



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:46 PM UTC

PDB ID : 7RIY / pdb\_00007riy  
Title : RNA polymerase II elongation complex with hairpin polyamide Py-Im 1, scaffold 2 soaked with UTP  
Authors : Oh, J.; Dervan, P.B.; Wang, D.  
Deposited on : 2021-07-20  
Resolution : 3.70 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

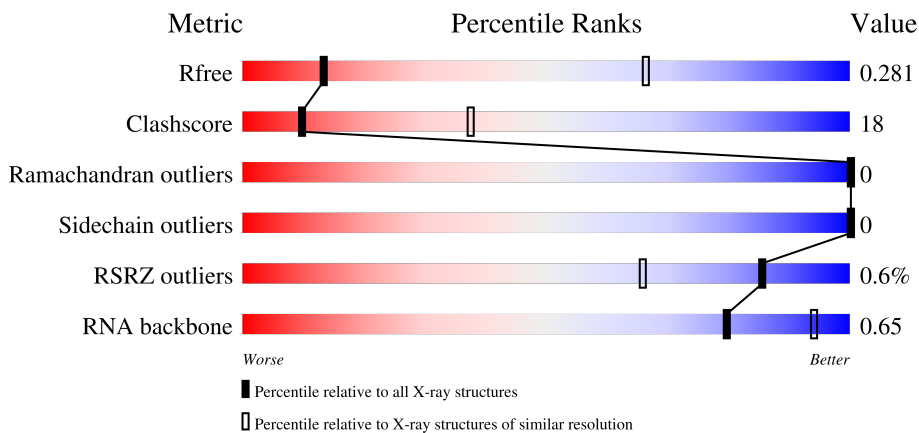
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






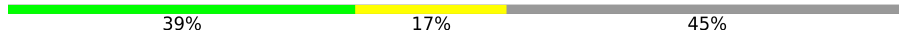


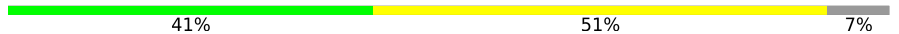

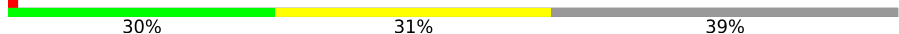
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)
RNA backbone	3983	1007 (4.30-3.08)

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  $\geq 3$ , 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	R	11	
2	T	30	
3	N	20	
4	A	1733	

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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 16 unique types of molecules in this entry. The entry contains 29168 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
			Total	C	N	O	P			
1	R	11	235	106	45	74	10	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	1384	10828	6831	1896	2041	60	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	1123	8859	5607	1552	1647	53	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

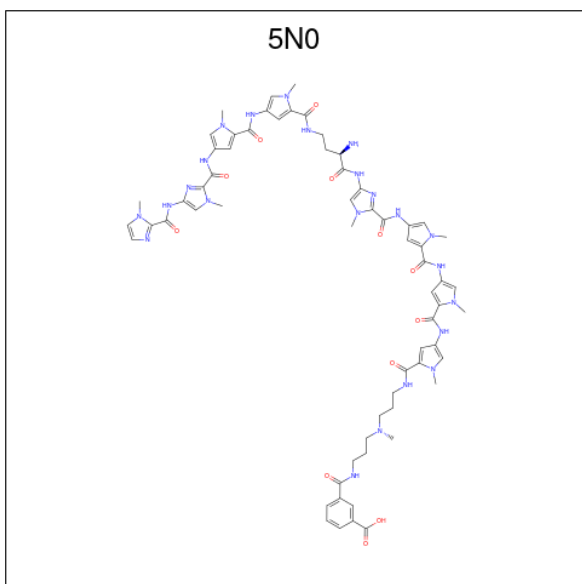
- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 14 is MAGNESIUM ION (CCD ID: 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-({(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}propyl)(methyl)amino]propyl}carbamoyl)benzoic acid (CCD ID: 5N0) (formula: C<sub>64</sub>H<sub>75</sub>N<sub>23</sub>O<sub>12</sub>) (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 (CCD ID: 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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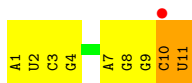
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
16	L	1	Total	Zn	0	0
			1	1		

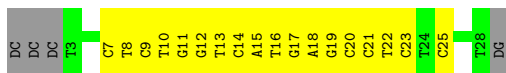
### 3 Residue-property plots [i](#)

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.

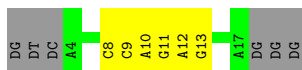
- Molecule 1: RNA



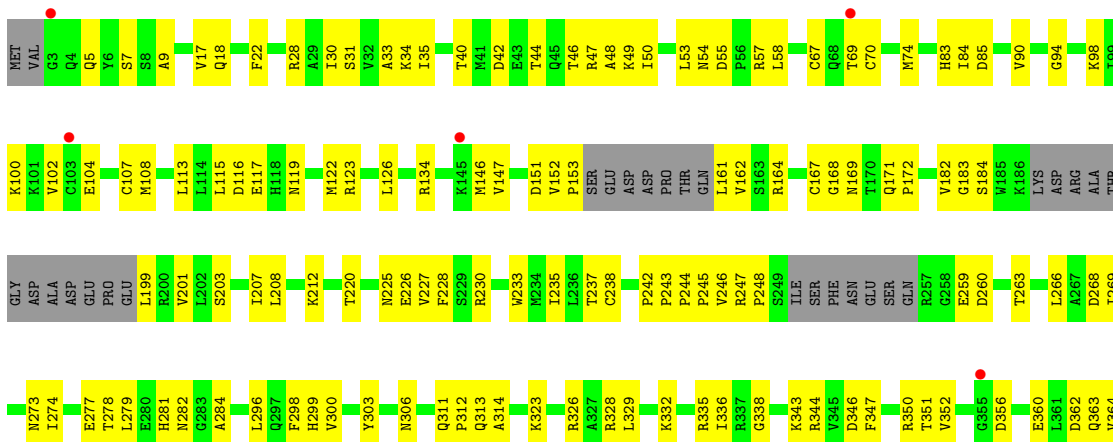
- Molecule 2: Template strand DNA



- Molecule 3: Non-template strand DNA



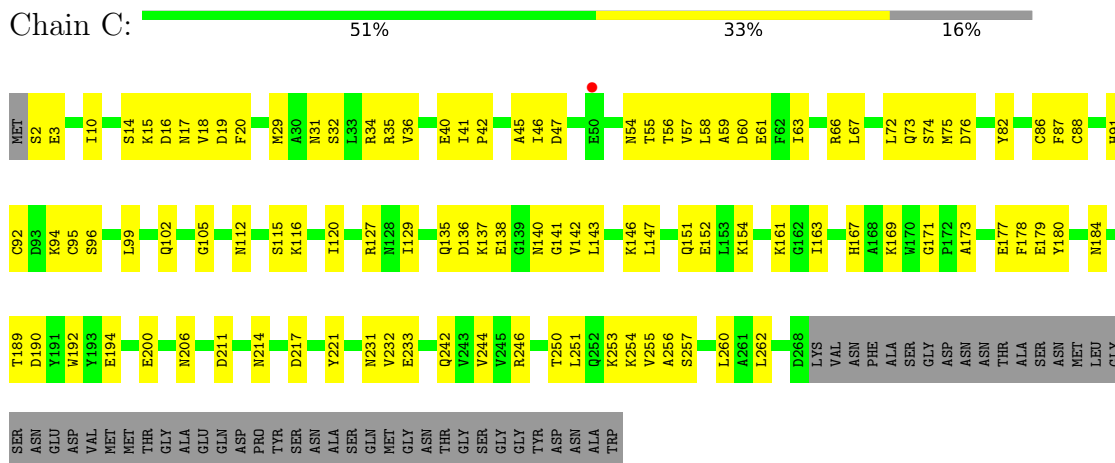
- Molecule 4: DNA-directed RNA polymerase II subunit RPB1



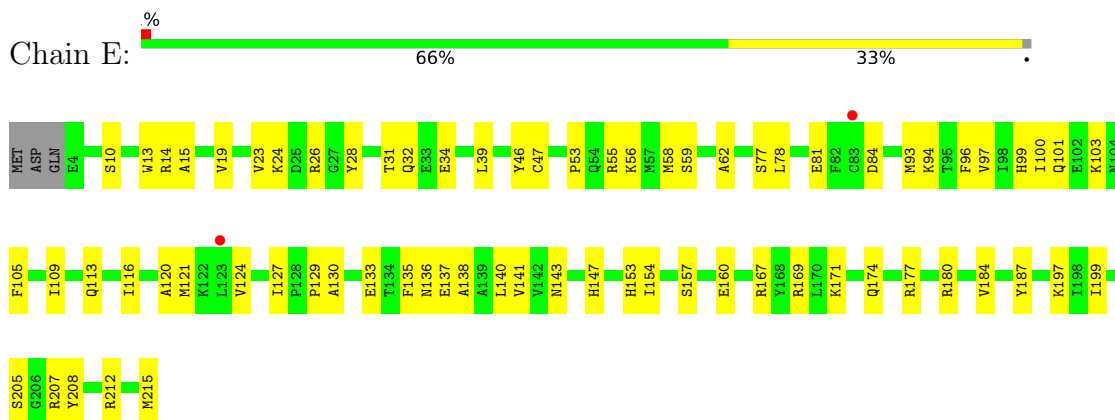
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THR	SER	GLY	GLY	THR	GLY	LEU	ASN	E1351	L1280	L1176	T1080	D985	K890	E795	F646	K567	M471	V366
PRO	PRO	GLY	THR	PRO	THR	ASP	THR	V1352	I1263	ASP	THR	K991	S882	E786	T649	S882	L472	P367
THR	PRO	GLY	THR	PRO	THR	GLU	PHE	V1355	M1287	GLU	PHE	L993	D884	K797	O650	K569	V474	K368
SER	PRO	ALA	ALA	TYR	ALA	ALA	ALA	V1356	I1271	GLU	ALA	L998	G888	V800	V653	L571	Y478	A371
PRO	PRO	VAL	VAL	TYR	GLY	GLU	ALA	A1357	T1272	GLU	ALA	R1001	S889	E807	N660	S573	M479	K372
THR	PRO	TYR	TYR	PRO	GLY	SER	VAL	M1364	L1273	GLN	GLY	R1002	D890	G574	G661	G574	A490	Y376
PRO	PRO	ALA	ALA	PRO	GLY	PHE	VAL	R1365	R1274	SER	VAL	G1002	F662	K575	F662	D483	P377	P377
ASN	PRO	ASP	PRO	PRO	ASP	ASP	ALA	R1366	G1275	ASP	SER	M1004	R898	O576	S663	O576	E378	E378
TYR	SER	GLU	GLU	TYR	GLU	GLN	K1092	V1276	V1276	GLN	K1092	M1004	D900	L806	D668	L577	M487	V379
SER	PRO	GLN	GLN	TYR	GLY	S1188	T1095	E1277	M1278	GLY	T1095	Q1008	L901	G807	S579	L576	M488	V380
PRO	PRO	LYS	LYS	PRO	THR	S1189	L1190	E1278	M1278	S1189	L902	R1012	L902	L808	D672	L582	V491	D386
PRO	PRO	ILE	ILE	PRO	THR	W1191	L1105	E1280	E1280	W1191	L1105	R1012	N903	L808	D672	L582	R387	R387
PRO	PRO	THR	THR	PRO	THR	L1192	M1106	R1281	R1281	L1192	M1106	T1016	T907	T809	T675	G585	S494	L388
PRO	PRO	GLU	GLU	PRO	GLU	L1193	V1107	K1286	K1286	L1193	V1107	L1021	T907	P810	T675	G585	E496	L388
PRO	PRO	ILE	ILE	PRO	GLU	R1194	K1112	K1286	K1286	R1194	K1112	L1021	Q926	E812	I683	H587	V392	V392
TYR	PRO	GLU	GLU	PRO	PHE	D1206	L1116	E1291	E1291	D1206	L1116	L1022	Q926	H816	K689	H587	P396	P396
PRO	PRO	ASP	ASP	PRO	GLY	P1292	L1117	P1292	P1292	P1292	L1117	R1023	L929	D592	D592	D592	R498	R498
PRO	PRO	GLN	GLN	PRO	GLY	V1212	T1118	G1296	G1296	V1212	T1118	S1025	D930	E500	E500	E500	K403	K403
PRO	PRO	GLY	GLY	PRO	GLU	R1215	Y1119	E1297	E1297	R1215	Y1119	L1026	D930	T595	T595	T595	R407	R407
PRO	PRO	VAL	VAL	PRO	GLY	I1216	L1120	F1389	F1389	I1216	L1120	A1027	R940	L597	A506	A506	D408	D408
PRO	PRO	THR	THR	PRO	THR	T1219	E1121	M1390	M1390	T1219	E1121	A1027	R940	S409	A506	A506	S409	S409
PRO	PRO	THR	THR	PRO	THR	P1122	P1122	L1397	L1397	P1122	P1122	R1029	R941	V507	V507	V507	V507	V507
PRO	PRO	TVR	TVR	PRO	GLY	A1125	A1125	M1398	M1398	A1125	A1125	R1030	F942	I424	I424	I424	I424	I424
PRO	PRO	ASN	ASN	PRO	GLY	L1224	L1224	R1399	R1399	L1224	L1224	V1031	F942	Q427	Q427	Q427	Q427	Q427
PRO	PRO	ASN	ASN	PRO	PHE	S1229	Q1130	C1400	C1400	S1229	Q1130	E1034	E945	Q515	Q515	Q515	Q515	Q515
PRO	PRO	GLU	GLU	PRO	GLY	E1230	A1131	F1402	F1402	E1230	A1131	A1041	E951	Q525	Q525	Q525	Q525	Q525
PRO	PRO	GLY	GLY	PRO	VAL	K1233	K1132	F1402	F1402	K1233	K1132	A1041	E951	D526	D526	D526	D526	D526
PRO	PRO	GLY	GLY	PRO	SER	L1236	L1133	E1403	E1403	L1236	L1133	W1044	E951	H435	H435	H435	H435	H435
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PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	F1410	F1410	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ALA	ALA	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ALA	ALA	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
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PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
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PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
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PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
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PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L1133	E1411	E1411	L1236	L1133	V1045	E951	H435	H435	H435	H435	H435
PRO	PRO	ASN	ASN	PRO	GLY	L1236	L113											



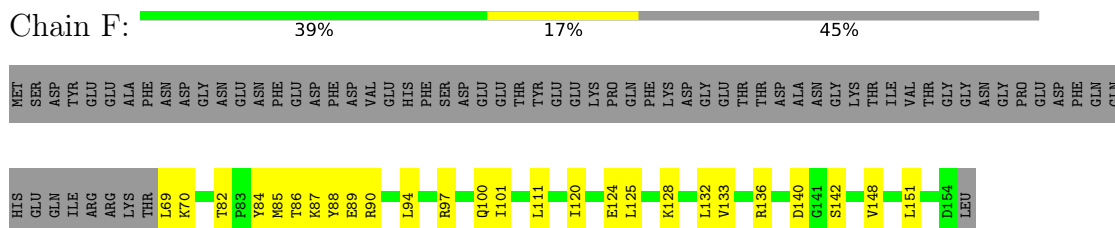
- Molecule 6: DNA-directed RNA polymerase II subunit RPB3



