Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 04:16 PM EDT

PDB ID	:	7RIP
Title	:	RNA polymerase II elongation complex with hairpin polyamide Py-Im 1, scaffold 1 soaked with CTP
Authors	:	Oh, J.; Dervan, P.B.; Wang, D.
Deposited on	:	2021-07-20
Resolution	:	3.30 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:

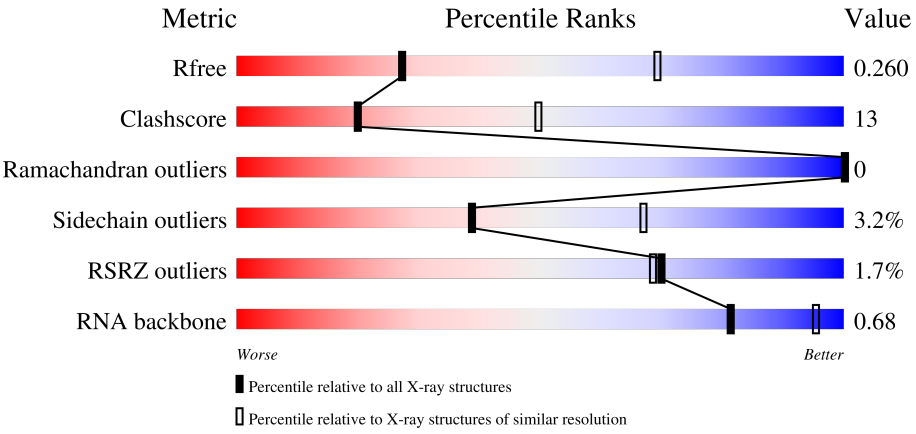
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	R	10	70% 30%
2	T	30	3% 27% 60% 13%
3	N	20	40% 30% 30%
4	A	1733	% 54% 24% · 20%

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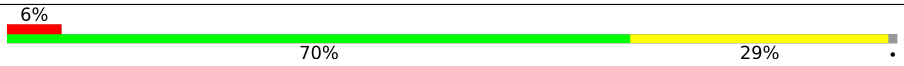
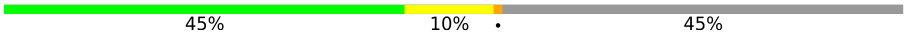
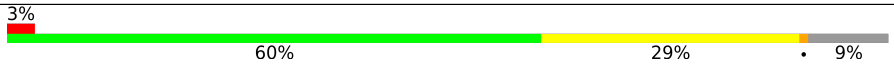
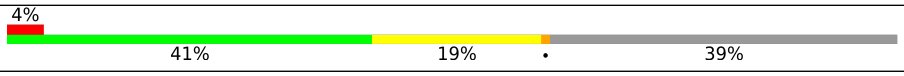
Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 29193 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			215	97	43	66	9			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	26	Total	C	N	O	P	0	0	0
			525	252	84	163	26			

- Molecule 3 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	14	Total	C	N	O	P	0	0	0
			293	138	63	78	14			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1384	Total	C	N	O	S	0	0	0
			10824	6829	1895	2040	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1129	Total	C	N	O	S	0	0	0
			8899	5630	1561	1655	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	212	Total	C	N	O	S	0	0	0
			1731	1100	305	315	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1064	670	179	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			952	585	173	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

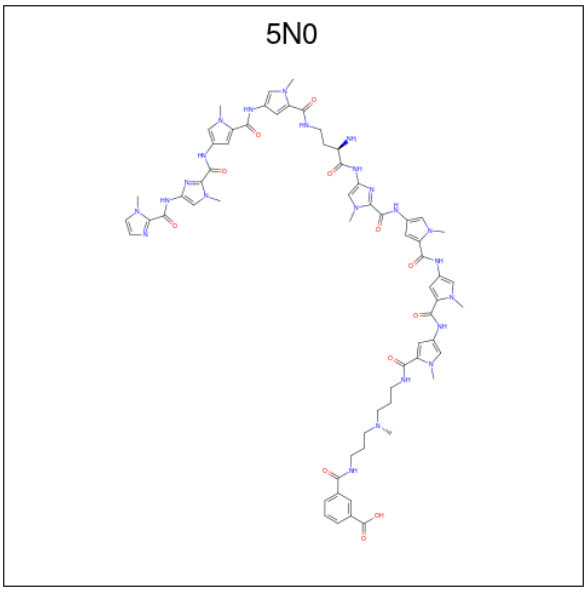
- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	R	1	Total Mg 1 1	0	0

- Molecule 15 is 3-({3-[(3-{[4-({4-[(4-{[4-({(2R)-2-amino-4-[(1-methyl-4-{[1-methyl-4-({1-methyl-4-[(1-methyl-1H-imidazole-2-carbonyl)amino]-1H-imidazole-2-carbonyl}amino)-1H-pyrrole-2-carbonyl]amino}-1H-pyrrole-2-carbonyl)amino]butanoyl}amino)-1-methyl-1H-imidazole-2-carbonyl]amino}-1-methyl-1H-pyrrole-2-carbonyl)amino]-1-methyl-1H-pyrrole-2-carbonyl}amino)-1-methyl-1H-pyrrole-2-carbonyl]amino}propyl)(methyl)amino]propyl}carbamoyl)benzoic acid (three-letter code: 5N0) (formula: $C_{64}H_{75}N_{23}O_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	T	1	Total C N O 99 64 23 12	0	0

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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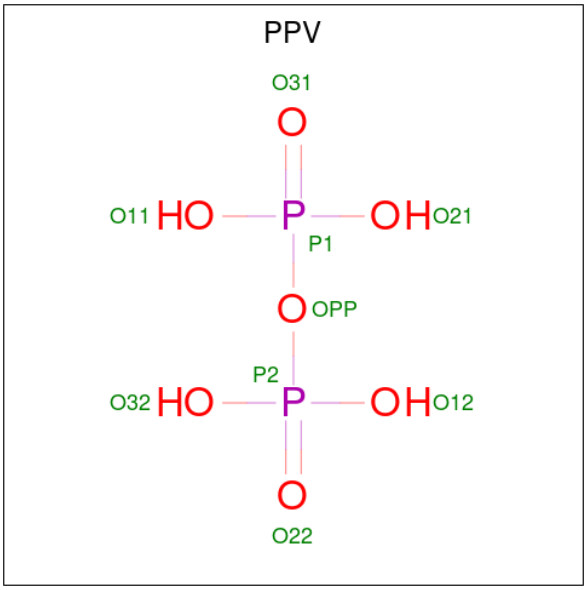
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	L	1	Total Zn 1 1	0	0

- Molecule 17 is PYROPHOSPHATE (three-letter code: PPV) (formula: $H_4O_7P_2$).



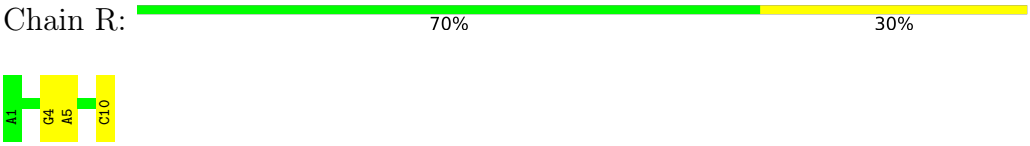
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	1	Total O P 9 7 2	0	0

3 Residue-property plots (i)

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

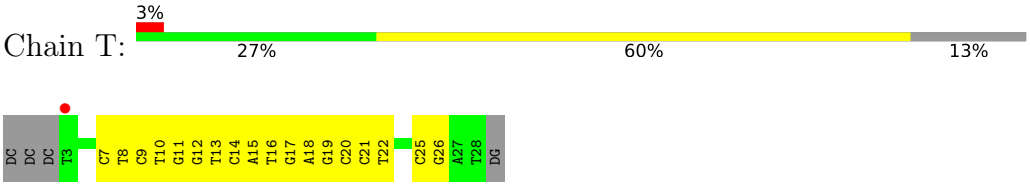
• Molecule 1: RNA

Chain R:



• Molecule 2: Template strand DNA

Chain T:

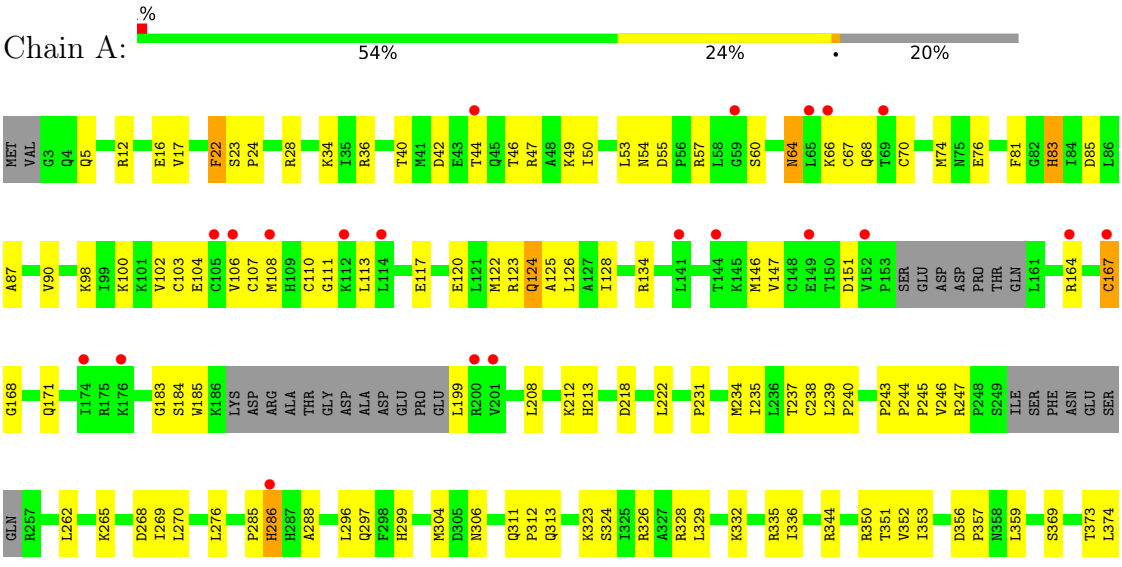


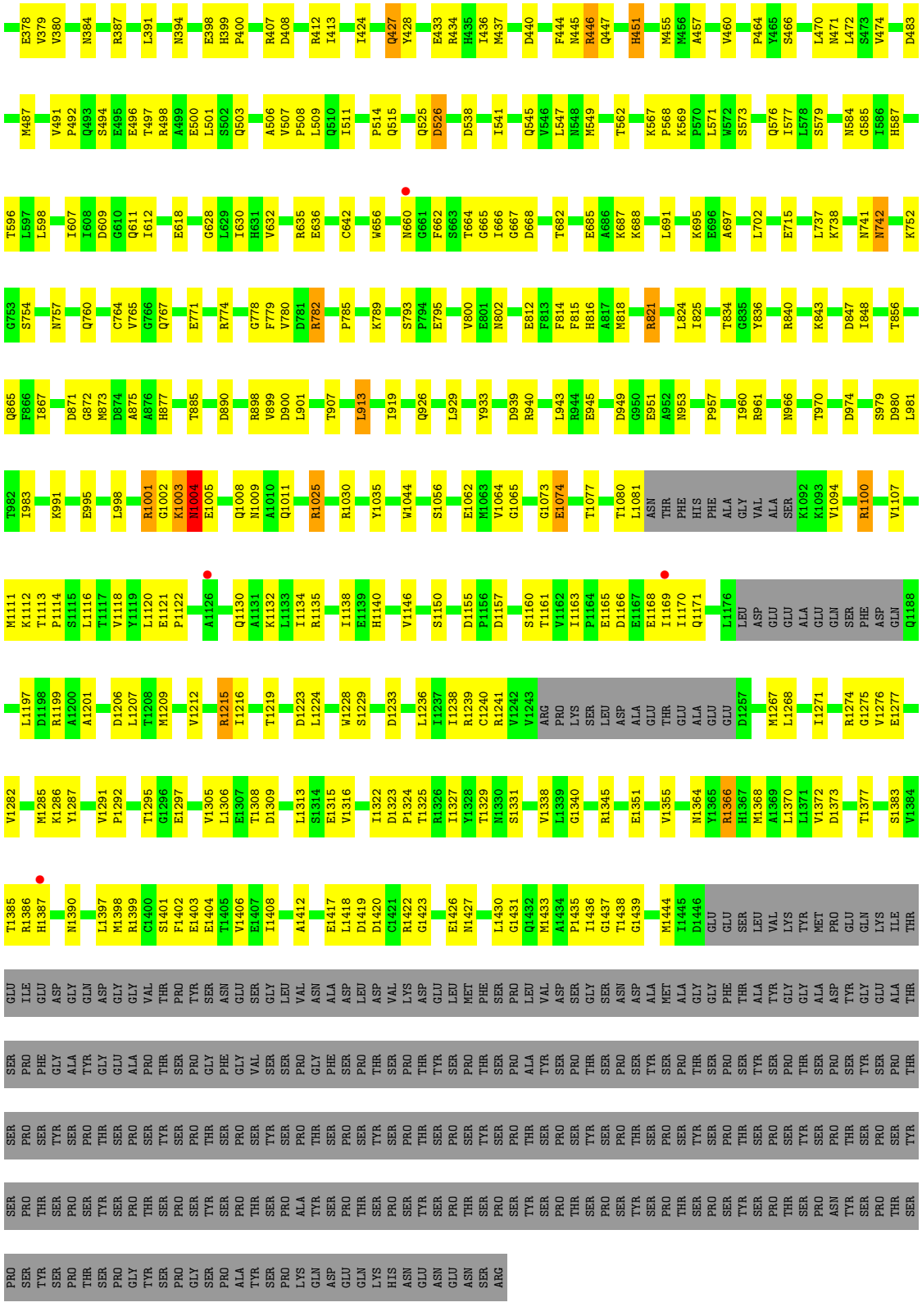
• Molecule 3: Non-template strand DNA

Chain N:

• Molecule 4: DNA-directed RNA polymerase II subunit RPB1

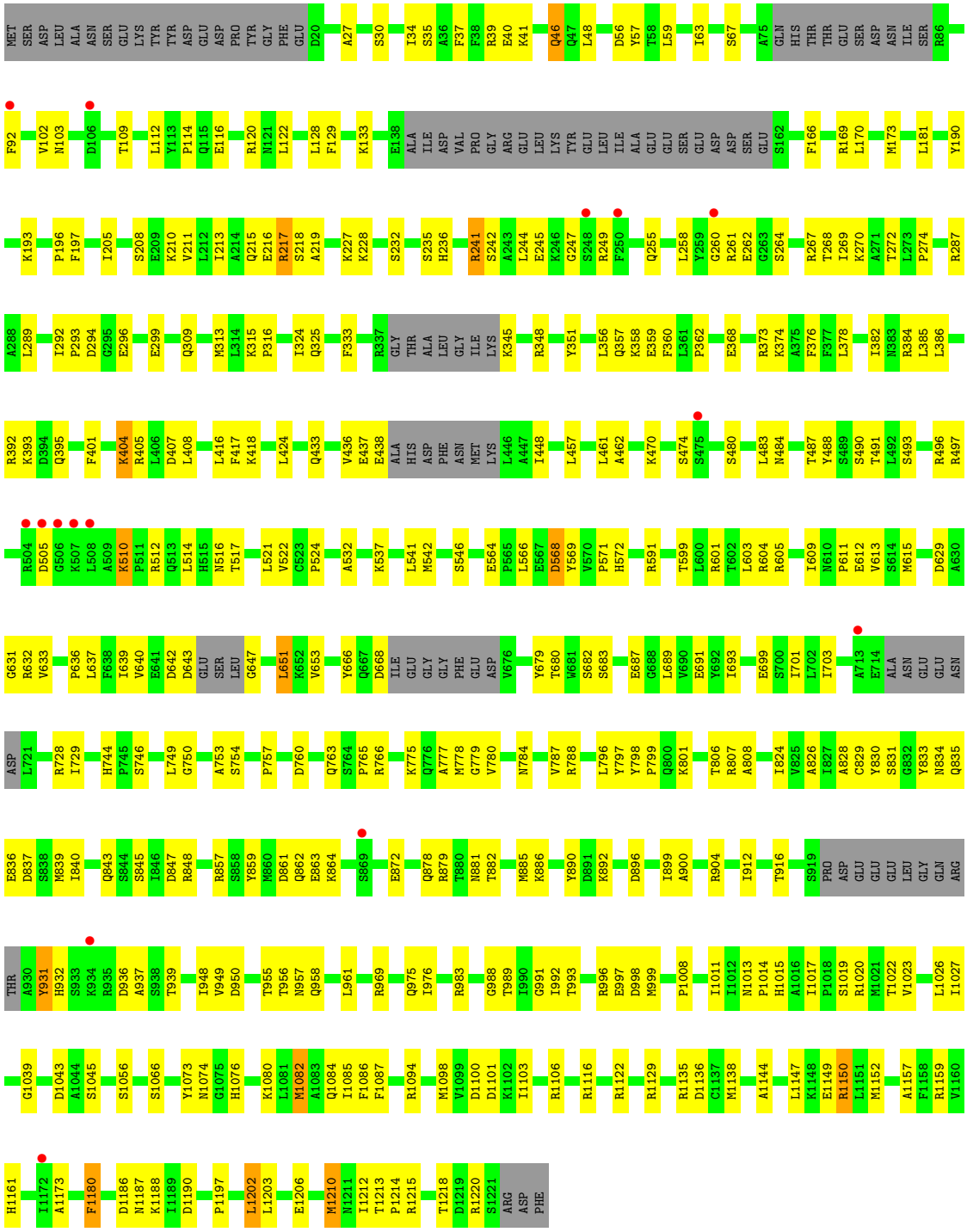
Chain A:





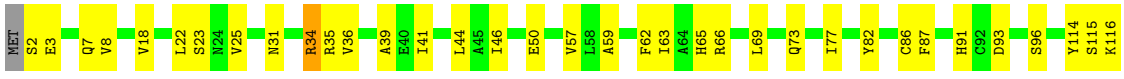
• Molecule 5: DNA-directed RNA polymerase II subunit RPB2

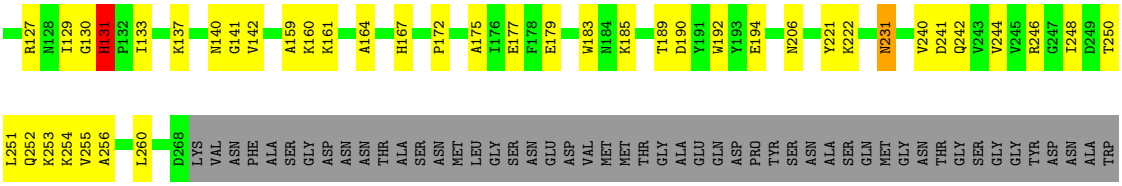
Chain B:



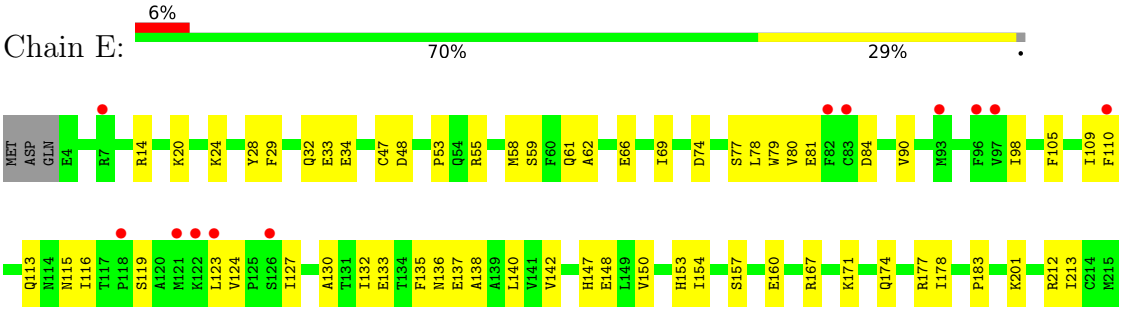
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

Chain C:

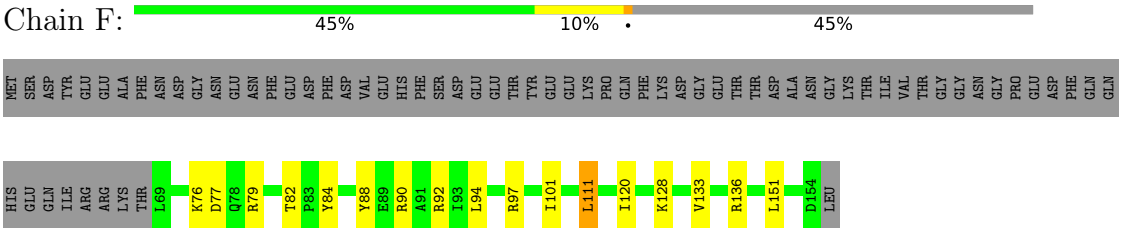




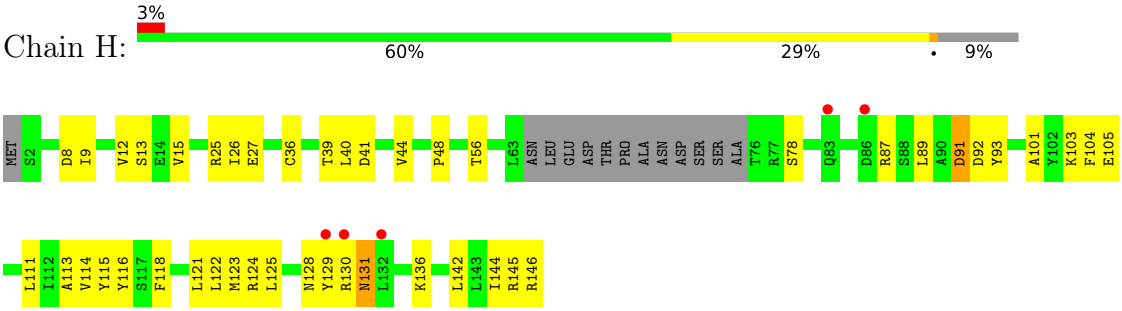
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



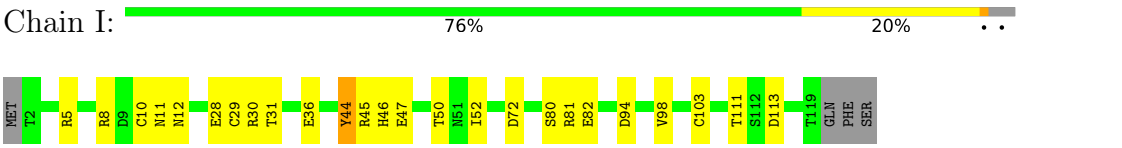
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



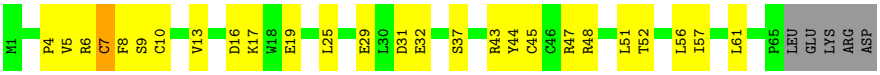
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



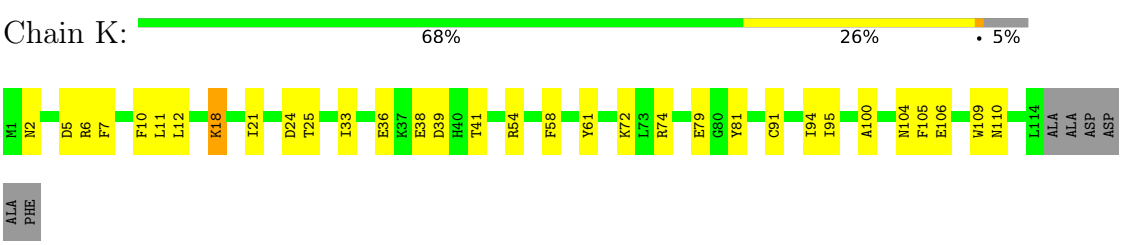
• Molecule 10: DNA-directed RNA polymerase II subunit RPB9



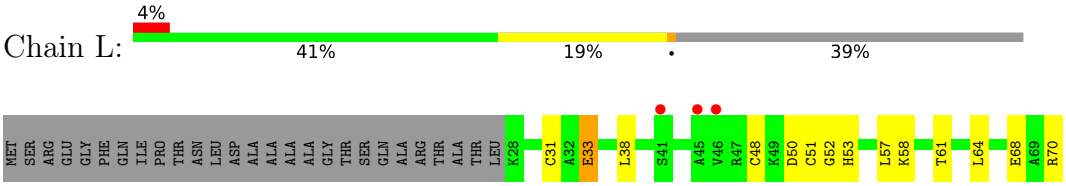
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



• Molecule 12: DNA-directed RNA polymerase II subunit RPB11



• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.16Å 223.04Å 193.46Å 90.00° 100.67° 90.00°	Depositor
Resolution (Å)	49.23 – 3.30 49.22 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.23-3.30) 99.9 (49.22-3.30)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.219 , 0.261 0.219 , 0.260	Depositor DCC
R_{free} test set	1942 reflections (1.85%)	wwPDB-VP
Wilson B-factor (Å^2)	91.0	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 58.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	29193	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 5N0, MG, PPV, 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	R	0.34	0/241	0.82	0/375
2	T	0.70	0/584	1.09	0/898
3	N	0.54	0/331	0.81	0/509
4	A	0.31	0/11016	0.60	11/14902 (0.1%)
5	B	0.29	0/9071	0.50	0/12242
6	C	0.34	0/2139	0.66	4/2899 (0.1%)
7	E	0.29	0/1767	0.46	0/2378
8	F	0.27	0/696	0.46	0/943
9	H	0.28	0/1082	0.52	0/1466
10	I	0.30	0/970	0.50	0/1308
11	J	0.29	0/541	0.52	0/727
12	K	0.31	0/937	0.55	0/1265
13	L	0.31	0/339	0.55	0/450
All	All	0.32	0/29714	0.58	15/40362 (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
4	A	0	2
6	C	0	2
All	All	0	4

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	64	ASN	CB-CG-OD1	29.19	179.97	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	64	ASN	CB-CG-ND2	-15.53	79.42	116.70
6	C	131	HIS	N-CA-CB	-14.04	85.34	110.60
4	A	1004	ASN	N-CA-CB	-13.60	86.12	110.60
6	C	131	HIS	CB-CG-CD2	-10.83	97.24	130.80
4	A	64	ASN	OD1-CG-ND2	-9.26	100.59	121.90
6	C	131	HIS	CB-CA-C	8.66	127.71	110.40
6	C	131	HIS	ND1-CG-CD2	-7.98	94.83	106.00
4	A	398	GLU	C-N-CA	6.98	139.14	121.70
4	A	446	ARG	NE-CZ-NH2	6.76	123.68	120.30
4	A	446	ARG	NE-CZ-NH1	-6.70	116.95	120.30
4	A	124	GLN	CG-CD-NE2	-5.62	103.20	116.70
4	A	1003	LYS	C-N-CA	5.42	135.26	121.70
4	A	1004	ASN	CB-CG-ND2	-5.38	103.78	116.70
4	A	1004	ASN	OD1-CG-ND2	-5.36	109.57	121.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1004	ASN	Sidechain
4	A	124	GLN	Sidechain
6	C	130	GLY	Peptide
6	C	131	HIS	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	R	215	0	111	2	0
2	T	525	0	297	22	0
3	N	293	0	156	5	0
4	A	10824	0	10869	317	0
5	B	8899	0	8854	251	0
6	C	2101	0	2056	62	0
7	E	1731	0	1758	35	0
8	F	684	0	692	14	0
9	H	1064	0	1029	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	952	0	897	17	0
11	J	532	0	542	21	0
12	K	919	0	929	34	0
13	L	337	0	352	8	0
14	R	1	0	0	0	0
15	T	99	0	0	2	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	B	9	0	0	0	0
All	All	29193	0	28542	725	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 13.

