



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2025 – 10:11 AM EDT

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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

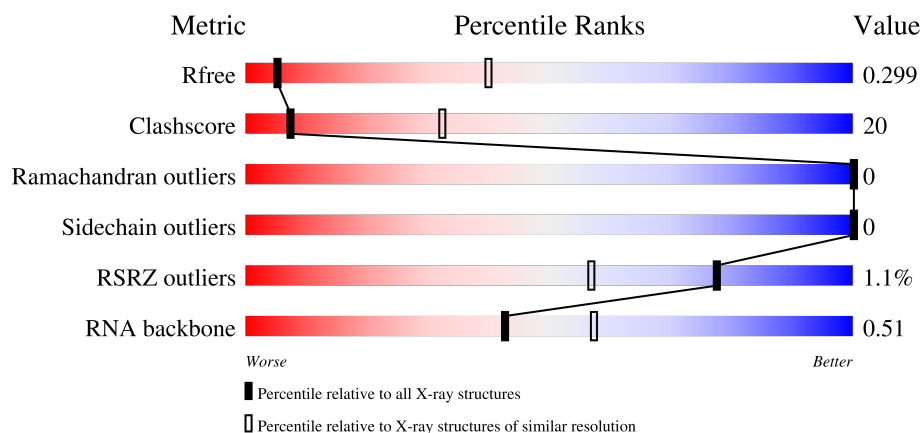
1 Overall quality at a glance

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}	164625	1563 (3.70-3.50)
Clashscore	180529	1665 (3.70-3.50)
Ramachandran outliers	177936	1641 (3.70-3.50)
Sidechain outliers	177891	1640 (3.70-3.50)
RSRZ outliers	164620	1562 (3.70-3.50)
RNA backbone	3690	1108 (4.20-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	<div> <div></div> <div>33%</div> <div>56%</div> <div>11%</div> </div>
2	T	29	<div> <div></div> <div>31%</div> <div>59%</div> <div>10%</div> </div>
3	N	18	<div> <div></div> <div>28%</div> <div>56%</div> <div>17%</div> </div>
4	A	1733	<div> <div></div> <div>45%</div> <div>35%</div> <div>20%</div> </div>

Continued on next page...

Continued from previous page...

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

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			

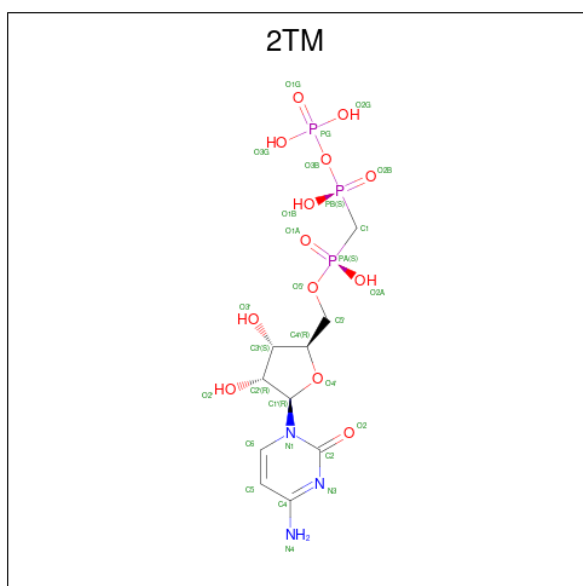
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

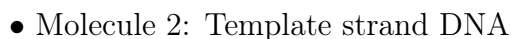
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

- 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).



