



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:13 AM UTC

PDB ID : 2E2I / pdb_00002e2i
Title : RNA polymerase II elongation complex in 5 mM Mg+2 with 2'-dGTP
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-14
Resolution : 3.41 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

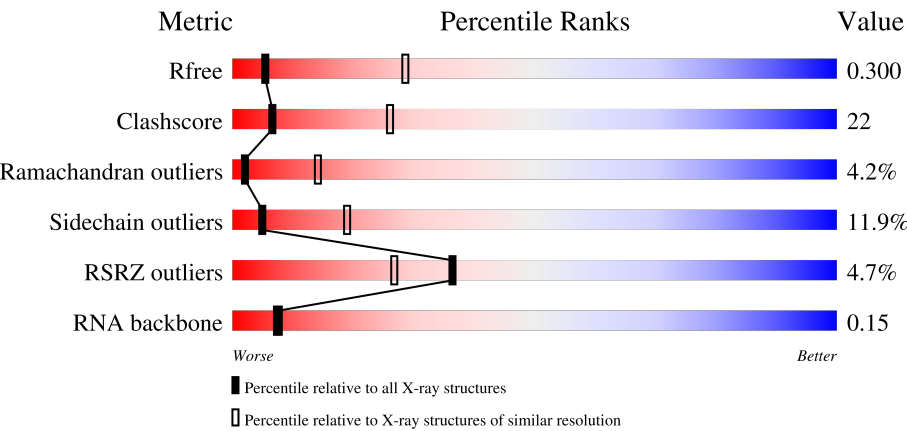
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)
RNA backbone	3983	1162 (3.84-3.00)

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	10	
2	T	28	
3	N	14	
4	A	1733	

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

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29722 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 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			216	98	45	64	9			

- Molecule 2 is a DNA chain called 28-MER DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	28	Total	C	N	O	P	0	0	0
			564	270	102	165	27			

- Molecule 3 is a DNA chain called 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1411	Total	C	N	O	S	0	0	0
			11098	6989	1944	2104	61			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1143	Total	C	N	O	S	0	0	0
			9092	5753	1595	1688	56			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			697	445	118	131	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	134	Total	C	N	O	S	0	0	0
			1076	678	181	212	5			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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 13.6 kDa polypeptide.

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 7.7 kDa polypeptide.

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

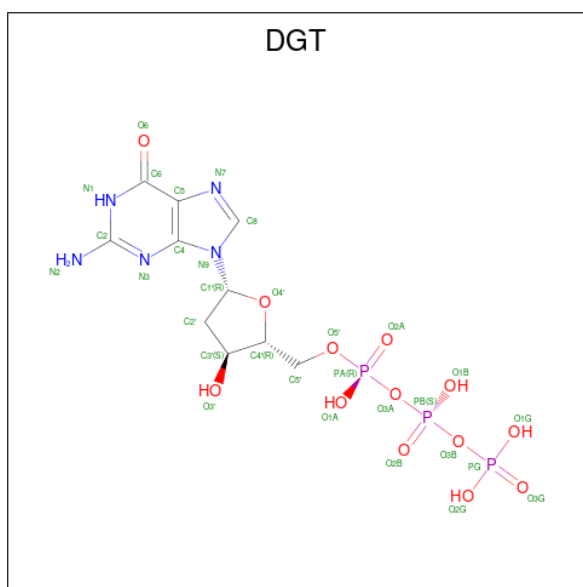
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
16	B	1	Total 62	C 20	N 10	O 26	P 6	0	1

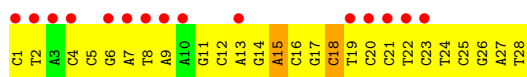
3 Residue-property plots

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.

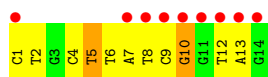
- Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'



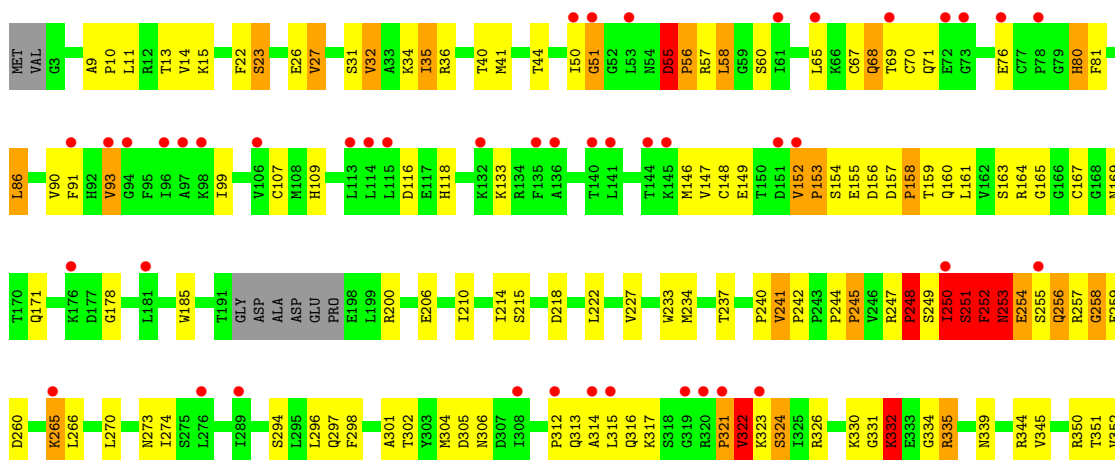
- Molecule 2: 28-MER DNA template strand



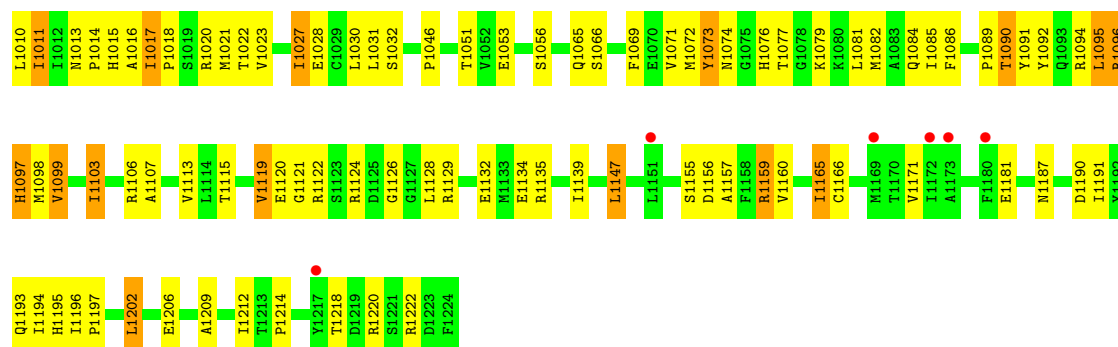
- Molecule 3: 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'



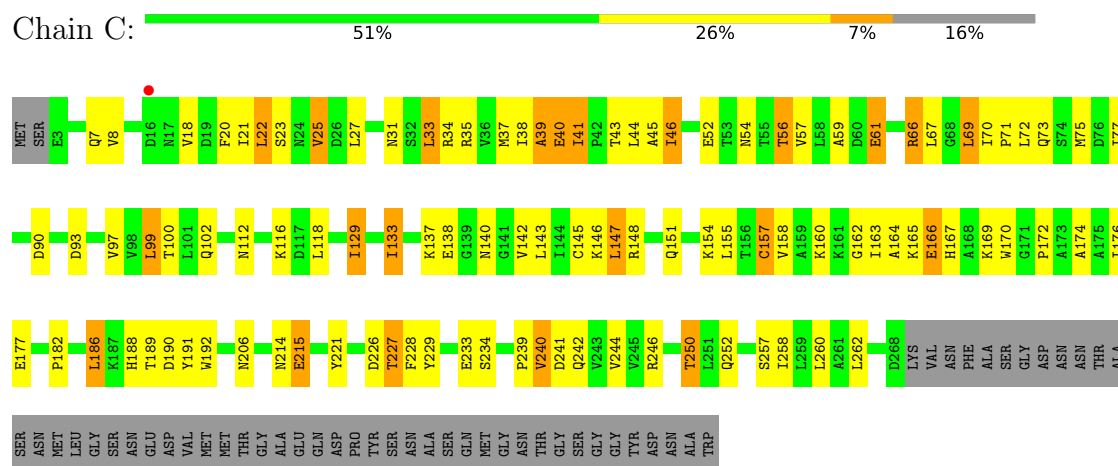
- Molecule 4: DNA-directed RNA polymerase II largest subunit



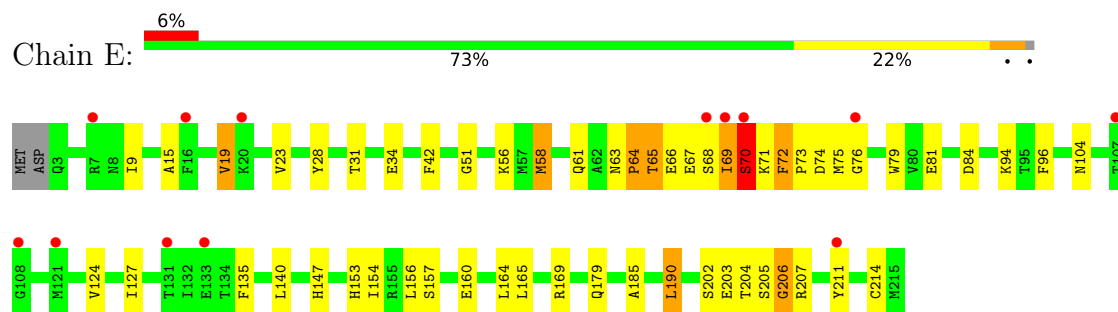
TYR	GLY	ASP	S1383	H1304	SER	T1095	M996	Y897	L808	T709	T596	V512	D438	I353
SER	ALA	GLY	V1384	V1305	PHE	L1101	M998	R896	T809	T709	L597	S513	R439	P357
PRO	THR	GLN	T1385	L1306	ASP	L1106	L998	R899	T809	R711	S599	N517	D440	N358
SER	GLY	ASP	G1388	T1308	Q1187	L1106	R1001	D900	E812	F714	L606	P519	L443	L359
PRO	ALA	GLY	F1389	M1312	L1193	M1106	G1002	L902	H816	V718	I607	G520	P444	E360
SER	THR	VAL	N1390	N1312	R1194	M1106	G1002	L902	A817	V718	I607	G520	L444	L361
TYR	THR	THR	R1391	L1314	D1198	M1112	V1015	T907	H816	V718	I607	G520	P444	L361
SER	PRO	PRO	S1392	S1314	R1199	K1112	V1015	L908	A817	V718	I607	G520	P444	L361
PRO	PRO	TYR	L1393	E1315	R1199	T1113	T1016	D909	R821	L722	D909	G522	Q447	Q363
THR	GLY	SER	T1394	V1316	A1200	P1114	L1017	D909	R821	L722	D909	G522	Q447	Q363
SER	PHE	ASN	G1395	V1316	A1201	S1115	C1018	L913	R821	L722	D909	G522	Q447	Q363
PRO	GLY	GLY	A1396	D1323	M1202	L1116	C1019	L914	R821	L722	D909	G522	Q447	Q363
SER	VAL	SER	L1397	F1324	M1202	T1117	C1019	S915	R821	L722	D909	G522	Q447	Q363
TYR	SER	GLY	M1398	R1325	K1205	V1118	A1027	S915	R821	L722	D909	G522	Q447	Q363
SER	SER	LEU	R1399	R1326	Y1119	Y1118	A1027	S915	R821	L722	D909	G522	Q447	Q363
PRO	PRO	ASN	C1400	I1327	T1219	L1120	R1029	T919	R821	L722	D909	G522	Q447	Q363
THR	GLY	VAL	Y1328	Y1328	F1220	L1120	R1029	T919	R821	L722	D909	G522	Q447	Q363
SER	PHE	ALA	T1329	T1329	L1224	H1124	V1031	K924	R821	L722	D909	G522	Q447	Q363
PRO	SER	ASP	E1403	T1333	F1225	A1125	R1036	K924	R821	L722	D909	G522	Q447	Q363
SER	PRO	LEU	V1406	D1334	F1225	A1125	R1036	K924	R821	L722	D909	G522	Q447	Q363
TYR	THR	ASP	E1407	D1334	F1225	A1125	R1036	K924	R821	L722	D909	G522	Q447	Q363
SER	SER	VAL	T1408	I1335	I1237	Q1128	L1046	L943	R821	L722	D909	G522	Q447	Q363
PRO	PRO	LYS	L1409	M1336	I1238	E1129	S1047	L943	R821	L722	D909	G522	Q447	Q363
THR	THR	ASP	F1410	E1337	R1239	Q1130	M1048	L943	R821	L722	D909	G522	Q447	Q363
SER	GLY	GLY	R1422	V1338	G1240	Q1130	M1048	L943	R821	L722	D909	G522	Q447	Q363
PRO	SER	LEU	G1423	L1339	R1241	I1134	F1053	R940	R821	L722	D909	G522	Q447	Q363
PRO	PRO	MET	V1424	G1340	V1242	I1138	L1054	R940	R821	L722	D909	G522	Q447	Q363
THR	THR	PHE	S1425	I1341	V1243	I1138	L1054	R940	R821	L722	D909	G522	Q447	Q363
PRO	PRO	SER	V1426	E1351	ARG	T1141	V1057	R940	R821	L722	D909	G522	Q447	Q363
THR	ALA	PRO	E1427	R1345	PRO	T1142	V1057	R940	R821	L722	D909	G522	Q447	Q363
SER	THR	LEU	N1428	A1346	LYS	T1142	V1057	R940	R821	L722	D909	G522	Q447	Q363
SER	THR	VAL	R1429	A1347	SER	T1142	V1057	R940	R821	L722	D909	G522	Q447	Q363
PRO	PRO	ASP	Q1432	I1348	LEU	A1149	P1060	Y948	R821	L722	D909	G522	Q447	Q363
THR	THR	SER	M1433	Y1349	ASP	S1150	G1061	Y948	R821	L722	D909	G522	Q447	Q363
PRO	PRO	GLY	E1436	K1350	ALA	E1151	E1062	Y954	R821	L722	D909	G522	Q447	Q363
THR	THR	ASN	G1437	E1351	GLY	I1152	M1063	P955	R821	L722	D909	G522	Q447	Q363
SER	PRO	ASN	T1438	V1352	THR	Y1153	G1064	P957	R821	L722	D909	G522	Q447	Q363
PRO	PRO	ASP	E1446	I1353	GLY	D1154	G1065	P958	R821	L722	D909	G522	Q447	Q363
THR	THR	ALA	S1449	N1354	ALA	D1155	V1066	P959	R821	L722	D909	G522	Q447	Q363
PRO	PRO	MET	E1448	V1355	E1255	P1156	L1067	P959	R821	L722	D909	G522	Q447	Q363
THR	THR	ALA	D1446	I1356	E1255	P1157	L1067	P959	R821	L722	D909	G522	Q447	Q363
PRO	PRO	GLY	E1447	D1359	M1259	P1158	T1077	P959	R821	L722	D909	G522	Q447	Q363
THR	THR	PHE	S1449	V1363	L1260	T1161	Q1078	Q959	R821	L722	D909	G522	Q447	Q363
PRO	PRO	THR	VAL	N1364	M1267	V1162	M1079	Q959	R821	L722	D909	G522	Q447	Q363
PRO	PRO	ALA	LYS	Y1365	I1271	I1163	T1080	Q959	R821	L722	D909	G522	Q447	Q363
THR	THR	GLY	TYR	R1366	T1272	L1172	L1081	Q959	R821	L722	D909	G522	Q447	Q363
SER	PRO	GLY	GLY	H1367	T1272	L1172	L1081	Q959	R821	L722	D909	G522	Q447	Q363
SER	THR	ALA	MET	M1368	I1279	H1173	THR	Q959	R821	L722	D909	G522	Q447	Q363
PRO	PRO	ASP	PRO	A1369	E1280	F1174	PHE	Q959	R821	L722	D909	G522	Q447	Q363
THR	THR	TYR	GLY	L1370	R1281	S1175	THR	Q959	R821	L722	D909	G522	Q447	Q363
SER	PRO	GLY	GLN	L1371	L1176	L1176	THR	Q959	R821	L722	D909	G522	Q447	Q363
PRO	PRO	GLY	LYS	L1372	ASP	LEU	THR	Q959	R821	L722	D909	G522	Q447	Q363
SER	PRO	ALA	ILE	D1373	GLY	GLY	THR	Q959	R821	L722	D909	G522	Q447	Q363
TYR	THR	THR	THR	T1376	V1291	GLY	THR	Q959	R821	L722	D909	G522	Q447	Q363
PRO	PRO	SER	GLY	T1376	V1291	GLY	THR	Q959	R821	L722	D909	G522	Q447	Q363
THR	THR	PHE	GLY	T1382	V1299	GLY	THR	Q959	R821	L722	D909	G522	Q447	Q363



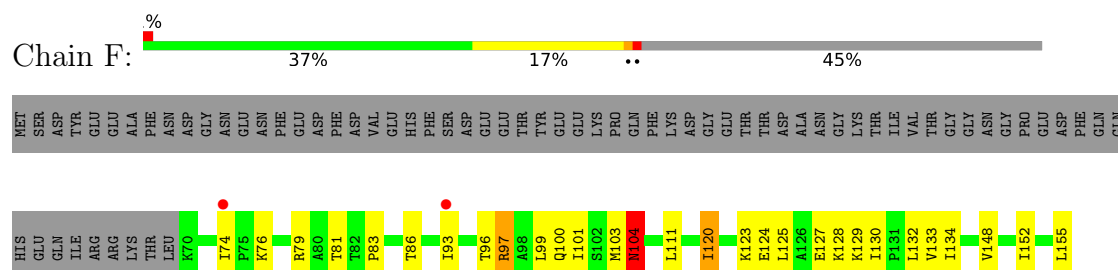
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide



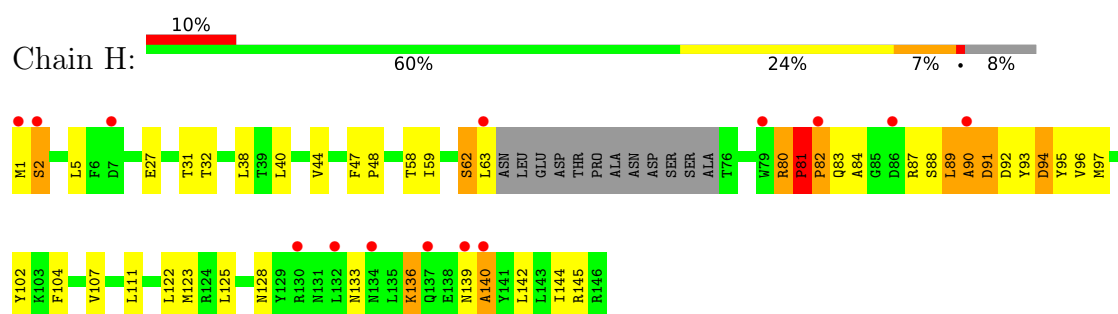
• Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