All (725) 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)
4:A:1329:THR:HG22	4:A:1331:SER:H	1.09	1.14
4:A:446:ARG:NH1	4:A:447:GLN:O	1.88	1.06
4:A:1003:LYS:C	4:A:1004:ASN:HD22	1.58	1.05
5:B:218:SER:OG	5:B:241:ARG:NH2	1.94	1.00
5:B:345:LYS:HG2	5:B:348:ARG:HH12	1.27	1.00
5:B:345:LYS:HG2	5:B:348:ARG:NH1	1.83	0.92
4:A:1111:MET:HG3	4:A:1114:PRO:HG3	1.53	0.90
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.54	0.90
4:A:1329:THR:HG22	4:A:1331:SER:N	1.90	0.87
12:K:10:PHE:CE1	12:K:11:LEU:HD13	2.09	0.86
11:J:10:CYS:SG	11:J:43:ARG:NH2	2.50	0.84
12:K:10:PHE:CD1	12:K:11:LEU:CD1	2.61	0.84
2:T:16:DT:H2'	2:T:17:DG:C8	2.13	0.82
12:K:10:PHE:CE1	12:K:11:LEU:CD1	2.64	0.81
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.14	0.80
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.14	0.80
4:A:329:LEU:HA	4:A:335:ARG:H	1.47	0.79
5:B:878:GLN:HB2	5:B:881:ASN:HB3	1.62	0.79
4:A:1004:ASN:OD1	7:E:167:ARG:NE	2.16	0.78
4:A:12:ARG:HD2	5:B:1218:THR:HG21	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:10:CYS:SG	10:I:31:THR:OG1	2.41	0.77
4:A:562:THR:O	4:A:576:GLN:NE2	2.18	0.77
9:H:103:LYS:HB3	9:H:115:TYR:HD1	1.50	0.77
4:A:771:GLU:OE2	5:B:510:LYS:NZ	2.18	0.77
4:A:525:GLN:HB2	5:B:1015:HIS:CD2	2.19	0.76
6:C:86:CYS:SG	6:C:87:PHE:N	2.59	0.76
10:I:50:THR:HG22	10:I:52:ILE:H	1.48	0.76
4:A:353:ILE:HG21	4:A:487:MET:HG3	1.66	0.76
13:L:38:LEU:HD21	13:L:48:CYS:HA	1.68	0.76
4:A:899:VAL:CG1	4:A:929:LEU:HD13	2.16	0.74
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.70	0.74
5:B:287:ARG:NH1	5:B:324:ILE:O	2.20	0.74
2:T:25:DC:OP1	5:B:857:ARG:NH2	2.21	0.74
4:A:42:ASP:HB2	4:A:50:ILE:HG23	1.69	0.74
4:A:107:CYS:SG	4:A:171:GLN:NE2	2.61	0.74
5:B:1082:MET:HA	6:C:189:THR:HA	1.68	0.74
4:A:877:HIS:CD2	4:A:1056:SER:HA	2.23	0.73
5:B:612:GLU:O	5:B:632:ARG:NH2	2.21	0.73
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.68	0.73
10:I:44:TYR:HE1	10:I:46:HIS:HB2	1.53	0.73
5:B:840:ILE:HG12	5:B:992:ILE:HG22	1.71	0.73
4:A:146:MET:HG3	4:A:147:VAL:HG23	1.71	0.73
4:A:378:GLU:OE2	4:A:387:ARG:NH2	2.22	0.72
4:A:335:ARG:NH1	5:B:1206:GLU:OE2	2.20	0.72
12:K:10:PHE:CD1	12:K:11:LEU:HD13	2.25	0.72
4:A:821:ARG:NH2	5:B:524:PRO:O	2.13	0.72
4:A:100:LYS:O	4:A:104:GLU:N	2.22	0.71
5:B:843:GLN:HG2	5:B:993:THR:HB	1.72	0.71
4:A:579:SER:HB3	4:A:611:GLN:HA	1.72	0.71
5:B:744:HIS:ND1	5:B:746:SER:OG	2.22	0.70
5:B:345:LYS:HA	5:B:348:ARG:NH1	2.06	0.70
4:A:738:LYS:NZ	6:C:194:GLU:O	2.17	0.70
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.73	0.70
5:B:629:ASP:O	5:B:632:ARG:NH1	2.25	0.70
5:B:643:ASP:O	5:B:647:GLY:N	2.25	0.70
5:B:824:ILE:HG22	5:B:1008:PRO:HA	1.74	0.70
4:A:55:ASP:O	4:A:57:ARG:N	2.23	0.70
5:B:205:ILE:HG13	5:B:461:LEU:HB3	1.73	0.70
4:A:1004:ASN:HD22	4:A:1004:ASN:N	1.90	0.70
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.24	0.69
2:T:19:DG:H2'	2:T:20:DC:H6	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:847:ASP:OD1	12:K:6:ARG:NH2	2.22	0.68
4:A:901:LEU:N	4:A:926:GLN:OE1	2.26	0.68
12:K:100:ALA:O	12:K:104:ASN:ND2	2.27	0.67
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.27	0.67
2:T:18:DA:H5"	2:T:19:DG:H5"	1.75	0.67
5:B:67:SER:HB2	5:B:92:PHE:HD1	1.60	0.67
11:J:9:SER:OG	11:J:48:ARG:NH2	2.27	0.67
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.77	0.67
4:A:765:VAL:HG22	4:A:800:VAL:HB	1.78	0.66
7:E:171:LYS:HB2	7:E:174:GLN:HG3	1.77	0.66
5:B:208:SER:OG	5:B:210:LYS:NZ	2.29	0.66
7:E:24:LYS:NZ	7:E:32:GLN:OE1	2.29	0.66
4:A:899:VAL:HG13	4:A:929:LEU:HD13	1.77	0.65
4:A:1166:ASP:HA	4:A:1169:ILE:HD13	1.78	0.65
4:A:848:ILE:HG21	4:A:1370:LEU:HD21	1.77	0.65
5:B:287:ARG:NH2	5:B:294:ASP:OD2	2.28	0.65
6:C:50:GLU:HB3	13:L:64:LEU:HD21	1.77	0.65
9:H:128:ASN:OD1	9:H:131:ASN:ND2	2.25	0.65
12:K:21:ILE:HG12	12:K:33:ILE:HG12	1.79	0.65
4:A:664:THR:HG21	5:B:1017:ILE:HG21	1.79	0.65
5:B:1186:ASP:OD1	5:B:1188:LYS:NZ	2.30	0.65
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.78	0.65
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.78	0.65
4:A:306:ASN:ND2	4:A:313:GLN:OE1	2.30	0.64
4:A:873:MET:HG3	4:A:957:PRO:HG3	1.79	0.64
5:B:103:ASN:ND2	5:B:109:THR:OG1	2.30	0.64
2:T:8:DT:H2"	2:T:9:DC:H2'	1.79	0.64
4:A:782:ARG:NH2	5:B:701:ILE:O	2.28	0.64
9:H:105:GLU:HB3	9:H:113:ALA:HB3	1.80	0.64
2:T:22:DT:OP1	4:A:344:ARG:NH1	2.30	0.63
5:B:496:ARG:HH12	5:B:541:LEU:HA	1.63	0.63
4:A:1003:LYS:C	4:A:1004:ASN:ND2	2.42	0.63
4:A:899:VAL:HG11	4:A:929:LEU:HD13	1.81	0.63
9:H:123:MET:HE3	9:H:142:LEU:HD11	1.80	0.63
4:A:1094:VAL:HA	4:A:1113:THR:HG21	1.79	0.63
5:B:299:GLU:OE1	5:B:572:HIS:ND1	2.32	0.63
7:E:177:ARG:O	7:E:212:ARG:NH2	2.31	0.63
5:B:245:GLU:O	5:B:249:ARG:NH2	2.31	0.63
5:B:835:GLN:HA	5:B:1013:ASN:HD22	1.64	0.63
5:B:766:ARG:HG3	5:B:1022:THR:HG22	1.80	0.63
6:C:2:SER:OG	6:C:3:GLU:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:208:LEU:HD23	4:A:235:ILE:HD11	1.80	0.62
5:B:1135:ARG:NH2	5:B:1136:ASP:OD1	2.32	0.62
4:A:526:ASP:HB2	5:B:835:GLN:CD	2.19	0.62
5:B:806:THR:HG22	5:B:808:ALA:H	1.65	0.62
5:B:325:GLN:NE2	10:I:12:ASN:OD1	2.33	0.62
5:B:604:ARG:NH2	5:B:613:VAL:O	2.27	0.62
5:B:219:ALA:HB2	5:B:405:ARG:HD3	1.80	0.62
2:T:13:DT:H2'	2:T:14:DC:C6	2.35	0.62
6:C:8:VAL:HG11	12:K:105:PHE:HD1	1.65	0.61
12:K:12:LEU:HD12	12:K:12:LEU:H	1.65	0.61
4:A:424:ILE:HD12	4:A:424:ILE:O	2.00	0.61
4:A:585:GLY:N	4:A:609:ASP:OD1	2.33	0.61
7:E:78:LEU:HD21	7:E:109:ILE:HD13	1.83	0.61
5:B:653:VAL:HG12	5:B:689:LEU:HB3	1.81	0.61
5:B:931:TYR:HD2	5:B:932:HIS:H	1.46	0.61
4:A:74:MET:O	5:B:1116:ARG:NH2	2.33	0.61
4:A:183:GLY:O	4:A:199:LEU:N	2.32	0.61
6:C:41:ILE:HG23	6:C:172:PRO:HG2	1.82	0.61
5:B:122:LEU:HD22	5:B:958:GLN:HG3	1.82	0.60
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.66	0.60
4:A:666:ILE:HG23	5:B:1026:LEU:HB2	1.84	0.60
4:A:785:PRO:HB2	5:B:703:ILE:HD12	1.84	0.60
4:A:1276:VAL:HG12	4:A:1277:GLU:H	1.66	0.60
4:A:1004:ASN:N	4:A:1004:ASN:ND2	2.48	0.60
12:K:106:GLU:O	12:K:110:ASN:ND2	2.35	0.60
5:B:957:ASN:OD1	5:B:961:LEU:N	2.33	0.59
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.83	0.59
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.82	0.59
5:B:260:GLY:HA3	5:B:267:ARG:HG2	1.83	0.59
10:I:98:VAL:HG11	10:I:113:ASP:HB2	1.83	0.59
4:A:1107:VAL:HG22	4:A:1383:SER:HB3	1.84	0.59
5:B:483:LEU:HD21	5:B:491:THR:HG23	1.83	0.59
6:C:35:ARG:NH1	12:K:39:ASP:OD1	2.35	0.59
9:H:12:VAL:HG13	9:H:26:ILE:HD11	1.85	0.59
5:B:778:MET:HE1	5:B:1094:ARG:HD3	1.84	0.59
5:B:828:ALA:O	5:B:834:ASN:ND2	2.35	0.58
6:C:246:ARG:O	6:C:250:THR:OG1	2.20	0.58
10:I:28:GLU:OE2	10:I:30:ARG:NH1	2.35	0.58
2:T:7:DC:H2"	2:T:8:DT:H5"	1.84	0.58
5:B:27:ALA:O	5:B:30:SER:OG	2.20	0.58
4:A:780:VAL:HG12	5:B:699:GLU:OE2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:77:ILE:HG13	6:C:161:LYS:HE3	1.85	0.58
12:K:10:PHE:CD1	12:K:11:LEU:HD12	2.38	0.58
4:A:1002:GLY:O	4:A:1008:GLN:NE2	2.35	0.58
4:A:1138:ILE:HD11	4:A:1316:VAL:HG13	1.85	0.58
7:E:47:CYS:HA	7:E:53:PRO:HA	1.86	0.58
9:H:87:ARG:HA	9:H:87:ARG:NH2	2.19	0.58
4:A:483:ASP:HA	5:B:988:GLY:HA2	1.86	0.58
4:A:1100:ARG:NH2	4:A:1351:GLU:OE2	2.36	0.58
4:A:1444:MET:HG3	8:F:133:VAL:HG13	1.85	0.57
5:B:896:ASP:OD2	13:L:58:LYS:NZ	2.36	0.57
3:N:8:DC:H2"	3:N:9:DC:H5"	1.85	0.57
4:A:76:GLU:OE2	5:B:1159:ARG:NH1	2.37	0.57
4:A:514:PRO:HB3	4:A:875:ALA:HB3	1.84	0.57
4:A:567:LYS:HB3	4:A:568:PRO:HD3	1.86	0.57
5:B:309:GLN:OE1	5:B:392:ARG:NH2	2.38	0.57
6:C:93:ASP:O	6:C:127:ARG:NH2	2.38	0.57
4:A:824:LEU:HD21	5:B:765:PRO:HB3	1.87	0.57
5:B:839:MET:HG2	5:B:989:THR:O	2.04	0.57
7:E:124:VAL:HG13	7:E:132:ILE:HB	1.85	0.57
4:A:1295:THR:HB	4:A:1297:GLU:OE2	2.04	0.57
4:A:46:THR:HG22	4:A:47:ARG:H	1.69	0.57
4:A:54:ASN:HB3	4:A:247:ARG:HH22	1.69	0.57
9:H:15:VAL:HB	9:H:26:ILE:HD13	1.87	0.57
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.85	0.57
4:A:90:VAL:HG21	4:A:296:LEU:HD12	1.87	0.56
4:A:662:PHE:O	5:B:828:ALA:HA	2.04	0.56
6:C:114:TYR:HB3	6:C:141:GLY:H	1.67	0.56
4:A:218:ASP:O	4:A:222:LEU:HB2	2.03	0.56
4:A:547:LEU:HD22	12:K:58:PHE:HD1	1.70	0.56
4:A:1130:GLN:O	4:A:1134:ILE:HG12	2.05	0.56
4:A:1224:LEU:HD11	4:A:1240:CYS:HB3	1.87	0.56
5:B:892:LYS:NZ	5:B:904:ARG:O	2.25	0.56
6:C:251:LEU:O	6:C:255:VAL:HG23	2.05	0.56
10:I:29:CYS:SG	10:I:31:THR:N	2.76	0.56
2:T:12:DG:H2"	2:T:13:DT:H5"	1.85	0.56
4:A:34:LYS:HG2	4:A:83:HIS:HE1	1.70	0.56
4:A:1005:GLU:O	4:A:1009:ASN:ND2	2.39	0.56
5:B:882:THR:OG1	5:B:885:MET:SD	2.64	0.56
8:F:76:LYS:HA	8:F:79:ARG:HD3	1.88	0.56
5:B:826:ALA:HB2	5:B:1087:PHE:HD1	1.71	0.56
5:B:899:ILE:HD13	5:B:949:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:635:ARG:NE	4:A:877:HIS:HB3	2.21	0.56
6:C:31:ASN:OD1	6:C:34:ARG:NH1	2.39	0.56
4:A:1155:ASP:OD2	4:A:1161:THR:OG1	2.17	0.55
5:B:912:ILE:HB	5:B:939:THR:HB	1.88	0.55
4:A:500:GLU:OE2	4:A:1438:THR:HG21	2.05	0.55
4:A:1161:THR:HG21	4:A:1166:ASP:HB2	1.88	0.55
5:B:470:LYS:HB2	5:B:474:SER:HB3	1.87	0.55
5:B:493:SER:OG	5:B:497:ARG:NH2	2.39	0.55
4:A:1420:ASP:OD1	4:A:1422:ARG:NH2	2.39	0.55
5:B:1020:ARG:HB2	5:B:1022:THR:HG23	1.88	0.55
4:A:464:PRO:O	12:K:2:ASN:HB3	2.07	0.55
4:A:929:LEU:HD11	4:A:983:ILE:HD13	1.89	0.55
2:T:18:DA:H2'	5:B:505:ASP:OD2	2.07	0.55
4:A:103:CYS:HA	4:A:106:VAL:HG12	1.88	0.55
5:B:213:ILE:O	5:B:215:GLN:OE1	2.24	0.55
4:A:113:LEU:HD23	4:A:113:LEU:H	1.71	0.55
4:A:151:ASP:OD1	4:A:164:ARG:N	2.34	0.55
4:A:304:MET:SD	5:B:1210:MET:HG3	2.47	0.55
4:A:541:ILE:HD12	4:A:577:ILE:HG21	1.88	0.55
4:A:697:ALA:HA	4:A:702:LEU:HD23	1.88	0.55
10:I:29:CYS:SG	10:I:30:ARG:N	2.80	0.55
4:A:246:VAL:O	4:A:328:ARG:NH1	2.33	0.55
4:A:503:GLN:OE1	8:F:90:ARG:NH2	2.40	0.55
6:C:254:LYS:NZ	12:K:38:GLU:OE1	2.38	0.55
9:H:40:LEU:HD13	9:H:123:MET:HB2	1.89	0.55
4:A:87:ALA:HB3	4:A:276:LEU:HD23	1.89	0.55
4:A:949:ASP:OD1	4:A:949:ASP:N	2.40	0.55
10:I:5:ARG:NH2	10:I:36:GLU:OE2	2.40	0.55
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.87	0.55
4:A:901:LEU:HA	4:A:907:THR:HG23	1.89	0.55
4:A:939:ASP:O	4:A:943:LEU:HG	2.07	0.55
8:F:82:THR:O	8:F:136:ARG:NH1	2.23	0.54
2:T:19:DG:H2'	2:T:20:DC:C6	2.38	0.54
4:A:526:ASP:OD1	5:B:835:GLN:HG3	2.07	0.54
5:B:847:ASP:HB3	6:C:167:HIS:CE1	2.42	0.54
5:B:1023:VAL:O	5:B:1027:ILE:HG13	2.07	0.54
13:L:51:CYS:SG	13:L:52:GLY:N	2.80	0.54
8:F:111:LEU:HD23	8:F:111:LEU:H	1.71	0.54
4:A:848:ILE:HB	4:A:1065:GLY:HA3	1.90	0.54
2:T:11:DG:H2"	2:T:12:DG:C8	2.41	0.54
4:A:67:CYS:HB3	4:A:70:CYS:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1206:ASP:OD1	4:A:1274:ARG:NH1	2.40	0.54
4:A:42:ASP:N	4:A:49:LYS:HA	2.22	0.54
4:A:369:SER:OG	12:K:2:ASN:OD1	2.25	0.54
4:A:379:VAL:O	4:A:384:ASN:ND2	2.39	0.54
5:B:211:VAL:O	5:B:480:SER:HA	2.07	0.54
13:L:68:GLU:CD	13:L:68:GLU:H	2.11	0.54
4:A:28:ARG:HH22	4:A:85:ASP:HB3	1.72	0.54
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.90	0.54
5:B:1187:ASN:ND2	5:B:1190:ASP:O	2.31	0.54
4:A:945:GLU:O	7:E:201:LYS:NZ	2.41	0.53
4:A:491:VAL:O	5:B:1150:ARG:NH2	2.41	0.53
9:H:87:ARG:HA	9:H:87:ARG:HH21	1.73	0.53
11:J:37:SER:OG	11:J:47:ARG:NH2	2.40	0.53
4:A:110:CYS:HB3	4:A:167:CYS:HB3	1.90	0.53
4:A:239:LEU:HD12	4:A:240:PRO:HD2	1.89	0.53
5:B:102:VAL:HG22	5:B:112:LEU:HB2	1.89	0.53