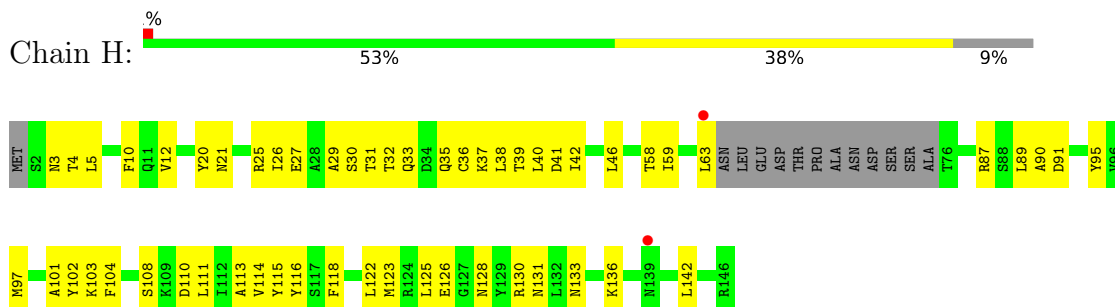
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



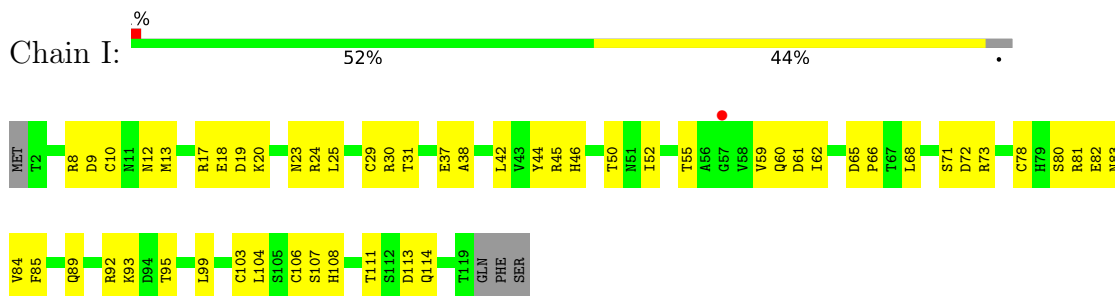
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



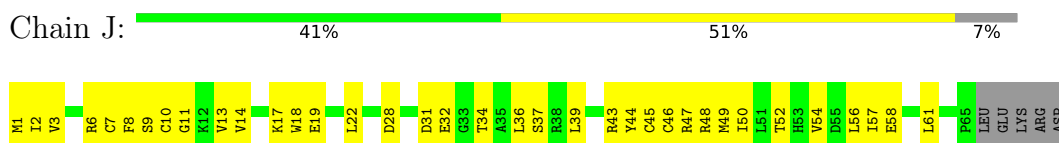
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



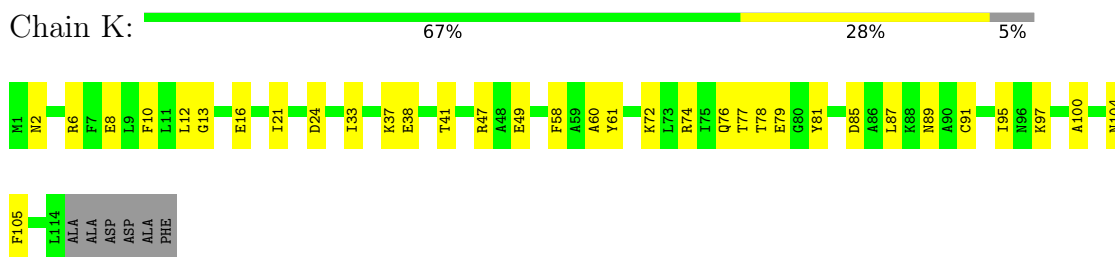
- Molecule 10: DNA-directed RNA polymerase II subunit RPB9



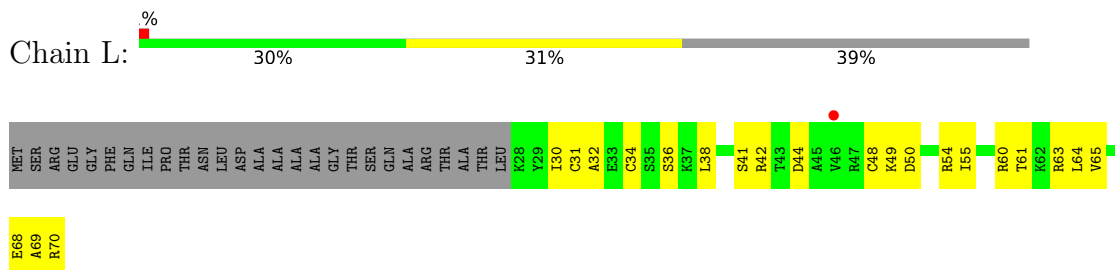
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- 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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.78Å 222.76Å 192.96Å 90.00° 100.54° 90.00°	Depositor
Resolution (Å)	49.53 – 3.70 49.53 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.53-3.70) 99.8 (49.53-3.70)	Depositor EDS
$R_{merge}$	0.52	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 3.67Å)	Xtrriage
Refinement program	PHENIX 1.13	Depositor
R, $R_{free}$	0.232 , 0.281 0.234 , 0.281	Depositor DCC
$R_{free}$ test set	2000 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	106.3	Xtrriage
Anisotropy	0.319	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 89.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	29168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 5N0, MG, 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	0.20	0/263	0.48	0/409
2	T	0.30	0/584	0.51	0/898
3	N	0.19	0/331	0.35	0/509
4	A	0.23	0/11020	0.42	0/14907
5	B	0.22	0/9030	0.42	0/12186
6	C	0.22	0/2139	0.41	0/2899
7	E	0.21	0/1767	0.41	0/2378
8	F	0.21	0/696	0.40	0/943
9	H	0.20	0/1082	0.44	0/1466
10	I	0.22	0/970	0.43	0/1308
11	J	0.23	0/541	0.43	0/727
12	K	0.23	0/937	0.41	0/1265
13	L	0.19	0/339	0.45	0/450
All	All	0.22	0/29699	0.42	0/40345

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	235	0	121	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	525	0	297	31	0
3	N	293	0	156	9	0
4	A	10828	0	10876	399	0
5	B	8859	0	8816	356	0
6	C	2101	0	2056	91	0
7	E	1731	0	1758	51	0
8	F	684	0	692	29	0
9	H	1064	0	1029	42	0
10	I	952	0	897	45	0
11	J	532	0	542	36	0
12	K	919	0	929	30	0
13	L	337	0	352	16	0
14	R	1	0	0	0	0
15	T	99	0	0	5	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
All	All	29168	0	28521	1011	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 18.

