



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:43 pm BST

PDB ID : 4BY1
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

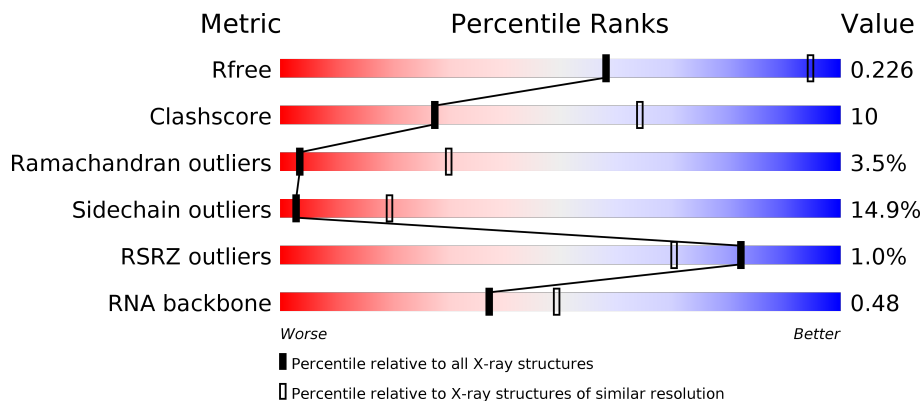
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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 on 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	 53% 24% 5% 18%
2	B	1224	 61% 25% 10%
3	C	318	 55% 26% 16%
4	D	221	 57% 22% 20%

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Mol	Chain	Length	Quality of chain
5	E	215	<p>71% 24% 5%</p>
6	F	155	<p>32% 21% 45%</p>
7	G	171	<p>60% 33% 7%</p>
8	H	146	<p>53% 31% 7% 9%</p>
9	I	122	<p>76% 19%</p>
10	J	70	<p>37% 43% 11% 7%</p>
11	K	120	<p>64% 29%</p>
12	L	70	<p>30% 26% 10% 34%</p>
13	N	14	<p>50% 21% 7% 21%</p>
14	P	11	<p>36% 27% 9% 18% 9%</p>
15	T	26	<p>58% 27% 8% 8%</p>
16	X	146	<p>42% 34% 21%</p>

2 Entry composition [i](#)

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1106	8793	5569	1538	1631	55	0	0	0

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

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

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	177	1356	840	241	273	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	P			
13	N	11	229	109	44	65	11	0	0	0

- 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
			Total	C	N	O	P			
14	P	10	215	96	41	68	10	0	0	0

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

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

- Molecule 16 is a protein called TRANSCRIPTION FACTOR BYE1.

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

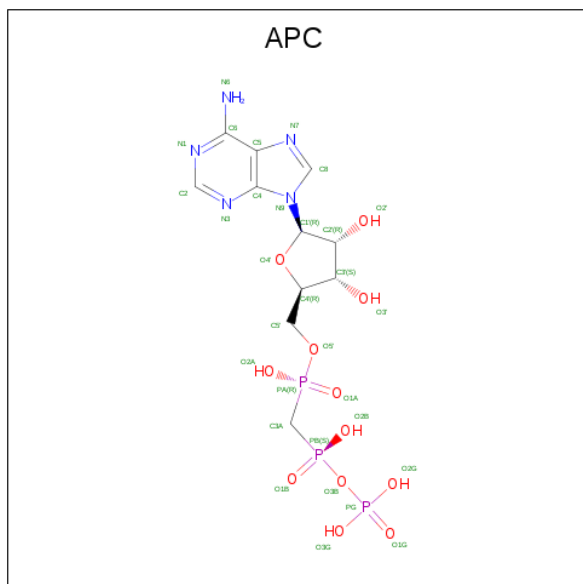
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 19 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