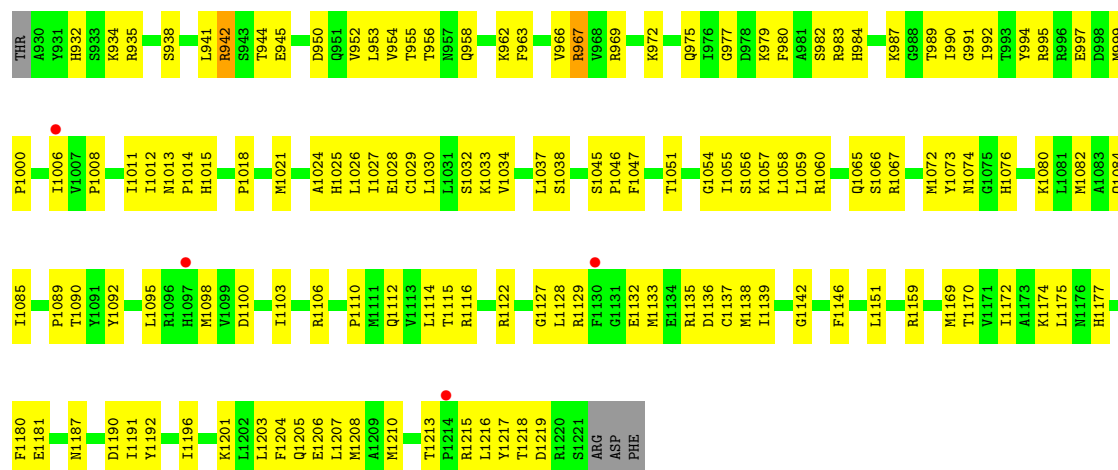
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
16	B	1	Total 29	C 10	N 3	O 13	P 3	0	0