All (1011) 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:446:ARG:NH2	4:A:480:ALA:HA	1.53	1.23
4:A:446:ARG:HH21	4:A:480:ALA:CA	1.76	0.98
4:A:446:ARG:HH21	4:A:480:ALA:HA	0.79	0.94
11:J:10:CYS:SG	11:J:43:ARG:NH2	2.46	0.89
4:A:1224:LEU:HD11	4:A:1240:CYS:HB3	1.57	0.84
4:A:757:ASN:HD22	5:B:1021:MET:HE2	1.44	0.82
5:B:118:ARG:NH1	5:B:209:GLU:OE1	2.12	0.82
4:A:848:ILE:HG21	4:A:1370:LEU:HD21	1.62	0.80
5:B:400:HIS:NE2	5:B:699:GLU:OE1	2.13	0.80
4:A:54:ASN:HD22	4:A:244:PRO:HG3	1.46	0.80
5:B:34:ILE:HG23	5:B:542:MET:HE3	1.64	0.80
4:A:7:SER:HA	5:B:1175:LEU:HD11	1.65	0.79
6:C:54:ASN:ND2	6:C:60:ASP:OD1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:43:ARG:NH2	11:J:46:CYS:SG	2.56	0.79
4:A:503:GLN:OE1	8:F:90:ARG:NH2	2.16	0.79
5:B:995:ARG:NH1	5:B:997:GLU:OE1	2.16	0.78
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.16	0.78
5:B:604:ARG:NH2	5:B:613:VAL:O	2.16	0.78
4:A:1385:THR:HG22	4:A:1386:ARG:H	1.47	0.78
4:A:1076:ALA:HA	4:A:1079:MET:HE2	1.64	0.77
6:C:17:ASN:HB3	6:C:233:GLU:HG2	1.68	0.76
7:E:14:ARG:HH11	7:E:141:VAL:HG12	1.51	0.76
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.66	0.76
4:A:738:LYS:HE3	6:C:194:GLU:HA	1.69	0.74
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	1.68	0.74
4:A:1437:GLY:HA3	8:F:88:TYR:HD2	1.53	0.74
10:I:111:THR:HG22	10:I:113:ASP:H	1.51	0.74
4:A:929:LEU:HD21	4:A:983:ILE:HG21	1.70	0.74
2:T:15:DA:H2'	2:T:16:DT:C6	2.23	0.74
4:A:55:ASP:O	4:A:57:ARG:N	2.21	0.73
4:A:800:VAL:HG13	4:A:812:GLU:HB3	1.70	0.73
2:T:21:DC:H5'	5:B:1129:ARG:HD3	1.70	0.73
9:H:128:ASN:OD1	9:H:131:ASN:ND2	2.21	0.73
5:B:1084:GLN:NE2	6:C:190:ASP:O	2.21	0.72
5:B:104:GLU:OE2	13:L:54:ARG:NH1	2.22	0.72
5:B:996:ARG:HH12	6:C:173:ALA:HB1	1.54	0.72
5:B:173:MET:O	5:B:176:SER:OG	2.05	0.72
5:B:834:ASN:HB3	5:B:840:ILE:HG13	1.68	0.72
4:A:608:ILE:HB	4:A:613:ILE:HD11	1.70	0.72
7:E:56:LYS:HE2	7:E:84:ASP:HB3	1.72	0.71
5:B:67:SER:HB2	5:B:92:PHE:HD1	1.54	0.71
4:A:506:ALA:HB3	4:A:509:LEU:HG	1.71	0.71
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.24	0.71
5:B:996:ARG:NH2	6:C:173:ALA:O	2.24	0.71
9:H:103:LYS:HB3	9:H:115:TYR:HD1	1.54	0.71
5:B:942:ARG:HB2	5:B:945:GLU:HG3	1.73	0.70
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.70	0.70
7:E:127:ILE:HG22	7:E:129:PRO:HD2	1.72	0.70
4:A:562:THR:O	4:A:576:GLN:NE2	2.24	0.70
6:C:86:CYS:SG	6:C:87:PHE:N	2.64	0.70
5:B:213:ILE:O	5:B:215:GLN:NE2	2.24	0.70
4:A:5:GLN:O	5:B:1159:ARG:NH2	2.26	0.69
2:T:7:DC:H2''	2:T:8:DT:H5''	1.74	0.69
4:A:660:ASN:ND2	5:B:1082:MET:HB3	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:636:GLU:OE2	4:A:966:ASN:ND2	2.25	0.69
5:B:287:ARG:NH1	5:B:324:ILE:O	2.24	0.69
12:K:58:PHE:HE2	12:K:74:ARG:HE	1.38	0.69
5:B:882:THR:OG1	5:B:885:MET:SD	2.51	0.69
6:C:40:GLU:OE1	6:C:254:LYS:HE2	1.93	0.69
4:A:167:CYS:SG	4:A:168:GLY:N	2.66	0.68
4:A:579:SER:HB3	4:A:612:ILE:HG22	1.76	0.68
4:A:67:CYS:HB3	4:A:70:CYS:HB3	1.76	0.68
4:A:183:GLY:O	4:A:199:LEU:N	2.27	0.68
4:A:134:ARG:NH2	4:A:220:THR:O	2.26	0.68
4:A:362:ASP:OD1	4:A:459:ARG:NH1	2.27	0.68
4:A:500:GLU:OE2	5:B:1145:SER:OG	2.11	0.67
5:B:332:ASP:OD1	5:B:348:ARG:NH2	2.27	0.67
4:A:1385:THR:HG22	4:A:1386:ARG:N	2.08	0.67
5:B:629:ASP:O	5:B:632:ARG:NH1	2.27	0.67
4:A:329:LEU:HA	4:A:335:ARG:H	1.60	0.67
4:A:1390:ASN:O	4:A:1399:ARG:NH1	2.27	0.67
4:A:281:HIS:ND1	4:A:282:ASN:OD1	2.27	0.67
4:A:17:VAL:HG22	5:B:1216:LEU:HD22	1.76	0.67
4:A:446:ARG:HB2	4:A:487:MET:HE2	1.76	0.67
5:B:287:ARG:NH2	5:B:294:ASP:OD2	2.28	0.67
5:B:613:VAL:HG23	5:B:628:THR:HG22	1.77	0.67
4:A:338:GLY:HA2	5:B:1129:ARG:HH22	1.59	0.67
4:A:983:ILE:HG23	4:A:1028:THR:HG21	1.75	0.67
11:J:9:SER:OG	11:J:48:ARG:NH2	2.27	0.67
9:H:37:LYS:H	9:H:126:GLU:HG2	1.60	0.67
5:B:892:LYS:NZ	5:B:904:ARG:O	2.28	0.67
4:A:146:MET:HG3	4:A:147:VAL:HG23	1.76	0.67
13:L:38:LEU:HD21	13:L:48:CYS:HA	1.75	0.67
2:T:13:DT:H2'	2:T:14:DC:C6	2.30	0.66
5:B:219:ALA:HB2	5:B:405:ARG:HD3	1.77	0.66
5:B:619:ILE:HD12	10:I:65:ASP:HB2	1.77	0.66
1:R:11:U:O2'	5:B:1019:SER:OG	2.11	0.66
4:A:1352:VAL:O	4:A:1356:ILE:HD13	1.94	0.66
12:K:100:ALA:O	12:K:104:ASN:ND2	2.28	0.66
5:B:744:HIS:ND1	5:B:746:SER:OG	2.25	0.66
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.78	0.66
5:B:824:ILE:HG22	5:B:1008:PRO:HA	1.76	0.66
5:B:29:ASP:OD2	5:B:655:LYS:NZ	2.21	0.65
6:C:40:GLU:OE1	6:C:254:LYS:CE	2.45	0.65
10:I:29:CYS:SG	10:I:30:ARG:N	2.68	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:2:SER:OG	6:C:3:GLU:N	2.29	0.65
4:A:1397:LEU:HB2	4:A:1426:GLU:HG3	1.77	0.65
4:A:1345:ARG:NH1	4:A:1373:ASP:OD1	2.25	0.65
4:A:660:ASN:HD21	5:B:1082:MET:HB3	1.61	0.65
6:C:16:ASP:OD2	6:C:135:GLN:NE2	2.29	0.65
1:R:3:C:H2'	1:R:4:G:C8	2.32	0.65
4:A:306:ASN:ND2	4:A:313:GLN:O	2.25	0.65
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.79	0.65
5:B:115:GLN:NE2	5:B:193:LYS:O	2.30	0.65
5:B:402:GLY:HA3	5:B:696:GLU:HG2	1.79	0.65
5:B:56:ASP:OD2	5:B:177:LYS:NZ	2.29	0.65
2:T:19:DG:H2'	2:T:20:DC:C6	2.31	0.64
5:B:216:GLU:OE1	5:B:537:LYS:NZ	2.31	0.64
5:B:232:SER:O	5:B:261:ARG:NH2	2.31	0.64
5:B:254:LEU:HD23	5:B:381:MET:HE1	1.78	0.64
7:E:177:ARG:O	7:E:212:ARG:NH2	2.29	0.64
8:F:82:THR:HG22	8:F:84:TYR:H	1.62	0.64
5:B:640:VAL:HA	5:B:651:LEU:HA	1.80	0.64
4:A:247:ARG:NH1	4:A:263:THR:OG1	2.31	0.64
5:B:176:SER:O	5:B:182:SER:OG	2.12	0.64
5:B:208:SER:OG	5:B:210:LYS:NZ	2.27	0.64
4:A:795:GLU:HG3	5:B:731:VAL:HG11	1.80	0.64
4:A:1276:VAL:HG12	4:A:1277:GLU:H	1.62	0.63
4:A:1341:ILE:HD13	4:A:1380:GLY:HA2	1.79	0.63
4:A:537:ARG:NH1	4:A:602:ASP:OD1	2.31	0.63
4:A:365:GLY:HA3	4:A:469:ARG:HB2	1.79	0.63
5:B:566:LEU:HD13	5:B:588:GLY:HA2	1.80	0.63
5:B:63:ILE:HA	5:B:421:PHE:HE2	1.63	0.63
7:E:24:LYS:NZ	7:E:32:GLN:OE1	2.26	0.63
13:L:34:CYS:SG	13:L:36:SER:OG	2.53	0.63
1:R:3:C:H2'	1:R:4:G:H8	1.61	0.63
5:B:496:ARG:NH1	5:B:540:SER:O	2.31	0.63
5:B:1006:ILE:HD11	11:J:43:ARG:HB3	1.80	0.63
4:A:456:MET:HE3	4:A:507:VAL:HG22	1.81	0.63
4:A:541:ILE:HD12	4:A:577:ILE:HG21	1.81	0.63
4:A:663:SER:O	4:A:742:ASN:ND2	2.32	0.63
4:A:1062:GLU:OE2	8:F:88:TYR:OH	2.16	0.63
6:C:169:LYS:NZ	13:L:69:ALA:O	2.25	0.63
4:A:153:PRO:HA	4:A:161:LEU:HB2	1.80	0.62
4:A:582:ILE:HG22	4:A:610:GLY:HA2	1.80	0.62
4:A:888:GLY:O	4:A:940:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:11:DG:H2''	2:T:12:DG:C8	2.34	0.62
4:A:825:ILE:HD13	5:B:512:ARG:HB2	1.81	0.62
5:B:680:THR:O	5:B:683:SER:OG	2.15	0.62
4:A:44:THR:OG1	4:A:46:THR:OG1	2.17	0.62
4:A:182:VAL:HG12	4:A:201:VAL:HA	1.81	0.62
4:A:547:LEU:HB3	12:K:58:PHE:HE1	1.63	0.62
4:A:882:SER:H	4:A:961:ARG:HH12	1.48	0.62
4:A:1165:GLU:OE2	4:A:1235:LYS:NZ	2.33	0.62
5:B:848:ARG:NH1	11:J:8:PHE:O	2.32	0.62
6:C:32:SER:OG	12:K:41:THR:O	2.16	0.62
4:A:807:GLY:HA2	5:B:761:HIS:CD2	2.35	0.62
4:A:1130:GLN:O	4:A:1134:ILE:HG12	1.99	0.62
5:B:612:GLU:O	5:B:632:ARG:NH2	2.32	0.62
2:T:22:DT:OP1	4:A:344:ARG:NH1	2.32	0.62
4:A:31:SER:O	5:B:1183:LYS:NZ	2.27	0.62
4:A:840:ARG:NH2	4:A:1106:ASN:OD1	2.32	0.62
2:T:19:DG:H2'	2:T:20:DC:H6	1.64	0.62
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.81	0.62
4:A:1212:VAL:O	4:A:1216:ILE:HG13	1.99	0.62
4:A:1312:ASN:ND2	4:A:1315:GLU:OE2	2.32	0.62
5:B:542:MET:HE1	5:B:743:ILE:HG21	1.81	0.62
10:I:44:TYR:HE1	10:I:46:HIS:HB2	1.64	0.62
4:A:445:ASN:HB2	4:A:455:MET:HG2	1.82	0.61
5:B:481:GLN:OE1	5:B:494:HIS:NE2	2.25	0.61
2:T:16:DT:H2'	2:T:17:DG:C8	2.35	0.61
5:B:519:TRP:CZ2	5:B:705:MET:HE1	2.35	0.61
2:T:17:DG:C2	2:T:18:DA:C8	2.89	0.61
5:B:1135:ARG:NH2	5:B:1136:ASP:OD1	2.31	0.61
6:C:242:GLN:OE1	6:C:246:ARG:NH2	2.33	0.61
7:E:47:CYS:HA	7:E:53:PRO:HA	1.80	0.61
5:B:255:GLN:H	5:B:272:THR:HG22	1.65	0.61
5:B:299:GLU:CD	5:B:572:HIS:HD1	2.09	0.61
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.35	0.61
13:L:32:ALA:HB3	13:L:55:ILE:HD12	1.82	0.61
6:C:66:ARG:NH1	6:C:143:LEU:O	2.33	0.61
7:E:26:ARG:NH2	7:E:133:GLU:OE1	2.29	0.61
4:A:1323:ASP:OD1	4:A:1325:THR:OG1	2.19	0.61
7:E:55:ARG:NH2	7:E:137:GLU:OE1	2.34	0.61
2:T:18:DA:H2'	2:T:18:DA:N3	2.16	0.61
4:A:407:ARG:NH2	4:A:409:SER:OG	2.33	0.61
5:B:117:ALA:HA	5:B:122:LEU:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1033:LYS:NZ	5:B:1087:PHE:O	2.32	0.61
6:C:184:ASN:ND2	6:C:189:THR:O	2.31	0.61
5:B:1082:MET:HA	6:C:189:THR:HA	1.82	0.60
8:F:128:LYS:NZ	8:F:151:LEU:O	2.33	0.60
4:A:1355:VAL:HG23	4:A:1356:ILE:HD12	1.82	0.60
5:B:309:GLN:OE1	5:B:392:ARG:NH2	2.34	0.60
8:F:97:ARG:NH2	8:F:124:GLU:OE2	2.29	0.60
5:B:822:ASN:O	11:J:48:ARG:NH1	2.32	0.60
4:A:367:PRO:HD2	4:A:370:ILE:HD12	1.84	0.60
4:A:713:SER:O	4:A:717:ASN:ND2	2.34	0.60
4:A:765:VAL:HG11	4:A:804:TYR:CD2	2.37	0.60
7:E:143:ASN:ND2	7:E:187:TYR:OH	2.35	0.60
5:B:851:PHE:HB3	5:B:1094:ARG:HD2	1.83	0.60
5:B:227:LYS:N	5:B:395:GLN:OE1	2.28	0.60
5:B:798:TYR:O	5:B:821:GLN:NE2	2.33	0.60
2:T:12:DG:H2''	2:T:13:DT:H5''	1.84	0.60
6:C:56:THR:HG22	6:C:147:LEU:HD21	1.83	0.60
4:A:369:SER:OG	12:K:2:ASN:OD1	2.19	0.60
4:A:1276:VAL:HB	4:A:1279:ILE:HD13	1.84	0.60
7:E:81:GLU:HB3	7:E:96:PHE:HE1	1.66	0.60
4:A:273:ASN:ND2	4:A:277:GLU:OE2	2.33	0.59
4:A:808:LEU:O	5:B:728:ARG:NH1	2.34	0.59
6:C:179:GLU:OE1	6:C:206:ASN:ND2	2.35	0.59
4:A:526:ASP:OD1	5:B:1013:ASN:ND2	2.31	0.59
5:B:384:ARG:NH2	5:B:623:GLU:OE2	2.34	0.59
4:A:771:GLU:N	4:A:822:GLU:OE2	2.33	0.59
5:B:259:TYR:HB2	5:B:268:THR:HG23	1.83	0.59
5:B:1213:THR:OG1	5:B:1215:ARG:NH2	2.35	0.59
10:I:50:THR:HG22	10:I:52:ILE:H	1.66	0.59
4:A:167:CYS:SG	4:A:169:ASN:ND2	2.64	0.59
4:A:306:ASN:ND2	4:A:313:GLN:OE1	2.35	0.59
5:B:519:TRP:HZ2	5:B:705:MET:HE1	1.68	0.59
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.83	0.59
5:B:759:PRO:HD2	5:B:1046:PRO:HG3	1.85	0.59
5:B:995:ARG:HD3	12:K:6:ARG:HH12	1.67	0.59
6:C:47:ASP:OD1	13:L:70:ARG:NH1	2.33	0.59
5:B:996:ARG:NH1	6:C:173:ALA:HB1	2.17	0.59
4:A:533:LYS:HE2	4:A:745:GLN:OE1	2.02	0.59
5:B:242:SER:HB2	5:B:362:PRO:HD2	1.85	0.59
6:C:17:ASN:HA	6:C:232:VAL:O	2.03	0.59
4:A:607:ILE:HG12	4:A:612:ILE:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:376:TYR:CZ	4:A:498:ARG:HD2	2.38	0.59
5:B:60:GLN:NE2	5:B:64:CYS:SG	2.76	0.59
5:B:179:CYS:O	5:B:182:SER:OG	2.21	0.59
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.83	0.59
5:B:499:ASN:OD1	5:B:500:THR:N	2.36	0.59
4:A:898:ARG:O	4:A:1029:ARG:NH1	2.35	0.59
4:A:74:MET:O	5:B:1116:ARG:NH2	2.36	0.59
4:A:351:THR:OG1	4:A:352:VAL:N	2.36	0.59
4:A:1165:GLU:OE1	4:A:1194:ARG:NH2	2.36	0.59
4:A:1276:VAL:HG11	4:A:1316:VAL:HG22	1.85	0.58
5:B:27:ALA:O	5:B:30:SER:OG	2.18	0.58
5:B:600:LEU:HB3	5:B:615:MET:HE3	1.85	0.58
5:B:797:TYR:O	11:J:1:MET:N	2.36	0.58
4:A:274:ILE:O	4:A:278:THR:OG1	2.18	0.58
4:A:707:GLY:O	4:A:1281:ARG:NH1	2.36	0.58
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.36	0.58
4:A:1351:GLU:O	4:A:1355:VAL:HG13	2.03	0.58
5:B:620:ARG:NH2	10:I:89:GLN:OE1	2.35	0.58
5:B:857:ARG:NH1	5:B:945:GLU:OE2	2.36	0.58
5:B:1082:MET:HG3	6:C:189:THR:HA	1.85	0.58
6:C:94:LYS:HA	6:C:127:ARG:HH22	1.67	0.58
7:E:113:GLN:HG3	7:E:137:GLU:HB2	1.85	0.58
4:A:979:SER:OG	4:A:980:ASP:N	2.34	0.58
5:B:653:VAL:HG12	5:B:689:LEU:HB3	1.84	0.58
4:A:810:PRO:HB2	5:B:705:MET:HE2	1.86	0.58
4:A:841:LEU:HD21	4:A:1105:LEU:HD22	1.85	0.58
10:I:18:GLU:OE2	10:I:20:LYS:NZ	2.31	0.58
10:I:59:VAL:H	10:I:62:ILE:HD13	1.69	0.58
8:F:97:ARG:NH1	8:F:100:GLN:OE1	2.27	0.58
9:H:33:GLN:HB3	9:H:35:GLN:HE22	1.69	0.58
10:I:29:CYS:SG	10:I:31:THR:N	2.73	0.58
4:A:961:ARG:HH11	4:A:1025:ARG:HH22	1.50	0.58
9:H:118:PHE:CZ	9:H:142:LEU:HD12	2.39	0.58
4:A:151:ASP:OD1	4:A:164:ARG:N	2.35	0.57
5:B:1073:TYR:CE2	5:B:1080:LYS:HG2	2.39	0.57
4:A:592:ASP:H	4:A:595:THR:HG21	1.67	0.57
5:B:41:LYS:NZ	5:B:692:TYR:OH	2.27	0.57
5:B:373:ARG:HE	5:B:567:GLU:CD	2.12	0.57
