



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 12:05 PM EDT

PDB ID : 8UKS / pdb_00008uks
Title : RNA polymerase II elongation complex with Fapy-dG lesion soaking with CTP before chemistry
Authors : Hou, P.; Oh, J.; Wang, D.
Deposited on : 2023-10-15
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

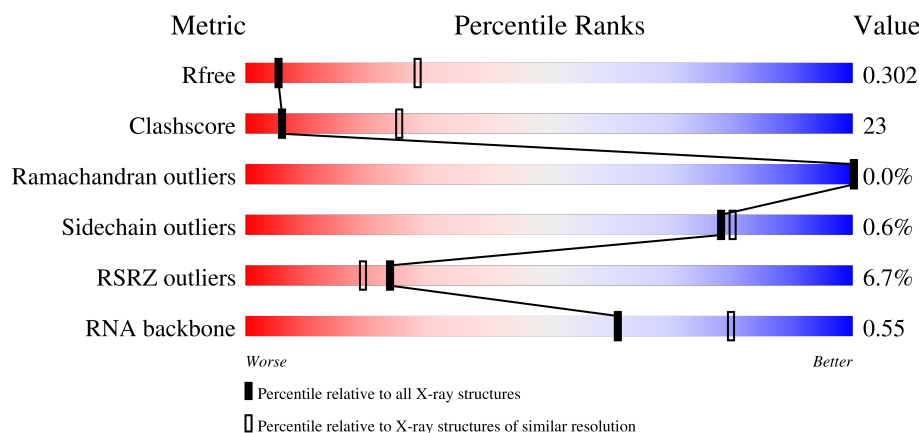
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.



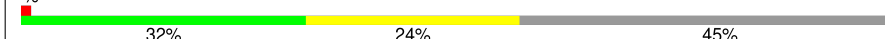
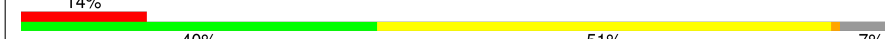
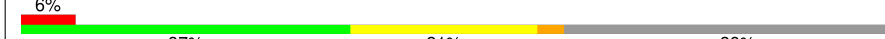
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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

Mol	Chain	Length	Quality of chain
1	R	9	
2	T	29	
3	N	18	
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

There are 16 unique types of molecules in this entry. The entry contains 29002 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	9	Total	C	N	O	P	0	0	0
			194	88	40	58	8			

- Molecule 2 is a DNA chain called tsDNA with Fapy-dG lesion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	24	Total	C	N	O	P	0	0	0
			481	230	76	151	24			

- Molecule 3 is a DNA chain called ntsDNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	13	Total	C	N	O	P	0	0	0
			275	128	61	73	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1385	Total	C	N	O	S	0	0	0
			10839	6837	1898	2044	60			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1123	Total	C	N	O	S	0	0	0
			8859	5607	1552	1647	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
			332	205	64	59	4			

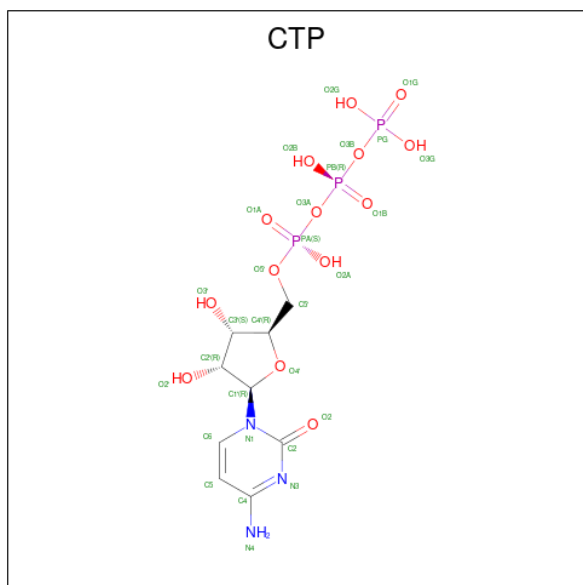
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total	Mg	0	0
			2	2		

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 16 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: C₉H₁₆N₃O₁₄P₃) (labeled as "Ligand of Interest" by depositor).

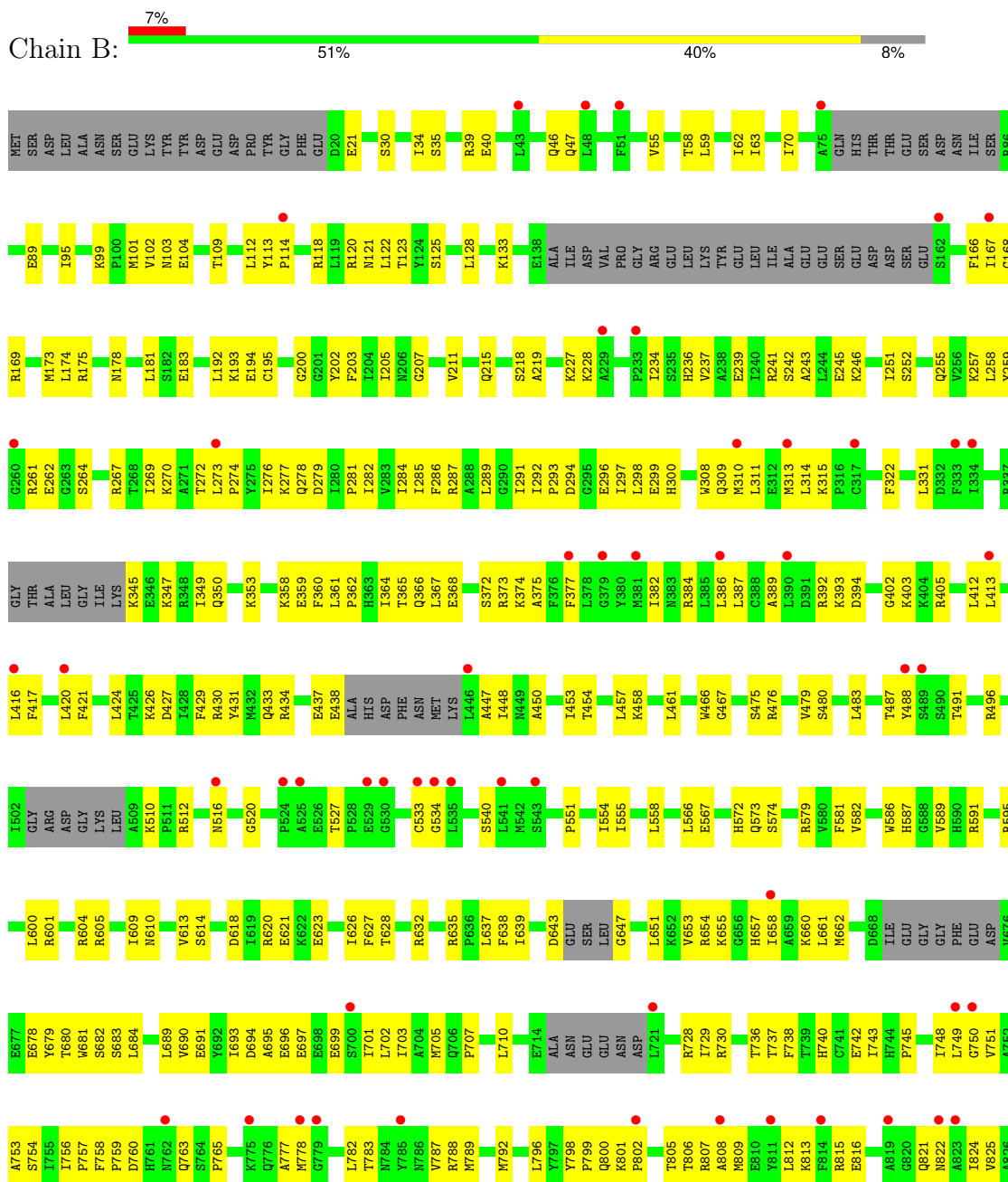


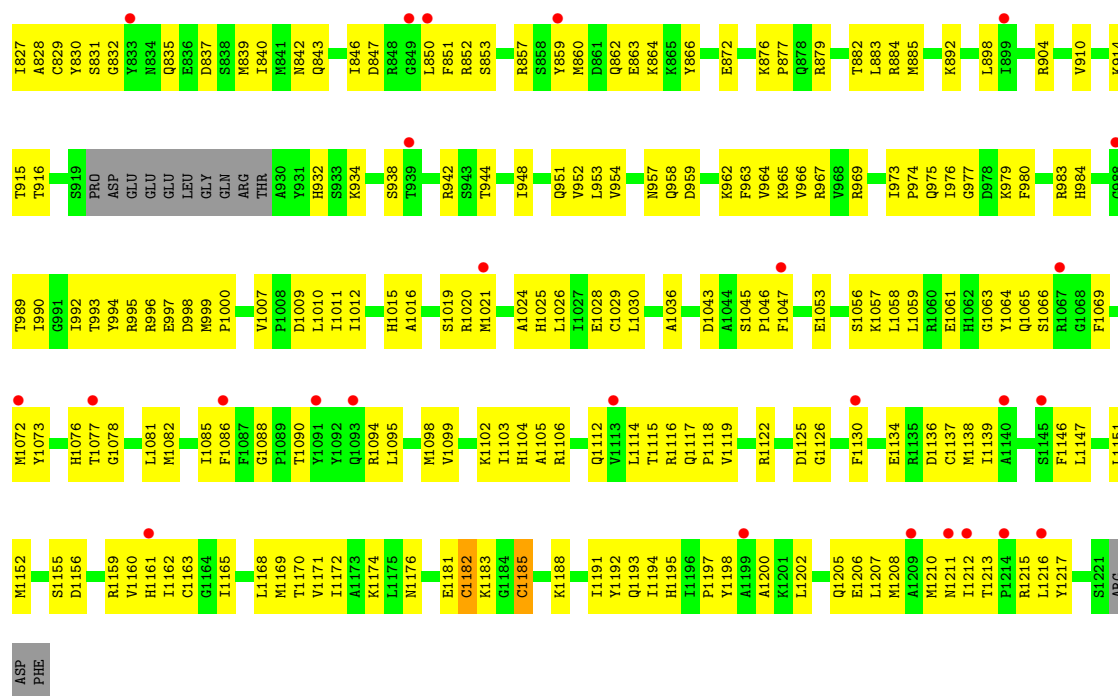
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	B	1	Total	C	N	O P	0	0
			29	9	3	14 3		

D1373	P1292	R1215	L1133	G1065	P978	D900	R826	M746	F662	K575	D483	V392	D307
V1374	K1300	I1216	I1134	V1066	L981	L901	T827	Y747	F662	K575	G484	V392	I308
M1375	M1300	Q1217	R1135	A1067	L982	L902	A828	M748	G665	Q576	N487	H399	Q311
T1376	E1303	Q1218	I1136	A1069	T983	N903	W829	S751	I666	I577	Y403	P312	P312
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T1382	V1305	L1224	T1141	S1071	V987	T907	T834	I756	D668	T582	L501	V405	L315
S1383	L1306	L1227	T1142	G1073	K991	L908	G835	W757	T669	P583	S502	R412	P321
V1384	T1308	I1227	K1143	T1077	D992	L913	G836	M758	I670	P583	Q503	R412	P321
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N1390	Y1154	E1234	Y1154	T1080	Q994	S915	R840	W761	G673	H587	C506	D414	S324
G1395	T1161	K1235	T1161	Q1079	E995	G916	L841	S762	P674	L588	A506	L415	I325
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L1397	E1166	K1237	E1166	Q1083	L997	L922	R843	Q767	M676	L598	P508	R420	A327
M1398	E1167	I1237	E1167	F1084	L998	L923	R844	Q768	E678	L598	Q510	R420	R328
R1399	D1166	C1240	D1166	H1085	V999	L928	R845	W769	T680	L598	V512	I424	K330
T1318	E1167	R1241	E1167	PHE	R1001	L929	R846	S770	E681	L598	V512	I424	G331
E1403	E1168	LYS	E1168	ALA	A1010	Q926	R847	I775	I683	K601	S513	L426	K332
E1404	I1169	GLY	I1169	GLY	Q1011	Q927	R851	A776	I683	D602	V512	L426	K332
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I1408	L1173	LYS	H1173	LYS	D1013	L929	Y852	F777	A776	I608	V512	L426	K330
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A1412	L1176	VAL	L1176	VAL	T1016	E932	G861	F779	K688	D609	P519	V442	R337
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C1421	L1176	VAL	L1176	VAL	T1016	E932	G861	F779	K688	D609	P519	V442	R337
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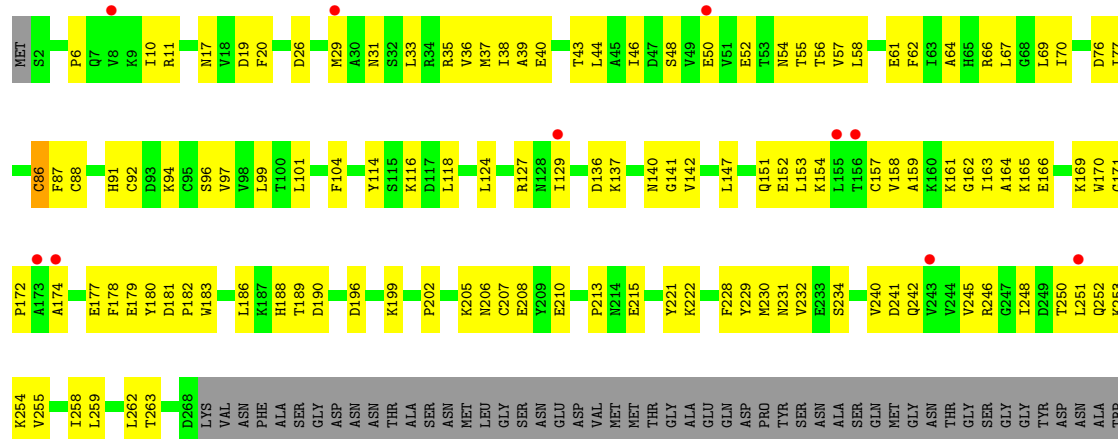
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- Molecule 5: DNA-directed RNA polymerase II subunit RPB2

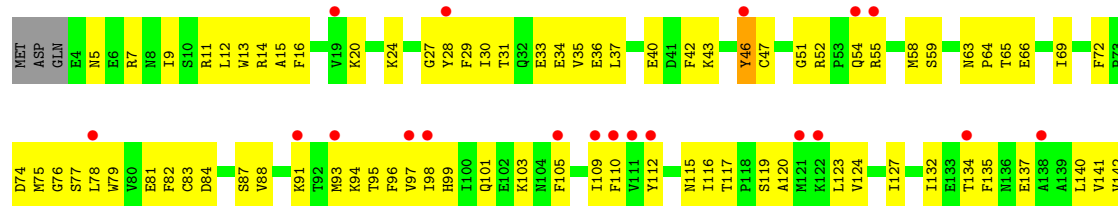


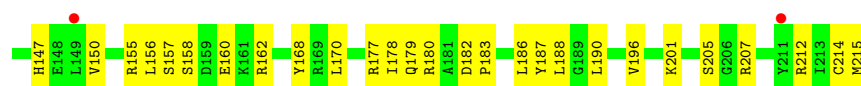


• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

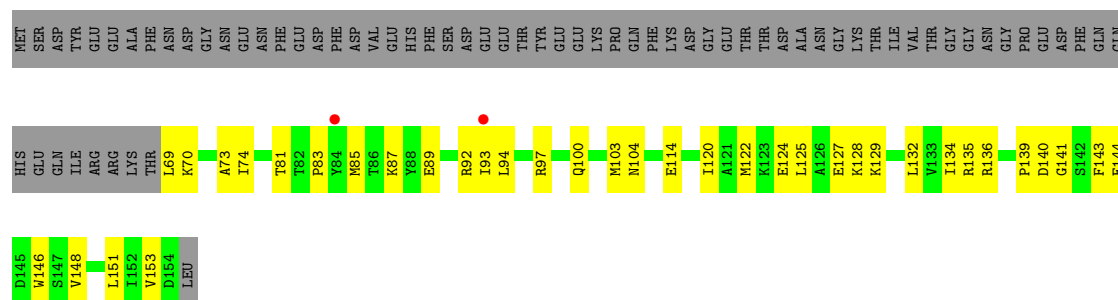
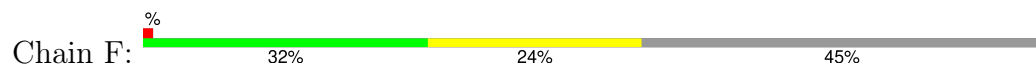


• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

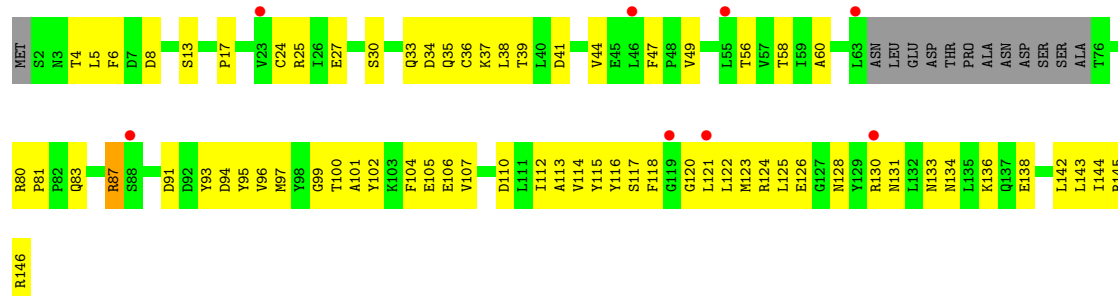
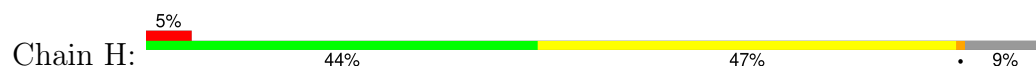




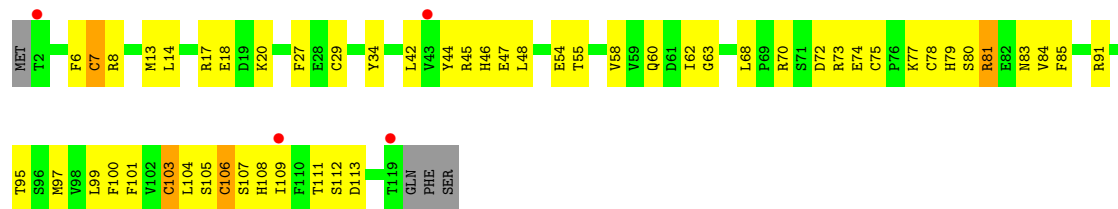
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



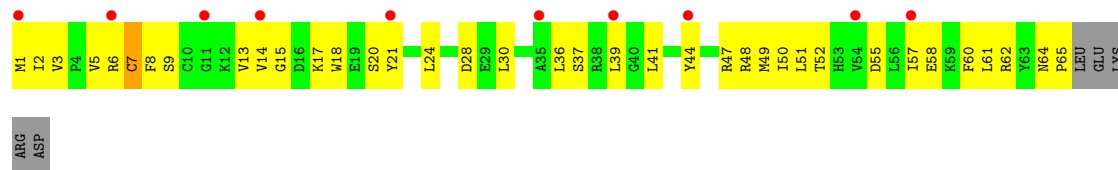
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