- Molecule 1: RNA

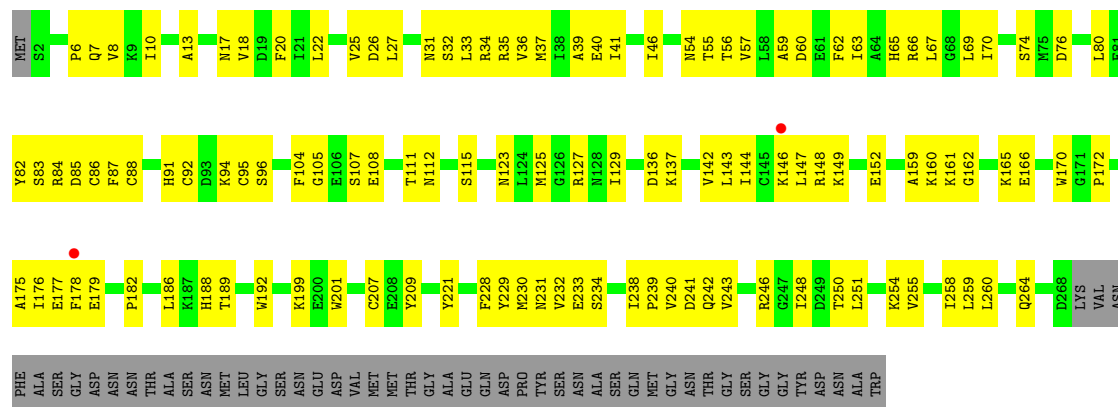


THR	ALA	SER	L1369	E1269	L1193	M1110	R1023	T907	T834	M746	Q650		M479	G395	I308
ALA	LEU	LEU	L1370	M1270	E1196	M1111	S1024	T914	T835	V747	R651		F482	F396	A309
GLY	VAL	VAL	L1371	T1271	L1197	T1112	R1025	S915	G835	M748	V652		D483		G310
GLY	TYR	TYR	L1372	T1272	L1198	T1113		G916	Y836		V653		P400		A314
ALA	MET	GLY	L1373	L1273	D1198	L1116	R1030	G916	Y837	S751	N654		D485	C401	
ASP	PRO	PRO	M1374	R1274	M1202	T1117	T1031		Q838	S754	F662		M487	A402	I325
TYR	GLY	GLY	M1375	G1275	M1203	T1118	E1034	T919	R839	F755	S663		M488		R326
GLY	GLY	GLY	L1276	K1205	K1206	V1119	Y1035	L920	R840	I756	S664			V405	
GLY	GLY	GLY	L1277	D1206	L1207	E1129	R1036	G921	L841	I757	G665			I406	
ALA	ILE	ALA	V1282	V1384	L1207	E1130	R1037	L925	V842	I758	I666		V491		K332
THR	THR	THR	K1290	K1386	M1209	A1131	M1048	Q926	L845	A759	A671		P492		R335
PRO	ILE	GLY	T1295	H1387	M1209	L1132	I1049	E932	E846	Q760	D672		E496		I336
PHE	GLY	GLY				L1133		Y933	D847				S799		R337
GLY	GLY	GLY	K1390	G1213	G1214	R1135	S1056	L936	I848	A763	T675		E497		G398
ALA	ALA	GLY	R1391	E1214	E1215	S1136	V1057	L936	M849	C764	M676		I413		N339
TYR	TYR	TYR	K1300	R1215	R1216	A1137	V1058		Y850	V765	I582		D414		L340
GLY	GLY	GLY	E1303	R1217	K1217	I1138	M1063	K941	Y851	G766	P583		L415		M341
GLY	GLY	GLY	L1397	K1218	Q1218	E1139	V1064	F942	Y852	Q767	I679		S418		G342
ALA	ALA	GLY	R1398	T1219	T1219	H1140	G1065	L943	D853	R774	T680		Q503		K343
PRO	PRO	THR	R1399	F1220	F1220	K1144	V1066	E945	R857	I775	A684		I424		R344
THR	THR	THR	V1311	F1221	F1221		L1067	E945	S859	F777	I683		M430		S348
SER	PRO	SER	V1316	N1222	N1222	I1148	Q1070	D949	V863	D781	K688		E433		A349
GLY	GLY	SER		D1223	D1223	E1151	S1071	A952	V863	R782	T694		R434		R350
PHE	GLY	ASN	V1319	L1224	L1224	I1152		Y953	F866	I783	P514		H435		T351
GLY	GLY	GLY	E1407	F1225	F1225	T1153	A1076	Y954	I867	L784	Q698		V352		V352
VAL	VAL	SER	L1408	V1226	V1226	Y1154	T1077	P955	Y868	P785	L701		M437		S354
SER	SER	GLY	L1409	I1227	I1227	P1155	M1078	L956	G869	H786	L701		G355		G355
LEU	LEU	LEU	F1410	W1228	W1228	P1156	M1079		E870		R711		P519		D356
PRO	PRO	VAL				D1157	T1080	T960	D871	K789	R711		G520		P357
GLY	GLY	ASN	A1416	K1235	K1235	D1157	L1081	R961	G872		F714		M521		E360
PHE	PHE	ALA		L1236	L1236	S1160	ASN	R962	M873	Y792	E715		L528		L361
SER	SER	ASP	D1419	T1237	T1237	T1161	THR	R963	D874		E715		P448		D362
PRO	PRO	LEU	D1420	I1238	I1238	V1162	PHE	L964	A875	K797	V718		S449		Q363
THR	THR	ASP	C1421	R1239	R1239	I1163	HIS	Q965	A876	G798			L450		V364
SER	SER	VAL	R1422	C1240	C1240	P1164	PHE	Q965	H877	F799	L722		H451		
PRO	PRO	LYS	M1336	R1241	R1241	E1165	GLY	Q968	I878	V900			K452		P367
THR	THR	ASP	E1426	V1242	V1242	D1166	ALA		E879		L722		M453		K368
TYR	TYR	GLY	N1427	V1243	V1243		GLY		K880	R806	R726		A457		S369
SER	SER	LEU	V1428	ARG	ARG	I1169	VAL	H975	Q881	R806	R726		H458		I370
PRO	PRO	MET	I1429	PRO	PRO	I1170	ALA		S882		D727		A457		A371
THR	THR	PHE	L1430	LYS	LYS	L1170	SER	Y986	L883	T809	A729		R459		K372
SER	SER	SER	G1431	SER	SER	L1176	K1092		D884	E812	G730		I463		L374
PRO	PRO	PRO	A1434	LEU	LEU	LEU	T1095	Y990	S885	F813	R731		P464		T375
ALA	ALA	VAL	P1435	ASP	ASP	ASP		X991	T885	F815	L732		V465		T375
SER	SER	GLY	I1436	GLY	GLY	GLY	V1098	D992	I886	F815	A733		S466		V360
PRO	PRO	GLY	G1437	THR	THR	GLY	P1099	L993	S889				N547		T381
THR	THR	SER	T1438	GLY	GLY	GLY	R1100	E995		M618	N736		N548		P382
SER	SER	SER		GLY	GLY	GLY	L1101	E995	R896	G819	L737		M549		Y383
PRO	PRO	ASN	F1441	ALA	ALA	ALA	K1102	L997	Y897	G820	K738		L550		
PRO	PRO	ASN	V1443	GLY	GLY	GLY	E1103		R898	R821	D739		N471		
TYR	TYR	ALA	W1444	THR	THR	PHE	L1105	R1001		L740	N741		V553		R387
SER	SER	MET	I1445	ALA	ALA	ASP	M1106	D1013	L901	L824	N741		P554		L388
PRO	PRO	ALA	I1446	ALA	ALA	Q1187	V1107		L902	I825	N742		D555		
THR	THR	GLY	D1446	GLY	GLY				N903	D826	V743		W556		L391
SER	SER	GLY	GLY	GLY	GLY	W1191	A1108	L1021		K648	K744				V392
PRO	PRO	PHE		PRO	PRO	L1192	K1109	L1022	H906	K830	Q745		P561		