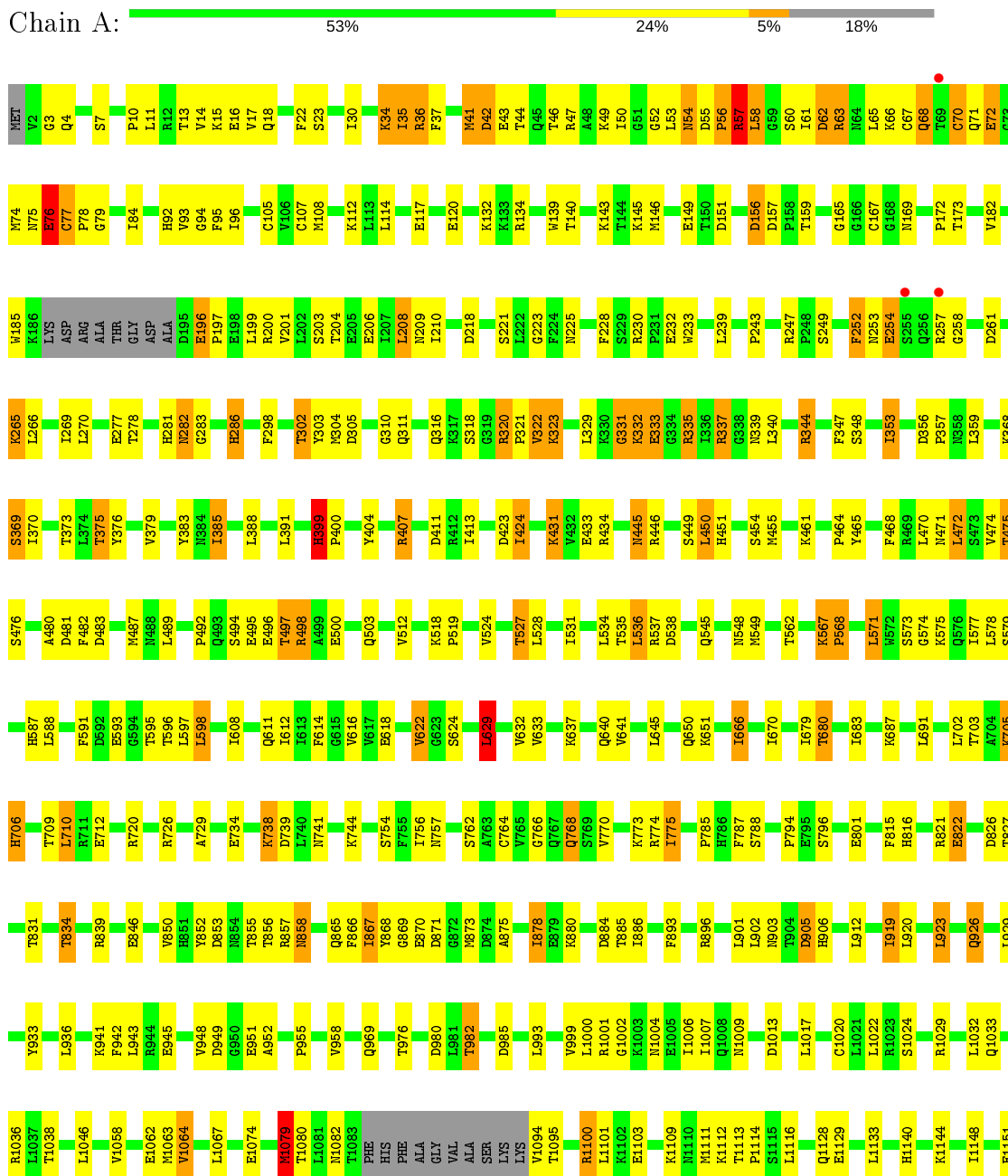


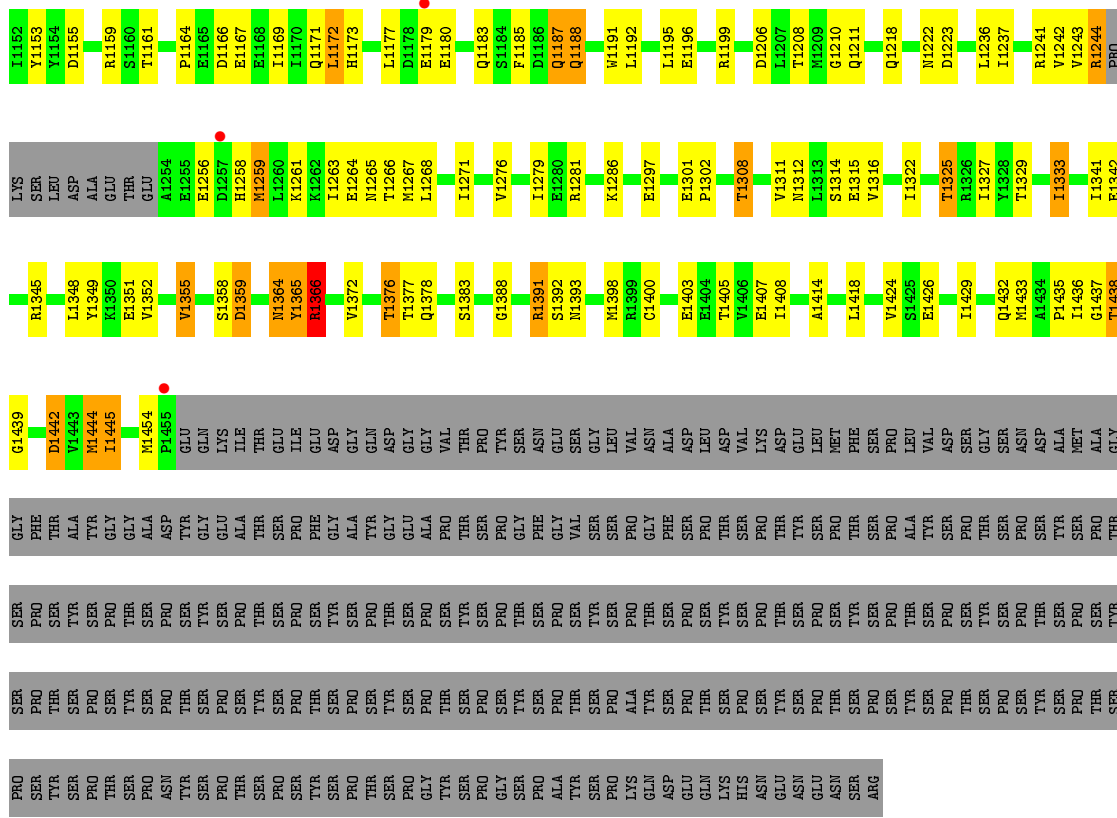
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	P	1	Total C N O P 31 11 5 12 3	0	0

3 Residue-property plots

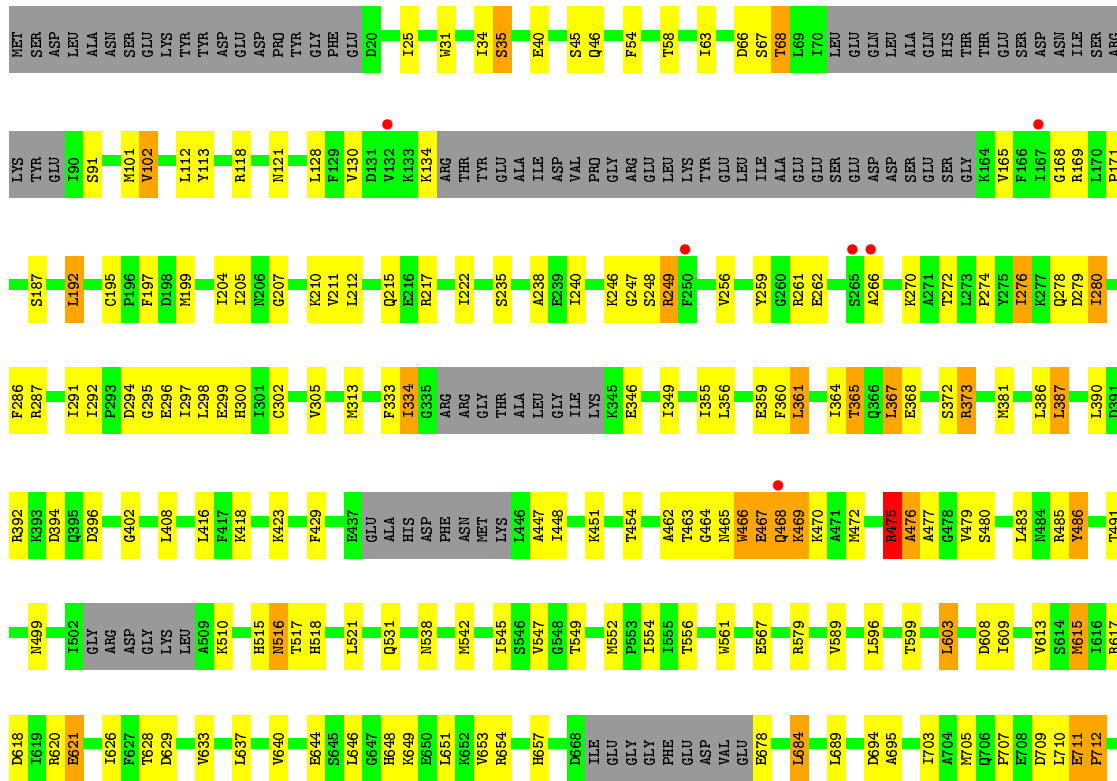
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

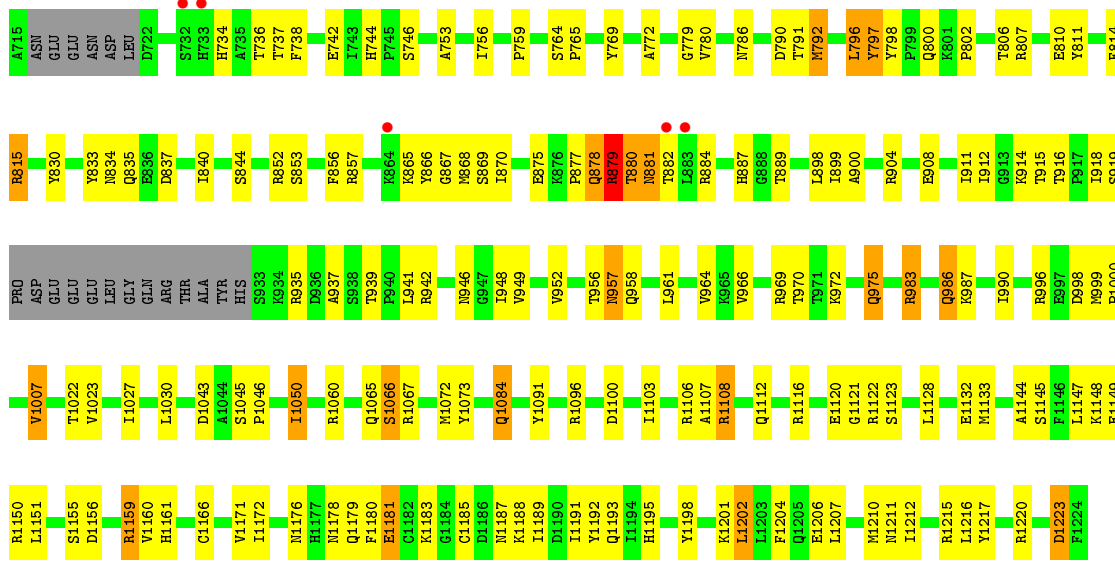
- Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