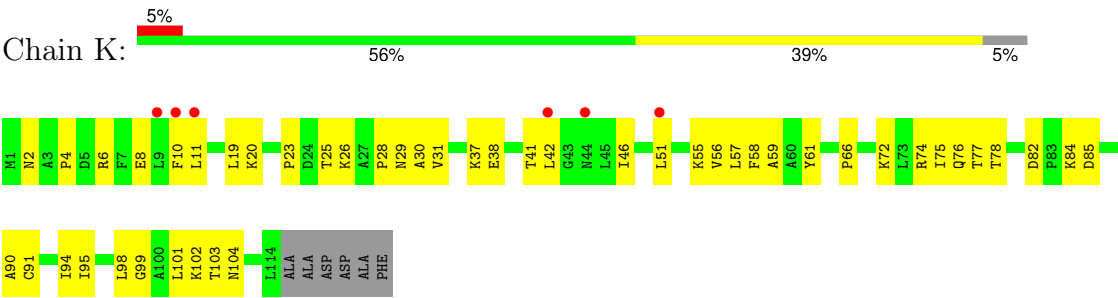
- Molecule 10: DNA-directed RNA polymerase II subunit RPB9



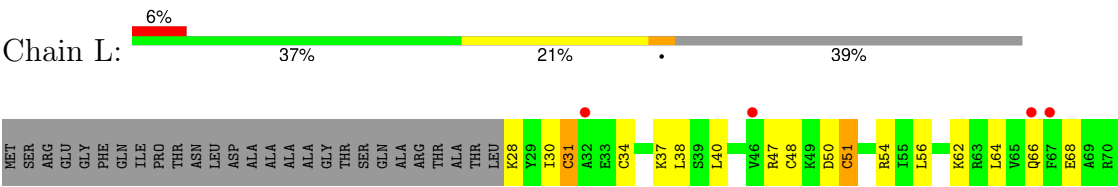
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



● 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, α , β , γ	157.12Å 221.63Å 189.96Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	47.76 – 3.40 47.76 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.76-3.40) 98.8 (47.76-3.40)	Depositor EDS
R_{merge}	0.52	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.267 , 0.301 0.267 , 0.302	Depositor DCC
R_{free} test set	2000 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å ²)	95.6	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 108.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29002	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, WVQ, CTP, 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	0.16	0/218	0.40	0/339
2	T	0.29	0/507	0.56	0/775
3	N	0.28	0/311	0.45	0/479
4	A	0.20	0/11033	0.48	0/14927
5	B	0.18	0/9030	0.45	0/12186
6	C	0.19	0/2139	0.42	0/2899
7	E	0.20	0/1767	0.46	0/2378
8	F	0.16	0/696	0.40	0/943
9	H	0.21	0/1082	0.51	0/1466
10	I	0.21	0/970	0.52	1/1308 (0.1%)
11	J	0.22	0/541	0.50	0/727
12	K	0.18	0/937	0.44	0/1265
13	L	0.20	0/333	0.47	0/442
All	All	0.20	0/29564	0.47	1/40134 (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
9	H	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	81	ARG	CB-CG-CD	6.96	127.32	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	H	87	ARG	Peptide

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	194	0	98	11	0
2	T	481	0	262	16	0
3	N	275	0	144	12	0
4	A	10839	0	10869	548	1
5	B	8859	0	8816	426	0
6	C	2101	0	2056	112	1
7	E	1731	0	1758	94	0
8	F	684	0	692	35	0
9	H	1064	0	1029	70	0
10	I	952	0	897	43	0
11	J	532	0	542	38	0
12	K	919	0	929	41	0
13	L	332	0	347	16	0
14	A	2	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	B	29	0	12	2	0
All	All	29002	0	28451	1310	1

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 23.

