



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:18 PM UTC

PDB ID : 9N5C / pdb_00009n5c
Title : RNA polymerase II elongation complex with 8-oxoG at +1 site, CMPCPP-bound
Authors : Oh, J.; Wang, D.
Deposited on : 2025-02-04
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

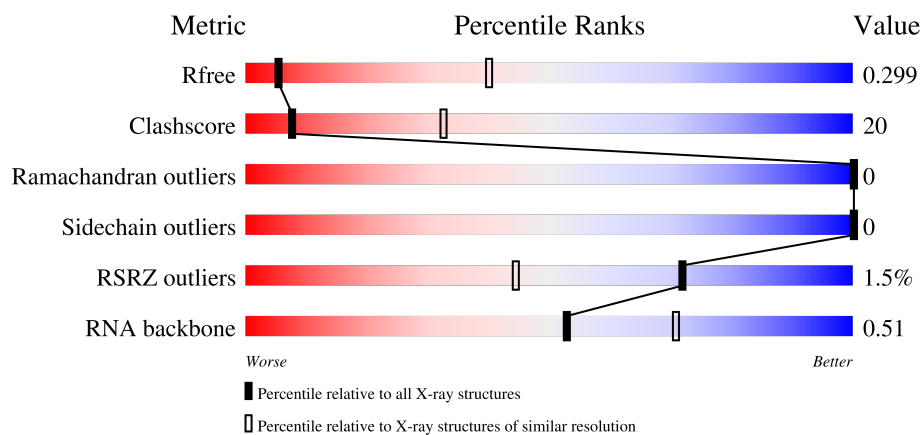
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	R	9	 33% 56% 11%
2	T	29	 31% 59% 10%
3	N	18	 28% 56% 17%
4	A	1733	 45% 35% 20%

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Mol	Chain	Length	Quality of chain
5	B	1224	2% 53% 38% 8%
6	C	318	% 47% 37% 16%
7	E	215	67% 32% .
8	F	155	32% 23% 45%
9	H	146	% 51% 40% 9%
10	I	122	54% 42% ..
11	J	70	3% 46% 47% 7%
12	K	120	% 61% 34% 5%
13	L	70	% 30% 31% 39%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29046 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
			199	88	40	62	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	26	Total	C	N	O	P	0	0	0
			521	250	80	165	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	15	Total	C	N	O	P	0	0	0
			317	148	71	83	15			

- 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
			10817	6824	1890	2043	60			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1121	Total	C	N	O	S	0	0	0
			8843	5598	1547	1645	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	213	Total	C	N	O	S	0	0	0
			1740	1105	307	317	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
			1052	664	173	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
			331	205	63	59	4			

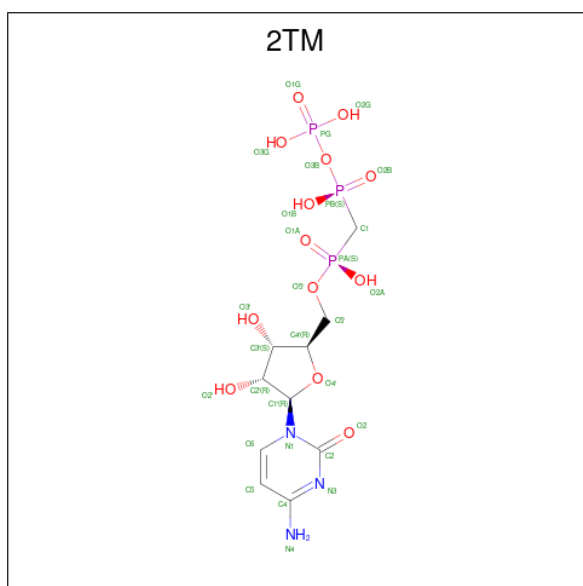
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (CCD ID: 2TM) (formula: C₁₀H₁₈N₃O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

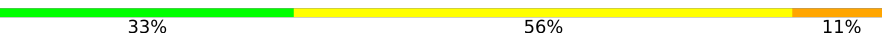


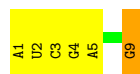
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	B	1	Total	C	N	O	P	0	0
			29	10	3	13	3		

3 Residue-property plots

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

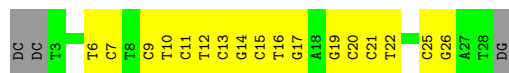
• Molecule 1: RNA

Chain R: 

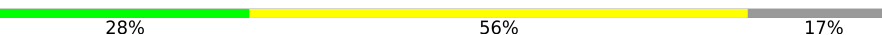


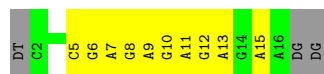
• Molecule 2: Template strand DNA

Chain T: 



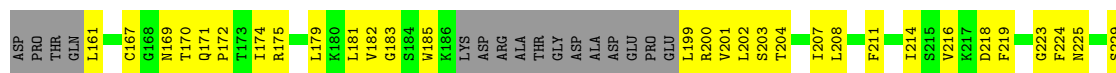
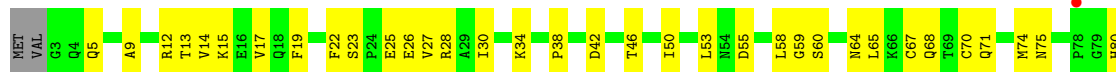
• Molecule 3: Non-template strand DNA

Chain N: 



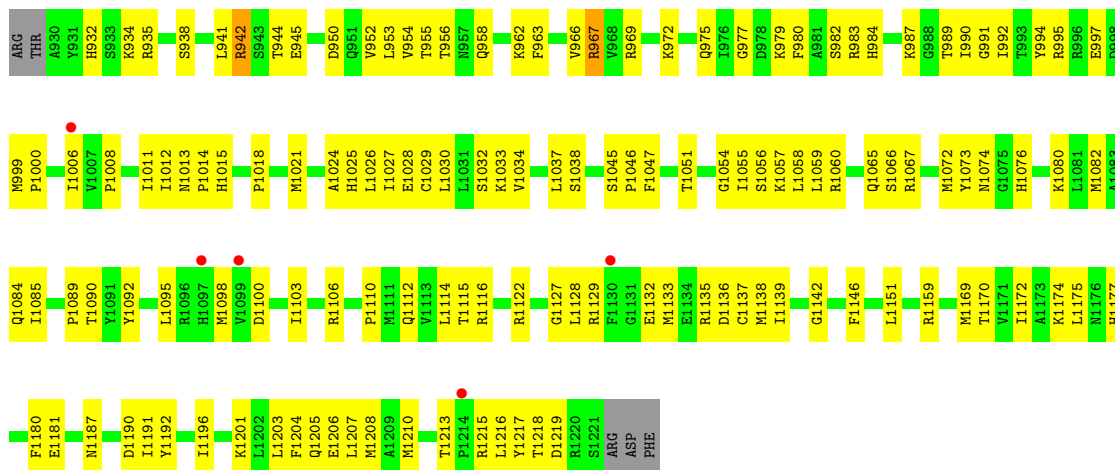
• Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain A: 

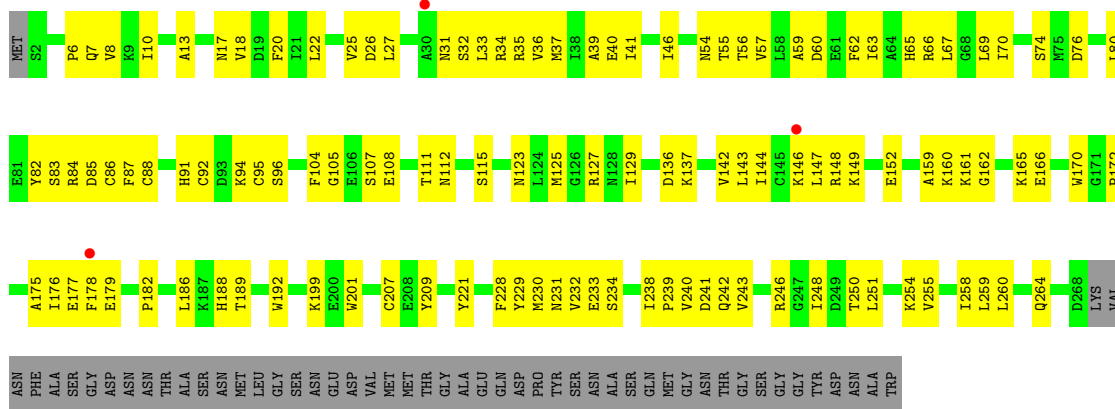


GLY	HI367	M1267	W1191	A1108	L1021	H906	K830	K744	N648	P561	Y478	V392	D305
PHE	M1368	L1268	L1192	K1109	L1022	T907	T834	Q745	I649	P561	M479	G395	I308
THR	E1269	N1270	L1193	M1110	R1023	T907	T834	M746	Q850	P561	M479	G396	A309
ALA	L1370	L1271	E1196	M1112	S1024	E914	T834	M747	K651	P561	F482	G310	G310
TYR	L1371	L1272	L1197	K1113	R1025	S915	Y836	M748	V653	P561	D483	H399	A314
GLY	D1373	L1273	D1374	T1113	R1030	G916	I837	S751	N654	P561	G484	P400	A314
ALA	V1374	G1275	M1202	L1116	V1031	G916	Q838	S754	F662	P561	D485	A401	I325
ASP	M1375	G1276	K1205	T1117	E1034	T919	R839	I756	S663	P561	E486	A402	R326
GLY	T1376	L1277	D1206	V1118	Y1035	G921	R840	I756	G663	P561	M487	V405	I326
GLY	S1383	L1278	L1207	E1129	R1036	L925	L841	N757	G665	P561	Q576	I406	K332
ALA	V1384	L1279	L1207	T1117	L1037	Q926	V842	I758	I666	P561	V491	G410	R335
THR	T1385	L1282	T1208	L1117	L1048	Q926	L845	A759	A671	P561	P492	D411	R336
SER	R1386	K1290	M1209	V1118	N1049	E932	D846	Q760	D672	P561	E496	R412	R337
PHE	H1387	T1295	G1213	L1132	T1048	Y933	D847	A763	A671	P561	S579	I413	G338
GLY	N1390	T1296	G1214	L1133	T1049	Y933	D847	A763	A671	P561	V580	I414	N339
ALA	R1391	K1300	E1215	R1135	S1056	L936	M849	V765	T675	P561	E501	I415	L340
TYR	A1396	E1303	I1216	S1136	V1057	L936	V850	V765	M676	P561	L501	L418	N341
GLY	L1397	L1217	E1138	A1137	V1058	K941	H851	Q766	T679	P561	Q503	S418	G342
ALA	M1398	Q1218	H1140	I1138	M1063	P942	Y852	Q767	T680	P561	Q503	I424	K343
PRO	R1399	T1219	E1140	E1139	V1064	L943	D853	I775	I683	P561	V507	I430	R344
THR	V1311	F1220	K1144	R944	V1065	E945	R857	A776	A684	P561	I511	V430	S348
SER	F1402	K1221	T1148	E945	L1067	E945	S859	F777	K688	P561	I511	A349	R350
PRO	E1403	N1222	I1148	D949	Q1070	D949	V863	D781	K688	P561	V512	E433	R351
GLY	V1406	D1223	E1151	A952	S1071	A952	V863	D781	K688	P561	I512	E433	R351
GLY	E1407	L1224	I1152	N953	S1071	N953	F866	T783	T694	P561	Q515	I436	V352
VAL	I1408	V1225	Y1153	Q954	A1076	Q954	I867	L784	Q698	P561	K518	M437	S354
SER	L1409	I1227	Y1154	P955	T1077	P955	I868	P785	L701	P561	P519	V442	G355
LEU	F1410	W1228	D1155	L956	Q1078	L956	G869	H786	L701	P561	C520	L443	D356
PRO	A1416	K1235	P1156	L960	M1079	L960	E870	I608	R711	P561	M521	L443	P357
GLY	A1416	L1236	L1081	R961	T1081	R961	G872	K789	R711	P561	M521	L443	P357
PHE	D1419	L1237	ASN	R962	ASN	R962	M873	Y792	F714	P561	L528	R446	E360
SER	I1433	I1238	THR	P963	THR	P963	D874	Y792	F714	P561	L528	R446	L361
PRO	C1421	R1239	PHE	P964	PHE	P964	A875	K797	E715	P561	I613	D447	D362
SER	R1422	C1240	HIS	Q965	HIS	Q965	A876	G798	E715	P561	I613	D447	D362
PRO	M1336	L1241	PHE	Q968	PHE	Q968	H877	F799	V718	P561	I613	D447	Q363
THR	E1426	V1242	ALA	Q968	ALA	Q968	I878	V800	L722	P561	I613	D447	V364
GLY	V1427	V1243	GLY	H975	GLY	H975	V880	R806	R726	P561	I613	D447	P367
SER	V1428	ARG	VAL	H975	VAL	H975	V880	R806	R726	P561	I613	D447	K368
PRO	I1429	PRO	ALA	H975	ALA	H975	V880	R806	R726	P561	I613	D447	S369
THR	G1430	LYS	ALA	H975	ALA	H975	V880	R806	R726	P561	I613	D447	I370
SER	G1431	SER	ALA	H975	ALA	H975	V880	R806	R726	P561	I613	D447	A371
PRO	R1345	LEU	ASP	H975	ASP	H975	V880	R806	R726	P561	I613	D447	K372
ALA	L1348	ASP	ALA	H975	ALA	H975	V880	R806	R726	P561	I613	D447	T373
SER	E1351	THR	GLU	H975	THR	H975	V880	R806	R726	P561	I613	D447	L374
THR	V1352	GLU	ALA	H975	GLU	H975	V880	R806	R726	P561	I613	D447	T374
SER	V1355	ALA	ALA	H975	ALA	H975	V880	R806	R726	P561	I613	D447	T375
PRO	I1356	GLU	GLN	H975	GLU	H975	V880	R806	R726	P561	I613	D447	V380
ASN	D1441	GLU	SER	H975	GLU	H975	V880	R806	R726	P561	I613	D447	T381
ASP	D1442	GLU	ASP	H975	GLU	H975	V880	R806	R726	P561	I613	D447	Y383
ALA	V1443	ASP	ASP	H975	GLU	H975	V880	R806	R726	P561	I613	D447	R387
THR	M1444	ALA	THR	H975	GLU	H975	V880	R806	R726	P561	I613	D447	L388
SER	I1445	ALA	ALA	H975	GLU	H975	V880	R806	R726	P561	I613	D447	L388
PRO	D1446	ALA	ALA	H975	GLU	H975	V880	R806	R726	P561	I613	D447	L391
THR	D1446	ALA	ALA	H975	GLU	H975	V880	R806	R726	P561	I613	D447	L391





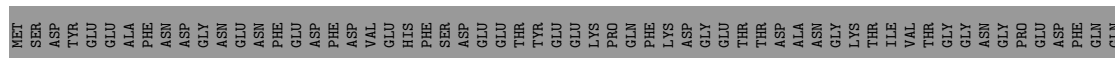
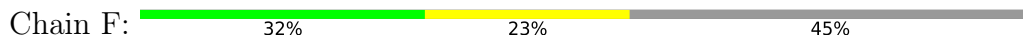
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

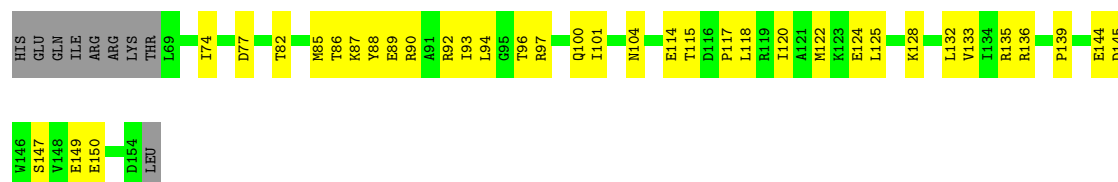


• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

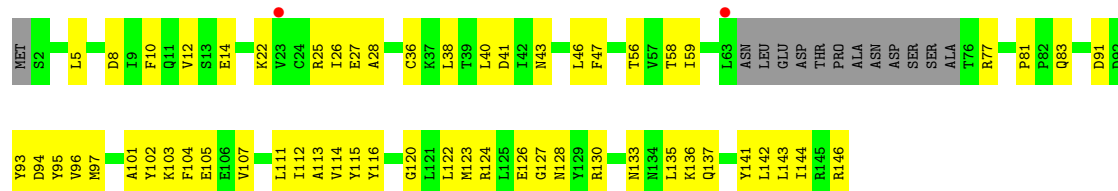


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

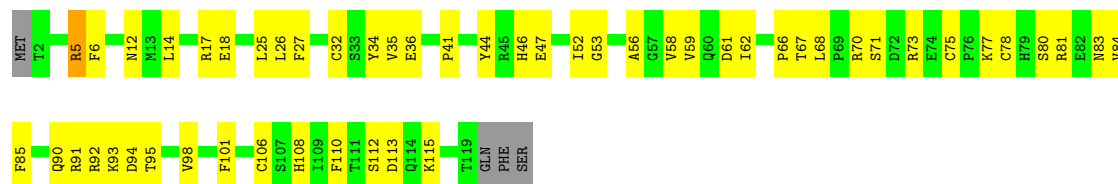




- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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