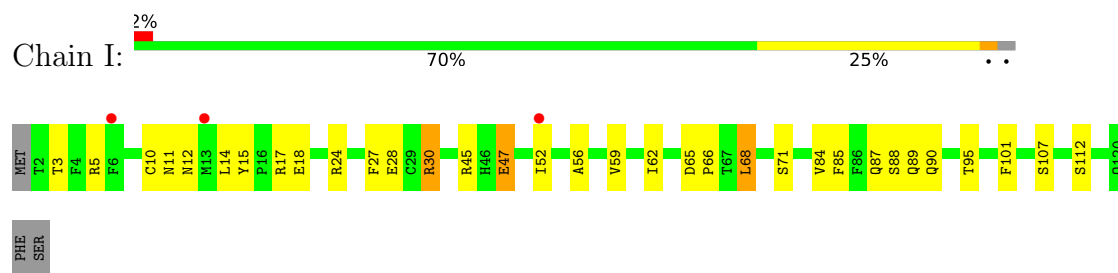
• Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



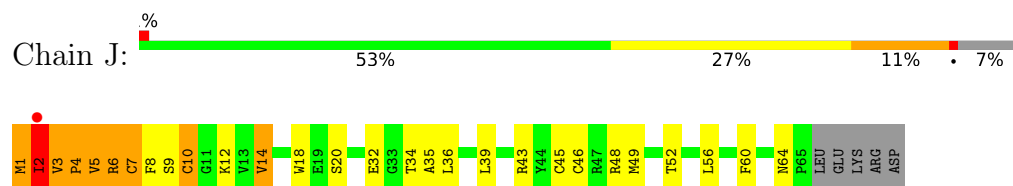
• Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



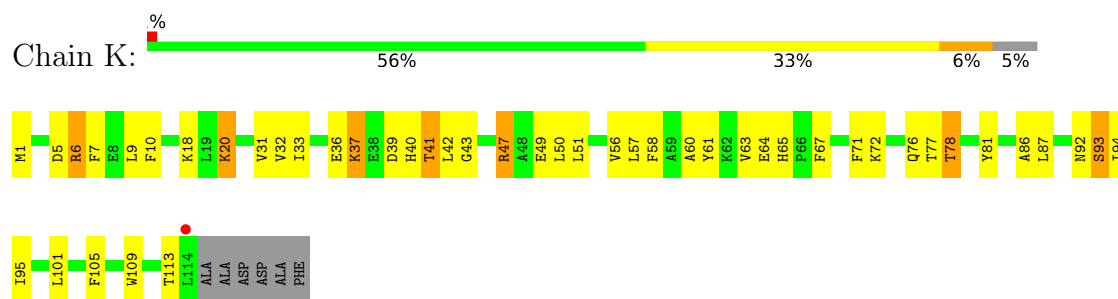
- Molecule 10: DNA-directed RNA polymerase II subunit 9



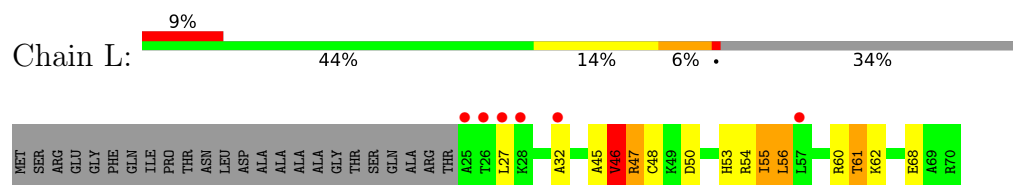
- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10



- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.68Å 223.52Å 193.94Å 90.00° 100.54° 90.00°	Depositor
Resolution (Å)	50.00 – 3.41 50.00 – 3.41	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-3.41) 98.0 (50.00-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.266 , 0.316 0.257 , 0.300	Depositor DCC
R_{free} test set	4732 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	92.7	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 81.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	29722	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, DGT

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	0.74	0/243	1.42	6/378 (1.6%)
2	T	0.37	0/631	1.07	9/970 (0.9%)
3	N	0.31	0/317	0.86	2/488 (0.4%)
4	A	0.82	4/11294 (0.0%)	1.07	32/15270 (0.2%)
5	B	0.99	9/9268 (0.1%)	1.19	47/12496 (0.4%)
6	C	0.87	1/2133 (0.0%)	1.09	5/2891 (0.2%)
7	E	0.64	0/1780	0.92	2/2395 (0.1%)
8	F	0.70	0/709	0.92	0/956
9	H	0.67	1/1094 (0.1%)	0.89	3/1480 (0.2%)
10	I	0.75	1/989 (0.1%)	0.90	2/1331 (0.2%)
11	J	1.00	1/541 (0.2%)	1.21	1/727 (0.1%)
12	K	0.82	1/937 (0.1%)	1.03	0/1265
13	L	1.04	0/365	1.17	0/485
All	All	0.86	18/30301 (0.1%)	1.09	109/41132 (0.3%)

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	7
5	B	0	11
7	E	0	1
11	J	0	2
All	All	0	21

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	507	VAL	CA-CB	8.35	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	846	ILE	CA-CB	-6.34	1.46	1.54
11	J	10	CYS	CA-CB	6.21	1.62	1.53
5	B	1027	ILE	CA-CB	-6.12	1.46	1.54
5	B	882	THR	CA-CB	6.09	1.62	1.53
5	B	882	THR	N-CA	5.92	1.53	1.46
4	A	1080	THR	CA-CB	5.87	1.62	1.53
10	I	52	ILE	CA-CB	5.80	1.60	1.53
9	H	81	PRO	CA-C	5.60	1.57	1.52
5	B	147	LEU	C-O	5.58	1.34	1.23
5	B	825	VAL	CA-CB	5.39	1.60	1.54
5	B	802	PRO	CA-C	5.38	1.59	1.52
5	B	993	THR	CA-C	5.35	1.59	1.53
6	C	61	GLU	CA-C	-5.31	1.45	1.52
4	A	878	ILE	CA-CB	-5.22	1.48	1.54
5	B	992	ILE	N-CA	-5.16	1.40	1.46
4	A	817	ALA	CA-CB	-5.14	1.44	1.53
12	K	39	ASP	CA-C	-5.01	1.48	1.53

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	635	ARG	CA-C-N	11.71	134.48	119.84
5	B	635	ARG	C-N-CA	11.71	134.48	119.84
1	R	9	G	C5'-C4'-C3'	-10.64	100.04	116.00
2	T	18	DC	C4'-C3'-O3'	9.94	124.90	110.00
11	J	9	SER	N-CA-C	8.83	120.91	111.28
2	T	28	DT	C1'-O4'-C4'	-8.30	97.25	109.70
6	C	39	ALA	N-CA-C	7.89	120.48	110.61
5	B	37	PHE	N-CA-C	-7.67	100.40	110.53
5	B	1009	ASP	N-CA-C	-7.20	103.96	112.89
4	A	672	ASP	N-CA-C	7.16	119.55	110.24
5	B	911	ILE	CB-CA-C	-7.11	103.37	111.55
1	R	9	G	P-O3'-C3'	-7.09	109.56	120.20
5	B	798	TYR	CA-C-N	6.94	128.51	119.84
5	B	798	TYR	C-N-CA	6.94	128.51	119.84
5	B	882	THR	N-CA-C	6.88	118.86	111.36
2	T	18	DC	O5'-C5'-C4'	6.86	121.08	110.80
2	T	18	DC	C4'-C3'-C2'	-6.85	92.13	102.40
5	B	678	GLU	N-CA-C	6.83	119.56	111.02
5	B	383	ASN	N-CA-C	-6.81	103.78	111.07
5	B	296	GLU	N-CA-C	-6.75	103.72	112.23
4	A	816	HIS	N-CA-C	-6.57	104.04	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	524	VAL	N-CA-C	6.49	118.06	108.45
5	B	835	GLN	N-CA-C	6.43	119.01	110.53
4	A	445	ASN	N-CA-C	6.30	119.41	110.14
5	B	764	SER	N-CA-C	6.26	123.64	109.81
4	A	1347	ALA	N-CA-C	-6.21	104.44	111.14
5	B	851	PHE	N-CA-C	6.21	120.19	112.24
2	T	18	DC	O4'-C4'-C3'	-6.20	96.09	105.40
10	I	68	LEU	CA-C-N	6.17	126.14	120.03
10	I	68	LEU	C-N-CA	6.17	126.14	120.03
5	B	488	TYR	N-CA-C	-6.13	104.71	111.82
5	B	970	THR	CB-CA-C	-6.05	99.09	110.16
4	A	666	ILE	N-CA-C	-6.04	103.35	111.44
5	B	966	VAL	CB-CA-C	-5.98	102.35	110.42
4	A	1445	ILE	N-CA-C	5.96	116.14	110.53
5	B	1071	VAL	CB-CA-C	-5.90	102.49	111.69
4	A	55	ASP	CA-C-N	5.82	127.12	119.84
4	A	55	ASP	C-N-CA	5.82	127.12	119.84
4	A	1389	PHE	N-CA-C	5.80	119.45	112.38
1	R	9	G	C2'-C3'-O3'	5.80	122.40	113.70
4	A	878	ILE	N-CA-C	5.77	117.94	109.63
6	C	69	LEU	N-CA-C	5.77	119.42	112.38
4	A	476	SER	CA-C-N	-5.76	113.69	119.56
4	A	476	SER	C-N-CA	-5.76	113.69	119.56
1	R	8	G	O3'-P-O5'	-5.74	95.39	104.00
9	H	80	ARG	CA-C-N	5.63	126.17	120.38
9	H	80	ARG	C-N-CA	5.63	126.17	120.38
2	T	18	DC	P-O5'-C5'	5.62	128.42	120.00
2	T	15	DA	P-O3'-C3'	5.61	128.62	120.20
4	A	567	LYS	CA-C-N	5.60	126.84	119.84
4	A	567	LYS	C-N-CA	5.60	126.84	119.84
6	C	174	ALA	CB-CA-C	-5.59	110.12	116.54
5	B	888	GLY	N-CA-C	5.57	121.66	112.30
9	H	92	ASP	N-CA-C	-5.57	106.28	112.57
2	T	18	DC	C1'-O4'-C4'	-5.56	101.36	109.70
4	A	375	THR	N-CA-C	5.56	117.24	108.96
2	T	18	DC	C5'-C4'-C3'	5.55	123.23	114.90
5	B	204	ILE	CB-CA-C	-5.54	102.94	110.42
5	B	552	MET	CA-C-N	-5.53	115.19	120.83
5	B	552	MET	C-N-CA	-5.53	115.19	120.83
5	B	570	VAL	CA-C-N	5.52	124.71	118.97
5	B	570	VAL	C-N-CA	5.52	124.71	118.97
4	A	886	ILE	N-CA-C	5.51	116.17	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	783	THR	CB-CA-C	-5.51	102.20	110.90
4	A	58	LEU	N-CA-C	5.50	117.14	111.03
4	A	1350	LYS	N-CA-C	-5.46	105.33	111.28
5	B	1119	VAL	N-CA-C	5.45	116.16	108.36
5	B	201	GLY	N-CA-C	-5.44	107.76	115.43
5	B	172	ILE	N-CA-C	5.43	115.68	107.75
6	C	93	ASP	N-CA-C	-5.43	106.66	113.28
4	A	562	THR	CA-C-N	5.41	125.17	119.76
4	A	562	THR	C-N-CA	5.41	125.17	119.76
5	B	25	ILE	CB-CA-C	-5.37	105.43	111.45
4	A	1356	ILE	CB-CA-C	-5.36	104.95	111.87
3	N	10	DG	P-O3'-C3'	5.35	128.22	120.20
4	A	867	ILE	N-CA-C	-5.34	100.54	108.45
5	B	1011	ILE	CB-CA-C	-5.34	104.05	110.99
5	B	975	GLN	CA-C-O	5.31	121.02	117.94
5	B	1103	ILE	CB-CA-C	-5.31	102.75	111.51
5	B	895	ASP	N-CA-C	5.28	117.78	111.71
5	B	825	VAL	N-CA-C	5.27	115.44	107.75
5	B	1090	THR	CB-CA-C	-5.26	102.56	110.24
3	N	5	DT	C1'-O4'-C4'	-5.26	101.81	109.70
1	R	9	G	C3'-C2'-O2'	5.25	118.58	110.70
5	B	636	PRO	CA-C-N	5.25	131.15	121.70
5	B	636	PRO	C-N-CA	5.25	131.15	121.70
4	A	474	VAL	N-CA-C	-5.24	107.19	112.17
5	B	983	ARG	N-CA-C	-5.24	106.65	112.57
5	B	230	ALA	N-CA-C	5.22	120.77	113.57
5	B	333	PHE	CA-C-N	5.20	131.06	121.70
5	B	333	PHE	C-N-CA	5.20	131.06	121.70
5	B	845	SER	CA-C-N	5.20	127.21	120.56
5	B	845	SER	C-N-CA	5.20	127.21	120.56
6	C	20	PHE	N-CA-C	5.18	116.95	109.07
4	A	746	MET	N-CA-C	-5.16	105.28	112.45
4	A	513	SER	CA-C-N	5.15	124.76	119.56
4	A	513	SER	C-N-CA	5.15	124.76	119.56
4	A	1352	VAL	N-CA-C	-5.15	105.82	110.82
5	B	66	ASP	N-CA-C	-5.12	105.33	112.30
7	E	63	ASN	CA-C-N	5.12	126.23	119.84
7	E	63	ASN	C-N-CA	5.12	126.23	119.84
5	B	767	ASN	N-CA-C	-5.09	105.82	112.23
4	A	1354	ASN	N-CA-C	5.09	116.83	111.28
5	B	167	ILE	CB-CA-C	-5.07	105.19	111.32
4	A	1036	ARG	N-CA-C	5.05	117.31	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	9	G	P-O5'-C5'	-5.03	113.35	120.90
5	B	99	LYS	CA-C-N	5.01	124.92	119.76
5	B	99	LYS	C-N-CA	5.01	124.92	119.76
4	A	163	SER	N-CA-C	5.01	117.91	109.95

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1175	SER	Peptide
4	A	248	PRO	Peptide
4	A	250	ILE	Peptide
4	A	251	SER	Peptide
4	A	252	PHE	Peptide
4	A	254	GLU	Peptide
4	A	460	VAL	Peptide
5	B	141	ASP	Peptide
5	B	143	PRO	Peptide
5	B	145	ARG	Peptide
5	B	502	ILE	Peptide
5	B	503	GLY	Peptide
5	B	504	ARG	Peptide
5	B	506	GLY	Peptide
5	B	508	LEU	Peptide
5	B	636	PRO	Peptide
5	B	71	LEU	Peptide
5	B	89	GLU	Peptide
7	E	70	SER	Peptide
11	J	3	VAL	Peptide
11	J	4	PRO	Peptide