All (1310) 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)
5:B:63:ILE:HD13	5:B:421:PHE:CE2	1.28	1.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:63:ILE:HD13	5:B:421:PHE:CZ	1.46	1.48
5:B:63:ILE:CD1	5:B:421:PHE:CE2	2.03	1.41
4:A:666:ILE:CD1	5:B:1030:LEU:HD22	1.55	1.35
5:B:63:ILE:CD1	5:B:421:PHE:HE2	1.38	1.34
5:B:63:ILE:HD12	5:B:421:PHE:HE2	1.21	1.04
4:A:666:ILE:CD1	5:B:1030:LEU:CD2	2.36	1.02
4:A:666:ILE:HD13	5:B:1030:LEU:CD2	1.90	1.01
5:B:63:ILE:CD1	5:B:421:PHE:CZ	2.35	0.97
4:A:666:ILE:HD13	5:B:1030:LEU:HD22	0.96	0.94
5:B:1182:CYS:SG	5:B:1185:CYS:HB2	2.09	0.93
4:A:666:ILE:HG22	5:B:1026:LEU:HB3	1.53	0.90
4:A:208:LEU:HB2	4:A:235:ILE:HD11	1.54	0.88
4:A:67:CYS:HB3	4:A:70:CYS:HB2	1.53	0.87
2:T:17:DG:H4'	4:A:1403:GLU:HG2	1.57	0.85
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.59	0.84
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.59	0.84
5:B:753:ALA:HA	5:B:756:ILE:HD12	1.59	0.83
9:H:97:MET:HE2	9:H:118:PHE:HB2	1.59	0.83
5:B:483:LEU:HD21	5:B:491:THR:HG23	1.61	0.82
4:A:1278:ASN:HB2	4:A:1312:ASN:HB2	1.62	0.81
8:F:135:ARG:NH1	8:F:143:PHE:CD1	2.48	0.81
11:J:21:TYR:HB2	11:J:39:LEU:HD11	1.61	0.81
4:A:202:LEU:HB3	4:A:207:ILE:HD11	1.62	0.81
13:L:47:ARG:HB3	13:L:54:ARG:HG2	1.63	0.81
4:A:597:LEU:HB3	9:H:102:TYR:HE2	1.45	0.80
4:A:392:VAL:HG11	4:A:424:ILE:HD11	1.62	0.79
9:H:39:THR:O	9:H:123:MET:HA	1.81	0.79
9:H:83:GLN:H	9:H:87:ARG:HE	1.29	0.79
4:A:666:ILE:HD11	5:B:1030:LEU:CD2	2.14	0.78
4:A:269:ILE:HG12	4:A:299:HIS:HB3	1.65	0.78
4:A:443:LEU:HD21	4:A:455:MET:HB3	1.67	0.77
4:A:1127:ASP:HB3	4:A:1130:GLN:HB3	1.65	0.77
6:C:177:GLU:O	6:C:230:MET:HA	1.85	0.77
4:A:786:HIS:HE1	5:B:742:GLU:HG3	1.48	0.77
5:B:239:GLU:HG2	5:B:255:GLN:HG2	1.67	0.77
9:H:38:LEU:HA	9:H:124:ARG:O	1.85	0.76
4:A:885:THR:HG23	4:A:1024:SER:HB3	1.68	0.76
5:B:661:LEU:HD11	5:B:684:LEU:HD11	1.68	0.76
4:A:209:ASN:O	4:A:213:HIS:ND1	2.15	0.76
5:B:394:ASP:HB2	10:I:91:ARG:HD2	1.67	0.75
5:B:63:ILE:HD13	5:B:421:PHE:HZ	1.40	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:315:LEU:HA	4:A:321:PRO:HA	1.69	0.74
4:A:484:GLY:H	5:B:989:THR:HG23	1.51	0.74
5:B:218:SER:O	5:B:241:ARG:NH1	2.21	0.74
5:B:384:ARG:NH2	5:B:623:GLU:OE2	2.21	0.74
5:B:431:TYR:HA	5:B:434:ARG:HE	1.52	0.74
5:B:102:VAL:HG22	5:B:112:LEU:HB2	1.69	0.73
5:B:287:ARG:HG3	5:B:292:ILE:HD13	1.69	0.73
5:B:789:MET:HE2	5:B:967:ARG:HB2	1.71	0.73
4:A:50:ILE:HG23	4:A:52:GLY:H	1.53	0.73
4:A:968:GLN:HA	4:A:973:ILE:HD12	1.68	0.73
5:B:310:MET:HG3	5:B:386:LEU:HD12	1.71	0.73
7:E:29:PHE:HB2	7:E:65:THR:HG22	1.71	0.72
5:B:420:LEU:HB3	5:B:453:ILE:HD13	1.69	0.72
5:B:680:THR:HG23	5:B:683:SER:H	1.53	0.72
4:A:535:THR:O	4:A:575:LYS:NZ	2.20	0.72
4:A:672:ASP:H	4:A:736:ASN:HD21	1.36	0.72
9:H:128:ASN:O	9:H:131:ASN:ND2	2.22	0.72
5:B:293:PRO:HB2	5:B:296:GLU:HB2	1.72	0.72
4:A:898:ARG:HH12	4:A:929:LEU:HB3	1.55	0.72
5:B:710:LEU:HD21	5:B:738:PHE:HB2	1.72	0.72
5:B:751:VAL:HG23	5:B:812:LEU:HD22	1.71	0.71
7:E:168:TYR:HB3	7:E:170:LEU:HD23	1.72	0.71
4:A:598:LEU:HB3	9:H:25:ARG:HH12	1.54	0.71
4:A:698:GLN:HG2	10:I:99:LEU:HG	1.73	0.71
4:A:946:VAL:HG22	7:E:201:LYS:HD3	1.71	0.71
5:B:736:THR:HG21	10:I:70:ARG:HD2	1.72	0.71
6:C:147:LEU:HD22	6:C:151:GLN:HB3	1.73	0.71
4:A:761:MET:HE2	5:B:1021:MET:HG2	1.73	0.70
5:B:104:GLU:OE2	5:B:120:ARG:NH2	2.23	0.70
10:I:7:CYS:HB2	10:I:34:TYR:HD2	1.56	0.70
13:L:38:LEU:HD12	13:L:56:LEU:HD11	1.71	0.70
3:N:4:DG:H2''	3:N:5:DC:C5	2.26	0.70
4:A:846:GLU:HA	4:A:1066:VAL:HG22	1.74	0.70
4:A:1128:GLN:HE21	4:A:1304:TRP:HE1	1.38	0.70
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.73	0.70
9:H:37:LYS:H	9:H:126:GLU:HB2	1.57	0.70
4:A:103:CYS:HA	4:A:106:VAL:HG12	1.75	0.69
5:B:123:THR:HG23	5:B:205:ILE:HA	1.74	0.69
5:B:215:GLN:HE21	5:B:476:ARG:HD2	1.57	0.69
5:B:728:ARG:HD2	5:B:730:ARG:HH21	1.56	0.69
5:B:860:MET:HG3	5:B:965:LYS:HE3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:28:LYS:N	13:L:38:LEU:O	2.25	0.69
4:A:914:GLU:HG2	4:A:978:PRO:HB2	1.74	0.69
7:E:127:ILE:HB	7:E:132:ILE:HD11	1.72	0.69
9:H:113:ALA:HB1	9:H:124:ARG:HH12	1.55	0.69
4:A:71:GLN:HE22	5:B:1176:ASN:HB2	1.58	0.69
5:B:996:ARG:HG3	5:B:1007:VAL:HG21	1.73	0.69
4:A:1282:VAL:HG13	4:A:1308:THR:HG22	1.74	0.69
4:A:1424:VAL:HG22	4:A:1436:ILE:HD11	1.74	0.69
4:A:997:LEU:O	4:A:1011:GLN:NE2	2.26	0.69
5:B:128:LEU:HB2	5:B:168:GLY:O	1.93	0.69
9:H:95:TYR:HB3	9:H:144:ILE:HB	1.75	0.69
4:A:69:THR:HB	5:B:1172:ILE:HD12	1.75	0.68
4:A:583:PRO:HD3	4:A:645:LEU:HD13	1.75	0.68
4:A:767:GLN:HA	4:A:799:PHE:HA	1.73	0.68
4:A:1239:ARG:HH22	4:A:1241:ARG:HH21	1.39	0.68
4:A:1282:VAL:HG12	4:A:1306:LEU:HD22	1.74	0.68
5:B:574:SER:OG	5:B:591:ARG:NH2	2.27	0.68
4:A:203:SER:O	4:A:206:GLU:HG3	1.93	0.68
4:A:900:ASP:H	4:A:906:HIS:HB3	1.59	0.68
7:E:64:PRO:HD3	7:E:77:SER:H	1.59	0.68
5:B:651:LEU:O	5:B:654:ARG:NH1	2.27	0.68
5:B:969:ARG:NH1	6:C:61:GLU:OE1	2.26	0.68
5:B:703:ILE:HG22	5:B:740:HIS:HB2	1.75	0.68
4:A:1080:THR:O	4:A:1083:THR:OG1	2.12	0.67
10:I:6:PHE:HD1	10:I:13:MET:HA	1.58	0.67
4:A:618:GLU:OE1	4:A:620:LYS:N	2.27	0.67
4:A:782:ARG:NH2	5:B:699:GLU:O	2.28	0.67
4:A:351:THR:HG23	5:B:1103:ILE:HG12	1.77	0.66
2:T:6:DT:H2"	2:T:7:DC:C5	2.31	0.66
4:A:1325:THR:HA	7:E:147:HIS:HA	1.76	0.66
5:B:277:LYS:HG2	5:B:278:GLN:HG2	1.77	0.66
12:K:56:VAL:HG22	12:K:77:THR:HG22	1.78	0.66
4:A:587:HIS:HA	4:A:607:ILE:O	1.96	0.66
5:B:121:ASN:HA	5:B:207:GLY:HA3	1.77	0.66
4:A:117:GLU:HB2	4:A:126:LEU:HD11	1.78	0.66
4:A:214:ILE:HB	4:A:219:PHE:CE1	2.31	0.66
4:A:999:VAL:HG12	4:A:1000:LEU:HD12	1.77	0.66
5:B:133:LYS:HA	5:B:133:LYS:HE3	1.78	0.66
4:A:102:VAL:HG12	4:A:135:PHE:CZ	2.31	0.66
4:A:711:ARG:HD2	10:I:95:THR:HB	1.77	0.66
7:E:179:GLN:HG3	7:E:182:ASP:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:86:CYS:SG	6:C:87:PHE:N	2.68	0.65
4:A:308:ILE:HG13	4:A:312:PRO:HD2	1.77	0.65
5:B:1104:HIS:NE2	5:B:1126:GLY:O	2.29	0.65
7:E:11:ARG:HE	7:E:141:VAL:HG21	1.61	0.65
12:K:25:THR:HG22	12:K:26:LYS:HG3	1.77	0.65
5:B:653:VAL:HA	5:B:689:LEU:HD22	1.78	0.65
7:E:40:GLU:HA	7:E:43:LYS:HE2	1.79	0.65
4:A:183:GLY:O	4:A:199:LEU:N	2.29	0.65
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.62	0.65
4:A:1397:LEU:HB2	4:A:1426:GLU:HG2	1.79	0.65
4:A:214:ILE:HB	4:A:219:PHE:HE1	1.62	0.65
5:B:1115:THR:HB	5:B:1117:GLN:HG3	1.79	0.65
4:A:1329:THR:HG22	4:A:1331:SER:H	1.62	0.65
5:B:1104:HIS:HB2	5:B:1122:ARG:HB2	1.78	0.65
13:L:34:CYS:HB3	13:L:51:CYS:HB3	1.79	0.65
5:B:166:PHE:HZ	5:B:169:ARG:HG2	1.62	0.65
5:B:219:ALA:N	5:B:403:LYS:O	2.28	0.65
6:C:11:ARG:NH1	6:C:206:ASN:OD1	2.30	0.65
4:A:845:LEU:HD12	4:A:1069:ALA:HB2	1.77	0.64
4:A:306:ASN:H	4:A:324:SER:HB2	1.62	0.64
4:A:1290:LYS:HA	4:A:1300:LYS:HA	1.79	0.64
10:I:17:ARG:HE	10:I:18:GLU:H	1.43	0.64
5:B:1043:ASP:OD1	5:B:1045:SER:OG	2.15	0.64
9:H:106:GLU:HG3	9:H:112:ILE:HD13	1.80	0.64
5:B:789:MET:HG2	5:B:967:ARG:HD3	1.79	0.64
6:C:101:LEU:HB2	6:C:118:LEU:HD23	1.79	0.64
9:H:105:GLU:HG3	9:H:113:ALA:HB3	1.78	0.64
4:A:1129:GLU:HA	4:A:1132:LYS:HD2	1.80	0.64
5:B:40:GLU:OE1	5:B:682:SER:N	2.30	0.64
6:C:142:VAL:HG23	11:J:15:GLY:HA3	1.80	0.64
4:A:1016:THR:HG21	7:E:207:ARG:HE	1.62	0.64
11:J:13:VAL:O	11:J:17:LYS:NZ	2.24	0.64
9:H:97:MET:HE1	9:H:121:LEU:HB2	1.80	0.64
4:A:102:VAL:HG12	4:A:135:PHE:HZ	1.61	0.64
5:B:952:VAL:HG22	5:B:966:VAL:HG22	1.79	0.64
6:C:88:CYS:HB3	6:C:92:CYS:HB3	1.78	0.64
4:A:117:GLU:HA	4:A:122:MET:HG3	1.80	0.63
4:A:176:LYS:HG3	4:A:181:LEU:HG	1.79	0.63
12:K:30:ALA:HA	12:K:75:ILE:O	1.98	0.63
5:B:308:TRP:H	5:B:308:TRP:CD1	2.14	0.63
5:B:604:ARG:NH2	5:B:613:VAL:O	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:32:VAL:HA	5:B:1183:LYS:HE2	1.81	0.63
5:B:424:LEU:HD11	5:B:448:ILE:HG13	1.79	0.63
4:A:1209:MET:HE2	4:A:1238:ILE:HD11	1.79	0.63
4:A:563:PRO:HG2	4:A:566:ILE:HG12	1.81	0.63
4:A:674:PRO:HA	4:A:677:ARG:HD3	1.81	0.63
4:A:1224:LEU:HD21	4:A:1240:CYS:HB3	1.80	0.63
5:B:114:PRO:HG3	5:B:181:LEU:HD11	1.81	0.63
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.81	0.63
4:A:569:LYS:NZ	6:C:221:TYR:O	2.32	0.63
4:A:1122:PRO:HD3	4:A:1323:ASP:HB2	1.81	0.63
4:A:1079:MET:HE1	4:A:1359:ASP:HA	1.81	0.62
5:B:1078:GLY:N	6:C:31:ASN:HD22	1.96	0.62
7:E:5:ASN:HB3	7:E:52:ARG:HH22	1.64	0.62
11:J:7:CYS:HA	11:J:49:MET:HE3	1.81	0.62
5:B:215:GLN:HG3	5:B:476:ARG:HE	1.63	0.62
2:T:8:DT:H2"	2:T:9:DC:C5	2.34	0.62
4:A:153:PRO:HB3	4:A:161:LEU:HD21	1.81	0.62
4:A:527:THR:HG21	4:A:650:GLN:HG2	1.81	0.62
10:I:58:VAL:HA	10:I:62:ILE:HD12	1.82	0.62
4:A:361:LEU:HB2	4:A:471:ASN:HD22	1.64	0.62
4:A:1142:THR:HG23	4:A:1145:SER:H	1.65	0.62
5:B:361:LEU:HD21	5:B:377:PHE:HB3	1.81	0.62
5:B:951:GLN:OE1	5:B:967:ARG:NH2	2.33	0.62
6:C:36:VAL:HA	6:C:40:GLU:HG2	1.81	0.62
4:A:870:GLU:OE2	4:A:1345:ARG:NH2	2.33	0.62
5:B:350:GLN:HA	5:B:353:LYS:HD3	1.81	0.62
4:A:116:ASP:O	4:A:118:HIS:ND1	2.33	0.61
4:A:517:ASN:OD1	4:A:1364:ASN:ND2	2.32	0.61
7:E:158:SER:O	7:E:162:ARG:HG3	2.00	0.61
7:E:177:ARG:HG2	7:E:215:MET:HE3	1.82	0.61
9:H:114:VAL:HB	9:H:125:LEU:HB2	1.83	0.61
12:K:28:PRO:HG2	12:K:76:GLN:HE22	1.65	0.61
4:A:265:LYS:O	4:A:269:ILE:HG13	2.01	0.61
5:B:979:LYS:HB3	5:B:1095:LEU:HB2	1.81	0.61
5:B:1181:GLU:HA	5:B:1188:LYS:HG2	1.82	0.61
5:B:827:ILE:HG23	5:B:1012:ILE:HG13	1.82	0.61
11:J:14:VAL:HB	11:J:50:ILE:HD11	1.83	0.61
4:A:30:ILE:HG23	5:B:1170:THR:HG23	1.83	0.61
4:A:1383:SER:OG	4:A:1387:HIS:O	2.19	0.61
9:H:96:VAL:HA	9:H:142:LEU:O	2.00	0.61
4:A:463:ILE:HD13	4:A:469:ARG:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:36:VAL:HG13	6:C:40:GLU:HB2	1.82	0.61
4:A:362:ASP:OD2	4:A:459:ARG:NH1	2.34	0.60
4:A:1430:LEU:HB3	4:A:1432:GLN:HG3	1.82	0.60
4:A:704:ALA:HB2	4:A:710:LEU:HD13	1.84	0.60
4:A:569:LYS:HE2	6:C:221:TYR:HB2	1.81	0.60
5:B:627:PHE:O	5:B:632:ARG:NH1	2.34	0.60
4:A:1399:ARG:HH21	4:A:1408:ILE:HG23	1.65	0.60
7:E:91:LYS:O	7:E:95:THR:HG23	2.02	0.60
5:B:915:THR:HG21	5:B:934:LYS:HE3	1.82	0.60
4:A:147:VAL:HB	4:A:170:THR:HA	1.83	0.60
5:B:291:ILE:HG21	5:B:300:HIS:HD2	1.66	0.60
3:N:3:DA:H1'	3:N:4:DG:H5'	1.84	0.60
5:B:243:ALA:HB2	5:B:251:ILE:HG12	1.84	0.60
7:E:47:CYS:HB3	7:E:51:GLY:HA2	1.82	0.60
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.65	0.60
4:A:131:SER:HB2	4:A:223:GLY:HA3	1.84	0.60
8:F:124:GLU:HG3	8:F:129:LYS:HB2	1.83	0.60
4:A:34:LYS:HD2	4:A:83:HIS:NE2	2.16	0.59
5:B:847:ASP:OD2	12:K:6:ARG:NH2	2.35	0.59
12:K:84:LYS:H	12:K:84:LYS:HD2	1.67	0.59
2:T:8:DT:O2	3:N:12:DG:N2	2.35	0.59
4:A:405:VAL:HG23	4:A:415:LEU:HD21	1.84	0.59
5:B:749:LEU:HD22	5:B:753:ALA:HB1	1.82	0.59
4:A:840:ARG:HD2	4:A:1384:VAL:HG23	1.83	0.59
5:B:1156:ASP:HB2	5:B:1198:TYR:HB3	1.84	0.59
6:C:94:LYS:HD2	6:C:127:ARG:HH12	1.67	0.59
4:A:25:GLU:HA	4:A:28:ARG:HE	1.68	0.59
4:A:128:ILE:HB	4:A:134:ARG:HB2	1.84	0.59
5:B:274:PRO:HG2	5:B:359:GLU:HB3	1.85	0.59
2:T:25:DC:H2'	2:T:26:DG:H8	1.67	0.59
7:E:79:TRP:HB2	7:E:105:PHE:HD2	1.67	0.59
1:R:2:U:H2'	1:R:3:C:C6	2.38	0.59
4:A:1352:VAL:O	4:A:1356:ILE:HG12	2.02	0.59
5:B:30:SER:OG	5:B:743:ILE:O	2.17	0.59
5:B:754:SER:HB2	5:B:812:LEU:HD11	1.83	0.59
4:A:330:LYS:HZ3	4:A:1405:THR:H	1.49	0.59
4:A:334:GLY:O	4:A:338:GLY:N	2.34	0.59
5:B:361:LEU:HD23	5:B:364:ILE:HG13	1.83	0.59
6:C:250:THR:HA	6:C:253:LYS:HD2	1.85	0.59
7:E:28:TYR:OH	7:E:76:GLY:N	2.35	0.59
5:B:843:GLN:N	5:B:994:TYR:O	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.35	0.59
13:L:38:LEU:HD13	13:L:40:LEU:HD21	1.84	0.59
7:E:72:PHE:HE2	7:E:155:ARG:HE	1.51	0.59
10:I:73:ARG:O	10:I:83:ASN:ND2	2.36	0.59
4:A:578:LEU:O	4:A:582:ILE:HG13	2.03	0.58
5:B:476:ARG:HG3	5:B:479:VAL:HG22	1.84	0.58
5:B:778:MET:HE2	5:B:1094:ARG:HB3	1.84	0.58
3:N:6:DG:H2''	3:N:7:DA:C8	2.38	0.58
4:A:180:LYS:HD2	4:A:201:VAL:HB	1.84	0.58
4:A:344:ARG:O	5:B:1155:SER:OG	2.17	0.58
4:A:335:ARG:HD3	5:B:1202:LEU:HD22	1.86	0.58
5:B:957:ASN:ND2	5:B:959:ASP:H	2.02	0.58
4:A:994:GLN:HG2	4:A:1022:LEU:HD23	1.86	0.58
13:L:30:ILE:HG12	13:L:37:LYS:HG3	1.84	0.58
2:T:25:DC:H2'	2:T:26:DG:C8	2.39	0.58
4:A:598:LEU:HD21	9:H:124:ARG:HB2	1.84	0.58
4:A:975:HIS:HA	4:A:1036:ARG:HG3	1.85	0.58
5:B:349:ILE:HG22	5:B:353:LYS:HD2	1.86	0.58
9:H:93:TYR:HA	9:H:145:ARG:HD3	1.86	0.58
6:C:11:ARG:HH12	6:C:229:TYR:HB3	1.69	0.58
4:A:517:ASN:ND2	4:A:875:ALA:O	2.36	0.58
5:B:118:ARG:NH2	5:B:194:GLU:OE1	2.36	0.58
4:A:203:SER:O	4:A:207:ILE:HD12	2.04	0.58
4:A:451:HIS:CE1	4:A:515:GLN:HE22	2.22	0.58
5:B:837:ASP:OD2	5:B:1020:ARG:NH1	2.37	0.58
7:E:20:LYS:HZ3	7:E:37:LEU:HD22	1.68	0.57
4:A:122:MET:HE2	4:A:141:LEU:HD12	1.87	0.57
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.85	0.57
4:A:666:ILE:HD11	5:B:1030:LEU:HD21	1.84	0.57
4:A:1169:ILE:HA	4:A:1172:LEU:HD12	1.85	0.57
5:B:308:TRP:HH2	10:I:47:GLU:HG3	1.69	0.57
4:A:387:ARG:O	4:A:391:LEU:HG	2.05	0.57
4:A:782:ARG:HH11	5:B:702:LEU:HD12	1.68	0.57
4:A:1398:MET:HE2	4:A:1423:GLY:HA3	1.86	0.57
5:B:825:VAL:HG13	5:B:1010:LEU:HB3	1.86	0.57
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.87	0.57
4:A:802:ASN:OD1	5:B:729:ILE:N	2.37	0.57
4:A:1013:ASP:HB3	7:E:207:ARG:HB3	1.86	0.57
5:B:384:ARG:HA	5:B:387:LEU:HD12	1.85	0.57
4:A:901:LEU:HB2	4:A:926:GLN:HB2	1.85	0.57
8:F:89:GLU:HG2	8:F:134:ILE:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:702:LEU:HD22	4:A:710:LEU:HD11	1.85	0.57
4:A:813:PHE:HE2	5:B:749:LEU:HD21	1.70	0.57
4:A:975:HIS:O	4:A:1036:ARG:NH1	2.37	0.57
4:A:1331:SER:OG	4:A:1334:ASP:OD1	2.18	0.57
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.86	0.57
5:B:1112:GLN:HG2	5:B:1119:VAL:HG12	1.86	0.57
7:E:24:LYS:NZ	7:E:30:ILE:O	2.35	0.57
4:A:328:ARG:HD3	4:A:335:ARG:HH21	1.69	0.57
4:A:779:PHE:CE2	4:A:785:PRO:HD3	2.40	0.57
5:B:796:LEU:HD23	5:B:799:PRO:HA	1.87	0.57
10:I:84:VAL:HG23	10:I:104:LEU:HD21	1.87	0.57
11:J:37:SER:OG	11:J:47:ARG:NH2	2.37	0.57
4:A:236:LEU:HD21	5:B:1211:ASN:HB2	1.87	0.57
4:A:380:VAL:HG12	4:A:388:LEU:HD12	1.86	0.57
4:A:550:LEU:HD21	4:A:561:PRO:HD2	1.85	0.57
4:A:1434:ALA:HB1	4:A:1436:ILE:HD13	1.87	0.57
5:B:802:PRO:HG2	5:B:805:THR:HG22	1.87	0.57
5:B:857:ARG:HD2	5:B:942:ARG:HH21	1.69	0.57
4:A:451:HIS:HE1	4:A:515:GLN:HE22	1.53	0.57
7:E:205:SER:OG	7:E:207:ARG:O	2.17	0.57
4:A:265:LYS:HB2	4:A:322:VAL:HG11	1.86	0.57
12:K:51:LEU:HD22	12:K:59:ALA:HB3	1.86	0.57
4:A:71:GLN:HB2	5:B:1174:LYS:NZ	2.20	0.56
4:A:1303:GLU:OE2	4:A:1326:ARG:NH1	2.36	0.56
5:B:944:THR:HG21	5:B:1122:ARG:HH22	1.69	0.56
11:J:55:ASP:OD1	11:J:57:ILE:HG22	2.05	0.56
5:B:416:LEU:HD21	5:B:467:GLY:HA2	1.88	0.56
5:B:453:ILE:O	5:B:457:LEU:HG	2.04	0.56
5:B:1072:MET:HG3	5:B:1085:ILE:HB	1.86	0.56
10:I:42:LEU:HD21	10:I:45:ARG:HB2	1.86	0.56
4:A:23:SER:HB2	4:A:233:TRP:CZ2	2.40	0.56
4:A:175:ARG:NH1	4:A:176:LYS:O	2.38	0.56
4:A:464:PRO:HB2	12:K:4:PRO:HD3	1.87	0.56
4:A:630:ILE:HG23	4:A:642:CYS:SG	2.45	0.56
5:B:1152:MET:HE1	5:B:1195:HIS:HB3	1.88	0.56
4:A:42:ASP:HB3	4:A:46:THR:HB	1.86	0.56
12:K:55:LYS:HB3	12:K:78:THR:HG22	1.88	0.56
4:A:91:PHE:HB3	4:A:235:ILE:HG22	1.88	0.56
4:A:512:VAL:HA	4:A:519:PRO:HA	1.88	0.56
4:A:1291:VAL:HG22	4:A:1292:PRO:HD2	1.88	0.56
9:H:128:ASN:OD1	9:H:131:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:976:ILE:HD11	5:B:993:THR:HG22	1.86	0.56
6:C:58:LEU:HD21	11:J:57:ILE:HD12	1.87	0.56
4:A:381:THR:HA	8:F:104:ASN:HD21	1.70	0.56
4:A:513:SER:OG	4:A:515:GLN:O	2.17	0.56
4:A:1081:LEU:HD22	16:B:1301:CTP:H2'	1.87	0.56
4:A:1134:ILE:O	4:A:1138:ILE:HG22	2.05	0.56
5:B:806:THR:HG22	5:B:808:ALA:H	1.71	0.56
4:A:464:PRO:O	12:K:2:ASN:HB3	2.05	0.56
4:A:868:TYR:CZ	4:A:1366:ARG:HD3	2.41	0.56
6:C:50:GLU:HG2	13:L:66:GLN:HA	1.88	0.56
9:H:47:PHE:HB2	9:H:95:TYR:HD2	1.71	0.56
10:I:60:GLN:OE1	10:I:107:SER:OG	2.24	0.56
4:A:586:ILE:HD13	4:A:633:VAL:HG22	1.87	0.56
4:A:613:ILE:HG21	9:H:102:TYR:HB3	1.88	0.56
4:A:1198:ASP:OD1	4:A:1200:ALA:N	2.39	0.56
4:A:1138:ILE:HG23	4:A:1282:VAL:HG21	1.87	0.55
6:C:76:ASP:HB2	6:C:129:ILE:HG12	1.88	0.55
9:H:101:ALA:HA	9:H:116:TYR:HA	1.88	0.55
10:I:14:LEU:HB3	10:I:27:PHE:HB3	1.87	0.55
4:A:881:GLN:NE2	4:A:958:VAL:O	2.36	0.55
5:B:173:MET:HB2	5:B:203:PHE:HE1	1.70	0.55
7:E:43:LYS:O	7:E:47:CYS:N	2.27	0.55
6:C:104:PHE:HD2	6:C:152:GLU:HB2	1.71	0.55
5:B:35:SER:O	5:B:39:ARG:HG3	2.06	0.55
4:A:537:ARG:NH1	9:H:120:GLY:O	2.37	0.55
8:F:74:ILE:HG21	8:F:144:GLU:HG2	1.88	0.55
4:A:18:GLN:HE22	4:A:1416:ALA:HB1	1.71	0.55
4:A:924:LYS:O	4:A:927:VAL:HG22	2.07	0.55
4:A:1193:LEU:HB2	4:A:1260:LEU:HD11	1.87	0.55
7:E:78:LEU:HD11	7:E:109:ILE:HG12	1.88	0.55
10:I:44:TYR:CE2	10:I:46:HIS:HB2	2.42	0.55
4:A:151:ASP:OD1	4:A:163:SER:HA	2.06	0.55
4:A:1329:THR:H	4:A:1335:ILE:HD11	1.72	0.55
5:B:745:PRO:O	5:B:748:ILE:HG12	2.06	0.55
4:A:956:LEU:HD22	4:A:1021:LEU:HD22	1.89	0.55
7:E:20:LYS:NZ	7:E:37:LEU:HD22	2.21	0.55
9:H:17:PRO:HA	9:H:24:CYS:SG	2.47	0.55
10:I:8:ARG:O	10:I:8:ARG:NH1	2.33	0.55
4:A:404:TYR:HD2	4:A:412:ARG:HG2	1.72	0.55
4:A:1267:MET:HA	4:A:1271:ILE:HG12	1.88	0.55
4:A:1376:THR:O	7:E:212:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1168:LEU:HD23	5:B:1208:MET:HE3	1.89	0.55
6:C:116:LYS:HD3	6:C:140:ASN:HA	1.88	0.55
4:A:231:PRO:HA	4:A:234:MET:HG3	1.88	0.54
4:A:666:ILE:HG22	5:B:1026:LEU:CB	2.33	0.54
4:A:1227:ILE:HG13	4:A:1239:ARG:HB2	1.87	0.54
5:B:175:ARG:HG2	5:B:200:GLY:HA3	1.88	0.54
5:B:750:GLY:O	5:B:754:SER:OG	2.18	0.54
5:B:1082:MET:HE3	6:C:190:ASP:HB2	1.88	0.54
8:F:148:VAL:HA	8:F:151:LEU:HD12	1.89	0.54
6:C:142:VAL:HG21	11:J:5:VAL:HG13	1.90	0.54
4:A:1433:MET:SD	8:F:92:ARG:NH2	2.81	0.54
5:B:358:LYS:HA	5:B:366:GLN:HG2	1.88	0.54
5:B:579:ARG:HH21	5:B:623:GLU:HG3	1.73	0.54
5:B:1099:VAL:O	5:B:1103:ILE:HG13	2.07	0.54
9:H:30:SER:HB2	9:H:36:CYS:HB3	1.88	0.54
9:H:39:THR:HB	9:H:124:ARG:HB3	1.89	0.54
4:A:67:CYS:HB3	4:A:70:CYS:CB	2.32	0.54
4:A:879:GLU:OE2	4:A:962:ARG:NH2	2.38	0.54
4:A:672:ASP:H	4:A:736:ASN:ND2	2.05	0.54
4:A:929:LEU:HD21	4:A:983:ILE:HG23	1.89	0.54
5:B:281:PRO:HD2	5:B:284:ILE:HD12	1.89	0.54
6:C:178:PHE:HE1	6:C:228:PHE:HB3	1.73	0.54
4:A:446:ARG:HE	4:A:448:PRO:HD2	1.73	0.54
4:A:667:GLY:HA2	4:A:670:ILE:HG13	1.88	0.54
4:A:1099:PRO:O	4:A:1103:GLU:HG3	2.08	0.54
8:F:81:THR:OG1	8:F:144:GLU:OE2	2.25	0.54
4:A:5:GLN:H	5:B:1159:ARG:HH22	1.55	0.54
4:A:130:ASP:OD2	4:A:133:LYS:HG3	2.07	0.54
5:B:852:ARG:HD3	5:B:973:ILE:HG12	1.90	0.54
11:J:36:LEU:HD11	11:J:51:LEU:HD13	1.90	0.54
5:B:1207:LEU:HD22	5:B:1212:ILE:HD11	1.88	0.54
10:I:80:SER:OG	10:I:105:SER:OG	2.24	0.54
13:L:50:ASP:OD1	13:L:50:ASP:N	2.39	0.54
4:A:9:ALA:HB3	5:B:1193:GLN:HG3	1.90	0.54
4:A:343:LYS:NZ	5:B:1151:LEU:O	2.28	0.54
4:A:528:LEU:O	4:A:531:ILE:HG22	2.08	0.54
4:A:608:ILE:HB	4:A:613:ILE:HD11	1.90	0.54
4:A:1096:SER:HB3	4:A:1100:ARG:HB2	1.90	0.54
11:J:20:SER:O	11:J:24:LEU:HD12	2.08	0.54
4:A:399:HIS:HD2	4:A:435:HIS:HB3	1.73	0.53
4:A:606:LEU:HG	4:A:613:ILE:HD13	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1279:ILE:HA	4:A:1310:GLY:HA3	1.90	0.53
10:I:55:THR:HG21	10:I:109:ILE:HG21	1.90	0.53
4:A:306:ASN:N	4:A:324:SER:HB2	2.23	0.53
5:B:466:TRP:NE1	5:B:479:VAL:HG11	2.23	0.53
5:B:614:SER:H	5:B:632:ARG:HH12	1.57	0.53
4:A:362:ASP:N	4:A:362:ASP:OD1	2.41	0.53
5:B:245:GLU:OE2	5:B:246:LYS:NZ	2.40	0.53
7:E:55:ARG:HG2	7:E:82:PHE:HB3	1.90	0.53
8:F:74:ILE:HG13	8:F:144:GLU:HG2	1.90	0.53
4:A:353:ILE:HG22	4:A:468:PHE:HB2	1.90	0.53
4:A:830:LYS:HD2	4:A:1098:VAL:HG11	1.90	0.53
4:A:837:ILE:O	4:A:841:LEU:HG	2.09	0.53
5:B:101:MET:HA	5:B:112:LEU:H	1.73	0.53
5:B:977:GLY:HA2	5:B:989:THR:HB	1.90	0.53
5:B:1114:LEU:HG	5:B:1202:LEU:HD11	1.90	0.53
4:A:1140:HIS:HA	4:A:1275:GLY:HA3	1.90	0.53
5:B:788:ARG:O	5:B:967:ARG:NH1	2.41	0.53
5:B:1016:ALA:O	5:B:1020:ARG:HG2	2.08	0.53
7:E:99:HIS:O	7:E:103:LYS:HG2	2.08	0.53
9:H:125:LEU:C	9:H:130:ARG:HH21	2.17	0.53
4:A:113:LEU:HD22	4:A:218:ASP:HB2	1.90	0.53
4:A:884:ASP:HB2	4:A:1024:SER:HB2	1.90	0.53
4:A:1289:ARG:CZ	4:A:1326:ARG:HH21	2.22	0.53
6:C:46:ILE:HG12	6:C:157:CYS:HB3	1.90	0.53
4:A:961:ARG:O	4:A:965:GLN:HG3	2.07	0.53
12:K:57:LEU:N	12:K:76:GLN:O	2.42	0.53
4:A:99:ILE:HG12	4:A:211:PHE:HE2	1.73	0.53
5:B:128:LEU:O	5:B:167:ILE:N	2.42	0.53
5:B:846:ILE:HD13	5:B:974:PRO:HB2	1.91	0.53
4:A:942:PHE:O	4:A:946:VAL:HG23	2.09	0.52
8:F:81:THR:HG21	8:F:136:ARG:HD3	1.90	0.52
2:T:8:DT:OP2	2:T:8:DT:H2'	2.09	0.52
4:A:361:LEU:HA	4:A:471:ASN:HB2	1.91	0.52
4:A:758:ILE:O	4:A:762:SER:HB2	2.08	0.52
5:B:63:ILE:HD12	5:B:421:PHE:CE2	2.11	0.52
5:B:236:HIS:CE1	5:B:389:ALA:HA	2.44	0.52
3:N:11:DA:H2''	3:N:12:DG:C8	2.44	0.52
4:A:115:LEU:HD12	4:A:116:ASP:H	1.75	0.52
4:A:1051:ALA:O	4:A:1055:ARG:HG3	2.09	0.52
7:E:93:MET:HE2	7:E:124:VAL:HG22	1.90	0.52
4:A:575:LYS:HB3	4:A:612:ILE:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.90	0.52
6:C:6:PRO:O	12:K:104:ASN:ND2	2.42	0.52
6:C:99:LEU:HB3	6:C:118:LEU:HD22	1.91	0.52
12:K:10:PHE:HB3	12:K:11:LEU:HD22	1.90	0.52
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.42	0.52
5:B:1058:LEU:HA	5:B:1061:GLU:OE1	2.09	0.52
6:C:251:LEU:HD23	12:K:98:LEU:HD21	1.92	0.52
4:A:340:LEU:HB3	4:A:1429:ILE:HG13	1.90	0.52
4:A:932:GLU:O	4:A:936:LEU:HG	2.10	0.52
4:A:1289:ARG:NH2	4:A:1326:ARG:HH21	2.07	0.52
4:A:185:TRP:HB3	4:A:199:LEU:HD22	1.92	0.52
4:A:277:GLU:O	4:A:280:GLU:HG3	2.09	0.52
4:A:455:MET:HE3	5:B:1138:MET:HE3	1.92	0.52
4:A:662:PHE:HE2	4:A:746:MET:HE2	1.74	0.52
4:A:1195:LEU:HB2	4:A:1238:ILE:HB	1.89	0.52
5:B:1116:ARG:HG3	5:B:1198:TYR:CD1	2.44	0.52
7:E:83:CYS:HB2	7:E:110:PHE:CZ	2.44	0.52
10:I:73:ARG:HH12	10:I:112:SER:HA	1.73	0.52
4:A:504:LEU:HD22	8:F:87:LYS:HG3	1.90	0.52
4:A:1268:LEU:HD22	10:I:48:LEU:HD11	1.92	0.52
5:B:167:ILE:HG22	5:B:448:ILE:HD11	1.92	0.52
5:B:983:ARG:NH2	5:B:1028:GLU:OE2	2.43	0.52
7:E:109:ILE:HD12	7:E:135:PHE:HE2	1.74	0.52
10:I:74:GLU:HB3	10:I:81:ARG:NH1	2.24	0.52
2:T:20:DC:H2'	2:T:21:DC:C6	2.45	0.52
4:A:662:PHE:O	5:B:828:ALA:HA	2.10	0.52
4:A:857:ARG:HD3	4:A:861:GLY:O	2.10	0.52
9:H:93:TYR:CD2	9:H:145:ARG:HB2	2.44	0.52
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.91	0.52
6:C:245:VAL:HA	6:C:248:ILE:HD12	1.91	0.52
4:A:1289:ARG:HD2	4:A:1290:LYS:N	2.25	0.51
5:B:258:LEU:HD11	5:B:267:ARG:HB3	1.91	0.51
4:A:472:LEU:HD13	5:B:835:GLN:CD	2.35	0.51
5:B:863:GLU:HG3	5:B:962:LYS:HB3	1.92	0.51
7:E:29:PHE:HB3	7:E:63:ASN:OD1	2.10	0.51
4:A:1313:LEU:HB3	4:A:1338:VAL:HG21	1.91	0.51
5:B:125:SER:OG	5:B:169:ARG:HB3	2.09	0.51
7:E:5:ASN:HB3	7:E:52:ARG:NH2	2.26	0.51
4:A:355:GLY:HA3	4:A:482:PHE:CZ	2.46	0.51
4:A:403:LYS:HB3	4:A:404:TYR:HD1	1.75	0.51
4:A:550:LEU:HD12	4:A:577:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:827:THR:HG23	4:A:1081:LEU:HA	1.93	0.51
5:B:613:VAL:HG22	5:B:628:THR:HA	1.92	0.51
8:F:140:ASP:OD1	8:F:141:GLY:N	2.43	0.51
13:L:37:LYS:H	13:L:37:LYS:HD2	1.75	0.51
4:A:729:ALA:HA	4:A:732:LEU:HD12	1.93	0.51
4:A:1390:ASN:HD21	4:A:1403:GLU:H	1.58	0.51
9:H:34:ASP:O	9:H:37:LYS:NZ	2.44	0.51
10:I:85:PHE:HD2	10:I:99:LEU:HD13	1.75	0.51
11:J:3:VAL:HG11	11:J:18:TRP:HB2	1.92	0.51
4:A:109:HIS:HE1	4:A:185:TRP:HZ2	1.59	0.51
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.91	0.51
4:A:960:ILE:O	4:A:964:ILE:HG12	2.11	0.51
5:B:291:ILE:HG12	5:B:300:HIS:CD2	2.46	0.51
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.46	0.51
5:B:839:MET:HB2	5:B:1010:LEU:HD21	1.93	0.51
5:B:915:THR:HB	5:B:934:LYS:HB3	1.93	0.51
9:H:33:GLN:HB3	9:H:35:GLN:HE22	1.75	0.51
4:A:353:ILE:HG21	4:A:487:MET:HB2	1.93	0.51
4:A:365:GLY:HA3	4:A:469:ARG:HB2	1.92	0.51
5:B:475:SER:HB3	5:B:476:ARG:NH1	2.26	0.51
5:B:758:PHE:HB2	5:B:1024:ALA:HB1	1.92	0.51
4:A:706:HIS:NE2	4:A:1139:GLU:OE2	2.31	0.51
5:B:1000:PRO:HB2	5:B:1072:MET:HE3	1.93	0.51
5:B:1162:ILE:HG22	5:B:1192:TYR:HB2	1.93	0.51
6:C:55:THR:HB	6:C:151:GLN:HG2	1.92	0.51
4:A:1348:LEU:HB3	4:A:1372:VAL:HG22	1.93	0.50
5:B:322:PHE:CE1	10:I:13:MET:HG2	2.46	0.50
5:B:572:HIS:ND1	5:B:573:GLN:HG2	2.26	0.50
7:E:42:PHE:HE1	7:E:58:MET:HE1	1.76	0.50
9:H:13:SER:N	9:H:27:GLU:O	2.44	0.50
10:I:17:ARG:HE	10:I:18:GLU:N	2.08	0.50
10:I:111:THR:HG22	10:I:113:ASP:H	1.75	0.50
4:A:109:HIS:CE1	4:A:169:ASN:HB3	2.45	0.50
4:A:903:ASN:O	4:A:907:THR:OG1	2.25	0.50
5:B:193:LYS:NZ	11:J:65:PRO:HG3	2.27	0.50
5:B:426:LYS:O	5:B:430:ARG:HG3	2.11	0.50
9:H:81:PRO:O	9:H:83:GLN:NE2	2.44	0.50
4:A:230:ARG:HG3	4:A:233:TRP:CE2	2.46	0.50
5:B:360:PHE:CE1	5:B:361:LEU:HD13	2.46	0.50
5:B:579:ARG:HG2	5:B:586:TRP:CZ2	2.46	0.50
5:B:601:ARG:O	5:B:605:ARG:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1077:THR:C	6:C:31:ASN:HD22	2.19	0.50
5:B:1172:ILE:HG13	5:B:1181:GLU:HG2	1.93	0.50
9:H:95:TYR:HE1	9:H:97:MET:HG3	1.76	0.50
4:A:326:ARG:HB2	4:A:1406:VAL:HG21	1.92	0.50
4:A:899:VAL:HG21	4:A:908:LEU:HG	1.94	0.50
4:A:1364:ASN:OD1	4:A:1366:ARG:HG2	2.11	0.50
5:B:403:LYS:NZ	5:B:696:GLU:OE2	2.44	0.50
5:B:1171:VAL:HA	5:B:1181:GLU:O	2.11	0.50
6:C:196:ASP:OD2	6:C:199:LYS:NZ	2.44	0.50
4:A:993:LEU:HB2	4:A:1046:LEU:HG	1.94	0.50
5:B:99:LYS:NZ	5:B:183:GLU:OE2	2.40	0.50
5:B:211:VAL:O	5:B:480:SER:HA	2.12	0.50
5:B:1181:GLU:HB3	5:B:1188:LYS:NZ	2.27	0.50
6:C:97:VAL:HG21	6:C:129:ILE:HG22	1.94	0.50
7:E:110:PHE:HD2	7:E:112:TYR:CZ	2.30	0.50
4:A:1170:ILE:HA	4:A:1173:HIS:NE2	2.27	0.50
5:B:551:PRO:O	5:B:555:ILE:HG13	2.11	0.50
6:C:255:VAL:HG22	12:K:42:LEU:HD11	1.94	0.50
7:E:59:SER:HB3	7:E:81:GLU:HA	1.94	0.50
7:E:179:GLN:HA	7:E:215:MET:HB2	1.93	0.50
4:A:1118:VAL:HB	4:A:1306:LEU:O	2.11	0.50
4:A:1234:GLU:C	4:A:1235:LYS:HD3	2.37	0.50
9:H:83:GLN:O	9:H:87:ARG:HG2	2.11	0.50
12:K:23:PRO:HA	12:K:31:VAL:HG23	1.93	0.50
2:T:15:DC:H1'	2:T:16:DT:C6	2.47	0.50
4:A:43:GLU:HG2	4:A:44:THR:HG23	1.94	0.50
4:A:598:LEU:HB3	9:H:25:ARG:NH1	2.26	0.50
4:A:883:LEU:H	4:A:952:ALA:HB1	1.77	0.50
4:A:1070:GLN:HE22	5:B:1137:CYS:HA	1.76	0.50
4:A:1109:LYS:CD	4:A:1109:LYS:H	2.25	0.50
9:H:41:ASP:HB2	9:H:121:LEU:HB3	1.94	0.50
4:A:96:ILE:HA	4:A:99:ILE:HB	1.94	0.50
4:A:662:PHE:CE2	4:A:746:MET:HE2	2.47	0.50
5:B:566:LEU:HD21	5:B:586:TRP:CE2	2.47	0.50
5:B:1063:GLY:O	6:C:202:PRO:HG3	2.12	0.50
6:C:205:LYS:O	6:C:208:GLU:HG2	2.12	0.50
7:E:12:LEU:HD21	7:E:55:ARG:HH12	1.77	0.50
4:A:71:GLN:HB2	5:B:1174:LYS:HZ2	1.77	0.49
4:A:451:HIS:CE1	4:A:515:GLN:NE2	2.80	0.49
4:A:545:GLN:HG2	4:A:549:MET:HE3	1.94	0.49
4:A:1128:GLN:H	4:A:1128:GLN:CD	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:205:ILE:HG13	5:B:461:LEU:HB3	1.94	0.49
5:B:259:TYR:CE1	5:B:270:LYS:HB2	2.47	0.49
5:B:496:ARG:NH1	5:B:540:SER:O	2.42	0.49
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.47	0.49
6:C:258:ILE:HG13	12:K:19:LEU:HD21	1.94	0.49
9:H:99:GLY:HA3	9:H:118:PHE:HD1	1.77	0.49
4:A:265:LYS:HG3	4:A:303:TYR:HB2	1.93	0.49
4:A:787:PHE:CE2	4:A:796:SER:HA	2.47	0.49
4:A:1209:MET:SD	4:A:1236:LEU:HB3	2.51	0.49
5:B:431:TYR:HD1	5:B:434:ARG:HH21	1.60	0.49
6:C:248:ILE:O	6:C:252:GLN:HG3	2.13	0.49
9:H:110:ASP:HA	9:H:128:ASN:HD22	1.77	0.49
4:A:1063:MET:SD	4:A:1436:ILE:HG13	2.52	0.49
4:A:569:LYS:HD3	6:C:221:TYR:HD2	1.77	0.49
4:A:608:ILE:HG23	4:A:969:GLN:OE1	2.12	0.49
4:A:613:ILE:HG23	9:H:117:SER:HB3	1.94	0.49
4:A:697:ALA:HA	4:A:702:LEU:HD12	1.94	0.49
4:A:851:HIS:HE1	4:A:1422:ARG:HH22	1.59	0.49
4:A:867:ILE:HG13	4:A:870:GLU:HA	1.94	0.49
4:A:1212:VAL:O	4:A:1216:ILE:HG13	2.12	0.49
5:B:980:PHE:CE1	5:B:990:ILE:HD11	2.48	0.49
7:E:156:LEU:HD22	7:E:160:GLU:HB3	1.94	0.49
11:J:8:PHE:H	11:J:49:MET:HE3	1.78	0.49
12:K:90:ALA:O	12:K:94:ILE:HG13	2.12	0.49
4:A:182:VAL:HB	4:A:201:VAL:HG12	1.93	0.49
5:B:882:THR:OG1	5:B:885:MET:SD	2.69	0.49
5:B:1059:LEU:HD23	5:B:1065:GLN:O	2.11	0.49
7:E:13:TRP:HB2	7:E:42:PHE:CE2	2.47	0.49
7:E:81:GLU:HG3	7:E:110:PHE:HE1	1.78	0.49
4:A:50:ILE:HG23	4:A:52:GLY:N	2.25	0.49
4:A:783:THR:O	5:B:516:ASN:ND2	2.36	0.49
4:A:869:GLY:HA2	4:A:1366:ARG:HB3	1.95	0.49
5:B:261:ARG:O	5:B:264:SER:OG	2.28	0.49
5:B:322:PHE:CZ	10:I:13:MET:HG2	2.47	0.49
5:B:757:PRO:HD3	5:B:983:ARG:HB3	1.95	0.49
8:F:132:LEU:O	8:F:148:VAL:HG23	2.12	0.49
5:B:405:ARG:CZ	5:B:632:ARG:HG2	2.43	0.49
5:B:527:THR:OG1	5:B:534:GLY:N	2.42	0.49
5:B:1098:MET:H	5:B:1102:LYS:HZ3	1.61	0.49
10:I:85:PHE:CD2	10:I:99:LEU:HD13	2.48	0.49
4:A:18:GLN:NE2	4:A:1416:ALA:HB1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:70:CYS:O	4:A:72:GLU:HG2	2.13	0.49
4:A:636:GLU:OE2	4:A:966:ASN:ND2	2.45	0.49
4:A:836:TYR:O	4:A:840:ARG:HG3	2.12	0.49
5:B:693:ILE:HG23	5:B:697:GLU:HG2	1.94	0.49
7:E:190:LEU:HD11	7:E:196:VAL:HG13	1.93	0.49
5:B:693:ILE:HG21	5:B:701:ILE:HD13	1.93	0.49
12:K:91:CYS:O	12:K:95:ILE:HG13	2.13	0.49
4:A:1345:ARG:NH1	4:A:1373:ASP:OD1	2.46	0.49
5:B:309:GLN:O	5:B:313:MET:HG3	2.13	0.49
5:B:792:MET:SD	5:B:857:ARG:NH1	2.85	0.49
7:E:72:PHE:CZ	7:E:157:SER:HA	2.48	0.49
7:E:178:ILE:HG23	7:E:214:CYS:HA	1.95	0.49
4:A:526:ASP:HB2	5:B:835:GLN:NE2	2.28	0.48
4:A:903:ASN:HB3	4:A:906:HIS:HB2	1.95	0.48
5:B:807:ARG:HG3	5:B:1045:SER:OG	2.13	0.48
6:C:245:VAL:HG13	12:K:102:LYS:HG3	1.95	0.48
7:E:16:PHE:CD2	7:E:20:LYS:HE2	2.48	0.48
4:A:304:MET:SD	5:B:1210:MET:HG2	2.53	0.48
4:A:852:TYR:OH	8:F:89:GLU:OE2	2.23	0.48
5:B:30:SER:O	5:B:34:ILE:HG13	2.14	0.48
5:B:311:LEU:O	5:B:315:LYS:HG3	2.13	0.48
5:B:475:SER:HB3	5:B:476:ARG:HH11	1.77	0.48
5:B:600:LEU:HD22	5:B:609:ILE:HD11	1.94	0.48
8:F:85:MET:HG2	8:F:89:GLU:HB3	1.95	0.48
9:H:115:TYR:CE1	9:H:124:ARG:HD2	2.48	0.48
4:A:325:ILE:O	4:A:329:LEU:HG	2.12	0.48
4:A:981:LEU:HG	4:A:1039:LYS:HA	1.96	0.48
5:B:778:MET:HE1	5:B:1094:ARG:HD3	1.94	0.48
5:B:979:LYS:HD3	5:B:1095:LEU:HD12	1.94	0.48
6:C:46:ILE:HA	6:C:159:ALA:HA	1.95	0.48
12:K:29:ASN:H	12:K:76:GLN:HE22	1.61	0.48
4:A:1096:SER:CB	4:A:1100:ARG:HB2	2.42	0.48
5:B:104:GLU:HG3	13:L:54:ARG:NH1	2.29	0.48