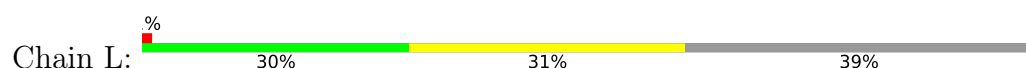
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

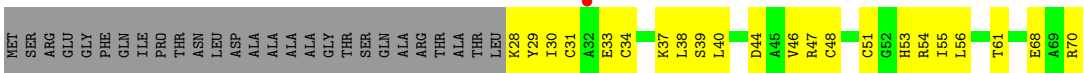


- Molecule 12: DNA-directed RNA polymerase II subunit RPB11



- 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	162.64Å 222.99Å 192.26Å 90.00° 98.55° 90.00°	Depositor
Resolution (Å)	48.77 – 3.60 48.77 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.77-3.60) 99.4 (48.77-3.60)	Depositor EDS
R_{merge}	0.51	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.252 , 0.297 0.253 , 0.299	Depositor DCC
R_{free} test set	2000 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å ²)	103.1	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 117.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	29046	wwPDB-VP
Average B, all atoms (Å ²)	124.0	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: ZN, 2TM, 8OG, MG

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	0.18	0/223	0.39	0/345
2	T	0.22	0/551	0.48	0/843
3	N	0.22	0/359	0.42	0/553
4	A	0.17	0/11009	0.41	0/14897
5	B	0.15	0/9014	0.37	0/12165
6	C	0.16	0/2139	0.39	0/2899
7	E	0.14	0/1776	0.36	0/2390
8	F	0.12	0/696	0.35	0/943
9	H	0.16	0/1070	0.45	0/1452
10	I	0.17	0/970	0.45	0/1308
11	J	0.19	0/541	0.48	0/727
12	K	0.17	0/937	0.42	0/1265
13	L	0.13	0/333	0.46	0/443
All	All	0.16	0/29618	0.40	0/40230

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	2
5	B	0	3
9	H	0	1
10	I	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	412	ARG	Sidechain
4	A	726	ARG	Sidechain
5	B	857	ARG	Sidechain
5	B	942	ARG	Sidechain
5	B	967	ARG	Sidechain
9	H	77	ARG	Sidechain
10	I	5	ARG	Sidechain

5.2 Too-close contacts

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	199	0	98	8	0
2	T	521	0	297	14	0
3	N	317	0	166	12	0
4	A	10817	0	10839	521	0
5	B	8843	0	8799	363	0
6	C	2101	0	2058	102	0
7	E	1740	0	1766	48	0
8	F	684	0	692	29	0
9	H	1052	0	1007	56	0
10	I	952	0	904	48	1
11	J	532	0	543	38	0
12	K	919	0	929	41	0
13	L	331	0	343	16	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	B	29	0	14	1	0
All	All	29046	0	28455	1157	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 20.