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	216	0	109	13	0
2	T	564	0	316	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	284	0	161	19	0
4	A	11098	0	11174	450	0
5	B	9092	0	9135	520	0
6	C	2095	0	2051	96	0
7	E	1744	0	1772	47	0
8	F	697	0	720	20	0
9	H	1076	0	1052	35	0
10	I	971	0	928	17	0
11	J	532	0	542	51	0
12	K	919	0	929	40	0
13	L	363	0	388	6	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	62	0	24	2	0
All	All	29722	0	29301	1276	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1276) 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:69:LEU:HG	5:B:70:ILE:CG2	1.32	1.55
2:T:19:DT:H2'	2:T:20:DC:C6	1.41	1.51
5:B:142:VAL:CG1	5:B:144:GLY:HA3	1.43	1.45
5:B:142:VAL:HG13	5:B:144:GLY:CA	1.57	1.34
5:B:69:LEU:CA	5:B:70:ILE:HB	1.58	1.28
5:B:70:ILE:N	5:B:89:GLU:HG3	1.53	1.24
6:C:66:ARG:NH2	11:J:2:ILE:HG13	1.54	1.21
4:A:255:SER:HA	4:A:256:GLN:CB	1.72	1.18
5:B:341:LEU:HB3	5:B:342:GLY:HA2	1.19	1.16
2:T:18:DC:H5''	2:T:19:DT:OP1	1.44	1.16
2:T:19:DT:C2'	2:T:20:DC:C6	2.30	1.15
4:A:253:ASN:HA	4:A:255:SER:HB3	1.29	1.14
5:B:69:LEU:HG	5:B:70:ILE:HG21	1.22	1.13
5:B:504:ARG:HG2	5:B:505:ASP:H	1.00	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:341:LEU:CB	5:B:342:GLY:HA2	1.78	1.12
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.29	1.12
5:B:89:GLU:HA	5:B:90:ILE:HB	1.32	1.12
4:A:567:LYS:HB2	4:A:568:PRO:HD2	1.19	1.11
5:B:69:LEU:CG	5:B:70:ILE:CG2	2.27	1.11
5:B:142:VAL:CG2	5:B:143:PRO:HD2	1.80	1.10
4:A:253:ASN:CA	4:A:255:SER:HB3	1.80	1.10
5:B:287:ARG:HD3	5:B:292:ILE:HA	1.34	1.09
6:C:66:ARG:HH21	11:J:2:ILE:CG1	1.63	1.09
4:A:256:GLN:N	4:A:257:ARG:HA	1.59	1.08
4:A:567:LYS:CB	4:A:568:PRO:HD2	1.83	1.08
5:B:69:LEU:HA	5:B:70:ILE:CB	1.73	1.08
5:B:636:PRO:HB2	5:B:637:LEU:HA	1.10	1.08
5:B:143:PRO:HB2	5:B:144:GLY:HA2	1.29	1.07
5:B:145:ARG:HB2	5:B:146:GLU:HB2	1.26	1.07
5:B:142:VAL:HG22	5:B:143:PRO:CD	1.83	1.07
5:B:502:ILE:N	5:B:502:ILE:HD12	1.68	1.07
5:B:334:ILE:HA	5:B:335:GLY:C	1.79	1.06
5:B:955:THR:HG22	5:B:956:THR:H	1.20	1.06
2:T:20:DC:C2'	2:T:21:DC:H5''	1.86	1.06
5:B:89:GLU:CD	5:B:89:GLU:H	1.55	1.06
4:A:446:ARG:HB2	4:A:487:MET:HE3	1.38	1.05
4:A:255:SER:CA	4:A:256:GLN:HB2	1.79	1.05
4:A:1364:ASN:ND2	4:A:1366:ARG:HG2	1.69	1.05
5:B:69:LEU:HG	5:B:70:ILE:HG22	1.06	1.03
5:B:636:PRO:HB2	5:B:637:LEU:CA	1.87	1.03
4:A:1356:ILE:HG13	4:A:1368:MET:HE2	1.40	1.03
5:B:88:TYR:CD2	5:B:136:THR:HG23	1.93	1.02
6:C:57:VAL:HG11	11:J:60:PHE:HB3	1.40	1.00
5:B:504:ARG:CG	5:B:505:ASP:H	1.74	1.00
5:B:519:TRP:HZ2	5:B:705:MET:HE1	1.21	0.99
4:A:255:SER:HA	4:A:256:GLN:HB2	0.99	0.99
2:T:18:DC:H2''	2:T:19:DT:H5'	1.42	0.99
5:B:145:ARG:HB2	5:B:146:GLU:CB	1.92	0.99
5:B:341:LEU:HB3	5:B:342:GLY:CA	1.93	0.98
2:T:18:DC:C2'	2:T:19:DT:H5'	1.93	0.97
5:B:504:ARG:HG2	5:B:505:ASP:N	1.78	0.97
5:B:69:LEU:CG	5:B:70:ILE:HG22	1.93	0.97
4:A:253:ASN:N	4:A:255:SER:HB3	1.80	0.97
2:T:19:DT:H2''	2:T:20:DC:H5'	1.43	0.96
4:A:153:PRO:HD2	4:A:154:SER:HA	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:89:GLU:CA	5:B:90:ILE:HB	1.96	0.95
4:A:868:TYR:HE1	4:A:1064:VAL:HG11	1.29	0.94
4:A:1364:ASN:HD22	4:A:1366:ARG:HG2	1.32	0.94
5:B:70:ILE:N	5:B:89:GLU:CG	2.30	0.94
2:T:19:DT:H2'	2:T:20:DC:C5	2.02	0.94
5:B:72:GLU:OE2	5:B:73:GLN:HB2	1.70	0.92
5:B:635:ARG:HB2	5:B:636:PRO:HD2	1.52	0.92
5:B:71:LEU:HD13	5:B:71:LEU:O	1.69	0.92
2:T:27:DA:N1	4:A:252:PHE:CE1	2.38	0.92
4:A:1118:VAL:HG23	4:A:1306:LEU:HB2	1.51	0.92
5:B:69:LEU:HA	5:B:70:ILE:HB	0.92	0.91
5:B:899:ILE:HG21	5:B:949:VAL:HG21	1.51	0.91
4:A:316:GLN:HB3	4:A:317:LYS:HB2	1.51	0.91
11:J:8:PHE:H	11:J:49:MET:HE3	1.36	0.90
5:B:143:PRO:HB2	5:B:144:GLY:CA	2.01	0.90
6:C:66:ARG:HH11	6:C:66:ARG:CG	1.84	0.90
2:T:20:DC:H2'	2:T:21:DC:C5'	2.02	0.89
5:B:976:ILE:O	5:B:990:ILE:HB	1.71	0.89
5:B:287:ARG:HG3	5:B:287:ARG:HH11	1.37	0.89
5:B:70:ILE:CA	5:B:89:GLU:HG3	2.03	0.89
5:B:848:ARG:HH22	5:B:996:ARG:NH1	1.71	0.89
4:A:565:ILE:HG23	4:A:567:LYS:HE3	1.55	0.88
5:B:69:LEU:CB	5:B:70:ILE:HB	2.02	0.88
2:T:19:DT:H2''	2:T:20:DC:C5'	2.02	0.88
2:T:18:DC:H3'	2:T:19:DT:H72	1.56	0.88
2:T:27:DA:N1	4:A:252:PHE:CZ	2.42	0.88
11:J:35:ALA:O	11:J:39:LEU:HD12	1.73	0.88
4:A:1017:LEU:HD12	7:E:206:GLY:H	1.38	0.87
7:E:65:THR:HA	7:E:66:GLU:C	2.00	0.87
5:B:798:TYR:HE2	11:J:2:ILE:HG22	1.39	0.87
4:A:1406:VAL:HA	4:A:1409:LEU:HD12	1.57	0.87
5:B:69:LEU:CA	5:B:70:ILE:CB	2.43	0.86
4:A:107:CYS:HA	4:A:171:GLN:HE21	1.39	0.86
4:A:1118:VAL:HG12	4:A:1327:ILE:HD12	1.56	0.86
6:C:66:ARG:NH2	11:J:2:ILE:HG23	1.91	0.86
5:B:519:TRP:CZ2	5:B:705:MET:HE1	2.12	0.85
2:T:19:DT:C2'	2:T:20:DC:H6	1.80	0.85
5:B:139:ALA:N	5:B:140:ILE:HA	1.88	0.85
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.59	0.85
5:B:879:ARG:O	5:B:882:THR:HG22	1.76	0.85
5:B:1084:GLN:HE22	6:C:191:TYR:HA	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:145:ARG:CB	5:B:146:GLU:HB2	2.07	0.84
2:T:18:DC:C5'	2:T:19:DT:OP1	2.22	0.84
4:A:51:GLY:HA2	4:A:56:PRO:HG3	1.57	0.84
5:B:141:ASP:O	5:B:142:VAL:HB	1.76	0.84
5:B:1084:GLN:NE2	6:C:191:TYR:HA	1.92	0.84
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.58	0.84
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.57	0.84
7:E:67:GLU:CB	7:E:68:SER:HA	2.08	0.84
5:B:69:LEU:CG	5:B:70:ILE:HG21	1.98	0.83
3:N:1:DC:H4'	3:N:2:DT:OP1	1.76	0.83
2:T:19:DT:H2'	2:T:20:DC:H6	1.02	0.83
5:B:502:ILE:N	5:B:502:ILE:CD1	2.41	0.83
5:B:338:GLY:HA2	5:B:340:ALA:H	1.43	0.83
4:A:450:LEU:HD12	4:A:450:LEU:H	1.44	0.83
5:B:70:ILE:HG23	5:B:70:ILE:O	1.79	0.83
8:F:97:ARG:HD2	8:F:101:ILE:HD11	1.59	0.83
5:B:88:TYR:CE2	5:B:136:THR:HG23	2.13	0.82
5:B:839:MET:HE1	5:B:980:PHE:HB2	1.61	0.82
6:C:73:GLN:HE21	6:C:75:MET:H	1.27	0.82
5:B:334:ILE:HA	5:B:335:GLY:O	1.77	0.82
7:E:72:PHE:H	7:E:73:PRO:HA	1.43	0.82
4:A:1323:ASP:OD1	4:A:1325:THR:HG22	1.80	0.82
5:B:89:GLU:CD	5:B:89:GLU:N	2.30	0.82
2:T:20:DC:C2'	2:T:21:DC:C5'	2.56	0.82
3:N:7:DA:C2'	3:N:8:DT:H71	2.09	0.81
4:A:256:GLN:N	4:A:257:ARG:CA	2.42	0.81
4:A:901:LEU:H	4:A:926:GLN:HE21	1.28	0.81
4:A:754:SER:H	4:A:757:ASN:HD22	1.24	0.81
5:B:136:THR:HB	5:B:137:TYR:HA	1.61	0.81
5:B:25:ILE:HD11	5:B:653:VAL:HB	1.61	0.81
4:A:256:GLN:H	4:A:257:ARG:HA	1.46	0.81
1:R:8:G:N2	2:T:22:DT:N3	2.29	0.80
5:B:142:VAL:CG1	5:B:144:GLY:CA	2.31	0.80
5:B:504:ARG:CG	5:B:505:ASP:N	2.36	0.79
6:C:43:THR:HG22	6:C:44:LEU:H	1.46	0.79
5:B:142:VAL:HG22	5:B:143:PRO:HD2	0.89	0.79
5:B:378:LEU:O	5:B:378:LEU:HG	1.79	0.79
4:A:316:GLN:HB3	4:A:317:LYS:CB	2.12	0.79
6:C:66:ARG:NH1	11:J:5:VAL:HG23	1.97	0.79
2:T:14:DG:C2	2:T:15:DA:N6	2.49	0.79
2:T:20:DC:H2''	2:T:21:DC:H5''	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:253:ASN:N	4:A:255:SER:CB	2.44	0.79
4:A:885:THR:O	4:A:940:ARG:HG3	1.82	0.79
5:B:287:ARG:HG3	5:B:287:ARG:NH1	1.95	0.79
5:B:71:LEU:O	5:B:71:LEU:CD1	2.30	0.79
4:A:1105:LEU:HD23	4:A:1384:VAL:HG21	1.65	0.78
6:C:66:ARG:NH2	11:J:2:ILE:CG2	2.46	0.78
4:A:90:VAL:HG13	4:A:297:GLN:NE2	1.98	0.78
5:B:72:GLU:CD	5:B:73:GLN:N	2.41	0.78
4:A:401:GLY:O	4:A:435:HIS:CD2	2.37	0.78
5:B:802:PRO:HB3	5:B:1091:TYR:CD1	2.18	0.78
5:B:798:TYR:CE2	11:J:2:ILE:HG22	2.18	0.78
3:N:8:DT:H2''	3:N:9:DC:O5'	1.82	0.78
5:B:1187:ASN:HD21	5:B:1190:ASP:HB3	1.48	0.78
6:C:66:ARG:CZ	11:J:2:ILE:HG21	2.14	0.77
5:B:726:ALA:HB1	5:B:1051:THR:HG21	1.65	0.77
6:C:182:PRO:HG3	6:C:206:ASN:O	1.84	0.77
5:B:472:ALA:HB3	5:B:473:MET:HE3	1.65	0.77
3:N:7:DA:H2''	3:N:8:DT:H71	1.66	0.77
2:T:20:DC:H2'	2:T:21:DC:H5'	1.66	0.77
9:H:81:PRO:CB	9:H:82:PRO:HD2	2.14	0.77
5:B:72:GLU:OE2	5:B:73:GLN:CB	2.32	0.77
5:B:766:ARG:NH2	5:B:1020:ARG:HD3	1.99	0.76
6:C:99:LEU:HD12	6:C:118:LEU:HD22	1.67	0.76
6:C:66:ARG:CZ	11:J:2:ILE:CG2	2.63	0.76
6:C:69:LEU:HD12	11:J:6:ARG:HD3	1.67	0.76
5:B:501:PRO:C	5:B:502:ILE:HD12	2.09	0.76
4:A:153:PRO:CD	4:A:154:SER:HA	2.15	0.76
5:B:955:THR:HG22	5:B:956:THR:N	2.00	0.76
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.68	0.76
4:A:567:LYS:HB2	4:A:568:PRO:CD	2.09	0.75
5:B:344:LYS:HA	5:B:345:LYS:HB3	1.68	0.75
4:A:351:THR:HG22	4:A:352:VAL:N	2.02	0.75
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.21	0.75
4:A:1356:ILE:HG13	4:A:1368:MET:CE	2.15	0.74
6:C:66:ARG:HH21	11:J:2:ILE:HG13	0.70	0.74
2:T:25:DC:H2''	2:T:26:DG:O5'	1.86	0.74
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.19	0.74
4:A:445:ASN:HB3	4:A:455:MET:HG2	1.69	0.74
5:B:329:THR:HA	5:B:332:ASP:HB3	1.70	0.74
5:B:955:THR:HG23	13:L:54:ARG:O	1.86	0.74
2:T:18:DC:H2'	2:T:19:DT:C6	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:654:ARG:H	5:B:657:HIS:HD2	1.33	0.74
5:B:862:GLN:HG2	5:B:963:PHE:HB2	1.68	0.74
5:B:744:HIS:HD2	5:B:746:SER:H	1.36	0.73
13:L:60:ARG:HG3	13:L:61:THR:H	1.51	0.73
6:C:165:LYS:O	12:K:6:ARG:NH1	2.21	0.73
5:B:70:ILE:HA	5:B:89:GLU:CG	2.18	0.73
4:A:1175:SER:OG	4:A:1176:LEU:C	2.31	0.73
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.71	0.73
7:E:75:MET:CB	7:E:76:GLY:HA2	2.19	0.72
4:A:157:ASP:HB3	4:A:158:PRO:HD3	1.71	0.72
4:A:1015:VAL:HG12	4:A:1019:CYS:SG	2.29	0.72
5:B:71:LEU:HD22	5:B:72:GLU:HB2	1.70	0.72
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.54	0.72
5:B:137:TYR:CD2	5:B:138:GLU:HG2	2.25	0.72
4:A:345:VAL:HG12	5:B:1155:SER:HB2	1.70	0.72
5:B:69:LEU:C	5:B:89:GLU:CG	2.62	0.72
5:B:247:GLY:HA2	5:B:418:LYS:HZ1	1.53	0.72
2:T:27:DA:N1	4:A:252:PHE:HE1	1.86	0.72
4:A:401:GLY:C	4:A:435:HIS:CD2	2.68	0.72
4:A:567:LYS:CB	4:A:568:PRO:CD	2.63	0.72
5:B:89:GLU:O	5:B:135:ARG:NH1	2.23	0.72
6:C:66:ARG:NH1	6:C:66:ARG:HG2	2.04	0.72
4:A:741:ASN:HD22	4:A:744:LYS:H	1.35	0.71
5:B:1077:THR:HG23	5:B:1079:LYS:H	1.53	0.71
4:A:351:THR:HG22	4:A:352:VAL:H	1.55	0.71
5:B:756:ILE:HG12	5:B:770:GLN:HG2	1.72	0.71
5:B:287:ARG:HD3	5:B:292:ILE:CA	2.16	0.71
5:B:1106:ARG:HD3	5:B:1126:GLY:O	1.90	0.71
2:T:22:DT:H2'	2:T:23:DC:O4'	1.89	0.71
6:C:112:ASN:ND2	6:C:146:LYS:HG2	2.05	0.71
4:A:249:SER:O	4:A:250:ILE:CG1	2.38	0.71
5:B:906:SER:HB3	5:B:946:ASN:HB2	1.70	0.71
5:B:88:TYR:HD2	5:B:136:THR:HG23	1.52	0.71
11:J:8:PHE:N	11:J:49:MET:HE3	2.06	0.71
4:A:901:LEU:H	4:A:926:GLN:NE2	1.86	0.71
5:B:992:ILE:HD11	12:K:67:PHE:CE2	2.26	0.70
5:B:200:GLY:HA2	5:B:202:TYR:CE2	2.26	0.70
4:A:511:ILE:HA	4:A:521:MET:HE2	1.74	0.70
4:A:834:THR:HG21	4:A:1077:THR:HA	1.73	0.70
5:B:955:THR:CG2	5:B:956:THR:H	2.01	0.70
5:B:1084:GLN:OE1	5:B:1084:GLN:N	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:89:GLU:HA	5:B:90:ILE:CB	2.14	0.70
6:C:242:GLN:HE21	6:C:246:ARG:HE	1.38	0.70
4:A:14:VAL:HB	4:A:1432:GLN:HE22	1.56	0.70
4:A:511:ILE:HG12	4:A:521:MET:CE	2.21	0.70
4:A:133:LYS:HG2	4:A:1391:ARG:HH21	1.55	0.70
4:A:518:LYS:HB2	4:A:519:PRO:HD2	1.74	0.70
5:B:68:THR:O	5:B:69:LEU:HB3	1.92	0.70
5:B:334:ILE:CA	5:B:335:GLY:C	2.62	0.70
5:B:542:MET:HG3	5:B:747:MET:CE	2.21	0.70
6:C:66:ARG:HH11	6:C:66:ARG:HG2	1.54	0.70
5:B:72:GLU:CA	5:B:72:GLU:OE1	2.40	0.70
5:B:345:LYS:H	5:B:348:ARG:H	1.40	0.70
4:A:249:SER:O	4:A:250:ILE:HG13	1.92	0.70
4:A:387:ARG:HH12	4:A:437:MET:HE1	1.56	0.69
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.73	0.69
5:B:69:LEU:C	5:B:89:GLU:HG2	2.18	0.69
7:E:67:GLU:OE1	7:E:67:GLU:HA	1.92	0.69
4:A:302:THR:HA	4:A:305:ASP:O	1.91	0.69
5:B:70:ILE:HA	5:B:89:GLU:HG3	1.75	0.69
4:A:645:LEU:HD11	4:A:649:ILE:HD11	1.75	0.69
4:A:608:ILE:O	4:A:609:ASP:O	2.11	0.69
5:B:542:MET:HE1	5:B:743:ILE:HB	1.75	0.69
4:A:533:LYS:HE3	4:A:745:GLN:HE22	1.58	0.69
5:B:544:CYS:HB2	5:B:634:TYR:CE1	2.28	0.69
4:A:344:ARG:NH2	5:B:1120:GLU:HG3	2.08	0.68
5:B:145:ARG:HB2	5:B:146:GLU:CG	2.23	0.68
4:A:1134:ILE:O	4:A:1138:ILE:HG12	1.92	0.68
4:A:998:LEU:HD12	4:A:1001:ARG:HG3	1.74	0.68
7:E:67:GLU:HB3	7:E:69:ILE:HA	1.75	0.68
5:B:72:GLU:OE1	5:B:72:GLU:HA	1.93	0.68
5:B:515:HIS:HD2	5:B:517:THR:OG1	1.76	0.68
6:C:233:GLU:OE2	11:J:43:ARG:NH2	2.26	0.68
5:B:140:ILE:HG13	5:B:141:ASP:OD1	1.93	0.68
5:B:70:ILE:CA	5:B:89:GLU:CG	2.70	0.68
5:B:71:LEU:HD13	5:B:71:LEU:C	2.19	0.67
5:B:143:PRO:CB	5:B:144:GLY:HA2	2.15	0.67
6:C:66:ARG:HH12	11:J:5:VAL:HG23	1.59	0.67
4:A:91:PHE:H	4:A:297:GLN:HE22	1.42	0.67
4:A:567:LYS:CG	4:A:568:PRO:HD2	2.23	0.67
9:H:1:MET:HE3	9:H:2:SER:OG	1.94	0.67
4:A:55:ASP:H	4:A:56:PRO:HD2	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:142:VAL:HG11	5:B:144:GLY:HA3	1.68	0.67
2:T:15:DA:C2	2:T:16:DC:C5	2.83	0.67
5:B:837:ASP:HB3	5:B:1020:ARG:NH2	2.10	0.67
3:N:7:DA:H2''	3:N:8:DT:C6	2.28	0.67
5:B:783:THR:HG22	5:B:783:THR:O	1.96	0.66
6:C:71:PRO:HB2	6:C:133:ILE:HD12	1.76	0.66
9:H:62:SER:OG	9:H:63:LEU:N	2.27	0.66
4:A:607:ILE:HG12	4:A:612:ILE:HG22	1.75	0.66
5:B:976:ILE:HG23	5:B:977:GLY:H	1.58	0.66
7:E:157:SER:OG	7:E:160:GLU:HG3	1.96	0.66
1:R:8:G:N2	2:T:22:DT:H3	1.93	0.66
4:A:252:PHE:HA	4:A:253:ASN:OD1	1.95	0.66
4:A:1064:VAL:HG12	4:A:1370:LEU:HD22	1.78	0.66
5:B:72:GLU:OE2	5:B:73:GLN:CG	2.43	0.66
4:A:251:SER:O	4:A:253:ASN:HB3	1.96	0.66
4:A:500:GLU:O	4:A:500:GLU:HG2	1.96	0.66
5:B:848:ARG:NH2	5:B:996:ARG:NH1	2.44	0.66
4:A:244:PRO:HB2	4:A:245:PRO:HD3	1.78	0.66
4:A:888:GLY:O	4:A:940:ARG:NH2	2.28	0.66
4:A:993:LEU:HD22	4:A:1046:LEU:HG	1.78	0.66
5:B:1032:SER:HB3	5:B:1089:PRO:HB2	1.78	0.66
4:A:381:THR:OG1	4:A:382:PRO:HD2	1.95	0.66
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.76	0.66
5:B:88:TYR:CE2	5:B:136:THR:CG2	2.78	0.66
5:B:341:LEU:HB2	5:B:342:GLY:HA2	1.75	0.66
4:A:534:LEU:O	4:A:574:GLY:HA3	1.96	0.66
4:A:1339:LEU:HD13	7:E:147:HIS:CD2	2.31	0.66
4:A:1364:ASN:HD21	4:A:1366:ARG:NH1	1.93	0.66
5:B:114:PRO:HG3	5:B:181:LEU:HD11	1.78	0.66
5:B:287:ARG:NE	5:B:292:ILE:O	2.29	0.65
5:B:766:ARG:HH22	5:B:1020:ARG:HD3	1.57	0.65
12:K:65:HIS:HD2	12:K:67:PHE:H	1.44	0.65
5:B:70:ILE:O	5:B:71:LEU:CB	2.44	0.65
5:B:341:LEU:CB	5:B:342:GLY:CA	2.62	0.65
5:B:254:LEU:CD2	5:B:381:MET:HE1	2.26	0.65
7:E:75:MET:HB2	7:E:76:GLY:HA2	1.78	0.65
5:B:25:ILE:HG22	5:B:29:ASP:HB2	1.78	0.65
4:A:858:ASN:C	4:A:858:ASN:HD22	2.02	0.65
5:B:980:PHE:O	5:B:981:ALA:HB2	1.96	0.65
2:T:4:DC:H2''	2:T:5:DC:O5'	1.96	0.65
4:A:164:ARG:HB3	4:A:165:GLY:HA2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:70:ILE:CG2	5:B:70:ILE:O	2.45	0.65
5:B:125:SER:HB3	5:B:171:PRO:HA	1.79	0.65
7:E:202:SER:OG	7:E:204:THR:HG22	1.97	0.65
6:C:66:ARG:HE	11:J:2:ILE:HG12	1.61	0.65
5:B:216:GLU:HB3	5:B:500:THR:HG23	1.79	0.64