4:A:1118:VAL:HG22	4:A:1327:ILE:HD11	1.86	0.57
4:A:343:LYS:NZ	5:B:1156:ASP:OD2	2.37	0.57
4:A:515:GLN:HB2	4:A:1071:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:960:ILE:HG23	4:A:964:ILE:HD13	1.86	0.57
5:B:25:ILE:HG21	5:B:653:VAL:HG23	1.86	0.57
5:B:128:LEU:HD21	5:B:170:LEU:HB2	1.85	0.57
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.87	0.57
4:A:40:THR:HA	4:A:53:LEU:HD23	1.85	0.57
4:A:446:ARG:NH2	4:A:479:ASN:O	2.36	0.57
8:F:111:LEU:HD23	8:F:111:LEU:H	1.70	0.57
12:K:85:ASP:O	12:K:89:ASN:ND2	2.33	0.57
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.86	0.57
7:E:99:HIS:CD2	7:E:103:LYS:HG3	2.39	0.57
4:A:596:THR:HG22	4:A:598:LEU:H	1.68	0.57
4:A:884:ASP:OD2	4:A:1030:ARG:NH2	2.29	0.57
5:B:1023:VAL:HG12	5:B:1027:ILE:HD11	1.87	0.57
2:T:10:DT:O4	3:N:9:DC:N4	2.38	0.57
4:A:42:ASP:HA	4:A:50:ILE:HG13	1.85	0.57
4:A:1002:GLY:O	4:A:1008:GLN:NE2	2.34	0.57
7:E:136:ASN:OD1	7:E:138:ALA:N	2.34	0.57
4:A:663:SER:HB2	5:B:1085:ILE:HA	1.86	0.57
4:A:939:ASP:OD2	4:A:1023:ARG:NH1	2.37	0.57
2:T:9:DC:H2''	2:T:10:DT:H71	1.85	0.56
3:N:11:DG:H2'	3:N:12:DA:C8	2.40	0.56
5:B:770:GLN:O	5:B:770:GLN:NE2	2.39	0.56
4:A:903:ASN:O	4:A:907:THR:OG1	2.20	0.56
7:E:78:LEU:HD21	7:E:109:ILE:HD13	1.87	0.56
4:A:1303:GLU:OE2	4:A:1326:ARG:NH1	2.39	0.56
4:A:525:GLN:HB2	5:B:1015:HIS:CD2	2.41	0.56
5:B:1020:ARG:HB2	5:B:1022:THR:HG23	1.86	0.56
11:J:37:SER:OG	11:J:47:ARG:NH2	2.39	0.56
4:A:226:GLU:HG3	4:A:227:VAL:HG23	1.87	0.56
9:H:87:ARG:HA	9:H:87:ARG:HH21	1.69	0.56
5:B:308:TRP:HA	5:B:311:LEU:HD12	1.87	0.56
10:I:92:ARG:O	10:I:95:THR:OG1	2.22	0.56
4:A:1364:ASN:OD1	4:A:1366:ARG:HG2	2.06	0.56
5:B:235:SER:OG	5:B:236:HIS:ND1	2.38	0.56
4:A:563:PRO:HB3	4:A:572:TRP:CE2	2.41	0.56
10:I:19:ASP:O	10:I:23:ASN:HA	2.06	0.56
4:A:848:ILE:HB	4:A:1065:GLY:HA3	1.88	0.55
5:B:1094:ARG:NH1	5:B:1098:MET:SD	2.73	0.55
5:B:1163:CYS:SG	5:B:1187:ASN:ND2	2.73	0.55
12:K:21:ILE:HG12	12:K:33:ILE:HG12	1.88	0.55
4:A:1436:ILE:O	4:A:1440:ALA:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:116:ASP:OD2	4:A:117:GLU:N	2.38	0.55
4:A:1012:ARG:O	4:A:1016:THR:OG1	2.23	0.55
5:B:299:GLU:OE1	5:B:572:HIS:ND1	2.37	0.55
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.40	0.55
4:A:746:MET:SD	5:B:1015:HIS:ND1	2.74	0.55
5:B:221:ASN:OD1	5:B:243:ALA:N	2.32	0.55
5:B:307:ASP:OD1	5:B:392:ARG:NH1	2.30	0.55
5:B:788:ARG:NH1	5:B:790:ASP:OD2	2.36	0.55
5:B:1034:VAL:O	5:B:1038:SER:OG	2.21	0.55
6:C:167:HIS:ND1	6:C:169:LYS:HG2	2.22	0.55
4:A:464:PRO:HG2	4:A:465:TYR:HD1	1.72	0.55
4:A:645:LEU:HD12	4:A:645:LEU:O	2.07	0.55
4:A:1067:LEU:O	4:A:1071:SER:OG	2.20	0.55
5:B:213:ILE:HD12	5:B:497:ARG:HB3	1.89	0.55
4:A:360:GLU:N	4:A:363:GLN:OE1	2.36	0.55
5:B:546:SER:OG	5:B:631:GLY:N	2.40	0.55
5:B:969:ARG:NH1	6:C:61:GLU:OE2	2.37	0.55
5:B:519:TRP:NE1	5:B:742:GLU:OE1	2.34	0.54
9:H:63:LEU:HB3	9:H:90:ALA:HB2	1.87	0.54
4:A:961:ARG:NH1	4:A:1025:ARG:HH22	2.04	0.54
5:B:210:LYS:HE2	5:B:462:ALA:HA	1.88	0.54
6:C:256:ALA:O	6:C:260:LEU:HG	2.06	0.54
5:B:862:GLN:O	5:B:914:LYS:NZ	2.30	0.54
10:I:72:ASP:O	10:I:81:ARG:NH2	2.27	0.54
2:T:25:DC:OP1	5:B:942:ARG:NH2	2.40	0.54
4:A:631:HIS:CE1	4:A:879:GLU:HG2	2.41	0.54
5:B:63:ILE:HA	5:B:421:PHE:CE2	2.42	0.54
10:I:73:ARG:O	10:I:83:ASN:ND2	2.41	0.54
5:B:976:ILE:HA	5:B:990:ILE:HG22	1.90	0.54
5:B:978:ASP:OD2	5:B:1094:ARG:NH2	2.41	0.54
9:H:5:LEU:HG	9:H:133:ASN:HB3	1.87	0.54
2:T:16:DT:C2	2:T:17:DG:C8	2.95	0.54
4:A:1329:THR:HG22	4:A:1331:SER:H	1.71	0.54
4:A:1385:THR:HG22	4:A:1386:ARG:HG2	1.90	0.54
6:C:88:CYS:HB3	6:C:92:CYS:HB3	1.89	0.54
6:C:116:LYS:HD3	6:C:140:ASN:HA	1.89	0.54
6:C:214:ASN:HB2	6:C:217:ASP:CG	2.33	0.54
4:A:446:ARG:NH2	4:A:480:ALA:CA	2.48	0.54
5:B:1186:ASP:OD1	5:B:1188:LYS:NZ	2.37	0.54
7:E:180:ARG:N	7:E:215:MET:OXT	2.41	0.54
5:B:423:LYS:NZ	5:B:468:GLU:OE1	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:646:PHE:O	4:A:650:GLN:HG3	2.09	0.54
4:A:1215:ARG:NH1	4:A:1272:THR:O	2.41	0.54
4:A:119:ASN:OD1	4:A:122:MET:N	2.37	0.53
4:A:547:LEU:HB3	12:K:58:PHE:CE1	2.43	0.53
4:A:1095:THR:HG21	4:A:1112:LYS:HB2	1.90	0.53
10:I:85:PHE:CD1	10:I:99:LEU:HD13	2.43	0.53
4:A:758:ILE:O	4:A:762:SER:OG	2.26	0.53
4:A:1166:ASP:HA	4:A:1169:ILE:HD13	1.90	0.53
5:B:487:THR:OG1	5:B:777:ALA:O	2.24	0.53
5:B:599:THR:O	5:B:603:LEU:HG	2.07	0.53
5:B:640:VAL:HG22	5:B:651:LEU:HB3	1.90	0.53
5:B:864:LYS:N	5:B:872:GLU:OE1	2.41	0.53
5:B:1074:ASN:OD1	5:B:1076:HIS:N	2.40	0.53
4:A:172:PRO:HB2	4:A:183:GLY:HA3	1.90	0.53
4:A:1140:HIS:CE1	4:A:1272:THR:HG22	2.43	0.53
5:B:483:LEU:HD21	5:B:491:THR:HG23	1.90	0.53
9:H:27:GLU:OE2	9:H:38:LEU:O	2.26	0.53
4:A:46:THR:HG22	4:A:47:ARG:H	1.73	0.53
4:A:113:LEU:HD23	4:A:113:LEU:H	1.72	0.53
4:A:810:PRO:CB	5:B:705:MET:HE2	2.38	0.53
5:B:899:ILE:HD11	5:B:903:VAL:HG11	1.91	0.53
6:C:251:LEU:O	6:C:255:VAL:HG23	2.09	0.53
7:E:101:GLN:O	7:E:101:GLN:NE2	2.37	0.53
9:H:30:SER:OG	9:H:36:CYS:SG	2.61	0.53
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.44	0.53
6:C:92:CYS:SG	6:C:94:LYS:HG3	2.48	0.53
7:E:62:ALA:HB3	7:E:78:LEU:HD12	1.90	0.53
5:B:544:CYS:HB2	5:B:634:TYR:CE1	2.43	0.53
5:B:553:PRO:O	5:B:557:PHE:N	2.38	0.53
5:B:1116:ARG:HD2	5:B:1198:TYR:CG	2.43	0.53
4:A:152:VAL:O	4:A:162:VAL:N	2.42	0.53
5:B:217:ARG:NH1	5:B:407:ASP:OD1	2.41	0.53
5:B:944:THR:HG21	5:B:1122:ARG:NH1	2.23	0.53
5:B:1187:ASN:ND2	5:B:1190:ASP:O	2.36	0.53
4:A:881:GLN:HE22	4:A:958:VAL:C	2.17	0.52
10:I:92:ARG:HD2	10:I:93:LYS:H	1.74	0.52
4:A:350:ARG:HD2	5:B:1128:LEU:HD11	1.89	0.52
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.91	0.52
12:K:12:LEU:HD12	12:K:12:LEU:H	1.74	0.52
4:A:628:GLY:O	4:A:632:VAL:HG23	2.09	0.52
4:A:1297:GLU:OE2	4:A:1297:GLU:N	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1169:MET:HE1	5:B:1201:LYS:HA	1.91	0.52
4:A:858:ASN:HD21	4:A:860:LEU:HB2	1.75	0.52
4:A:944:ARG:NH2	4:A:1296:GLY:O	2.30	0.52
5:B:118:ARG:HH21	5:B:194:GLU:CD	2.17	0.52
7:E:171:LYS:HB3	7:E:174:GLN:HG3	1.91	0.52
4:A:649:ILE:O	4:A:653:VAL:HG23	2.09	0.52
4:A:1140:HIS:HE1	4:A:1272:THR:HG22	1.72	0.52
6:C:112:ASN:ND2	11:J:19:GLU:OE2	2.43	0.52
4:A:545:GLN:O	4:A:549:MET:HG3	2.09	0.52
10:I:10:CYS:SG	10:I:31:THR:OG1	2.67	0.52
4:A:108:MET:SD	4:A:108:MET:N	2.82	0.52
4:A:336:ILE:HG21	4:A:1401:SER:HA	1.92	0.52
4:A:804:TYR:OH	4:A:816:HIS:NE2	2.31	0.52
4:A:931:GLU:OE2	4:A:991:LYS:NZ	2.37	0.52
4:A:1116:LEU:HD13	4:A:1329:THR:OG1	2.10	0.52
5:B:384:ARG:HH22	5:B:621:GLU:HG2	1.74	0.52
6:C:34:ARG:HD2	6:C:178:PHE:CD1	2.45	0.52
5:B:847:ASP:OD2	12:K:6:ARG:NH2	2.43	0.51
4:A:866:PHE:N	7:E:208:TYR:OH	2.42	0.51
5:B:120:ARG:HB2	5:B:122:LEU:HG	1.91	0.51
5:B:861:ASP:OD1	5:B:862:GLN:N	2.37	0.51
9:H:25:ARG:HD2	9:H:39:THR:HG22	1.92	0.51
4:A:534:LEU:O	4:A:574:GLY:HA3	2.10	0.51
4:A:697:ALA:HA	4:A:702:LEU:HD23	1.93	0.51
5:B:429:PHE:O	5:B:433:GLN:HG3	2.10	0.51
5:B:635:ARG:NH1	5:B:742:GLU:OE2	2.36	0.51
5:B:780:VAL:HG21	11:J:56:LEU:HD11	1.93	0.51
1:R:1:A:H2'	1:R:2:U:C6	2.46	0.51
4:A:873:MET:HG3	4:A:957:PRO:HG3	1.93	0.51
5:B:130:VAL:HG23	5:B:132:VAL:HG23	1.93	0.51
8:F:94:LEU:HD21	8:F:125:LEU:HD22	1.93	0.51
4:A:35:ILE:O	4:A:84:ILE:HD13	2.11	0.51
4:A:311:GLN:N	4:A:312:PRO:HD3	2.26	0.51
5:B:497:ARG:HH21	5:B:538:ASN:HD21	1.57	0.51
10:I:72:ASP:N	10:I:72:ASP:OD1	2.43	0.51
4:A:900:ASP:O	4:A:907:THR:OG1	2.28	0.51
5:B:325:GLN:OE1	10:I:12:ASN:ND2	2.44	0.51
4:A:1118:VAL:HA	4:A:1327:ILE:HG13	1.93	0.51
4:A:806:ARG:NH1	5:B:725:PRO:O	2.42	0.51
8:F:90:ARG:O	8:F:94:LEU:HG	2.11	0.51
4:A:469:ARG:NH2	5:B:991:GLY:O	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:807:ARG:HG2	5:B:1045:SER:HB3	1.93	0.50
9:H:103:LYS:HB3	9:H:115:TYR:CD1	2.39	0.50
4:A:323:LYS:HE2	4:A:328:ARG:HG3	1.93	0.50
4:A:483:ASP:HB2	5:B:987:LYS:HB2	1.92	0.50
4:A:585:GLY:N	4:A:609:ASP:OD1	2.43	0.50
5:B:864:LYS:NZ	5:B:872:GLU:OE2	2.31	0.50
10:I:19:ASP:HB3	10:I:24:ARG:HB2	1.93	0.50
2:T:17:DG:N3	2:T:18:DA:C8	2.79	0.50
4:A:9:ALA:O	5:B:1193:GLN:NE2	2.27	0.50
4:A:569:LYS:HD2	4:A:571:LEU:HD11	1.93	0.50
8:F:128:LYS:NZ	8:F:148:VAL:O	2.27	0.50
4:A:122:MET:O	4:A:126:LEU:HG	2.12	0.50
4:A:738:LYS:NZ	6:C:194:GLU:O	2.33	0.50
4:A:881:GLN:NE2	4:A:958:VAL:O	2.34	0.50
4:A:1021:LEU:HD11	4:A:1025:ARG:NH1	2.26	0.50
4:A:1235:LYS:HB3	4:A:1237:ILE:HD11	1.92	0.50
10:I:68:LEU:HB3	10:I:84:VAL:HG13	1.94	0.50
4:A:557:ASP:OD1	4:A:559:VAL:N	2.44	0.50
4:A:662:PHE:O	5:B:828:ALA:HA	2.11	0.50
5:B:31:TRP:CE3	5:B:34:ILE:HD12	2.46	0.50
5:B:273:LEU:HB2	5:B:276:ILE:HB	1.92	0.50
10:I:103:CYS:SG	10:I:104:LEU:N	2.84	0.50
3:N:10:DA:H2"	3:N:11:DG:C8	2.47	0.50
4:A:350:ARG:NH1	4:A:488:ASN:OD1	2.45	0.50
4:A:629:LEU:O	4:A:633:VAL:HG23	2.12	0.50
10:I:71:SER:HB3	10:I:85:PHE:CD2	2.47	0.50
2:T:18:DA:H5"	4:A:332:LYS:NZ	2.27	0.50
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.11	0.50
4:A:843:LYS:NZ	4:A:1401:SER:OG	2.34	0.50
5:B:977:GLY:HA3	5:B:1099:VAL:HG21	1.93	0.50
7:E:77:SER:HB2	7:E:105:PHE:CD2	2.46	0.50
10:I:25:LEU:HB3	10:I:38:ALA:HB2	1.93	0.50
13:L:42:ARG:N	13:L:44:ASP:OD2	2.42	0.50
4:A:601:LYS:HB2	4:A:603:ASN:OD1	2.12	0.50
5:B:846:ILE:O	5:B:852:ARG:NH2	2.44	0.50
5:B:1168:LEU:HD23	5:B:1208:MET:HE2	1.93	0.50
6:C:20:PHE:HE2	6:C:232:VAL:HG23	1.77	0.50
4:A:266:LEU:HD11	4:A:303:TYR:CE1	2.47	0.49
4:A:881:GLN:HE21	4:A:956:LEU:HB2	1.77	0.49
6:C:40:GLU:OE1	6:C:254:LYS:HE3	2.12	0.49
9:H:32:THR:HG22	9:H:32:THR:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:44:TYR:CE1	10:I:46:HIS:HB2	2.46	0.49
4:A:744:LYS:HZ2	4:A:748:MET:HE3	1.77	0.49
6:C:34:ARG:HD2	6:C:178:PHE:HD1	1.76	0.49
9:H:29:ALA:HA	9:H:37:LYS:HA	1.93	0.49
9:H:113:ALA:HA	9:H:125:LEU:O	2.11	0.49
15:T:101:5N0:N23	3:N:11:DG:H1'	2.28	0.49
5:B:216:GLU:OE1	5:B:500:THR:OG1	2.22	0.49
2:T:16:DT:H2'	2:T:17:DG:H8	1.75	0.49
4:A:237:THR:OG1	4:A:238:CYS:N	2.45	0.49
4:A:343:LYS:NZ	5:B:1197:PRO:HB3	2.28	0.49
4:A:526:ASP:CG	5:B:1013:ASN:HD21	2.21	0.49
4:A:966:ASN:HB3	4:A:1044:TRP:HH2	1.76	0.49
4:A:974:ASP:HA	9:H:136:LYS:HE3	1.94	0.49
4:A:1063:MET:HE2	4:A:1436:ILE:HD12	1.93	0.49
4:A:1051:ALA:O	4:A:1055:ARG:HG3	2.12	0.49
8:F:82:THR:O	8:F:136:ARG:NH1	2.25	0.49
4:A:1229:SER:OG	4:A:1230:GLU:N	2.46	0.49
5:B:102:VAL:HG13	5:B:112:LEU:HB2	1.95	0.49
7:E:94:LYS:HA	7:E:97:VAL:HG22	1.95	0.49
10:I:8:ARG:NE	10:I:9:ASP:OD1	2.37	0.49
10:I:78:CYS:SG	10:I:80:SER:OG	2.63	0.49
11:J:2:ILE:HG12	11:J:3:VAL:H	1.77	0.49
11:J:10:CYS:SG	11:J:11:GLY:N	2.85	0.49
4:A:538:ASP:OD2	9:H:21:ASN:N	2.41	0.49
4:A:1027:ALA:HB3	4:A:1030:ARG:HB2	1.94	0.49
5:B:614:SER:OG	5:B:627:PHE:HB2	2.12	0.49
5:B:944:THR:HG21	5:B:1122:ARG:HH12	1.77	0.49
5:B:406:LEU:N	5:B:631:GLY:O	2.42	0.49
5:B:496:ARG:HH12	5:B:541:LEU:HA	1.77	0.49
5:B:878:GLN:HB2	5:B:881:ASN:HB3	1.94	0.49
6:C:66:ARG:NH2	11:J:3:VAL:O	2.38	0.49
11:J:9:SER:HB2	11:J:45:CYS:HB2	1.94	0.49
11:J:44:TYR:O	11:J:48:ARG:HG2	2.13	0.49
4:A:378:GLU:OE1	4:A:434:ARG:NE	2.45	0.49
4:A:550:LEU:HD23	4:A:556:TRP:CZ2	2.48	0.49
4:A:998:LEU:HD12	4:A:1001:ARG:HH11	1.77	0.49
4:A:1412:ALA:HA	4:A:1417:GLU:HG3	1.94	0.49
5:B:41:LYS:HB3	5:B:45:SER:OG	2.12	0.49
4:A:901:LEU:HA	4:A:907:THR:HG23	1.95	0.48
4:A:1027:ALA:O	4:A:1031:VAL:HG23	2.13	0.48
5:B:168:GLY:HA2	5:B:450:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:384:ARG:NH2	5:B:621:GLU:HG2	2.28	0.48
5:B:861:ASP:OD1	5:B:914:LYS:NZ	2.35	0.48
6:C:105:GLY:N	6:C:151:GLN:O	2.41	0.48
4:A:100:LYS:O	4:A:104:GLU:N	2.46	0.48
4:A:107:CYS:SG	4:A:171:GLN:NE2	2.86	0.48
4:A:208:LEU:HD21	4:A:212:LYS:HE3	1.95	0.48
4:A:1206:ASP:OD1	4:A:1274:ARG:NH1	2.46	0.48
5:B:1152:MET:O	5:B:1157:ALA:HB2	2.13	0.48
6:C:102:GLN:HB3	6:C:154:LYS:HG3	1.95	0.48