All (1157) 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:863:GLU:HG3	5:B:962:LYS:HB2	1.46	0.97
9:H:36:CYS:HA	9:H:126:GLU:O	1.67	0.94
11:J:21:TYR:HB2	11:J:39:LEU:HD11	1.50	0.92
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.03	0.91
5:B:101:MET:HG2	5:B:111:ALA:HA	1.57	0.87
4:A:68:GLN:NE2	4:A:70:CYS:SG	2.49	0.86
4:A:877:HIS:HD2	4:A:1056:SER:HA	1.40	0.86
5:B:128:LEU:HB2	5:B:168:GLY:O	1.76	0.85
4:A:1224:LEU:HD21	4:A:1240:CYS:HB3	1.58	0.84
5:B:999:MET:HE3	5:B:1000:PRO:HD2	1.58	0.84
4:A:350:ARG:HB2	5:B:1128:LEU:HD21	1.59	0.83
4:A:1397:LEU:HB2	4:A:1426:GLU:HG3	1.61	0.83
4:A:613:ILE:HG21	9:H:102:TYR:HB3	1.61	0.83
4:A:1227:ILE:HD11	4:A:1239:ARG:HH11	1.43	0.82
4:A:326:ARG:HG3	4:A:1406:VAL:HG21	1.62	0.82
5:B:857:ARG:HH22	5:B:942:ARG:HD2	1.45	0.81
4:A:30:ILE:HD12	5:B:1170:THR:HG21	1.63	0.81
5:B:1172:ILE:HD11	5:B:1181:GLU:HG2	1.63	0.81
4:A:285:PRO:HB2	4:A:288:ALA:HB3	1.61	0.81
5:B:857:ARG:NH1	5:B:945:GLU:OE1	2.13	0.81
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.61	0.80
4:A:174:ILE:HD11	4:A:181:LEU:HB2	1.62	0.80
4:A:12:ARG:HD2	5:B:1218:THR:HG21	1.65	0.79
5:B:287:ARG:NH2	5:B:294:ASP:OD1	2.15	0.79
5:B:497:ARG:HH22	5:B:775:LYS:HE2	1.48	0.79
9:H:96:VAL:HA	9:H:142:LEU:O	1.82	0.79
5:B:402:GLY:O	5:B:405:ARG:NH1	2.15	0.78
5:B:365:THR:HG21	5:B:370:PHE:HB2	1.64	0.78
5:B:287:ARG:NH1	5:B:324:ILE:O	2.17	0.78
5:B:173:MET:HE3	5:B:201:GLY:HA2	1.64	0.78
11:J:17:LYS:HB3	11:J:39:LEU:HD13	1.65	0.77
4:A:809:THR:HG22	5:B:730:ARG:HH11	1.49	0.77
4:A:767:GLN:HA	4:A:799:PHE:HA	1.67	0.77
6:C:86:CYS:SG	6:C:87:PHE:N	2.58	0.77
4:A:598:LEU:HD21	9:H:124:ARG:HB2	1.66	0.77
5:B:840:ILE:HG12	5:B:1011:ILE:HB	1.67	0.76
4:A:512:VAL:HA	4:A:519:PRO:HA	1.67	0.76
6:C:165:LYS:O	12:K:6:ARG:NH2	2.19	0.76
4:A:1100:ARG:NH1	4:A:1351:GLU:OE2	2.19	0.75
4:A:200:ARG:HH21	4:A:202:LEU:HA	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:859:SER:O	4:A:1422:ARG:NH1	2.20	0.74
4:A:108:MET:SD	4:A:108:MET:N	2.53	0.74
4:A:1390:ASN:O	4:A:1399:ARG:NH1	2.19	0.74
4:A:1136:SER:O	4:A:1274:ARG:NH1	2.20	0.74
5:B:848:ARG:HD2	11:J:8:PHE:HA	1.69	0.74
5:B:984:HIS:NE2	5:B:1028:GLU:OE1	2.19	0.74
4:A:464:PRO:HB2	12:K:4:PRO:HD3	1.69	0.74
4:A:14:VAL:HA	5:B:1218:THR:HA	1.70	0.73
4:A:361:LEU:HB2	4:A:471:ASN:HD22	1.52	0.73
6:C:22:LEU:HG	6:C:25:VAL:HG21	1.71	0.73
4:A:131:SER:HB2	4:A:223:GLY:HA3	1.69	0.73
5:B:736:THR:HG23	5:B:737:THR:HG23	1.71	0.73
5:B:243:ALA:HA	5:B:251:ILE:HG12	1.69	0.73
6:C:34:ARG:HD2	6:C:178:PHE:CE2	2.24	0.72
4:A:225:ASN:HB3	4:A:229:SER:H	1.54	0.72
4:A:975:HIS:HA	4:A:1036:ARG:HG3	1.69	0.72
5:B:1060:ARG:NH1	6:C:199:LYS:O	2.22	0.72
13:L:30:ILE:HG12	13:L:37:LYS:HB3	1.72	0.72
5:B:1174:LYS:HB2	5:B:1177:HIS:HB2	1.70	0.72
6:C:56:THR:HG22	6:C:147:LEU:HD21	1.72	0.72
4:A:337:ARG:NH2	5:B:1132:GLU:OE1	2.23	0.72
4:A:1348:LEU:HD23	4:A:1372:VAL:HG13	1.71	0.71
4:A:1290:LYS:HG2	4:A:1300:LYS:HG2	1.73	0.71
5:B:1054:GLY:HA2	5:B:1057:LYS:HD2	1.70	0.71
9:H:95:TYR:HE1	9:H:97:MET:HG3	1.54	0.71
5:B:848:ARG:NH1	11:J:8:PHE:O	2.22	0.71
5:B:102:VAL:HG22	5:B:112:LEU:HB2	1.72	0.71
5:B:979:LYS:HG2	5:B:1095:LEU:HD12	1.71	0.71
4:A:608:ILE:HB	4:A:613:ILE:HD11	1.72	0.71
9:H:25:ARG:NH2	9:H:122:LEU:HB2	2.06	0.71
6:C:46:ILE:HA	6:C:159:ALA:HA	1.72	0.70
5:B:694:ASP:OD1	5:B:695:ALA:N	2.25	0.70
10:I:92:ARG:NH1	10:I:93:LYS:HG3	2.06	0.70
5:B:1103:ILE:O	5:B:1122:ARG:NH1	2.23	0.70
5:B:365:THR:HG22	5:B:374:LYS:HE3	1.73	0.70
4:A:821:ARG:NH2	5:B:524:PRO:O	2.25	0.69
4:A:963:ILE:HD11	4:A:1048:ASN:HB3	1.75	0.69
5:B:613:VAL:HA	5:B:632:ARG:HH22	1.58	0.69
6:C:148:ARG:HH12	11:J:64:ASN:HA	1.56	0.69
4:A:806:ARG:NH1	5:B:725:PRO:O	2.26	0.69
4:A:344:ARG:HH11	5:B:1129:ARG:HB2	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1215:ARG:NH2	4:A:1274:ARG:HB3	2.07	0.69
12:K:91:CYS:HA	12:K:94:ILE:HD12	1.75	0.69
5:B:1112:GLN:OE1	5:B:1115:THR:N	2.25	0.69
6:C:54:ASN:ND2	6:C:60:ASP:OD1	2.20	0.69
5:B:276:ILE:HD11	5:B:355:ILE:HD13	1.74	0.69
5:B:1072:MET:HG3	5:B:1085:ILE:HB	1.74	0.69
2:T:25:DC:H2''	2:T:26:DG:H5'	1.74	0.68
4:A:956:LEU:HD13	4:A:1021:LEU:HD22	1.75	0.68
11:J:36:LEU:HD13	11:J:47:ARG:HG2	1.74	0.68
4:A:5:GLN:O	5:B:1159:ARG:NH2	2.25	0.68
4:A:332:LYS:HG2	4:A:337:ARG:HE	1.56	0.68
6:C:55:THR:OG1	6:C:152:GLU:N	2.26	0.68
6:C:35:ARG:O	6:C:39:ALA:HB3	1.94	0.68
4:A:1399:ARG:HB3	4:A:1408:ILE:HD13	1.74	0.68
4:A:286:HIS:CG	4:A:287:HIS:H	2.11	0.68
5:B:325:GLN:NE2	10:I:12:ASN:OD1	2.27	0.68
5:B:1076:HIS:O	6:C:31:ASN:ND2	2.26	0.68
5:B:1135:ARG:O	5:B:1139:ILE:HG13	1.93	0.68
3:N:9:DA:H2''	3:N:10:DG:C8	2.29	0.67
5:B:298:LEU:HD22	5:B:314:LEU:HD13	1.75	0.67
5:B:618:ASP:HB3	5:B:621:GLU:HB2	1.76	0.67
4:A:399:HIS:HA	4:A:401:GLY:H	1.58	0.67
9:H:115:TYR:CE1	9:H:124:ARG:HG3	2.30	0.67
8:F:94:LEU:HD21	8:F:125:LEU:HD23	1.76	0.67
4:A:821:ARG:O	4:A:825:ILE:HG12	1.93	0.67
5:B:1065:GLN:HE22	5:B:1067:ARG:HG2	1.59	0.67
4:A:848:ILE:HG22	4:A:1064:VAL:HG23	1.76	0.67
7:E:117:THR:HG23	7:E:120:ALA:H	1.59	0.67
4:A:1239:ARG:HH12	4:A:1241:ARG:HH12	1.43	0.67
4:A:449:SER:HB2	5:B:1133:MET:HG2	1.76	0.67
10:I:5:ARG:NH1	10:I:36:GLU:OE2	2.28	0.67
4:A:569:LYS:HG2	4:A:570:PRO:HD2	1.77	0.66
6:C:76:ASP:HB2	6:C:129:ILE:HG13	1.77	0.66
5:B:483:LEU:HD21	5:B:491:THR:HG23	1.77	0.66
4:A:102:VAL:O	4:A:106:VAL:HG13	1.96	0.66
4:A:1013:ASP:HB3	7:E:207:ARG:HG3	1.76	0.66
4:A:92:HIS:HB2	4:A:236:LEU:HD11	1.77	0.66
4:A:117:GLU:HG2	4:A:123:ARG:HG3	1.76	0.66
4:A:382:PRO:HD3	8:F:104:ASN:HD21	1.60	0.66
4:A:1352:VAL:O	4:A:1356:ILE:HG12	1.96	0.66
4:A:179:LEU:HD22	4:A:297:GLN:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:972:LYS:HD3	5:B:1098:MET:HE3	1.77	0.66
4:A:1215:ARG:O	4:A:1219:THR:HG23	1.96	0.65
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.77	0.65
6:C:179:GLU:HB3	6:C:229:TYR:HB2	1.78	0.65
4:A:137:ALA:O	4:A:141:LEU:HG	1.97	0.65
4:A:901:LEU:HA	4:A:907:THR:HG23	1.77	0.65
6:C:82:TYR:HB2	6:C:85:ASP:HB2	1.79	0.65
6:C:8:VAL:HG23	12:K:101:LEU:HD21	1.77	0.65
4:A:839:ARG:HH12	4:A:1402:PHE:HA	1.62	0.65
6:C:6:PRO:HB2	12:K:101:LEU:HD23	1.79	0.65
9:H:40:LEU:HD13	9:H:123:MET:HB2	1.78	0.65
4:A:786:HIS:HE1	5:B:742:GLU:HG3	1.62	0.65
4:A:607:ILE:HG12	4:A:612:ILE:HG22	1.78	0.64
7:E:21:GLU:HG3	7:E:35:VAL:HG11	1.80	0.64
5:B:357:GLN:HG2	5:B:358:LYS:HG3	1.79	0.64
5:B:952:VAL:HG22	5:B:966:VAL:HG22	1.79	0.64
5:B:1187:ASN:HD21	5:B:1190:ASP:C	2.06	0.64
4:A:242:PRO:O	4:A:247:ARG:NH2	2.31	0.64
5:B:822:ASN:O	11:J:48:ARG:NH1	2.31	0.64
5:B:275:TYR:HD2	5:B:359:GLU:HG2	1.63	0.64
5:B:1132:GLU:HA	5:B:1135:ARG:HG2	1.80	0.64
4:A:760:GLN:OE1	4:A:765:VAL:HG23	1.97	0.64
5:B:570:VAL:HG23	5:B:573:GLN:HB2	1.80	0.64
5:B:627:PHE:O	5:B:632:ARG:NH2	2.31	0.64
6:C:41:ILE:HG21	6:C:172:PRO:HG3	1.80	0.64
8:F:85:MET:HG2	8:F:89:GLU:HG3	1.80	0.64
4:A:367:PRO:HD2	4:A:370:ILE:HD12	1.79	0.64
4:A:1107:VAL:HG22	4:A:1383:SER:HB3	1.78	0.63
5:B:542:MET:HE3	5:B:636:PRO:HG2	1.80	0.63
5:B:806:THR:H	5:B:809:MET:HE3	1.63	0.63
6:C:177:GLU:HG3	6:C:231:ASN:HB3	1.80	0.63
4:A:308:ILE:HG22	4:A:310:GLY:H	1.64	0.63
4:A:881:GLN:HB2	4:A:956:LEU:HD12	1.80	0.63
5:B:416:LEU:HD23	5:B:457:LEU:HD23	1.79	0.63
4:A:877:HIS:CD2	4:A:1056:SER:HA	2.27	0.63
5:B:733:HIS:CE1	5:B:738:PHE:HZ	2.17	0.63
4:A:368:LYS:HG2	4:A:372:LYS:HE3	1.81	0.63
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.81	0.63
4:A:265:LYS:O	4:A:269:ILE:HG12	1.99	0.63
5:B:857:ARG:HG2	5:B:859:TYR:CZ	2.33	0.62
4:A:392:VAL:HG13	4:A:415:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:757:PRO:HG2	5:B:984:HIS:CE1	2.34	0.62
8:F:97:ARG:O	8:F:101:ILE:HG13	1.99	0.62
3:N:5:DC:N4	3:N:6:DG:O6	2.33	0.62
4:A:106:VAL:O	4:A:171:GLN:NE2	2.32	0.62
4:A:1192:LEU:HD11	4:A:1239:ARG:HB3	1.80	0.62
4:A:1239:ARG:HH22	4:A:1241:ARG:HH22	1.45	0.62
6:C:17:ASN:ND2	6:C:233:GLU:OE2	2.18	0.62
4:A:961:ARG:HE	4:A:1025:ARG:HH22	1.48	0.62
4:A:1217:LYS:HZ2	4:A:1222:ASN:H	1.47	0.62
4:A:846:GLU:HA	4:A:1066:VAL:HG22	1.81	0.62
9:H:130:ARG:HD3	9:H:133:ASN:HB3	1.82	0.62
4:A:1129:GLU:HA	4:A:1132:LYS:HD2	1.82	0.62
4:A:849:MET:HB2	4:A:1063:MET:SD	2.40	0.62
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.82	0.62
5:B:680:THR:HG23	5:B:683:SER:H	1.64	0.62
7:E:124:VAL:HA	7:E:132:ILE:HD12	1.82	0.62
4:A:391:LEU:HD22	4:A:400:PRO:HB2	1.81	0.62
5:B:45:SER:HA	5:B:48:LEU:HD12	1.82	0.62
4:A:1441:PHE:HE1	8:F:92:ARG:HD3	1.65	0.61
4:A:303:TYR:CZ	4:A:325:ILE:HD11	2.36	0.61
4:A:360:GLU:HB2	4:A:363:GLN:HG3	1.82	0.61
5:B:828:ALA:O	5:B:834:ASN:ND2	2.33	0.61
4:A:337:ARG:HD2	4:A:839:ARG:HH21	1.64	0.61
4:A:1212:VAL:HG13	4:A:1273:LEU:HD11	1.82	0.61
5:B:437:GLU:OE1	5:B:437:GLU:N	2.33	0.61
4:A:742:ASN:HA	4:A:745:GLN:HG3	1.82	0.61
11:J:9:SER:OG	11:J:48:ARG:NH2	2.34	0.61
11:J:20:SER:O	11:J:24:LEU:HG	2.00	0.61
11:J:31:ASP:OD1	11:J:32:GLU:N	2.33	0.61
4:A:765:VAL:HG13	4:A:800:VAL:HB	1.83	0.61
4:A:1162:VAL:HG23	4:A:1163:ILE:HD12	1.83	0.60
4:A:1364:ASN:OD1	4:A:1366:ARG:HG2	2.01	0.60
5:B:801:LYS:HG2	11:J:52:THR:HA	1.82	0.60
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.81	0.60
4:A:1025:ARG:HG3	4:A:1030:ARG:HH22	1.66	0.60
5:B:915:THR:HB	5:B:934:LYS:HB3	1.82	0.60
3:N:12:DG:H1'	3:N:13:DA:N7	2.16	0.60
4:A:800:VAL:HG13	4:A:812:GLU:HB3	1.82	0.60
4:A:169:ASN:HD21	4:A:185:TRP:HZ2	1.48	0.60
4:A:994:GLN:HE22	4:A:1023:ARG:HH21	1.49	0.60
5:B:638:PHE:O	5:B:740:HIS:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:75:CYS:HB2	10:I:110:PHE:CE1	2.35	0.60
12:K:32:VAL:HG22	12:K:74:ARG:HB2	1.83	0.60
12:K:55:LYS:HD2	12:K:81:TYR:HD2	1.65	0.60
4:A:289:ILE:O	4:A:293:GLU:HG3	2.02	0.60
4:A:1227:ILE:HD11	4:A:1239:ARG:NH1	2.15	0.60
5:B:522:VAL:HG11	5:B:537:LYS:HD2	1.83	0.60
10:I:52:ILE:O	10:I:90:GLN:NE2	2.34	0.60
1:R:4:G:H2'	1:R:5:A:H8	1.67	0.60
4:A:13:THR:HG23	4:A:15:LYS:HZ2	1.66	0.60
16:B:2101:2TM:H10	16:B:2101:2TM:O2A	2.02	0.60
6:C:177:GLU:O	6:C:230:MET:HA	2.01	0.60
6:C:260:LEU:HG	6:C:264:GLN:HE21	1.67	0.60
8:F:128:LYS:HD2	8:F:149:GLU:HA	1.84	0.60
4:A:216:VAL:HA	4:A:219:PHE:CE2	2.37	0.60
6:C:36:VAL:HA	6:C:40:GLU:HG3	1.84	0.60
7:E:55:ARG:NH2	7:E:137:GLU:OE1	2.35	0.60
6:C:27:LEU:HD12	6:C:228:PHE:HE2	1.67	0.59
3:N:11:DA:H3'	3:N:12:DG:H2'	1.84	0.59
4:A:737:LEU:HD11	4:A:758:ILE:HG21	1.83	0.59
4:A:1155:ASP:OD2	4:A:1161:THR:OG1	2.14	0.59
5:B:211:VAL:HG21	5:B:483:LEU:HD12	1.82	0.59
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.84	0.59
7:E:127:ILE:O	7:E:127:ILE:HG13	2.01	0.59
10:I:59:VAL:HG12	10:I:61:ASP:H	1.65	0.59
10:I:92:ARG:HG2	10:I:92:ARG:HH11	1.66	0.59
5:B:262:GLU:HA	5:B:267:ARG:HH21	1.67	0.59
5:B:1034:VAL:HG22	5:B:1059:LEU:HD13	1.85	0.59
5:B:257:LYS:HD3	5:B:272:THR:HG23	1.84	0.59
6:C:251:LEU:O	6:C:255:VAL:HG23	2.02	0.59
5:B:63:ILE:HA	5:B:421:PHE:HE2	1.68	0.59
9:H:107:VAL:HG13	9:H:113:ALA:HB2	1.85	0.59
4:A:1436:ILE:O	4:A:1438:THR:N	2.36	0.58
3:N:11:DA:H2'	3:N:12:DG:C8	2.38	0.58
6:C:242:GLN:HB3	6:C:246:ARG:NH1	2.18	0.58
4:A:59:GLY:HA2	4:A:67:CYS:HB2	1.86	0.58
4:A:606:LEU:O	4:A:613:ILE:N	2.36	0.58
5:B:412:LEU:HD22	5:B:466:TRP:CD1	2.38	0.58
8:F:122:MET:O	8:F:125:LEU:HG	2.02	0.58
4:A:82:GLY:O	4:A:240:PRO:HA	2.03	0.58
4:A:279:LEU:HD12	4:A:285:PRO:HD3	1.86	0.58
4:A:941:LYS:O	4:A:945:GLU:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:275:TYR:CD2	5:B:359:GLU:HG2	2.38	0.58
6:C:31:ASN:O	6:C:34:ARG:HG2	2.03	0.58
13:L:38:LEU:HD11	13:L:48:CYS:HA	1.86	0.58
4:A:1063:MET:HG3	5:B:1139:ILE:HG22	1.85	0.58
4:A:93:VAL:HA	4:A:96:ILE:HD12	1.85	0.57
4:A:553:VAL:HB	4:A:556:TRP:HB2	1.86	0.57
5:B:332:ASP:OD1	5:B:348:ARG:NH2	2.37	0.57
6:C:92:CYS:N	6:C:95:CYS:SG	2.77	0.57
12:K:47:ARG:HH11	12:K:47:ARG:HG2	1.69	0.57
4:A:1099:PRO:O	4:A:1103:GLU:HG3	2.04	0.57
4:A:1214:GLU:OE1	4:A:1218:GLN:NE2	2.37	0.57
5:B:291:ILE:HG12	5:B:300:HIS:NE2	2.20	0.57
5:B:400:HIS:HB3	5:B:403:LYS:HG2	1.86	0.57
5:B:878:GLN:OE1	5:B:880:THR:OG1	2.22	0.57
7:E:112:TYR:HB3	7:E:116:ILE:HD11	1.85	0.57
9:H:101:ALA:HA	9:H:116:TYR:HA	1.86	0.57
4:A:336:ILE:HD11	5:B:1203:LEU:HD13	1.86	0.57
4:A:919:ILE:HD11	4:A:925:LEU:HG	1.87	0.57
5:B:128:LEU:O	5:B:167:ILE:N	2.37	0.57
4:A:350:ARG:HH12	4:A:447:GLN:HG2	1.70	0.57
7:E:59:SER:HB3	7:E:81:GLU:HA	1.85	0.57
2:T:9:DC:H2'	2:T:10:DT:H71	1.86	0.57
4:A:153:PRO:HA	4:A:161:LEU:HD13	1.86	0.57
5:B:555:ILE:HD12	5:B:555:ILE:H	1.70	0.57
4:A:1070:GLN:HE22	5:B:1137:CYS:HA	1.69	0.57
4:A:1267:MET:HA	4:A:1271:ILE:HG12	1.85	0.57
7:E:96:PHE:O	7:E:100:ILE:HG12	2.05	0.57
4:A:185:TRP:HB3	4:A:199:LEU:HG	1.86	0.57
4:A:1335:ILE:HG23	4:A:1339:LEU:HD12	1.86	0.57
6:C:66:ARG:HE	11:J:5:VAL:HG13	1.70	0.57
7:E:86:PRO:HA	7:E:113:GLN:HE22	1.68	0.57
10:I:92:ARG:HD3	10:I:94:ASP:H	1.69	0.57
4:A:1445:ILE:HA	8:F:132:LEU:HA	1.86	0.57
6:C:209:TYR:HD2	6:C:229:TYR:HE2	1.53	0.57
6:C:240:VAL:O	6:C:243:VAL:HG22	2.05	0.57
4:A:781:ASP:HB2	4:A:789:LYS:HG2	1.86	0.56
5:B:308:TRP:HH2	10:I:47:GLU:HG3	1.70	0.56
5:B:364:ILE:HD13	5:B:585:VAL:HG13	1.86	0.56
4:A:13:THR:HG23	4:A:15:LYS:NZ	2.21	0.56
4:A:840:ARG:HB3	4:A:1384:VAL:HG12	1.88	0.56
4:A:1267:MET:HA	4:A:1271:ILE:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:164:LYS:H	5:B:164:LYS:HD3	1.70	0.56
4:A:672:ASP:H	4:A:736:ASN:HD21	1.54	0.56
4:A:1100:ARG:O	4:A:1104:ILE:HG13	2.05	0.56
4:A:1220:PHE:CE1	4:A:1224:LEU:CD2	2.89	0.56
4:A:671:ALA:HB3	4:A:676:MET:HE2	1.88	0.56
4:A:1118:VAL:HA	4:A:1327:ILE:HG13	1.87	0.56