5:B:766:ARG:NH2	5:B:1020:ARG:CD	2.60	0.64
4:A:255:SER:CA	4:A:256:GLN:CB	2.55	0.64
4:A:535:THR:O	4:A:575:LYS:HE2	1.97	0.64
5:B:286:PHE:HB3	5:B:297:ILE:HD12	1.78	0.64
5:B:843:GLN:HA	5:B:846:ILE:HD12	1.79	0.64
2:T:14:DG:N2	2:T:15:DA:H62	1.94	0.64
6:C:46:ILE:CG2	6:C:157:CYS:HB3	2.27	0.64
5:B:70:ILE:O	5:B:71:LEU:HG	1.98	0.64
5:B:71:LEU:CD1	5:B:71:LEU:C	2.71	0.64
6:C:66:ARG:HH11	6:C:66:ARG:HG3	1.62	0.64
5:B:70:ILE:H	5:B:89:GLU:HG3	1.60	0.64
5:B:502:ILE:HG22	5:B:503:GLY:N	2.12	0.64
9:H:63:LEU:C	9:H:90:ALA:HB3	2.23	0.64
5:B:71:LEU:O	5:B:88:TYR:N	2.30	0.64
7:E:67:GLU:HB2	7:E:68:SER:HA	1.80	0.64
2:T:8:DT:H2''	2:T:9:DA:O5'	1.97	0.64
4:A:608:ILE:O	4:A:609:ASP:C	2.41	0.64
5:B:327:ARG:O	5:B:330:ALA:HB3	1.97	0.64
6:C:27:LEU:HD12	6:C:228:PHE:HE2	1.62	0.64
10:I:68:LEU:HB3	10:I:84:VAL:HG13	1.79	0.63
4:A:690:VAL:HG22	4:A:718:VAL:HG13	1.79	0.63
3:N:7:DA:H2''	3:N:8:DT:C7	2.28	0.63
5:B:141:ASP:OD1	5:B:141:ASP:N	2.30	0.63
4:A:1152:ILE:HG12	4:A:1260:LEU:HD23	1.79	0.63
5:B:502:ILE:HD12	5:B:502:ILE:H	1.61	0.63
5:B:843:GLN:O	5:B:843:GLN:HG3	1.98	0.63
4:A:215:SER:HB3	4:A:218:ASP:CG	2.24	0.63
4:A:567:LYS:HG3	4:A:568:PRO:CD	2.29	0.63
4:A:1364:ASN:HD21	4:A:1366:ARG:HH11	1.43	0.63
5:B:46:GLN:OE1	5:B:408:LEU:HD21	1.99	0.63
4:A:637:LYS:HB3	4:A:641:VAL:HG11	1.81	0.63
5:B:635:ARG:CB	5:B:636:PRO:HD2	2.20	0.63
8:F:132:LEU:O	8:F:148:VAL:HG23	1.99	0.63
5:B:69:LEU:CD1	5:B:70:ILE:HG21	2.29	0.63
5:B:72:GLU:OE1	5:B:72:GLU:C	2.42	0.63
5:B:1016:ALA:CB	5:B:1020:ARG:HH21	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:874:ASP:CA	4:A:1058:VAL:HG23	2.29	0.62
7:E:42:PHE:HZ	7:E:58:MET:HE2	1.63	0.62
4:A:255:SER:C	4:A:257:ARG:HA	2.23	0.62
4:A:1118:VAL:CG2	4:A:1306:LEU:HB2	2.29	0.62
5:B:634:TYR:CE1	5:B:692:TYR:CD1	2.87	0.62
4:A:23:SER:O	4:A:27:VAL:HG23	1.99	0.62
5:B:1084:GLN:NE2	6:C:192:TRP:H	1.98	0.62
4:A:741:ASN:ND2	4:A:744:LYS:H	1.96	0.62
5:B:58:THR:O	5:B:62:ILE:HG12	1.99	0.62
3:N:7:DA:H2''	3:N:8:DT:C5	2.35	0.62
4:A:901:LEU:HD22	4:A:919:ILE:HG22	1.81	0.62
4:A:330:LYS:HG2	4:A:331:GLY:H	1.65	0.61
5:B:889:THR:HG22	5:B:891:ASP:HB2	1.82	0.61
5:B:1084:GLN:HE22	6:C:192:TRP:H	1.46	0.61
10:I:15:TYR:CD1	10:I:30:ARG:HD3	2.35	0.61
5:B:504:ARG:HD2	5:B:504:ARG:C	2.25	0.61
6:C:241:ASP:HB3	12:K:109:TRP:CE2	2.35	0.61
4:A:32:VAL:O	4:A:57:ARG:HD2	2.00	0.61
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.31	0.61
6:C:73:GLN:HE21	6:C:75:MET:N	1.95	0.61
3:N:12:DT:H2''	3:N:13:DA:C8	2.36	0.61
5:B:515:HIS:H	5:B:518:HIS:CD2	2.19	0.61
6:C:46:ILE:HG23	6:C:157:CYS:HB3	1.82	0.61
7:E:15:ALA:O	7:E:19:VAL:HG23	2.00	0.61
9:H:38:LEU:HD13	9:H:125:LEU:HD13	1.83	0.61
5:B:70:ILE:O	5:B:71:LEU:HB3	2.01	0.61
4:A:389:THR:OG1	4:A:426:LEU:HD12	2.01	0.61
3:N:7:DA:C2'	3:N:8:DT:C7	2.78	0.61
4:A:955:PRO:O	4:A:956:LEU:HG	2.00	0.61
5:B:542:MET:HE2	5:B:747:MET:HG3	1.83	0.61
6:C:66:ARG:NH2	11:J:2:ILE:CG1	2.39	0.61
9:H:82:PRO:O	9:H:83:GLN:HB2	1.99	0.61
5:B:72:GLU:OE2	5:B:73:GLN:HG3	2.01	0.60
2:T:8:DT:C2'	2:T:9:DA:C8	2.84	0.60
5:B:975:GLN:HG2	5:B:976:ILE:H	1.66	0.60
7:E:67:GLU:HB3	7:E:68:SER:HA	1.81	0.60
9:H:38:LEU:HD11	9:H:123:MET:HE2	1.83	0.60
9:H:81:PRO:HB2	9:H:82:PRO:HD2	1.82	0.60
2:T:18:DC:H2''	2:T:19:DT:C5'	2.26	0.60
5:B:89:GLU:CB	5:B:90:ILE:HB	2.31	0.60
5:B:1017:ILE:H	5:B:1018:PRO:HD2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:19:DT:H2''	2:T:20:DC:O4'	2.01	0.60
2:T:27:DA:N1	4:A:252:PHE:HZ	1.96	0.60
5:B:464:GLY:HA2	5:B:479:VAL:O	2.01	0.60
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.01	0.60
6:C:33:LEU:HD12	6:C:37:MET:HE2	1.84	0.60
2:T:19:DT:C2'	2:T:20:DC:H5'	2.26	0.60
3:N:4:DC:H2''	3:N:5:DT:OP2	2.02	0.60
4:A:1333:ILE:O	4:A:1337:GLU:HG3	2.02	0.60
5:B:482:VAL:O	5:B:483:LEU:C	2.43	0.60
3:N:7:DA:H2'	3:N:8:DT:H71	1.82	0.60
5:B:256:VAL:HG11	5:B:382:ILE:HD13	1.83	0.60
4:A:915:SER:O	4:A:919:ILE:HG12	2.02	0.60
5:B:744:HIS:CD2	5:B:746:SER:OG	2.54	0.59
5:B:344:LYS:HB3	5:B:345:LYS:O	2.02	0.59
5:B:678:GLU:O	5:B:678:GLU:HG2	2.01	0.59
10:I:17:ARG:HH12	10:I:28:GLU:CD	2.10	0.59
4:A:996:ASN:HA	4:A:998:LEU:HD23	1.83	0.59
9:H:139:ASN:O	9:H:140:ALA:HB3	2.02	0.59
2:T:18:DC:H3'	2:T:19:DT:C7	2.32	0.59
4:A:805:LEU:HG	4:A:805:LEU:O	2.02	0.59
4:A:567:LYS:HG3	4:A:568:PRO:HG2	1.83	0.59
4:A:834:THR:HG21	4:A:1077:THR:CA	2.33	0.59
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.84	0.59
5:B:847:ASP:HB3	6:C:167:HIS:CE1	2.38	0.59
4:A:34:LYS:HD3	4:A:36:ARG:HH22	1.67	0.59
4:A:351:THR:HG21	4:A:466:SER:O	2.03	0.59
4:A:1174:PHE:HB3	4:A:1175:SER:HB3	1.85	0.59
5:B:504:ARG:C	5:B:504:ARG:CD	2.73	0.59
4:A:351:THR:HG23	5:B:1103:ILE:HG12	1.83	0.59
12:K:65:HIS:CD2	12:K:67:PHE:HB2	2.37	0.59
13:L:32:ALA:HB3	13:L:55:ILE:HD12	1.85	0.59
5:B:136:THR:HB	5:B:137:TYR:CA	2.33	0.59
5:B:211:VAL:O	5:B:480:SER:HA	2.03	0.59
7:E:135:PHE:HB3	7:E:140:LEU:HD11	1.84	0.59
5:B:287:ARG:HH11	5:B:287:ARG:CG	2.11	0.59
5:B:507:LYS:O	5:B:508:LEU:HB2	2.01	0.59
5:B:732:SER:HB2	5:B:734:HIS:CD2	2.38	0.59
5:B:70:ILE:CD1	5:B:70:ILE:C	2.76	0.58
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.85	0.58
6:C:67:LEU:HD11	6:C:155:LEU:HD13	1.85	0.58
5:B:411:PRO:HA	5:B:414:ALA:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:573:SER:O	4:A:576:GLN:HB2	2.04	0.58
4:A:675:THR:O	4:A:679:ILE:HG13	2.04	0.58
5:B:839:MET:HE1	5:B:980:PHE:CB	2.33	0.58
4:A:1116:LEU:HD13	4:A:1329:THR:HG23	1.85	0.58
5:B:248:SER:O	5:B:249:ARG:HB2	2.01	0.58
5:B:370:PHE:HD2	5:B:373:ARG:HG3	1.68	0.58
12:K:81:TYR:HE2	12:K:86:ALA:HB2	1.68	0.58
5:B:139:ALA:N	5:B:140:ILE:CA	2.63	0.58
5:B:142:VAL:HG13	5:B:144:GLY:HA3	0.66	0.58
4:A:618:GLU:HG3	4:A:620:LYS:H	1.69	0.58
4:A:1422:ARG:HH21	5:B:1220:ARG:HD2	1.68	0.58
5:B:834:ASN:HB3	5:B:840:ILE:HD12	1.86	0.58
5:B:977:GLY:H	5:B:1099:VAL:HG21	1.69	0.58
4:A:1339:LEU:CD1	7:E:147:HIS:CD2	2.87	0.58
5:B:361:LEU:O	5:B:363:HIS:O	2.22	0.58
5:B:504:ARG:HD2	5:B:505:ASP:N	2.18	0.58
5:B:610:ASN:HB3	5:B:613:VAL:HG23	1.86	0.58
5:B:1073:TYR:N	5:B:1073:TYR:CD1	2.70	0.58
7:E:64:PRO:HB3	7:E:75:MET:HG3	1.86	0.58
4:A:148:CYS:SG	4:A:167:CYS:HB3	2.44	0.58
4:A:874:ASP:HA	4:A:1058:VAL:HG23	1.86	0.57
5:B:1106:ARG:HG3	5:B:1107:ALA:N	2.18	0.57
4:A:549:MET:SD	4:A:577:ILE:HD13	2.44	0.57
5:B:89:GLU:HB2	5:B:90:ILE:O	2.04	0.57
5:B:1084:GLN:HE22	6:C:192:TRP:N	2.02	0.57
9:H:47:PHE:HB3	9:H:95:TYR:HD1	1.69	0.57
4:A:622:VAL:HG22	4:A:622:VAL:O	2.04	0.57
11:J:2:ILE:HG23	11:J:3:VAL:O	2.04	0.57
4:A:672:ASP:H	4:A:736:ASN:HD21	1.52	0.57
11:J:32:GLU:O	11:J:36:LEU:HD23	2.04	0.57
4:A:767:GLN:HG3	4:A:768:GLN:N	2.20	0.57
5:B:542:MET:HG3	5:B:747:MET:HE3	1.85	0.57
2:T:16:DC:H2'	2:T:17:DG:C8	2.40	0.57
2:T:18:DC:C3'	2:T:19:DT:H5'	2.34	0.57
4:A:483:ASP:HA	5:B:988:GLY:HA2	1.87	0.57
6:C:147:LEU:HB3	6:C:151:GLN:HB2	1.87	0.57
4:A:55:ASP:O	4:A:57:ARG:N	2.38	0.57
5:B:176:SER:O	5:B:182:SER:HB3	2.04	0.57
4:A:466:SER:HB3	5:B:1103:ILE:HD11	1.87	0.57
4:A:793:SER:HB2	4:A:794:PRO:HD2	1.86	0.57
5:B:287:ARG:NH1	5:B:324:ILE:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:66:ARG:NE	11:J:2:ILE:HG21	2.19	0.57
4:A:240:PRO:HG2	5:B:1209:ALA:HA	1.87	0.57
4:A:1193:LEU:HD21	4:A:1267:MET:HE2	1.85	0.57
5:B:70:ILE:HA	5:B:89:GLU:CD	2.29	0.57
5:B:195:CYS:HB3	5:B:782:LEU:HD22	1.86	0.57
5:B:344:LYS:HB3	5:B:345:LYS:C	2.29	0.57
5:B:519:TRP:HZ2	5:B:705:MET:CE	2.07	0.57
4:A:1128:GLN:HB3	4:A:1304:TRP:NE1	2.20	0.57
2:T:8:DT:H2"	2:T:9:DA:C8	2.39	0.56
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.86	0.56
4:A:253:ASN:O	4:A:253:ASN:ND2	2.38	0.56
5:B:90:ILE:O	5:B:90:ILE:HG22	2.04	0.56
5:B:881:ASN:HB2	5:B:933:SER:OG	2.05	0.56
5:B:69:LEU:HG	5:B:70:ILE:CB	2.25	0.56
4:A:265:LYS:HD3	4:A:313:GLN:HE22	1.69	0.56
5:B:1004:GLU:O	6:C:177:GLU:HG2	2.05	0.56
2:T:23:DC:C4	2:T:24:DT:H73	2.40	0.56
4:A:1161:THR:HG22	4:A:1163:ILE:N	2.20	0.56
5:B:502:ILE:HG22	5:B:503:GLY:H	1.70	0.56
5:B:174:LEU:HD22	5:B:204:ILE:HD11	1.88	0.56
5:B:756:ILE:HG12	5:B:770:GLN:CG	2.35	0.56
5:B:837:ASP:HB3	5:B:1020:ARG:HH22	1.70	0.56
4:A:335:ARG:HA	4:A:339:ASN:HB2	1.88	0.56
4:A:357:PRO:HD2	5:B:833:TYR:CZ	2.41	0.56
4:A:894:GLU:C	4:A:896:ARG:H	2.12	0.56
4:A:1364:ASN:HD21	4:A:1366:ARG:HG2	1.64	0.56
5:B:70:ILE:O	5:B:71:LEU:CG	2.53	0.56
5:B:975:GLN:HG2	5:B:976:ILE:N	2.20	0.56
11:J:7:CYS:HB2	11:J:49:MET:HG2	1.86	0.56
4:A:68:GLN:HG3	4:A:68:GLN:O	2.05	0.56
12:K:61:TYR:HA	12:K:72:LYS:O	2.05	0.56
4:A:380:VAL:HG23	4:A:430:TRP:O	2.06	0.56
4:A:853:ASP:C	4:A:855:THR:H	2.13	0.56
5:B:798:TYR:HE2	11:J:2:ILE:CG2	2.15	0.56
5:B:805:THR:HG22	5:B:809:MET:SD	2.46	0.56
9:H:81:PRO:HB3	9:H:82:PRO:HD2	1.87	0.56
6:C:8:VAL:HG11	12:K:105:PHE:HD1	1.70	0.56
9:H:81:PRO:CB	9:H:82:PRO:CD	2.83	0.56
9:H:104:PHE:CE1	9:H:136:LYS:HG3	2.41	0.56
5:B:471:LYS:HD2	5:B:471:LYS:O	2.06	0.55
4:A:531:ILE:HG13	4:A:653:VAL:HG21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:868:TYR:HE1	4:A:1064:VAL:CG1	2.13	0.55
5:B:142:VAL:HG21	5:B:145:ARG:CG	2.36	0.55
5:B:654:ARG:H	5:B:657:HIS:CD2	2.20	0.55
2:T:1:DC:H2'	2:T:2:DT:C7	2.37	0.55
5:B:217:ARG:NH1	5:B:407:ASP:OD1	2.40	0.55
4:A:841:LEU:HD21	4:A:1105:LEU:HD21	1.88	0.55
4:A:1017:LEU:HB2	7:E:205:SER:HA	1.87	0.55
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.89	0.55
4:A:1053:PHE:O	4:A:1056:SER:N	2.36	0.55
5:B:71:LEU:N	5:B:71:LEU:HD12	2.21	0.55
5:B:408:LEU:HD22	5:B:545:ILE:HD13	1.88	0.55
6:C:7:GLN:HB2	6:C:23:SER:HB2	1.87	0.55
4:A:849:MET:CE	4:A:1061:GLY:HA2	2.37	0.55
5:B:72:GLU:OE1	5:B:73:GLN:HG2	2.05	0.55
5:B:848:ARG:NH1	11:J:8:PHE:O	2.33	0.55
5:B:975:GLN:N	5:B:978:ASP:OD2	2.40	0.55
7:E:42:PHE:HZ	7:E:58:MET:CE	2.18	0.55
12:K:49:GLU:HG3	12:K:94:ILE:HG13	1.89	0.55
2:T:5:DC:H2''	2:T:6:DG:C8	2.42	0.55
2:T:16:DC:C2'	2:T:17:DG:C8	2.90	0.55
4:A:116:ASP:HB2	4:A:118:HIS:HD2	1.71	0.55
5:B:797:TYR:O	11:J:1:MET:HG2	2.06	0.55
6:C:166:GLU:HG3	12:K:10:PHE:HZ	1.71	0.55
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.87	0.55
1:R:9:G:N2	2:T:20:DC:O2	2.40	0.55
4:A:775:ILE:HG13	4:A:798:GLY:HA3	1.89	0.55
2:T:27:DA:C6	4:A:252:PHE:HE1	2.25	0.55
5:B:801:LYS:O	11:J:52:THR:HG23	2.07	0.55
5:B:944:THR:HG21	5:B:1122:ARG:HH12	1.71	0.55
2:T:5:DC:C2	2:T:6:DG:C5	2.95	0.55
4:A:1364:ASN:ND2	4:A:1366:ARG:H	2.06	0.55
5:B:119:LEU:HD22	5:B:953:LEU:HD11	1.88	0.55
5:B:1017:ILE:HB	5:B:1018:PRO:HD3	1.88	0.55
4:A:249:SER:O	4:A:250:ILE:HG12	2.07	0.54
5:B:363:HIS:O	5:B:364:ILE:HB	2.07	0.54
5:B:978:ASP:HB2	5:B:980:PHE:HE1	1.72	0.54
2:T:1:DC:H2''	2:T:2:DT:C6	2.42	0.54
4:A:499:ALA:C	4:A:501:LEU:H	2.12	0.54
4:A:828:ALA:HB1	5:B:530:GLY:HA2	1.88	0.54
5:B:113:TYR:O	5:B:114:PRO:C	2.50	0.54
6:C:66:ARG:NH2	11:J:3:VAL:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:2:SER:HB3	9:H:62:SER:OG	2.07	0.54
5:B:72:GLU:CD	5:B:72:GLU:C	2.73	0.54
6:C:226:ASP:O	6:C:227:THR:HB	2.07	0.54
4:A:821:ARG:HH11	4:A:821:ARG:HB2	1.71	0.54
4:A:1017:LEU:CD1	7:E:206:GLY:H	2.13	0.54
5:B:504:ARG:CD	5:B:505:ASP:N	2.69	0.54
7:E:205:SER:OG	7:E:205:SER:O	2.19	0.54
4:A:596:THR:C	4:A:598:LEU:H	2.16	0.54
5:B:542:MET:HG3	5:B:747:MET:HE2	1.88	0.54
5:B:803:LEU:H	5:B:822:ASN:HD21	1.54	0.54
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.89	0.54
5:B:292:ILE:HD11	5:B:327:ARG:HG2	1.89	0.54
5:B:515:HIS:H	5:B:518:HIS:HD2	1.53	0.54
9:H:89:LEU:HB2	9:H:91:ASP:OD2	2.07	0.54
4:A:523:ILE:HG22	4:A:528:LEU:HD23	1.90	0.54
5:B:765:PRO:O	5:B:768:THR:HB	2.07	0.54
4:A:512:VAL:HA	4:A:519:PRO:HA	1.90	0.54
4:A:541:ILE:HD11	4:A:577:ILE:HG12	1.87	0.54
4:A:669:THR:O	4:A:762:SER:HB3	2.08	0.54
4:A:901:LEU:N	4:A:926:GLN:HE21	2.03	0.54
4:A:778:GLY:HA3	5:B:516:ASN:ND2	2.23	0.54
5:B:141:ASP:O	5:B:142:VAL:CB	2.49	0.54
6:C:252:GLN:HG3	12:K:95:ILE:HG23	1.88	0.54
4:A:440:ASP:O	4:A:460:VAL:HG23	2.08	0.54
4:A:559:VAL:HG12	4:A:559:VAL:O	2.07	0.54
5:B:778:MET:HE1	5:B:1094:ARG:HH11	1.72	0.54
7:E:153:HIS:O	7:E:154:ILE:HD13	2.08	0.54
1:R:9:G:C8	1:R:9:G:H5"	2.44	0.53
5:B:119:LEU:HD22	5:B:953:LEU:CD1	2.37	0.53
6:C:22:LEU:HD22	6:C:25:VAL:HG21	1.90	0.53
1:R:10:A:H2	2:T:19:DT:O2	1.90	0.53
2:T:21:DC:C6	2:T:22:DT:H72	2.43	0.53
4:A:248:PRO:O	4:A:260:ASP:HB2	2.07	0.53
6:C:18:VAL:HG23	6:C:240:VAL:HB	1.90	0.53
3:N:9:DC:C4	3:N:10:DG:C6	2.97	0.53
4:A:567:LYS:HG3	4:A:568:PRO:HD2	1.90	0.53
4:A:1363:VAL:HG12	4:A:1364:ASN:N	2.23	0.53
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.91	0.53
4:A:836:TYR:CZ	4:A:840:ARG:HD2	2.42	0.53
5:B:142:VAL:CG2	5:B:145:ARG:HH11	2.22	0.53
2:T:21:DC:N1	2:T:22:DT:H72	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.91	0.53
4:A:1328:TYR:CZ	4:A:1350:LYS:HD3	2.44	0.53
5:B:370:PHE:CD2	5:B:373:ARG:HG3	2.44	0.53
4:A:471:ASN:O	4:A:474:VAL:HG12	2.09	0.53
5:B:911:ILE:HG21	5:B:966:VAL:HG11	1.89	0.53
5:B:815:ARG:HB2	5:B:816:GLU:OE2	2.08	0.53
5:B:976:ILE:HG23	5:B:977:GLY:N	2.24	0.53
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.90	0.53
12:K:65:HIS:HD2	12:K:67:PHE:HB2	1.74	0.53
4:A:582:ILE:HD12	4:A:629:LEU:HD11	1.90	0.53
5:B:142:VAL:CG2	5:B:145:ARG:HG2	2.38	0.53
5:B:825:VAL:HG22	5:B:1010:LEU:HB3	1.90	0.53
5:B:969:ARG:HH21	6:C:59:ALA:HB1	1.73	0.53
11:J:8:PHE:CD1	11:J:49:MET:HE1	2.43	0.53
4:A:67:CYS:O	4:A:70:CYS:SG	2.67	0.53
4:A:1156:PRO:O	4:A:1158:PRO:HD3	2.09	0.53
5:B:692:TYR:HD2	5:B:692:TYR:N	2.06	0.53
6:C:73:GLN:NE2	6:C:75:MET:HB2	2.24	0.53
4:A:1149:ALA:HA	10:I:47:GLU:HA	1.91	0.53
4:A:1364:ASN:ND2	4:A:1366:ARG:HH11	2.06	0.53
7:E:72:PHE:H	7:E:73:PRO:CA	2.19	0.53
12:K:81:TYR:CE2	12:K:86:ALA:HB2	2.44	0.53
5:B:344:LYS:HA	5:B:345:LYS:CB	2.37	0.52
5:B:692:TYR:N	5:B:692:TYR:CD2	2.77	0.52
5:B:899:ILE:CG2	5:B:949:VAL:HG21	2.32	0.52
5:B:978:ASP:OD1	5:B:1098:MET:HB3	2.09	0.52
6:C:233:GLU:HG2	6:C:234:SER:H	1.74	0.52
2:T:8:DT:H2'	2:T:9:DA:C8	2.44	0.52
4:A:1398:MET:HE2	4:A:1423:GLY:HA3	1.91	0.52
5:B:72:GLU:CD	5:B:73:GLN:CG	2.83	0.52
5:B:476:ARG:C	5:B:478:GLY:N	2.67	0.52
5:B:521:LEU:CD2	5:B:635:ARG:HD3	2.39	0.52
5:B:839:MET:CE	5:B:980:PHE:HB2	2.34	0.52
9:H:95:TYR:HE2	9:H:97:MET:SD	2.32	0.52
5:B:971:THR:OG1	6:C:61:GLU:HG3	2.09	0.52
6:C:229:TYR:CD1	6:C:229:TYR:N	2.77	0.52
8:F:101:ILE:HD13	8:F:120:ILE:HG22	1.91	0.52
4:A:1064:VAL:CG1	4:A:1370:LEU:HD22	2.39	0.52
5:B:345:LYS:N	5:B:348:ARG:H	2.07	0.52
2:T:6:DG:H1	3:N:9:DC:H42	1.56	0.52