5:B:995:ARG:HD3	6:C:165:LYS:HA	1.95	0.48
6:C:52:GLU:HG3	6:C:154:LYS:HB2	1.95	0.48
6:C:54:ASN:OD1	6:C:56:THR:HG22	2.14	0.48
9:H:107:VAL:HG23	9:H:113:ALA:HB2	1.95	0.48
9:H:116:TYR:HB2	9:H:123:MET:HG2	1.96	0.48
11:J:20:SER:C	11:J:24:LEU:HD12	2.38	0.48
2:T:13:DC:C2	2:T:14:DG:N7	2.82	0.48
4:A:57:ARG:HA	4:A:67:CYS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:298:PHE:HE1	4:A:312:PRO:HB2	1.78	0.48
7:E:79:TRP:HB2	7:E:105:PHE:CD2	2.47	0.48
11:J:28:ASP:HB2	11:J:30:LEU:HG	1.96	0.48
4:A:575:LYS:O	4:A:579:SER:OG	2.28	0.48
4:A:1120:LEU:HD11	4:A:1130:GLN:HG2	1.95	0.48
5:B:345:LYS:HG2	5:B:347:LYS:HE3	1.94	0.48
7:E:55:ARG:HD3	7:E:83:CYS:O	2.14	0.48
13:L:68:GLU:CD	13:L:68:GLU:H	2.22	0.48
4:A:442:VAL:O	4:A:457:ALA:HA	2.13	0.48
4:A:782:ARG:NH1	5:B:701:ILE:O	2.29	0.48
4:A:1111:MET:SD	4:A:1330:ASN:ND2	2.87	0.48
7:E:20:LYS:NZ	7:E:34:GLU:O	2.31	0.48
9:H:118:PHE:CE2	9:H:142:LEU:HD12	2.49	0.48
4:A:95:PHE:HE2	5:B:1211:ASN:HD22	1.62	0.48
4:A:1239:ARG:HH22	4:A:1241:ARG:NH2	2.10	0.48
4:A:1281:ARG:NH2	4:A:1309:ASP:OD1	2.47	0.48
5:B:128:LEU:HB3	5:B:167:ILE:HG13	1.95	0.48
5:B:610:ASN:HB3	5:B:613:VAL:HG23	1.96	0.48
5:B:618:ASP:OD2	5:B:621:GLU:HB2	2.14	0.48
10:I:77:LYS:HB3	10:I:108:HIS:ND1	2.28	0.48
4:A:744:LYS:O	4:A:748:MET:HG3	2.14	0.48
4:A:1050:GLU:O	4:A:1054:LEU:HG	2.13	0.48
4:A:1431:GLY:HA3	5:B:1197:PRO:HD3	1.96	0.48
5:B:1082:MET:HA	6:C:189:THR:HA	1.96	0.48
12:K:82:ASP:HB3	12:K:85:ASP:HB2	1.94	0.48
4:A:303:TYR:CE1	4:A:325:ILE:HD11	2.49	0.48
5:B:58:THR:O	5:B:62:ILE:HG12	2.14	0.48
7:E:97:VAL:O	7:E:101:GLN:HG3	2.14	0.48
4:A:1205:LYS:HA	4:A:1205:LYS:HD3	1.59	0.47
5:B:331:LEU:HD13	5:B:349:ILE:HG23	1.96	0.47
5:B:998:ASP:HB3	5:B:1076:HIS:HE1	1.79	0.47
7:E:103:LYS:HB3	7:E:105:PHE:CG	2.49	0.47
9:H:125:LEU:O	9:H:130:ARG:NH2	2.42	0.47
4:A:181:LEU:HB2	4:A:202:LEU:HD22	1.96	0.47
4:A:420:ARG:O	4:A:424:ILE:HG23	2.13	0.47
4:A:479:ASN:ND2	4:A:1078:GLN:OE1	2.41	0.47
4:A:929:LEU:HD21	4:A:983:ILE:CG2	2.44	0.47
5:B:953:LEU:O	5:B:964:VAL:HA	2.15	0.47
7:E:15:ALA:HA	7:E:140:LEU:O	2.14	0.47
7:E:20:LYS:HD2	7:E:35:VAL:HA	1.95	0.47
4:A:70:CYS:SG	4:A:80:HIS:CE1	3.06	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:122:MET:O	4:A:126:LEU:HG	2.14	0.47
4:A:226:GLU:O	4:A:230:ARG:NH1	2.47	0.47
4:A:506:ALA:H	4:A:509:LEU:HD12	1.79	0.47
4:A:541:ILE:HG22	4:A:545:GLN:HB3	1.96	0.47
4:A:579:SER:OG	4:A:612:ILE:HG22	2.14	0.47
5:B:122:LEU:HD11	5:B:958:GLN:H	1.79	0.47
5:B:832:GLY:O	5:B:835:GLN:HG3	2.13	0.47
6:C:43:THR:HB	6:C:170:TRP:O	2.13	0.47
7:E:94:LYS:O	7:E:98:ILE:HG12	2.14	0.47
4:A:845:LEU:HD23	4:A:1374:VAL:HG21	1.95	0.47
4:A:1116:LEU:HD12	4:A:1311:VAL:HA	1.95	0.47
5:B:637:LEU:HD23	5:B:742:GLU:HA	1.96	0.47
4:A:230:ARG:HG3	4:A:233:TRP:CD2	2.49	0.47
4:A:343:LYS:HG2	5:B:1117:GLN:HE22	1.77	0.47
5:B:402:GLY:O	5:B:405:ARG:NH1	2.47	0.47
6:C:26:ASP:OD1	6:C:26:ASP:N	2.44	0.47
6:C:46:ILE:O	6:C:169:LYS:NZ	2.41	0.47
4:A:761:MET:HA	4:A:804:TYR:HB2	1.96	0.47
4:A:898:ARG:NH2	4:A:933:TYR:HB2	2.29	0.47
6:C:124:LEU:O	6:C:127:ARG:HG2	2.13	0.47
9:H:56:THR:HB	9:H:145:ARG:HB3	1.96	0.47
4:A:477:PRO:HG3	4:A:521:MET:HE2	1.97	0.47
4:A:519:PRO:O	4:A:624:SER:HB2	2.15	0.47
4:A:557:ASP:OD1	4:A:559:VAL:N	2.48	0.47
4:A:588:LEU:H	4:A:607:ILE:HB	1.79	0.47
4:A:1012:ARG:O	4:A:1016:THR:OG1	2.33	0.47
5:B:1130:PHE:CE1	5:B:1134:GLU:HB3	2.50	0.47
6:C:241:ASP:OD1	6:C:242:GLN:N	2.46	0.47
6:C:259:LEU:O	6:C:263:THR:HG23	2.15	0.47
7:E:12:LEU:HD22	7:E:137:GLU:OE2	2.15	0.47
7:E:87:SER:HA	7:E:115:ASN:O	2.15	0.47
9:H:93:TYR:CD2	9:H:143:LEU:HB3	2.49	0.47
4:A:25:GLU:CD	4:A:25:GLU:H	2.23	0.47
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.55	0.47
4:A:752:LYS:HG2	5:B:1015:HIS:O	2.14	0.47
4:A:898:ARG:NH1	4:A:929:LEU:HB3	2.28	0.47
4:A:987:VAL:O	4:A:991:LYS:HG3	2.14	0.47
5:B:655:LYS:HD2	5:B:655:LYS:O	2.15	0.47
6:C:10:ILE:HA	6:C:20:PHE:HA	1.96	0.47
1:R:4:G:H2'	1:R:5:A:C8	2.50	0.47
6:C:162:GLY:HA3	6:C:170:TRP:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:30:SER:CB	9:H:36:CYS:HB3	2.45	0.47
9:H:91:ASP:HB2	9:H:93:TYR:CD1	2.50	0.47
3:N:12:DG:H2"	3:N:13:DA:N7	2.30	0.47
4:A:682:THR:HG21	4:A:728:LYS:HD2	1.96	0.47
5:B:273:LEU:HB2	5:B:276:ILE:HB	1.96	0.47
6:C:11:ARG:N	6:C:19:ASP:O	2.48	0.47
6:C:54:ASN:OD1	6:C:153:LEU:HD12	2.15	0.47
6:C:259:LEU:HA	6:C:262:LEU:HD12	1.96	0.47
7:E:7:ARG:O	7:E:11:ARG:HG3	2.14	0.47
4:A:143:LYS:HD2	4:A:143:LYS:C	2.40	0.46
4:A:689:LYS:O	4:A:693:VAL:HG23	2.15	0.46
4:A:1067:LEU:O	4:A:1071:SER:OG	2.30	0.46
5:B:59:LEU:HD23	5:B:417:PHE:CE2	2.49	0.46
5:B:166:PHE:CZ	5:B:169:ARG:HG2	2.47	0.46
5:B:488:TYR:HE2	5:B:813:LYS:HB2	1.80	0.46
6:C:91:HIS:CE1	6:C:158:VAL:HG11	2.49	0.46
9:H:117:SER:HB2	9:H:122:LEU:HD23	1.97	0.46
4:A:351:THR:HG21	4:A:466:SER:O	2.14	0.46
5:B:298:LEU:HG	5:B:314:LEU:HD13	1.96	0.46
5:B:368:GLU:N	5:B:368:GLU:OE1	2.48	0.46
7:E:46:TYR:HE1	7:E:54:GLN:O	1.97	0.46
4:A:108:MET:HG2	4:A:210:ILE:HG12	1.98	0.46
4:A:1442:ASP:HB2	8:F:135:ARG:HB2	1.97	0.46
5:B:857:ARG:HG2	5:B:859:TYR:CZ	2.51	0.46
5:B:975:GLN:O	5:B:990:ILE:HD12	2.15	0.46
7:E:55:ARG:N	7:E:84:ASP:OD2	2.41	0.46
10:I:20:LYS:H	10:I:20:LYS:HD2	1.80	0.46
10:I:85:PHE:HB3	10:I:101:PHE:CD2	2.50	0.46
4:A:224:PHE:HB3	4:A:229:SER:O	2.14	0.46
4:A:549:MET:HE1	4:A:656:TRP:CD1	2.46	0.46
4:A:1412:ALA:HA	4:A:1415:SER:HB2	1.98	0.46
5:B:759:PRO:HD2	5:B:1046:PRO:HG3	1.97	0.46
5:B:798:TYR:CZ	6:C:62:PHE:HE1	2.34	0.46
6:C:17:ASN:HA	6:C:232:VAL:O	2.15	0.46
6:C:91:HIS:ND1	6:C:158:VAL:HG11	2.29	0.46
7:E:14:ARG:HB3	7:E:141:VAL:O	2.15	0.46
7:E:69:ILE:HA	7:E:72:PHE:O	2.15	0.46
8:F:73:ALA:HA	8:F:143:PHE:CE1	2.50	0.46
11:J:48:ARG:NH1	11:J:49:MET:HE1	2.30	0.46
5:B:360:PHE:CE2	5:B:374:LYS:HB3	2.50	0.46
6:C:234:SER:HB3	6:C:240:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:56:VAL:HA	12:K:77:THR:HA	1.98	0.46
4:A:272:ALA:HB3	4:A:296:LEU:HD23	1.98	0.46
4:A:324:SER:O	4:A:328:ARG:HG3	2.15	0.46
4:A:820:GLY:O	4:A:824:LEU:HG	2.16	0.46
5:B:103:ASN:HA	5:B:109:THR:HA	1.97	0.46
5:B:227:LYS:HG2	5:B:236:HIS:CD2	2.51	0.46
5:B:1160:VAL:HG11	5:B:1169:MET:SD	2.55	0.46
6:C:248:ILE:HG21	12:K:102:LYS:HB2	1.98	0.46
7:E:52:ARG:HD2	7:E:52:ARG:HA	1.58	0.46
4:A:19:PHE:HB3	4:A:1413:GLY:HA2	1.97	0.46
4:A:795:GLU:H	4:A:795:GLU:CD	2.24	0.46
5:B:579:ARG:NH2	5:B:623:GLU:HG3	2.31	0.46
5:B:883:LEU:HD12	5:B:884:ARG:H	1.81	0.46
6:C:254:LYS:NZ	12:K:38:GLU:OE2	2.36	0.46
10:I:6:PHE:CD1	10:I:13:MET:HA	2.45	0.46
10:I:78:CYS:SG	10:I:106:CYS:HB3	2.54	0.46
4:A:30:ILE:HD12	5:B:1170:THR:HG21	1.96	0.46
4:A:575:LYS:HE2	9:H:120:GLY:HA3	1.98	0.46
4:A:1323:ASP:OD2	4:A:1325:THR:OG1	2.33	0.46
6:C:36:VAL:HG22	6:C:40:GLU:HG3	1.98	0.46
7:E:187:TYR:HD2	7:E:188:LEU:HD22	1.79	0.46
8:F:128:LYS:NZ	8:F:151:LEU:O	2.40	0.46
4:A:800:VAL:HG22	4:A:812:GLU:HG2	1.97	0.46
4:A:923:LEU:O	4:A:927:VAL:HG13	2.16	0.46
4:A:997:LEU:HB3	4:A:1053:PHE:CE1	2.51	0.46
4:A:1300:LYS:HD2	4:A:1300:LYS:O	2.16	0.46
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.98	0.46
4:A:1395:GLY:O	4:A:1399:ARG:NH1	2.48	0.46
5:B:582:VAL:HB	5:B:587:HIS:CD2	2.51	0.46
6:C:29:MET:HE3	6:C:29:MET:HB2	1.82	0.46
6:C:66:ARG:O	6:C:70:ILE:HG13	2.16	0.46
6:C:91:HIS:HB3	6:C:96:SER:OG	2.16	0.46
9:H:91:ASP:HB2	9:H:93:TYR:HD1	1.81	0.46
4:A:977:LYS:HA	4:A:977:LYS:HD3	1.68	0.45
5:B:286:PHE:CE1	5:B:375:ALA:HB1	2.52	0.45
5:B:487:THR:OG1	5:B:777:ALA:O	2.33	0.45
7:E:66:GLU:O	7:E:69:ILE:HG12	2.16	0.45
8:F:94:LEU:HD13	8:F:122:MET:HG2	1.97	0.45
4:A:9:ALA:HA	5:B:1191:ILE:HG13	1.99	0.45
4:A:99:ILE:HG23	4:A:211:PHE:CZ	2.51	0.45
4:A:605:MET:SD	4:A:615:GLY:HA3	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:643:ASP:HB3	5:B:647:GLY:HA3	1.97	0.45
5:B:760:ASP:OD1	5:B:760:ASP:N	2.49	0.45
5:B:1168:LEU:HD23	5:B:1208:MET:CE	2.46	0.45
10:I:72:ASP:OD1	10:I:72:ASP:N	2.48	0.45
11:J:58:GLU:O	11:J:62:ARG:HG2	2.16	0.45
4:A:446:ARG:NH1	4:A:480:ALA:HA	2.31	0.45
4:A:508:PRO:HA	4:A:511:ILE:HG13	1.97	0.45
4:A:537:ARG:HH12	9:H:122:LEU:HD11	1.81	0.45
4:A:598:LEU:HD13	9:H:39:THR:HG21	1.98	0.45
4:A:1220:PHE:CD2	4:A:1224:LEU:HB3	2.51	0.45
5:B:55:VAL:O	5:B:59:LEU:HD12	2.16	0.45
5:B:883:LEU:HB2	5:B:932:HIS:HB3	1.98	0.45
5:B:954:VAL:HA	5:B:963:PHE:O	2.16	0.45
6:C:11:ARG:NH1	6:C:229:TYR:HB3	2.31	0.45
6:C:35:ARG:HA	6:C:38:ILE:HD12	1.99	0.45
6:C:163:ILE:HG13	6:C:166:GLU:H	1.81	0.45
12:K:99:GLY:O	12:K:103:THR:HG23	2.16	0.45
4:A:354:SER:O	4:A:469:ARG:HA	2.16	0.45
4:A:501:LEU:HD21	5:B:1146:PHE:CD2	2.51	0.45
4:A:1303:GLU:CD	4:A:1326:ARG:HH12	2.24	0.45
11:J:64:ASN:N	11:J:65:PRO:HD2	2.31	0.45
2:T:12:DT:H3'	2:T:13:DC:C6	2.51	0.45
4:A:22:PHE:CD2	5:B:1213:THR:HG22	2.52	0.45
4:A:230:ARG:HB2	4:A:233:TRP:CG	2.52	0.45
5:B:310:MET:O	5:B:314:LEU:HG	2.17	0.45
9:H:4:THR:HA	9:H:60:ALA:HA	1.98	0.45
9:H:80:ARG:HG2	9:H:87:ARG:NH2	2.32	0.45
11:J:9:SER:HB3	11:J:48:ARG:HH22	1.82	0.45
4:A:226:GLU:O	4:A:230:ARG:HG2	2.16	0.45
4:A:527:THR:O	4:A:653:VAL:HG11	2.16	0.45
4:A:733:ALA:O	4:A:737:LEU:HG	2.16	0.45
4:A:842:VAL:HG11	5:B:1136:ASP:CG	2.42	0.45
4:A:1031:VAL:HG13	4:A:1037:LEU:HD22	1.97	0.45
4:A:1111:MET:HE3	4:A:1111:MET:HB2	1.69	0.45
6:C:48:SER:HB3	6:C:158:VAL:HB	1.99	0.45
6:C:62:PHE:O	6:C:66:ARG:HG3	2.17	0.45
8:F:97:ARG:HA	8:F:100:GLN:HG2	1.98	0.45
2:T:6:DT:H2''	2:T:7:DC:C4	2.51	0.45
4:A:120:GLU:HB2	4:A:123:ARG:HH21	1.81	0.45
4:A:370:ILE:HD13	5:B:1105:ALA:HB2	1.98	0.45
4:A:813:PHE:CE2	5:B:749:LEU:HD21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:925:LEU:HD21	4:A:984:LYS:HB2	1.97	0.45
5:B:269:ILE:HG21	5:B:382:ILE:HG23	1.99	0.45
5:B:365:THR:CG2	5:B:367:LEU:HG	2.46	0.45
8:F:97:ARG:HE	8:F:124:GLU:CD	2.24	0.45
9:H:37:LYS:HB2	9:H:126:GLU:HG3	1.99	0.45
9:H:44:VAL:HG12	9:H:49:VAL:HG22	1.99	0.45
4:A:445:ASN:HA	4:A:454:SER:O	2.17	0.45
4:A:827:THR:O	4:A:831:THR:HG23	2.16	0.45
6:C:76:ASP:C	6:C:129:ILE:HD11	2.42	0.45
6:C:182:PRO:HB2	6:C:207:CYS:SG	2.56	0.45
7:E:31:THR:HG22	7:E:33:GLU:H	1.82	0.45
8:F:83:PRO:HA	8:F:146:TRP:CZ3	2.52	0.45
8:F:100:GLN:HA	8:F:103:MET:HB2	1.98	0.45
12:K:61:TYR:HA	12:K:72:LYS:O	2.17	0.45
4:A:109:HIS:CG	4:A:169:ASN:HB3	2.52	0.45
4:A:146:MET:HG2	4:A:170:THR:OG1	2.17	0.45
4:A:270:LEU:O	4:A:274:ILE:HG12	2.16	0.45
4:A:311:GLN:N	4:A:312:PRO:HD3	2.31	0.45
4:A:676:MET:O	4:A:680:THR:HG23	2.17	0.45
4:A:693:VAL:HG21	4:A:721:PHE:HE2	1.82	0.45
4:A:1209:MET:HE3	4:A:1212:VAL:HB	1.97	0.45
5:B:193:LYS:HZ3	11:J:65:PRO:HG3	1.82	0.45
5:B:1163:CYS:HB2	5:B:1171:VAL:HG13	1.99	0.45
7:E:36:GLU:HG2	7:E:36:GLU:O	2.16	0.45
9:H:94:ASP:HB3	9:H:146:ARG:NH1	2.31	0.45
9:H:100:THR:HA	9:H:138:GLU:O	2.16	0.45
4:A:466:SER:HB3	5:B:1103:ILE:HD11	1.98	0.45
4:A:535:THR:HG21	4:A:617:VAL:H	1.81	0.45
4:A:857:ARG:HG2	4:A:863:VAL:HA	1.98	0.45
4:A:1398:MET:HG2	4:A:1426:GLU:OE2	2.17	0.45
5:B:21:GLU:O	5:B:654:ARG:HB3	2.16	0.45
5:B:1215:ARG:HB3	5:B:1217:TYR:CE1	2.52	0.45
6:C:20:PHE:CE1	6:C:230:MET:HB2	2.52	0.45
10:I:74:GLU:OE1	10:I:79:HIS:HA	2.17	0.45
4:A:1169:ILE:HD12	4:A:1229:SER:HB3	2.00	0.44
4:A:1235:LYS:HD3	4:A:1235:LYS:N	2.32	0.44
5:B:373:ARG:HG2	5:B:566:LEU:HB2	1.98	0.44
5:B:678:GLU:OE2	5:B:680:THR:HB	2.17	0.44
5:B:1036:ALA:O	11:J:47:ARG:HD3	2.16	0.44
5:B:1072:MET:HB2	5:B:1085:ILE:HD12	1.99	0.44
5:B:1165:ILE:HB	5:B:1185:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:44:LEU:HB2	6:C:77:ILE:HD13	1.99	0.44
4:A:243:PRO:HG2	4:A:246:VAL:HG23	2.00	0.44
4:A:515:GLN:OE1	4:A:1071:SER:HA	2.17	0.44
5:B:392:ARG:HG2	5:B:393:LYS:NZ	2.33	0.44
7:E:72:PHE:HB3	7:E:74:ASP:OD1	2.17	0.44
7:E:190:LEU:HD12	7:E:214:CYS:HB2	2.00	0.44
8:F:125:LEU:HD21	8:F:153:VAL:HG11	1.98	0.44
9:H:5:LEU:HD23	9:H:134:ASN:HA	1.98	0.44
4:A:212:LYS:HA	4:A:212:LYS:HD2	1.82	0.44
4:A:375:THR:HA	4:A:434:ARG:O	2.17	0.44
4:A:777:PHE:CD1	4:A:783:THR:HG23	2.53	0.44
5:B:778:MET:HE2	5:B:778:MET:HB2	1.76	0.44
5:B:824:ILE:O	5:B:1009:ASP:N	2.50	0.44
5:B:876:LYS:HG3	5:B:877:PRO:HD2	1.99	0.44
5:B:892:LYS:NZ	5:B:904:ARG:O	2.45	0.44
3:N:6:DG:H2''	3:N:7:DA:N7	2.31	0.44
4:A:108:MET:H	4:A:171:GLN:CD	2.25	0.44
4:A:913:LEU:HD12	4:A:914:GLU:N	2.33	0.44
7:E:120:ALA:O	7:E:124:VAL:HG23	2.15	0.44
4:A:53:LEU:HD23	4:A:53:LEU:HA	1.78	0.44
4:A:403:LYS:HB3	4:A:404:TYR:CD1	2.53	0.44
4:A:465:TYR:CD2	5:B:976:ILE:HD13	2.53	0.44
4:A:579:SER:HB3	4:A:611:GLN:HA	1.99	0.44
4:A:598:LEU:O	9:H:122:LEU:HD13	2.18	0.44
4:A:891:ALA:HA	4:A:894:GLU:HG2	2.00	0.44
4:A:1132:LYS:HE2	4:A:1284:MET:HE1	2.00	0.44
4:A:1411:GLU:O	4:A:1415:SER:N	2.41	0.44
5:B:510:LYS:HE2	5:B:510:LYS:HB2	1.79	0.44
5:B:976:ILE:HA	5:B:990:ILE:HB	1.98	0.44
6:C:67:LEU:HA	6:C:70:ILE:HD12	1.98	0.44
6:C:242:GLN:HB3	6:C:246:ARG:NH1	2.32	0.44
4:A:830:LYS:HB3	4:A:1080:THR:CG2	2.48	0.44
4:A:1220:PHE:HZ	4:A:1267:MET:HE2	1.83	0.44
5:B:554:ILE:O	5:B:558:LEU:HG	2.18	0.44
5:B:620:ARG:HD3	10:I:68:LEU:HD11	1.98	0.44
5:B:976:ILE:HD12	5:B:976:ILE:H	1.83	0.44
6:C:10:ILE:HG12	6:C:20:PHE:HB3	1.99	0.44
6:C:104:PHE:CD2	6:C:152:GLU:HB2	2.51	0.44
7:E:96:PHE:CE2	7:E:110:PHE:HB2	2.53	0.44
3:N:3:DA:H2''	3:N:4:DG:H2'	1.99	0.44
4:A:343:LYS:HG2	5:B:1117:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:702:LEU:HD23	4:A:703:THR:H	1.81	0.44
4:A:777:PHE:HB3	4:A:782:ARG:N	2.33	0.44
4:A:782:ARG:HG3	4:A:789:LYS:HA	1.98	0.44
4:A:974:ASP:OD2	9:H:136:LYS:NZ	2.39	0.44
6:C:258:ILE:HG23	12:K:19:LEU:HD11	1.99	0.44
1:R:9:G:H21	4:A:447:GLN:HB2	1.83	0.44
4:A:328:ARG:HB3	4:A:335:ARG:HH21	1.82	0.44
4:A:1381:LEU:HD23	4:A:1381:LEU:HA	1.84	0.44
5:B:842:ASN:HA	5:B:999:MET:HE3	2.00	0.44
6:C:6:PRO:HB2	12:K:101:LEU:HB2	1.99	0.44
6:C:55:THR:OG1	6:C:152:GLU:N	2.38	0.44
7:E:93:MET:HE3	7:E:97:VAL:HG23	1.99	0.44
10:I:54:GLU:HB2	10:I:100:PHE:CZ	2.53	0.44
1:R:4:G:H2'	1:R:5:A:H8	1.83	0.44
4:A:242:PRO:O	4:A:247:ARG:NH2	2.48	0.44
4:A:1165:GLU:O	4:A:1169:ILE:HG12	2.18	0.44
5:B:582:VAL:HG22	5:B:626:ILE:HB	2.00	0.44
5:B:658:ILE:HG22	5:B:662:MET:HE2	1.99	0.44
9:H:104:PHE:CE1	9:H:114:VAL:HG13	2.52	0.44
2:T:8:DT:C2	3:N:12:DG:N2	2.86	0.43
4:A:35:ILE:O	4:A:84:ILE:HD13	2.18	0.43
4:A:635:ARG:CZ	4:A:877:HIS:HA	2.48	0.43
4:A:1284:MET:HG3	4:A:1306:LEU:HD21	2.00	0.43
4:A:1333:ILE:O	4:A:1337:GLU:HG2	2.18	0.43
5:B:572:HIS:CE1	5:B:573:GLN:HG2	2.53	0.43
5:B:778:MET:CE	5:B:853:SER:HB3	2.48	0.43
5:B:783:THR:HA	11:J:60:PHE:HE1	1.82	0.43
5:B:851:PHE:CG	5:B:980:PHE:HE2	2.36	0.43
5:B:1106:ARG:CZ	5:B:1118:PRO:HB3	2.48	0.43
4:A:996:ASN:O	4:A:997:LEU:HD23	2.19	0.43
5:B:113:TYR:CD2	5:B:192:LEU:HD22	2.53	0.43
5:B:195:CYS:SG	5:B:782:LEU:HD22	2.58	0.43
6:C:31:ASN:OD1	6:C:35:ARG:HD2	2.18	0.43
6:C:50:GLU:OE1	13:L:64:LEU:HB3	2.18	0.43
6:C:177:GLU:HG3	6:C:231:ASN:HB3	1.99	0.43
7:E:183:PRO:HA	7:E:186:LEU:HD12	2.01	0.43
1:R:5:A:H2'	1:R:6:G:H8	1.83	0.43
4:A:120:GLU:HA	4:A:123:ARG:HE	1.82	0.43
4:A:1105:LEU:HB3	4:A:1384:VAL:CG2	2.49	0.43
5:B:203:PHE:CZ	5:B:413:LEU:HD11	2.52	0.43
5:B:816:GLU:OE1	5:B:816:GLU:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:31:CYS:HB2	13:L:56:LEU:HA	2.00	0.43
2:T:12:DT:H3'	2:T:13:DC:C5	2.53	0.43
3:N:5:DC:P	4:A:1109:LYS:HZ1	2.41	0.43
4:A:37:PHE:H	4:A:52:GLY:HA3	1.84	0.43
4:A:101:LYS:HD2	4:A:139:TRP:CZ2	2.53	0.43
4:A:668:ASP:HB3	4:A:743:VAL:HG23	2.00	0.43
4:A:843:LYS:HD2	4:A:843:LYS:HA	1.82	0.43
4:A:892:ALA:O	4:A:896:ARG:HG3	2.19	0.43
5:B:579:ARG:HA	5:B:589:VAL:HG12	1.99	0.43
6:C:182:PRO:HD2	6:C:210:GLU:OE1	2.18	0.43
6:C:251:LEU:O	6:C:255:VAL:HG23	2.18	0.43
7:E:147:HIS:HB3	7:E:150:VAL:HG23	2.01	0.43
8:F:69:LEU:HB3	8:F:70:LYS:H	1.74	0.43
5:B:99:LYS:HD3	5:B:178:ASN:O	2.18	0.43
5:B:203:PHE:HZ	5:B:413:LEU:HD11	1.83	0.43
5:B:289:LEU:HD13	5:B:375:ALA:HB2	1.99	0.43
5:B:595:ARG:HE	5:B:595:ARG:HB2	1.65	0.43
5:B:992:ILE:HD11	12:K:66:PRO:HB2	1.99	0.43
5:B:1205:GLN:HA	5:B:1208:MET:HB2	2.01	0.43
6:C:77:ILE:N	6:C:129:ILE:HD11	2.34	0.43
7:E:79:TRP:CE2	7:E:81:GLU:HB2	2.53	0.43
9:H:37:LYS:N	9:H:126:GLU:HB2	2.29	0.43
5:B:429:PHE:O	5:B:433:GLN:HG2	2.17	0.43
5:B:620:ARG:HH11	10:I:68:LEU:HD11	1.82	0.43
5:B:904:ARG:HG2	5:B:948:ILE:HG13	1.99	0.43
7:E:119:SER:O	7:E:123:LEU:HG	2.18	0.43
11:J:1:MET:HE2	11:J:60:PHE:CE2	2.54	0.43
12:K:42:LEU:HD12	12:K:42:LEU:HA	1.83	0.43
1:R:2:U:H2'	1:R:3:C:H6	1.81	0.43
4:A:1209:MET:HB2	4:A:1236:LEU:HD22	2.00	0.43
5:B:431:TYR:CD2	5:B:447:ALA:HB2	2.53	0.43
5:B:1147:LEU:O	5:B:1151:LEU:HB2	2.18	0.43
7:E:9:ILE:HG21	7:E:43:LYS:HG2	2.00	0.43
4:A:399:HIS:NE2	4:A:436:ILE:O	2.52	0.43
4:A:515:GLN:C	4:A:517:ASN:H	2.26	0.43
4:A:665:GLY:HA3	5:B:1069:PHE:CZ	2.54	0.43
4:A:1154:TYR:HB2	4:A:1191:TRP:CZ3	2.53	0.43
5:B:168:GLY:HA2	5:B:450:ALA:HB1	2.00	0.43
5:B:269:ILE:O	5:B:282:ILE:HG12	2.19	0.43
5:B:427:ASP:HA	5:B:430:ARG:HG3	1.99	0.43
5:B:437:GLU:HB2	5:B:438:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1029:CYS:HB3	5:B:1088:GLY:HA3	2.00	0.43
5:B:1106:ARG:HD2	5:B:1125:ASP:O	2.19	0.43
5:B:1138:MET:HE2	5:B:1138:MET:HA	2.00	0.43
12:K:20:LYS:HE3	12:K:20:LYS:HB3	1.87	0.43
4:A:113:LEU:HB3	4:A:218:ASP:OD1	2.18	0.43
4:A:357:PRO:HG2	5:B:831:SER:O	2.19	0.43
4:A:426:LEU:HD23	4:A:426:LEU:HA	1.86	0.43
4:A:575:LYS:HB3	4:A:612:ILE:CG2	2.49	0.43
4:A:710:LEU:HD12	4:A:710:LEU:HA	1.83	0.43
4:A:752:LYS:HE3	5:B:1019:SER:OG	2.19	0.43
4:A:1279:ILE:HG21	4:A:1282:VAL:HG22	2.01	0.43
5:B:604:ARG:NH2	5:B:614:SER:HA	2.33	0.43
5:B:839:MET:HG2	5:B:989:THR:O	2.19	0.43
5:B:839:MET:SD	5:B:980:PHE:HB2	2.59	0.43
4:A:242:PRO:C	4:A:247:ARG:HH12	2.27	0.43
4:A:268:ASP:HA	4:A:271:LYS:HG2	2.01	0.43
4:A:546:VAL:O	4:A:550:LEU:HD13	2.19	0.43
4:A:825:ILE:O	4:A:829:VAL:HG12	2.18	0.43
5:B:879:ARG:HA	5:B:885:MET:SD	2.59	0.43
5:B:910:VAL:HG11	5:B:938:SER:HB3	2.00	0.43
5:B:957:ASN:HB3	5:B:963:PHE:CD1	2.54	0.43
5:B:996:ARG:NH1	6:C:174:ALA:O	2.52	0.43
5:B:1138:MET:HB3	5:B:1147:LEU:HG	2.01	0.43
7:E:112:TYR:HE1	7:E:134:THR:HA	1.83	0.43
8:F:89:GLU:O	8:F:93:ILE:HG12	2.19	0.43
8:F:136:ARG:HB2	8:F:144:GLU:O	2.18	0.43
9:H:112:ILE:HG13	9:H:131:ASN:ND2	2.34	0.43
10:I:97:MET:HE2	10:I:97:MET:HB3	1.93	0.43
1:R:8:G:H2'	1:R:9:G:C8	2.54	0.42
2:T:26:DG:H3'	2:T:27:DA:H8	1.84	0.42
4:A:302:THR:HA	4:A:305:ASP:O	2.18	0.42
4:A:582:ILE:HB	4:A:610:GLY:O	2.19	0.42
4:A:814:PHE:CE1	4:A:818:MET:HE2	2.54	0.42
4:A:1038:THR:OG1	4:A:1040:GLN:HG2	2.19	0.42
4:A:1238:ILE:HD13	4:A:1238:ILE:HA	1.81	0.42
5:B:976:ILE:HD11	5:B:993:THR:CG2	2.49	0.42
6:C:180:TYR:HB3	6:C:228:PHE:CD2	2.53	0.42
11:J:17:LYS:HB3	11:J:39:LEU:HD22	2.01	0.42
4:A:105:CYS:HA	4:A:142:CYS:HB3	1.99	0.42
4:A:114:LEU:HG	4:A:148:CYS:SG	2.59	0.42
4:A:131:SER:HB2	4:A:223:GLY:CA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:756:ILE:O	4:A:760:GLN:HG3	2.18	0.42
5:B:123:THR:OG1	5:B:458:LYS:NZ	2.46	0.42
5:B:169:ARG:HB2	5:B:454:THR:HG23	2.01	0.42
5:B:657:HIS:CD2	5:B:689:LEU:HD11	2.54	0.42
5:B:1161:HIS:HA	5:B:1192:TYR:O	2.18	0.42
6:C:31:ASN:OD1	6:C:31:ASN:C	2.62	0.42
6:C:64:ALA:HA	6:C:67:LEU:HD12	2.00	0.42
5:B:174:LEU:HD22	5:B:202:TYR:CE2	2.53	0.42
5:B:291:ILE:HG12	5:B:300:HIS:NE2	2.34	0.42
5:B:736:THR:HG23	5:B:737:THR:HG23	2.00	0.42
5:B:745:PRO:HB2	5:B:1047:PHE:CD2	2.54	0.42
6:C:181:ASP:OD2	6:C:186:LEU:HB2	2.19	0.42
7:E:81:GLU:HB3	7:E:110:PHE:HD1	1.84	0.42
9:H:102:TYR:CZ	9:H:115:TYR:HB3	2.54	0.42
10:I:63:GLY:O	10:I:70:ARG:NH2	2.53	0.42
12:K:59:ALA:HA	12:K:74:ARG:O	2.19	0.42
4:A:863:VAL:HG23	7:E:170:LEU:HD11	2.02	0.42
4:A:939:ASP:OD2	4:A:1023:ARG:NH1	2.49	0.42
5:B:63:ILE:CD1	5:B:421:PHE:HZ	2.06	0.42
5:B:1064:TYR:CZ	11:J:44:TYR:HE2	2.37	0.42
1:R:7:A:H2'	1:R:8:G:H8	1.84	0.42
4:A:1035:TYR:HB2	4:A:1037:LEU:HD13	2.02	0.42
5:B:262:GLU:CD	5:B:262:GLU:H	2.27	0.42
5:B:1106:ARG:HH12	5:B:1119:VAL:HG22	1.84	0.42
5:B:1159:ARG:HA	5:B:1194:ILE:O	2.20	0.42
11:J:17:LYS:HB3	11:J:39:LEU:HD13	2.02	0.42
3:N:4:DG:H2''	3:N:5:DC:C6	2.55	0.42
4:A:901:LEU:HA	4:A:907:THR:HG23	2.02	0.42
4:A:941:LYS:HA	4:A:941:LYS:HD3	1.94	0.42
4:A:1161:THR:OG1	4:A:1167:GLU:HG2	2.19	0.42
5:B:392:ARG:HG2	5:B:393:LYS:HZ3	1.84	0.42
6:C:136:ASP:OD1	6:C:137:LYS:N	2.53	0.42
10:I:106:CYS:SG	10:I:108:HIS:HB2	2.60	0.42
4:A:33:ALA:C	4:A:34:LYS:HD3	2.45	0.42
4:A:122:MET:HE1	4:A:138:ILE:HA	2.00	0.42
4:A:1170:ILE:HD13	4:A:1173:HIS:NE2	2.35	0.42
6:C:36:VAL:HG23	12:K:41:THR:HG21	2.02	0.42
4:A:128:ILE:H	4:A:134:ARG:NH1	2.17	0.42
4:A:130:ASP:OD2	4:A:132:LYS:HE2	2.20	0.42
4:A:335:ARG:NE	5:B:1206:GLU:OE2	2.53	0.42
4:A:445:ASN:OD1	4:A:455:MET:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:679:ILE:HG21	4:A:763:ALA:HB1	2.02	0.42
4:A:786:HIS:HA	5:B:703:ILE:O	2.20	0.42
4:A:1063:MET:HG3	5:B:1139:ILE:HG22	2.02	0.42
4:A:1143:LEU:HD23	4:A:1267:MET:HG2	2.02	0.42
4:A:1215:ARG:HA	4:A:1218:GLN:OE1	2.20	0.42
4:A:1442:ASP:O	8:F:135:ARG:N	2.49	0.42
5:B:193:LYS:HG2	5:B:787:VAL:HG11	2.02	0.42
5:B:821:GLN:OE1	5:B:850:LEU:HD12	2.18	0.42
5:B:984:HIS:NE2	5:B:1028:GLU:OE1	2.52	0.42
6:C:164:ALA:HB2	6:C:171:GLY:CA	2.50	0.42
4:A:340:LEU:HD21	5:B:1200:ALA:HB2	2.00	0.42
4:A:684:ALA:O	4:A:688:LYS:HG2	2.20	0.42
4:A:1129:GLU:CD	4:A:1129:GLU:H	2.28	0.42
5:B:1162:ILE:HG22	5:B:1192:TYR:CB	2.49	0.42
10:I:80:SER:HB2	10:I:103:CYS:SG	2.60	0.42
4:A:92:HIS:HB2	4:A:236:LEU:HD11	2.01	0.42
4:A:675:THR:HG21	4:A:736:ASN:HB2	2.02	0.42
4:A:757:ASN:HA	5:B:1021:MET:SD	2.60	0.42
4:A:919:ILE:O	4:A:922:ASP:HB2	2.20	0.42
5:B:1025:HIS:CE1	5:B:1090:THR:HG21	2.54	0.42
9:H:102:TYR:CE1	9:H:122:LEU:HD23	2.55	0.42
4:A:547:LEU:HD22	12:K:58:PHE:CD1	2.55	0.41
4:A:775:ILE:HG21	4:A:815:PHE:CD1	2.55	0.41
4:A:1121:GLU:HB3	4:A:1321:GLY:C	2.45	0.41
4:A:1135:ARG:O	4:A:1139:GLU:HB2	2.20	0.41
4:A:1279:ILE:HG21	4:A:1308:THR:HB	2.02	0.41
4:A:1284:MET:HB3	4:A:1304:TRP:CZ3	2.55	0.41
5:B:299:GLU:OE1	5:B:572:HIS:HD2	2.03	0.41
5:B:466:TRP:HE1	5:B:479:VAL:HG11	1.85	0.41
5:B:801:LYS:N	11:J:52:THR:O	2.38	0.41
5:B:957:ASN:HB3	5:B:963:PHE:CE1	2.55	0.41
9:H:113:ALA:HB1	9:H:124:ARG:NH1	2.28	0.41
4:A:208:LEU:HB2	4:A:235:ILE:CD1	2.37	0.41
4:A:517:ASN:HB3	4:A:878:ILE:O	2.20	0.41
4:A:915:SER:O	4:A:919:ILE:N	2.50	0.41
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	2.01	0.41
5:B:694:ASP:OD1	5:B:695:ALA:N	2.50	0.41
5:B:1081:LEU:HA	5:B:1081:LEU:HD23	1.72	0.41
16:B:1301:CTP:H6	16:B:1301:CTP:H5'1	1.84	0.41
6:C:69:LEU:HD13	11:J:6:ARG:HD2	2.01	0.41
7:E:97:VAL:HG13	7:E:127:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:5:LEU:HG	9:H:133:ASN:O	2.20	0.41
4:A:244:PRO:HA	4:A:247:ARG:HG2	2.02	0.41
4:A:345:VAL:HG23	4:A:348:SER:HB3	2.02	0.41
4:A:630:ILE:HD12	4:A:630:ILE:H	1.84	0.41
4:A:1213:GLY:HA2	4:A:1216:ILE:HD12	2.01	0.41
4:A:1371:LEU:O	4:A:1375:MET:HG3	2.20	0.41
5:B:175:ARG:HD2	5:B:175:ARG:HA	1.83	0.41
5:B:255:GLN:HB2	5:B:272:THR:HG22	2.02	0.41
5:B:806:THR:HG23	5:B:1045:SER:HA	2.02	0.41
5:B:847:ASP:O	5:B:852:ARG:NH2	2.54	0.41
5:B:866:TYR:OH	5:B:916:THR:HB	2.19	0.41
7:E:27:GLY:O	7:E:65:THR:HG23	2.20	0.41
7:E:168:TYR:CB	7:E:170:LEU:HD23	2.46	0.41
11:J:41:LEU:O	11:J:47:ARG:HG3	2.21	0.41
2:T:16:DT:H2"	2:T:17:DG:C8	2.55	0.41
4:A:442:VAL:HG11	4:A:489:LEU:HD21	2.02	0.41
4:A:665:GLY:HA2	5:B:1086:PHE:CD2	2.55	0.41
4:A:671:ALA:HB3	4:A:676:MET:HE2	2.03	0.41
4:A:685:GLU:O	4:A:689:LYS:HG2	2.19	0.41
4:A:956:LEU:HD13	4:A:1021:LEU:HD22	2.01	0.41
4:A:1141:THR:HB	4:A:1273:LEU:O	2.19	0.41
5:B:281:PRO:O	5:B:285:ILE:HG13	2.20	0.41
5:B:384:ARG:HA	5:B:384:ARG:HD2	1.77	0.41
5:B:697:GLU:O	5:B:701:ILE:HG23	2.20	0.41
5:B:801:LYS:HG2	11:J:52:THR:HA	2.03	0.41
5:B:809:MET:HE1	5:B:983:ARG:NH1	2.35	0.41
5:B:839:MET:HE2	5:B:839:MET:HB3	1.88	0.41
5:B:862:GLN:O	5:B:914:LYS:HE2	2.20	0.41
8:F:74:ILE:HD13	8:F:74:ILE:HA	1.92	0.41
8:F:127:GLU:HB3	8:F:129:LYS:HG2	2.03	0.41
4:A:332:LYS:HA	4:A:337:ARG:HD3	2.02	0.41
4:A:436:ILE:HG22	4:A:460:VAL:HG11	2.03	0.41
4:A:457:ALA:O	4:A:507:VAL:HG23	2.21	0.41
4:A:526:ASP:HB3	4:A:657:LEU:HD23	2.02	0.41
4:A:1188:GLN:N	4:A:1243:VAL:O	2.54	0.41
5:B:228:LYS:HD2	5:B:228:LYS:HA	1.95	0.41
5:B:242:SER:HB2	5:B:362:PRO:HD2	2.03	0.41
5:B:257:LYS:HG3	5:B:259:TYR:CE1	2.56	0.41
5:B:822:ASN:O	11:J:48:ARG:HD2	2.20	0.41
7:E:40:GLU:H	7:E:40:GLU:HG3	1.69	0.41
7:E:93:MET:HE1	7:E:96:PHE:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:215:MET:HE2	7:E:215:MET:HA	2.02	0.41
8:F:97:ARG:NH1	8:F:100:GLN:OE1	2.53	0.41
12:K:8:GLU:O	12:K:37:LYS:HE3	2.21	0.41
1:R:3:C:H2'	1:R:4:G:C8	2.55	0.41
1:R:5:A:H2'	1:R:6:G:C8	2.56	0.41
4:A:305:ASP:CG	4:A:326:ARG:HD3	2.46	0.41
4:A:583:PRO:O	4:A:610:GLY:HA3	2.20	0.41
4:A:768:GLN:HG2	4:A:816:HIS:HA	2.01	0.41
4:A:915:SER:C	4:A:919:ILE:HG12	2.46	0.41
4:A:1352:VAL:HG12	4:A:1368:MET:HE3	2.01	0.41
5:B:245:GLU:HG2	5:B:246:LYS:N	2.34	0.41
5:B:259:TYR:HE1	5:B:270:LYS:HB2	1.86	0.41
5:B:372:SER:OG	5:B:567:GLU:HA	2.20	0.41
5:B:1073:TYR:OH	6:C:179:GLU:HA	2.21	0.41
6:C:183:TRP:CG	6:C:213:PRO:HD3	2.56	0.41
7:E:74:ASP:OD1	7:E:75:MET:N	2.54	0.41
7:E:178:ILE:HB	7:E:212:ARG:HD3	2.03	0.41
9:H:6:PHE:CZ	9:H:8:ASP:HB2	2.55	0.41
12:K:11:LEU:C	12:K:37:LYS:HG2	2.45	0.41
12:K:72:LYS:HE2	12:K:72:LYS:HB2	1.67	0.41
13:L:28:LYS:HB3	13:L:28:LYS:HE3	1.83	0.41
13:L:38:LEU:HD21	13:L:48:CYS:HB3	2.02	0.41
4:A:17:VAL:HG22	5:B:1216:LEU:HG	2.02	0.41
4:A:91:PHE:CE1	4:A:96:ILE:HD12	2.56	0.41
4:A:260:ASP:HB3	4:A:263:THR:OG1	2.21	0.41
4:A:800:VAL:HG13	4:A:812:GLU:CD	2.44	0.41
4:A:1312:ASN:O	4:A:1316:VAL:HG23	2.21	0.41
5:B:59:LEU:HB3	5:B:95:ILE:HG21	2.01	0.41
5:B:294:ASP:HA	5:B:297:ILE:HD12	2.02	0.41
5:B:377:PHE:HE1	5:B:581:PHE:HE2	1.68	0.41
5:B:643:ASP:HB3	5:B:647:GLY:CA	2.50	0.41
5:B:864:LYS:H	5:B:872:GLU:HB2	1.85	0.41
5:B:997:GLU:HB2	6:C:35:ARG:HG2	2.02	0.41
5:B:1053:GLU:HB3	5:B:1057:LYS:NZ	2.35	0.41
6:C:222:LYS:HA	6:C:222:LYS:HD2	1.84	0.41
11:J:58:GLU:H	11:J:58:GLU:HG2	1.61	0.41
4:A:14:VAL:HG21	5:B:1216:LEU:HB3	2.01	0.41
4:A:122:MET:HE1	4:A:138:ILE:HG12	2.02	0.41
4:A:206:GLU:HA	4:A:209:ASN:ND2	2.35	0.41
4:A:343:LYS:NZ	5:B:1197:PRO:HB3	2.36	0.41
4:A:738:LYS:HB2	4:A:740:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:810:PRO:HG2	5:B:705:MET:HG2	2.03	0.41
4:A:963:ILE:HG22	4:A:1045:VAL:HG22	2.03	0.41
4:A:1130:GLN:O	4:A:1134:ILE:HG12	2.21	0.41
5:B:638:PHE:O	5:B:740:HIS:HB3	2.20	0.41
5:B:800:GLN:HE22	11:J:49:MET:HA	1.86	0.41
7:E:112:TYR:CG	7:E:116:ILE:HG12	2.56	0.41
8:F:136:ARG:HB2	8:F:144:GLU:HB2	2.03	0.41
4:A:601:LYS:HB2	4:A:603:ASN:OD1	2.21	0.41
4:A:896:ARG:NH2	4:A:1034:GLU:OE2	2.54	0.41
4:A:1314:SER:HA	4:A:1317:MET:HE2	2.01	0.41
5:B:272:THR:HB	5:B:279:ASP:OD1	2.20	0.41
5:B:566:LEU:HD23	5:B:566:LEU:HA	1.82	0.41
5:B:660:LYS:HB3	5:B:679:TYR:CD2	2.56	0.41
5:B:808:ALA:O	5:B:812:LEU:HG	2.21	0.41
5:B:984:HIS:CD2	5:B:1025:HIS:HA	2.55	0.41
6:C:114:TYR:HB3	6:C:141:GLY:H	1.85	0.41
6:C:171:GLY:HA2	6:C:172:PRO:HD3	1.91	0.41
6:C:250:THR:O	6:C:254:LYS:HG3	2.21	0.41
11:J:2:ILE:HD12	11:J:57:ILE:HD13	2.02	0.41
12:K:29:ASN:HB2	12:K:76:GLN:HE21	1.86	0.41
13:L:62:LYS:HE3	13:L:62:LYS:HB3	1.77	0.41
3:N:11:DA:O5'	3:N:11:DA:H8	2.04	0.41
4:A:17:VAL:HG23	4:A:1421:CYS:SG	2.61	0.41
4:A:137:ALA:O	4:A:141:LEU:HG	2.21	0.41
4:A:414:ASP:O	4:A:418:SER:HB2	2.20	0.41
4:A:880:LYS:HD2	4:A:953:ASN:HB3	2.03	0.41
4:A:1194:ARG:HG2	4:A:1237:ILE:HD11	2.03	0.41
4:A:1412:ALA:O	4:A:1416:ALA:N	2.53	0.41
5:B:412:LEU:HB3	5:B:466:TRP:CZ2	2.56	0.41
5:B:512:ARG:HD3	5:B:533:CYS:O	2.21	0.41
5:B:520:GLY:HA3	5:B:635:ARG:HH21	1.86	0.41
5:B:572:HIS:HD1	5:B:573:GLN:HG2	1.86	0.41
6:C:57:VAL:HG21	11:J:57:ILE:HG13	2.03	0.41
12:K:42:LEU:HG	12:K:46:ILE:HD11	2.03	0.41
4:A:757:ASN:O	4:A:761:MET:HG3	2.21	0.40
4:A:916:GLY:HA2	4:A:919:ILE:HB	2.03	0.40
4:A:1202:MET:HE3	4:A:1202:MET:HB3	1.80	0.40
4:A:1329:THR:HG22	4:A:1331:SER:N	2.33	0.40
4:A:1438:THR:HA	4:A:1441:PHE:CZ	2.56	0.40
5:B:234:ILE:HD12	5:B:237:VAL:HG22	2.03	0.40
5:B:815:ARG:H	5:B:815:ARG:HG3	1.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:898:LEU:HD22	5:B:964:VAL:HG11	2.02	0.40
6:C:77:ILE:HD11	6:C:161:LYS:HG3	2.03	0.40
1:R:7:A:H2'	1:R:8:G:C8	2.56	0.40
4:A:80:HIS:CD2	4:A:80:HIS:N	2.90	0.40
4:A:259:GLU:HB3	4:A:264:PHE:CE1	2.56	0.40
4:A:587:HIS:CE1	4:A:609:ASP:H	2.39	0.40
4:A:1318:THR:HG22	7:E:142:VAL:HG23	2.03	0.40
5:B:70:ILE:HG13	5:B:89:GLU:HA	2.03	0.40
5:B:613:VAL:HA	5:B:632:ARG:HH22	1.86	0.40
5:B:681:TRP:CH2	5:B:690:VAL:HG11	2.56	0.40
6:C:215:GLU:HA	6:C:215:GLU:OE1	2.22	0.40
7:E:79:TRP:CZ2	7:E:81:GLU:HB2	2.57	0.40
4:A:138:ILE:O	4:A:142:CYS:HB2	2.22	0.40
4:A:851:HIS:ND1	8:F:139:PRO:HG3	2.37	0.40
5:B:63:ILE:HD12	5:B:63:ILE:HA	1.91	0.40
5:B:377:PHE:CE1	5:B:581:PHE:HE2	2.39	0.40
5:B:651:LEU:HD21	5:B:707:PRO:HB3	2.03	0.40
7:E:88:VAL:O	7:E:117:THR:HG23	2.21	0.40
7:E:180:ARG:HD2	7:E:180:ARG:HA	1.90	0.40
8:F:135:ARG:NH1	8:F:143:PHE:HD1	2.13	0.40
4:A:864:ILE:H	4:A:864:ILE:HG12	1.70	0.40
4:A:1335:ILE:HG23	4:A:1339:LEU:HD12	2.04	0.40
5:B:46:GLN:OE1	5:B:47:GLN:HG2	2.20	0.40
6:C:33:LEU:CD2	6:C:37:MET:HE2	2.51	0.40
7:E:116:ILE:H	7:E:116:ILE:HG13	1.73	0.40
9:H:101:ALA:HB2	9:H:116:TYR:CZ	2.56	0.40
11:J:57:ILE:O	11:J:61:LEU:HG	2.21	0.40
4:A:248:PRO:HD2	4:A:260:ASP:OD2	2.22	0.40
4:A:259:GLU:HB3	4:A:264:PHE:CZ	2.57	0.40
4:A:915:SER:O	4:A:919:ILE:HG12	2.21	0.40
4:A:958:VAL:O	4:A:960:ILE:HD12	2.22	0.40
4:A:1111:MET:HB3	4:A:1114:PRO:HG3	2.03	0.40
5:B:102:VAL:HA	5:B:169:ARG:HH12	1.87	0.40
5:B:237:VAL:HG12	5:B:239:GLU:HG3	2.03	0.40
5:B:242:SER:OG	5:B:252:SER:O	2.39	0.40
7:E:103:LYS:HB3	7:E:105:PHE:CD2	2.57	0.40
8:F:114:GLU:HB2	8:F:120:ILE:HD11	2.03	0.40
10:I:77:LYS:HG3	10:I:78:CYS:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:418:SER:OG	6:C:87:PHE:O[2_555]	2.12	0.08