5:B:44:VAL:HG11	5:B:495:LEU:HD13	1.87	0.56
1:R:1:A:P	5:B:1112:GLN:HE21	2.28	0.56
5:B:33:VAL:HG21	5:B:638:PHE:HZ	1.70	0.56
5:B:857:ARG:NH2	5:B:942:ARG:HD2	2.16	0.56
5:B:911:ILE:HG13	5:B:912:ILE:HD12	1.88	0.56
13:L:33:GLU:HB2	13:L:51:CYS:SG	2.46	0.56
4:A:497:THR:HG23	5:B:1146:PHE:HB2	1.88	0.56
4:A:837:ILE:O	4:A:841:LEU:HG	2.05	0.56
6:C:107:SER:OG	6:C:111:THR:OG1	2.24	0.56
4:A:472:LEU:HD12	4:A:650:GLN:HE21	1.70	0.56
4:A:1345:ARG:HG3	4:A:1372:VAL:HG12	1.88	0.56
4:A:370:ILE:HG22	4:A:374:LEU:HD12	1.88	0.55
10:I:75:CYS:HB2	10:I:110:PHE:CD1	2.41	0.55
5:B:995:ARG:HB3	5:B:997:GLU:OE1	2.07	0.55
6:C:82:TYR:HD1	6:C:161:LYS:HB3	1.71	0.55
2:T:20:DC:H2"	2:T:21:DC:C6	2.42	0.55
4:A:1206:ASP:O	4:A:1274:ARG:NH2	2.36	0.55
5:B:414:ALA:O	5:B:418:LYS:HG3	2.07	0.55
5:B:451:LYS:O	5:B:455:SER:N	2.34	0.55
9:H:14:GLU:HG3	9:H:27:GLU:HB3	1.87	0.55
6:C:254:LYS:HD3	12:K:42:LEU:HD21	1.89	0.55
9:H:105:GLU:HG2	9:H:113:ALA:HB3	1.89	0.55
4:A:84:ILE:HG22	4:A:239:LEU:HB3	1.88	0.55
4:A:91:PHE:N	4:A:297:GLN:OE1	2.36	0.55
4:A:344:ARG:NH1	5:B:1129:ARG:HB2	2.19	0.55
7:E:101:GLN:HB2	7:E:127:ILE:HD13	1.86	0.55
8:F:133:VAL:HG23	8:F:147:SER:HA	1.89	0.55
4:A:302:THR:HA	4:A:305:ASP:O	2.07	0.55
4:A:1215:ARG:HD2	4:A:1273:LEU:HA	1.87	0.55
5:B:1204:PHE:O	5:B:1208:MET:HG3	2.06	0.55
7:E:20:LYS:NZ	7:E:34:GLU:O	2.35	0.55
13:L:28:LYS:HG3	13:L:39:SER:O	2.06	0.55
4:A:172:PRO:HB2	4:A:183:GLY:HA3	1.89	0.55
4:A:528:LEU:O	4:A:531:ILE:HG22	2.07	0.55
5:B:121:ASN:HA	5:B:207:GLY:HA3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:301:ILE:HG21	5:B:314:LEU:HD21	1.88	0.55
10:I:14:LEU:HD22	10:I:27:PHE:HB3	1.89	0.55
7:E:116:ILE:HG22	7:E:117:THR:H	1.71	0.55
3:N:8:DG:H5''	4:A:175:ARG:HH12	1.71	0.55
4:A:269:ILE:HD13	4:A:299:HIS:HB3	1.88	0.55
4:A:383:TYR:HB3	8:F:115:THR:HB	1.89	0.55
4:A:1274:ARG:HD2	4:A:1274:ARG:O	2.07	0.55
5:B:880:THR:O	5:B:932:HIS:ND1	2.40	0.55
10:I:106:CYS:SG	10:I:108:HIS:HB2	2.47	0.55
4:A:949:ASP:OD1	4:A:949:ASP:N	2.40	0.54
5:B:635:ARG:NH1	5:B:742:GLU:OE2	2.33	0.54
5:B:656:GLY:O	5:B:660:LYS:HG3	2.07	0.54
4:A:122:MET:HE1	4:A:138:ILE:HA	1.90	0.54
4:A:548:ASN:OD1	12:K:47:ARG:NE	2.40	0.54
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.43	0.54
5:B:830:TYR:OH	5:B:1074:ASN:OD1	2.24	0.54
12:K:21:ILE:HG12	12:K:33:ILE:HG12	1.89	0.54
4:A:897:TYR:OH	4:A:1030:ARG:NH1	2.41	0.54
5:B:115:GLN:O	5:B:119:LEU:HG	2.07	0.54
5:B:780:VAL:HG23	5:B:817:LEU:HG	1.89	0.54
9:H:95:TYR:CE1	9:H:97:MET:HG3	2.38	0.54
4:A:42:ASP:OD1	4:A:42:ASP:N	2.38	0.54
5:B:1082:MET:HA	6:C:189:THR:HA	1.89	0.54
4:A:182:VAL:HG23	4:A:201:VAL:HA	1.88	0.54
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.89	0.54
5:B:487:THR:OG1	5:B:777:ALA:O	2.20	0.54
6:C:94:LYS:HA	6:C:127:ARG:HH22	1.73	0.54
4:A:547:LEU:HD22	12:K:58:PHE:CD2	2.43	0.54
5:B:175:ARG:HG2	5:B:200:GLY:HA3	1.89	0.54
5:B:754:SER:HB2	5:B:812:LEU:HD11	1.89	0.54
4:A:1161:THR:HG21	4:A:1166:ASP:HB2	1.88	0.54
3:N:15:DA:OP1	7:E:117:THR:OG1	2.25	0.54
4:A:650:GLN:O	4:A:654:ASN:ND2	2.41	0.54
4:A:789:LYS:HD2	10:I:67:THR:HB	1.90	0.54
4:A:836:TYR:OH	4:A:1403:GLU:OE1	2.25	0.54
5:B:1112:GLN:HE22	5:B:1114:LEU:HB3	1.72	0.54
3:N:8:DG:H2''	3:N:9:DA:C8	2.43	0.54
4:A:528:LEU:HD23	4:A:751:SER:HA	1.90	0.54
4:A:575:LYS:HB3	4:A:612:ILE:HD11	1.89	0.54
10:I:78:CYS:C	10:I:80:SER:H	2.14	0.54
1:R:4:G:H2'	1:R:5:A:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:714:PHE:O	4:A:718:VAL:HG23	2.08	0.53
4:A:1076:ALA:HA	4:A:1079:MET:HE3	1.90	0.53
5:B:757:PRO:HG3	5:B:983:ARG:NE	2.23	0.53
4:A:1205:LYS:HB2	4:A:1207:LEU:HG	1.89	0.53
4:A:1333:ILE:O	4:A:1337:GLU:HG3	2.08	0.53
5:B:48:LEU:HA	5:B:173:MET:HE1	1.90	0.53
5:B:658:ILE:HA	5:B:661:LEU:HD12	1.91	0.53
6:C:39:ALA:HB1	6:C:165:LYS:HG2	1.89	0.53
4:A:350:ARG:NH1	4:A:447:GLN:HG2	2.24	0.53
4:A:600:PRO:HA	9:H:25:ARG:NH1	2.23	0.53
4:A:1427:ASN:HB2	4:A:1434:ALA:HB2	1.91	0.53
4:A:451:HIS:HB3	4:A:453:MET:HE2	1.90	0.53
4:A:756:ILE:O	4:A:760:GLN:HG3	2.08	0.53
4:A:1116:LEU:HD22	4:A:1311:VAL:HG23	1.91	0.53
5:B:872:GLU:HB3	5:B:914:LYS:HD2	1.91	0.53
6:C:74:SER:HB2	6:C:238:ILE:HD11	1.88	0.53
4:A:543:LEU:HA	4:A:546:VAL:HG22	1.90	0.53
4:A:1220:PHE:CE1	4:A:1224:LEU:HD22	2.43	0.53
5:B:449:ASN:HD21	5:B:451:LYS:HB3	1.74	0.53
8:F:101:ILE:HB	8:F:117:PRO:HB3	1.91	0.53
9:H:102:TYR:CZ	9:H:115:TYR:HB3	2.43	0.53
12:K:30:ALA:HA	12:K:75:ILE:O	2.09	0.53
5:B:416:LEU:HD22	5:B:466:TRP:CZ3	2.44	0.53
7:E:86:PRO:HA	7:E:113:GLN:NE2	2.24	0.53
9:H:146:ARG:HD2	9:H:146:ARG:H	1.74	0.53
5:B:41:LYS:HB3	5:B:45:SER:HB3	1.90	0.53
5:B:728:ARG:HH12	5:B:760:ASP:HB2	1.74	0.53
5:B:955:THR:HB	13:L:55:ILE:HA	1.90	0.53
4:A:1213:GLY:HA2	4:A:1216:ILE:HD12	1.90	0.53
4:A:1263:ILE:O	4:A:1267:MET:HG3	2.09	0.53
4:A:820:GLY:O	4:A:824:LEU:HG	2.09	0.53
4:A:884:ASP:HB3	4:A:896:ARG:HH12	1.74	0.53
4:A:961:ARG:HD2	4:A:1025:ARG:HH12	1.74	0.52
5:B:1006:ILE:HG12	11:J:45:CYS:SG	2.49	0.52
12:K:57:LEU:N	12:K:76:GLN:O	2.42	0.52
13:L:46:VAL:O	13:L:54:ARG:HA	2.09	0.52
4:A:857:ARG:HD3	4:A:863:VAL:HG22	1.91	0.52
5:B:195:CYS:SG	5:B:783:THR:OG1	2.64	0.52
5:B:681:TRP:CH2	5:B:690:VAL:HG11	2.45	0.52
6:C:115:SER:HB3	6:C:142:VAL:HG12	1.92	0.52
7:E:179:GLN:HB2	7:E:182:ASP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:32:GLU:O	11:J:36:LEU:HG	2.09	0.52
4:A:1022:LEU:HD11	4:A:1049:ILE:HD13	1.90	0.52
5:B:733:HIS:CE1	5:B:738:PHE:CZ	2.98	0.52
4:A:1024:SER:OG	4:A:1025:ARG:HD2	2.10	0.52
4:A:727:ASP:O	4:A:731:ARG:HG2	2.09	0.52
4:A:883:LEU:H	4:A:952:ALA:HB1	1.74	0.52
5:B:637:LEU:HD21	5:B:742:GLU:HG2	1.90	0.52
6:C:162:GLY:HA3	6:C:170:TRP:CD2	2.45	0.52
4:A:361:LEU:HA	4:A:471:ASN:HB2	1.92	0.52
5:B:839:MET:O	5:B:991:GLY:N	2.35	0.52
4:A:30:ILE:HG23	5:B:1170:THR:HG23	1.91	0.52
4:A:181:LEU:HD12	4:A:202:LEU:HB2	1.93	0.52
4:A:286:HIS:CG	4:A:287:HIS:N	2.77	0.51
4:A:882:SER:H	4:A:961:ARG:NH2	2.07	0.51
5:B:215:GLN:HE22	5:B:479:VAL:HG13	1.75	0.51
7:E:13:TRP:HB2	7:E:42:PHE:CD2	2.46	0.51
9:H:104:PHE:HE1	9:H:114:VAL:HG13	1.74	0.51
4:A:598:LEU:O	9:H:122:LEU:HD12	2.10	0.51
5:B:398:ARG:O	5:B:404:LYS:NZ	2.28	0.51
4:A:357:PRO:HG3	5:B:831:SER:O	2.10	0.51
4:A:679:ILE:O	4:A:683:ILE:HG12	2.10	0.51
4:A:932:GLU:O	4:A:936:LEU:HG	2.10	0.51
5:B:422:LYS:O	5:B:426:LYS:HG3	2.10	0.51
4:A:457:ALA:O	4:A:507:VAL:HG23	2.10	0.51
4:A:518:LYS:HE2	4:A:624:SER:O	2.10	0.51
4:A:569:LYS:NZ	6:C:221:TYR:O	2.42	0.51
4:A:942:PHE:HD1	4:A:943:LEU:HD23	1.75	0.51
10:I:32:CYS:SG	10:I:34:TYR:HB3	2.51	0.51
11:J:21:TYR:CZ	11:J:25:LEU:HD11	2.45	0.51
12:K:99:GLY:HA2	12:K:102:LYS:HD2	1.91	0.51
4:A:666:ILE:HG22	5:B:1026:LEU:HB3	1.91	0.51
12:K:99:GLY:O	12:K:102:LYS:HG2	2.10	0.51
4:A:336:ILE:O	4:A:341:MET:HG2	2.10	0.51
4:A:550:LEU:HD21	4:A:561:PRO:HD2	1.91	0.51
4:A:744:LYS:O	4:A:748:MET:HG3	2.11	0.51
4:A:1220:PHE:CZ	4:A:1224:LEU:HD22	2.46	0.51
4:A:353:ILE:HG21	4:A:487:MET:HB2	1.91	0.51
4:A:541:ILE:HG22	4:A:545:GLN:HB2	1.93	0.51
4:A:1134:ILE:O	4:A:1138:ILE:HG22	2.10	0.51
4:A:1436:ILE:HG22	5:B:1142:GLY:HA2	1.93	0.51
5:B:173:MET:HB2	5:B:203:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:400:PRO:HB3	4:A:437:MET:SD	2.50	0.51
4:A:550:LEU:HD11	4:A:577:ILE:HD12	1.92	0.51
5:B:213:ILE:HG21	5:B:499:ASN:HB2	1.92	0.51
9:H:103:LYS:O	9:H:115:TYR:HB2	2.10	0.51
4:A:82:GLY:HA3	4:A:241:VAL:HG22	1.93	0.51
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.93	0.51
4:A:631:HIS:CE1	4:A:879:GLU:HG2	2.46	0.51
4:A:1063:MET:HE2	4:A:1436:ILE:HG23	1.91	0.51
5:B:1051:THR:HG23	5:B:1054:GLY:H	1.74	0.51
6:C:108:GLU:HG2	6:C:149:LYS:HD2	1.93	0.51
5:B:826:ALA:HB3	5:B:1011:ILE:HD13	1.93	0.51
11:J:13:VAL:O	11:J:17:LYS:NZ	2.28	0.51
12:K:99:GLY:O	12:K:103:THR:HG23	2.11	0.51
2:T:14:DG:H2"	2:T:15:DC:C5	2.45	0.50
4:A:538:ASP:OD1	9:H:22:LYS:HB2	2.12	0.50
4:A:546:VAL:HG11	4:A:572:TRP:HB2	1.91	0.50
4:A:619:LYS:O	4:A:623:GLY:N	2.44	0.50
5:B:803:LEU:HD13	5:B:1032:SER:HB3	1.92	0.50
5:B:997:GLU:HG2	6:C:39:ALA:HB2	1.93	0.50
2:T:6:DT:H2"	2:T:7:DC:C5	2.46	0.50
4:A:1341:ILE:HG13	4:A:1376:THR:HG23	1.94	0.50
5:B:230:ALA:O	5:B:261:ARG:NH2	2.44	0.50
9:H:81:PRO:HB2	9:H:83:GLN:HG3	1.93	0.50
13:L:68:GLU:O	13:L:70:ARG:NH1	2.45	0.50
4:A:414:ASP:O	4:A:418:SER:HB2	2.11	0.50
4:A:1390:ASN:HD21	4:A:1402:PHE:HB3	1.76	0.50
5:B:60:GLN:OE1	5:B:94:LYS:HA	2.11	0.50
5:B:212:LEU:HD23	5:B:466:TRP:HZ2	1.75	0.50
5:B:1206:GLU:O	5:B:1210:MET:HG2	2.11	0.50
4:A:434:ARG:HH12	4:A:437:MET:HE3	1.76	0.50
6:C:35:ARG:NE	12:K:41:THR:OG1	2.39	0.50
7:E:151:PRO:HD2	7:E:153:HIS:CE1	2.46	0.50
10:I:71:SER:HB3	10:I:85:PHE:CD1	2.46	0.50
4:A:19:PHE:O	4:A:1416:ALA:HA	2.12	0.50
5:B:125:SER:HB2	5:B:169:ARG:HB3	1.93	0.50
5:B:843:GLN:N	5:B:994:TYR:O	2.27	0.50
5:B:856:PHE:CE1	5:B:969:ARG:HG3	2.47	0.50
9:H:91:ASP:HB3	9:H:143:LEU:HD23	1.92	0.50
10:I:98:VAL:HG11	10:I:113:ASP:HB2	1.93	0.50
13:L:40:LEU:HB2	13:L:44:ASP:OD2	2.10	0.50
4:A:907:THR:HG21	4:A:920:LEU:HG	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:316:PRO:HA	5:B:319:GLU:HG3	1.93	0.50
4:A:83:HIS:NE2	4:A:85:ASP:OD1	2.45	0.50
4:A:170:THR:HG1	4:A:185:TRP:CD1	2.29	0.50
12:K:61:TYR:HA	12:K:72:LYS:O	2.12	0.50
4:A:1130:GLN:O	4:A:1134:ILE:HG12	2.12	0.50
5:B:879:ARG:HA	5:B:885:MET:HE2	1.93	0.50
4:A:471:ASN:OD1	4:A:650:GLN:NE2	2.36	0.50
4:A:579:SER:HA	4:A:582:ILE:HG13	1.93	0.50
4:A:1095:THR:OG1	4:A:1100:ARG:NH2	2.44	0.50
5:B:104:GLU:OE1	13:L:47:ARG:NH2	2.45	0.50
5:B:129:PHE:HA	5:B:166:PHE:HA	1.93	0.50
5:B:383:ASN:O	5:B:387:LEU:HG	2.11	0.50
6:C:88:CYS:SG	6:C:92:CYS:N	2.85	0.50
9:H:8:ASP:HB3	9:H:10:PHE:CE1	2.46	0.50
4:A:402:ALA:O	4:A:415:LEU:HD12	2.11	0.49
4:A:729:ALA:HB1	4:A:763:ALA:HB1	1.94	0.49
4:A:1332:PHE:CE1	4:A:1351:GLU:HB2	2.46	0.49
4:A:1390:ASN:HA	4:A:1399:ARG:HG2	1.94	0.49
5:B:992:ILE:HG12	5:B:994:TYR:CE1	2.46	0.49
5:B:1135:ARG:HG3	5:B:1136:ASP:N	2.27	0.49
2:T:16:DT:H2'	2:T:17:DG:C8	2.47	0.49
9:H:25:ARG:HH21	9:H:122:LEU:HB2	1.76	0.49
5:B:273:LEU:HD12	5:B:276:ILE:HD13	1.94	0.49
4:A:531:ILE:O	4:A:535:THR:OG1	2.24	0.49
4:A:841:LEU:HD23	4:A:1384:VAL:HG11	1.94	0.49
4:A:986:ILE:O	4:A:990:VAL:HG23	2.12	0.49
5:B:424:LEU:O	5:B:428:ILE:HG13	2.11	0.49
4:A:826:ASP:O	4:A:830:LYS:HG2	2.11	0.49
5:B:60:GLN:NE2	5:B:64:CYS:SG	2.86	0.49
6:C:10:ILE:HA	6:C:20:PHE:HA	1.95	0.49
9:H:112:ILE:HG22	9:H:127:GLY:O	2.12	0.49
5:B:215:GLN:NE2	5:B:479:VAL:HG22	2.27	0.49
5:B:657:HIS:HA	5:B:660:LYS:HD3	1.94	0.49
9:H:124:ARG:NH1	9:H:126:GLU:HB2	2.28	0.49
8:F:135:ARG:NH2	8:F:145:ASP:OD2	2.46	0.49
9:H:136:LYS:HG3	9:H:136:LYS:O	2.12	0.49
10:I:83:ASN:OD1	10:I:101:PHE:HB3	2.13	0.49
4:A:26:GLU:O	4:A:30:ILE:HG12	2.12	0.49
4:A:777:PHE:HA	4:A:783:THR:HA	1.94	0.49
4:A:848:ILE:HG21	4:A:1370:LEU:HD11	1.95	0.49
4:A:903:ASN:HB3	4:A:906:HIS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:62:PHE:CE1	6:C:66:ARG:HD2	2.48	0.49
7:E:96:PHE:CZ	7:E:110:PHE:HB2	2.48	0.49
4:A:112:LYS:HZ1	4:A:167:CYS:H	1.61	0.49
4:A:541:ILE:HD11	4:A:574:GLY:HA2	1.95	0.49
5:B:104:GLU:CD	5:B:120:ARG:HH22	2.21	0.49
5:B:226:PHE:CZ	5:B:398:ARG:HG3	2.48	0.49
10:I:68:LEU:O	10:I:70:ARG:NH2	2.45	0.49
4:A:96:ILE:HA	4:A:99:ILE:HB	1.95	0.49
4:A:340:LEU:HD12	4:A:1429:ILE:HA	1.94	0.49
4:A:542:GLU:O	4:A:546:VAL:HG13	2.12	0.49
5:B:199:MET:SD	5:B:199:MET:N	2.80	0.49
5:B:603:LEU:HB2	5:B:609:ILE:HD12	1.94	0.49
7:E:161:LYS:HG3	7:E:195:VAL:HG21	1.95	0.49
12:K:47:ARG:HG2	12:K:47:ARG:NH1	2.25	0.49
4:A:1095:THR:OG1	4:A:1100:ARG:HD3	2.13	0.48
5:B:35:SER:O	5:B:39:ARG:HG3	2.13	0.48
5:B:574:SER:HA	5:B:591:ARG:HH21	1.77	0.48
5:B:1025:HIS:CE1	5:B:1090:THR:HG21	2.48	0.48
9:H:59:ILE:HA	9:H:141:TYR:O	2.13	0.48
4:A:792:TYR:HA	4:A:797:LYS:HD3	1.95	0.48
4:A:992:ASP:HA	4:A:995:GLU:OE2	2.13	0.48
4:A:1130:GLN:HA	4:A:1133:LEU:HD12	1.95	0.48
4:A:1282:VAL:HG22	4:A:1308:THR:HG22	1.95	0.48
4:A:1419:ASP:OD1	4:A:1426:GLU:HG2	2.12	0.48
6:C:143:LEU:HD21	6:C:146:LYS:HZ3	1.78	0.48
8:F:114:GLU:HB2	8:F:120:ILE:HD11	1.95	0.48
4:A:471:ASN:O	4:A:474:VAL:HG12	2.12	0.48
4:A:711:ARG:HH11	10:I:95:THR:HB	1.78	0.48
5:B:48:LEU:O	5:B:52:ASN:ND2	2.46	0.48
5:B:827:ILE:HG12	5:B:1012:ILE:HD11	1.96	0.48
5:B:950:ASP:HB3	5:B:967:ARG:HG2	1.95	0.48
9:H:115:TYR:HE1	9:H:124:ARG:HG3	1.75	0.48
10:I:77:LYS:HB3	10:I:106:CYS:SG	2.53	0.48
4:A:25:GLU:CD	4:A:25:GLU:H	2.21	0.48
4:A:457:ALA:HB2	4:A:501:LEU:HD12	1.94	0.48
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.13	0.48
4:A:1213:GLY:HA3	4:A:1228:TRP:CZ3	2.47	0.48
7:E:99:HIS:CE1	7:E:103:LYS:HG3	2.49	0.48
4:A:122:MET:O	4:A:126:LEU:HG	2.12	0.48
4:A:1303:GLU:CD	4:A:1326:ARG:HH12	2.21	0.48
5:B:276:ILE:HG12	5:B:334:ILE:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:544:CYS:HB2	5:B:634:TYR:CZ	2.48	0.48
5:B:488:TYR:O	5:B:492:LEU:HD12	2.13	0.48
4:A:350:ARG:NH1	4:A:488:ASN:OD1	2.36	0.48
4:A:587:HIS:HA	4:A:607:ILE:O	2.14	0.48
4:A:675:THR:O	4:A:679:ILE:HG12	2.13	0.48
5:B:23:ALA:HB3	5:B:655:LYS:HG3	1.94	0.48
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.96	0.48
5:B:493:SER:OG	5:B:526:GLU:OE2	2.26	0.48
5:B:899:ILE:HD11	5:B:903:VAL:HG11	1.96	0.48
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.95	0.48
12:K:100:ALA:O	12:K:104:ASN:ND2	2.47	0.48
4:A:1153:TYR:HD2	10:I:41:PRO:HB2	1.78	0.48
4:A:1338:VAL:HG12	4:A:1339:LEU:HG	1.95	0.48
5:B:129:PHE:CE2	5:B:166:PHE:HB2	2.49	0.48
6:C:57:VAL:HG11	11:J:60:PHE:HB3	1.94	0.48
