	101	LEU
11	K	108	GLU
11	K	113	THR
12	L	27	LEU
12	L	30	ILE
12	L	38	LEU
12	L	43	THR
12	L	44	ASP
12	L	46	VAL
12	L	54	ARG
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	62	LYS
12	L	65	VAL
12	L	68	GLU
16	X	232	GLU
16	X	243	LYS
16	X	247	THR
16	X	252	PHE

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Mol	Chain	Res	Type
16	X	253	ILE
16	X	284	GLU
16	X	286	LEU
16	X	292	ASN
16	X	303	THR
16	X	304	GLU
16	X	306	VAL
16	X	319	LEU
16	X	321	LEU
16	X	333	ASN
16	X	335	LEU
16	X	345	ASN
16	X	347	ASP
16	X	358	ILE
16	X	360	LEU
16	X	364	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	54	ASN
1	A	71	GLN
1	A	75	ASN
1	A	92	HIS
1	A	225	ASN
1	A	253	ASN
1	A	256	GLN
1	A	281	HIS
1	A	282	ASN
1	A	339	ASN
1	A	358	ASN
1	A	425	GLN
1	A	451	HIS
1	A	471	ASN
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	548	ASN
1	A	603	ASN
1	A	611	GLN
1	A	650	GLN

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Mol	Chain	Res	Type
1	A	660	ASN
1	A	698	GLN
1	A	717	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	903	ASN
1	A	965	GLN
1	A	994	GLN
1	A	1171	GLN
1	A	1258	HIS
1	A	1265	ASN
1	A	1278	ASN
1	A	1312	ASN
1	A	1364	ASN
1	A	1378	GLN
1	A	1390	ASN
1	A	1432	GLN
2	B	47	GLN
2	B	103	ASN
2	B	110	HIS
2	B	115	GLN
2	B	236	HIS
2	B	325	GLN
2	B	357	GLN
2	B	366	GLN
2	B	395	GLN
2	B	468	GLN
2	B	481	GLN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	573	GLN
2	B	587	HIS
2	B	657	HIS
2	B	733	HIS
2	B	744	HIS
2	B	767	ASN
2	B	842	ASN

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Mol	Chain	Res	Type
2	B	957	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1025	HIS
2	B	1065	GLN
2	B	1112	GLN
2	B	1161	HIS
2	B	1176	ASN
2	B	1178	ASN
2	B	1179	GLN
2	B	1195	HIS
3	C	7	GLN
3	C	17	ASN
3	C	65	HIS
3	C	123	ASN
3	C	135	GLN
3	C	151	GLN
3	C	184	ASN
3	C	203	GLN
3	C	231	ASN
3	C	242	GLN
3	C	264	GLN
4	D	37	GLN
4	D	39	ASN
4	D	41	GLN
4	D	132	GLN
4	D	157	GLN
4	D	173	HIS
4	D	179	GLN
5	E	5	ASN
5	E	136	ASN
5	E	147	HIS
5	E	179	GLN
7	G	10	ASN
7	G	14	HIS
7	G	96	GLN
7	G	102	GLN
7	G	122	ASN
7	G	131	GLN
7	G	153	GLN
8	H	35	GLN
8	H	133	ASN

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Mol	Chain	Res	Type
9	I	11	ASN
9	I	23	ASN
9	I	114	GLN
10	J	26	GLN
11	K	65	HIS
12	L	66	GLN
16	X	312	ASN
16	X	337	ASN
16	X	345	ASN
16	X	362	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	10/11 (90%)	4 (40%)	1 (10%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	3	C
14	P	4	G
14	P	5	A
14	P	9	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	2	U