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	1371/1733 (79%)	1338 (98%)	32 (2%)	1 (0%)	48	78
5	B	1103/1224 (90%)	1086 (98%)	17 (2%)	0	100	100
6	C	265/318 (83%)	261 (98%)	4 (2%)	0	100	100
7	E	210/215 (98%)	205 (98%)	5 (2%)	0	100	100
8	F	84/155 (54%)	82 (98%)	2 (2%)	0	100	100
9	H	129/146 (88%)	128 (99%)	1 (1%)	0	100	100
10	I	116/122 (95%)	112 (97%)	4 (3%)	0	100	100
11	J	63/70 (90%)	63 (100%)	0	0	100	100
12	K	112/120 (93%)	110 (98%)	2 (2%)	0	100	100
13	L	41/70 (59%)	41 (100%)	0	0	100	100
All	All	3494/4173 (84%)	3426 (98%)	67 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	484	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1195/1520 (79%)	1189 (100%)	6 (0%)	81	81
5	B	955/1061 (90%)	953 (100%)	2 (0%)	87	85
6	C	235/274 (86%)	234 (100%)	1 (0%)	84	83
7	E	193/197 (98%)	192 (100%)	1 (0%)	81	81
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	116/128 (91%)	115 (99%)	1 (1%)	70	76
10	I	110/116 (95%)	105 (96%)	5 (4%)	24	51
11	J	60/65 (92%)	59 (98%)	1 (2%)	53	67
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	36/57 (63%)	34 (94%)	2 (6%)	19	46
All	All	3072/3657 (84%)	3053 (99%)	19 (1%)	78	80