7:E:121:MET:HA	7:E:124:VAL:HG23	1.95	0.48
4:A:440:ASP:O	4:A:460:VAL:HG23	2.13	0.48
4:A:464:PRO:O	12:K:2:ASN:HB3	2.13	0.48
4:A:494:SER:HB3	4:A:496:GLU:OE1	2.14	0.48
4:A:1152:ILE:HB	10:I:44:TYR:HB3	1.94	0.48
5:B:376:PHE:HE2	5:B:569:TYR:HD2	1.60	0.48
5:B:437:GLU:N	5:B:437:GLU:OE1	2.47	0.48
5:B:883:LEU:HD12	5:B:884:ARG:H	1.78	0.48
10:I:82:GLU:OE1	10:I:82:GLU:N	2.45	0.48
4:A:1066:VAL:O	4:A:1070:GLN:HG3	2.13	0.48
4:A:1239:ARG:HH12	4:A:1241:ARG:HH12	1.61	0.48
4:A:1444:MET:HG3	8:F:133:VAL:HG13	1.95	0.48
5:B:1084:GLN:NE2	5:B:1084:GLN:H	2.11	0.48
9:H:10:PHE:CD2	9:H:38:LEU:HD22	2.49	0.48
9:H:12:VAL:HG13	9:H:26:ILE:HD11	1.94	0.48
4:A:22:PHE:CD1	5:B:1213:THR:HG22	2.48	0.48
4:A:1224:LEU:HD12	4:A:1241:ARG:O	2.13	0.48
5:B:638:PHE:HB2	5:B:741:CYS:O	2.13	0.48
6:C:246:ARG:O	6:C:250:THR:OG1	2.30	0.48
9:H:104:PHE:HD2	9:H:114:VAL:HG22	1.78	0.48
10:I:82:GLU:HB3	10:I:104:LEU:HD12	1.96	0.48
11:J:14:VAL:HA	11:J:17:LYS:HD2	1.96	0.48
4:A:396:PRO:HB3	4:A:403:LYS:HA	1.96	0.48
5:B:402:GLY:O	5:B:405:ARG:NH1	2.47	0.48
5:B:936:ASP:OD1	5:B:937:ALA:N	2.46	0.48
11:J:32:GLU:O	11:J:36:LEU:HG	2.13	0.48
4:A:900:ASP:OD1	4:A:926:GLN:NE2	2.47	0.48
4:A:982:THR:N	4:A:985:ASP:OD2	2.47	0.48
5:B:242:SER:OG	5:B:252:SER:O	2.21	0.48
5:B:1080:LYS:HG3	6:C:180:TYR:OH	2.13	0.48
6:C:92:CYS:N	6:C:95:CYS:SG	2.86	0.48
4:A:259:GLU:OE1	4:A:260:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:544:ASP:N	4:A:544:ASP:OD1	2.45	0.48
4:A:1070:GLN:HE22	5:B:1137:CYS:HA	1.79	0.48
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.96	0.48
4:A:809:THR:OG1	4:A:812:GLU:OE1	2.32	0.48
5:B:114:PRO:HG2	5:B:181:LEU:HD11	1.95	0.48
4:A:1116:LEU:HB3	4:A:1308:THR:OG1	2.13	0.48
7:E:31:THR:HB	7:E:34:GLU:HB2	1.96	0.48
4:A:447:GLN:HG2	5:B:1134:GLU:OE2	2.13	0.47
4:A:1120:LEU:HD13	4:A:1304:TRP:O	2.14	0.47
4:A:1423:GLY:O	4:A:1427:ASN:ND2	2.47	0.47
5:B:470:LYS:O	5:B:474:SER:OG	2.30	0.47
5:B:792:MET:SD	5:B:857:ARG:NH2	2.87	0.47
5:B:1030:LEU:O	5:B:1034:VAL:HG23	2.14	0.47
5:B:1213:THR:OG1	5:B:1213:THR:O	2.31	0.47
6:C:163:ILE:HD11	12:K:10:PHE:CE1	2.49	0.47
4:A:974:ASP:OD1	4:A:977:LYS:HG2	2.14	0.47
4:A:1107:VAL:HG22	4:A:1383:SER:HB3	1.96	0.47
5:B:705:MET:HE3	5:B:745:PRO:HB3	1.96	0.47
5:B:60:GLN:NE2	5:B:60:GLN:O	2.46	0.47
4:A:18:GLN:HG2	4:A:228:PHE:CE1	2.49	0.47
5:B:737:THR:OG1	5:B:737:THR:O	2.32	0.47
8:F:86:THR:O	8:F:89:GLU:HG2	2.14	0.47
9:H:104:PHE:HE1	9:H:136:LYS:HB3	1.78	0.47
4:A:545:GLN:HG2	4:A:549:MET:HE3	1.94	0.47
4:A:842:VAL:HG11	5:B:1136:ASP:CG	2.39	0.47
5:B:334:ILE:HG21	5:B:348:ARG:HB3	1.97	0.47
5:B:365:THR:HG21	5:B:370:PHE:HD1	1.79	0.47
12:K:49:GLU:OE2	12:K:97:LYS:NZ	2.32	0.47
4:A:225:ASN:OD1	4:A:227:VAL:N	2.44	0.47
4:A:768:GLN:HG3	4:A:816:HIS:HA	1.96	0.47
4:A:1060:PRO:HD2	8:F:86:THR:HG21	1.96	0.47
5:B:183:GLU:N	5:B:183:GLU:OE2	2.47	0.47
6:C:254:LYS:O	6:C:257:SER:OG	2.30	0.47
8:F:87:LYS:HE3	8:F:88:TYR:HE1	1.80	0.47
2:T:16:DT:C2	2:T:17:DG:N7	2.82	0.47
4:A:1132:LYS:HD3	4:A:1135:ARG:NH1	2.29	0.47
4:A:1153:TYR:HB2	4:A:1192:LEU:HD23	1.96	0.47
4:A:1168:GLU:HA	4:A:1171:GLN:HB3	1.97	0.47
5:B:115:GLN:O	5:B:119:LEU:HG	2.15	0.47
5:B:408:LEU:HG	5:B:409:ALA:H	1.79	0.47
6:C:171:GLY:C	6:C:173:ALA:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:153:HIS:C	7:E:154:ILE:HD12	2.39	0.47
8:F:85:MET:HG3	8:F:89:GLU:HG3	1.97	0.47
8:F:132:LEU:O	8:F:148:VAL:HG23	2.15	0.47
12:K:24:ASP:OD2	12:K:74:ARG:HD2	2.14	0.47
4:A:42:ASP:N	4:A:49:LYS:HA	2.30	0.47
4:A:268:ASP:HB3	4:A:299:HIS:CE1	2.50	0.47
4:A:457:ALA:O	4:A:507:VAL:HG23	2.14	0.47
5:B:634:TYR:HA	5:B:694:ASP:HA	1.96	0.47
5:B:762:ASN:HD21	5:B:1024:ALA:HB3	1.80	0.47
5:B:1009:ASP:OD2	11:J:48:ARG:NH2	2.48	0.47
5:B:1143:ALA:HB1	5:B:1146:PHE:HB3	1.96	0.47
7:E:28:TYR:CE1	7:E:78:LEU:HG	2.49	0.47
5:B:112:LEU:HD21	5:B:117:ALA:HB2	1.95	0.47
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.96	0.47
6:C:73:GLN:OE1	6:C:75:MET:N	2.42	0.47
4:A:203:SER:O	4:A:207:ILE:HG13	2.15	0.47
4:A:840:ARG:HD2	4:A:1402:PHE:HZ	1.79	0.47
12:K:91:CYS:O	12:K:95:ILE:HG13	2.15	0.47
4:A:117:GLU:O	4:A:123:ARG:HD3	2.15	0.46
4:A:618:GLU:O	4:A:622:VAL:HG12	2.14	0.46
4:A:1030:ARG:NE	4:A:1034:GLU:OE1	2.44	0.46
4:A:1206:ASP:O	4:A:1274:ARG:NH1	2.45	0.46
5:B:552:MET:HB3	5:B:553:PRO:HD3	1.98	0.46
5:B:816:GLU:N	5:B:816:GLU:OE1	2.48	0.46
5:B:1073:TYR:CD2	5:B:1080:LYS:HG2	2.50	0.46
4:A:592:ASP:O	4:A:595:THR:OG1	2.22	0.46
4:A:1151:GLU:HG2	10:I:45:ARG:HG3	1.98	0.46
4:A:1193:LEU:HB2	4:A:1260:LEU:HD21	1.97	0.46
4:A:1312:ASN:O	4:A:1316:VAL:HG23	2.15	0.46
6:C:57:VAL:HG23	6:C:58:LEU:HD23	1.98	0.46
7:E:19:VAL:O	7:E:23:VAL:HG22	2.16	0.46
4:A:537:ARG:HB2	9:H:20:TYR:CE2	2.50	0.46
7:E:93:MET:HB2	7:E:120:ALA:HB1	1.96	0.46
2:T:14:DC:H1'	2:T:15:DA:H1'	1.97	0.46
4:A:328:ARG:HD3	5:B:1206:GLU:OE1	2.15	0.46
4:A:526:ASP:HB2	5:B:835:GLN:CD	2.41	0.46
5:B:40:GLU:OE1	5:B:682:SER:OG	2.24	0.46
5:B:412:LEU:HB3	5:B:466:TRP:CZ2	2.50	0.46
5:B:681:TRP:CH2	5:B:690:VAL:HG11	2.50	0.46
10:I:17:ARG:HG3	10:I:18:GLU:N	2.29	0.46
5:B:863:GLU:OE2	5:B:874:PHE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:42:ASP:HB2	4:A:50:ILE:HG23	1.98	0.46
5:B:872:GLU:HG2	5:B:916:THR:HB	1.97	0.46
5:B:1182:CYS:HB3	5:B:1187:ASN:HB3	1.98	0.46
6:C:59:ALA:O	6:C:63:ILE:HG13	2.16	0.46
12:K:61:TYR:HA	12:K:72:LYS:O	2.15	0.46
3:N:12:DA:H2''	3:N:13:DG:C8	2.51	0.46
4:A:122:MET:HE3	4:A:122:MET:HA	1.96	0.46
5:B:387:LEU:HD23	5:B:387:LEU:HA	1.77	0.46
5:B:542:MET:HB3	5:B:636:PRO:HD2	1.98	0.46
6:C:91:HIS:HB2	6:C:96:SER:OG	2.15	0.46
4:A:541:ILE:HD13	4:A:549:MET:HE1	1.98	0.46
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.56	0.46
4:A:672:ASP:OD1	4:A:675:THR:OG1	2.21	0.46
4:A:1338:VAL:HG12	4:A:1339:LEU:HD23	1.98	0.46
4:A:1355:VAL:O	4:A:1358:SER:OG	2.34	0.46
5:B:357:GLN:NE2	5:B:368:GLU:HB3	2.31	0.46
6:C:115:SER:OG	6:C:141:GLY:HA3	2.16	0.46
4:A:668:ASP:OD1	6:C:192:TRP:NE1	2.49	0.46
4:A:1437:GLY:HA3	8:F:88:TYR:CD2	2.43	0.46
5:B:1074:ASN:OD1	5:B:1075:GLY:N	2.48	0.46
6:C:36:VAL:HG23	12:K:41:THR:HG21	1.97	0.46
5:B:221:ASN:O	5:B:584:GLY:HA3	2.16	0.46
5:B:770:GLN:OE1	5:B:983:ARG:HA	2.15	0.46
5:B:936:ASP:OD1	5:B:938:SER:OG	2.26	0.46
5:B:1165:ILE:O	5:B:1217:TYR:OH	2.31	0.46
5:B:652:LYS:HB3	5:B:689:LEU:HD22	1.98	0.45
5:B:661:LEU:HD23	5:B:661:LEU:HA	1.65	0.45
5:B:797:TYR:HB3	5:B:798:TYR:CD1	2.51	0.45
6:C:254:LYS:NZ	12:K:38:GLU:OE1	2.49	0.45
7:E:167:ARG:HA	7:E:167:ARG:HD3	1.68	0.45
11:J:18:TRP:CE2	11:J:22:LEU:HD11	2.51	0.45
13:L:61:THR:HB	13:L:63:ARG:HG3	1.98	0.45
4:A:445:ASN:O	4:A:487:MET:HG2	2.17	0.45
4:A:494:SER:O	4:A:498:ARG:HG3	2.16	0.45
9:H:41:ASP:OD1	9:H:122:LEU:N	2.49	0.45
1:R:1:A:H2'	1:R:2:U:H6	1.80	0.45
4:A:364:VAL:HG12	4:A:458:HIS:HB3	1.97	0.45
4:A:741:ASN:O	4:A:745:GLN:HG3	2.16	0.45
4:A:980:ASP:N	4:A:980:ASP:OD1	2.49	0.45
4:A:1385:THR:CG2	4:A:1386:ARG:H	2.22	0.45
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:279:LEU:HB3	4:A:284:ALA:HB2	1.98	0.45
4:A:1120:LEU:HD22	4:A:1125:ALA:HA	1.97	0.45
5:B:629:ASP:OD2	5:B:630:ALA:N	2.49	0.45
5:B:843:GLN:N	5:B:994:TYR:O	2.37	0.45
5:B:1159:ARG:HH12	5:B:1175:LEU:HD22	1.82	0.45
7:E:46:TYR:CE2	7:E:58:MET:HA	2.52	0.45
4:A:464:PRO:HG2	4:A:465:TYR:CD1	2.52	0.45
4:A:605:MET:HE3	4:A:621:THR:HG21	1.97	0.45
4:A:771:GLU:OE2	5:B:510:LYS:NZ	2.48	0.45
5:B:1037:LEU:HD21	11:J:44:TYR:HD2	1.81	0.45
10:I:60:GLN:NE2	10:I:107:SER:OG	2.46	0.45
13:L:64:LEU:HD22	13:L:65:VAL:H	1.82	0.45
4:A:34:LYS:HG2	4:A:83:HIS:HE1	1.82	0.45
4:A:365:GLY:N	4:A:469:ARG:O	2.37	0.45
4:A:1331:SER:OG	4:A:1334:ASP:OD2	2.28	0.45
5:B:315:LYS:HG3	10:I:13:MET:HE1	1.97	0.45
5:B:898:LEU:HD13	5:B:964:VAL:HG11	1.98	0.45
6:C:54:ASN:OD1	6:C:56:THR:OG1	2.19	0.45
4:A:28:ARG:HH22	4:A:85:ASP:HB3	1.82	0.45
4:A:69:THR:HG22	5:B:1174:LYS:HD3	1.97	0.45
4:A:392:VAL:HG11	4:A:424:ILE:HG12	1.98	0.45
4:A:1263:ILE:O	4:A:1267:MET:HG3	2.17	0.45
5:B:493:SER:OG	5:B:497:ARG:NH2	2.49	0.45
5:B:1076:HIS:O	6:C:31:ASN:ND2	2.47	0.45
9:H:102:TYR:CE2	9:H:115:TYR:HB3	2.51	0.45
4:A:836:TYR:OH	4:A:1403:GLU:OE2	2.28	0.45
4:A:1068:ALA:O	4:A:1072:ILE:HG13	2.16	0.45
5:B:554:ILE:O	5:B:558:LEU:N	2.46	0.45
6:C:143:LEU:HD21	6:C:146:LYS:HE3	1.99	0.45
4:A:619:LYS:O	4:A:623:GLY:N	2.35	0.45
4:A:960:ILE:HG21	4:A:1025:ARG:HG2	1.97	0.45
5:B:493:SER:OG	5:B:775:LYS:HE2	2.17	0.45
2:T:22:DT:H2'	2:T:23:DC:H6	1.81	0.45
4:A:28:ARG:HH12	4:A:85:ASP:HB3	1.81	0.45
4:A:94:GLY:HA3	4:A:1410:PHE:CD1	2.51	0.45
4:A:471:ASN:OD1	4:A:472:LEU:N	2.50	0.45
4:A:606:LEU:HB3	4:A:614:PHE:CE1	2.52	0.45
4:A:941:LYS:HA	4:A:941:LYS:HD3	1.54	0.45
4:A:1239:ARG:HH12	4:A:1241:ARG:HH22	1.64	0.45
4:A:1325:THR:HA	7:E:147:HIS:HA	1.97	0.45
5:B:67:SER:HB2	5:B:92:PHE:CD1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:325:GLN:HE21	5:B:325:GLN:HB2	1.63	0.45
5:B:371:GLU:CD	5:B:371:GLU:H	2.25	0.45
5:B:778:MET:CE	5:B:1094:ARG:HD3	2.47	0.45
5:B:936:ASP:OD1	5:B:938:SER:N	2.45	0.45
6:C:82:TYR:CE2	6:C:161:LYS:HG2	2.52	0.45
7:E:184:VAL:HA	7:E:187:TYR:HB3	1.99	0.45
4:A:711:ARG:HH12	10:I:95:THR:HB	1.82	0.44
4:A:841:LEU:HD21	4:A:1105:LEU:CD2	2.46	0.44
5:B:104:GLU:OE1	5:B:120:ARG:NH2	2.47	0.44
5:B:1153:GLU:OE1	5:B:1153:GLU:N	2.51	0.44
6:C:31:ASN:O	6:C:35:ARG:HG3	2.16	0.44
7:E:99:HIS:HD2	7:E:103:LYS:HG3	1.80	0.44
12:K:47:ARG:HD3	12:K:60:ALA:HA	1.98	0.44
13:L:68:GLU:HB2	13:L:70:ARG:HG3	1.99	0.44
4:A:951:GLU:O	4:A:954:TRP:NE1	2.30	0.44
5:B:301:ILE:HD13	5:B:382:ILE:HG21	1.99	0.44
5:B:881:ASN:O	5:B:932:HIS:HA	2.17	0.44
7:E:127:ILE:HB	7:E:130:ALA:HB3	1.98	0.44
2:T:10:DT:H2"	2:T:11:DG:C8	2.52	0.44
15:T:101:5N0:O5	4:A:1387:HIS:NE2	2.47	0.44
4:A:571:LEU:HD22	9:H:46:LEU:HD11	1.99	0.44
4:A:714:PHE:O	4:A:718:VAL:HG23	2.17	0.44
4:A:874:ASP:OD1	4:A:875:ALA:N	2.50	0.44
4:A:1267:MET:HA	4:A:1271:ILE:HD13	1.99	0.44
4:A:1291:VAL:HG22	4:A:1292:PRO:HD2	1.99	0.44
5:B:282:ILE:HG13	5:B:283:VAL:N	2.32	0.44
6:C:136:ASP:OD1	6:C:137:LYS:N	2.50	0.44
8:F:140:ASP:CG	8:F:142:SER:HG	2.23	0.44
4:A:17:VAL:HG23	4:A:1421:CYS:SG	2.58	0.44
2:T:15:DA:H2"	15:T:101:5N0:C22	2.47	0.44
4:A:841:LEU:HD23	4:A:1384:VAL:HG11	1.99	0.44
6:C:29:MET:HE3	6:C:29:MET:HB2	1.85	0.44
6:C:115:SER:HB3	6:C:142:VAL:HG22	2.00	0.44
10:I:55:THR:HG22	10:I:55:THR:O	2.17	0.44
5:B:310:MET:HG3	5:B:386:LEU:HD13	2.00	0.44
5:B:635:ARG:HH22	5:B:742:GLU:CD	2.25	0.44
5:B:770:GLN:HG2	5:B:983:ARG:O	2.17	0.44
5:B:786:ASN:OD1	5:B:967:ARG:NH2	2.50	0.44
5:B:834:ASN:O	5:B:1013:ASN:HB2	2.17	0.44
6:C:99:LEU:HD13	6:C:120:ILE:HA	2.00	0.44
4:A:550:LEU:HD12	4:A:577:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:63:LEU:HB3	9:H:90:ALA:CB	2.47	0.44
9:H:101:ALA:HB2	9:H:116:TYR:HE2	1.83	0.44
5:B:1023:VAL:O	5:B:1027:ILE:HG13	2.17	0.44
5:B:1159:ARG:HD3	5:B:1161:HIS:HE1	1.83	0.44
4:A:298:PHE:CE2	4:A:314:ALA:HB2	2.52	0.44
4:A:567:LYS:HB3	4:A:568:PRO:HD3	2.00	0.44
4:A:683:ILE:HD13	4:A:683:ILE:HA	1.89	0.44
4:A:1156:PRO:HA	4:A:1190:PRO:HB3	2.00	0.44
12:K:78:THR:HG22	12:K:79:GLU:H	1.83	0.44
4:A:707:GLY:O	4:A:1281:ARG:HD2	2.18	0.43
4:A:993:LEU:HD22	4:A:1046:LEU:HG	2.00	0.43
5:B:751:VAL:HG23	5:B:812:LEU:HD13	2.00	0.43
5:B:766:ARG:HG3	5:B:1022:THR:HG22	1.99	0.43
5:B:1072:MET:HE2	5:B:1085:ILE:HD12	1.99	0.43
7:E:100:ILE:HD13	7:E:100:ILE:HA	1.85	0.43
2:T:8:DT:H2''	2:T:9:DC:H5'	1.99	0.43
4:A:534:LEU:HD11	4:A:541:ILE:HD11	2.00	0.43
4:A:870:GLU:HG2	7:E:208:TYR:CD2	2.53	0.43
4:A:380:VAL:HG12	4:A:388:LEU:HD13	2.00	0.43
5:B:357:GLN:HE22	5:B:368:GLU:HB3	1.83	0.43
5:B:360:PHE:CE2	5:B:361:LEU:HD13	2.53	0.43
7:E:135:PHE:HD2	7:E:140:LEU:HD11	1.83	0.43
1:R:7:A:H2'	1:R:8:G:H8	1.84	0.43
4:A:608:ILE:HD13	4:A:608:ILE:HA	1.89	0.43