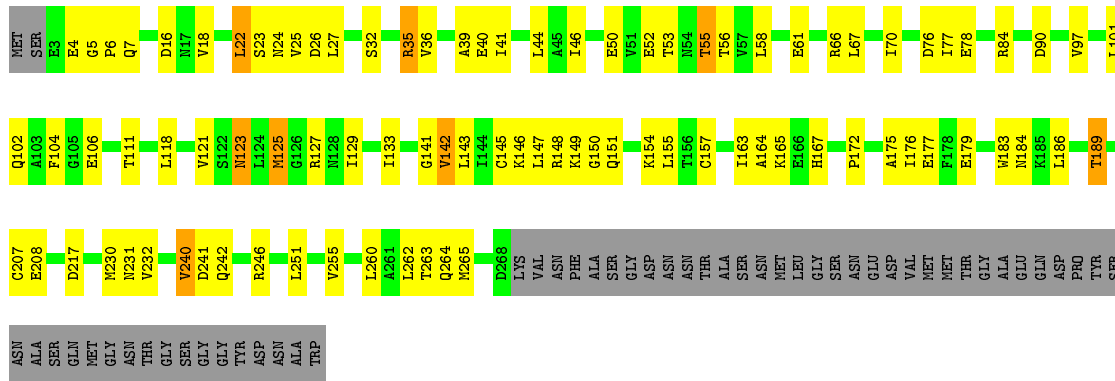


• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

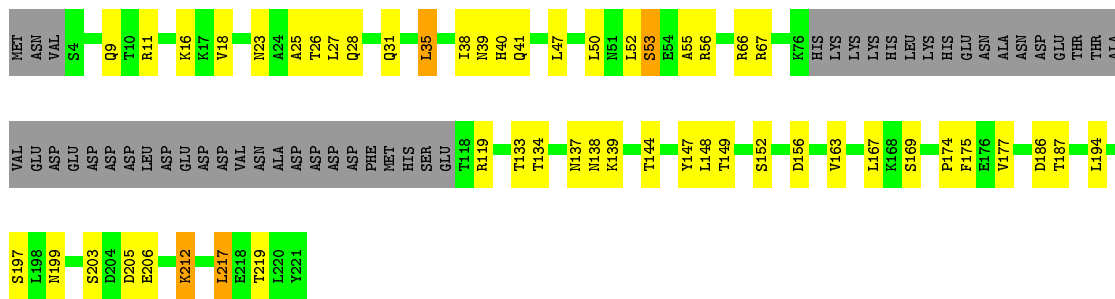




• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

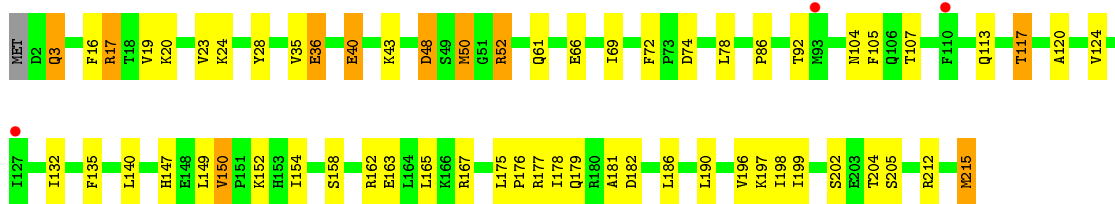


• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4



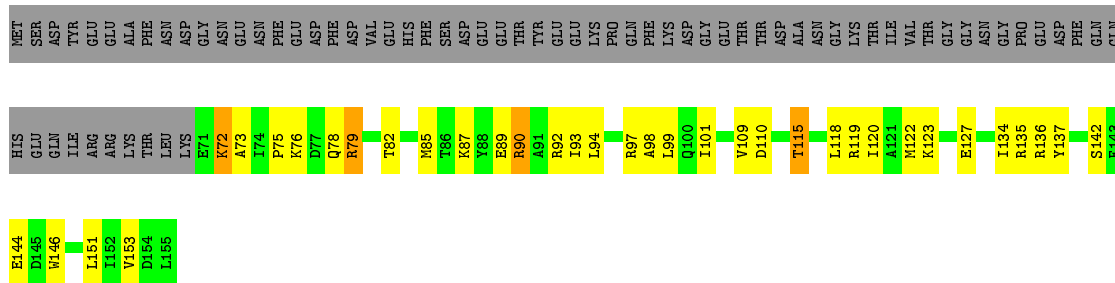
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1





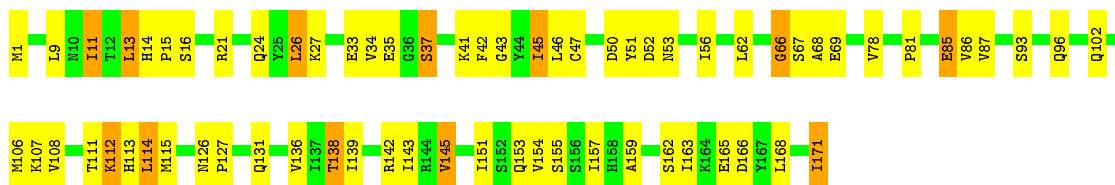
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F: 32% 21% 45%



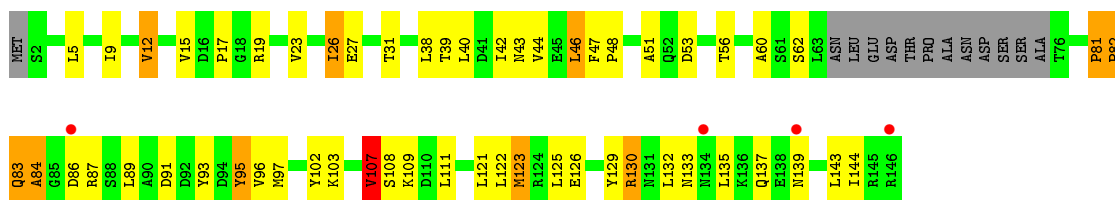
- Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G: 60% 33% 7%



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

Chain H: 3% 53% 31% 7% 9%

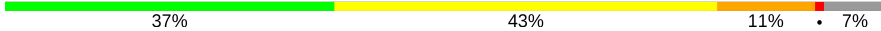


- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I: 3% 76% 19%



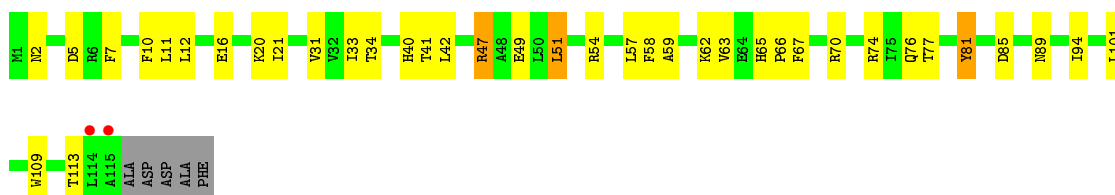
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:  37% 43% 11% 7%

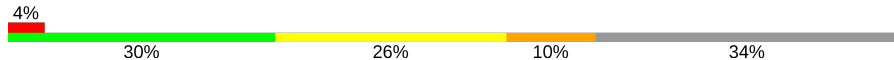


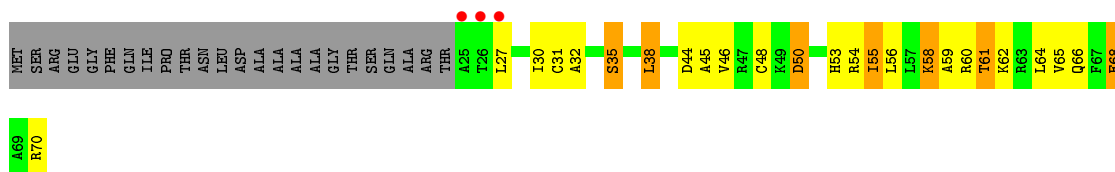
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:  2% 64% 29%



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

Chain L:  4% 30% 26% 10% 34%



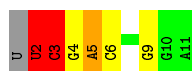
- Molecule 13: 5'-D(*AP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*TP)-3'