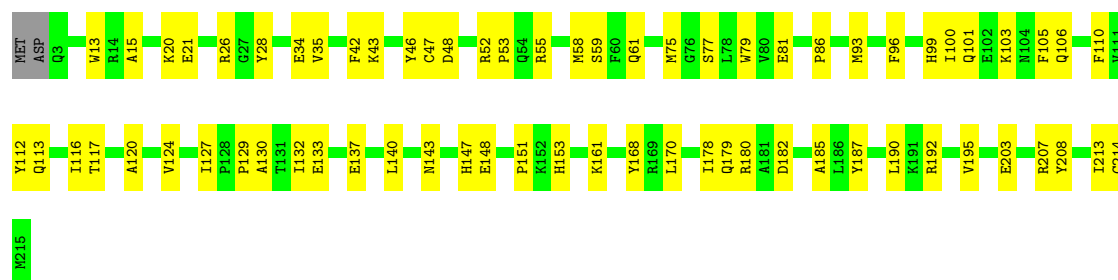




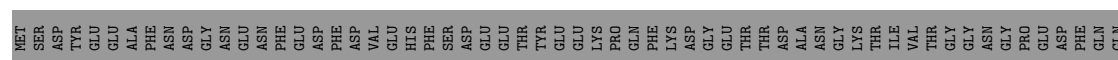
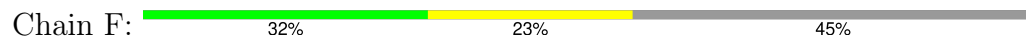
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