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	14,15	18,21,22	1.57	4 (22%)	25,30,33	2.46	10 (40%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C4-N3	-3.31	1.32	1.38
15	T	22	BRU	C6-N1	-3.23	1.32	1.38
15	T	22	BRU	C2-N3	-2.84	1.33	1.38
15	T	22	BRU	C2-N1	2.70	1.42	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C5-C4-N3	4.56	118.59	113.34
15	T	22	BRU	C4-N3-C2	-4.54	121.39	127.34
15	T	22	BRU	O4-C4-C5	-4.39	120.20	125.80
15	T	22	BRU	BR-C5-C4	4.38	123.06	118.02
15	T	22	BRU	N3-C2-N1	4.27	120.45	114.89
15	T	22	BRU	O4'-C1'-N1	3.54	114.14	107.86
15	T	22	BRU	C1'-N1-C2	3.16	123.84	117.66
15	T	22	BRU	C1'-N1-C6	-3.15	115.45	120.74
15	T	22	BRU	O2-C2-N3	-2.80	116.32	121.49
15	T	22	BRU	BR-C5-C6	-2.10	117.71	120.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	22	BRU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	APC	P	12	18	29,33,33	1.90	8 (27%)	44,52,52	2.06	9 (20%)

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	APC	P	12	18	-	6/19/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	12	APC	C5-C4	4.90	1.47	1.39
19	P	12	APC	PA-O1A	4.46	1.62	1.51
19	P	12	APC	C5-C6	3.42	1.50	1.41
19	P	12	APC	PB-O3B	3.25	1.62	1.58
19	P	12	APC	PA-O2A	-3.16	1.48	1.56
19	P	12	APC	C8-N7	2.56	1.36	1.31
19	P	12	APC	PB-O2B	2.14	1.61	1.56
19	P	12	APC	C5-N7	-2.10	1.35	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	P	12	APC	C5-C4-N3	-6.91	117.20	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	P	12	APC	C4-C5-N7	-4.93	104.95	110.58
19	P	12	APC	N3-C4-N9	4.61	135.00	127.17
19	P	12	APC	C2-N3-C4	4.37	122.50	111.83
19	P	12	APC	N3-C2-N1	-3.54	123.23	128.58
19	P	12	APC	C5-N7-C8	3.29	108.62	103.45
19	P	12	APC	C6-C5-N7	3.01	137.89	132.09
19	P	12	APC	PB-O3B-PG	-2.36	123.99	132.45
19	P	12	APC	C2'-C1'-N9	-2.06	108.19	113.30

There are no chirality outliers.

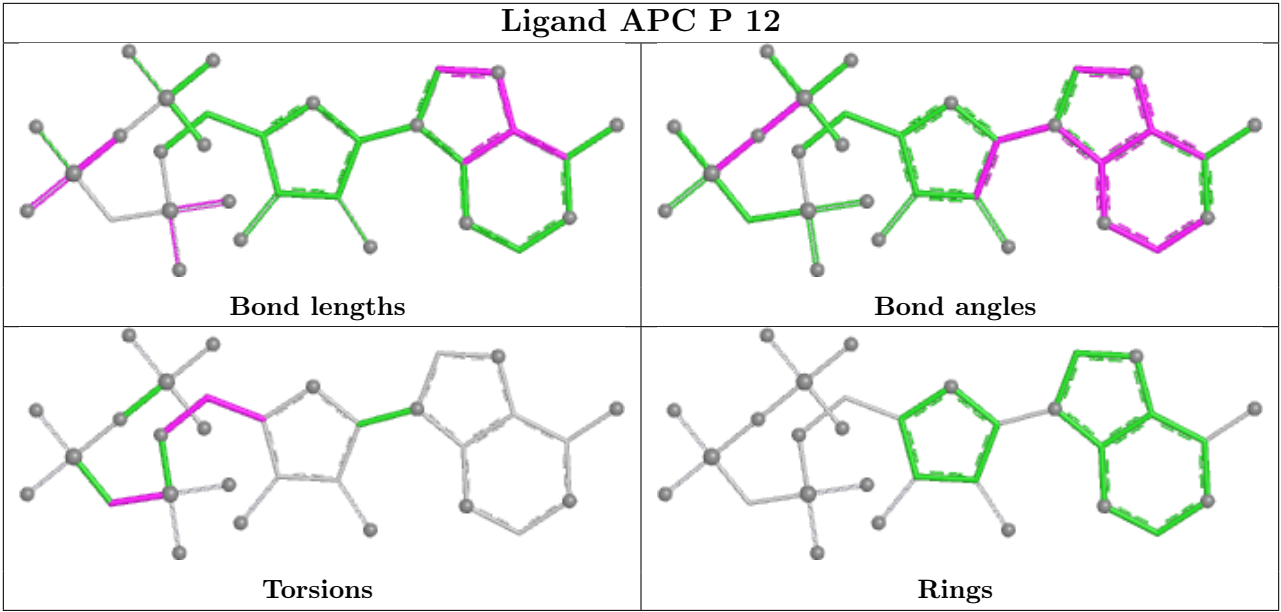
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	P	12	APC	PB-C3A-PA-O1A
19	P	12	APC	PB-C3A-PA-O2A
19	P	12	APC	PB-C3A-PA-O5'
19	P	12	APC	O4'-C4'-C5'-O5'
19	P	12	APC	C3'-C4'-C5'-O5'
19	P	12	APC	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	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	3.57