Chain N:  50% 21% 7% 21%



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

Chain P:  36% 27% 9% 18% 9%

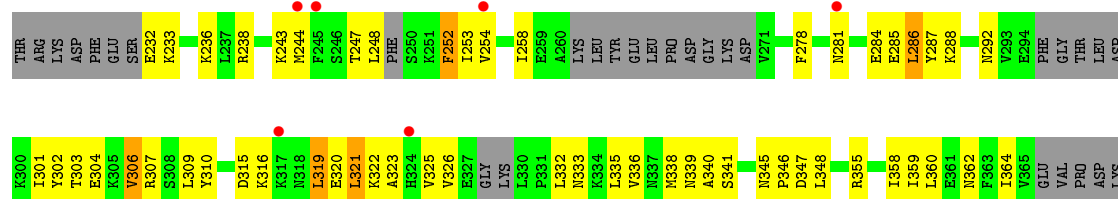
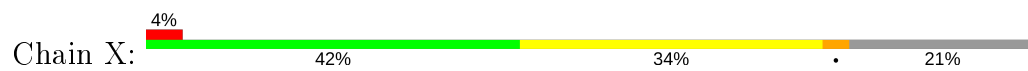


- Molecule 15: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP *TP*TP*CP*CP*BRUP*GP*GP*TP*CP*AP*AP*T)-3'

Chain T:  58% 27% 8% 8%



- 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) 100.0 (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)	Xtrriage
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	Xtrriage
Anisotropy	0.211	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 113.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
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	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/11431	0.81	9/15462 (0.1%)
2	B	0.50	0/8963	0.77	1/12085 (0.0%)
3	C	0.48	0/2133	0.75	0/2891
4	D	0.51	0/1365	0.80	2/1837 (0.1%)
5	E	0.49	0/1788	0.71	0/2406
6	F	0.58	0/700	0.80	0/945
7	G	0.50	0/1368	0.79	0/1844
8	H	0.48	0/1086	0.80	0/1470
9	I	0.47	0/989	0.72	0/1331
10	J	0.52	0/541	0.85	0/727
11	K	0.45	0/938	0.68	0/1267
12	L	0.59	0/365	0.97	0/485
13	N	1.09	0/257	1.07	1/395 (0.3%)
14	P	1.35	1/240 (0.4%)	1.04	1/372 (0.3%)
15	T	1.25	1/512 (0.2%)	1.06	0/783
16	X	0.54	0/963	0.77	0/1287
All	All	0.55	2/33639 (0.0%)	0.80	14/45587 (0.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	2	U	C3'-O3'	6.44	1.51	1.42
15	T	27	DA	C3'-O3'	5.33	1.50	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	HIS	N-CA-CB	7.16	123.48	110.60
1	A	56	PRO	C-N-CA	6.69	138.42	121.70
4	D	25	ALA	C-N-CA	5.76	136.11	121.70
1	A	3	GLY	C-N-CA	5.59	135.67	121.70
1	A	223	GLY	C-N-CA	5.46	135.35	121.70
1	A	331	GLY	N-CA-C	5.37	126.53	113.10
4	D	26	THR	N-CA-C	-5.31	96.66	111.00
14	P	2	U	P-O3'-C3'	5.20	125.94	119.70
13	N	6	DG	O4'-C1'-N9	5.18	111.62	108.00
1	A	57	ARG	C-N-CA	5.14	134.54	121.70
1	A	252	PHE	C-N-CA	5.08	134.40	121.70
2	B	880	THR	C-N-CA	5.08	134.39	121.70
1	A	310	GLY	C-N-CA	5.06	134.36	121.70
1	A	1063	MET	C-N-CA	5.06	134.35	121.70