4:A:662:PHE:CE1	4:A:742:ASN:HB3	2.54	0.43
5:B:1024:ALA:HA	5:B:1027:ILE:HD12	2.00	0.43
12:K:8:GLU:O	12:K:37:LYS:HE3	2.19	0.43
2:T:13:DT:H2''	2:T:14:DC:H5'	2.00	0.43
4:A:689:LYS:HE2	4:A:721:PHE:CZ	2.53	0.43
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.19	0.43
11:J:31:ASP:OD1	11:J:34:THR:OG1	2.24	0.43
12:K:58:PHE:HB3	12:K:76:GLN:HB3	2.00	0.43
4:A:881:GLN:OE1	4:A:959:ASN:HA	2.18	0.43
5:B:37:PHE:CE1	5:B:41:LYS:HD2	2.53	0.43
5:B:546:SER:OG	5:B:632:ARG:N	2.50	0.43
5:B:586:TRP:NE1	5:B:588:GLY:O	2.45	0.43
6:C:136:ASP:OD1	6:C:138:GLU:N	2.42	0.43
8:F:87:LYS:HG3	8:F:88:TYR:HD1	1.84	0.43
4:A:744:LYS:NZ	4:A:748:MET:HE3	2.32	0.43
4:A:765:VAL:CG2	4:A:800:VAL:HB	2.48	0.43
4:A:853:ASP:OD1	4:A:855:THR:OG1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1355:VAL:HG23	4:A:1356:ILE:CD1	2.49	0.43
5:B:640:VAL:HG13	5:B:650:GLU:C	2.44	0.43
5:B:890:TYR:CZ	5:B:910:VAL:HG21	2.54	0.43
5:B:972:LYS:NZ	5:B:1101:ASP:OD2	2.38	0.43
8:F:140:ASP:OD1	8:F:142:SER:OG	2.30	0.43
4:A:456:MET:HB2	4:A:478:TYR:OH	2.18	0.43
4:A:1229:SER:OG	4:A:1233:ASP:OD1	2.37	0.43
5:B:334:ILE:HD13	5:B:352:ALA:HB2	2.00	0.43
5:B:759:PRO:CD	5:B:1046:PRO:HG3	2.49	0.43
4:A:538:ASP:HB2	9:H:20:TYR:HD2	1.84	0.43
4:A:1138:ILE:O	4:A:1276:VAL:HG23	2.19	0.43
5:B:66:ASP:OD2	5:B:422:LYS:NZ	2.34	0.43
5:B:567:GLU:OE2	5:B:567:GLU:N	2.48	0.43
5:B:946:ASN:O	5:B:970:THR:OG1	2.31	0.43
7:E:169:ARG:HB3	8:F:140:ASP:HB3	2.01	0.43
9:H:40:LEU:HG	9:H:42:ILE:HG12	2.01	0.43
10:I:80:SER:OG	10:I:103:CYS:SG	2.77	0.43
11:J:17:LYS:HB3	11:J:39:LEU:HD13	2.01	0.43
12:K:13:GLY:H	12:K:16:GLU:HB2	1.83	0.43
15:T:101:5N0:C35	3:N:8:DC:H1'	2.49	0.43
4:A:1001:ARG:HH21	8:F:82:THR:HA	1.83	0.43
5:B:239:GLU:HA	5:B:254:LEU:O	2.19	0.43
7:E:10:SER:O	7:E:14:ARG:HG3	2.18	0.43
7:E:205:SER:O	7:E:207:ARG:N	2.50	0.43
10:I:42:LEU:HD11	10:I:45:ARG:HB2	2.00	0.43
5:B:34:ILE:O	5:B:37:PHE:HB3	2.19	0.42
5:B:401:PHE:HB2	5:B:517:THR:OG1	2.19	0.42
6:C:19:ASP:HB2	6:C:231:ASN:OD1	2.19	0.42
5:B:261:ARG:NE	5:B:262:GLU:OE2	2.48	0.42
5:B:757:PRO:HG2	5:B:984:HIS:HE1	1.84	0.42
5:B:961:LEU:HD23	5:B:961:LEU:HA	1.77	0.42
6:C:56:THR:HG22	6:C:147:LEU:CD2	2.49	0.42
6:C:60:ASP:OD2	13:L:60:ARG:NH1	2.44	0.42
6:C:92:CYS:SG	6:C:94:LYS:N	2.90	0.42
11:J:57:ILE:O	11:J:61:LEU:HG	2.19	0.42
3:N:11:DG:H2''	3:N:12:DA:H5'	2.00	0.42
4:A:33:ALA:HB2	4:A:58:LEU:HD21	2.02	0.42
4:A:268:ASP:HB3	4:A:299:HIS:NE2	2.34	0.42
4:A:775:ILE:HD13	4:A:775:ILE:HA	1.92	0.42
4:A:899:VAL:HG13	4:A:929:LEU:HD13	2.00	0.42
6:C:40:GLU:CD	6:C:254:LYS:HE3	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:42:ASP:N	4:A:48:ALA:O	2.45	0.42
4:A:248:PRO:O	4:A:260:ASP:HB2	2.19	0.42
4:A:298:PHE:CZ	4:A:314:ALA:HB2	2.54	0.42
4:A:711:ARG:NH1	10:I:95:THR:HB	2.35	0.42
5:B:105:SER:HB2	5:B:958:GLN:O	2.19	0.42
6:C:262:LEU:HD11	12:K:87:LEU:HD23	2.00	0.42
9:H:108:SER:HB2	9:H:111:LEU:HB2	2.01	0.42
13:L:30:ILE:HG22	13:L:31:CYS:O	2.19	0.42
4:A:115:LEU:HD12	4:A:119:ASN:HB2	2.02	0.42
4:A:372:LYS:O	4:A:435:HIS:NE2	2.52	0.42
4:A:942:PHE:O	4:A:945:GLU:HG2	2.19	0.42
4:A:1004:ASN:ND2	7:E:167:ARG:HD2	2.35	0.42
5:B:100:PRO:O	5:B:180:TYR:OH	2.27	0.42
5:B:899:ILE:O	5:B:952:VAL:HG21	2.19	0.42
5:B:1006:ILE:HG23	11:J:45:CYS:HB3	2.02	0.42
4:A:34:LYS:HG2	4:A:83:HIS:CE1	2.55	0.42
4:A:90:VAL:HG21	4:A:296:LEU:HD12	2.01	0.42
4:A:449:SER:OG	5:B:1134:GLU:HG3	2.20	0.42
4:A:775:ILE:O	4:A:797:LYS:NZ	2.32	0.42
5:B:373:ARG:HA	5:B:566:LEU:HD23	2.02	0.42
5:B:405:ARG:NE	5:B:632:ARG:HB3	2.35	0.42
5:B:782:LEU:HD23	5:B:782:LEU:HA	1.82	0.42
5:B:1215:ARG:C	5:B:1216:LEU:HD23	2.45	0.42
6:C:76:ASP:C	6:C:129:ILE:HD11	2.44	0.42
7:E:14:ARG:NH1	7:E:141:VAL:HG12	2.28	0.42
9:H:3:ASN:CG	9:H:4:THR:H	2.28	0.42
9:H:40:LEU:HD13	9:H:123:MET:HB2	2.00	0.42
10:I:113:ASP:OD1	10:I:114:GLN:N	2.53	0.42
4:A:230:ARG:HD3	4:A:233:TRP:CH2	2.55	0.42
4:A:550:LEU:HD23	4:A:556:TRP:CH2	2.55	0.42
5:B:848:ARG:HD2	11:J:8:PHE:HA	2.01	0.42
6:C:73:GLN:OE1	6:C:74:SER:N	2.52	0.42
5:B:1174:LYS:NZ	5:B:1179:GLN:OE1	2.33	0.42
9:H:27:GLU:OE1	9:H:39:THR:HG23	2.19	0.42
5:B:900:ALA:HB3	13:L:61:THR:CG2	2.50	0.42
5:B:994:TYR:HB2	5:B:999:MET:HE1	2.02	0.42
11:J:7:CYS:SG	11:J:9:SER:N	2.92	0.42
11:J:54:VAL:HG12	11:J:56:LEU:HG	2.01	0.42
12:K:77:THR:OG1	12:K:81:TYR:O	2.38	0.42
3:N:12:DA:H4'	3:N:13:DG:OP2	2.16	0.42
4:A:98:LYS:O	4:A:102:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:436:ILE:HD11	4:A:491:VAL:HG11	2.02	0.42
5:B:273:LEU:HD23	5:B:273:LEU:HA	1.87	0.42
6:C:178:PHE:HD2	6:C:179:GLU:N	2.18	0.42
7:E:197:LYS:HE2	7:E:199:ILE:HD11	2.02	0.42
2:T:14:DC:H2''	2:T:15:DA:O4'	2.20	0.41
4:A:30:ILE:HD13	4:A:30:ILE:HA	1.91	0.41
4:A:471:ASN:O	4:A:474:VAL:HG12	2.19	0.41
4:A:1143:LEU:O	4:A:1147:THR:OG1	2.36	0.41
5:B:486:TYR:OH	5:B:794:ASN:ND2	2.52	0.41
5:B:912:ILE:HB	5:B:939:THR:HB	2.01	0.41
6:C:18:VAL:O	6:C:231:ASN:HA	2.20	0.41
8:F:69:LEU:HB3	8:F:70:LYS:H	1.50	0.41
8:F:87:LYS:HG3	8:F:88:TYR:CD1	2.55	0.41
9:H:110:ASP:C	9:H:128:ASN:HD22	2.28	0.41
10:I:106:CYS:SG	10:I:108:HIS:HB2	2.59	0.41
13:L:41:SER:N	13:L:44:ASP:OD2	2.52	0.41
4:A:346:ASP:HB3	5:B:1108:ARG:H	1.85	0.41
4:A:853:ASP:OD2	4:A:857:ARG:NH2	2.49	0.41
5:B:258:LEU:HD13	5:B:269:ILE:HG12	2.02	0.41
5:B:526:GLU:OE2	5:B:538:ASN:ND2	2.54	0.41
6:C:14:SER:OG	6:C:15:LYS:N	2.53	0.41
6:C:244:VAL:HG11	12:K:105:PHE:CE2	2.54	0.41
4:A:380:VAL:HG21	4:A:427:GLN:O	2.21	0.41
4:A:573:SER:O	4:A:577:ILE:HG22	2.20	0.41
4:A:1319:VAL:HB	4:A:1322:ILE:HD13	2.02	0.41
5:B:351:TYR:O	5:B:355:ILE:HG13	2.19	0.41
5:B:356:LEU:HD13	5:B:356:LEU:HA	1.82	0.41
5:B:786:ASN:O	5:B:967:ARG:NH2	2.41	0.41
5:B:954:VAL:HG22	5:B:964:VAL:HG13	2.01	0.41
4:A:242:PRO:HB2	4:A:246:VAL:HG21	2.03	0.41
4:A:347:PHE:HB2	5:B:1150:ARG:HH22	1.86	0.41
4:A:569:LYS:HE2	6:C:221:TYR:HB2	2.02	0.41
4:A:1022:LEU:HD12	4:A:1022:LEU:HA	1.91	0.41
4:A:1420:ASP:OD2	4:A:1422:ARG:NH2	2.53	0.41
4:A:1436:ILE:HG22	4:A:1437:GLY:H	1.86	0.41
5:B:275:TYR:HE2	5:B:359:GLU:HG3	1.86	0.41
5:B:797:TYR:OH	5:B:971:THR:OG1	2.31	0.41
5:B:1159:ARG:HD3	5:B:1161:HIS:CE1	2.55	0.41
7:E:23:VAL:O	7:E:28:TYR:HB2	2.20	0.41
2:T:17:DG:C4	2:T:18:DA:C8	3.09	0.41
4:A:273:ASN:O	4:A:277:GLU:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:587:HIS:NE2	4:A:969:GLN:HG3	2.36	0.41
4:A:802:ASN:ND2	5:B:729:ILE:O	2.37	0.41
4:A:890:ASP:OD2	4:A:940:ARG:NH1	2.54	0.41
4:A:1121:GLU:HG3	4:A:1122:PRO:HD2	2.01	0.41
5:B:500:THR:HG22	5:B:502:ILE:HG22	2.02	0.41
5:B:666:TYR:O	5:B:668:ASP:N	2.51	0.41
5:B:1060:ARG:NH1	6:C:200:GLU:O	2.54	0.41
6:C:46:ILE:HD13	6:C:67:LEU:O	2.21	0.41
7:E:157:SER:N	7:E:160:GLU:OE1	2.43	0.41
11:J:6:ARG:HD3	11:J:13:VAL:HG12	2.03	0.41
4:A:388:LEU:HD22	4:A:432:VAL:HG11	2.03	0.41
4:A:820:GLY:O	4:A:824:LEU:HG	2.20	0.41
4:A:825:ILE:CD1	5:B:512:ARG:HB2	2.48	0.41
5:B:408:LEU:C	5:B:412:LEU:HD12	2.45	0.41
11:J:50:ILE:HD13	11:J:50:ILE:HA	1.88	0.41
4:A:352:VAL:HG21	5:B:1099:VAL:HG22	2.01	0.41
7:E:13:TRP:CE3	7:E:39:LEU:HD13	2.56	0.41
1:R:10:C:H42	2:T:19:DG:H1	1.67	0.41
5:B:46:GLN:H	5:B:46:GLN:HG3	1.65	0.41
5:B:365:THR:HG21	5:B:370:PHE:CD1	2.56	0.41
5:B:394:ASP:OD1	5:B:395:GLN:N	2.50	0.41
5:B:620:ARG:NH1	10:I:68:LEU:HD21	2.36	0.41
9:H:25:ARG:HD2	9:H:39:THR:CG2	2.50	0.41
9:H:26:ILE:HD12	9:H:26:ILE:HA	1.90	0.41
9:H:130:ARG:H	9:H:130:ARG:HE	1.69	0.41
10:I:37:GLU:HG2	10:I:38:ALA:H	1.86	0.41
3:N:11:DG:H2'	3:N:12:DA:H8	1.84	0.41
4:A:184:SER:O	4:A:199:LEU:N	2.53	0.41
4:A:208:LEU:HD23	4:A:235:ILE:HD11	2.02	0.41
4:A:364:VAL:CG1	4:A:458:HIS:HB3	2.50	0.41
4:A:455:MET:HE3	5:B:1138:MET:HE2	2.03	0.41
4:A:550:LEU:HD12	4:A:577:ILE:CD1	2.50	0.41
4:A:1384:VAL:HA	4:A:1389:PHE:CE2	2.56	0.41
4:A:1441:PHE:HZ	8:F:89:GLU:HA	1.86	0.41
5:B:301:ILE:HG21	5:B:314:LEU:HD11	2.02	0.41
5:B:582:VAL:HA	5:B:626:ILE:O	2.21	0.41
5:B:598:GLU:O	5:B:602:THR:OG1	2.31	0.41
5:B:771:SER:O	5:B:775:LYS:HE3	2.21	0.41
6:C:253:LYS:HB2	6:C:253:LYS:HE3	1.76	0.41
7:E:55:ARG:HD2	7:E:84:ASP:HA	2.02	0.41
7:E:59:SER:HB3	7:E:81:GLU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:31:THR:C	9:H:33:GLN:H	2.29	0.41
11:J:28:ASP:OD1	11:J:28:ASP:N	2.54	0.41
4:A:1286:LYS:HE2	4:A:1286:LYS:HB2	1.75	0.41
5:B:737:THR:OG1	10:I:66:PRO:O	2.36	0.41
6:C:10:ILE:HD11	12:K:105:PHE:CE1	2.55	0.41
7:E:99:HIS:CD2	7:E:99:HIS:C	2.98	0.41
7:E:116:ILE:HD13	7:E:121:MET:SD	2.61	0.41
8:F:101:ILE:HD13	8:F:120:ILE:HG22	2.02	0.41
2:T:13:DT:H1'	15:T:101:5N0:N6	2.36	0.40
4:A:269:ILE:HD11	4:A:300:VAL:HA	2.03	0.40
4:A:825:ILE:O	4:A:829:VAL:HG23	2.22	0.40
4:A:1041:ALA:O	4:A:1045:VAL:HG23	2.21	0.40
4:A:1105:LEU:HD23	4:A:1384:VAL:HG21	2.03	0.40
5:B:512:ARG:H	5:B:512:ARG:HG3	1.55	0.40
5:B:760:ASP:OD1	5:B:760:ASP:N	2.50	0.40
5:B:975:GLN:HG2	5:B:976:ILE:H	1.86	0.40
5:B:1015:HIS:O	5:B:1018:PRO:HD2	2.21	0.40
9:H:95:TYR:CE1	9:H:97:MET:HG3	2.56	0.40
13:L:49:LYS:HG3	13:L:50:ASP:OD1	2.22	0.40
2:T:19:DG:H5'	4:A:832:ALA:O	2.21	0.40
4:A:356:ASP:HB2	4:A:469:ARG:HE	1.86	0.40
4:A:442:VAL:HG12	4:A:491:VAL:HG22	2.03	0.40
4:A:598:LEU:O	9:H:122:LEU:HD12	2.20	0.40
5:B:299:GLU:OE1	5:B:572:HIS:N	2.47	0.40
5:B:586:TRP:CD1	5:B:588:GLY:H	2.39	0.40
5:B:789:MET:HE3	5:B:789:MET:HB3	1.93	0.40
5:B:1010:LEU:HD23	5:B:1010:LEU:HA	1.89	0.40
6:C:41:ILE:HA	6:C:42:PRO:HD3	1.95	0.40
11:J:1:MET:H3	11:J:1:MET:HG2	1.80	0.40
13:L:31:CYS:SG	13:L:32:ALA:N	2.94	0.40
4:A:279:LEU:HD13	4:A:279:LEU:HA	1.93	0.40
4:A:335:ARG:HE	4:A:335:ARG:HB2	1.61	0.40
5:B:726:ALA:HB2	5:B:1053:GLU:HG3	2.03	0.40
5:B:801:LYS:HE2	11:J:52:THR:HA	2.04	0.40
5:B:821:GLN:HB2	5:B:851:PHE:CE2	2.56	0.40
6:C:211:ASP:OD1	6:C:211:ASP:N	2.54	0.40
9:H:89:LEU:HB2	9:H:91:ASP:OD2	2.21	0.40
4:A:543:LEU:O	4:A:547:LEU:HG	2.22	0.40
4:A:1215:ARG:O	4:A:1219:THR:OG1	2.38	0.40
4:A:1436:ILE:O	4:A:1439:GLY:N	2.54	0.40
5:B:835:GLN:O	5:B:838:SER:OG	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:40:GLU:OE2	6:C:254:LYS:HE3	2.21	0.40
7:E:15:ALA:HA	7:E:140:LEU:O	2.22	0.40
8:F:97:ARG:HA	8:F:97:ARG:HD2	1.89	0.40
9:H:58:THR:C	9:H:59:ILE:HD12	2.47	0.40
10:I:61:ASP:OD1	10:I:61:ASP:N	2.54	0.40
11:J:49:MET:HE3	11:J:49:MET:HB3	1.63	0.40
4:A:1327:ILE:O	7:E:147:HIS:NE2	2.52	0.40
5:B:373:ARG:NE	5:B:567:GLU:OE2	2.54	0.40
5:B:825:VAL:HG21	5:B:1092:TYR:CE1	2.56	0.40
5:B:847:ASP:O	5:B:852:ARG:NH2	2.54	0.40
5:B:977:GLY:HA2	5:B:989:THR:OG1	2.21	0.40
6:C:55:THR:OG1	6:C:152:GLU:N	2.37	0.40
6:C:146:LYS:NZ	11:J:58:GLU:OE2	2.45	0.40
10:I:59:VAL:C	10:I:61:ASP:H	2.30	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%)	1264 (92%)	106 (8%)	0	100	100
5	B	1103/1224 (90%)	1030 (93%)	73 (7%)	0	100	100
6	C	265/318 (83%)	245 (92%)	20 (8%)	0	100	100
7	E	210/215 (98%)	196 (93%)	14 (7%)	0	100	100
8	F	84/155 (54%)	78 (93%)	6 (7%)	0	100	100
9	H	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
10	I	116/122 (95%)	104 (90%)	12 (10%)	0	100	100
11	J	63/70 (90%)	57 (90%)	6 (10%)	0	100	100
12	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	L	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	3493/4173 (84%)	3239 (93%)	254 (7%)	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	1194/1520 (79%)	1194 (100%)	0	100	100
5	B	955/1061 (90%)	955 (100%)	0	100	100
6	C	235/274 (86%)	235 (100%)	0	100	100
7	E	193/197 (98%)	193 (100%)	0	100	100
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	116/128 (91%)	116 (100%)	0	100	100
10	I	110/116 (95%)	110 (100%)	0	100	100
11	J	60/65 (92%)	60 (100%)	0	100	100
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	37/57 (65%)	37 (100%)	0	100	100
All	All	3072/3657 (84%)	3072 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	18	GLN
4	A	92	HIS
4	A	339	ASN
4	A	394	ASN
4	A	397	ASN