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	1427/1733 (82%)	-0.25	13 (0%) 81 56	58, 108, 175, 232	0
2	B	1106/1224 (90%)	-0.09	29 (2%) 57 33	65, 120, 181, 216	0
3	C	266/318 (83%)	-0.34	0 100 100	81, 109, 151, 180	0
4	D	177/221 (80%)	-0.04	8 (4%) 38 21	85, 123, 173, 199	0
5	E	214/215 (99%)	-0.25	1 (0%) 87 66	83, 139, 189, 210	0
6	F	85/155 (54%)	-0.47	0 100 100	68, 91, 124, 144	0
7	G	171/171 (100%)	-0.23	0 100 100	79, 108, 151, 169	0
8	H	133/146 (91%)	0.20	5 (3%) 44 25	118, 153, 189, 226	0
9	I	119/122 (97%)	0.10	3 (2%) 58 34	117, 159, 198, 220	0
10	J	65/70 (92%)	-0.33	0 100 100	88, 105, 148, 160	0
11	K	115/120 (95%)	-0.30	3 (2%) 57 33	77, 106, 155, 173	0
12	L	46/70 (65%)	0.69	5 (10%) 10 9	105, 175, 195, 205	0
13	N	11/14 (78%)	0.93	0 100 100	176, 194, 264, 267	0
14	P	10/11 (90%)	0.24	2 (20%) 3 3	85, 113, 169, 174	0
15	T	23/26 (88%)	0.37	1 (4%) 40 22	83, 148, 246, 258	0
16	X	116/146 (79%)	0.88	14 (12%) 8 7	163, 195, 212, 220	0
All	All	4084/4762 (85%)	-0.14	84 (2%) 63 37	58, 118, 189, 267	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	8.4
2	B	335	GLY	5.2
11	K	115	ALA	4.8
1	A	1177	LEU	4.6
16	X	291	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	65	LEU	4.2
8	H	63	LEU	4.1
2	B	446	LEU	3.9
11	K	114	LEU	3.7
1	A	69	THR	3.6
1	A	1254	ALA	3.6
2	B	469	LYS	3.5
2	B	266	ALA	3.5
4	D	14	ARG	3.5
12	L	27	LEU	3.5
2	B	251	ILE	3.4
4	D	24	ALA	3.3
12	L	26	THR	3.3
8	H	86	ASP	3.2
12	L	28	LYS	3.1
16	X	323	ALA	3.1
16	X	300	LYS	3.1
2	B	231	PRO	3.1
2	B	881	ASN	3.0
2	B	1224	PHE	3.0
2	B	265	SER	3.0
16	X	244	MET	2.9
14	P	2	U	2.9
4	D	15	LEU	2.9
12	L	25	ALA	2.8
2	B	486	TYR	2.8
2	B	731	VAL	2.8
4	D	4	SER	2.8
12	L	46	VAL	2.8
1	A	2	VAL	2.7
2	B	70	ILE	2.7
8	H	139	ASN	2.7
16	X	301	ILE	2.7
2	B	509	ALA	2.7
16	X	320	GLU	2.7
2	B	323	VAL	2.6
16	X	255	PRO	2.6
16	X	321	LEU	2.6
2	B	502	ILE	2.6
2	B	883	LEU	2.6
14	P	3	C	2.5
16	X	254	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
16	X	325	VAL	2.5
2	B	715	ALA	2.5
15	T	6	DC	2.5
1	A	186	LYS	2.4
16	X	365	VAL	2.4
1	A	1083	THR	2.4
2	B	709	ASP	2.4
2	B	880	THR	2.4
16	X	330	LEU	2.4
2	B	249	ARG	2.4
2	B	919	SER	2.3
4	D	9	GLN	2.3
2	B	108	VAL	2.3
2	B	134	LYS	2.3
4	D	173	HIS	2.3
1	A	311	GLN	2.3
11	K	14	GLU	2.3
2	B	734	HIS	2.3
16	X	271	VAL	2.3
1	A	3	GLY	2.2
4	D	5	THR	2.2
2	B	262	GLU	2.2
8	H	84	ALA	2.2
9	I	52	ILE	2.2
2	B	732	SER	2.2
1	A	1179	GLU	2.2
8	H	132	LEU	2.2
5	E	110	PHE	2.1
9	I	47	GLU	2.1
4	D	76	LYS	2.1
16	X	313	LEU	2.1
1	A	1257	ASP	2.0
9	I	118	ARG	2.0
2	B	164	LYS	2.0
1	A	1217	LYS	2.0
2	B	250	PHE	2.0
1	A	640	GLN	2.0