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	284	0
2	B	8793	0	8824	166	0
3	C	2095	0	2051	49	0
4	D	1356	0	1319	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1752	0	1776	40	0
6	F	688	0	707	22	0
7	G	1340	0	1357	35	0
8	H	1068	0	1040	38	0
9	I	971	0	927	8	0
10	J	532	0	542	24	0
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	23	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	656	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 (656) 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:CG1	2:B:1172:ILE:CD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:H:95:TYR:HE1	8:H:97:MET:HG3	1.44	0.82
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.62	0.81
2:B:516:ASN:HD22	2:B:516:ASN:H	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: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:41:MET:HA	1:A:50:ILE:H	1.48	0.79
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.18	0.79
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.48	0.79
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.63	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
10:J:48:ARG:HE	10:J:49:MET:HE2	1.49	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:B:853:SER:HB3	2:B:972:LYS:HB2	1.79	0.64
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.62	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:H	3:C:46:ILE:HD12	1.64	0.62
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.81	0.62
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.82	0.62
1:A:754:SER:H	1:A:757:ASN:HD22	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1:MET:HE3	7:G:81:PRO:HA	1.85	0.58
1:A:34:LYS:HG3	1:A:36:ARG:HH21	1.68	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
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.05	0.56
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.39	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
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:106:MET:HG3	7:G:157:ILE:O	2.06	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
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
2:B:516:ASN:ND2	2:B:516:ASN:H	2.03	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:399:HIS:HB3	1:A:400:PRO:HD3	1.88	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:143:LEU:HG	10:J:2:ILE:HD11	1.88	0.55
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
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.90	0.54
1:A:35:ILE:HG13	1:A:56:PRO:HG2	1.90	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
1:A:63:ARG:H	1:A:74:MET:HE2	1.72	0.53
3:C:251:LEU:O	3:C:255:VAL:HG23	2.08	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
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.90	0.53
1:A:567:LYS:CB	8:H:95:TYR:HA	2.38	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
8:H:23:VAL:HG12	8:H:43:ASN:HA	1.91	0.53
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.90	0.52
1:A:225:ASN:ND2	1:A:228:PHE:H	2.00	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:182:VAL:HG22	1:A:201:VAL:HG22	1.91	0.51
1:A:42:ASP:HA	1:A:46:THR:O	2.10	0.51
1:A:687:LYS:HG2	1:A:794:PRO:HG2	1.92	0.51
1:A:68:GLN:OE1	1:A:70:CYS:HB3	2.10	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:313:MET:HE3	2:B:386:LEU:HD22	1.93	0.51
2:B:900:ALA:CB	12:L:61:THR:HG23	2.40	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:614:PHE:HB3	8:H:122:LEU:HD21	1.92	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
3:C:163:ILE:HD12	3:C:165:LYS:HB2	1.93	0.50
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.93	0.50
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.94	0.50
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
1:A:67:CYS:C	1:A:68:GLN:HG3	2.30	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
2:B:1185:CYS:C	2:B:1187:ASN:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:710:LEU:HD12	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:534:LEU:O	1:A:574:GLY:HA3	2.11	0.49
1:A:55:ASP:OD2	1:A:55:ASP:O	2.30	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:868:TYR:CD2	1:A:1058:VAL:HG21	2.48	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
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
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
1:A:738:LYS:HA	8:H:19:ARG:HH22	1.77	0.49
5:E:179:GLN:HE21	5:E:181:ALA:HB3	1.77	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:61:ILE:HG22	1:A:62:ASP:N	2.27	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
2:B:463:THR:C	2:B:465:ASN:H	2.17	0.49
5:E:197:LYS:HD3	5:E:199:ILE:HD11	1.95	0.49
1:A:1129:GLU:O	1:A:1133:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1256:GLU:HA	1:A:1259:MET:HB2	1.94	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
3:C:84:ARG:HD3	11:K:11:LEU:HD21	1.95	0.49
1:A:831:THR:O	1:A:834:THR:HG22	2.13	0.48
1:A:304:MET:HG2	2:B:1210:MET:HG2	1.95	0.48
1:A:1079:MET:HE3	1:A:1359:ASP:HB2	1.96	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
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
10:J:48:ARG:HE	10:J:49:MET:CE	2.23	0.48
16:X:326:VAL:HG13	16:X:332:LEU:HD11	1.96	0.48
1:A:1032:LEU:O	1:A:1036:ARG:HD2	2.14	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
3:C:148:ARG:HD3	3:C:149:LYS:HG3	1.96	0.48
3:C:55:THR:HB	3:C:151:GLN:HA	1.95	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:1084:GLN:OE1	3:C:189:THR:HG22	2.14	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
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:1244:ARG:HG3	1:A:1244:ARG:O	2.14	0.47
1:A:266:LEU:HA	1:A:269:ILE:HD12	1.96	0.47
2:B:259:TYR:CE1	2:B:270:LYS:HB2	2.49	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: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
1:A:77:CYS:SG	1:A:78:PRO:O	2.73	0.47
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:768:GLN:HB3	1:A:775:ILE:HD11	1.96	0.47
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.96	0.47
1:A:1116:LEU:HB2	1:A:1311:VAL:HG22	1.95	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
8:H:82:PRO:C	8:H:84:ALA:H	2.19	0.47
15:T:20:DC:H6	15:T:20:DC:H5''	1.80	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
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.97	0.47
1:A:464:PRO:HD2	11:K:67:PHE:HD2	1.79	0.47
1:A:335:ARG:HD3	2:B:1202:LEU:HD13	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
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
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.97	0.46
1:A:323:LYS:N	1:A:323:LYS:HE2	2.30	0.46
1:A:56:PRO:HD3	1:A:58:LEU:HG	1.96	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
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:512:VAL:HA	1:A:519:PRO:HA	1.98	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:1121:GLY:HA2	15:T:22:BRU:OP1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.85	0.46
5:E:178:ILE:HB	5:E:212:ARG:HD3	1.98	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:356:ASP:OD2	11:K:65:HIS:HE1	1.99	0.46
1:A:379:VAL:HG22	1:A:431:LYS:HG3	1.97	0.46
1:A:49:LYS:HZ3	1:A:61:ILE:N	2.13	0.46
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.15	0.46
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.97	0.46
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.51	0.46
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.97	0.46
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.97	0.46
1:A:787:PHE:CE2	1:A:796:SER:HA	2.51	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: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
1:A:503:GLN:NE2	6:F:90:ARG:HH21	2.14	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:168:GLY:HA2	2:B:454:THR:OG1	2.16	0.45
2:B:802:PRO:HD3	2:B:814:PHE:HE1	1.82	0.45
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:527:THR:HG21	1:A:650:GLN:HA	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.32	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
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:1444:MET:HE1	6:F:135:ARG:HB2	1.97	0.45
1:A:709:THR:HB	1:A:712:GLU:H	1.81	0.45
1:A:404:TYR:HE2	2:B:1108:ARG:HH22	1.64	0.45
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.52	0.45
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.99	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
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.97	0.44
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.99	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:1198:TYR:O	2:B:1201:LYS:HB3	2.17	0.44
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.99	0.44
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:993:LEU:HD23	1:A:1022:LEU:HD21	1.99	0.44
1:A:1079:MET:CE	1:A:1359:ASP:HB2	2.47	0.44
1:A:344:ARG:CZ	2:B:1120:GLU:HG3	2.48	0.44
1:A:49:LYS:NZ	1:A:60:SER:HA	2.32	0.44
1:A:754:SER:N	1:A:757:ASN:HD22	2.11	0.44
7:G:62:LEU:HD21	7:G:69:GLU:HB2	2.00	0.44
8:H:89:LEU:C	8:H:91:ASP:H	2.21	0.44
10:J:7:CYS:HA	10:J:49:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:35:ARG:HB2	11:K:41:THR:HG23	2.00	0.44
16:X:355:ARG:O	16:X:359:ILE:HG12	2.17	0.44
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.18	0.44
1:A:41:MET:HA	1:A:50:ILE:N	2.26	0.44
1:A:741:ASN:HB3	1:A:744:LYS:HB2	2.00	0.44
1:A:332:LYS:H	1:A:337:ARG:CB	2.31	0.44
1:A:17:VAL:HG22	2:B:1216:LEU:HD23	2.00	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
7:G:112:LYS:HA	7:G:115:MET:HE3	1.99	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:164:ALA:HA	3:C:167:HIS:O	2.18	0.43
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.17	0.43
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.00	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
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: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
3:C:44:LEU:HB2	3:C:77:ILE:HD13	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:1161:THR:HG21	1:A:1166:ASP:HB2	1.99	0.43
1:A:856:THR:HB	1:A:865:GLN:HB2	2.01	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:1116:LEU:HB3	1:A:1308:THR:OG1	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	6:F:97:ARG:HD2	1.81	0.43
16:X:278:PHE:HA	16:X:281:ASN:HB2	1.99	0.43
1:A:1172:LEU:HD12	16:X:310:TYR:CE2	2.54	0.43
1:A:337:ARG:HD3	2:B:1132:GLU:OE2	2.19	0.43
2:B:296:GLU:O	2:B:300:HIS:HD2	2.02	0.43
1:A:1444:MET:HE3	6:F:135:ARG:HB2	1.99	0.43
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.99	0.43
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.54	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:1151:GLU:HG2	9:I:45:ARG:HG3	2.01	0.43
1:A:34:LYS:HG3	1:A:36:ARG:NH2	2.33	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
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: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
1:A:71:GLN:HE22	2:B:1176:ASN:HB2	1.84	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:680:THR:HA	1:A:683:ILE:HD12	2.01	0.42
1:A:75:ASN:O	1:A:76:GLU:HB2	2.19	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
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:102:TYR:OH	8:H:122:LEU:HD22	2.18	0.42
8:H:42:ILE:HG23	8:H:95:TYR:HE2	1.85	0.42
1:A:302:THR:HA	1:A:305:ASP:O	2.20	0.42
4:D:167:LEU:HB3	4:D:177:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:LEU:HD11	4:D:174:PRO:HD2	2.01	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: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
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
6:F:101:ILE:HD13	6:F:120:ILE:HG22	2.02	0.42
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.88	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
3:C:67:LEU:HD11	3:C:155:LEU:HD13	2.02	0.42
1:A:1325:THR:HA	5:E:147:HIS:HA	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
2:B:165:VAL:HG11	2:B:448:ILE:HD13	2.02	0.42
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
8:H:135:LEU:C	8:H:137:GLN:H	2.22	0.42
15:T:27:DA:H2''	15:T:28:DT:O5'	2.19	0.42
1:A:705:LYS:HA	16:X:362:ASN:HA	2.02	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
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: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
3:C:22:LEU:HD13	3:C:230:MET:HE3	2.01	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:1345:ARG:HG2	1:A:1372:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ASN:O	1:A:474:VAL:HG12	2.20	0.41
1:A:53:LEU:O	1:A:54:ASN:C	2.59	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:1208:THR:HG22	1:A:1210:GLY:H	1.84	0.41
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.54	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: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:HG13	2:B:280:ILE:H	1.48	0.41
6:F:94:LEU:HD23	6:F:94:LEU:HA	1.89	0.41
7:G:13:LEU:HA	7:G:13:LEU:HD23	1.82	0.41
10:J:23:ASN:O	10:J:27:GLU:HB2	2.21	0.41
1:A:1109:LYS:HD2	1:A:1333:ILE:HD13	2.03	0.41
1:A:446:ARG:HB2	1:A:487:MET:SD	2.61	0.41
1:A:591:PHE:HA	1:A:595:THR:HB	2.03	0.41
1:A:596:THR:C	1:A:598:LEU:H	2.22	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:1017:LEU:O	1:A:1020:CYS:HB2	2.21	0.41
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.21	0.41
3:C:184:ASN:HD21	3:C:189:THR:H	1.67	0.41
3:C:6:PRO:HA	3:C:24:ASN:HB3	2.02	0.41
4:D:56:ARG:HB2	4:D:148:LEU:HD22	2.01	0.41
1:A:1327:ILE:O	5:E:147:HIS:HE1	2.02	0.41
10:J:36:LEU:HD23	10:J:41:LEU:HD13	2.02	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
2:B:361:LEU:HD11	2:B:381:MET:HE1	2.02	0.41
2:B:618:ASP:OD1	2:B:621:GLU:HB2	2.21	0.41
7:G:102:GLN:HE22	7:G:107:LYS:HE2	1.85	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:705:MET:N	2:B:710:LEU:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:GLU:HA	1:A:1236:LEU:O	2.20	0.41
1:A:376:TYR:CE1	1:A:498:ARG:HD2	2.56	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:1333:ILE:H	1:A:1333:ILE:HG13	1.62	0.40
1:A:134:ARG:HD2	1:A:221:SER:O	2.21	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:HA	2:B:387:LEU:HD12	1.91	0.40
5:E:135:PHE:HB3	5:E:140:LEU:CD1	2.48	0.40
5:E:17:ARG:O	5:E:20:LYS:HB2	2.22	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
2:B:313:MET:HE2	2:B:390:LEU:HG	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
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%)	3	27
2	B	1086/1224 (89%)	949 (87%)	99 (9%)	38 (4%)	3	30
3	C	264/318 (83%)	229 (87%)	31 (12%)	4 (2%)	10	47
4	D	173/221 (78%)	155 (90%)	11 (6%)	7 (4%)	3	26
5	E	212/215 (99%)	199 (94%)	11 (5%)	2 (1%)	17	57
6	F	83/155 (54%)	75 (90%)	7 (8%)	1 (1%)	13	51
7	G	169/171 (99%)	153 (90%)	14 (8%)	2 (1%)	13	51
8	H	129/146 (88%)	102 (79%)	18 (14%)	9 (7%)	1	14
9	I	117/122 (96%)	93 (80%)	23 (20%)	1 (1%)	17	57
10	J	63/70 (90%)	51 (81%)	6 (10%)	6 (10%)	0	8
11	K	113/120 (94%)	106 (94%)	6 (5%)	1 (1%)	17	57
12	L	44/70 (63%)	33 (75%)	3 (7%)	8 (18%)	0	2
16	X	106/146 (73%)	90 (85%)	9 (8%)	7 (7%)	1	16
All	All	3978/4711 (84%)	3458 (87%)	380 (10%)	140 (4%)	3	30