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	67	CYS
4	A	70	CYS
4	A	77	CYS
4	A	80	HIS
4	A	148	CYS
4	A	167	CYS
5	B	1182	CYS
5	B	1185	CYS
6	C	86	CYS
7	E	46	TYR
9	H	58	THR
10	I	7	CYS
10	I	29	CYS
10	I	75	CYS
10	I	103	CYS
10	I	106	CYS
11	J	7	CYS
13	L	31	CYS
13	L	51	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	18	GLN
4	A	71	GLN
4	A	75	ASN
4	A	124	GLN
4	A	171	GLN
4	A	209	ASN
4	A	313	GLN
4	A	358	ASN
4	A	363	GLN
4	A	493	GLN
4	A	515	GLN
4	A	654	ASN
4	A	851	HIS
4	A	881	GLN
4	A	906	HIS
4	A	935	GLN
4	A	953	ASN
4	A	1128	GLN
4	A	1211	GLN
4	A	1390	ASN
5	B	52	ASN
5	B	215	GLN
5	B	236	HIS
5	B	300	HIS
5	B	481	GLN
5	B	572	HIS
5	B	592	ASN
5	B	733	HIS
5	B	786	ASN
5	B	800	GLN
5	B	957	ASN
5	B	1076	HIS
5	B	1117	GLN
5	B	1211	ASN
6	C	24	ASN
6	C	31	ASN
6	C	91	HIS
6	C	135	GLN
9	H	35	GLN
9	H	128	ASN
9	H	131	ASN
9	H	134	ASN
10	I	11	ASN