5:B:976:ILE:HD11	5:B:992:ILE:HA	1.91	0.53
9:H:44:VAL:HG13	9:H:48:PRO:HA	1.90	0.53
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	1.89	0.53
6:C:31:ASN:O	6:C:35:ARG:HG3	2.08	0.53
4:A:1215:ARG:O	4:A:1219:THR:OG1	2.24	0.53
8:F:82:THR:HG22	8:F:84:TYR:H	1.74	0.53
4:A:1132:LYS:HD3	4:A:1135:ARG:HH11	1.74	0.53
9:H:113:ALA:HA	9:H:125:LEU:O	2.09	0.53
4:A:44:THR:OG1	4:A:46:THR:OG1	2.27	0.53
4:A:306:ASN:H	4:A:324:SER:HB3	1.73	0.53
4:A:793:SER:OG	4:A:795:GLU:OE1	2.23	0.53
4:A:821:ARG:NH1	4:A:821:ARG:HB2	2.24	0.53
5:B:232:SER:O	5:B:261:ARG:NH2	2.41	0.53
5:B:834:ASN:O	5:B:1013:ASN:HB2	2.09	0.53
4:A:351:THR:OG1	4:A:352:VAL:N	2.42	0.53
4:A:951:GLU:OE2	4:A:953:ASN:ND2	2.41	0.53
9:H:92:ASP:OD1	9:H:92:ASP:N	2.33	0.53
4:A:506:ALA:HB3	4:A:509:LEU:HG	1.91	0.52
4:A:966:ASN:HB3	4:A:1044:TRP:HH2	1.74	0.52
10:I:111:THR:HG22	10:I:113:ASP:H	1.73	0.52
4:A:455:MET:CE	5:B:1138:MET:HG2	2.38	0.52
4:A:840:ARG:HD2	4:A:1402:PHE:HZ	1.74	0.52
5:B:261:ARG:H	5:B:264:SER:HB3	1.73	0.52
10:I:72:ASP:O	10:I:81:ARG:NH2	2.32	0.52
4:A:246:VAL:HG12	4:A:328:ARG:HH22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:434:ARG:NH1	4:A:440:ASP:OD2	2.39	0.52
4:A:455:MET:HE3	5:B:1138:MET:HG2	1.91	0.52
5:B:680:THR:O	5:B:683:SER:OG	2.23	0.52
9:H:105:GLU:N	9:H:113:ALA:O	2.35	0.52
4:A:1423:GLY:O	4:A:1427:ASN:ND2	2.42	0.52
6:C:116:LYS:HD3	6:C:140:ASN:HA	1.91	0.52
7:E:28:TYR:CE1	7:E:78:LEU:HG	2.45	0.52
4:A:1351:GLU:O	4:A:1355:VAL:HG13	2.09	0.52
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.91	0.52
9:H:41:ASP:HB2	9:H:121:LEU:HB3	1.91	0.52
4:A:525:GLN:NE2	5:B:836:GLU:OE1	2.42	0.52
4:A:596:THR:HG22	4:A:598:LEU:H	1.75	0.52
5:B:34:ILE:HG12	5:B:542:MET:HE3	1.91	0.52
5:B:345:LYS:HA	5:B:348:ARG:CZ	2.40	0.52
5:B:955:THR:OG1	5:B:956:THR:N	2.42	0.52
7:E:55:ARG:HH22	7:E:113:GLN:HG3	1.75	0.52
4:A:391:LEU:HD11	4:A:437:MET:HE1	1.91	0.51
7:E:77:SER:HB2	7:E:105:PHE:CD2	2.45	0.51
5:B:484:ASN:OD1	5:B:490:SER:HB2	2.10	0.51
13:L:33:GLU:HG3	13:L:53:HIS:CE1	2.45	0.51
4:A:856:THR:HB	4:A:865:GLN:HB2	1.93	0.51
4:A:1062:GLU:OE2	8:F:88:TYR:OH	2.26	0.51
4:A:691:LEU:HD22	4:A:695:LYS:HE2	1.92	0.51
5:B:864:LYS:NZ	5:B:872:GLU:OE2	2.33	0.51
5:B:904:ARG:HG2	5:B:948:ILE:HG12	1.92	0.51
10:I:82:GLU:OE1	10:I:82:GLU:N	2.43	0.51
4:A:399:HIS:CD2	4:A:400:PRO:HA	2.46	0.51
5:B:289:LEU:HD21	5:B:356:LEU:HD12	1.92	0.51
6:C:7:GLN:HB3	6:C:23:SER:HB2	1.93	0.51
4:A:128:ILE:HG23	4:A:134:ARG:HB2	1.93	0.51
5:B:255:GLN:H	5:B:272:THR:HG22	1.75	0.51
5:B:1039:GLY:HA2	11:J:51:LEU:HD22	1.93	0.51
7:E:136:ASN:OD1	7:E:138:ALA:N	2.37	0.51
9:H:118:PHE:CZ	9:H:142:LEU:HD12	2.45	0.51
10:I:44:TYR:CE1	10:I:46:HIS:HB2	2.41	0.51
4:A:412:ARG:NH2	4:A:433:GLU:OE2	2.43	0.51
4:A:974:ASP:HA	9:H:136:LYS:HE3	1.93	0.51
4:A:108:MET:SD	4:A:108:MET:N	2.83	0.51
4:A:1080:THR:OG1	4:A:1081:LEU:N	2.44	0.51
5:B:244:LEU:HD12	5:B:244:LEU:H	1.76	0.51
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:56:THR:HB	9:H:145:ARG:HB3	1.93	0.51
4:A:122:MET:O	4:A:126:LEU:HG	2.10	0.51
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.46	0.51
5:B:235:SER:HG	5:B:236:HIS:CE1	2.29	0.51
5:B:1017:ILE:HD12	5:B:1026:LEU:HD21	1.93	0.51
5:B:268:THR:OG1	5:B:270:LYS:NZ	2.43	0.50
5:B:512:ARG:HH21	5:B:532:ALA:H	1.59	0.50
4:A:899:VAL:HG13	4:A:899:VAL:O	2.11	0.50
4:A:1267:MET:HA	4:A:1271:ILE:HD13	1.92	0.50
7:E:62:ALA:HB3	7:E:78:LEU:HD12	1.93	0.50
2:T:21:DC:H5'	5:B:1129:ARG:HD3	1.93	0.50
4:A:451:HIS:CE1	4:A:1074:GLU:HG3	2.46	0.50
4:A:508:PRO:HA	4:A:511:ILE:HG13	1.93	0.50
4:A:715:GLU:OE2	4:A:774:ARG:NH1	2.45	0.50
4:A:779:PHE:CZ	5:B:517:THR:HA	2.47	0.50
9:H:89:LEU:HD13	9:H:91:ASP:O	2.12	0.50
12:K:91:CYS:O	12:K:95:ILE:HG13	2.12	0.50
5:B:830:TYR:O	5:B:831:SER:OG	2.20	0.50
5:B:843:GLN:CG	5:B:993:THR:HB	2.41	0.50
7:E:157:SER:N	7:E:160:GLU:OE1	2.37	0.50
5:B:1101:ASP:O	5:B:1122:ARG:NH1	2.44	0.50
6:C:62:PHE:HE2	6:C:66:ARG:HD2	1.76	0.50
5:B:997:GLU:CD	5:B:997:GLU:H	2.15	0.50
2:T:25:DC:H2"	2:T:26:DG:H5'	1.94	0.50
4:A:90:VAL:HG11	4:A:297:GLN:HA	1.94	0.50
4:A:466:SER:HB3	5:B:1103:ILE:HD11	1.93	0.49
4:A:497:THR:OG1	5:B:1149:GLU:OE2	2.28	0.49
7:E:14:ARG:HH11	7:E:142:VAL:HG23	1.77	0.49
10:I:45:ARG:NH1	10:I:47:GLU:OE2	2.45	0.49
12:K:5:ASP:HB3	12:K:7:PHE:CE2	2.47	0.49
4:A:1224:LEU:HD12	4:A:1241:ARG:O	2.12	0.49
5:B:313:MET:O	5:B:316:PRO:HD2	2.12	0.49
4:A:208:LEU:HD21	4:A:212:LYS:HE3	1.95	0.49
4:A:687:LYS:NZ	4:A:795:GLU:OE2	2.45	0.49
4:A:42:ASP:HA	4:A:50:ILE:HG13	1.94	0.49
4:A:357:PRO:HD2	5:B:833:TYR:CZ	2.47	0.49
4:A:737:LEU:HD22	4:A:741:ASN:ND2	2.28	0.49
4:A:1398:MET:O	4:A:1401:SER:OG	2.30	0.49
9:H:8:ASP:OD1	9:H:129:TYR:OH	2.21	0.49
4:A:167:CYS:SG	4:A:168:GLY:N	2.85	0.49
4:A:541:ILE:HD13	4:A:549:MET:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1436:ILE:HG22	4:A:1437:GLY:H	1.77	0.49
5:B:1073:TYR:CE2	5:B:1080:LYS:HG2	2.47	0.49
6:C:179:GLU:OE1	6:C:206:ASN:ND2	2.44	0.49
9:H:8:ASP:OD2	9:H:9:ILE:N	2.45	0.49
10:I:94:ASP:OD1	10:I:94:ASP:N	2.44	0.49
4:A:800:VAL:HG13	4:A:812:GLU:HB3	1.94	0.49
5:B:640:VAL:HA	5:B:651:LEU:HA	1.95	0.49
8:F:128:LYS:NZ	8:F:151:LEU:O	2.46	0.49
9:H:93:TYR:CD2	9:H:145:ARG:HB2	2.47	0.49
11:J:13:VAL:O	11:J:17:LYS:NZ	2.46	0.49
4:A:664:THR:OG1	5:B:1014:PRO:HB3	2.13	0.49
4:A:821:ARG:HG3	4:A:825:ILE:HD11	1.94	0.49
5:B:357:GLN:HA	5:B:374:LYS:NZ	2.28	0.49
5:B:780:VAL:HG11	11:J:56:LEU:HD13	1.95	0.49
6:C:115:SER:OG	6:C:141:GLY:HA3	2.12	0.49
2:T:18:DA:C5'	2:T:19:DG:H5"	2.43	0.49
4:A:1118:VAL:HA	4:A:1327:ILE:HG13	1.93	0.49
5:B:487:THR:OG1	5:B:777:ALA:O	2.30	0.49
6:C:41:ILE:HD12	6:C:246:ARG:HB3	1.94	0.49
6:C:167:HIS:CD2	13:L:70:ARG:HB3	2.47	0.49
11:J:7:CYS:SG	11:J:9:SER:N	2.86	0.49
4:A:960:ILE:HG21	4:A:1025:ARG:HG2	1.95	0.48
4:A:979:SER:OG	4:A:980:ASP:N	2.44	0.48
4:A:1163:ILE:HG22	4:A:1165:GLU:H	1.77	0.48
5:B:217:ARG:NH1	5:B:407:ASP:OD1	2.46	0.48
5:B:313:MET:HE2	5:B:386:LEU:HD22	1.95	0.48
5:B:546:SER:OG	5:B:631:GLY:N	2.46	0.48
4:A:34:LYS:HG2	4:A:83:HIS:CE1	2.48	0.48
4:A:607:ILE:HA	4:A:612:ILE:HA	1.95	0.48
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.93	0.48
2:T:8:DT:H1'	2:T:9:DC:H5'	1.95	0.48
3:N:15:DG:H2"	3:N:16:DA:C8	2.48	0.48
4:A:268:ASP:HB3	4:A:299:HIS:CD2	2.49	0.48
4:A:834:THR:HG21	4:A:1077:THR:HA	1.95	0.48
5:B:48:LEU:HD23	5:B:173:MET:SD	2.53	0.48
5:B:797:TYR:HB3	5:B:798:TYR:CD1	2.48	0.48
3:N:8:DC:H2"	3:N:9:DC:C6	2.48	0.48
4:A:457:ALA:O	4:A:507:VAL:HG23	2.14	0.48
4:A:665:GLY:HA2	5:B:1086:PHE:CG	2.48	0.48
5:B:59:LEU:HD11	5:B:417:PHE:CZ	2.48	0.48
4:A:814:PHE:CE1	5:B:514:LEU:HD21	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1140:HIS:HA	4:A:1275:GLY:HA3	1.95	0.48
4:A:1373:ASP:O	4:A:1377:THR:N	2.45	0.48
5:B:1074:ASN:OD1	5:B:1076:HIS:N	2.44	0.48
4:A:1345:ARG:NH1	4:A:1373:ASP:OD1	2.42	0.48
2:T:20:DC:OP1	4:A:332:LYS:HD3	2.12	0.48
4:A:444:PHE:HE2	4:A:470:LEU:HD23	1.79	0.48
5:B:345:LYS:CG	5:B:348:ARG:NH1	2.65	0.48
5:B:487:THR:HG22	5:B:488:TYR:H	1.78	0.48
5:B:778:MET:CE	5:B:1094:ARG:HD3	2.43	0.48
4:A:336:ILE:HD11	5:B:1203:LEU:HD13	1.94	0.48
6:C:241:ASP:HB3	12:K:109:TRP:CE2	2.49	0.48
4:A:980:ASP:N	4:A:980:ASP:OD1	2.46	0.48
5:B:358:LYS:HG2	5:B:359:GLU:HG2	1.96	0.48
5:B:404:LYS:O	5:B:405:ARG:HD2	2.14	0.48
7:E:79:TRP:CZ3	7:E:81:GLU:HB2	2.48	0.48
12:K:79:GLU:OE1	12:K:79:GLU:N	2.41	0.48
4:A:1364:ASN:OD1	4:A:1366:ARG:HG2	2.13	0.48
4:A:1412:ALA:HA	4:A:1417:GLU:HG3	1.95	0.48
5:B:603:LEU:HB3	5:B:609:ILE:HG13	1.95	0.48
3:N:11:DG:H8	3:N:11:DG:H5"	1.79	0.47
1:R:4:G:H2'	1:R:5:A:C8	2.49	0.47
4:A:494:SER:HB3	4:A:496:GLU:OE1	2.14	0.47
6:C:69:LEU:O	11:J:6:ARG:NH1	2.42	0.47
9:H:13:SER:OG	9:H:27:GLU:O	2.22	0.47
12:K:24:ASP:OD1	12:K:25:THR:N	2.47	0.47
4:A:1140:HIS:ND1	4:A:1276:VAL:O	2.46	0.47
6:C:114:TYR:CG	6:C:140:ASN:HB3	2.48	0.47
4:A:445:ASN:OD1	4:A:446:ARG:N	2.47	0.47
4:A:802:ASN:OD1	5:B:729:ILE:N	2.30	0.47
5:B:258:LEU:HB2	5:B:385:LEU:HD21	1.97	0.47
5:B:1213:THR:OG1	5:B:1215:ARG:NH2	2.48	0.47
6:C:256:ALA:O	6:C:260:LEU:HG	2.14	0.47
5:B:197:PHE:O	5:B:488:TYR:OH	2.18	0.47
8:F:101:ILE:HD13	8:F:120:ILE:HG22	1.96	0.47
6:C:62:PHE:CE2	6:C:66:ARG:HD2	2.50	0.47
4:A:311:GLN:N	4:A:312:PRO:HD3	2.30	0.47
5:B:848:ARG:HH22	5:B:996:ARG:NH1	2.13	0.47
7:E:20:LYS:NZ	7:E:34:GLU:O	2.43	0.47
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.95	0.47
5:B:274:PRO:HG2	5:B:359:GLU:HB3	1.97	0.47
5:B:1152:MET:O	5:B:1157:ALA:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:55:ARG:HA	7:E:58:MET:HG3	1.97	0.47
4:A:54:ASN:HD22	4:A:244:PRO:HG3	1.79	0.47
4:A:1438:THR:HG23	8:F:92:ARG:HB2	1.96	0.47
7:E:59:SER:HA	7:E:80:VAL:O	2.14	0.47
4:A:470:LEU:HD21	4:A:487:MET:HE3	1.97	0.47
5:B:210:LYS:HE2	5:B:462:ALA:HA	1.97	0.47
5:B:760:ASP:OD1	5:B:760:ASP:N	2.41	0.47
6:C:22:LEU:HG	6:C:25:VAL:HG21	1.96	0.47
9:H:111:LEU:HD23	9:H:111:LEU:HA	1.82	0.47
9:H:115:TYR:HE2	9:H:124:ARG:HB2	1.80	0.47
5:B:798:TYR:CD2	11:J:4:PRO:HG3	2.50	0.46
5:B:470:LYS:O	5:B:474:SER:OG	2.19	0.46
5:B:599:THR:O	5:B:603:LEU:HG	2.15	0.46
4:A:628:GLY:O	4:A:632:VAL:HG23	2.14	0.46
4:A:1168:GLU:HA	4:A:1171:GLN:HB3	1.95	0.46
8:F:97:ARG:HD2	8:F:97:ARG:HA	1.66	0.46
4:A:898:ARG:HB2	4:A:933:TYR:CE1	2.51	0.46
4:A:1345:ARG:HG2	4:A:1372:VAL:HG12	1.98	0.46
4:A:1398:MET:N	4:A:1426:GLU:OE2	2.46	0.46
5:B:872:GLU:HG2	5:B:916:THR:HB	1.97	0.46
9:H:105:GLU:OE1	9:H:124:ARG:NH1	2.48	0.46
5:B:564:GLU:OE2	5:B:591:ARG:NH2	2.45	0.46
6:C:44:LEU:HD12	6:C:160:LYS:O	2.15	0.46
4:A:16:GLU:HG2	4:A:1418:LEU:HD11	1.97	0.46
4:A:1297:GLU:OE2	4:A:1297:GLU:N	2.46	0.46
4:A:1397:LEU:HD12	4:A:1426:GLU:HG3	1.97	0.46
5:B:1103:ILE:O	5:B:1122:ARG:HD2	2.16	0.46
5:B:357:GLN:OE1	5:B:368:GLU:N	2.49	0.46
5:B:493:SER:OG	5:B:775:LYS:HE2	2.14	0.46
9:H:101:ALA:HB2	9:H:116:TYR:CE2	2.51	0.46
4:A:60:SER:OG	4:A:66:LYS:O	2.29	0.46
5:B:56:ASP:HB2	5:B:57:TYR:CD1	2.51	0.46
5:B:393:LYS:HD2	5:B:393:LYS:HA	1.75	0.46
6:C:175:ALA:HB2	11:J:10:CYS:HB2	1.98	0.46
12:K:91:CYS:HA	12:K:94:ILE:HD12	1.98	0.46
4:A:451:HIS:NE2	4:A:515:GLN:OE1	2.43	0.46
4:A:573:SER:O	4:A:577:ILE:HG22	2.16	0.46
4:A:961:ARG:HH11	4:A:1025:ARG:HH22	1.63	0.46
5:B:784:ASN:OD1	5:B:788:ARG:HD2	2.16	0.46
4:A:545:GLN:O	4:A:549:MET:HG3	2.16	0.46
5:B:1213:THR:OG1	5:B:1213:THR:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:7:PHE:O	12:K:11:LEU:HB2	2.16	0.46
12:K:61:TYR:HA	12:K:72:LYS:O	2.16	0.46
4:A:335:ARG:NH1	5:B:1202:LEU:HD13	2.31	0.45
4:A:630:ILE:HG23	4:A:642:CYS:SG	2.56	0.45
5:B:975:GLN:NE2	5:B:1100:ASP:OD2	2.44	0.45
4:A:913:LEU:HD21	4:A:981:LEU:O	2.16	0.45
4:A:1212:VAL:O	4:A:1216:ILE:HG13	2.17	0.45
5:B:828:ALA:HB2	5:B:1085:ILE:HD13	1.99	0.45
5:B:1135:ARG:HG3	5:B:1147:LEU:HD21	1.98	0.45
4:A:587:HIS:HA	4:A:607:ILE:O	2.16	0.45
5:B:242:SER:HB2	5:B:362:PRO:HD2	1.98	0.45
5:B:416:LEU:HD23	5:B:457:LEU:HD23	1.98	0.45
5:B:826:ALA:HB2	5:B:1087:PHE:CD1	2.52	0.45
5:B:1173:ALA:HB1	5:B:1180:PHE:HD2	1.81	0.45
4:A:636:GLU:OE2	4:A:966:ASN:ND2	2.49	0.45
4:A:1366:ARG:HG2	4:A:1366:ARG:H	1.54	0.45
5:B:227:LYS:N	5:B:395:GLN:OE1	2.47	0.45
5:B:1043:ASP:OD1	5:B:1045:SER:OG	2.30	0.45
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.17	0.45