4:A:901:LEU:HD12	4:A:926:GLN:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1111:MET:HE2	4:A:1114:PRO:HA	1.89	0.52
5:B:760:ASP:OD1	5:B:760:ASP:N	2.43	0.52
5:B:1081:LEU:HD13	5:B:1085:ILE:HD11	1.90	0.52
1:R:10:A:C2	2:T:19:DT:O2	2.63	0.52
4:A:855:THR:HG23	4:A:857:ARG:HG3	1.91	0.52
4:A:1436:ILE:O	4:A:1437:GLY:C	2.52	0.52
5:B:333:PHE:H	5:B:334:ILE:HB	1.75	0.52
8:F:111:LEU:HD12	8:F:111:LEU:H	1.74	0.52
4:A:464:PRO:O	4:A:465:TYR:HB2	2.09	0.52
11:J:6:ARG:HA	11:J:12:LYS:O	2.09	0.52
2:T:18:DC:C4'	2:T:19:DT:OP1	2.57	0.52
2:T:24:DT:OP1	5:B:857:ARG:NH2	2.43	0.52
4:A:511:ILE:HG12	4:A:521:MET:HE1	1.92	0.52
4:A:829:VAL:HG12	4:A:830:LYS:N	2.24	0.52
4:A:1017:LEU:HD12	7:E:206:GLY:N	2.18	0.52
5:B:238:ALA:HB3	5:B:256:VAL:HB	1.92	0.52
5:B:1016:ALA:HB1	5:B:1020:ARG:HH21	1.74	0.52
6:C:40:GLU:HA	6:C:163:ILE:HG23	1.92	0.51
8:F:76:LYS:O	8:F:79:ARG:NE	2.42	0.51
9:H:5:LEU:HD22	9:H:133:ASN:O	2.10	0.51
4:A:401:GLY:C	4:A:435:HIS:HD2	2.17	0.51
4:A:567:LYS:HG3	4:A:568:PRO:CG	2.39	0.51
4:A:567:LYS:HB3	9:H:96:VAL:H	1.76	0.51
4:A:714:PHE:O	4:A:718:VAL:HG23	2.09	0.51
4:A:1363:VAL:HB	4:A:1368:MET:HE3	1.92	0.51
5:B:63:ILE:O	5:B:67:SER:HB2	2.10	0.51
5:B:69:LEU:CA	5:B:89:GLU:HG2	2.40	0.51
5:B:600:LEU:O	5:B:615:MET:HE1	2.10	0.51
4:A:1055:ARG:HD3	8:F:155:LEU:O	2.10	0.51
5:B:484:ASN:C	5:B:484:ASN:HD22	2.19	0.51
2:T:22:DT:OP2	5:B:1121:GLY:HA2	2.10	0.51
5:B:530:GLY:O	5:B:531:GLN:C	2.54	0.51
4:A:302:THR:OG1	4:A:306:ASN:HB3	2.11	0.51
5:B:510:LYS:CD	5:B:511:PRO:HD2	2.41	0.51
2:T:19:DT:C2'	2:T:20:DC:C5'	2.81	0.51
3:N:1:DC:H6	3:N:1:DC:O5'	1.93	0.51
4:A:344:ARG:HA	5:B:1129:ARG:HA	1.92	0.51
4:A:523:ILE:HG23	4:A:527:THR:HB	1.93	0.51
4:A:1348:LEU:O	4:A:1352:VAL:HG23	2.11	0.51
5:B:569:TYR:CE1	5:B:589:VAL:HG21	2.46	0.51
8:F:93:ILE:HD11	8:F:134:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:330:LYS:HG2	4:A:331:GLY:N	2.26	0.51
4:A:728:LYS:O	4:A:732:LEU:HB2	2.11	0.51
5:B:526:GLU:HG3	5:B:771:SER:HB3	1.93	0.51
2:T:5:DC:C2	2:T:6:DG:C6	2.98	0.51
4:A:899:VAL:HB	4:A:929:LEU:HD12	1.91	0.51
5:B:788:ARG:NH1	5:B:790:ASP:OD2	2.44	0.51
4:A:93:VAL:HG23	4:A:304:MET:HE3	1.92	0.51
4:A:253:ASN:ND2	4:A:253:ASN:C	2.68	0.51
4:A:642:CYS:O	4:A:645:LEU:HB3	2.10	0.51
5:B:89:GLU:O	5:B:89:GLU:OE1	2.29	0.51
5:B:115:GLN:HG3	5:B:119:LEU:HD12	1.93	0.51
5:B:143:PRO:CB	5:B:144:GLY:CA	2.73	0.51
4:A:26:GLU:O	4:A:27:VAL:C	2.53	0.50
4:A:445:ASN:CB	4:A:455:MET:HG2	2.38	0.50
4:A:567:LYS:CG	4:A:568:PRO:CD	2.88	0.50
4:A:1116:LEU:HB2	4:A:1308:THR:OG1	2.10	0.50
5:B:476:ARG:O	5:B:478:GLY:N	2.44	0.50
5:B:1084:GLN:HE22	6:C:191:TYR:CA	2.16	0.50
4:A:828:ALA:CB	5:B:530:GLY:HA2	2.41	0.50
5:B:142:VAL:HG21	5:B:145:ARG:HH11	1.76	0.50
4:A:544:ASP:HB2	12:K:47:ARG:NH2	2.26	0.50
4:A:645:LEU:CD1	4:A:649:ILE:HD11	2.41	0.50
5:B:20:ASP:OD2	5:B:21:GLU:N	2.44	0.50
5:B:37:PHE:O	5:B:38:PHE:HB2	2.12	0.50
5:B:41:LYS:O	5:B:45:SER:HB3	2.12	0.50
9:H:59:ILE:HG12	9:H:142:LEU:HD12	1.93	0.50
13:L:60:ARG:HG3	13:L:61:THR:N	2.23	0.50
4:A:93:VAL:HG22	4:A:301:ALA:HA	1.93	0.50
4:A:840:ARG:NH2	4:A:1106:ASN:OD1	2.45	0.50
4:A:1397:LEU:O	4:A:1400:CYS:HB2	2.11	0.50
5:B:488:TYR:HE2	5:B:813:LYS:HB2	1.76	0.50
9:H:40:LEU:HD13	9:H:123:MET:HE3	1.93	0.50
10:I:68:LEU:HD13	10:I:84:VAL:HG11	1.94	0.50
4:A:23:SER:HB2	4:A:233:TRP:CE2	2.46	0.50
5:B:142:VAL:HG11	5:B:144:GLY:C	2.36	0.50
5:B:502:ILE:CD1	5:B:502:ILE:H	2.22	0.50
4:A:316:GLN:H	4:A:317:LYS:HB3	1.76	0.50
4:A:407:ARG:HD3	4:A:413:ILE:HD11	1.93	0.50
4:A:606:LEU:HD11	4:A:608:ILE:HD11	1.93	0.50
5:B:476:ARG:C	5:B:478:GLY:H	2.20	0.50
6:C:41:ILE:HG13	6:C:172:PRO:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:19:DT:H3'	2:T:19:DT:H6	1.77	0.50
4:A:353:ILE:HD13	4:A:487:MET:SD	2.52	0.50
4:A:472:LEU:HD11	5:B:835:GLN:HB3	1.94	0.50
5:B:1017:ILE:HB	5:B:1018:PRO:CD	2.42	0.50
8:F:127:GLU:O	8:F:129:LYS:N	2.45	0.50
4:A:249:SER:O	4:A:250:ILE:O	2.30	0.50
5:B:25:ILE:CG2	5:B:29:ASP:HB2	2.41	0.50
5:B:260:GLY:O	5:B:267:ARG:HD3	2.11	0.50
5:B:801:LYS:O	11:J:52:THR:CG2	2.60	0.50
5:B:1051:THR:HG22	5:B:1053:GLU:H	1.76	0.50
7:E:31:THR:OG1	7:E:34:GLU:HB2	2.12	0.50
9:H:139:ASN:O	9:H:140:ALA:CB	2.59	0.50
4:A:256:GLN:HA	4:A:257:ARG:HG3	1.93	0.49
4:A:257:ARG:O	4:A:258:GLY:O	2.30	0.49
4:A:446:ARG:HD2	4:A:478:TYR:O	2.12	0.49
4:A:907:THR:HG22	4:A:908:LEU:H	1.76	0.49
5:B:732:SER:HB2	5:B:734:HIS:HD2	1.77	0.49
5:B:998:ASP:HB3	5:B:1076:HIS:CE1	2.47	0.49
5:B:1134:GLU:CD	5:B:1134:GLU:N	2.70	0.49
8:F:97:ARG:HD2	8:F:101:ILE:CD1	2.36	0.49
4:A:546:VAL:HG13	4:A:577:ILE:HG21	1.94	0.49
6:C:241:ASP:HB3	12:K:109:TRP:CZ2	2.47	0.49
6:C:67:LEU:HA	6:C:70:ILE:CD1	2.42	0.49
4:A:557:ASP:OD2	4:A:559:VAL:HB	2.12	0.49
5:B:338:GLY:HA2	5:B:340:ALA:N	2.20	0.49
5:B:365:THR:HG21	5:B:370:PHE:HB2	1.95	0.49
5:B:706:GLN:O	5:B:710:LEU:HB2	2.12	0.49
6:C:35:ARG:HB2	12:K:41:THR:HG23	1.93	0.49
11:J:7:CYS:HA	11:J:49:MET:HG2	1.94	0.49
5:B:145:ARG:N	5:B:146:GLU:HB2	2.28	0.49
7:E:23:VAL:O	7:E:28:TYR:HB2	2.12	0.49
12:K:49:GLU:HG3	12:K:94:ILE:CG1	2.43	0.49
2:T:11:DG:H2''	2:T:12:DC:OP2	2.13	0.49
4:A:58:LEU:HD23	4:A:80:HIS:O	2.13	0.49
4:A:55:ASP:N	4:A:56:PRO:HD2	2.27	0.49
5:B:137:TYR:CE2	5:B:138:GLU:HG2	2.47	0.49
11:J:10:CYS:HB3	11:J:45:CYS:SG	2.52	0.49
2:T:15:DA:H4'	2:T:16:DC:OP1	2.13	0.49
2:T:23:DC:N4	2:T:24:DT:H73	2.28	0.49
4:A:562:THR:HG23	4:A:563:PRO:HD2	1.95	0.49
4:A:722:LEU:HD22	4:A:799:PHE:CG	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:2:U:H2'	1:R:3:C:H6	1.78	0.49
4:A:81:PHE:HE1	5:B:1209:ALA:HB2	1.77	0.49
4:A:754:SER:N	4:A:757:ASN:HD22	2.02	0.49
5:B:636:PRO:CB	5:B:637:LEU:CA	2.76	0.49
4:A:868:TYR:CE1	4:A:1064:VAL:HG21	2.48	0.49
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.46	0.49
3:N:7:DA:H2'	3:N:8:DT:C7	2.41	0.48
4:A:540:PHE:HB3	4:A:571:LEU:HD23	1.94	0.48
4:A:1105:LEU:HB3	4:A:1384:VAL:CG2	2.44	0.48
5:B:323:VAL:C	5:B:324:ILE:HG13	2.38	0.48
5:B:333:PHE:N	5:B:334:ILE:O	2.47	0.48
5:B:473:MET:C	5:B:475:SER:H	2.21	0.48
5:B:521:LEU:HD21	5:B:635:ARG:HD3	1.95	0.48
11:J:20:SER:HB3	11:J:39:LEU:HD21	1.95	0.48
2:T:26:DG:N2	2:T:27:DA:H1'	2.28	0.48
4:A:255:SER:HB2	4:A:256:GLN:C	2.38	0.48
4:A:323:LYS:O	4:A:324:SER:CB	2.61	0.48
4:A:450:LEU:H	4:A:450:LEU:CD1	2.19	0.48
4:A:666:ILE:HD11	5:B:1030:LEU:HD13	1.96	0.48
4:A:1064:VAL:HG12	4:A:1370:LEU:CD2	2.42	0.48
5:B:219:ALA:HB2	5:B:405:ARG:HG2	1.95	0.48
5:B:744:HIS:CD2	5:B:745:PRO:HD2	2.49	0.48
1:R:8:G:H1	2:T:21:DC:N4	2.11	0.48
4:A:206:GLU:O	4:A:210:ILE:HG12	2.13	0.48
4:A:535:THR:HG23	4:A:575:LYS:HG2	1.94	0.48
4:A:894:GLU:O	4:A:896:ARG:N	2.45	0.48
4:A:1394:THR:HG22	4:A:1395:GLY:N	2.28	0.48
7:E:64:PRO:O	7:E:65:THR:HG22	2.14	0.48
4:A:548:ASN:HD21	12:K:47:ARG:CD	2.26	0.48
4:A:908:LEU:O	4:A:909:ASP:C	2.56	0.48
5:B:377:PHE:C	5:B:379:GLY:H	2.20	0.48
9:H:89:LEU:O	9:H:91:ASP:N	2.45	0.48
1:R:8:G:H1	2:T:21:DC:H42	1.61	0.48
3:N:5:DT:H2''	3:N:6:DT:OP2	2.14	0.48
4:A:508:PRO:O	4:A:511:ILE:HG13	2.14	0.48
4:A:901:LEU:HA	4:A:907:THR:HG23	1.94	0.48
5:B:70:ILE:C	5:B:70:ILE:HD12	2.39	0.48
5:B:527:THR:OG1	5:B:528:PRO:HD2	2.13	0.48
5:B:995:ARG:HB2	5:B:995:ARG:CZ	2.42	0.48
6:C:57:VAL:HG11	11:J:60:PHE:CB	2.28	0.48
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:94:ASP:N	9:H:94:ASP:OD1	2.47	0.48
5:B:214:ALA:O	5:B:498:THR:HA	2.14	0.48
5:B:743:ILE:O	5:B:744:HIS:HB2	2.13	0.48
5:B:843:GLN:HB2	5:B:993:THR:OG1	2.14	0.48
6:C:66:ARG:HE	11:J:2:ILE:CG1	2.25	0.48
10:I:68:LEU:HB3	10:I:84:VAL:CG1	2.41	0.48
4:A:455:MET:HE1	5:B:1134:GLU:HB3	1.96	0.48
4:A:1141:THR:CG2	4:A:1205:LYS:HD3	2.44	0.48
5:B:142:VAL:CG1	5:B:144:GLY:C	2.86	0.48
1:R:5:A:H2'	1:R:6:G:C8	2.49	0.47
5:B:72:GLU:CG	5:B:73:GLN:H	2.27	0.47
5:B:1023:VAL:HG12	5:B:1027:ILE:HD11	1.96	0.47
6:C:239:PRO:HB2	6:C:241:ASP:OD1	2.14	0.47
2:T:18:DC:C3'	2:T:19:DT:H72	2.38	0.47
4:A:573:SER:H	4:A:576:GLN:HG3	1.78	0.47
4:A:661:GLY:O	4:A:662:PHE:HB2	2.15	0.47
5:B:254:LEU:HD22	5:B:381:MET:HE1	1.96	0.47
5:B:756:ILE:O	5:B:759:PRO:HD3	2.14	0.47
12:K:63:VAL:HG23	12:K:63:VAL:O	2.14	0.47
4:A:350:ARG:HB2	5:B:1128:LEU:HD11	1.97	0.47
4:A:406:ILE:HB	4:A:431:LYS:HB2	1.95	0.47
4:A:438:ASP:HA	4:A:460:VAL:O	2.14	0.47
4:A:531:ILE:HD13	4:A:617:VAL:CG1	2.44	0.47
4:A:1027:ALA:O	4:A:1031:VAL:HG23	2.14	0.47
4:A:1120:LEU:HB3	4:A:1124:HIS:O	2.14	0.47
5:B:71:LEU:HD13	5:B:72:GLU:HB2	1.96	0.47
5:B:642:ASP:O	5:B:644:GLU:N	2.32	0.47
5:B:1134:GLU:CD	5:B:1134:GLU:H	2.21	0.47
4:A:159:THR:HA	4:A:160:GLN:HB2	1.96	0.47
5:B:256:VAL:HG12	5:B:385:LEU:HD22	1.96	0.47
5:B:1135:ARG:HG3	5:B:1147:LEU:HD21	1.97	0.47
2:T:12:DC:H2''	2:T:13:DA:C8	2.49	0.47
4:A:158:PRO:HG2	4:A:160:GLN:NE2	2.30	0.47
4:A:847:ASP:OD1	4:A:847:ASP:N	2.34	0.47
8:F:152:ILE:HD12	8:F:152:ILE:N	2.30	0.47
4:A:253:ASN:N	4:A:255:SER:HB2	2.26	0.47
4:A:947:PHE:CD2	4:A:954:TRP:CZ2	3.03	0.47
16:B:1308[A]:DGT:H8	16:B:1308[A]:DGT:H5'	1.97	0.47
2:T:5:DC:H1'	2:T:6:DG:C8	2.50	0.47
4:A:159:THR:CA	4:A:160:GLN:HB2	2.45	0.47
4:A:353:ILE:HG22	4:A:468:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:618:GLU:O	4:A:622:VAL:HG12	2.15	0.47
5:B:142:VAL:HG21	5:B:145:ARG:HG2	1.97	0.47
6:C:257:SER:HA	6:C:260:LEU:HG	1.96	0.47
7:E:67:GLU:CB	7:E:68:SER:CA	2.87	0.47
10:I:14:LEU:HB3	10:I:27:PHE:HB3	1.97	0.47
12:K:36:GLU:O	12:K:37:LYS:C	2.57	0.47
4:A:665:GLY:HA2	5:B:1086:PHE:CD1	2.50	0.47
4:A:1094:VAL:HA	4:A:1113:THR:HG21	1.96	0.47
4:A:1280:GLU:HB3	4:A:1281:ARG:H	1.59	0.47
4:A:1436:ILE:O	4:A:1438:THR:N	2.48	0.47
5:B:501:PRO:CA	5:B:502:ILE:HD12	2.44	0.47
5:B:766:ARG:NH2	5:B:1020:ARG:HB3	2.30	0.47
5:B:778:MET:HE1	5:B:1094:ARG:HD3	1.96	0.47
6:C:99:LEU:N	6:C:157:CYS:O	2.39	0.47
5:B:69:LEU:CB	5:B:70:ILE:CB	2.83	0.47
9:H:2:SER:HB3	9:H:62:SER:CB	2.45	0.47
4:A:1397:LEU:HB2	4:A:1426:GLU:HG2	1.97	0.47
6:C:56:THR:HG21	6:C:145:CYS:SG	2.55	0.47
11:J:5:VAL:O	11:J:6:ARG:O	2.33	0.47
12:K:47:ARG:HD2	12:K:60:ALA:HA	1.97	0.47
4:A:672:ASP:HB3	4:A:675:THR:OG1	2.15	0.46
5:B:482:VAL:C	5:B:483:LEU:O	2.58	0.46
4:A:567:LYS:O	4:A:569:LYS:N	2.48	0.46
4:A:690:VAL:CG2	4:A:718:VAL:HG13	2.45	0.46
4:A:1349:TYR:HB2	4:A:1372:VAL:HG21	1.98	0.46
5:B:378:LEU:O	5:B:382:ILE:HG12	2.16	0.46
5:B:698:GLU:HA	5:B:701:ILE:CD1	2.46	0.46
6:C:46:ILE:HG21	6:C:157:CYS:HB3	1.97	0.46
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.79	0.46
4:A:215:SER:O	4:A:218:ASP:HB2	2.16	0.46
4:A:532:ARG:HH12	4:A:745:GLN:HE21	1.62	0.46
4:A:568:PRO:CB	6:C:221:TYR:CE1	2.98	0.46
4:A:947:PHE:HE2	7:E:203:GLU:HB2	1.80	0.46
4:A:1155:ASP:OD1	4:A:1162:VAL:HG23	2.15	0.46
5:B:283:VAL:HG21	5:B:321:GLY:HA3	1.96	0.46
5:B:291:ILE:HD12	5:B:291:ILE:N	2.31	0.46
4:A:568:PRO:HB3	6:C:221:TYR:CE1	2.50	0.46
4:A:587:HIS:NE2	4:A:969:GLN:HG2	2.31	0.46
4:A:1015:VAL:O	4:A:1016:THR:C	2.58	0.46
5:B:1020:ARG:NH1	16:B:1308[A]:DGT:O1B	2.45	0.46
4:A:1352:VAL:O	4:A:1355:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:294:SER:O	4:A:298:PHE:HB2	2.16	0.46
5:B:315:LYS:N	5:B:316:PRO:HD2	2.31	0.46
5:B:377:PHE:C	5:B:379:GLY:N	2.74	0.46
5:B:493:SER:HB3	5:B:751:VAL:HB	1.96	0.46
5:B:864:LYS:HD3	5:B:870:ILE:O	2.16	0.46
7:E:61:GLN:HB3	7:E:79:TRP:HE3	1.81	0.46
4:A:109:HIS:CD2	4:A:169:ASN:HD21	2.33	0.46
4:A:821:ARG:HB2	4:A:821:ARG:NH1	2.30	0.46
5:B:984:HIS:HE1	5:B:1028:GLU:OE2	1.98	0.46
4:A:424:ILE:HD12	4:A:424:ILE:O	2.15	0.46
4:A:567:LYS:NZ	9:H:95:TYR:CZ	2.70	0.46
5:B:258:LEU:HB2	5:B:385:LEU:HD21	1.97	0.46
5:B:615:MET:HG2	5:B:626:ILE:HG23	1.98	0.46
5:B:634:TYR:CE1	5:B:692:TYR:HD1	2.31	0.46
12:K:92:ASN:HA	12:K:95:ILE:HD12	1.97	0.46
2:T:13:DA:C2	3:N:2:DT:O2	2.69	0.46
2:T:22:DT:H6	2:T:22:DT:H3'	1.80	0.46
5:B:102:VAL:HG23	5:B:112:LEU:HD22	1.97	0.46
5:B:145:ARG:CA	5:B:146:GLU:HB2	2.45	0.46
4:A:855:THR:HG21	4:A:857:ARG:HE	1.81	0.46
4:A:1155:ASP:OD2	4:A:1161:THR:HA	2.16	0.46
5:B:544:CYS:HB2	5:B:634:TYR:CZ	2.51	0.46
2:T:6:DG:N2	2:T:7:DA:C2	2.84	0.45
4:A:296:LEU:O	4:A:296:LEU:HG	2.16	0.45
4:A:596:THR:C	4:A:598:LEU:N	2.74	0.45
4:A:800:VAL:HA	4:A:812:GLU:HG2	1.98	0.45
4:A:1111:MET:HG3	4:A:1114:PRO:HG3	1.96	0.45
5:B:142:VAL:HG11	5:B:144:GLY:CA	2.34	0.45
5:B:1157:ALA:H	5:B:1197:PRO:HA	1.82	0.45
1:R:6:G:H2'	1:R:7:A:C8	2.52	0.45
5:B:108:VAL:HG12	5:B:109:THR:H	1.81	0.45
5:B:841:MET:HG2	5:B:846:ILE:HD11	1.96	0.45
8:F:93:ILE:CD1	8:F:134:ILE:HD11	2.46	0.45
9:H:84:ALA:HA	9:H:87:ARG:HB2	1.98	0.45
9:H:104:PHE:CZ	9:H:136:LYS:HA	2.52	0.45
4:A:365:GLY:O	4:A:468:PHE:HA	2.15	0.45
4:A:662:PHE:O	5:B:828:ALA:HA	2.16	0.45
5:B:176:SER:O	5:B:182:SER:CB	2.63	0.45
5:B:783:THR:O	5:B:783:THR:CG2	2.62	0.45
6:C:148:ARG:H	6:C:151:GLN:HG3	1.81	0.45
4:A:361:LEU:HD22	4:A:646:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:662:PHE:HD2	5:B:829:CYS:SG	2.39	0.45
5:B:72:GLU:OE1	5:B:73:GLN:CG	2.64	0.45
5:B:254:LEU:HD23	5:B:381:MET:HE1	1.97	0.45
5:B:741:CYS:SG	5:B:742:GLU:N	2.89	0.45
6:C:31:ASN:O	6:C:34:ARG:HB3	2.16	0.45
12:K:65:HIS:CD2	12:K:67:PHE:H	2.29	0.45
2:T:16:DC:H2"	2:T:17:DG:C8	2.51	0.45
2:T:19:DT:C6	2:T:20:DC:C5	3.04	0.45
4:A:249:SER:C	4:A:250:ILE:O	2.59	0.45
4:A:455:MET:CE	5:B:1134:GLU:HB3	2.46	0.45
4:A:1194:ARG:HH21	4:A:1237:ILE:HD13	1.80	0.45
5:B:212:LEU:HD21	5:B:461:LEU:HD11	1.99	0.45
5:B:321:GLY:C	5:B:323:VAL:H	2.24	0.45
5:B:361:LEU:N	5:B:362:PRO:HD3	2.32	0.45
5:B:1119:VAL:O	5:B:1126:GLY:HA3	2.16	0.45
11:J:32:GLU:O	11:J:36:LEU:CD2	2.64	0.45
4:A:672:ASP:H	4:A:736:ASN:ND2	2.11	0.45
5:B:100:PRO:HA	5:B:126:SER:HB3	1.99	0.45
7:E:68:SER:HA	7:E:69:ILE:HA	1.65	0.45
12:K:57:LEU:HB2	12:K:76:GLN:HG2	1.98	0.45
4:A:765:VAL:HG22	4:A:800:VAL:HB	1.98	0.45
4:A:897:TYR:CD2	4:A:936:LEU:HD13	2.52	0.45
4:A:1239:ARG:HH12	4:A:1241:ARG:HH12	1.64	0.45
5:B:1072:MET:HB2	5:B:1085:ILE:HD12	1.99	0.45
7:E:75:MET:CB	7:E:76:GLY:CA	2.94	0.45
9:H:80:ARG:HA	9:H:81:PRO:HD3	1.66	0.45
12:K:40:HIS:O	12:K:41:THR:C	2.60	0.45
4:A:691:LEU:HD11	4:A:695:LYS:HZ1	1.81	0.45
4:A:1127:ASP:HB3	4:A:1130:GLN:HB3	1.99	0.45
5:B:326:ASP:OD1	5:B:329:THR:OG1	2.33	0.45
4:A:241:VAL:HA	4:A:242:PRO:HD2	1.86	0.45
4:A:873:MET:HG2	4:A:957:PRO:HG3	1.98	0.45
4:A:1154:TYR:CE1	10:I:18:GLU:HG3	2.52	0.45
5:B:193:LYS:HB3	5:B:787:VAL:HG11	1.99	0.45
5:B:292:ILE:H	5:B:293:PRO:HD3	1.82	0.45
5:B:1013:ASN:OD1	5:B:1014:PRO:HD2	2.17	0.45
8:F:99:LEU:HD13	8:F:99:LEU:O	2.17	0.45