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [i](#)

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%)	1042 (83%)	207 (17%)	2	15
2	B	960/1061 (90%)	827 (86%)	133 (14%)	3	22
3	C	234/274 (85%)	205 (88%)	29 (12%)	4	26
4	D	140/200 (70%)	123 (88%)	17 (12%)	5	26
5	E	196/197 (100%)	176 (90%)	20 (10%)	7	34
6	F	75/137 (55%)	64 (85%)	11 (15%)	3	20
7	G	152/152 (100%)	130 (86%)	22 (14%)	3	20
8	H	117/128 (91%)	100 (86%)	17 (14%)	3	20
9	I	113/116 (97%)	98 (87%)	15 (13%)	4	23
10	J	60/65 (92%)	46 (77%)	14 (23%)	1	5
11	K	99/102 (97%)	87 (88%)	12 (12%)	5	26
12	L	40/57 (70%)	28 (70%)	12 (30%)	0	2
16	X	107/136 (79%)	88 (82%)	19 (18%)	2	11
All	All	3542/4145 (86%)	3014 (85%)	528 (15%)	3	19

All (528) 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	22	PHE
1	A	30	ILE
1	A	34	LYS
1	A	36	ARG
1	A	41	MET
1	A	42	ASP
1	A	62	ASP
1	A	63	ARG
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS
1	A	76	GLU
1	A	77	CYS
1	A	93	VAL

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Mol	Chain	Res	Type
1	A	96	ILE
1	A	107	CYS
1	A	114	LEU
1	A	117	GLU
1	A	120	GLU
1	A	132	LYS
1	A	145	LYS
1	A	146	MET
1	A	149	GLU
1	A	151	ASP
1	A	156	ASP
1	A	157	ASP
1	A	159	THR
1	A	173	THR
1	A	196	GLU
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	252	PHE
1	A	254	GLU
1	A	261	ASP
1	A	265	LYS
1	A	282	ASN
1	A	286	HIS
1	A	302	THR
1	A	303	TYR
1	A	316	GLN
1	A	320	ARG
1	A	323	LYS
1	A	329	LEU
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	369	SER
1	A	373	THR
1	A	375	THR

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Mol	Chain	Res	Type
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	445	ASN
1	A	449	SER
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	461	LYS
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	518	LYS
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	640	GLN
1	A	645	LEU
1	A	651	LYS
1	A	666	ILE

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Mol	Chain	Res	Type
1	A	680	THR
1	A	691	LEU
1	A	702	LEU
1	A	705	LYS
1	A	706	HIS
1	A	710	LEU
1	A	720	ARG
1	A	734	GLU
1	A	738	LYS
1	A	756	ILE
1	A	762	SER
1	A	764	CYS
1	A	768	GLN
1	A	773	LYS
1	A	774	ARG
1	A	788	SER
1	A	821	ARG
1	A	822	GLU
1	A	826	ASP
1	A	834	THR
1	A	839	ARG
1	A	858	ASN
1	A	867	ILE
1	A	878	ILE
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	969	GLN
1	A	976	THR
1	A	980	ASP
1	A	982	THR
1	A	1001	ARG
1	A	1009	ASN
1	A	1013	ASP
1	A	1024	SER

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Mol	Chain	Res	Type
1	A	1029	ARG
1	A	1038	THR
1	A	1062	GLU
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	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	1187	GLN
1	A	1195	LEU
1	A	1199	ARG
1	A	1218	GLN
1	A	1222	ASN
1	A	1223	ASP
1	A	1237	ILE
1	A	1242	VAL
1	A	1244	ARG
1	A	1259	MET
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	1297	GLU
1	A	1301	GLU
1	A	1308	THR
1	A	1314	SER
1	A	1315	GLU
1	A	1322	ILE
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE

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Mol	Chain	Res	Type
1	A	1341	ILE
1	A	1355	VAL
1	A	1358	SER
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1376	THR
1	A	1383	SER
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1407	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	1454	MET
2	B	25	ILE
2	B	35	SER
2	B	40	GLU
2	B	46	GLN
2	B	63	ILE
2	B	66	ASP
2	B	101	MET
2	B	102	VAL
2	B	128	LEU
2	B	130	VAL
2	B	134	LYS
2	B	169	ARG
2	B	192	LEU
2	B	199	MET
2	B	217	ARG
2	B	222	ILE
2	B	240	ILE
2	B	262	GLU
2	B	272	THR
2	B	276	ILE
2	B	278	GLN

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Mol	Chain	Res	Type
2	B	279	ASP
2	B	280	ILE
2	B	294	ASP
2	B	299	GLU
2	B	302	CYS
2	B	305	VAL
2	B	361	LEU
2	B	365	THR
2	B	372	SER
2	B	373	ARG
2	B	387	LEU
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	472	MET
2	B	475	ARG
2	B	485	ARG
2	B	486	TYR
2	B	510	LYS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	554	ILE
2	B	556	THR
2	B	561	TRP
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

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Mol	Chain	Res	Type
2	B	644	GLU
2	B	646	LEU
2	B	653	VAL
2	B	678	GLU
2	B	684	LEU
2	B	694	ASP
2	B	709	ASP
2	B	734	HIS
2	B	736	THR
2	B	742	GLU
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	796	LEU
2	B	797	TYR
2	B	806	THR
2	B	815	ARG
2	B	830	TYR
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	887	HIS
2	B	889	THR
2	B	908	GLU
2	B	915	THR
2	B	916	THR
2	B	942	ARG
2	B	946	ASN
2	B	956	THR
2	B	957	ASN
2	B	958	GLN
2	B	970	THR
2	B	975	GLN
2	B	983	ARG
2	B	986	GLN
2	B	998	ASP
2	B	1007	VAL
2	B	1045	SER
2	B	1050	ILE

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Mol	Chain	Res	Type
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
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	1178	ASN
2	B	1179	GLN
2	B	1183	LYS
2	B	1189	ILE
2	B	1195	HIS
2	B	1202	LEU
2	B	1211	ASN
2	B	1212	ILE
2	B	1220	ARG
2	B	1223	ASP
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	35	ARG
3	C	40	GLU
3	C	53	THR
3	C	55	THR
3	C	56	THR
3	C	76	ASP
3	C	78	GLU
3	C	102	GLN