4:A:125:ALA:O	4:A:128:ILE:HG22	2.15	0.45
4:A:668:ASP:OD1	6:C:192:TRP:NE1	2.49	0.45
4:A:867:ILE:HG22	4:A:872:GLY:N	2.32	0.45
5:B:401:PHE:HD2	5:B:521:LEU:HD12	1.81	0.45
2:T:13:DT:H1'	15:T:101:5N0:C15	2.46	0.45
4:A:815:PHE:HA	4:A:818:MET:HE3	1.98	0.45
5:B:637:LEU:HD12	5:B:693:ILE:HG13	1.99	0.45
9:H:115:TYR:CE2	9:H:124:ARG:HB2	2.52	0.45
12:K:7:PHE:HB2	12:K:11:LEU:HD22	1.98	0.45
12:K:18:LYS:HE2	12:K:36:GLU:O	2.17	0.45
8:F:90:ARG:O	8:F:94:LEU:HG	2.17	0.45
4:A:237:THR:OG1	4:A:238:CYS:N	2.50	0.45
4:A:1431:GLY:HA3	5:B:1197:PRO:HD3	1.98	0.45
5:B:879:ARG:HA	5:B:885:MET:HG3	1.99	0.45
4:A:5:GLN:O	5:B:1159:ARG:NH2	2.50	0.45
4:A:472:LEU:HD13	5:B:835:GLN:HE22	1.82	0.45
4:A:666:ILE:HG23	5:B:1026:LEU:CB	2.45	0.45
6:C:222:LYS:HD3	6:C:222:LYS:HA	1.71	0.45
7:E:90:VAL:HB	7:E:119:SER:HB2	1.98	0.45
4:A:1282:VAL:HG22	4:A:1308:THR:HG22	1.99	0.44
5:B:376:PHE:CE2	5:B:569:TYR:HD2	2.35	0.44
5:B:749:LEU:HD22	5:B:753:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:184:SER:O	4:A:199:LEU:N	2.51	0.44
4:A:1121:GLU:HG3	4:A:1122:PRO:HD2	1.98	0.44
5:B:1023:VAL:HG12	5:B:1027:ILE:HD11	1.99	0.44
4:A:471:ASN:O	4:A:474:VAL:HG12	2.17	0.44
4:A:1116:LEU:O	4:A:1308:THR:HG23	2.17	0.44
5:B:129:PHE:HE2	5:B:166:PHE:HB2	1.82	0.44
2:T:13:DT:H1'	15:T:101:5N0:C14	2.47	0.44
4:A:269:ILE:HG12	4:A:299:HIS:HB3	2.00	0.44
4:A:329:LEU:HB3	4:A:335:ARG:HB3	1.99	0.44
4:A:666:ILE:HD12	4:A:667:GLY:N	2.32	0.44
4:A:991:LYS:O	4:A:995:GLU:HG2	2.18	0.44
4:A:1207:LEU:HD23	4:A:1207:LEU:HA	1.84	0.44
6:C:114:TYR:OH	11:J:19:GLU:OE2	2.23	0.44
4:A:457:ALA:HB2	4:A:501:LEU:HD12	1.99	0.44
4:A:900:ASP:O	4:A:907:THR:OG1	2.36	0.44
5:B:424:LEU:HD11	5:B:448:ILE:HG23	1.99	0.44
11:J:9:SER:HB2	11:J:45:CYS:HB2	2.00	0.44
5:B:216:GLU:OE1	5:B:537:LYS:NZ	2.51	0.44
5:B:437:GLU:HG2	5:B:438:GLU:HG3	2.00	0.44
4:A:1073:GLY:O	4:A:1077:THR:HG23	2.18	0.44
4:A:1228:TRP:HB3	4:A:1238:ILE:HG12	2.00	0.44
11:J:16:ASP:OD1	11:J:16:ASP:N	2.48	0.44
4:A:1435:PRO:HA	4:A:1439:GLY:O	2.17	0.44
5:B:128:LEU:HD21	5:B:170:LEU:HB2	2.00	0.44
5:B:750:GLY:O	5:B:754:SER:OG	2.26	0.44
5:B:936:ASP:OD1	5:B:937:ALA:N	2.51	0.44
7:E:133:GLU:HB3	7:E:135:PHE:HE1	1.83	0.44
2:T:15:DA:H3'	2:T:16:DT:C6	2.54	0.43
4:A:472:LEU:HD13	5:B:835:GLN:NE2	2.33	0.43
4:A:1368:MET:O	4:A:1372:VAL:HG23	2.18	0.43
5:B:114:PRO:HG2	5:B:181:LEU:HD11	2.00	0.43
6:C:57:VAL:HG21	11:J:57:ILE:HG13	2.00	0.43
4:A:1120:LEU:O	4:A:1323:ASP:HB2	2.18	0.43
4:A:53:LEU:HG	4:A:54:ASN:H	1.83	0.43
4:A:998:LEU:HD13	4:A:1001:ARG:HG3	2.00	0.43
5:B:487:THR:HG22	5:B:488:TYR:N	2.33	0.43
5:B:1076:HIS:O	6:C:31:ASN:ND2	2.51	0.43
9:H:41:ASP:OD1	9:H:122:LEU:N	2.48	0.43
4:A:1004:ASN:OD1	7:E:167:ARG:CD	2.66	0.43
4:A:1112:LYS:HE3	4:A:1112:LYS:HB3	1.85	0.43
4:A:1322:ILE:O	4:A:1324:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:261:ARG:HG3	5:B:262:GLU:H	1.83	0.43
5:B:522:VAL:HG11	5:B:537:LYS:HB3	2.01	0.43
4:A:17:VAL:O	4:A:1419:ASP:N	2.49	0.43
4:A:754:SER:N	4:A:757:ASN:OD1	2.50	0.43
6:C:115:SER:HB3	6:C:142:VAL:HG22	2.00	0.43
4:A:57:ARG:O	4:A:68:GLN:HB2	2.19	0.43
4:A:1285:MET:HG3	4:A:1286:LYS:H	1.84	0.43
4:A:1386:ARG:HG3	4:A:1387:HIS:CE1	2.53	0.43
5:B:437:GLU:OE1	5:B:437:GLU:N	2.49	0.43
5:B:950:ASP:HB2	5:B:969:ARG:HB3	1.99	0.43
6:C:65:HIS:O	6:C:69:LEU:HD23	2.19	0.43
7:E:178:ILE:N	7:E:213:ILE:O	2.41	0.43
11:J:44:TYR:HA	11:J:47:ARG:HB2	2.01	0.43
4:A:24:PRO:O	4:A:28:ARG:HG3	2.18	0.43
4:A:630:ILE:HD12	4:A:630:ILE:H	1.84	0.43
5:B:299:GLU:HG3	5:B:571:PRO:HG2	1.99	0.43
6:C:59:ALA:O	6:C:63:ILE:HG13	2.19	0.43
2:T:9:DC:H2"	2:T:10:DT:H71	1.99	0.43
4:A:120:GLU:HG3	4:A:123:ARG:NH2	2.34	0.43
5:B:35:SER:O	5:B:39:ARG:HG2	2.18	0.43
5:B:483:LEU:CD2	5:B:491:THR:HG23	2.49	0.43
5:B:1084:GLN:NE2	6:C:190:ASP:O	2.38	0.43
6:C:46:ILE:HD12	6:C:46:ILE:H	1.82	0.43
6:C:91:HIS:HB2	6:C:96:SER:OG	2.18	0.43
7:E:115:ASN:OD1	7:E:116:ILE:N	2.52	0.43
1:R:4:G:H2'	1:R:5:A:H8	1.83	0.43
4:A:821:ARG:HB2	4:A:821:ARG:HH11	1.84	0.43
5:B:37:PHE:O	5:B:41:LYS:HG3	2.18	0.43
4:A:268:ASP:HB3	4:A:299:HIS:NE2	2.33	0.43
4:A:466:SER:O	5:B:1103:ILE:HD11	2.19	0.43
4:A:607:ILE:HG12	4:A:612:ILE:HG22	2.01	0.43
4:A:966:ASN:HB3	4:A:1044:TRP:CH2	2.53	0.43
5:B:103:ASN:OD1	5:B:169:ARG:NH1	2.49	0.43
5:B:345:LYS:HA	5:B:348:ARG:HD3	2.01	0.43
6:C:46:ILE:HA	6:C:159:ALA:HA	1.99	0.43
4:A:359:LEU:HD23	4:A:359:LEU:HA	1.83	0.42
4:A:660:ASN:OD1	5:B:1082:MET:HB2	2.19	0.42
4:A:767:GLN:NE2	4:A:774:ARG:HG2	2.34	0.42
5:B:433:GLN:O	5:B:436:VAL:HG13	2.19	0.42
5:B:779:GLY:HA2	5:B:796:LEU:HB2	2.01	0.42
5:B:801:LYS:O	11:J:52:THR:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:861:ASP:OD1	5:B:862:GLN:N	2.45	0.42
6:C:252:GLN:HG3	12:K:95:ILE:HG23	2.01	0.42
6:C:253:LYS:HE3	6:C:253:LYS:HB2	1.77	0.42
4:A:1166:ASP:O	4:A:1170:ILE:HG13	2.19	0.42
4:A:1199:ARG:HG2	4:A:1236:LEU:HD23	2.00	0.42
7:E:135:PHE:HB3	7:E:140:LEU:HD11	2.00	0.42
4:A:117:GLU:O	4:A:123:ARG:HD3	2.18	0.42
4:A:1385:THR:HG22	4:A:1386:ARG:H	1.85	0.42
5:B:247:GLY:HA2	5:B:418:LYS:HE3	2.01	0.42
5:B:405:ARG:HH21	5:B:629:ASP:HB3	1.83	0.42
5:B:837:ASP:O	5:B:988:GLY:HA3	2.18	0.42
5:B:857:ARG:HD3	5:B:859:TYR:CZ	2.54	0.42
5:B:1039:GLY:O	11:J:32:GLU:HB2	2.20	0.42
4:A:1064:VAL:HG23	4:A:1370:LEU:HD11	2.01	0.42
4:A:1239:ARG:HH12	4:A:1241:ARG:HH12	1.68	0.42
5:B:190:TYR:CZ	5:B:196:PRO:HG2	2.54	0.42
6:C:129:ILE:HD13	6:C:129:ILE:HA	1.84	0.42
4:A:285:PRO:HG2	4:A:288:ALA:HB2	2.02	0.42
4:A:843:LYS:HD3	4:A:843:LYS:HA	1.90	0.42
4:A:1239:ARG:HH22	4:A:1241:ARG:HH12	1.67	0.42
5:B:293:PRO:HB2	10:I:11:ASN:HB3	2.01	0.42
5:B:357:GLN:HA	5:B:374:LYS:HZ2	1.84	0.42
5:B:604:ARG:HG3	5:B:611:PRO:HA	2.01	0.42
6:C:183:TRP:HB2	6:C:185:LYS:HG3	2.01	0.42
11:J:5:VAL:HG12	11:J:6:ARG:HG2	2.01	0.42
4:A:391:LEU:HD22	4:A:400:PRO:O	2.19	0.42
4:A:1157:ASP:OD1	4:A:1160:SER:N	2.45	0.42
7:E:74:ASP:OD1	7:E:74:ASP:N	2.53	0.42
6:C:244:VAL:O	6:C:248:ILE:HG13	2.20	0.42
7:E:61:GLN:HE21	7:E:105:PHE:HZ	1.66	0.42
9:H:104:PHE:HD2	9:H:114:VAL:HG22	1.84	0.42
3:N:10:DA:H2"	3:N:11:DG:C8	2.55	0.42
4:A:407:ARG:HD3	4:A:413:ILE:HD11	2.01	0.42
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.60	0.42
4:A:1386:ARG:HD3	4:A:1403:GLU:OE1	2.19	0.42
5:B:757:PRO:HD3	5:B:983:ARG:HD2	2.02	0.42
9:H:40:LEU:HD13	9:H:123:MET:HE3	2.01	0.42
4:A:752:LYS:HG2	5:B:1019:SER:HB2	2.02	0.42
4:A:778:GLY:HA3	5:B:516:ASN:HB2	2.01	0.42
4:A:885:THR:HG22	4:A:940:ARG:HB2	2.01	0.42
7:E:153:HIS:C	7:E:154:ILE:HD12	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:22:PHE:CD1	5:B:1213:THR:HG22	2.53	0.42
4:A:1118:VAL:HG22	4:A:1327:ILE:HD11	2.02	0.42
5:B:63:ILE:O	5:B:67:SER:HB3	2.20	0.42
5:B:315:LYS:HB3	5:B:316:PRO:HD3	2.02	0.42
5:B:384:ARG:HD2	5:B:384:ARG:HA	1.73	0.42
6:C:36:VAL:HG23	12:K:41:THR:HG21	2.01	0.42
9:H:142:LEU:HD22	9:H:144:ILE:CD1	2.50	0.42
4:A:369:SER:O	4:A:373:THR:OG1	2.33	0.41
5:B:236:HIS:HB2	5:B:385:LEU:HD11	2.01	0.41
4:A:380:VAL:HG23	4:A:428:TYR:HA	2.02	0.41
4:A:440:ASP:O	4:A:460:VAL:HG23	2.21	0.41
4:A:890:ASP:OD2	4:A:940:ARG:NH1	2.53	0.41
4:A:1313:LEU:HD12	4:A:1338:VAL:HG11	2.02	0.41
4:A:1404:GLU:O	4:A:1408:ILE:HG12	2.19	0.41
5:B:1094:ARG:NH1	5:B:1098:MET:SD	2.84	0.41
2:T:10:DT:H2"	2:T:11:DG:C8	2.55	0.41
4:A:40:THR:HA	4:A:53:LEU:HD23	2.02	0.41
4:A:662:PHE:CZ	4:A:742:ASN:HB3	2.55	0.41
4:A:1291:VAL:HG22	4:A:1292:PRO:HD2	2.02	0.41
5:B:116:GLU:OE2	5:B:120:ARG:NH1	2.53	0.41
5:B:666:TYR:O	5:B:668:ASP:N	2.52	0.41
4:A:569:LYS:HD2	4:A:571:LEU:HD11	2.01	0.41
4:A:1003:LYS:O	4:A:1004:ASN:ND2	2.51	0.41
4:A:1146:VAL:HG12	4:A:1201:ALA:HB1	2.02	0.41
4:A:1430:LEU:HD23	4:A:1430:LEU:HA	1.83	0.41
5:B:360:PHE:HE2	5:B:374:LYS:HB3	1.85	0.41
5:B:378:LEU:O	5:B:382:ILE:HG13	2.20	0.41
10:I:80:SER:OG	10:I:103:CYS:SG	2.78	0.41
4:A:111:GLY:HA3	4:A:213:HIS:O	2.21	0.41
4:A:494:SER:O	4:A:498:ARG:HG3	2.20	0.41
4:A:569:LYS:NZ	6:C:221:TYR:O	2.48	0.41
5:B:40:GLU:OE2	5:B:682:SER:N	2.46	0.41
5:B:46:GLN:H	5:B:46:GLN:HG3	1.62	0.41
4:A:262:LEU:HD13	4:A:323:LYS:HE2	2.01	0.41
4:A:374:LEU:O	4:A:436:ILE:HD13	2.21	0.41
4:A:501:LEU:HD13	4:A:501:LEU:HA	1.95	0.41
4:A:547:LEU:HD22	12:K:58:PHE:CD1	2.52	0.41
4:A:901:LEU:HG	4:A:929:LEU:HD12	2.02	0.41
4:A:1229:SER:OG	4:A:1233:ASP:OD1	2.34	0.41
5:B:521:LEU:HD13	5:B:633:VAL:HB	2.02	0.41
6:C:82:TYR:HD2	6:C:161:LYS:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:98:ILE:HD13	7:E:98:ILE:HA	1.89	0.41
11:J:57:ILE:O	11:J:61:LEU:HG	2.20	0.41
4:A:54:ASN:HB3	4:A:247:ARG:NH2	2.35	0.41
4:A:780:VAL:HG13	4:A:789:LYS:HE2	2.01	0.41
4:A:1433:MET:HG3	5:B:1144:ALA:HB1	2.01	0.41
6:C:73:GLN:HA	6:C:133:ILE:HD11	2.03	0.41
7:E:136:ASN:OD1	7:E:137:GLU:N	2.53	0.41
4:A:380:VAL:HG21	4:A:427:GLN:O	2.21	0.41
4:A:98:LYS:O	4:A:102:VAL:HG12	2.21	0.41
4:A:1268:LEU:HD23	4:A:1268:LEU:HA	1.83	0.41
5:B:568:ASP:OD1	5:B:568:ASP:N	2.54	0.41
5:B:636:PRO:HA	5:B:691:GLU:O	2.21	0.41
5:B:1084:GLN:OE1	6:C:192:TRP:N	2.35	0.41
6:C:242:GLN:O	6:C:246:ARG:HB2	2.21	0.41
7:E:147:HIS:HB3	7:E:150:VAL:HG23	2.03	0.41
9:H:25:ARG:HD2	9:H:39:THR:HG22	2.02	0.41
4:A:525:GLN:H	4:A:525:GLN:HG2	1.62	0.41
4:A:966:ASN:O	4:A:970:THR:OG1	2.29	0.41
11:J:25:LEU:O	11:J:29:GLU:HA	2.21	0.41
4:A:919:ILE:HA	4:A:919:ILE:HD12	1.87	0.40
4:A:1025:ARG:HE	4:A:1030:ARG:HH12	1.69	0.40
4:A:1287:TYR:CD1	4:A:1305:VAL:HG21	2.56	0.40
6:C:18:VAL:HG23	6:C:240:VAL:HG21	2.04	0.40
9:H:103:LYS:HB3	9:H:115:TYR:CD1	2.41	0.40
4:A:286:HIS:ND1	4:A:286:HIS:N	2.69	0.40
4:A:492:PRO:HB3	4:A:497:THR:HG22	2.04	0.40
4:A:1325:THR:O	7:E:148:GLU:HG3	2.22	0.40
4:A:1437:GLY:HA3	8:F:88:TYR:CD2	2.57	0.40
5:B:807:ARG:H	5:B:1045:SER:HB3	1.86	0.40
6:C:62:PHE:O	6:C:66:ARG:HG3	2.21	0.40
8:F:77:ASP:N	8:F:77:ASP:OD1	2.51	0.40
9:H:103:LYS:HD2	9:H:103:LYS:HA	1.89	0.40
4:A:760:GLN:NE2	4:A:765:VAL:O	2.41	0.40
4:A:1197:LEU:HD12	4:A:1209:MET:SD	2.60	0.40
5:B:193:LYS:HB3	5:B:787:VAL:HG11	2.03	0.40
7:E:66:GLU:HA	7:E:69:ILE:HG12	2.03	0.40
7:E:127:ILE:HB	7:E:130:ALA:HB3	2.03	0.40
12:K:10:PHE:CE1	12:K:11:LEU:HD11	2.55	0.40
12:K:24:ASP:OD2	12:K:74:ARG:HD2	2.21	0.40
4:A:231:PRO:HA	4:A:234:MET:HG3	2.03	0.40
5:B:408:LEU:HD12	5:B:408:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:601:ARG:HG3	5:B:615:MET:HE2	2.04	0.40
5:B:886:LYS:HB2	5:B:890:TYR:OH	2.21	0.40
4:A:682:THR:O	4:A:685:GLU:HG2	2.22	0.40
5:B:679:TYR:OH	5:B:687:GLU:OE1	2.34	0.40
5:B:845:SER:HB2	11:J:8:PHE:HB3	2.02	0.40
5:B:976:ILE:HD13	5:B:991:GLY:O	2.21	0.40
6:C:41:ILE:CD1	6:C:246:ARG:HB3	2.52	0.40
12:K:58:PHE:HE2	12:K:74:ARG:HE	1.66	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	
4	A	1370/1733 (79%)	1290 (94%)	80 (6%)	0	100	100
5	B	1111/1224 (91%)	1057 (95%)	54 (5%)	0	100	100
6	C	265/318 (83%)	253 (96%)	12 (4%)	0	100	100
7	E	210/215 (98%)	198 (94%)	12 (6%)	0	100	100
8	F	84/155 (54%)	81 (96%)	3 (4%)	0	100	100
9	H	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
10	I	116/122 (95%)	112 (97%)	4 (3%)	0	100	100
11	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
12	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
13	L	41/70 (59%)	41 (100%)	0	0	100	100
All	All	3501/4173 (84%)	3320 (95%)	181 (5%)	0	100	100