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Mol	Chain	Res	Type
12	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	7/9 (77%)	2 (28%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	5	A

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	WVQ	T	19	2	19,24,25	3.68	7 (36%)	18,33,36	1.54	3 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WVQ	T	19	2	-	4/6/40/41	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	WVQ	C5-N7	13.00	1.47	1.28
2	T	19	WVQ	C4-N9	4.91	1.46	1.35
2	T	19	WVQ	C2-N2	4.20	1.45	1.34
2	T	19	WVQ	C6-C5	-4.01	1.36	1.47
2	T	19	WVQ	C6-N1	-3.19	1.32	1.38
2	T	19	WVQ	O6-C6	-2.73	1.18	1.23
2	T	19	WVQ	C5-C4	-2.09	1.37	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	WVQ	N3-C2-N1	-4.47	119.36	126.44
2	T	19	WVQ	N2-C2-N3	2.35	120.31	116.57
2	T	19	WVQ	N2-C2-N1	2.10	120.33	117.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	WVQ	C3'-C4'-C5'-O5'
2	T	19	WVQ	O4'-C4'-C5'-O5'
2	T	19	WVQ	C4'-C5'-O5'-P
2	T	19	WVQ	O4'-C1'-N9-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 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	$\# Z > 2$
16	CTP	B	1301	14	29,30,30	1.04	2 (6%)	43,47,47	0.94	2 (4%)