4:A:40:THR:HG22	4:A:41:MET:HG3	1.99	0.45
4:A:901:LEU:HB2	4:A:926:GLN:HG2	1.98	0.45
4:A:981:LEU:HD13	4:A:986:ILE:HD11	1.98	0.45
4:A:982:THR:C	4:A:984:LYS:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:373:ARG:HD3	5:B:567:GLU:OE2	2.16	0.45
5:B:826:ALA:O	5:B:1011:ILE:HA	2.17	0.45
5:B:898:LEU:HD11	5:B:964:VAL:HG21	1.98	0.45
5:B:1074:ASN:OD1	5:B:1076:HIS:HB2	2.17	0.45
12:K:77:THR:HG21	12:K:81:TYR:HD2	1.82	0.45
4:A:457:ALA:O	4:A:507:VAL:HG23	2.17	0.44
4:A:849:MET:HE1	4:A:1061:GLY:HA2	1.98	0.44
4:A:1392:SER:O	4:A:1394:THR:N	2.49	0.44
5:B:338:GLY:CA	5:B:340:ALA:H	2.23	0.44
5:B:475:SER:C	5:B:477:ALA:N	2.76	0.44
5:B:510:LYS:HA	5:B:510:LYS:HD3	1.66	0.44
5:B:1095:LEU:C	5:B:1096:ARG:O	2.60	0.44
4:A:915:SER:O	4:A:919:ILE:CG1	2.64	0.44
5:B:145:ARG:CB	5:B:146:GLU:CB	2.77	0.44
5:B:836:GLU:O	5:B:837:ASP:OD2	2.35	0.44
2:T:20:DC:H4'	4:A:447:GLN:OE1	2.17	0.44
3:N:8:DT:C2'	3:N:9:DC:O5'	2.56	0.44
4:A:447:GLN:HG2	5:B:1134:GLU:OE2	2.17	0.44
4:A:1364:ASN:HD22	4:A:1366:ARG:H	1.64	0.44
4:A:1448:GLU:HA	4:A:1449:SER:HA	1.49	0.44
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.52	0.44
6:C:46:ILE:O	6:C:169:LYS:HE3	2.17	0.44
7:E:179:GLN:HA	7:E:179:GLN:OE1	2.18	0.44
11:J:2:ILE:HD12	11:J:2:ILE:HA	1.68	0.44
4:A:35:ILE:HG13	4:A:241:VAL:HG21	1.98	0.44
4:A:982:THR:C	4:A:984:LYS:H	2.25	0.44
5:B:1073:TYR:N	5:B:1073:TYR:HD1	2.16	0.44
4:A:65:LEU:O	4:A:71:GLN:HA	2.18	0.44
4:A:265:LYS:NZ	4:A:322:VAL:HB	2.31	0.44
4:A:360:GLU:HB2	4:A:363:GLN:OE1	2.18	0.44
4:A:391:LEU:O	4:A:394:ASN:N	2.51	0.44
5:B:286:PHE:HB3	5:B:297:ILE:CD1	2.44	0.44
7:E:69:ILE:O	7:E:70:SER:HB2	2.18	0.44
8:F:103:MET:O	8:F:104:ASN:C	2.61	0.44
4:A:322:VAL:HB	4:A:323:LYS:H	1.56	0.44
4:A:849:MET:HE3	4:A:1061:GLY:HA2	1.99	0.44
5:B:71:LEU:O	5:B:71:LEU:HD12	2.15	0.44
5:B:850:LEU:HB2	11:J:8:PHE:CG	2.53	0.44
11:J:32:GLU:CD	11:J:32:GLU:H	2.25	0.44
4:A:443:LEU:HD11	4:A:455:MET:HB3	2.00	0.44
4:A:548:ASN:HD21	12:K:47:ARG:NE	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1151:GLU:HG2	10:I:45:ARG:HG3	2.00	0.44
5:B:333:PHE:CD1	5:B:333:PHE:O	2.70	0.44
5:B:428:ILE:HD11	5:B:448:ILE:HA	2.00	0.44
5:B:800:GLN:HB3	11:J:52:THR:HG22	1.99	0.44
6:C:46:ILE:H	6:C:46:ILE:HG12	1.57	0.44
7:E:42:PHE:CZ	7:E:58:MET:HE2	2.48	0.44
9:H:1:MET:CE	9:H:2:SER:OG	2.63	0.44
2:T:15:DA:H1'	2:T:16:DC:O5'	2.17	0.44
4:A:107:CYS:CA	4:A:171:GLN:HE21	2.19	0.44
4:A:1399:ARG:NH1	4:A:1408:ILE:HD12	2.33	0.44
5:B:114:PRO:HB2	5:B:118:ARG:NH2	2.32	0.44
5:B:802:PRO:HB3	5:B:1091:TYR:CG	2.53	0.44
8:F:97:ARG:NH1	8:F:100:GLN:OE1	2.51	0.44
11:J:1:MET:N	11:J:56:LEU:H	2.16	0.44
12:K:20:LYS:NZ	12:K:20:LYS:HB2	2.33	0.44
4:A:313:GLN:HG2	4:A:314:ALA:H	1.83	0.44
5:B:287:ARG:HA	5:B:291:ILE:O	2.17	0.44
5:B:333:PHE:N	5:B:334:ILE:HB	2.31	0.44
7:E:205:SER:O	7:E:207:ARG:N	2.50	0.44
4:A:11:LEU:HD13	5:B:1195:HIS:HD2	1.81	0.43
4:A:456:MET:HB2	4:A:478:TYR:OH	2.18	0.43
4:A:524:VAL:HG12	4:A:525:GLN:HG3	2.00	0.43
4:A:577:ILE:H	4:A:577:ILE:HG13	1.57	0.43
5:B:291:ILE:HG22	5:B:297:ILE:HD13	2.00	0.43
5:B:507:LYS:O	5:B:507:LYS:HG3	2.18	0.43
5:B:788:ARG:HH12	5:B:790:ASP:CG	2.26	0.43
5:B:800:GLN:O	5:B:1091:TYR:HE1	2.00	0.43
7:E:81:GLU:HB3	7:E:96:PHE:HE1	1.83	0.43
4:A:247:ARG:N	4:A:248:PRO:HD3	2.33	0.43
4:A:754:SER:O	4:A:757:ASN:HB2	2.18	0.43
4:A:983:ILE:O	4:A:983:ILE:HG22	2.17	0.43
4:A:1345:ARG:HG3	4:A:1376:THR:HG21	1.99	0.43
5:B:240:ILE:HG23	5:B:240:ILE:O	2.18	0.43
5:B:1013:ASN:HD21	5:B:1015:HIS:HD2	1.66	0.43
5:B:1202:LEU:HD12	5:B:1206:GLU:CD	2.44	0.43
4:A:51:GLY:CA	4:A:56:PRO:HG3	2.39	0.43
4:A:332:LYS:C	4:A:334:GLY:H	2.27	0.43
4:A:1064:VAL:HG12	4:A:1064:VAL:O	2.18	0.43
5:B:570:VAL:HA	5:B:571:PRO:HD3	1.77	0.43
2:T:19:DT:H2''	2:T:20:DC:C4'	2.47	0.43
4:A:11:LEU:HA	5:B:1193:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:93:VAL:CG2	4:A:301:ALA:HA	2.49	0.43
4:A:618:GLU:HG3	4:A:619:LYS:N	2.33	0.43
5:B:213:ILE:O	5:B:215:GLN:HG2	2.18	0.43
5:B:504:ARG:CD	5:B:505:ASP:H	2.28	0.43
5:B:526:GLU:HG2	5:B:538:ASN:ND2	2.33	0.43
5:B:913:GLY:HA2	5:B:938:SER:OG	2.18	0.43
4:A:244:PRO:HB2	4:A:245:PRO:CD	2.48	0.43
4:A:401:GLY:O	4:A:435:HIS:HD2	1.96	0.43
5:B:72:GLU:CG	5:B:73:GLN:N	2.78	0.43
5:B:142:VAL:CG2	5:B:143:PRO:CD	2.67	0.43
5:B:475:SER:O	5:B:477:ALA:N	2.51	0.43
6:C:37:MET:O	6:C:38:ILE:C	2.62	0.43
8:F:83:PRO:HB2	8:F:152:ILE:HD13	1.98	0.43
2:T:21:DC:H2"	2:T:22:DT:OP2	2.19	0.43
4:A:407:ARG:HG2	4:A:430:TRP:CZ2	2.53	0.43
4:A:1369:ALA:O	4:A:1373:ASP:HB2	2.18	0.43
5:B:412:LEU:HD23	5:B:412:LEU:HA	1.58	0.43
2:T:9:DA:N1	3:N:7:DA:C2	2.87	0.43
12:K:49:GLU:C	12:K:51:LEU:H	2.26	0.43
4:A:9:ALA:HA	4:A:10:PRO:HD3	1.89	0.43
4:A:116:ASP:C	4:A:118:HIS:H	2.27	0.43
4:A:252:PHE:HA	4:A:253:ASN:CG	2.44	0.43
4:A:315:LEU:HA	4:A:316:GLN:HA	1.81	0.43
4:A:840:ARG:HE	4:A:1385:THR:HG23	1.84	0.43
4:A:1093:LYS:HD2	4:A:1281:ARG:NH2	2.34	0.43
4:A:1267:MET:HA	4:A:1271:ILE:HG12	2.01	0.43
4:A:1352:VAL:O	4:A:1353:TYR:C	2.62	0.43
4:A:1390:ASN:O	4:A:1399:ARG:HD2	2.19	0.43
6:C:66:ARG:CZ	11:J:2:ILE:HG23	2.38	0.43
4:A:253:ASN:HA	4:A:254:GLU:HA	1.52	0.43
4:A:316:GLN:N	4:A:317:LYS:HB3	2.34	0.43
4:A:323:LYS:O	4:A:324:SER:HB3	2.19	0.43
4:A:1117:THR:N	4:A:1328:TYR:O	2.47	0.43
5:B:100:PRO:N	5:B:126:SER:HB3	2.34	0.43
4:A:444:PHE:HE2	4:A:470:LEU:CD2	2.32	0.43
4:A:586:ILE:HD13	4:A:586:ILE:HA	1.86	0.43
4:A:1410:PHE:HD1	5:B:1212:ILE:HD11	1.84	0.43
5:B:416:LEU:HD11	5:B:460:ALA:HB3	2.01	0.43
5:B:882:THR:HB	5:B:934:LYS:O	2.19	0.43
5:B:944:THR:HG21	5:B:1122:ARG:NH1	2.33	0.43
11:J:6:ARG:H	11:J:14:VAL:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:321:PRO:O	4:A:322:VAL:HG13	2.19	0.42
5:B:142:VAL:CG2	5:B:145:ARG:CG	2.97	0.42
5:B:185:THR:OG1	5:B:188:ASP:OD2	2.37	0.42
5:B:416:LEU:HD13	5:B:457:LEU:HD23	2.00	0.42
5:B:506:GLY:O	5:B:507:LYS:HB3	2.19	0.42
5:B:642:ASP:HB3	5:B:649:LYS:HG3	2.01	0.42
5:B:654:ARG:HA	5:B:654:ARG:HD3	1.84	0.42
5:B:998:ASP:HB3	5:B:1076:HIS:HE1	1.84	0.42
7:E:94:LYS:HE2	7:E:94:LYS:HA	2.01	0.42
4:A:99:ILE:HG13	4:A:234:MET:SD	2.59	0.42
4:A:849:MET:HE3	4:A:1061:GLY:CA	2.50	0.42
4:A:1312:ASN:CG	4:A:1312:ASN:O	2.60	0.42
4:A:1394:THR:HG22	4:A:1395:GLY:H	1.84	0.42
5:B:334:ILE:HD13	5:B:335:GLY:O	2.19	0.42
5:B:428:ILE:HD13	5:B:428:ILE:HA	1.86	0.42
5:B:475:SER:C	5:B:477:ALA:H	2.26	0.42
5:B:510:LYS:HD2	5:B:511:PRO:HD2	2.01	0.42
6:C:8:VAL:HG11	12:K:105:PHE:CD1	2.53	0.42
1:R:8:G:N2	2:T:22:DT:C4	2.86	0.42
2:T:12:DC:C2'	2:T:13:DA:C8	3.02	0.42
4:A:482:PHE:O	5:B:989:THR:HG23	2.19	0.42
4:A:1101:LEU:HG	4:A:1105:LEU:CD1	2.49	0.42
5:B:137:TYR:CG	5:B:138:GLU:N	2.87	0.42
5:B:344:LYS:O	5:B:347:LYS:HB2	2.18	0.42
5:B:377:PHE:O	5:B:380:TYR:N	2.51	0.42
5:B:450:ALA:O	5:B:452:THR:N	2.51	0.42
5:B:488:TYR:CE2	5:B:813:LYS:HB2	2.53	0.42
5:B:809:MET:HA	5:B:812:LEU:HB2	2.01	0.42
5:B:850:LEU:HB2	11:J:8:PHE:CD1	2.54	0.42
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.18	0.42
2:T:18:DC:H2'	2:T:19:DT:C5	2.55	0.42
4:A:156:ASP:HA	4:A:157:ASP:HA	1.75	0.42
4:A:599:SER:OG	4:A:614:PHE:CD2	2.67	0.42
4:A:760:GLN:HG2	4:A:765:VAL:HA	2.02	0.42
5:B:89:GLU:N	5:B:89:GLU:OE2	2.35	0.42
5:B:189:LEU:HD23	5:B:189:LEU:HA	1.81	0.42
5:B:291:ILE:HG12	5:B:300:HIS:CD2	2.54	0.42
5:B:333:PHE:H	5:B:334:ILE:CA	2.32	0.42
6:C:100:THR:CG2	6:C:102:GLN:HE21	2.32	0.42
8:F:93:ILE:HD11	8:F:134:ILE:CD1	2.49	0.42
5:B:48:LEU:HD23	5:B:48:LEU:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:144:GLY:HA2	5:B:145:ARG:HA	1.49	0.42
5:B:834:ASN:HB2	5:B:839:MET:HA	2.02	0.42
5:B:848:ARG:HH22	5:B:996:ARG:HH12	1.63	0.42
6:C:66:ARG:CZ	11:J:2:ILE:HG13	2.39	0.42
9:H:44:VAL:HG12	9:H:44:VAL:O	2.20	0.42
12:K:77:THR:CG2	12:K:81:TYR:HD2	2.32	0.42
2:T:20:DC:H2'	2:T:21:DC:H5''	1.63	0.42
4:A:334:GLY:O	4:A:335:ARG:C	2.62	0.42
4:A:367:PRO:HG2	4:A:370:ILE:HD12	2.00	0.42
4:A:405:VAL:HG23	4:A:415:LEU:HD11	2.02	0.42
4:A:535:THR:HG21	4:A:617:VAL:H	1.84	0.42
5:B:386:LEU:O	5:B:390:LEU:HD12	2.19	0.42
5:B:507:LYS:O	5:B:508:LEU:CB	2.68	0.42
4:A:253:ASN:CA	4:A:255:SER:CB	2.74	0.42
5:B:600:LEU:HD23	5:B:600:LEU:HA	1.71	0.42
5:B:785:TYR:CD1	5:B:785:TYR:C	2.97	0.42
6:C:262:LEU:HD11	12:K:87:LEU:HD23	2.01	0.42
4:A:335:ARG:HE	4:A:335:ARG:HB2	1.63	0.42
4:A:518:LYS:HB2	4:A:519:PRO:CD	2.48	0.42
4:A:544:ASP:HB2	12:K:47:ARG:HH21	1.85	0.42
4:A:960:ILE:O	4:A:961:ARG:C	2.62	0.42
4:A:1174:PHE:HA	4:A:1175:SER:HA	1.62	0.42
5:B:71:LEU:HD22	5:B:72:GLU:HG2	2.02	0.42
5:B:164:LYS:NZ	5:B:443:ASN:HB3	2.35	0.42
5:B:603:LEU:HB3	5:B:609:ILE:HG12	2.01	0.42
5:B:610:ASN:OD1	5:B:612:GLU:HB3	2.20	0.42
9:H:44:VAL:HG13	9:H:48:PRO:HA	2.01	0.42
9:H:91:ASP:HA	9:H:93:TYR:HD1	1.85	0.42
4:A:351:THR:CG2	4:A:352:VAL:N	2.71	0.42
4:A:894:GLU:C	4:A:896:ARG:N	2.78	0.42
4:A:1029:ARG:HG3	4:A:1029:ARG:HH11	1.85	0.42
4:A:1060:PRO:HD2	8:F:86:THR:HG21	2.02	0.42
5:B:142:VAL:HG13	5:B:143:PRO:N	2.33	0.42
6:C:246:ARG:O	6:C:250:THR:OG1	2.33	0.42
7:E:71:LYS:HB3	7:E:75:MET:H	1.84	0.42
4:A:15:LYS:HD3	4:A:15:LYS:HA	1.84	0.42
4:A:152:VAL:HA	4:A:153:PRO:HA	1.77	0.42
4:A:249:SER:C	4:A:250:ILE:CG1	2.92	0.42
2:T:5:DC:H2''	2:T:6:DG:N7	2.35	0.41
4:A:153:PRO:O	4:A:161:LEU:HA	2.21	0.41
4:A:414:ASP:OD1	4:A:416:ARG:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:512:VAL:O	4:A:512:VAL:HG12	2.18	0.41
5:B:560:GLU:O	5:B:561:TRP:CD1	2.72	0.41
10:I:87:GLN:O	10:I:88:SER:C	2.63	0.41
4:A:316:GLN:HB3	4:A:317:LYS:HB3	2.00	0.41
4:A:366:VAL:HA	4:A:367:PRO:HD2	1.83	0.41
4:A:853:ASP:O	4:A:855:THR:N	2.53	0.41
5:B:552:MET:N	5:B:553:PRO:CD	2.83	0.41
5:B:641:GLU:C	5:B:643:ASP:H	2.29	0.41
5:B:744:HIS:HA	5:B:745:PRO:HD3	1.84	0.41
6:C:163:ILE:HD13	12:K:10:PHE:CE1	2.55	0.41
10:I:71:SER:HB3	10:I:85:PHE:CD2	2.55	0.41
2:T:1:DC:H2'	2:T:2:DT:H71	2.02	0.41
4:A:86:LEU:HA	4:A:273:ASN:HD21	1.85	0.41
4:A:1048:ASN:H	4:A:1048:ASN:HD22	1.69	0.41
4:A:1079:MET:HG2	4:A:1359:ASP:CG	2.45	0.41
5:B:737:THR:HB	10:I:66:PRO:HB3	2.02	0.41
4:A:722:LEU:HD22	4:A:799:PHE:CD1	2.56	0.41
4:A:886:ILE:HG23	4:A:944:ARG:HG2	2.02	0.41
4:A:1066:VAL:HG21	5:B:1139:ILE:HG21	2.02	0.41
4:A:1198:ASP:O	4:A:1202:MET:HG2	2.20	0.41
5:B:284:ILE:O	5:B:285:ILE:C	2.64	0.41
5:B:487:THR:HG22	5:B:488:TYR:H	1.86	0.41
5:B:804:GLY:O	5:B:983:ARG:NH2	2.53	0.41
7:E:56:LYS:HG3	7:E:84:ASP:OD1	2.20	0.41
9:H:93:TYR:CD2	9:H:145:ARG:HB3	2.56	0.41
4:A:313:GLN:HG2	4:A:314:ALA:N	2.36	0.41
4:A:871:ASP:HB3	7:E:204:THR:OG1	2.20	0.41
4:A:924:LYS:HE3	4:A:924:LYS:HB2	1.86	0.41
5:B:510:LYS:HD3	5:B:511:PRO:HD2	2.03	0.41
12:K:7:PHE:C	12:K:9:LEU:H	2.29	0.41
2:T:23:DC:C4	2:T:24:DT:C7	3.03	0.41
4:A:185:TRP:CZ3	4:A:200:ARG:HB3	2.55	0.41
4:A:825:ILE:HD13	4:A:825:ILE:HA	1.91	0.41
4:A:1433:MET:HE2	4:A:1433:MET:HB3	1.98	0.41
5:B:542:MET:HE3	5:B:636:PRO:HG3	2.03	0.41
5:B:822:ASN:HD22	11:J:52:THR:HG21	1.85	0.41
5:B:860:MET:SD	5:B:861:ASP:N	2.94	0.41
6:C:39:ALA:HA	6:C:164:ALA:HB3	2.02	0.41
6:C:44:LEU:HD12	6:C:160:LYS:O	2.21	0.41
7:E:190:LEU:HB3	7:E:214:CYS:SG	2.60	0.41
13:L:46:VAL:HB	13:L:47:ARG:H	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:253:ASN:C	4:A:253:ASN:HD22	2.27	0.41
5:B:977:GLY:C	5:B:1099:VAL:HG22	2.45	0.41
5:B:1132:GLU:H	5:B:1132:GLU:HG3	1.66	0.41
8:F:96:THR:O	8:F:96:THR:HG22	2.21	0.41
9:H:102:TYR:OH	9:H:122:LEU:HD22	2.20	0.41
10:I:56:ALA:HB3	10:I:89:GLN:HG3	2.01	0.41
12:K:92:ASN:O	12:K:93:SER:C	2.63	0.41
4:A:929:LEU:HD21	4:A:983:ILE:CG2	2.51	0.41
2:T:21:DC:C2	2:T:22:DT:C4	3.09	0.41
2:T:23:DC:O2	2:T:23:DC:H2'	2.21	0.41
4:A:399:HIS:CB	4:A:400:PRO:HD3	2.49	0.41
4:A:531:ILE:HD13	4:A:617:VAL:HG11	2.01	0.41
4:A:568:PRO:HB2	6:C:221:TYR:CE1	2.56	0.41
4:A:711:ARG:HH12	10:I:95:THR:HB	1.86	0.41
4:A:1287:TYR:CD2	4:A:1305:VAL:HB	2.56	0.41
5:B:142:VAL:HG13	5:B:144:GLY:N	2.26	0.41
5:B:345:LYS:H	5:B:348:ARG:N	2.13	0.41
5:B:500:THR:HA	5:B:501:PRO:HD3	1.85	0.41
5:B:523:CYS:SG	5:B:750:GLY:N	2.92	0.41
5:B:636:PRO:O	5:B:691:GLU:C	2.63	0.41
6:C:112:ASN:HD22	6:C:146:LYS:HG2	1.84	0.41
12:K:43:GLY:HA2	12:K:71:PHE:CE1	2.55	0.41
4:A:407:ARG:HH11	4:A:413:ILE:HD11	1.86	0.41
4:A:473:SER:OG	4:A:522:GLY:O	2.38	0.41
5:B:623:GLU:OE1	5:B:625:LYS:HE2	2.21	0.41
5:B:845:SER:HB3	5:B:850:LEU:HD22	2.03	0.41
5:B:975:GLN:CG	5:B:976:ILE:H	2.29	0.41
6:C:52:GLU:OE2	6:C:154:LYS:HG2	2.21	0.41
6:C:54:ASN:OD1	6:C:56:THR:OG1	2.39	0.41
12:K:57:LEU:HD21	12:K:78:THR:HG23	2.02	0.41
4:A:15:LYS:O	5:B:1220:ARG:NH1	2.54	0.40
4:A:382:PRO:CA	4:A:428:TYR:HE1	2.34	0.40
4:A:873:MET:HE3	4:A:957:PRO:HG3	2.03	0.40
5:B:724:ASP:HA	5:B:725:PRO:HD3	1.96	0.40
5:B:973:ILE:HG22	5:B:974:PRO:HD2	2.02	0.40
6:C:226:ASP:O	6:C:227:THR:CB	2.69	0.40
11:J:1:MET:HE2	11:J:1:MET:HB2	1.86	0.40
13:L:55:ILE:O	13:L:56:LEU:HB2	2.21	0.40
2:T:5:DC:N3	2:T:6:DG:C6	2.89	0.40
4:A:362:ASP:OD2	4:A:459:ARG:HD3	2.21	0.40
4:A:586:ILE:HG13	4:A:633:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:885:THR:HG22	4:A:940:ARG:HB2	2.03	0.40
5:B:982:SER:HB3	5:B:1092:TYR:CE1	2.56	0.40
6:C:56:THR:CG2	6:C:147:LEU:HD23	2.51	0.40
6:C:162:GLY:HA3	6:C:170:TRP:CE2	2.57	0.40
7:E:164:LEU:HD13	7:E:211:TYR:CE2	2.56	0.40
10:I:68:LEU:HD23	10:I:68:LEU:HA	1.77	0.40
11:J:1:MET:O	11:J:2:ILE:O	2.39	0.40
1:R:7:A:H5"	1:R:8:G:OP2	2.21	0.40
4:A:858:ASN:C	4:A:858:ASN:ND2	2.73	0.40
5:B:69:LEU:CB	5:B:70:ILE:CG2	2.98	0.40
5:B:128:LEU:HB2	5:B:167:ILE:O	2.21	0.40
5:B:174:LEU:HA	5:B:174:LEU:HD12	1.68	0.40
5:B:842:ASN:O	5:B:846:ILE:HG13	2.22	0.40
6:C:97:VAL:HG21	6:C:129:ILE:HG23	2.03	0.40
10:I:65:ASP:HA	10:I:66:PRO:HD3	1.92	0.40
4:A:533:LYS:HE3	4:A:745:GLN:NE2	2.32	0.40
4:A:900:ASP:HA	4:A:926:GLN:NE2	2.37	0.40
4:A:1060:PRO:HD2	8:F:86:THR:CG2	2.51	0.40
4:A:1141:THR:HG21	4:A:1205:LYS:HD3	2.04	0.40
4:A:1428:VAL:HG22	5:B:1147:LEU:HD11	2.02	0.40
5:B:879:ARG:HB3	5:B:880:THR:H	1.39	0.40
5:B:884:ARG:O	5:B:936:ASP:HB3	2.21	0.40
5:B:1069:PHE:HA	5:B:1085:ILE:O	2.22	0.40
7:E:204:THR:HG23	7:E:205:SER:N	2.36	0.40
8:F:124:GLU:O	8:F:130:ILE:HG13	2.21	0.40
4:A:535:THR:HG21	4:A:617:VAL:HG23	2.03	0.40
4:A:1366:ARG:HG2	4:A:1366:ARG:H	1.68	0.40
5:B:457:LEU:HD23	5:B:457:LEU:HA	1.97	0.40
5:B:788:ARG:NH1	5:B:790:ASP:CG	2.79	0.40
5:B:1010:LEU:HA	5:B:1010:LEU:HD12	1.61	0.40
7:E:190:LEU:HD13	7:E:190:LEU:HA	1.95	0.40
9:H:82:PRO:O	9:H:83:GLN:CB	2.68	0.40