There are no Ramachandran outliers to report.

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
4	A	1193/1520 (78%)	1149 (96%)	44 (4%)	34 63
5	B	958/1061 (90%)	933 (97%)	25 (3%)	46 71
6	C	235/274 (86%)	231 (98%)	4 (2%)	60 78
7	E	193/197 (98%)	187 (97%)	6 (3%)	40 67
8	F	73/137 (53%)	72 (99%)	1 (1%)	67 82
9	H	116/128 (91%)	110 (95%)	6 (5%)	23 54
10	I	110/116 (95%)	108 (98%)	2 (2%)	59 78
11	J	60/65 (92%)	58 (97%)	2 (3%)	38 66
12	K	99/102 (97%)	96 (97%)	3 (3%)	41 68
13	L	37/57 (65%)	33 (89%)	4 (11%)	6 24
All	All	3074/3657 (84%)	2977 (97%)	97 (3%)	39 67

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	22	PHE
4	A	23	SER
4	A	36	ARG
4	A	64	ASN
4	A	81	PHE
4	A	83	HIS
4	A	167	CYS
4	A	185	TRP
4	A	265	LYS
4	A	270	LEU
4	A	286	HIS
4	A	350	ARG
4	A	356	ASP
4	A	394	ASN
4	A	408	ASP
4	A	427	GLN