4:A:1370:LEU:O	4:A:1374:VAL:HG23	2.14	0.48
5:B:380:TYR:O	5:B:384:ARG:HG2	2.14	0.48
5:B:877:PRO:HB2	5:B:882:THR:OG1	2.12	0.48
3:N:12:DG:H1'	3:N:13:DA:C8	2.49	0.48
4:A:368:LYS:HB2	4:A:368:LYS:HE3	1.74	0.48
4:A:630:ILE:HG23	4:A:642:CYS:SG	2.53	0.48
4:A:960:ILE:HG22	4:A:964:ILE:HD13	1.95	0.48
5:B:273:LEU:HB3	5:B:276:ILE:HB	1.95	0.48
13:L:28:LYS:HB2	13:L:29:TYR:CD2	2.49	0.48
4:A:1368:MET:O	4:A:1372:VAL:HG23	2.13	0.47
4:A:1387:HIS:HA	4:A:1391:ARG:HE	1.79	0.47
6:C:32:SER:HA	12:K:41:THR:HG23	1.95	0.47
5:B:232:SER:H	5:B:261:ARG:HH21	1.61	0.47
5:B:980:PHE:CE1	5:B:990:ILE:HD11	2.49	0.47
1:R:9:G:O2'	4:A:446:ARG:NH2	2.47	0.47
4:A:848:ILE:HB	4:A:1065:GLY:HA3	1.97	0.47
4:A:1148:ILE:HD11	4:A:1198:ASP:HA	1.95	0.47
5:B:769:TYR:O	5:B:773:MET:HG3	2.15	0.47
1:R:1:A:H2'	1:R:2:U:C6	2.49	0.47
4:A:82:GLY:CA	4:A:241:VAL:HG22	2.44	0.47
4:A:1166:ASP:O	4:A:1170:ILE:HG12	2.14	0.47
4:A:1316:VAL:O	4:A:1319:VAL:HG12	2.14	0.47
8:F:89:GLU:O	8:F:93:ILE:HG12	2.14	0.47
4:A:89:PRO:HB2	4:A:204:THR:HG22	1.96	0.47
4:A:93:VAL:HG13	4:A:301:ALA:HB1	1.95	0.47
4:A:351:THR:HG22	5:B:1103:ILE:HG23	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:618:GLU:OE1	4:A:620:LYS:N	2.45	0.47
4:A:1325:THR:HA	7:E:147:HIS:HA	1.95	0.47
5:B:824:ILE:HG22	5:B:1008:PRO:HA	1.95	0.47
6:C:57:VAL:HG21	11:J:60:PHE:HB3	1.97	0.47
7:E:143:ASN:ND2	7:E:187:TYR:OH	2.41	0.47
1:R:2:U:H2'	1:R:3:C:C6	2.50	0.47
4:A:1111:MET:HE2	4:A:1331:SER:HA	1.96	0.47
10:I:85:PHE:HB3	10:I:101:PHE:CD2	2.50	0.47
2:T:11:DC:H2''	2:T:12:DT:H72	1.96	0.47
4:A:19:PHE:HA	5:B:1213:THR:O	2.15	0.47
4:A:23:SER:HB2	4:A:233:TRP:CZ2	2.50	0.47
4:A:80:HIS:CE1	5:B:1172:ILE:HG22	2.49	0.47
4:A:271:LYS:O	4:A:274:ILE:HG22	2.15	0.47
4:A:361:LEU:HD12	4:A:473:SER:HB2	1.96	0.47
4:A:483:ASP:O	5:B:989:THR:HG23	2.15	0.47
4:A:496:GLU:O	4:A:500:GLU:HG3	2.14	0.47
4:A:1165:GLU:OE1	4:A:1235:LYS:HD2	2.14	0.47
5:B:863:GLU:HG2	5:B:874:PHE:CE2	2.49	0.47
5:B:1030:LEU:O	5:B:1034:VAL:HG23	2.14	0.47
6:C:59:ALA:O	6:C:63:ILE:HG13	2.15	0.47
6:C:83:SER:OG	6:C:160:LYS:HB3	2.15	0.47
7:E:15:ALA:HA	7:E:140:LEU:O	2.15	0.47
10:I:75:CYS:HB3	10:I:78:CYS:SG	2.54	0.47
12:K:21:ILE:HG23	12:K:31:VAL:HG21	1.96	0.47
12:K:42:LEU:O	12:K:46:ILE:HG13	2.14	0.47
12:K:58:PHE:O	12:K:75:ILE:HA	2.15	0.47
5:B:833:TYR:O	5:B:838:SER:OG	2.33	0.47
2:T:20:DC:H2''	2:T:21:DC:H6	1.80	0.47
4:A:70:CYS:SG	4:A:80:HIS:NE2	2.75	0.47
4:A:364:VAL:HG12	4:A:459:ARG:O	2.15	0.47
4:A:434:ARG:NH1	4:A:437:MET:HE3	2.30	0.47
4:A:754:SER:N	4:A:757:ASN:OD1	2.48	0.47
5:B:905:VAL:HG12	5:B:941:LEU:HD22	1.96	0.47
6:C:112:ASN:HB3	6:C:143:LEU:HD13	1.95	0.47
6:C:250:THR:O	6:C:254:LYS:HG3	2.15	0.47
12:K:7:PHE:HA	12:K:10:PHE:CE1	2.49	0.47
4:A:243:PRO:HG2	5:B:1205:GLN:NE2	2.30	0.47
4:A:337:ARG:NH2	4:A:839:ARG:HE	2.12	0.47
4:A:1325:THR:HG22	7:E:148:GLU:HG3	1.97	0.47
5:B:604:ARG:HH11	5:B:691:GLU:HG2	1.79	0.47
5:B:697:GLU:O	5:B:701:ILE:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:850:LEU:HB2	11:J:8:PHE:CD2	2.50	0.47
4:A:798:GLY:HA2	4:A:815:PHE:CD2	2.50	0.46
4:A:1095:THR:HG23	4:A:1113:THR:HB	1.97	0.46
5:B:556:THR:O	5:B:560:GLU:HG2	2.15	0.46
5:B:637:LEU:HD13	5:B:693:ILE:HD12	1.96	0.46
5:B:864:LYS:H	5:B:872:GLU:HB2	1.80	0.46
5:B:1219:ASP:OD1	5:B:1219:ASP:N	2.45	0.46
5:B:170:LEU:HD12	5:B:171:PRO:HD2	1.97	0.46
5:B:900:ALA:HB3	13:L:61:THR:OG1	2.15	0.46
4:A:742:ASN:O	4:A:746:MET:HE3	2.15	0.46
4:A:882:SER:O	4:A:1025:ARG:NH2	2.49	0.46
4:A:1001:ARG:NH2	8:F:82:THR:OG1	2.49	0.46
6:C:7:GLN:N	6:C:7:GLN:OE1	2.48	0.46
10:I:17:ARG:O	10:I:25:LEU:HD12	2.16	0.46
12:K:49:GLU:HG3	12:K:94:ILE:HG13	1.97	0.46
4:A:13:THR:O	4:A:15:LYS:NZ	2.32	0.46
4:A:112:LYS:NZ	4:A:148:CYS:SG	2.69	0.46
4:A:200:ARG:NH2	4:A:203:SER:H	2.13	0.46
4:A:354:SER:O	4:A:469:ARG:HA	2.16	0.46
4:A:387:ARG:O	4:A:391:LEU:HG	2.16	0.46
4:A:565:ILE:HG21	9:H:46:LEU:HD13	1.97	0.46
4:A:722:LEU:HD13	4:A:799:PHE:HB2	1.96	0.46
4:A:775:ILE:HG13	4:A:798:GLY:HA3	1.97	0.46
4:A:1396:ALA:HA	4:A:1399:ARG:HE	1.81	0.46
5:B:351:TYR:CZ	5:B:355:ILE:HD11	2.50	0.46
5:B:597:MET:SD	5:B:624:LEU:HD11	2.55	0.46
5:B:745:PRO:HB2	5:B:1047:PHE:CD2	2.51	0.46
5:B:1084:GLN:NE2	6:C:189:THR:OG1	2.48	0.46
6:C:248:ILE:HG23	12:K:98:LEU:HB3	1.98	0.46
11:J:1:MET:HE2	11:J:60:PHE:CE2	2.51	0.46
4:A:42:ASP:HA	4:A:50:ILE:HB	1.97	0.46
4:A:592:ASP:N	4:A:592:ASP:OD1	2.48	0.46
4:A:825:ILE:HD12	5:B:512:ARG:HB3	1.95	0.46
4:A:1157:ASP:HB3	4:A:1160:SER:O	2.16	0.46
5:B:24:PRO:HB3	5:B:650:GLU:CD	2.40	0.46
5:B:750:GLY:O	5:B:754:SER:OG	2.28	0.46
5:B:876:LYS:NZ	5:B:890:TYR:O	2.48	0.46
10:I:44:TYR:CZ	10:I:46:HIS:HB2	2.51	0.46
4:A:443:LEU:HD12	4:A:501:LEU:HD11	1.96	0.46
4:A:447:GLN:OE1	4:A:447:GLN:HA	2.15	0.46
4:A:738:LYS:HB2	4:A:740:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.48	0.46
10:I:62:ILE:HG23	10:I:68:LEU:CD1	2.46	0.46
10:I:73:ARG:HH12	10:I:112:SER:HA	1.80	0.46
4:A:570:PRO:HB2	4:A:572:TRP:CZ3	2.51	0.46
4:A:1129:GLU:O	4:A:1133:LEU:HG	2.16	0.46
5:B:706:GLN:HG2	5:B:708:GLU:OE2	2.15	0.46
5:B:850:LEU:HB2	11:J:8:PHE:CG	2.50	0.46
10:I:78:CYS:HB3	10:I:106:CYS:HB2	1.70	0.46
4:A:632:VAL:O	4:A:636:GLU:HG3	2.16	0.46
4:A:733:ALA:O	4:A:737:LEU:HG	2.16	0.46
4:A:866:PHE:N	7:E:208:TYR:OH	2.42	0.46
5:B:186:GLU:HA	5:B:189:LEU:HD12	1.97	0.46
7:E:106:GLN:HA	7:E:130:ALA:HA	1.98	0.46
9:H:130:ARG:CD	9:H:133:ASN:HB3	2.45	0.46
4:A:219:PHE:HB2	4:A:231:PRO:HG2	1.97	0.46
5:B:352:ALA:HA	5:B:355:ILE:HD12	1.98	0.46
5:B:886:LYS:HE2	5:B:938:SER:HB2	1.97	0.46
5:B:953:LEU:HA	13:L:56:LEU:O	2.16	0.46
5:B:1106:ARG:NH2	5:B:1110:PRO:O	2.40	0.46
6:C:36:VAL:HG21	6:C:251:LEU:HD13	1.97	0.46
6:C:239:PRO:O	6:C:243:VAL:HG13	2.16	0.46
7:E:48:ASP:OD1	7:E:52:ARG:N	2.49	0.46
2:T:21:DC:H2'	2:T:22:DT:C6	2.51	0.46
4:A:114:LEU:HD22	4:A:114:LEU:H	1.81	0.46
4:A:1220:PHE:HE1	4:A:1224:LEU:HD23	1.81	0.46
4:A:113:LEU:HD23	4:A:218:ASP:HA	1.98	0.45
4:A:262:LEU:O	4:A:266:LEU:HG	2.16	0.45
4:A:482:PHE:CD2	5:B:836:GLU:HB2	2.51	0.45
4:A:1224:LEU:HD12	4:A:1241:ARG:C	2.41	0.45
5:B:639:ILE:HD13	5:B:740:HIS:CD2	2.51	0.45
5:B:773:MET:SD	5:B:987:LYS:HG2	2.56	0.45
6:C:69:LEU:HD12	11:J:6:ARG:HG3	1.99	0.45
9:H:111:LEU:HA	9:H:128:ASN:HB3	1.97	0.45
4:A:868:TYR:CD2	4:A:1058:VAL:HG11	2.50	0.45
5:B:118:ARG:HA	5:B:207:GLY:HA2	1.99	0.45
5:B:1033:LYS:O	5:B:1037:LEU:HG	2.15	0.45
5:B:1106:ARG:HD3	5:B:1127:GLY:CA	2.46	0.45
8:F:85:MET:HE2	8:F:90:ARG:HA	1.97	0.45
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.98	0.45
4:A:151:ASP:OD1	4:A:161:LEU:N	2.49	0.45
4:A:941:LYS:HG3	4:A:942:PHE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:954:TRP:CZ3	7:E:203:GLU:HG3	2.52	0.45
4:A:1144:LYS:HD2	4:A:1269:GLU:OE1	2.17	0.45
8:F:96:THR:O	8:F:100:GLN:HG3	2.16	0.45
12:K:60:ALA:O	12:K:73:LEU:HA	2.16	0.45
4:A:71:GLN:HE22	5:B:1177:HIS:CG	2.35	0.45
4:A:442:VAL:O	4:A:457:ALA:HA	2.17	0.45
4:A:809:THR:HG22	5:B:730:ARG:NH1	2.26	0.45
4:A:825:ILE:HD13	5:B:533:CYS:HB3	1.97	0.45
4:A:898:ARG:HB2	4:A:933:TYR:CE1	2.51	0.45
5:B:69:LEU:HB3	5:B:429:PHE:CD1	2.51	0.45
5:B:1073:TYR:CE2	5:B:1080:LYS:HG3	2.52	0.45
7:E:127:ILE:C	7:E:129:PRO:HD2	2.42	0.45
4:A:757:ASN:HD22	5:B:1021:MET:HE2	1.81	0.45
5:B:1175:LEU:HA	5:B:1180:PHE:HE1	1.81	0.45
5:B:1215:ARG:HH21	5:B:1215:ARG:HG3	1.82	0.45
7:E:20:LYS:HB3	7:E:35:VAL:HG22	1.98	0.45
9:H:47:PHE:HB3	9:H:95:TYR:HD2	1.82	0.45
4:A:211:PHE:HA	4:A:214:ILE:HG12	1.99	0.45
4:A:335:ARG:HA	4:A:339:ASN:HB2	1.98	0.45
4:A:375:THR:OG1	4:A:433:GLU:HB3	2.17	0.45
4:A:406:ILE:CD1	4:A:412:ARG:HH11	2.29	0.45
4:A:666:ILE:CG2	5:B:1026:LEU:HB3	2.47	0.45
5:B:365:THR:HG21	5:B:370:PHE:CB	2.42	0.45
5:B:496:ARG:HH12	5:B:540:SER:C	2.24	0.45
6:C:136:ASP:OD1	6:C:137:LYS:N	2.50	0.45
13:L:51:CYS:SG	13:L:53:HIS:HB2	2.56	0.45
4:A:531:ILE:HD12	4:A:653:VAL:HG21	1.99	0.45
4:A:830:LYS:O	4:A:834:THR:OG1	2.26	0.45
4:A:1332:PHE:HE1	4:A:1351:GLU:HB2	1.80	0.45
5:B:234:ILE:HD12	5:B:257:LYS:HB3	1.97	0.45
5:B:1055:ILE:HA	5:B:1058:LEU:HD12	1.99	0.45
11:J:14:VAL:HB	11:J:50:ILE:HD11	1.98	0.45
12:K:6:ARG:HB3	12:K:6:ARG:NH1	2.31	0.45
4:A:782:ARG:NH2	5:B:698:GLU:O	2.49	0.45
4:A:815:PHE:HA	4:A:818:MET:HG3	1.99	0.45
6:C:6:PRO:O	12:K:104:ASN:ND2	2.50	0.45
7:E:77:SER:HB2	7:E:105:PHE:HA	1.99	0.45
11:J:7:CYS:HB2	11:J:49:MET:HG3	1.99	0.45
4:A:100:LYS:O	4:A:104:GLU:N	2.48	0.45
4:A:482:PHE:N	5:B:836:GLU:O	2.50	0.45
4:A:555:ASP:OD1	4:A:555:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:583:PRO:HD3	4:A:645:LEU:HD13	1.98	0.45
4:A:65:LEU:HD12	4:A:65:LEU:H	1.82	0.45
4:A:545:GLN:O	4:A:549:MET:HG3	2.16	0.45
11:J:10:CYS:SG	11:J:43:ARG:NH2	2.90	0.45
4:A:17:VAL:HG23	4:A:1421:CYS:SG	2.57	0.44
4:A:42:ASP:OD2	4:A:46:THR:OG1	2.33	0.44
4:A:406:ILE:HG22	4:A:410:GLY:HA2	1.99	0.44
4:A:954:TRP:CE3	4:A:955:PRO:HD2	2.52	0.44
4:A:1148:ILE:N	4:A:1196:GLU:O	2.51	0.44
5:B:187:SER:O	5:B:191:LYS:HG3	2.17	0.44
5:B:944:THR:HG23	5:B:945:GLU:OE2	2.17	0.44
9:H:94:ASP:HB3	9:H:146:ARG:NE	2.32	0.44
10:I:26:LEU:HD13	10:I:35:VAL:HG11	1.98	0.44
4:A:91:PHE:CE1	4:A:204:THR:HG23	2.53	0.44
5:B:394:ASP:OD2	10:I:91:ARG:HG3	2.17	0.44
5:B:806:THR:HG23	5:B:1045:SER:HA	1.99	0.44
5:B:861:ASP:OD1	5:B:862:GLN:N	2.50	0.44
6:C:91:HIS:HB2	6:C:96:SER:OG	2.18	0.44
6:C:104:PHE:HD1	6:C:105:GLY:N	2.15	0.44
9:H:41:ASP:CG	9:H:122:LEU:H	2.24	0.44
4:A:353:ILE:HD12	4:A:470:LEU:HD21	1.99	0.44
4:A:395:GLY:O	4:A:401:GLY:HA3	2.17	0.44
4:A:412:ARG:O	4:A:413:ILE:HD13	2.18	0.44
5:B:261:ARG:HD3	5:B:261:ARG:HA	1.64	0.44
5:B:637:LEU:HD23	5:B:742:GLU:HA	1.99	0.44
5:B:651:LEU:HG	5:B:710:LEU:HD22	1.99	0.44
5:B:737:THR:O	10:I:66:PRO:HB3	2.18	0.44
6:C:34:ARG:HB2	6:C:176:ILE:CD1	2.47	0.44
8:F:147:SER:OG	8:F:150:GLU:HG3	2.18	0.44
4:A:71:GLN:O	4:A:71:GLN:HG2	2.18	0.44
4:A:901:LEU:N	4:A:926:GLN:OE1	2.50	0.44
4:A:1212:VAL:O	4:A:1216:ILE:HG13	2.17	0.44
5:B:612:GLU:HG2	5:B:632:ARG:NH1	2.33	0.44
6:C:36:VAL:HG22	6:C:40:GLU:HG3	1.99	0.44
7:E:93:MET:HE3	7:E:93:MET:HA	1.99	0.44
7:E:178:ILE:HG22	7:E:213:ILE:O	2.18	0.44
4:A:14:VAL:HG11	5:B:1216:LEU:HB3	2.00	0.44
4:A:86:LEU:C	4:A:88:LYS:H	2.25	0.44
4:A:442:VAL:HG12	4:A:491:VAL:HG22	1.99	0.44
4:A:483:ASP:OD1	4:A:484:GLY:N	2.47	0.44
8:F:93:ILE:HG23	8:F:132:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:124:ARG:HH12	9:H:126:GLU:HB2	1.82	0.44
4:A:12:ARG:HG3	5:B:1192:TYR:CD2	2.53	0.44
4:A:405:VAL:C	4:A:406:ILE:HD13	2.42	0.44
4:A:731:ARG:HG3	4:A:731:ARG:HH11	1.82	0.44
4:A:1220:PHE:CE1	4:A:1224:LEU:HB3	2.52	0.44
4:A:1333:ILE:HG13	4:A:1337:GLU:OE2	2.17	0.44
4:A:1407:GLU:HA	4:A:1410:PHE:HD1	1.83	0.44
5:B:639:ILE:HG22	5:B:652:LYS:HG3	1.99	0.44
11:J:2:ILE:HG13	11:J:3:VAL:N	2.33	0.44
4:A:954:TRP:HE3	4:A:955:PRO:HD2	1.83	0.44
4:A:1427:ASN:O	4:A:1431:GLY:N	2.51	0.44
5:B:428:ILE:O	5:B:432:MET:HG3	2.18	0.44
5:B:495:LEU:HD23	5:B:495:LEU:HA	1.73	0.44
5:B:642:ASP:OD1	5:B:649:LYS:HE3	2.17	0.44
5:B:759:PRO:HD2	5:B:1046:PRO:HG3	2.00	0.44
11:J:57:ILE:O	11:J:61:LEU:N	2.50	0.44
1:R:9:G:O2'	4:A:485:ASP:OD1	2.34	0.44
4:A:152:VAL:O	4:A:161:LEU:N	2.50	0.44
5:B:361:LEU:HD13	5:B:364:ILE:HG13	2.00	0.44
6:C:41:ILE:CG2	6:C:172:PRO:HG3	2.46	0.44
6:C:92:CYS:HB3	6:C:95:CYS:HB3	1.99	0.44
8:F:86:THR:O	8:F:89:GLU:HG2	2.18	0.44
4:A:886:ILE:HD12	4:A:943:LEU:HB3	2.00	0.44
4:A:1202:MET:HE2	4:A:1209:MET:HG2	1.99	0.44
4:A:1368:MET:HE3	4:A:1368:MET:HB2	1.86	0.44
5:B:288:ALA:HB1	5:B:331:LEU:HD23	2.00	0.44
5:B:1169:MET:H	5:B:1169:MET:HG2	1.63	0.44
6:C:234:SER:HB3	6:C:240:VAL:HG12	2.00	0.44
6:C:260:LEU:HG	6:C:264:GLN:NE2	2.33	0.44
10:I:106:CYS:HB3	10:I:108:HIS:H	1.82	0.44
11:J:21:TYR:O	11:J:25:LEU:HG	2.17	0.44
4:A:336:ILE:HD11	5:B:1203:LEU:HD22	1.99	0.43
4:A:1165:GLU:H	4:A:1165:GLU:HG3	1.62	0.43
4:A:1202:MET:HE3	4:A:1202:MET:HB3	1.80	0.43
5:B:1100:ASP:HA	5:B:1103:ILE:HG12	2.00	0.43
4:A:248:PRO:HG3	5:B:1114:LEU:HD22	1.99	0.43
4:A:337:ARG:HD2	4:A:839:ARG:NH2	2.31	0.43
4:A:392:VAL:HG12	4:A:424:ILE:HD13	2.00	0.43
4:A:513:SER:OG	4:A:515:GLN:O	2.23	0.43
4:A:672:ASP:H	4:A:736:ASN:ND2	2.16	0.43
5:B:878:GLN:CD	5:B:881:ASN:HB2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:18:VAL:HG23	6:C:240:VAL:HG21	2.00	0.43
12:K:18:LYS:HG3	12:K:19:LEU:HG	1.99	0.43
4:A:540:PHE:HE2	9:H:43:ASN:HD22	1.66	0.43
4:A:783:THR:O	5:B:516:ASN:ND2	2.52	0.43
4:A:834:THR:HG21	4:A:1077:THR:HG22	2.00	0.43
5:B:728:ARG:HD2	5:B:730:ARG:NH1	2.33	0.43
5:B:795:ILE:HG21	11:J:1:MET:HE3	1.99	0.43
5:B:796:LEU:HB2	5:B:799:PRO:HG3	2.00	0.43
5:B:982:SER:HB2	5:B:1092:TYR:CZ	2.53	0.43
6:C:6:PRO:CB	12:K:101:LEU:HD23	2.48	0.43
6:C:241:ASP:OD1	6:C:241:ASP:N	2.52	0.43
13:L:31:CYS:HB3	13:L:34:CYS:SG	2.58	0.43
4:A:821:ARG:NH1	4:A:821:ARG:HB2	2.33	0.43
4:A:965:GLN:HA	4:A:968:GLN:OE1	2.19	0.43
4:A:1192:LEU:HD12	4:A:1240:CYS:O	2.19	0.43
5:B:31:TRP:O	5:B:34:ILE:HB	2.19	0.43
5:B:122:LEU:HD11	5:B:958:GLN:HB3	2.00	0.43
5:B:424:LEU:HD11	5:B:449:ASN:O	2.17	0.43
5:B:683:SER:O	5:B:687:GLU:N	2.37	0.43
4:A:648:ASN:O	4:A:652:VAL:HG23	2.19	0.43
5:B:204:ILE:C	5:B:205:ILE:HD13	2.44	0.43
5:B:1196:ILE:HD11	5:B:1201:LYS:HB2	2.01	0.43
6:C:37:MET:HB3	6:C:37:MET:HE2	1.79	0.43
6:C:254:LYS:NZ	12:K:38:GLU:OE1	2.46	0.43
8:F:97:ARG:HE	8:F:124:GLU:CD	2.26	0.43
4:A:1151:GLU:HB3	4:A:1153:TYR:CE1	2.53	0.43
5:B:751:VAL:HG23	5:B:812:LEU:HD22	2.01	0.43
6:C:34:ARG:HD2	6:C:178:PHE:HE2	1.78	0.43
7:E:112:TYR:CB	7:E:116:ILE:HD11	2.47	0.43