There are no symmetry-related clashes.

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	1401/1733 (81%)	1186 (85%)	160 (11%)	55 (4%)	2	15
5	B	1129/1224 (92%)	938 (83%)	133 (12%)	58 (5%)	1	11
6	C	264/318 (83%)	226 (86%)	33 (12%)	5 (2%)	6	26
7	E	211/215 (98%)	176 (83%)	29 (14%)	6 (3%)	4	19
8	F	84/155 (54%)	74 (88%)	7 (8%)	3 (4%)	2	16
9	H	130/146 (89%)	104 (80%)	21 (16%)	5 (4%)	2	15
10	I	117/122 (96%)	95 (81%)	19 (16%)	3 (3%)	4	21
11	J	63/70 (90%)	55 (87%)	4 (6%)	4 (6%)	1	7
12	K	112/120 (93%)	102 (91%)	8 (7%)	2 (2%)	6	26
13	L	44/70 (63%)	30 (68%)	7 (16%)	7 (16%)	0	0
All	All	3555/4173 (85%)	2986 (84%)	421 (12%)	148 (4%)	2	14

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	50	ILE
4	A	55	ASP
4	A	56	PRO
4	A	250	ILE
4	A	312	PRO
4	A	321	PRO
4	A	322	VAL
4	A	335	ARG
4	A	399	HIS
4	A	424	ILE
4	A	609	ASP
4	A	854	ASN
4	A	1393	ASN
4	A	1446	ASP
5	B	70	ILE
5	B	71	LEU
5	B	72	GLU
5	B	249	ARG
5	B	451	LYS
5	B	469	GLN