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Mol	Chain	Res	Type
4	A	660	ASN
4	A	858	ASN
4	A	1009	ASN
4	A	1011	GLN
4	A	1140	HIS
4	A	1427	ASN
5	B	60	GLN
5	B	325	GLN
5	B	357	GLN
5	B	538	ASN
5	B	835	GLN
5	B	932	HIS
5	B	1093	GLN
5	B	1161	HIS
5	B	1177	HIS
6	C	31	ASN
6	C	65	HIS
7	E	99	HIS
9	H	128	ASN
9	H	131	ASN
9	H	133	ASN
9	H	139	ASN
10	I	12	ASN
10	I	46	HIS
10	I	90	GLN
12	K	29	ASN
12	K	52	ASN
12	K	112	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	10/11 (90%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	10	C
1	R	11	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	9	G

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	5N0	T	101	-	100,107,107	2.82	51 (51%)	115,153,153	2.05	26 (22%)

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	5N0	T	101	-	-	13/92/92/92	0/9/9/9

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	101	5N0	C49-N23	8.35	1.47	1.33
15	T	101	5N0	C22-N10	7.97	1.47	1.33
15	T	101	5N0	C56-N25	6.25	1.47	1.33
15	T	101	5N0	C26-N14	6.13	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	101	5N0	C9-N3	6.08	1.49	1.39
15	T	101	5N0	C5-N3	5.74	1.48	1.37
15	T	101	5N0	C37-N19	5.38	1.47	1.37
15	T	101	5N0	C29-N14	5.30	1.47	1.39
15	T	101	5N0	C10-N6	5.26	1.47	1.37
15	T	101	5N0	C43-N21	5.24	1.47	1.37
15	T	101	5N0	C31-N17	5.05	1.47	1.37
15	T	101	5N0	C16-N8	5.00	1.47	1.37
15	T	101	5N0	C44-N22	-4.27	1.32	1.38
15	T	101	5N0	C31-C30	4.27	1.56	1.49
15	T	101	5N0	C10-C6	4.17	1.56	1.49
15	T	101	5N0	C5-C4	4.03	1.56	1.49
15	T	101	5N0	C39-N20	-3.86	1.33	1.38
15	T	101	5N0	C17-N9	-3.51	1.34	1.38
15	T	101	5N0	C11-N7	-3.49	1.34	1.38
15	T	101	5N0	C32-N18	-3.37	1.34	1.38
15	T	101	5N0	C32-C37	3.36	1.56	1.49
15	T	101	5N0	C11-C16	3.33	1.56	1.49
15	T	101	5N0	C17-C22	3.05	1.56	1.49
15	T	101	5N0	C39-C43	2.75	1.55	1.49
15	T	101	5N0	C44-C49	2.75	1.55	1.49
15	T	101	5N0	C6-N5	-2.72	1.33	1.37
15	T	101	5N0	C3-N2	-2.66	1.33	1.38
15	T	101	5N0	C28-C29	2.55	1.40	1.37
15	T	101	5N0	C2-N1	-2.47	1.33	1.37
15	T	101	5N0	O8-C43	-2.44	1.18	1.23
15	T	101	5N0	C4-N1	-2.42	1.33	1.37
15	T	101	5N0	C8-C9	2.41	1.39	1.37
15	T	101	5N0	O1-C5	-2.41	1.19	1.23
15	T	101	5N0	C59-C63	2.40	1.54	1.49
15	T	101	5N0	C42-N19	2.39	1.48	1.41
15	T	101	5N0	O7-C37	-2.38	1.19	1.23
15	T	101	5N0	O5-C26	-2.36	1.18	1.23
15	T	101	5N0	O3-C16	-2.34	1.19	1.23
15	T	101	5N0	O9-C49	-2.34	1.19	1.23
15	T	101	5N0	O2-C10	-2.33	1.19	1.23
15	T	101	5N0	C41-N20	-2.29	1.32	1.37
15	T	101	5N0	C21-N8	2.27	1.48	1.41
15	T	101	5N0	C14-N6	2.27	1.48	1.41
15	T	101	5N0	O6-C31	-2.22	1.19	1.23
15	T	101	5N0	C36-N17	2.22	1.48	1.41
15	T	101	5N0	O4-C22	-2.18	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	101	5N0	C30-N16	-2.17	1.34	1.37
15	T	101	5N0	C57-C56	2.16	1.55	1.50
15	T	101	5N0	C46-N22	-2.11	1.32	1.37
15	T	101	5N0	C48-N21	2.09	1.47	1.41
15	T	101	5N0	C8-N5	-2.04	1.32	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	101	5N0	C16-C11-N7	6.27	129.57	122.78
15	T	101	5N0	C37-C32-N18	5.55	128.80	122.78
15	T	101	5N0	C4-C5-N3	5.44	121.26	113.08
15	T	101	5N0	C22-C17-N9	5.36	128.59	122.78
15	T	101	5N0	N1-C4-N2	-5.31	108.41	111.40
15	T	101	5N0	C29-N15-C30	5.14	109.29	104.64
15	T	101	5N0	C24-C25-C26	-5.08	100.38	110.76
15	T	101	5N0	C9-N4-C6	5.00	109.17	104.64
15	T	101	5N0	C6-C10-N6	4.34	119.60	113.08
15	T	101	5N0	C3-N2-C4	4.08	109.11	105.08
15	T	101	5N0	C2-N1-C4	3.91	108.93	106.46
15	T	101	5N0	C43-C39-N20	3.88	126.98	122.78
15	T	101	5N0	C39-C43-N21	3.67	120.53	114.27
15	T	101	5N0	N3-C9-N4	3.43	127.09	118.64
15	T	101	5N0	C49-C44-N22	3.18	126.23	122.78
15	T	101	5N0	C2-C3-N2	-2.97	106.86	110.74
15	T	101	5N0	C19-N9-C17	2.87	111.36	109.03
15	T	101	5N0	C32-C37-N19	2.85	119.13	114.27
15	T	101	5N0	C15-C11-C16	-2.78	122.41	129.54
15	T	101	5N0	O4-C22-N10	-2.67	118.53	123.35
15	T	101	5N0	C35-C32-C37	-2.63	122.81	129.54
15	T	101	5N0	C31-C30-N15	-2.37	120.85	124.20
15	T	101	5N0	O8-C43-N21	-2.14	119.06	122.88
15	T	101	5N0	C11-C16-N8	2.12	117.89	114.27
15	T	101	5N0	N14-C29-N15	2.09	123.80	118.64
15	T	101	5N0	O11-C63-C59	2.03	120.04	114.84