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Mol	Chain	Res	Type
4	A	451	HIS
4	A	526	ASP
4	A	538	ASP
4	A	584	ASN
4	A	618	GLU
4	A	688	LYS
4	A	742	ASN
4	A	764	CYS
4	A	782	ARG
4	A	816	HIS
4	A	821	ARG
4	A	836	TYR
4	A	847	ASP
4	A	913	LEU
4	A	1001	ARG
4	A	1011	GLN
4	A	1025	ARG
4	A	1035	TYR
4	A	1074	GLU
4	A	1100	ARG
4	A	1150	SER
4	A	1215	ARG
4	A	1223	ASP
4	A	1309	ASP
4	A	1315	GLU
4	A	1366	ARG
4	A	1390	ASN
4	A	1399	ARG
5	B	46	GLN
5	B	133	LYS
5	B	217	ARG
5	B	228	LYS
5	B	241	ARG
5	B	333	PHE
5	B	351	TYR
5	B	404	LYS
5	B	510	LYS
5	B	568	ASP
5	B	605	ARG
5	B	642	ASP
5	B	651	LEU
5	B	728	ARG

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Mol	Chain	Res	Type
5	B	863	GLU
5	B	931	TYR
5	B	999	MET
5	B	1082	MET
5	B	1106	ARG
5	B	1150	ARG
5	B	1161	HIS
5	B	1180	PHE
5	B	1202	LEU
5	B	1210	MET
5	B	1220	ARG
6	C	34	ARG
6	C	131	HIS
6	C	137	LYS
6	C	231	ASN
7	E	29	PHE
7	E	33	GLU
7	E	48	ASP
7	E	84	ASP
7	E	110	PHE
7	E	123	LEU
8	F	111	LEU
9	H	36	CYS
9	H	78	SER
9	H	91	ASP
9	H	130	ARG
9	H	131	ASN
9	H	146	ARG
10	I	8	ARG
10	I	44	TYR
11	J	7	CYS
11	J	31	ASP
12	K	18	LYS
12	K	54	ARG
12	K	81	TYR
13	L	31	CYS
13	L	33	GLU
13	L	50	ASP
13	L	57	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	B	103	ASN
5	B	835	GLN
12	K	2	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	10	C

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	PPV	B	1301	-	6,8,8	0.75	0	13,13,13	1.09	0
15	5N0	T	101	-	93,107,107	2.34	32 (34%)	94,153,153	1.37	8 (8%)

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
17	PPV	B	1301	-	-	0/6/6/6	-
15	5N0	T	101	-	-	14/51/92/92	0/9/9/9