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Mol	Chain	Res	Type
3	C	106	GLU
3	C	111	THR
3	C	121	VAL
3	C	123	ASN
3	C	125	MET
3	C	127	ARG
3	C	133	ILE
3	C	186	LEU
3	C	189	THR
3	C	208	GLU
3	C	217	ASP
3	C	240	VAL
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	67	ARG
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	149	THR
4	D	156	ASP
4	D	187	THR
4	D	203	SER
4	D	205	ASP
4	D	206	GLU
4	D	212	LYS
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	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	104	ASN
5	E	107	THR
5	E	117	THR
5	E	150	VAL
5	E	165	LEU
5	E	175	LEU
5	E	190	LEU
5	E	202	SER
5	E	215	MET
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	87	LYS
6	F	90	ARG
6	F	92	ARG
6	F	109	VAL
6	F	115	THR
6	F	119	ARG
6	F	127	GLU
6	F	153	VAL
7	G	11	ILE
7	G	13	LEU
7	G	26	LEU
7	G	33	GLU
7	G	37	SER
7	G	45	ILE
7	G	47	CYS
7	G	52	ASP
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
7	G	143	ILE
7	G	145	VAL
7	G	151	ILE
7	G	153	GLN
7	G	155	SER
7	G	166	ASP

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Mol	Chain	Res	Type
7	G	171	ILE
8	H	12	VAL
8	H	26	ILE
8	H	27	GLU
8	H	31	THR
8	H	46	LEU
8	H	62	SER
8	H	83	GLN
8	H	86	ASP
8	H	95	TYR
8	H	103	LYS
8	H	107	VAL
8	H	109	LYS
8	H	111	LEU
8	H	123	MET
8	H	129	TYR
8	H	130	ARG
8	H	132	LEU
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	107	SER
9	I	108	HIS
10	J	2	ILE
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	23	ASN
10	J	26	GLN

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Mol	Chain	Res	Type
10	J	32	GLU
10	J	43	ARG
10	J	48	ARG
10	J	52	THR
10	J	54	VAL
11	K	31	VAL
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	54	ARG
11	K	62	LYS
11	K	74	ARG
11	K	81	TYR
11	K	85	ASP
11	K	89	ASN
11	K	101	LEU
11	K	113	THR
12	L	27	LEU
12	L	30	ILE
12	L	38	LEU
12	L	44	ASP
12	L	46	VAL
12	L	50	ASP
12	L	54	ARG
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	244	MET
16	X	247	THR
16	X	252	PHE
16	X	253	ILE
16	X	284	GLU
16	X	286	LEU
16	X	292	ASN
16	X	303	THR
16	X	306	VAL
16	X	319	LEU
16	X	321	LEU

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Mol	Chain	Res	Type
16	X	333	ASN
16	X	335	LEU
16	X	347	ASP
16	X	358	ILE
16	X	360	LEU
16	X	364	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	71	GLN
1	A	75	ASN
1	A	92	HIS
1	A	169	ASN
1	A	225	ASN
1	A	253	ASN
1	A	256	GLN
1	A	281	HIS
1	A	282	ASN
1	A	316	GLN
1	A	339	ASN
1	A	358	ASN
1	A	503	GLN
1	A	517	ASN
1	A	548	ASN
1	A	603	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	858	ASN
1	A	903	ASN
1	A	965	GLN
1	A	994	GLN
1	A	1270	ASN
1	A	1312	ASN
1	A	1364	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	215	GLN
2	B	300	HIS

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Mol	Chain	Res	Type
2	B	357	GLN
2	B	366	GLN
2	B	383	ASN
2	B	395	GLN
2	B	468	GLN
2	B	515	HIS
2	B	516	ASN
2	B	590	HIS
2	B	657	HIS
2	B	744	HIS
2	B	957	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1025	HIS
2	B	1161	HIS
2	B	1176	ASN
2	B	1177	HIS
3	C	7	GLN
3	C	73	GLN
3	C	102	GLN
3	C	112	ASN
3	C	123	ASN
3	C	203	GLN
3	C	242	GLN
3	C	264	GLN
4	D	23	ASN
4	D	37	GLN
4	D	39	ASN
4	D	173	HIS
5	E	136	ASN
5	E	147	HIS
5	E	179	GLN
7	G	14	HIS
7	G	102	GLN
7	G	131	GLN
7	G	153	GLN
8	H	133	ASN
9	I	12	ASN
10	J	26	GLN
11	K	65	HIS
16	X	312	ASN
16	X	345	ASN

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Mol	Chain	Res	Type
16	X	362	ASN

5.3.3 RNA [i](#)

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 [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	BRU	T	22	15,14	15,21,22	2.02	2 (13%)	17,30,33	2.21	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BRU	T	22	15,14	-	0/4/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C4-C5	6.92	1.47	1.38
15	T	22	BRU	C2-N3	-2.60	1.33	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C4-N3-C2	7.40	121.39	115.14
15	T	22	BRU	C5-C4-N3	-4.22	118.59	123.64
15	T	22	BRU	C2'-C1'-N1	-2.09	109.46	114.27

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 carbohydrates 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	27,33,33	1.74	7 (25%)	31,52,52	1.44	5 (16%)

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	-	6/15/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	12	APC	PA-O1A	4.37	1.62	1.51
19	P	12	APC	PA-O2A	-3.29	1.48	1.56
19	P	12	APC	PB-O3B	3.27	1.62	1.58
19	P	12	APC	PA-O5'	2.93	1.61	1.57
19	P	12	APC	C5-C4	2.61	1.47	1.40
19	P	12	APC	PB-O2B	2.23	1.61	1.56
19	P	12	APC	C2-N3	2.08	1.35	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	P	12	APC	C4-C5-N7	-4.27	104.95	109.40
19	P	12	APC	N3-C2-N1	-3.49	123.23	128.68
19	P	12	APC	PG-O3B-PB	-2.45	123.99	132.62
19	P	12	APC	C5-C6-N6	2.27	123.80	120.35
19	P	12	APC	C3'-C2'-C1'	2.07	104.09	100.98

There are no chirality outliers.

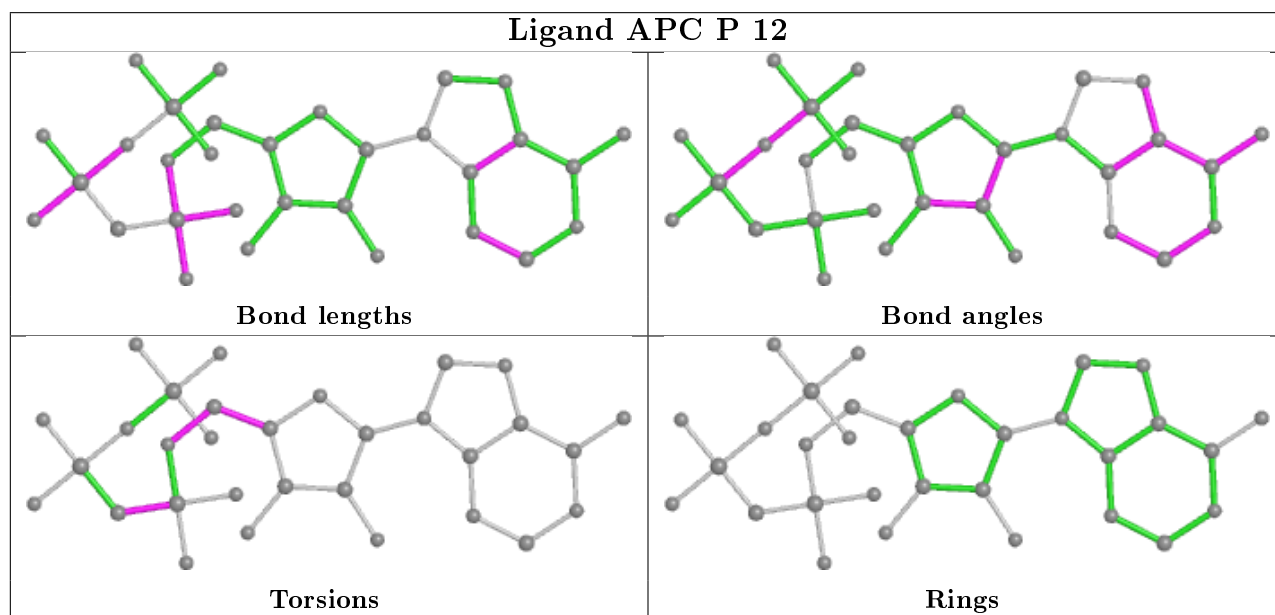
All (6) torsion outliers are listed below:

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 [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

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 i

6.1 Protein, DNA and RNA chains i

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%)	-0.24	6 (0%) 92 86	58, 108, 175, 232	0
2	B	1106/1224 (90%)	-0.19	11 (0%) 82 70	65, 120, 181, 216	0
3	C	266/318 (83%)	-0.30	0 100 100	81, 109, 151, 180	0
4	D	177/221 (80%)	-0.24	0 100 100	85, 123, 173, 199	0
5	E	214/215 (99%)	-0.16	3 (1%) 75 61	83, 139, 189, 210	0
6	F	85/155 (54%)	-0.40	0 100 100	68, 91, 124, 144	0
7	G	171/171 (100%)	-0.08	0 100 100	79, 108, 151, 169	0
8	H	133/146 (91%)	0.23	4 (3%) 50 34	118, 153, 189, 226	0
9	I	119/122 (97%)	0.04	4 (3%) 45 30	117, 159, 198, 220	0
10	J	65/70 (92%)	-0.43	0 100 100	88, 105, 148, 160	0
11	K	115/120 (95%)	-0.24	2 (1%) 70 55	77, 106, 155, 173	0
12	L	46/70 (65%)	0.56	3 (6%) 18 11	105, 175, 195, 205	0
13	N	11/14 (78%)	-0.16	0 100 100	176, 194, 264, 267	0
14	P	10/11 (90%)	-0.32	0 100 100	85, 113, 169, 174	0
15	T	23/26 (88%)	-0.15	0 100 100	83, 148, 246, 258	0
16	X	116/146 (79%)	0.35	6 (5%) 27 17	163, 195, 212, 220	0
All	All	4084/4762 (85%)	-0.18	39 (0%) 82 70	58, 118, 189, 267	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	6.0
8	H	86	ASP	4.4
12	L	25	ALA	4.4
11	K	115	ALA	4.0
12	L	26	THR	3.9

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Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	3.5
1	A	69	THR	3.4
9	I	119	THR	3.3
2	B	250	PHE	3.3
5	E	110	PHE	3.2
11	K	114	LEU	3.0
9	I	117	LYS	2.9
2	B	265	SER	2.8
2	B	883	LEU	2.6
8	H	134	ASN	2.5
16	X	317	LYS	2.5
2	B	167	ILE	2.5
8	H	146	ARG	2.4
2	B	732	SER	2.4
2	B	266	ALA	2.4
16	X	244	MET	2.4
16	X	324	HIS	2.3
5	E	93	MET	2.3
1	A	1455	PRO	2.3
1	A	1257	ASP	2.2
2	B	864	LYS	2.2
16	X	254	VAL	2.2
16	X	245	PHE	2.2
2	B	733	HIS	2.2
8	H	139	ASN	2.2
1	A	257	ARG	2.1
5	E	127	ILE	2.1
2	B	468	GLN	2.1
9	I	25	LEU	2.1
1	A	1179	GLU	2.0
16	X	281	ASN	2.0
1	A	255	SER	2.0
2	B	132	VAL	2.0
9	I	118	ARG	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(\AA^2)	Q<0.9
15	BRU	T	22	20/21	0.96	0.17	87,97,123,144	0

6.3 Carbohydrates [i](#)

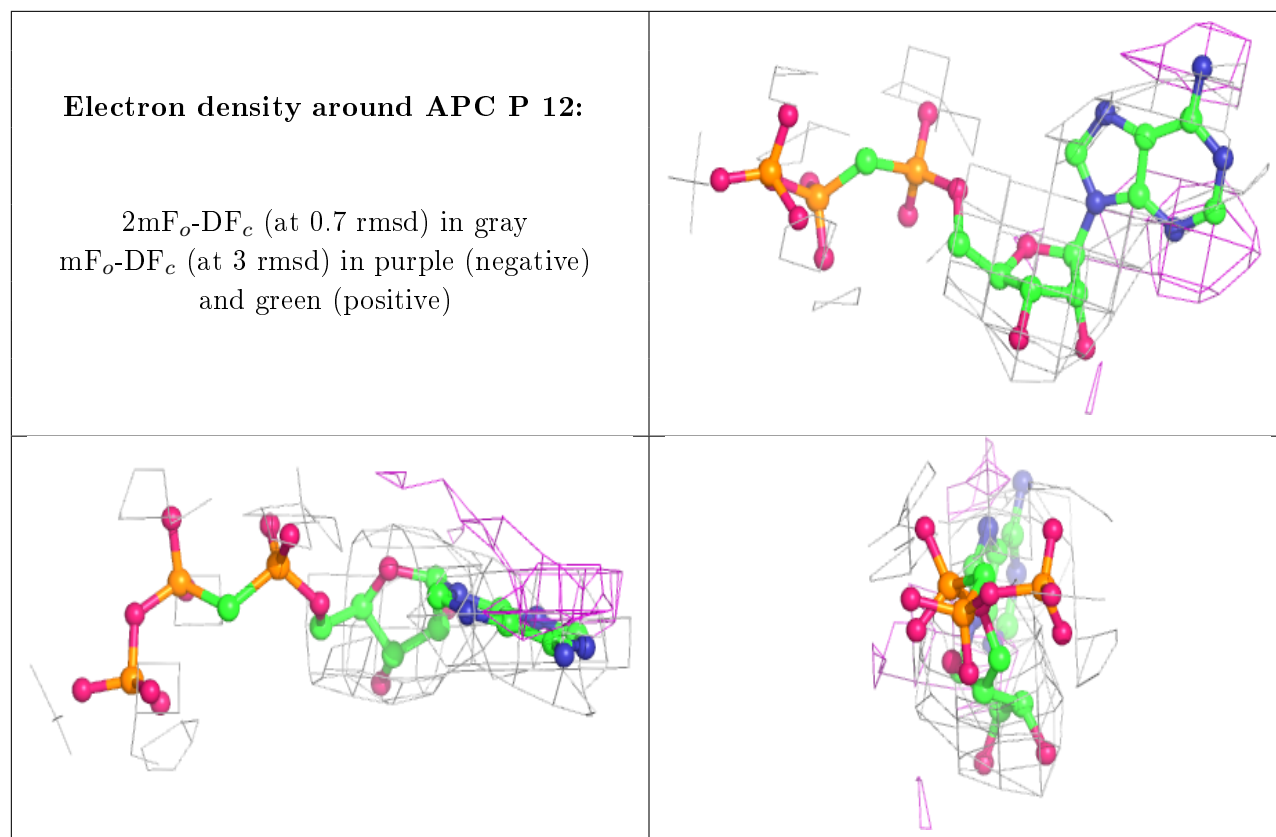
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
19	APC	P	12	31/31	0.83	0.28	102,118,169,170	0
17	ZN	I	1122	1/1	0.94	0.04	234,234,234,234	0
18	MG	A	2458	1/1	0.99	0.12	58,58,58,58	0
17	ZN	C	1269	1/1	0.99	0.11	92,92,92,92	0
17	ZN	I	1121	1/1	0.99	0.11	129,129,129,129	0
17	ZN	L	1071	1/1	0.99	0.04	192,192,192,192	0
17	ZN	A	2457	1/1	0.99	0.16	77,77,77,77	0
17	ZN	A	2456	1/1	0.99	0.06	128,128,128,128	0
17	ZN	J	1066	1/1	1.00	0.20	85,85,85,85	0
17	ZN	B	2225	1/1	1.00	0.18	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.