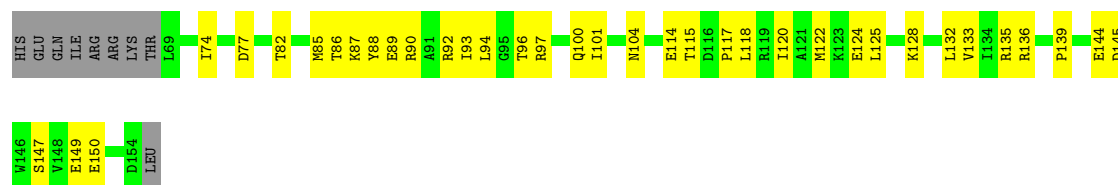


• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

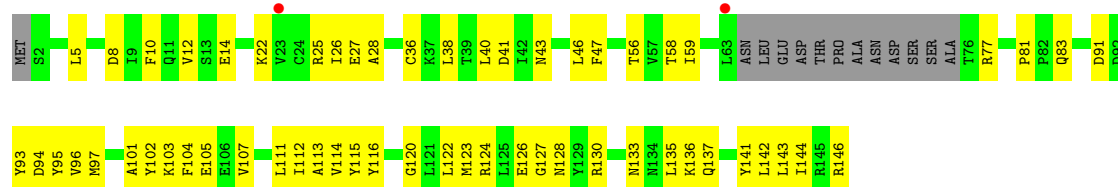


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

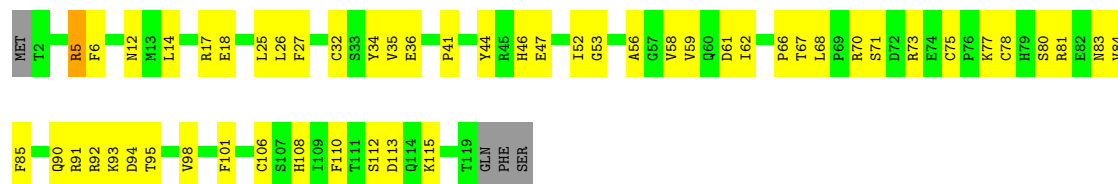




- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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



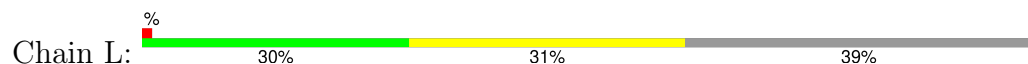
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



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



MET	SER	ARG	GLU	GLY	PHE	GLN	ILE	PRO	THR	ASN	LEU	ASP	ALA	ALA	ALA	GLY	THR	SER	GLN	ALA	ARG	THR	ALA	THR	LEU	K28	Y29	I30	C31	A32	E33	C34	K37	L38	S39	L40	D44	A45	V46	R47	C48	C51	G52	H53	R54	I55	L56	T61	E68	A69	R70
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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 , 117.6	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, 8OG, 2TM, 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:OH	5:B:1074:ASN:OD1	2.24	0.54
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.43	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 ⓘ

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

Continued on next page...

Continued from previous page...

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 ⓘ

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:

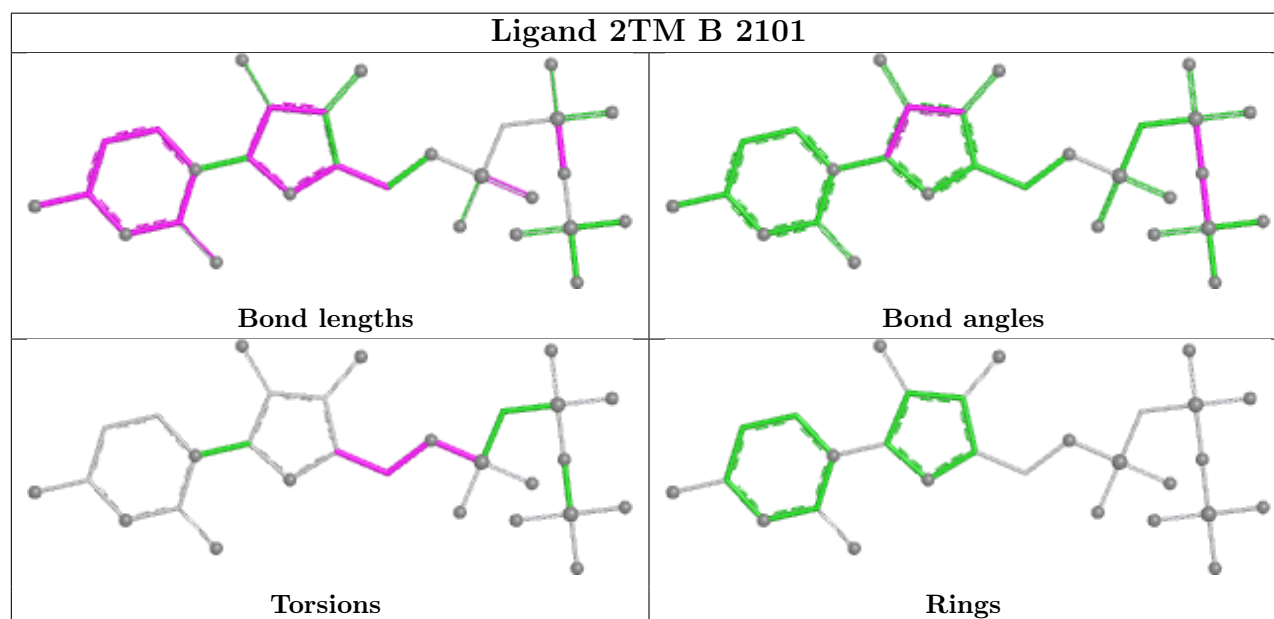
Mol	Chain	Res	Type	Atoms
16	B	2101	2TM	C3'-C4'-C5'-O5'
16	B	2101	2TM	O4'-C4'-C5'-O5'
16	B	2101	2TM	C5'-O5'-PA-O1A
16	B	2101	2TM	C4'-C5'-O5'-PA