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	101	5N0	C49-N23	6.42	1.47	1.33
15	T	101	5N0	C22-N10	6.22	1.47	1.33
15	T	101	5N0	C56-N25	6.16	1.47	1.33
15	T	101	5N0	C26-N14	5.33	1.47	1.35
15	T	101	5N0	C5-N3	4.67	1.48	1.35
15	T	101	5N0	C43-N21	4.56	1.47	1.35
15	T	101	5N0	C10-N6	4.54	1.47	1.35
15	T	101	5N0	C30-C31	4.47	1.57	1.53
15	T	101	5N0	C16-N8	4.46	1.47	1.35
15	T	101	5N0	C6-C10	4.43	1.57	1.53
15	T	101	5N0	C31-N17	4.35	1.47	1.35
15	T	101	5N0	C37-N19	4.27	1.47	1.35
15	T	101	5N0	C4-C5	3.77	1.56	1.53
15	T	101	5N0	C9-N3	3.61	1.48	1.40
15	T	101	5N0	C21-N8	3.55	1.48	1.41
15	T	101	5N0	C14-N6	3.40	1.48	1.41
15	T	101	5N0	C42-N19	3.31	1.48	1.41
15	T	101	5N0	C36-N17	3.27	1.48	1.41
15	T	101	5N0	C48-N21	3.17	1.48	1.41
15	T	101	5N0	C29-N14	3.11	1.47	1.40
15	T	101	5N0	C2-N1	-2.64	1.33	1.37
15	T	101	5N0	C59-C63	2.41	1.54	1.49
15	T	101	5N0	C57-C56	2.35	1.55	1.50
15	T	101	5N0	O5-C26	-2.17	1.19	1.23
15	T	101	5N0	O10-C56	-2.12	1.19	1.23
15	T	101	5N0	O9-C49	-2.12	1.19	1.23
15	T	101	5N0	C30-N15	-2.07	1.31	1.34
15	T	101	5N0	O8-C43	-2.06	1.19	1.23
15	T	101	5N0	O6-C31	-2.04	1.19	1.23
15	T	101	5N0	O7-C37	-2.04	1.19	1.23
15	T	101	5N0	O3-C16	-2.01	1.19	1.23
15	T	101	5N0	O2-C10	-2.01	1.19	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	101	5N0	C6-C10-N6	5.84	120.03	113.69
15	T	101	5N0	C4-C5-N3	4.55	118.63	113.69
15	T	101	5N0	C24-C25-C26	-3.62	103.02	110.85
15	T	101	5N0	C30-C31-N17	2.94	116.88	113.69
15	T	101	5N0	C19-N9-C17	2.68	111.50	108.65
15	T	101	5N0	O4-C22-N10	-2.27	118.09	122.61
15	T	101	5N0	C3-N2-C4	2.09	109.14	104.01
15	T	101	5N0	O11-C63-C59	2.07	120.21	114.85

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	101	5N0	C23-C24-C25-C26
15	T	101	5N0	C24-C25-C26-N14
15	T	101	5N0	C47-C44-C49-O9
15	T	101	5N0	C58-C59-C63-O12
15	T	101	5N0	C60-C59-C63-O11
15	T	101	5N0	C60-C59-C63-O12
15	T	101	5N0	C58-C59-C63-O11
15	T	101	5N0	C50-C51-C52-N24
15	T	101	5N0	N11-C25-C26-O5
15	T	101	5N0	C24-C25-C26-O5
15	T	101	5N0	N11-C25-C26-N14
15	T	101	5N0	C53-C54-C55-N25
15	T	101	5N0	N10-C23-C24-C25
15	T	101	5N0	C23-C24-C25-N11

There are no ring outliers.

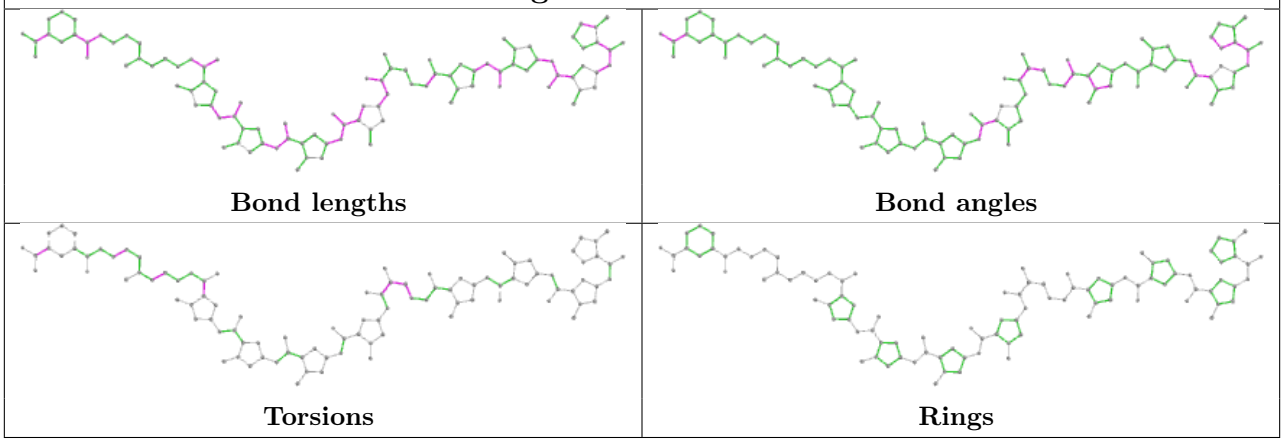
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	101	5N0	2	0

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 then 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.

Ligand 5N0 T 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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, 95^{th} 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	R	10/10 (100%)	-0.41	0 100 100	87, 103, 157, 163	0
2	T	26/30 (86%)	-0.10	1 (3%) 40 37	89, 211, 242, 259	0
3	N	14/20 (70%)	0.13	0 100 100	213, 220, 241, 246	0
4	A	1384/1733 (79%)	-0.10	25 (1%) 68 67	51, 105, 187, 235	0
5	B	1129/1224 (92%)	-0.07	15 (1%) 77 77	50, 88, 153, 189	0
6	C	267/318 (83%)	-0.31	0 100 100	59, 88, 128, 156	0
7	E	212/215 (98%)	0.04	12 (5%) 23 23	81, 149, 216, 230	0
8	F	86/155 (55%)	-0.29	0 100 100	74, 107, 153, 189	0
9	H	133/146 (91%)	0.19	5 (3%) 40 37	97, 138, 173, 195	0
10	I	118/122 (96%)	-0.29	0 100 100	71, 109, 146, 171	0
11	J	65/70 (92%)	-0.36	0 100 100	55, 81, 123, 141	0
12	K	114/120 (95%)	-0.27	0 100 100	67, 96, 128, 146	0
13	L	43/70 (61%)	0.20	3 (6%) 16 16	67, 143, 191, 209	0
All	All	3601/4233 (85%)	-0.10	61 (1%) 70 68	50, 101, 182, 259	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	106	ASP	4.9
7	E	93	MET	4.9
5	B	507	LYS	4.4
4	A	1387	HIS	4.3
5	B	869	SER	4.2
5	B	505	ASP	4.1
5	B	248	SER	4.1
5	B	508	LEU	4.1
5	B	504	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
7	E	126	SER	4.0
4	A	65	LEU	3.9
4	A	144	THR	3.7
13	L	45	ALA	3.6
4	A	69	THR	3.6
7	E	83	CYS	3.6
13	L	46	VAL	3.5
5	B	1172	ILE	3.4
7	E	110	PHE	3.4
4	A	152	VAL	3.1
4	A	286	HIS	3.1
7	E	121	MET	3.1
9	H	83	GLN	3.0
9	H	130	ARG	2.9
9	H	132	LEU	2.8
4	A	114	LEU	2.8
9	H	86	ASP	2.8
7	E	123	LEU	2.8
4	A	1126	ALA	2.7
4	A	141	LEU	2.7
5	B	506	GLY	2.7
7	E	122	LYS	2.7
5	B	475	SER	2.6
5	B	934	LYS	2.6
9	H	129	TYR	2.5
5	B	260	GLY	2.5
4	A	105	CYS	2.5
4	A	201	VAL	2.5
4	A	112	LYS	2.4
4	A	106	VAL	2.4
7	E	97	VAL	2.4
7	E	7	ARG	2.4
5	B	713	ALA	2.4
4	A	164	ARG	2.3
4	A	174	ILE	2.3
4	A	167	CYS	2.2
5	B	250	PHE	2.2
4	A	44	THR	2.2
4	A	59	GLY	2.2
4	A	1169	ILE	2.2
7	E	96	PHE	2.1
4	A	200	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	660	ASN	2.1
4	A	149	GLU	2.1
7	E	118	PRO	2.1
4	A	66	LYS	2.1
13	L	41	SER	2.1
5	B	92	PHE	2.1
4	A	176	LYS	2.0
7	E	82	PHE	2.0
4	A	108	MET	2.0
2	T	3	DT	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

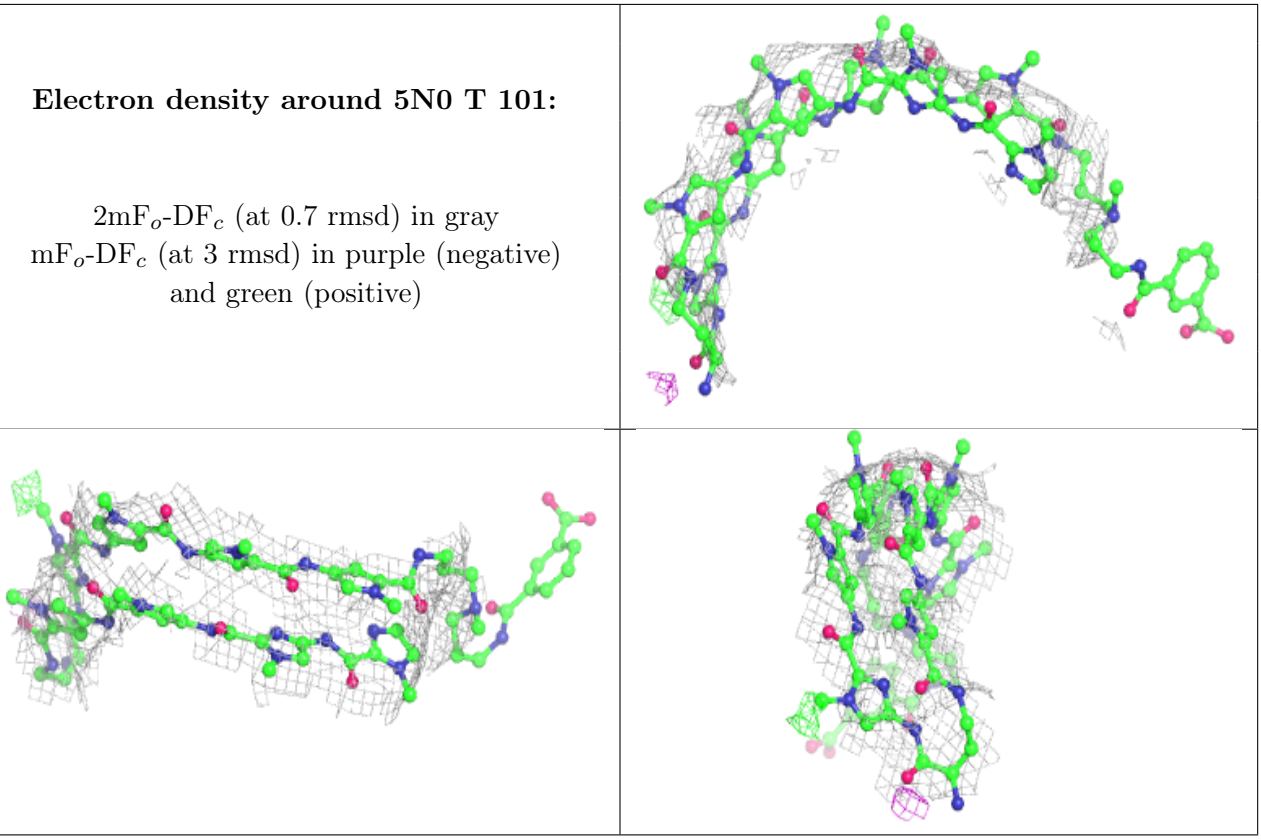
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	PPV	B	1301	9/9	0.73	0.33	175,175,175,175	0
15	5N0	T	101	99/99	0.80	0.36	184,225,251,258	0
16	ZN	A	1801	1/1	0.86	0.13	246,246,246,246	0
14	MG	R	2001	1/1	0.92	0.13	106,106,106,106	0
16	ZN	B	1302	1/1	0.94	0.09	184,184,184,184	0
16	ZN	L	101	1/1	0.96	0.04	164,164,164,164	0
16	ZN	C	401	1/1	0.97	0.13	82,82,82,82	0
16	ZN	J	101	1/1	0.97	0.21	77,77,77,77	0
16	ZN	I	201	1/1	0.98	0.14	97,97,97,97	0
16	ZN	I	202	1/1	0.99	0.15	93,93,93,93	0
16	ZN	A	1802	1/1	0.99	0.11	153,153,153,153	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 5N0 T 101:

$2mF_o$-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.