10:I:6:PHE:HB3	10:I:12:ASN:O	2.18	0.43
11:J:2:ILE:HG13	11:J:3:VAL:H	1.83	0.43
2:T:11:DC:H2"	2:T:12:DT:C7	2.48	0.43
4:A:535:THR:HG21	4:A:617:VAL:H	1.84	0.43
4:A:633:VAL:HG12	4:A:642:CYS:HB2	1.99	0.43
4:A:851:HIS:ND1	8:F:139:PRO:HG3	2.33	0.43
5:B:558:LEU:HB3	5:B:563:MET:HE3	2.01	0.43
5:B:760:ASP:OD1	5:B:760:ASP:N	2.51	0.43
6:C:17:ASN:HA	6:C:232:VAL:O	2.18	0.43
6:C:80:LEU:CD2	6:C:161:LYS:HB2	2.49	0.43
4:A:60:SER:OG	4:A:64:ASN:O	2.35	0.43
4:A:75:ASN:HA	5:B:1116:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:272:ALA:O	4:A:276:LEU:HG	2.18	0.43
4:A:472:LEU:HD12	4:A:650:GLN:NE2	2.32	0.43
4:A:956:LEU:HD23	4:A:956:LEU:HA	1.90	0.43
4:A:993:LEU:O	4:A:997:LEU:HG	2.19	0.43
5:B:1024:ALA:HA	5:B:1027:ILE:HD12	2.00	0.43
6:C:65:HIS:HD2	6:C:69:LEU:HD23	1.84	0.43
6:C:66:ARG:HH21	11:J:5:VAL:HG13	1.83	0.43
7:E:178:ILE:HG22	7:E:214:CYS:HA	2.00	0.43
9:H:107:VAL:HG23	9:H:111:LEU:HB3	2.01	0.43
12:K:85:ASP:OD1	12:K:85:ASP:N	2.52	0.43
4:A:511:ILE:HA	4:A:521:MET:HE3	2.01	0.43
5:B:95:ILE:HD13	5:B:130:VAL:HG13	2.01	0.43
5:B:860:MET:SD	5:B:963:PHE:CZ	3.12	0.43
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.53	0.43
7:E:79:TRP:NE1	7:E:81:GLU:OE1	2.48	0.43
9:H:25:ARG:HH22	9:H:122:LEU:HB2	1.83	0.43
2:T:17:DG:H1'	4:A:1386:ARG:NH2	2.34	0.43
4:A:224:PHE:CG	4:A:231:PRO:HG3	2.54	0.43
4:A:302:THR:OG1	4:A:314:ALA:HB2	2.19	0.43
4:A:367:PRO:HB2	4:A:370:ILE:HG13	2.00	0.43
4:A:578:LEU:O	4:A:582:ILE:HG13	2.19	0.43
4:A:889:SER:HB2	4:A:1295:THR:HG22	1.99	0.43
4:A:1443:VAL:HG13	8:F:132:LEU:HD13	2.00	0.43
5:B:229:ALA:O	5:B:232:SER:HB3	2.19	0.43
5:B:977:GLY:HA2	5:B:989:THR:HB	2.00	0.43
5:B:1203:LEU:O	5:B:1207:LEU:HG	2.19	0.43
9:H:58:THR:HB	9:H:143:LEU:HB2	2.01	0.43
4:A:28:ARG:HE	4:A:83:HIS:HE2	1.67	0.42
4:A:694:THR:HG22	4:A:698:GLN:HE21	1.84	0.42
5:B:792:MET:HG2	5:B:857:ARG:HD2	2.01	0.42
9:H:5:LEU:HB3	9:H:133:ASN:HD21	1.83	0.42
9:H:102:TYR:CE2	9:H:115:TYR:HB3	2.54	0.42
4:A:472:LEU:HD13	5:B:835:GLN:HE22	1.84	0.42
4:A:592:ASP:O	4:A:595:THR:OG1	2.26	0.42
4:A:701:LEU:HA	10:I:115:LYS:HE3	2.02	0.42
4:A:1140:HIS:HB2	4:A:1276:VAL:O	2.19	0.42
4:A:1151:GLU:O	4:A:1193:LEU:HD12	2.19	0.42
5:B:247:GLY:O	5:B:249:ARG:NH1	2.51	0.42
5:B:291:ILE:HG21	5:B:300:HIS:CD2	2.54	0.42
5:B:831:SER:OG	5:B:833:TYR:HD1	2.02	0.42
6:C:259:LEU:HD21	12:K:92:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:46:TYR:HD2	7:E:53:PRO:HB2	1.84	0.42
10:I:17:ARG:HD3	10:I:18:GLU:H	1.83	0.42
4:A:343:LYS:HD3	5:B:1151:LEU:HD13	2.01	0.42
4:A:380:VAL:HG22	4:A:430:TRP:O	2.19	0.42
4:A:399:HIS:HD2	4:A:435:HIS:HB3	1.84	0.42
4:A:437:MET:HE3	4:A:437:MET:HB2	1.64	0.42
4:A:1031:VAL:HG13	4:A:1037:LEU:HD12	2.01	0.42
5:B:599:THR:O	5:B:603:LEU:HG	2.19	0.42
5:B:899:ILE:O	5:B:952:VAL:HG21	2.20	0.42
5:B:984:HIS:CD2	5:B:1025:HIS:HA	2.55	0.42
5:B:1215:ARG:HB3	5:B:1217:TYR:HE1	1.84	0.42
6:C:70:ILE:HD11	6:C:144:ILE:CD1	2.50	0.42
7:E:61:GLN:HB2	7:E:79:TRP:CE3	2.54	0.42
9:H:135:LEU:HD12	9:H:136:LYS:H	1.85	0.42
10:I:101:PHE:CE1	10:I:112:SER:HB3	2.55	0.42
11:J:7:CYS:HB3	11:J:10:CYS:HB3	1.82	0.42
4:A:203:SER:O	4:A:207:ILE:HG22	2.19	0.42
4:A:208:LEU:HB2	4:A:235:ILE:HD11	2.01	0.42
4:A:388:LEU:O	4:A:392:VAL:HG23	2.19	0.42
5:B:551:PRO:O	5:B:555:ILE:HD12	2.19	0.42
5:B:826:ALA:HB3	5:B:1011:ILE:CD1	2.48	0.42
5:B:1172:ILE:HD12	5:B:1172:ILE:O	2.20	0.42
6:C:13:ALA:HB1	6:C:18:VAL:HG22	2.00	0.42
7:E:180:ARG:NH2	7:E:192:ARG:HB2	2.34	0.42
4:A:575:LYS:HE2	9:H:120:GLY:HA3	2.01	0.42
4:A:579:SER:HB3	4:A:611:GLN:HA	2.01	0.42
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.60	0.42
4:A:964:ILE:O	4:A:968:GLN:HG3	2.19	0.42
5:B:1138:MET:HG3	5:B:1146:PHE:HE1	1.85	0.42
6:C:166:GLU:HB2	12:K:10:PHE:CE1	2.55	0.42
6:C:175:ALA:HB3	11:J:43:ARG:NH1	2.34	0.42
9:H:12:VAL:HG23	9:H:26:ILE:HG23	2.01	0.42
3:N:8:DG:C5'	4:A:175:ARG:HH12	2.32	0.42
4:A:544:ASP:OD1	4:A:545:GLN:N	2.51	0.42
4:A:600:PRO:HA	9:H:25:ARG:HH12	1.84	0.42
4:A:684:ALA:O	4:A:688:LYS:HG2	2.20	0.42
4:A:842:VAL:HG11	5:B:1136:ASP:CG	2.45	0.42
5:B:227:LYS:H	5:B:395:GLN:CD	2.28	0.42
5:B:788:ARG:NH1	5:B:790:ASP:OD1	2.53	0.42
6:C:147:LEU:HD23	6:C:147:LEU:HA	1.73	0.42
9:H:93:TYR:HB3	9:H:144:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:49:GLU:HB3	12:K:90:ALA:HB1	2.01	0.42
4:A:107:CYS:HB3	4:A:110:CYS:O	2.20	0.42
4:A:286:HIS:O	4:A:289:ILE:HG22	2.19	0.42
4:A:353:ILE:CG2	4:A:487:MET:HB2	2.49	0.42
4:A:402:ALA:HB1	4:A:433:GLU:O	2.19	0.42
4:A:789:LYS:HD2	10:I:67:THR:CB	2.49	0.42
5:B:242:SER:N	5:B:252:SER:O	2.49	0.42
5:B:290:GLY:HA2	5:B:327:ARG:HD2	2.00	0.42
5:B:975:GLN:O	5:B:990:ILE:HD12	2.20	0.42
5:B:1006:ILE:HD13	11:J:44:TYR:CZ	2.55	0.42
6:C:192:TRP:O	6:C:201:TRP:NE1	2.51	0.42
1:R:1:A:OP2	5:B:1112:GLN:NE2	2.51	0.42
4:A:15:LYS:HE2	4:A:15:LYS:HB2	1.86	0.42
4:A:382:PRO:HD3	8:F:104:ASN:ND2	2.32	0.42
4:A:774:ARG:NH2	4:A:797:LYS:HG3	2.34	0.42
5:B:216:GLU:HB3	5:B:500:THR:HG23	2.00	0.42
5:B:858:SER:HA	5:B:966:VAL:O	2.20	0.42
9:H:38:LEU:HA	9:H:124:ARG:O	2.20	0.42
4:A:399:HIS:HA	4:A:401:GLY:N	2.29	0.42
4:A:446:ARG:HH21	4:A:485:ASP:CG	2.27	0.42
4:A:643:ALA:HA	4:A:646:PHE:HD2	1.84	0.42
4:A:1140:HIS:ND1	4:A:1277:GLU:HA	2.35	0.42
4:A:1220:PHE:HE1	4:A:1224:LEU:CD2	2.33	0.42
5:B:179:CYS:O	5:B:182:SER:OG	2.38	0.42
5:B:273:LEU:CB	5:B:276:ILE:HB	2.50	0.42
5:B:358:LYS:O	5:B:362:PRO:HB3	2.20	0.42
5:B:1112:GLN:HE22	5:B:1114:LEU:CB	2.33	0.42
6:C:46:ILE:HG13	6:C:159:ALA:HB2	2.02	0.42
7:E:77:SER:HB2	7:E:105:PHE:HD1	1.85	0.42
10:I:78:CYS:C	10:I:80:SER:N	2.78	0.42
4:A:9:ALA:HB2	5:B:1191:ILE:HD12	2.01	0.42
4:A:58:LEU:HD13	4:A:244:PRO:HD3	2.02	0.42
4:A:101:LYS:HB3	4:A:135:PHE:HZ	1.84	0.42
4:A:348:SER:HB3	5:B:1128:LEU:HB2	2.01	0.42
4:A:369:SER:O	4:A:373:THR:HG23	2.20	0.42
4:A:853:ASP:OD2	4:A:857:ARG:NH2	2.46	0.42
4:A:1226:VAL:HA	4:A:1239:ARG:O	2.20	0.42
4:A:1398:MET:HB2	4:A:1426:GLU:OE2	2.19	0.42
5:B:95:ILE:HD12	5:B:129:PHE:O	2.20	0.42
5:B:485:ARG:HD2	5:B:781:PHE:CD1	2.54	0.42
6:C:182:PRO:HB2	6:C:207:CYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:87:LYS:HE3	8:F:88:TYR:CE1	2.55	0.42
9:H:103:LYS:HD2	9:H:103:LYS:HA	1.71	0.42
10:I:58:VAL:HA	10:I:62:ILE:CD1	2.50	0.42
4:A:362:ASP:OD1	4:A:362:ASP:N	2.53	0.41
4:A:406:ILE:HD12	4:A:412:ARG:NH1	2.35	0.41
4:A:676:MET:O	4:A:680:THR:HG23	2.20	0.41
4:A:1030:ARG:HD2	4:A:1034:GLU:CD	2.45	0.41
5:B:1034:VAL:O	5:B:1038:SER:HB3	2.19	0.41
9:H:95:TYR:HE1	9:H:97:MET:CG	2.29	0.41
10:I:59:VAL:H	10:I:62:ILE:HD12	1.85	0.41
10:I:70:ARG:NE	10:I:84:VAL:HG12	2.35	0.41
13:L:46:VAL:O	13:L:47:ARG:HG3	2.19	0.41
4:A:239:LEU:HD12	4:A:240:PRO:HD2	2.02	0.41
4:A:492:PRO:HB3	4:A:497:THR:HG22	2.02	0.41
4:A:576:GLN:O	4:A:580:VAL:HG23	2.20	0.41
5:B:69:LEU:HD13	5:B:429:PHE:HB2	2.02	0.41
5:B:124:TYR:HB2	5:B:204:ILE:HB	2.01	0.41
5:B:416:LEU:HD22	5:B:466:TRP:HZ3	1.84	0.41
4:A:22:PHE:CD1	4:A:27:VAL:HG23	2.55	0.41
4:A:58:LEU:HD23	4:A:58:LEU:HA	1.73	0.41
4:A:274:ILE:HD12	4:A:274:ILE:HA	1.90	0.41
4:A:569:LYS:CE	6:C:221:TYR:HB2	2.50	0.41
4:A:1030:ARG:HA	4:A:1034:GLU:OE2	2.20	0.41
5:B:464:GLY:HA2	5:B:480:SER:HB3	2.02	0.41
5:B:918:ILE:HG21	5:B:935:ARG:HH11	1.85	0.41
5:B:1029:CYS:HA	5:B:1089:PRO:O	2.21	0.41
6:C:33:LEU:O	6:C:37:MET:HG3	2.19	0.41
7:E:26:ARG:NH2	7:E:133:GLU:OE1	2.29	0.41
8:F:77:ASP:OD1	8:F:77:ASP:N	2.42	0.41
8:F:118:LEU:O	8:F:122:MET:HG3	2.20	0.41
10:I:26:LEU:HD13	10:I:35:VAL:CG1	2.51	0.41
2:T:12:DT:H2''	2:T:13:DC:H5'	2.01	0.41
4:A:99:ILE:HD12	4:A:211:PHE:HE2	1.85	0.41
4:A:446:ARG:HD3	4:A:478:TYR:O	2.21	0.41
4:A:870:GLU:OE2	4:A:1365:TYR:OH	2.33	0.41
4:A:1036:ARG:HA	4:A:1036:ARG:HD3	1.76	0.41
4:A:1116:LEU:HD12	4:A:1328:TYR:O	2.20	0.41
5:B:834:ASN:O	5:B:1013:ASN:ND2	2.37	0.41
6:C:82:TYR:CD1	6:C:161:LYS:HB3	2.53	0.41
8:F:74:ILE:HB	8:F:144:GLU:HG2	2.03	0.41
9:H:101:ALA:HB2	9:H:116:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:873:MET:C	4:A:1058:VAL:HG13	2.45	0.41
4:A:1067:LEU:O	4:A:1071:SER:OG	2.35	0.41
4:A:1236:LEU:C	4:A:1237:ILE:HD13	2.45	0.41
5:B:333:PHE:C	5:B:334:ILE:HD12	2.45	0.41
6:C:123:ASN:OD1	6:C:125:MET:HG2	2.21	0.41
6:C:166:GLU:HB2	12:K:10:PHE:CZ	2.56	0.41
7:E:20:LYS:HE3	7:E:35:VAL:HA	2.02	0.41
7:E:46:TYR:HB2	7:E:58:MET:HE2	2.02	0.41
4:A:92:HIS:CG	4:A:95:PHE:HD2	2.38	0.41
5:B:797:TYR:HB3	5:B:798:TYR:CD1	2.55	0.41
9:H:56:THR:O	9:H:144:ILE:HA	2.21	0.41
4:A:38:PRO:HA	4:A:53:LEU:HD13	2.01	0.41
4:A:55:ASP:HA	4:A:58:LEU:HB2	2.01	0.41
4:A:535:THR:O	4:A:575:LYS:NZ	2.47	0.41
4:A:784:LEU:HD23	4:A:784:LEU:HA	1.88	0.41
5:B:195:CYS:SG	5:B:782:LEU:HD22	2.61	0.41
5:B:257:LYS:HE2	5:B:259:TYR:HE1	1.85	0.41
5:B:292:ILE:N	5:B:293:PRO:HD2	2.36	0.41
5:B:294:ASP:HB2	10:I:12:ASN:HA	2.01	0.41
5:B:450:ALA:O	5:B:453:ILE:HG22	2.21	0.41
5:B:592:ASN:N	5:B:593:PRO:HD3	2.34	0.41
5:B:597:MET:CG	5:B:601:ARG:HH21	2.33	0.41
9:H:12:VAL:HA	9:H:28:ALA:HB2	2.02	0.41
11:J:30:LEU:HD23	11:J:30:LEU:HA	1.85	0.41
4:A:34:LYS:HA	4:A:83:HIS:O	2.20	0.41
4:A:501:LEU:HD21	5:B:1146:PHE:CD2	2.56	0.41
4:A:688:LYS:HA	4:A:688:LYS:HD3	1.92	0.41
5:B:120:ARG:HB3	5:B:122:LEU:HD23	2.02	0.41
5:B:130:VAL:HG22	5:B:167:ILE:HG13	2.01	0.41
5:B:755:ILE:HD11	5:B:814:PHE:CG	2.56	0.41
5:B:821:GLN:OE1	5:B:850:LEU:HG	2.20	0.41
5:B:954:VAL:O	13:L:56:LEU:N	2.54	0.41
6:C:65:HIS:CD2	6:C:69:LEU:HD23	2.56	0.41
6:C:82:TYR:HE1	6:C:161:LYS:HG2	1.86	0.41
3:N:5:DC:OP2	4:A:1109:LYS:NZ	2.54	0.41
4:A:74:MET:HE3	4:A:74:MET:HB3	1.90	0.41
4:A:93:VAL:CG1	4:A:301:ALA:HB1	2.51	0.41
4:A:208:LEU:HD22	4:A:235:ILE:HD11	2.02	0.41
4:A:463:ILE:HD13	4:A:469:ARG:HG3	2.03	0.41
4:A:500:GLU:OE2	4:A:1438:THR:HG21	2.20	0.41
4:A:715:GLU:OE2	4:A:774:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1191:TRP:CD1	4:A:1191:TRP:H	2.39	0.41
5:B:856:PHE:HE1	5:B:969:ARG:HG3	1.85	0.41
5:B:1015:HIS:O	5:B:1018:PRO:HD2	2.20	0.41
6:C:67:LEU:HA	6:C:70:ILE:HG12	2.03	0.41
10:I:32:CYS:SG	10:I:34:TYR:N	2.94	0.41
10:I:53:GLY:HA2	10:I:56:ALA:HB2	2.03	0.41
10:I:58:VAL:HA	10:I:62:ILE:HD11	2.03	0.41
4:A:396:PRO:HD3	4:A:415:LEU:HB3	2.02	0.41
4:A:1351:GLU:O	4:A:1355:VAL:HG23	2.20	0.41
5:B:823:ALA:HA	11:J:48:ARG:HH12	1.86	0.41
9:H:135:LEU:O	9:H:137:GLN:N	2.47	0.41
12:K:38:GLU:OE1	12:K:42:LEU:HD23	2.21	0.41
4:A:598:LEU:HD23	4:A:598:LEU:HA	1.86	0.40
4:A:836:TYR:O	4:A:840:ARG:HG3	2.20	0.40
4:A:845:LEU:O	4:A:1065:GLY:HA3	2.21	0.40
4:A:852:TYR:CZ	8:F:136:ARG:HG2	2.55	0.40
5:B:944:THR:HG21	5:B:1122:ARG:HH21	1.86	0.40
5:B:1187:ASN:ND2	5:B:1190:ASP:O	2.54	0.40
7:E:168:TYR:HB3	7:E:170:LEU:HG	2.03	0.40
2:T:21:DC:H1'	4:A:447:GLN:HG3	2.02	0.40
4:A:23:SER:HB2	4:A:233:TRP:CE2	2.56	0.40
4:A:388:LEU:HD23	4:A:388:LEU:HA	1.93	0.40
4:A:1063:MET:HE2	4:A:1436:ILE:HA	2.03	0.40
4:A:1224:LEU:HD12	4:A:1242:VAL:HA	2.03	0.40
4:A:630:ILE:H	4:A:630:ILE:HD12	1.85	0.40
4:A:1116:LEU:HB3	4:A:1308:THR:OG1	2.21	0.40
4:A:1169:ILE:HG22	4:A:1227:ILE:HD12	2.03	0.40
5:B:98:THR:O	5:B:126:SER:HB2	2.22	0.40
5:B:238:ALA:HB3	5:B:256:VAL:HB	2.03	0.40
5:B:756:ILE:HG23	5:B:983:ARG:O	2.22	0.40
6:C:26:ASP:N	6:C:26:ASP:OD1	2.53	0.40
12:K:79:GLU:H	12:K:79:GLU:HG2	1.74	0.40
2:T:21:DC:H2''	4:A:447:GLN:HE21	1.86	0.40
3:N:6:DG:H2''	3:N:7:DA:C8	2.56	0.40
4:A:475:THR:O	4:A:479:ASN:N	2.55	0.40
4:A:914:GLU:H	4:A:914:GLU:HG2	1.75	0.40
4:A:916:GLY:O	4:A:919:ILE:HG22	2.22	0.40
4:A:1101:LEU:O	4:A:1105:LEU:HG	2.21	0.40
4:A:1402:PHE:CD2	4:A:1403:GLU:HG3	2.56	0.40
5:B:120:ARG:NE	5:B:956:THR:O	2.55	0.40
6:C:84:ARG:H	6:C:84:ARG:HG2	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:254:LYS:O	6:C:258:ILE:HG12	2.21	0.40
7:E:43:LYS:O	7:E:47:CYS:HB2	2.22	0.40
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.86	0.40
11:J:8:PHE:CD2	11:J:49:MET:HE1	2.56	0.40
4:A:664:THR:OG1	5:B:1014:PRO:HB3	2.22	0.40
4:A:814:PHE:CZ	5:B:514:LEU:HD11	2.57	0.40
5:B:579:ARG:HA	5:B:589:VAL:HG23	2.03	0.40
5:B:1106:ARG:HD3	5:B:1127:GLY:HA2	2.02	0.40
7:E:28:TYR:CZ	7:E:75:MET:HE2	2.56	0.40
9:H:25:ARG:HA	9:H:41:ASP:HA	2.04	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)
10:I:81:ARG:O	10:I:81:ARG:NH2[2_556]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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%)	1326 (97%)	45 (3%)	0	100	100
5	B	1101/1224 (90%)	1081 (98%)	20 (2%)	0	100	100
6	C	265/318 (83%)	259 (98%)	6 (2%)	0	100	100
7	E	211/215 (98%)	198 (94%)	13 (6%)	0	100	100
8	F	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
9	H	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
10	I	116/122 (95%)	113 (97%)	3 (3%)	0	100	100
11	J	63/70 (90%)	63 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	K	112/120 (93%)	111 (99%)	1 (1%)	0	100	100
13	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
All	All	3493/4173 (84%)	3397 (97%)	96 (3%)	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	1191/1520 (78%)	1191 (100%)	0	100	100
5	B	954/1061 (90%)	954 (100%)	0	100	100
6	C	235/274 (86%)	235 (100%)	0	100	100
7	E	194/197 (98%)	194 (100%)	0	100	100
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	114/128 (89%)	114 (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	36/57 (63%)	36 (100%)	0	100	100
All	All	3066/3657 (84%)	3066 (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 (32) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	71	GLN
4	A	273	ASN
4	A	427	GLN
4	A	447	GLN