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
16	CTP	B	1301	14	-	3/22/38/38	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1301	CTP	C4-N3	2.08	1.38	1.34
16	B	1301	CTP	PB-O3A	2.06	1.61	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1301	CTP	C3'-C2'-C1'	2.36	105.93	101.46
16	B	1301	CTP	N4-C4-N3	2.06	121.58	117.91

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	1301	CTP	C3'-C4'-C5'-O5'
16	B	1301	CTP	O4'-C4'-C5'-O5'
16	B	1301	CTP	PA-O3A-PB-O2B

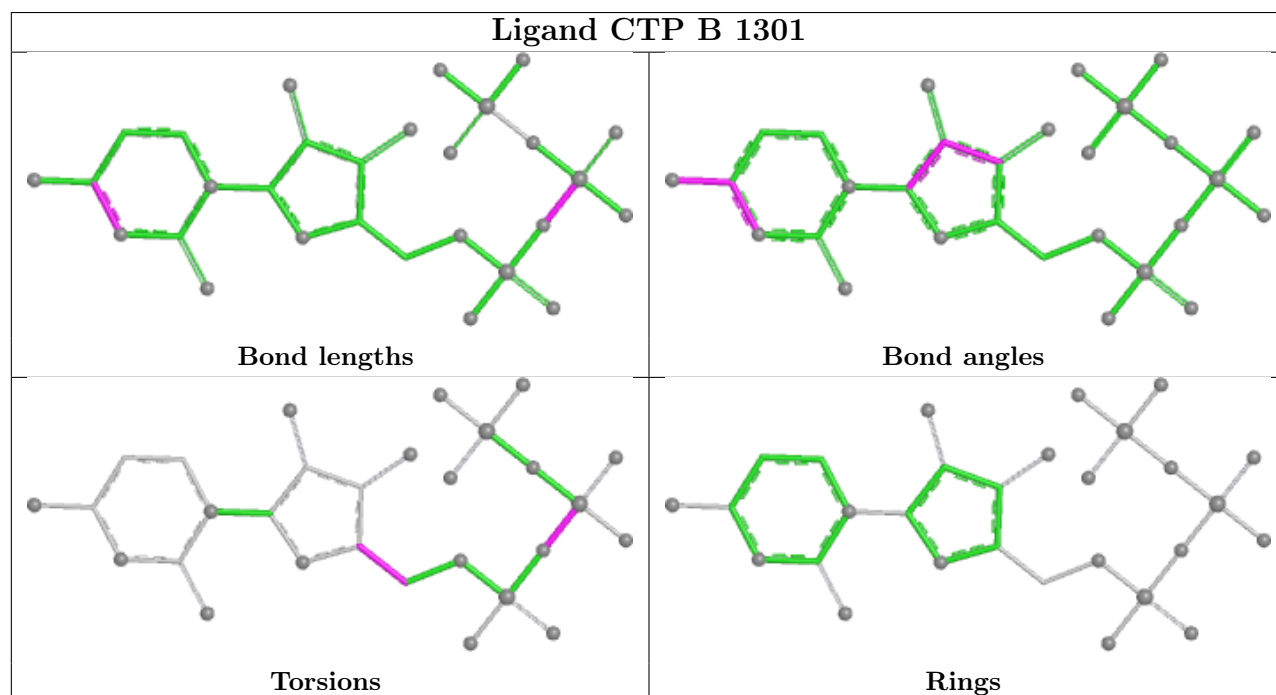
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1301	CTP	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 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	R	9/9 (100%)	-0.35	0	100	100	90, 102, 175, 216	0
2	T	23/29 (79%)	0.11	0	100	100	93, 172, 290, 313	0
3	N	13/18 (72%)	0.35	0	100	100	210, 238, 301, 324	0
4	A	1385/1733 (79%)	0.52	94 (6%)	23	19	58, 123, 197, 259	0
5	B	1123/1224 (91%)	0.54	80 (7%)	22	18	47, 109, 172, 231	0
6	C	267/318 (83%)	0.41	10 (3%)	45	32	56, 96, 155, 207	0
7	E	212/215 (98%)	0.58	21 (9%)	13	12	88, 159, 241, 308	0
8	F	86/155 (55%)	0.37	2 (2%)	61	46	91, 126, 166, 208	0
9	H	133/146 (91%)	0.40	8 (6%)	27	21	95, 143, 214, 310	0
10	I	118/122 (96%)	0.23	4 (3%)	48	35	90, 143, 191, 265	0
11	J	65/70 (92%)	0.65	10 (15%)	5	7	55, 96, 141, 175	0
12	K	114/120 (95%)	0.32	6 (5%)	32	24	60, 98, 143, 167	0
13	L	43/70 (61%)	0.63	4 (9%)	14	14	78, 184, 274, 324	0
All	All	3591/4229 (84%)	0.50	239 (6%)	24	19	47, 118, 206, 324	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	E	93	MET	6.3
8	F	84	TYR	5.4
4	A	1332	PHE	5.2
5	B	543	SER	5.0
4	A	642	CYS	5.0
5	B	533	CYS	4.8
5	B	420	LEU	4.4
8	F	93	ILE	4.4
11	J	54	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
4	A	328	ARG	4.3
5	B	310	MET	4.2
7	E	122	LYS	4.2
5	B	51	PHE	4.1
4	A	96	ILE	4.1
4	A	448	PRO	4.1
4	A	1010	ALA	4.0
5	B	386	LEU	4.0
4	A	997	LEU	4.0
5	B	814	PHE	3.9
7	E	111	VAL	3.9
4	A	1390	ASN	3.8
6	C	251	LEU	3.8
4	A	303	TYR	3.8
5	B	823	ALA	3.8
5	B	381	MET	3.8
12	K	42	LEU	3.7
4	A	815	PHE	3.7
5	B	1093	GLN	3.7
9	H	23	VAL	3.7
4	A	834	THR	3.6
5	B	811	TYR	3.6
4	A	144	THR	3.6
4	A	646	PHE	3.6
5	B	1209	ALA	3.6
13	L	32	ALA	3.6
4	A	1328	TYR	3.6
5	B	775	LYS	3.6
9	H	55	LEU	3.6
4	A	466	SER	3.5
13	L	67	PHE	3.5
5	B	534	GLY	3.5
5	B	413	LEU	3.4
4	A	1267	MET	3.4
5	B	658	ILE	3.4
7	E	97	VAL	3.4
4	A	341	MET	3.4
5	B	516	ASN	3.4
4	A	540	PHE	3.3
6	C	50	GLU	3.3
5	B	1072	MET	3.3
4	A	1429	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
7	E	112	TYR	3.3
6	C	173	ALA	3.3
5	B	48	LEU	3.3
12	K	11	LEU	3.2
5	B	1113	VAL	3.2
4	A	1072	ILE	3.2
5	B	849	GLY	3.2
5	B	273	LEU	3.2
4	A	1085	HIS	3.2
4	A	153	PRO	3.1
4	A	1018	PHE	3.1
5	B	1140	ALA	3.1
5	B	446	LEU	3.1
11	J	6	ARG	3.1
5	B	819	ALA	3.0
5	B	379	GLY	3.0
5	B	808	ALA	3.0
4	A	873	MET	3.0
5	B	1199	ALA	3.0
5	B	779	GLY	3.0
6	C	29	MET	3.0
5	B	390	LEU	3.0
5	B	899	ILE	3.0
5	B	1021	MET	3.0
5	B	700	SER	2.9
4	A	161	LEU	2.9
5	B	114	PRO	2.9
6	C	8	VAL	2.9
4	A	694	THR	2.9
5	B	1130	PHE	2.9
4	A	95	PHE	2.9
5	B	260	GLY	2.9
4	A	1410	PHE	2.9
4	A	62	ASP	2.8
5	B	762	ASN	2.8
5	B	1211	ASN	2.8
4	A	135	PHE	2.8
4	A	1317	MET	2.8
4	A	1396	ALA	2.8
5	B	525	ALA	2.8
5	B	802	PRO	2.8
5	B	167	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
5	B	333	PHE	2.8
5	B	1212	ILE	2.8
4	A	355	GLY	2.8
4	A	1077	THR	2.8
4	A	612	ILE	2.7
4	A	666	ILE	2.7
4	A	1026	LEU	2.7
5	B	1091	TYR	2.7
12	K	44	ASN	2.7
5	B	785	TYR	2.7
7	E	109	ILE	2.7
5	B	778	MET	2.7
4	A	830	LYS	2.6
5	B	489	SER	2.6
6	C	174	ALA	2.6
7	E	149	LEU	2.6
5	B	530	GLY	2.6
5	B	1077	THR	2.6
4	A	759	ALA	2.6
4	A	1434	ALA	2.6
5	B	75	ALA	2.6
9	H	88	SER	2.6
6	C	243	VAL	2.6
11	J	35	ALA	2.6
4	A	336	ILE	2.6
7	E	28	TYR	2.6
4	A	182	VAL	2.6
4	A	49	LYS	2.6
4	A	1195	LEU	2.6
5	B	317	CYS	2.5
11	J	21	TYR	2.5
4	A	1001	ARG	2.5
4	A	269	ILE	2.5
4	A	577	ILE	2.5
4	A	683	ILE	2.5
5	B	524	PRO	2.5
4	A	323	LYS	2.5
4	A	89	PRO	2.5
4	A	737	LEU	2.5
5	B	749	LEU	2.5
7	E	91	LYS	2.5
4	A	1073	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
4	A	698	GLN	2.5
4	A	1271	ILE	2.4
6	C	129	ILE	2.4
5	B	822	ASN	2.4
5	B	939	THR	2.4
11	J	39	LEU	2.4
5	B	162	SER	2.4
4	A	335	ARG	2.4
9	H	119	GLY	2.4
5	B	1047	PHE	2.4
4	A	306	ASN	2.4
4	A	960	ILE	2.4
4	A	847	ASP	2.4
13	L	66	GLN	2.4
12	K	9	LEU	2.4
4	A	1020	CYS	2.4
5	B	334	ILE	2.3
5	B	313	MET	2.3
9	H	63	LEU	2.3
5	B	535	LEU	2.3
10	I	2	THR	2.3
5	B	1086	PHE	2.3
5	B	233	PRO	2.3
4	A	1108	ALA	2.3
5	B	1145	SER	2.3
5	B	1161	HIS	2.3
4	A	1066	VAL	2.3
11	J	11	GLY	2.3
4	A	181	LEU	2.3
4	A	751	SER	2.3
10	I	109	ILE	2.2
4	A	1431	GLY	2.2
5	B	43	LEU	2.2
11	J	44	TYR	2.2
4	A	999	VAL	2.2
4	A	630	ILE	2.2
11	J	57	ILE	2.2
4	A	1306	LEU	2.2
5	B	488	TYR	2.2
11	J	14	VAL	2.2
4	A	447	GLN	2.2
4	A	1257	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
4	A	183	GLY	2.2
7	E	78	LEU	2.2
4	A	239	LEU	2.2
4	A	908	LEU	2.2
5	B	377	PHE	2.2
4	A	803	SER	2.2
7	E	54	GLN	2.2
7	E	98	ILE	2.2
4	A	443	LEU	2.2
5	B	721	LEU	2.2
12	K	10	PHE	2.2
4	A	322	VAL	2.1
7	E	211	TYR	2.1
4	A	710	LEU	2.1
9	H	130	ARG	2.1
4	A	17	VAL	2.1
5	B	833	TYR	2.1
7	E	46	TYR	2.1
6	C	155	LEU	2.1
12	K	51	LEU	2.1
5	B	750	GLY	2.1
5	B	1214	PRO	2.1
4	A	653	VAL	2.1
13	L	46	VAL	2.1
4	A	92	HIS	2.1
7	E	134	THR	2.1
5	B	1067	ARG	2.1
4	A	770	VAL	2.1
10	I	43	VAL	2.1
4	A	113	LEU	2.1
4	A	659	HIS	2.1
9	H	46	LEU	2.1
4	A	503	GLN	2.1
4	A	56	PRO	2.1
7	E	105	PHE	2.1
7	E	19	VAL	2.1
4	A	199	LEU	2.1
5	B	416	LEU	2.1
5	B	541	LEU	2.1
5	B	1216	LEU	2.1
6	C	156	THR	2.1
10	I	119	THR	2.1

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Mol	Chain	Res	Type	RSRZ
11	J	1	MET	2.1
4	A	258	GLY	2.1
4	A	872	GLY	2.1
4	A	925	LEU	2.0
9	H	121	LEU	2.0
7	E	121	MET	2.0
5	B	229	ALA	2.0
5	B	859	TYR	2.0
4	A	1065	GLY	2.0
5	B	529	GLU	2.0
7	E	138	ALA	2.0
4	A	19	PHE	2.0
4	A	105	CYS	2.0
4	A	219	PHE	2.0
5	B	988	GLY	2.0
7	E	110	PHE	2.0
7	E	55	ARG	2.0
4	A	1430	LEU	2.0
5	B	850	LEU	2.0
4	A	84	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	WVQ	T	19	23/24	0.81	0.12	104,114,138,142	0

6.3 Carbohydrates [i](#)

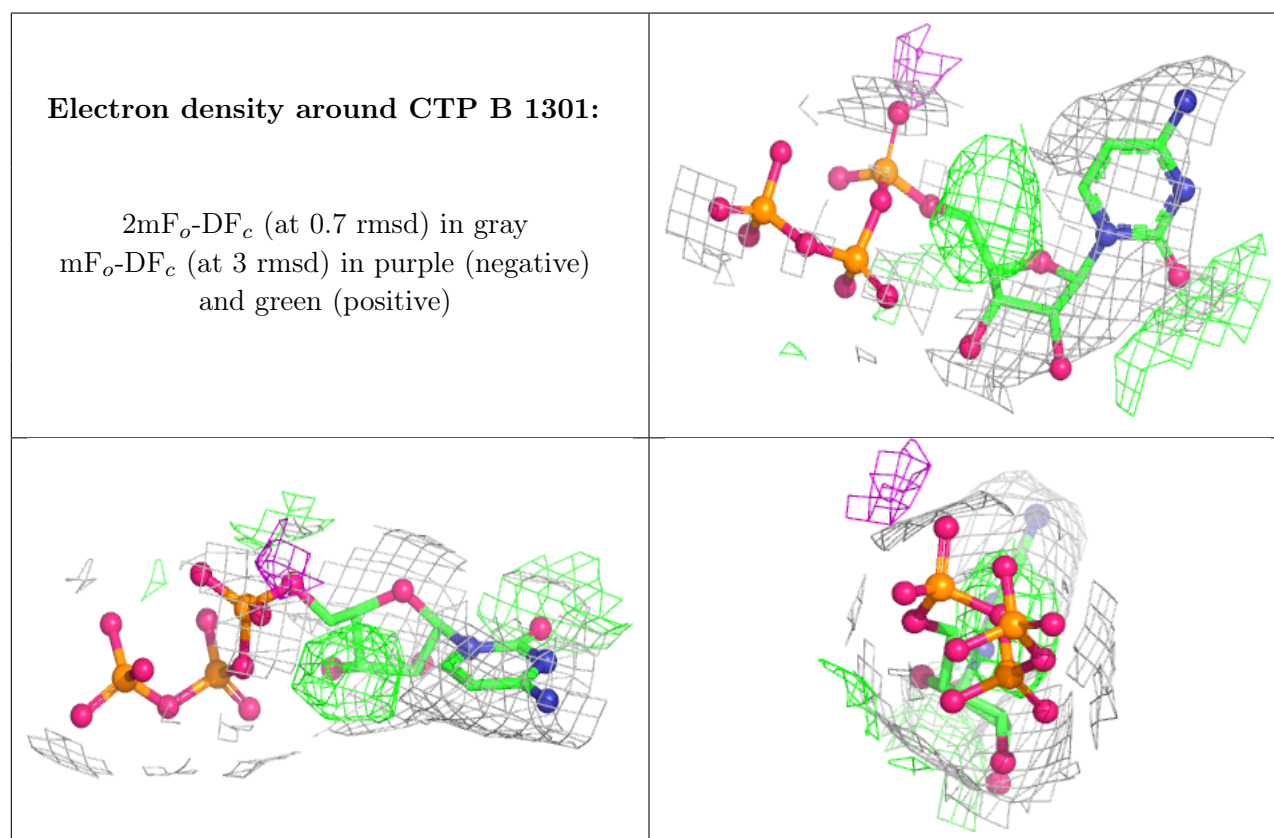
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	ZN	A	1802	1/1	0.80	0.08	315,315,315,315	0
16	CTP	B	1301	29/29	0.81	0.11	86,105,129,137	0
14	MG	A	1804	1/1	0.87	0.18	137,137,137,137	0
15	ZN	A	1803	1/1	0.90	0.07	165,165,165,165	0
15	ZN	L	101	1/1	0.91	0.06	310,310,310,310	0
14	MG	A	1801	1/1	0.95	0.06	141,141,141,141	0
15	ZN	B	1302	1/1	0.97	0.04	192,192,192,192	0
15	ZN	I	201	1/1	0.97	0.06	125,125,125,125	0
15	ZN	J	101	1/1	0.99	0.06	93,93,93,93	0
15	ZN	C	401	1/1	0.99	0.07	119,119,119,119	0
15	ZN	I	202	1/1	0.99	0.03	152,152,152,152	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 ⓘ

There are no such residues in this entry.