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%)	0.00	0 100 100	76, 86, 172, 223	0
2	T	25/29 (86%)	0.15	0 100 100	90, 188, 241, 268	0
3	N	15/18 (83%)	0.19	0 100 100	143, 205, 241, 253	0
4	A	1385/1733 (79%)	-0.07	16 (1%) 76 55	74, 121, 184, 241	0
5	B	1121/1224 (91%)	0.02	18 (1%) 70 49	52, 106, 170, 250	0
6	C	267/318 (83%)	-0.17	2 (0%) 84 67	73, 111, 158, 195	0
7	E	213/215 (99%)	-0.33	0 100 100	83, 144, 211, 252	0
8	F	86/155 (55%)	-0.25	0 100 100	76, 110, 158, 178	0
9	H	133/146 (91%)	-0.03	2 (1%) 71 51	106, 146, 202, 220	0
10	I	118/122 (96%)	-0.06	0 100 100	88, 137, 194, 229	0
11	J	65/70 (92%)	0.14	2 (3%) 51 33	65, 99, 134, 165	0
12	K	114/120 (95%)	-0.23	0 100 100	63, 103, 147, 185	0
13	L	43/70 (61%)	0.08	1 (2%) 61 41	93, 195, 256, 274	0
All	All	3594/4229 (84%)	-0.06	41 (1%) 77 57	52, 118, 188, 274	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	775	LYS	4.7
4	A	103	CYS	3.6
5	B	899	ILE	3.6
13	L	32	ALA	3.5
5	B	819	ALA	3.5
4	A	448	PRO	3.5
4	A	355	GLY	3.4
5	B	525	ALA	3.1
5	B	1130	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	B	386	LEU	2.8
5	B	754	SER	2.6
4	A	921	GLY	2.6
5	B	335	GLY	2.6
4	A	303	TYR	2.6
4	A	466	SER	2.6
9	H	63	LEU	2.5
5	B	533	CYS	2.4
4	A	144	THR	2.4
5	B	1097	HIS	2.4
6	C	178	PHE	2.3
4	A	104	GLU	2.3
4	A	447	GLN	2.3
9	H	23	VAL	2.3
5	B	1214	PRO	2.3
4	A	1267	MET	2.3
5	B	694	ASP	2.2
5	B	647	GLY	2.2
5	B	381	MET	2.2
5	B	1006	ILE	2.2
5	B	300	HIS	2.1
11	J	61	LEU	2.1
4	A	234	MET	2.1
4	A	873	MET	2.1
4	A	488	ASN	2.1
4	A	1098	VAL	2.1
5	B	751	VAL	2.1
4	A	503	GLN	2.0
5	B	806	THR	2.0
6	C	146	LYS	2.0
4	A	932	GLU	2.0
11	J	44	TYR	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](#)