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Mol	Chain	Res	Type
4	A	451	HIS
4	A	768	GLN
4	A	877	HIS
4	A	881	GLN
4	A	953	ASN
4	A	965	GLN
4	A	1173	HIS
4	A	1187	GLN
4	A	1222	ASN
5	B	206	ASN
5	B	469	GLN
5	B	481	GLN
5	B	733	HIS
5	B	835	GLN
5	B	975	GLN
5	B	986	GLN
5	B	1025	HIS
5	B	1117	GLN
6	C	65	HIS
6	C	264	GLN
7	E	99	HIS
7	E	101	GLN
7	E	104	ASN
8	F	104	ASN
9	H	33	GLN
9	H	134	ASN
10	I	46	HIS
13	L	53	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/9 (88%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	9	G

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	8OG	T	19	2	22,25,26	3.97	18 (81%)	26,37,40	1.50	5 (19%)

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	8OG	T	19	2	-	4/7/21/22	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	8OG	C8-N7	7.26	1.51	1.38
2	T	19	8OG	C8-N9	6.14	1.51	1.40
2	T	19	8OG	C2-N3	5.78	1.47	1.33
2	T	19	8OG	C4-N3	5.61	1.47	1.34
2	T	19	8OG	C2-N2	4.74	1.45	1.34
2	T	19	8OG	C5-C4	4.65	1.43	1.37
2	T	19	8OG	O4'-C1'	-4.60	1.32	1.42
2	T	19	8OG	O3'-C3'	4.31	1.52	1.43
2	T	19	8OG	C2-N1	3.97	1.47	1.37
2	T	19	8OG	C5-N7	3.96	1.44	1.37
2	T	19	8OG	C2'-C1'	3.82	1.62	1.52
2	T	19	8OG	C5-C6	3.20	1.51	1.41
2	T	19	8OG	C6-N1	3.10	1.44	1.38
2	T	19	8OG	C5'-C4'	-3.08	1.42	1.51
2	T	19	8OG	O8-C8	-2.63	1.18	1.23
2	T	19	8OG	O6-C6	-2.44	1.18	1.23
2	T	19	8OG	C3'-C4'	2.35	1.59	1.53
2	T	19	8OG	C4-N9	2.20	1.43	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	8OG	C2-N3-C4	3.63	118.55	112.30
2	T	19	8OG	C5-N7-C8	-2.77	105.65	109.47
2	T	19	8OG	O6-C6-C5	-2.57	121.06	127.26
2	T	19	8OG	C4-C5-N7	2.46	110.57	106.06
2	T	19	8OG	C5-C6-N1	2.24	118.29	112.13