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

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	0.97	0.07	87,97,123,144	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

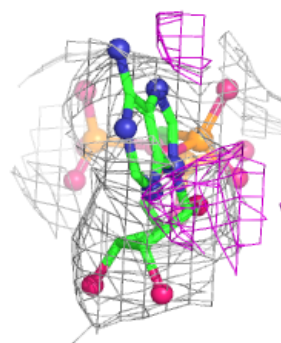
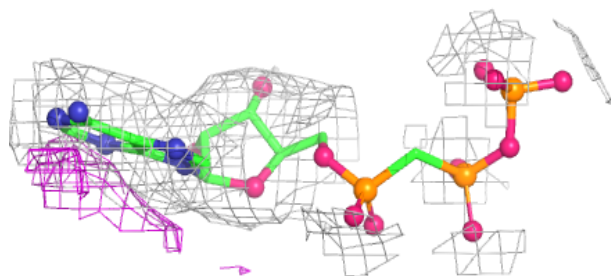
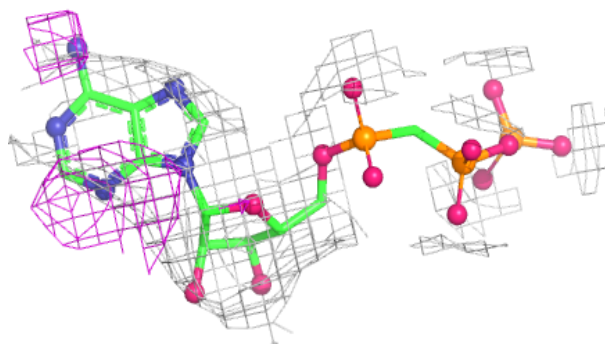
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	APC	P	12	31/31	0.92	0.10	102,118,169,170	0
17	ZN	I	1122	1/1	0.97	0.05	234,234,234,234	0
17	ZN	L	1071	1/1	0.99	0.03	192,192,192,192	0
17	ZN	C	1269	1/1	1.00	0.03	92,92,92,92	0
17	ZN	I	1121	1/1	1.00	0.04	129,129,129,129	0
17	ZN	A	2456	1/1	1.00	0.02	128,128,128,128	0
17	ZN	J	1066	1/1	1.00	0.01	85,85,85,85	0
17	ZN	A	2457	1/1	1.00	0.05	77,77,77,77	0
18	MG	A	2458	1/1	1.00	0.01	58,58,58,58	0
17	ZN	B	2225	1/1	1.00	0.03	92,92,92,92	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around APC P 12:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.