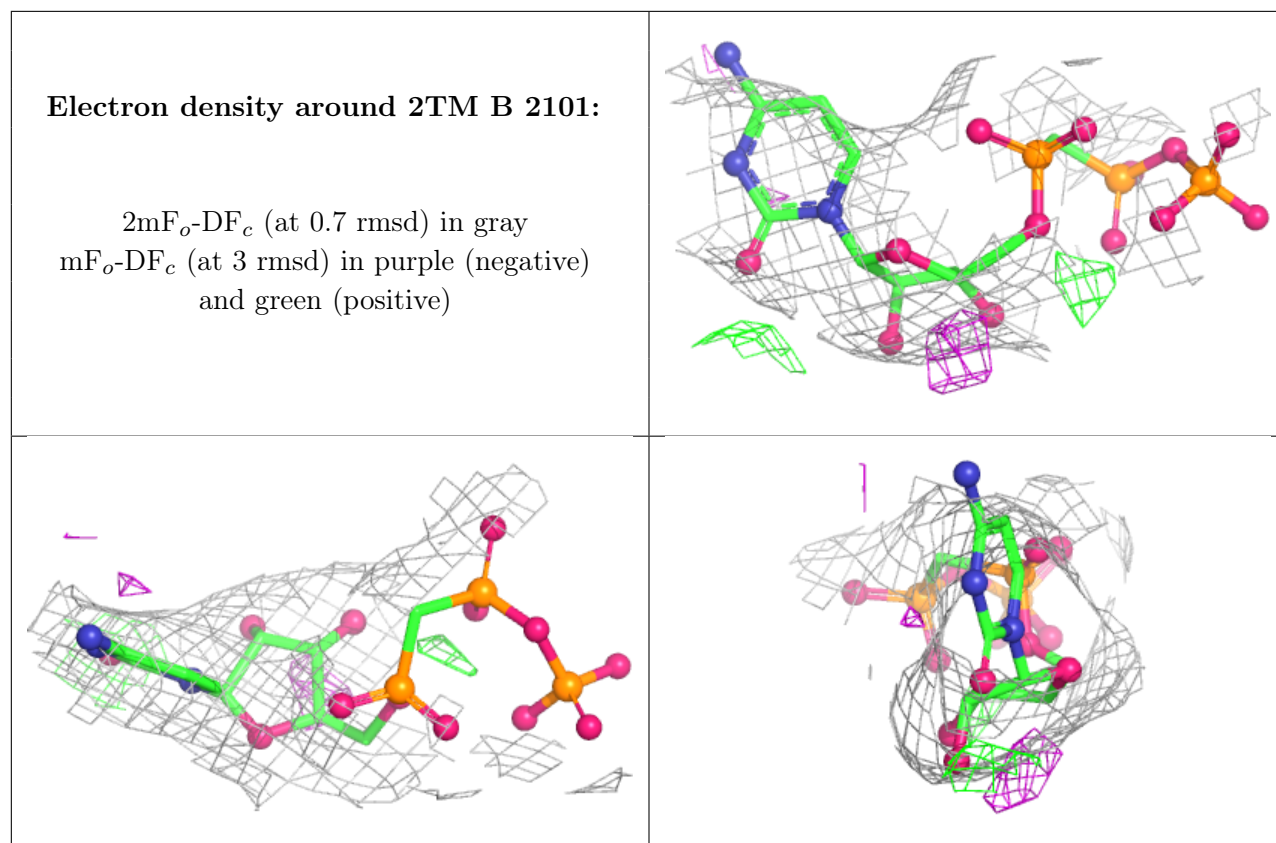
There are no oligosaccharides in this entry.

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(\AA^2)	Q<0.9
14	ZN	I	202	1/1	0.65	0.19	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	0.09	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.