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	8OG	O4'-C4'-C5'-O5'
2	T	19	8OG	C3'-C4'-C5'-O5'
2	T	19	8OG	C4'-C5'-O5'-P
2	T	19	8OG	C2'-C1'-N9-C8

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 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	$\# Z > 2$
16	2TM	B	2101	-	26,30,30	3.98	15 (57%)	39,47,47	0.96	2 (5%)

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	2TM	B	2101	-	-	4/19/38/38	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	2101	2TM	PB-O3B	7.73	1.67	1.58
16	B	2101	2TM	C2'-C3'	-7.14	1.34	1.53
16	B	2101	2TM	C2-N3	6.50	1.49	1.36
16	B	2101	2TM	O4'-C4'	6.38	1.59	1.45
16	B	2101	2TM	C6-C5	6.10	1.49	1.35
16	B	2101	2TM	C4-N4	5.69	1.47	1.33
16	B	2101	2TM	C4-N3	5.34	1.45	1.34
16	B	2101	2TM	O4'-C1'	-4.58	1.31	1.42
16	B	2101	2TM	C2-N1	4.50	1.49	1.40
16	B	2101	2TM	C5'-C4'	-4.44	1.38	1.51
16	B	2101	2TM	C2'-C1'	3.68	1.65	1.53
16	B	2101	2TM	O2-C2	-3.36	1.17	1.23
16	B	2101	2TM	C6-N1	3.09	1.45	1.38
16	B	2101	2TM	C5-C4	2.70	1.49	1.42
16	B	2101	2TM	PA-O2A	-2.08	1.51	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	2101	2TM	C3'-C2'-C1'	2.53	106.25	101.46
16	B	2101	2TM	PB-O3B-PG	-2.35	124.02	132.45

There are no chirality outliers.

All (4) torsion outliers are listed below:

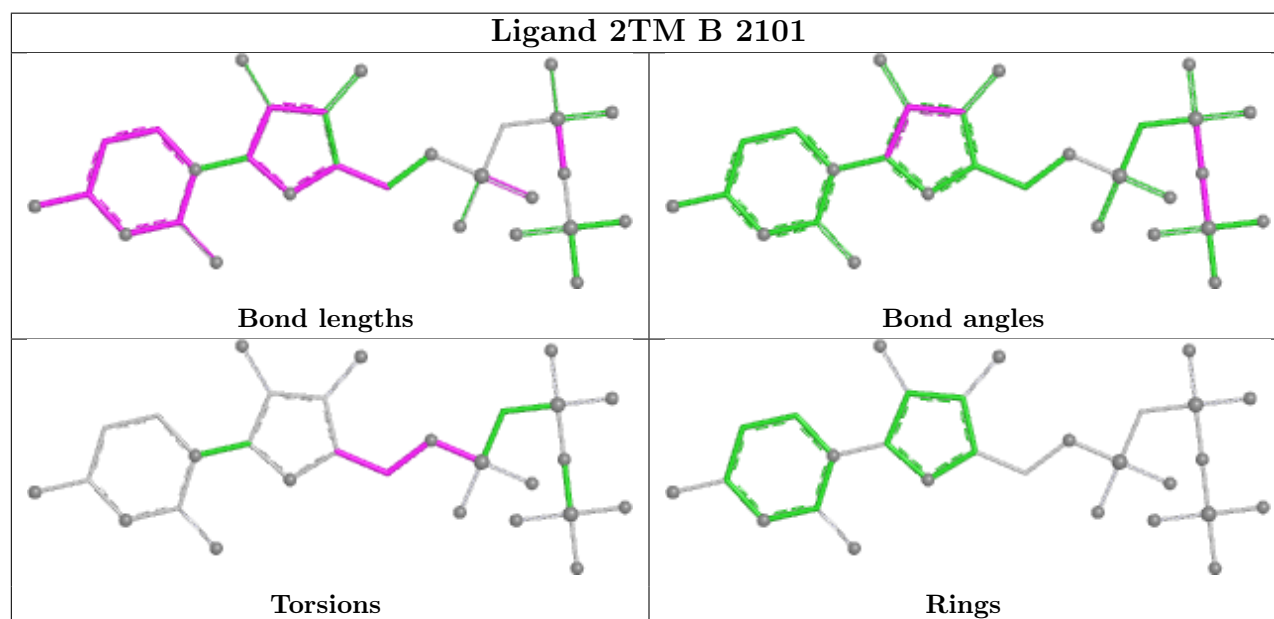
Mol	Chain	Res	Type	Atoms
16	B	2101	2TM	C3'-C4'-C5'-O5'
16	B	2101	2TM	O4'-C4'-C5'-O5'
16	B	2101	2TM	C5'-O5'-PA-O1A
16	B	2101	2TM	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	2101	2TM	1	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%)	0.19	0 100 100	76, 86, 172, 223	0
2	T	25/29 (86%)	0.33	0 100 100	90, 188, 241, 268	0
3	N	15/18 (83%)	0.35	0 100 100	143, 205, 241, 253	0
4	A	1385/1733 (79%)	0.09	21 (1%) 72 44	74, 121, 184, 241	0
5	B	1121/1224 (91%)	0.18	23 (2%) 63 37	52, 106, 170, 250	0
6	C	267/318 (83%)	-0.00	3 (1%) 78 52	73, 111, 158, 195	0
7	E	213/215 (99%)	-0.16	1 (0%) 87 66	83, 144, 211, 252	0
8	F	86/155 (55%)	-0.09	0 100 100	76, 110, 158, 178	0
9	H	133/146 (91%)	0.13	2 (1%) 72 44	106, 146, 202, 220	0
10	I	118/122 (96%)	0.10	0 100 100	88, 137, 194, 229	0
11	J	65/70 (92%)	0.30	2 (3%) 51 29	65, 99, 134, 165	0
12	K	114/120 (95%)	-0.07	1 (0%) 81 56	63, 103, 147, 185	0
13	L	43/70 (61%)	0.25	1 (2%) 61 35	93, 195, 256, 274	0
All	All	3594/4229 (84%)	0.10	54 (1%) 72 44	52, 118, 188, 274	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	775	LYS	4.8
4	A	103	CYS	4.0
13	L	32	ALA	3.7
5	B	819	ALA	3.7
4	A	448	PRO	3.6
4	A	355	GLY	3.6
5	B	899	ILE	3.6
5	B	525	ALA	3.3
5	B	1130	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
4	A	303	TYR	2.9
4	A	921	GLY	2.8
5	B	386	LEU	2.8
5	B	533	CYS	2.8
5	B	335	GLY	2.8
5	B	1097	HIS	2.6
9	H	63	LEU	2.6
4	A	104	GLU	2.6
9	H	23	VAL	2.5
6	C	178	PHE	2.5
5	B	754	SER	2.5
4	A	466	SER	2.4
5	B	1214	PRO	2.4
4	A	144	THR	2.4
4	A	447	GLN	2.4
5	B	300	HIS	2.4
4	A	1267	MET	2.4
5	B	694	ASP	2.4
5	B	381	MET	2.4
11	J	44	TYR	2.3
5	B	647	GLY	2.3
5	B	681	TRP	2.3
4	A	1098	VAL	2.3
5	B	751	VAL	2.3
5	B	1006	ILE	2.2
4	A	932	GLU	2.2
4	A	234	MET	2.2
5	B	1099	VAL	2.2
6	C	146	LYS	2.2
4	A	873	MET	2.2
5	B	830	TYR	2.2
11	J	61	LEU	2.2
4	A	137	ALA	2.1
4	A	503	GLN	2.1
5	B	806	THR	2.1
5	B	753	ALA	2.1
4	A	488	ASN	2.1
4	A	1410	PHE	2.1
5	B	384	ARG	2.1
12	K	11	LEU	2.1
7	E	93	MET	2.1
4	A	350	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	1282	VAL	2.0
4	A	78	PRO	2.0
6	C	30	ALA	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	8OG	T	19	23/24	0.88	0.11	88,96,112,144	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

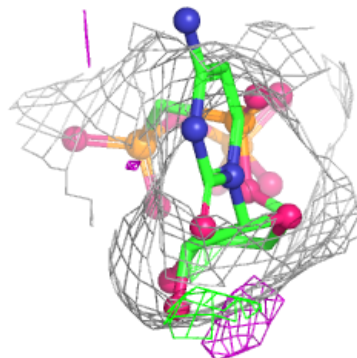
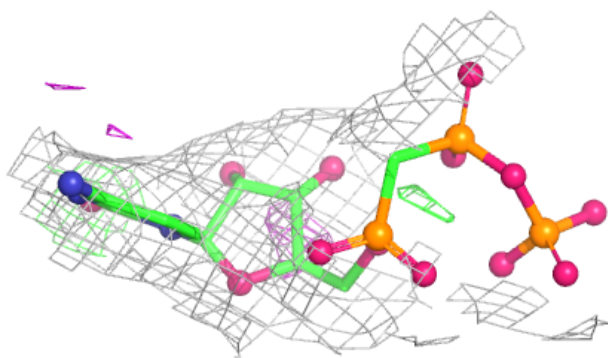
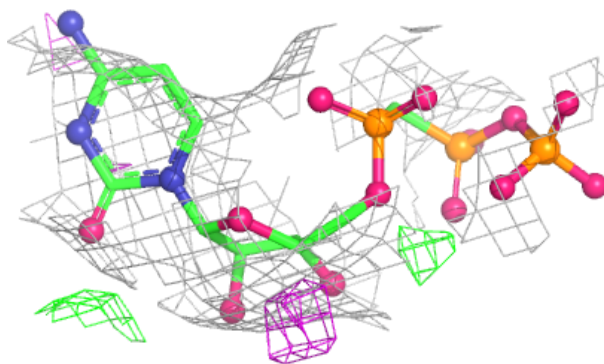
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	ZN	I	202	1/1	0.64	0.20	209,209,209,209	0
14	ZN	L	101	1/1	0.78	0.11	309,309,309,309	0
16	2TM	B	2101	29/29	0.87	0.09	38,77,133,172	0
14	ZN	A	1801	1/1	0.92	0.07	240,240,240,240	0
14	ZN	J	101	1/1	0.92	0.08	145,145,145,145	0
14	ZN	C	401	1/1	0.93	0.10	148,148,148,148	0
14	ZN	B	2102	1/1	0.98	0.04	163,163,163,163	0
15	MG	A	1803	1/1	0.98	0.05	62,62,62,62	0
14	ZN	A	1802	1/1	0.98	0.03	121,121,121,121	0
14	ZN	I	201	1/1	0.99	0.03	110,110,110,110	0

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

Electron density around 2TM B 2101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.