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	101	5N0	C23-C24-C25-C26
15	T	101	5N0	N22-C44-C49-O9

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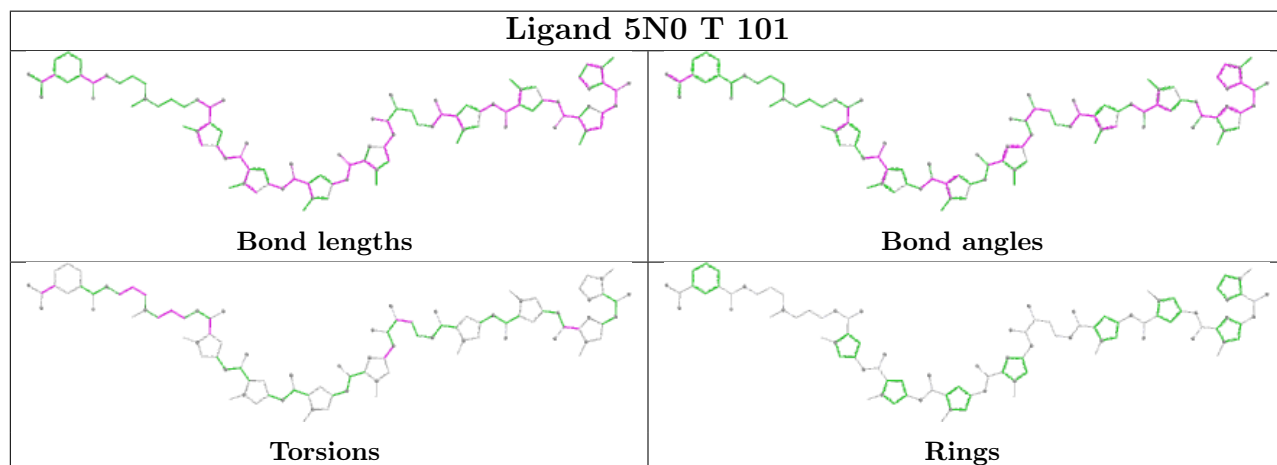
Mol	Chain	Res	Type	Atoms
15	T	101	5N0	N22-C44-C49-N23
15	T	101	5N0	C58-C59-C63-O11
15	T	101	5N0	C60-C59-C63-O12
15	T	101	5N0	C60-C59-C63-O11
15	T	101	5N0	C58-C59-C63-O12
15	T	101	5N0	C50-C51-C52-N24
15	T	101	5N0	C53-C54-C55-N25
15	T	101	5N0	N24-C53-C54-C55
15	T	101	5N0	N23-C50-C51-C52
15	T	101	5N0	C28-C29-N14-C26
15	T	101	5N0	O2-C10-C6-N4

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	101	5N0	5	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 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](#)

There are no chain breaks in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	R	11/11 (100%)	0.21	1 (9%) 15 13	116, 132, 191, 198	0
2	T	26/30 (86%)	0.41	0 100 100	118, 225, 252, 258	0
3	N	14/20 (70%)	0.20	0 100 100	229, 244, 260, 264	0
4	A	1384/1733 (79%)	0.02	9 (0%) 84 63	52, 113, 188, 236	0
5	B	1123/1224 (91%)	0.01	5 (0%) 88 72	55, 99, 153, 196	0
6	C	267/318 (83%)	-0.05	1 (0%) 88 72	67, 99, 136, 165	0
7	E	212/215 (98%)	-0.06	2 (0%) 81 58	96, 154, 209, 231	0
8	F	86/155 (55%)	-0.18	0 100 100	82, 114, 147, 186	0
9	H	133/146 (91%)	0.07	2 (1%) 72 46	106, 137, 170, 202	0
10	I	118/122 (96%)	-0.07	1 (0%) 82 60	83, 117, 150, 162	0
11	J	65/70 (92%)	0.02	0 100 100	73, 93, 151, 161	0
12	K	114/120 (95%)	-0.18	0 100 100	78, 105, 131, 153	0
13	L	43/70 (61%)	0.27	1 (2%) 61 38	92, 158, 222, 258	0
All	All	3596/4234 (84%)	-0.00	22 (0%) 85 66	52, 111, 185, 264	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	E	83	CYS	3.5
9	H	63	LEU	3.3
10	I	57	GLY	3.2
13	L	46	VAL	3.0
5	B	620	ARG	2.9
9	H	139	ASN	2.9
5	B	1172	ILE	2.7
5	B	106	ASP	2.5
4	A	365	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
5	B	335	GLY	2.4
6	C	50	GLU	2.4
1	R	10	C	2.4
4	A	69	THR	2.3
4	A	1081	LEU	2.2
5	B	467	GLY	2.2
4	A	386	ASP	2.2
4	A	355	GLY	2.2
4	A	1413	GLY	2.1
7	E	123	LEU	2.1
4	A	145	LYS	2.1
4	A	3	GLY	2.0
4	A	103	CYS	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](#)

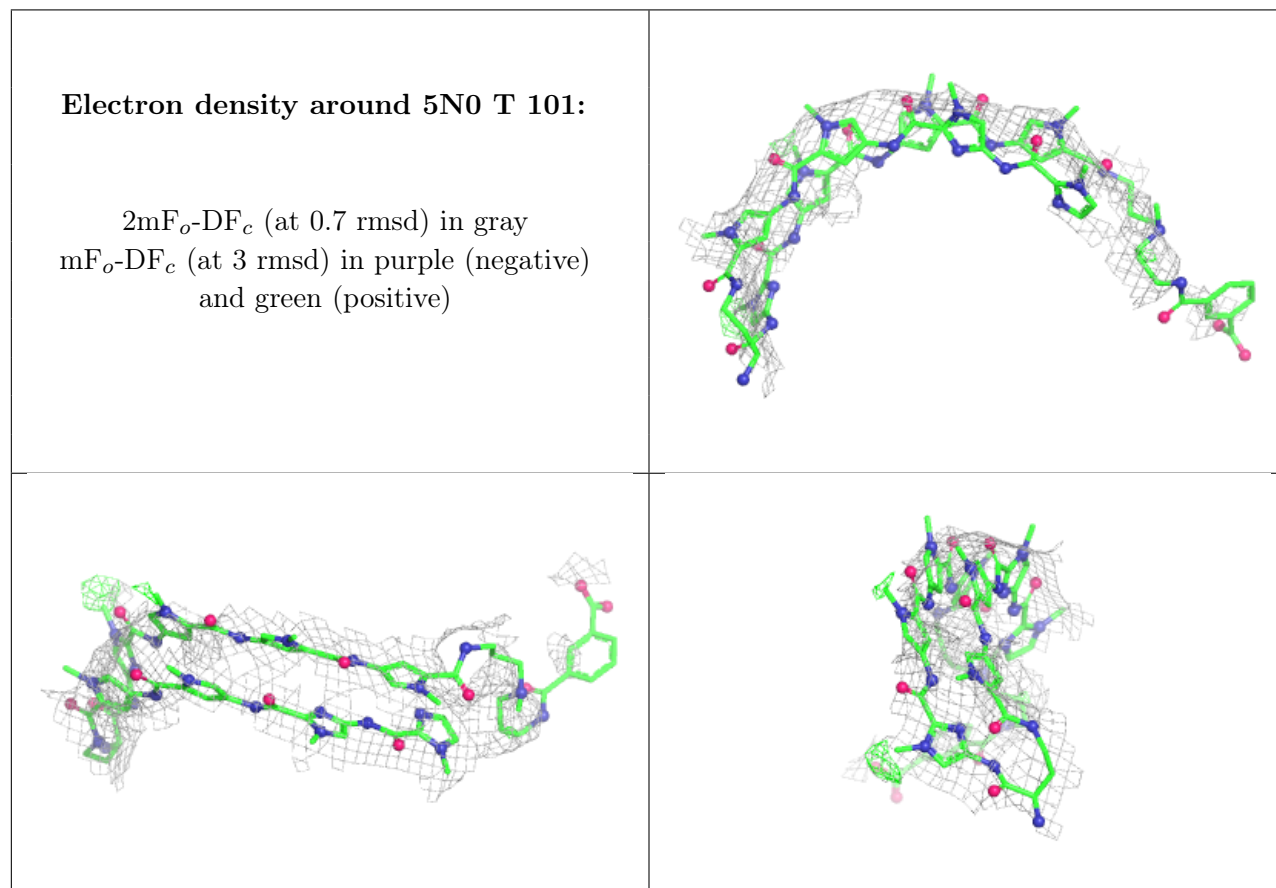
There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	5N0	T	101	99/99	0.71	0.12	198,236,262,264	0
14	MG	R	2001	1/1	0.80	0.26	141,141,141,141	0
16	ZN	A	1801	1/1	0.93	0.12	242,242,242,242	0
16	ZN	B	1301	1/1	0.93	0.07	195,195,195,195	0
16	ZN	L	101	1/1	0.96	0.08	182,182,182,182	0
16	ZN	A	1802	1/1	0.97	0.04	167,167,167,167	0
16	ZN	C	401	1/1	0.99	0.02	108,108,108,108	0
16	ZN	I	202	1/1	1.00	0.03	110,110,110,110	0
16	ZN	J	101	1/1	1.00	0.02	90,90,90,90	0
16	ZN	I	201	1/1	1.00	0.03	99,99,99,99	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.