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Mol	Chain	Res	Type
5	B	476	ARG
5	B	636	PRO
5	B	643	ASP
5	B	677	GLU
5	B	712	PRO
5	B	731	VAL
5	B	813	LYS
5	B	883	LEU
5	B	1156	ASP
5	B	1181	GLU
7	E	70	SER
7	E	72	PHE
7	E	206	GLY
10	I	3	THR
13	L	53	HIS
4	A	155	GLU
4	A	214	ILE
4	A	253	ASN
4	A	256	GLN
4	A	258	GLY
4	A	332	LYS
4	A	404	TYR
4	A	517	ASN
4	A	895	LYS
4	A	998	LEU
4	A	1403	GLU
4	A	1437	GLY
5	B	138	GLU
5	B	143	PRO
5	B	446	LEU
5	B	477	ALA
5	B	483	LEU
5	B	484	ASN
5	B	531	GLN
5	B	1096	ARG
8	F	128	LYS
11	J	2	ILE
11	J	6	ARG
13	L	45	ALA
13	L	46	VAL
13	L	55	ILE
4	A	27	VAL

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Mol	Chain	Res	Type
4	A	76	GLU
4	A	248	PRO
4	A	251	SER
4	A	324	SER
4	A	568	PRO
4	A	1173	HIS
4	A	1388	GLY
5	B	68	THR
5	B	69	LEU
5	B	142	VAL
5	B	146	GLU
5	B	277	LYS
5	B	322	PHE
5	B	338	GLY
5	B	367	LEU
5	B	468	GLU
5	B	474	SER
5	B	792	MET
5	B	1021	MET
5	B	1046	PRO
5	B	1165	ILE
6	C	214	ASN
6	C	215	GLU
7	E	64	PRO
9	H	81	PRO
9	H	82	PRO
9	H	128	ASN
9	H	140	ALA
10	I	47	GLU
12	K	37	LYS
12	K	50	LEU
13	L	50	ASP
4	A	152	VAL
4	A	178	GLY
4	A	245	PRO
4	A	926	GLN
4	A	1448	GLU
5	B	65	GLU
5	B	540	SER
5	B	648	HIS
5	B	981	ALA
5	B	1017	ILE

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Mol	Chain	Res	Type
5	B	1222	ARG
6	C	142	VAL
8	F	74	ILE
8	F	104	ASN
10	I	90	GLN
13	L	47	ARG
4	A	68	GLN
4	A	149	GLU
4	A	597	LEU
4	A	827	THR
4	A	846	GLU
4	A	958	VAL
4	A	1255	GLU
5	B	90	ILE
5	B	214	ALA
5	B	334	ILE
5	B	410	GLY
5	B	508	LEU
5	B	519	TRP
5	B	1171	VAL
6	C	90	ASP
6	C	227	THR
7	E	124	VAL
9	H	90	ALA
11	J	4	PRO
4	A	44	THR
4	A	51	GLY
4	A	1424	VAL
5	B	266	ALA
5	B	467	GLY
5	B	974	PRO
5	B	1097	HIS
11	J	5	VAL
13	L	56	LEU
4	A	153	PRO
7	E	51	GLY
4	A	35	ILE
4	A	567	LYS
5	B	114	PRO
4	A	983	ILE
5	B	901	PRO
4	A	484	GLY

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Mol	Chain	Res	Type
5	B	482	VAL
4	A	158	PRO

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	1233/1520 (81%)	1098 (89%)	135 (11%)	6	22
5	B	991/1061 (93%)	855 (86%)	136 (14%)	3	14
6	C	234/274 (85%)	203 (87%)	31 (13%)	4	15
7	E	195/197 (99%)	183 (94%)	12 (6%)	16	42
8	F	76/137 (56%)	69 (91%)	7 (9%)	8	29
9	H	118/128 (92%)	104 (88%)	14 (12%)	5	19
10	I	113/116 (97%)	104 (92%)	9 (8%)	11	35
11	J	60/65 (92%)	52 (87%)	8 (13%)	4	15
12	K	99/102 (97%)	82 (83%)	17 (17%)	2	9
13	L	40/57 (70%)	34 (85%)	6 (15%)	3	11
All	All	3159/3657 (86%)	2784 (88%)	375 (12%)	5	19

All (375) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	13	THR
4	A	22	PHE
4	A	23	SER
4	A	31	SER
4	A	32	VAL
4	A	60	SER
4	A	69	THR
4	A	80	HIS
4	A	86	LEU
4	A	93	VAL
4	A	146	MET

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Mol	Chain	Res	Type
4	A	147	VAL
4	A	222	LEU
4	A	227	VAL
4	A	237	THR
4	A	241	VAL
4	A	251	SER
4	A	252	PHE
4	A	253	ASN
4	A	259	GLU
4	A	265	LYS
4	A	266	LEU
4	A	270	LEU
4	A	274	ILE
4	A	322	VAL
4	A	332	LYS
4	A	359	LEU
4	A	375	THR
4	A	387	ARG
4	A	392	VAL
4	A	403	LYS
4	A	409	SER
4	A	413	ILE
4	A	424	ILE
4	A	437	MET
4	A	449	SER
4	A	450	LEU
4	A	454	SER
4	A	463	ILE
4	A	472	LEU
4	A	475	THR
4	A	486	GLU
4	A	491	VAL
4	A	501	LEU
4	A	505	CYS
4	A	509	LEU
4	A	512	VAL
4	A	513	SER
4	A	518	LYS
4	A	523	ILE
4	A	524	VAL
4	A	527	THR
4	A	528	LEU

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Mol	Chain	Res	Type
4	A	531	ILE
4	A	550	LEU
4	A	559	VAL
4	A	566	ILE
4	A	573	SER
4	A	576	GLN
4	A	577	ILE
4	A	595	THR
4	A	598	LEU
4	A	616	VAL
4	A	660	ASN
4	A	666	ILE
4	A	675	THR
4	A	690	VAL
4	A	691	LEU
4	A	702	LEU
4	A	709	THR
4	A	732	LEU
4	A	740	LEU
4	A	756	ILE
4	A	762	SER
4	A	765	VAL
4	A	771	GLU
4	A	773	LYS
4	A	775	ILE
4	A	783	THR
4	A	803	SER
4	A	805	LEU
4	A	808	LEU
4	A	809	THR
4	A	821	ARG
4	A	829	VAL
4	A	831	THR
4	A	855	THR
4	A	858	ASN
4	A	871	ASP
4	A	880	LYS
4	A	884	ASP
4	A	902	LEU
4	A	913	LEU
4	A	929	LEU
4	A	948	VAL

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Mol	Chain	Res	Type
4	A	982	THR
4	A	990	VAL
4	A	996	ASN
4	A	1001	ARG
4	A	1017	LEU
4	A	1029	ARG
4	A	1047	SER
4	A	1058	VAL
4	A	1067	LEU
4	A	1077	THR
4	A	1094	VAL
4	A	1095	THR
4	A	1113	THR
4	A	1118	VAL
4	A	1142	THR
4	A	1152	ILE
4	A	1172	LEU
4	A	1219	THR
4	A	1224	LEU
4	A	1259	MET
4	A	1272	THR
4	A	1279	ILE
4	A	1280	GLU
4	A	1291	VAL
4	A	1299	VAL
4	A	1308	THR
4	A	1314	SER
4	A	1316	VAL
4	A	1329	THR
4	A	1333	ILE
4	A	1335	ILE
4	A	1336	MET
4	A	1341	ILE
4	A	1359	ASP
4	A	1376	THR
4	A	1382	THR
4	A	1385	THR
4	A	1403	GLU
4	A	1436	ILE
4	A	1449	SER
5	B	21	GLU
5	B	28	GLU

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Mol	Chain	Res	Type
5	B	40	GLU
5	B	58	THR
5	B	63	ILE
5	B	70	ILE
5	B	71	LEU
5	B	72	GLU
5	B	73	GLN
5	B	89	GLU
5	B	90	ILE
5	B	94	LYS
5	B	98	THR
5	B	108	VAL
5	B	109	THR
5	B	134	LYS
5	B	140	ILE
5	B	141	ASP
5	B	142	VAL
5	B	145	ARG
5	B	194	GLU
5	B	217	ARG
5	B	225	VAL
5	B	234	ILE
5	B	239	GLU
5	B	250	PHE
5	B	264	SER
5	B	285	ILE
5	B	287	ARG
5	B	322	PHE
5	B	323	VAL
5	B	339	THR
5	B	343	ILE
5	B	365	THR
5	B	378	LEU
5	B	387	LEU
5	B	404	LYS
5	B	408	LEU
5	B	412	LEU
5	B	416	LEU
5	B	423	LYS
5	B	424	LEU
5	B	425	THR
5	B	445	LYS

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Mol	Chain	Res	Type
5	B	452	THR
5	B	453	ILE
5	B	463	THR
5	B	469	GLN
5	B	473	MET
5	B	474	SER
5	B	479	VAL
5	B	482	VAL
5	B	483	LEU
5	B	484	ASN
5	B	485	ARG
5	B	487	THR
5	B	500	THR
5	B	502	ILE
5	B	504	ARG
5	B	510	LYS
5	B	513	GLN
5	B	536	VAL
5	B	537	LYS
5	B	539	LEU
5	B	563	MET
5	B	570	VAL
5	B	574	SER
5	B	609	ILE
5	B	619	ILE
5	B	628	THR
5	B	637	LEU
5	B	658	ILE
5	B	676	VAL
5	B	692	TYR
5	B	694	ASP
5	B	701	ILE
5	B	729	ILE
5	B	731	VAL
5	B	737	THR
5	B	755	ILE
5	B	764	SER
5	B	790	ASP
5	B	791	THR
5	B	796	LEU
5	B	799	PRO
5	B	805	THR

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Mol	Chain	Res	Type
5	B	812	LEU
5	B	827	ILE
5	B	831	SER
5	B	850	LEU
5	B	878	GLN
5	B	879	ARG
5	B	880	THR
5	B	883	LEU
5	B	889	THR
5	B	905	VAL
5	B	906	SER
5	B	911	ILE
5	B	916	THR
5	B	936	ASP
5	B	945	GLU
5	B	958	GLN
5	B	963	PHE
5	B	964	VAL
5	B	967	ARG
5	B	969	ARG
5	B	973	ILE
5	B	983	ARG
5	B	986	GLN
5	B	992	ILE
5	B	993	THR
5	B	997	GLU
5	B	999	MET
5	B	1007	VAL
5	B	1022	THR
5	B	1031	LEU
5	B	1065	GLN
5	B	1073	TYR
5	B	1082	MET
5	B	1090	THR
5	B	1095	LEU
5	B	1097	HIS
5	B	1099	VAL
5	B	1113	VAL
5	B	1115	THR
5	B	1124	ARG
5	B	1147	LEU
5	B	1159	ARG

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Mol	Chain	Res	Type
5	B	1160	VAL
5	B	1165	ILE
5	B	1166	CYS
5	B	1191	ILE
5	B	1194	ILE
5	B	1196	ILE
5	B	1202	LEU
5	B	1218	THR
6	C	21	ILE
6	C	22	LEU
6	C	25	VAL
6	C	33	LEU
6	C	40	GLU
6	C	41	ILE
6	C	46	ILE
6	C	56	THR
6	C	66	ARG
6	C	77	ILE
6	C	99	LEU
6	C	116	LYS
6	C	129	ILE
6	C	133	ILE
6	C	137	LYS
6	C	138	GLU
6	C	140	ASN
6	C	143	LEU
6	C	147	LEU
6	C	157	CYS
6	C	158	VAL
6	C	166	GLU
6	C	176	ILE
6	C	186	LEU
6	C	189	THR
6	C	190	ASP
6	C	215	GLU
6	C	240	VAL
6	C	244	VAL
6	C	250	THR
6	C	258	ILE
7	E	9	ILE
7	E	19	VAL
7	E	58	MET

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Mol	Chain	Res	Type
7	E	65	THR
7	E	69	ILE
7	E	74	ASP
7	E	104	ASN
7	E	127	ILE
7	E	156	LEU
7	E	165	LEU
7	E	169	ARG
7	E	190	LEU
8	F	81	THR
8	F	97	ARG
8	F	104	ASN
8	F	120	ILE
8	F	123	LYS
8	F	125	LEU
8	F	133	VAL
9	H	2	SER
9	H	27	GLU
9	H	31	THR
9	H	32	THR
9	H	58	THR
9	H	62	SER
9	H	88	SER
9	H	89	LEU
9	H	91	ASP
9	H	94	ASP
9	H	107	VAL
9	H	111	LEU
9	H	136	LYS
9	H	144	ILE
10	I	5	ARG
10	I	10	CYS
10	I	11	ASN
10	I	12	ASN
10	I	24	ARG
10	I	30	ARG
10	I	59	VAL
10	I	62	ILE
10	I	107	SER
11	J	1	MET
11	J	2	ILE
11	J	7	CYS

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Mol	Chain	Res	Type
11	J	14	VAL
11	J	34	THR
11	J	46	CYS
11	J	48	ARG
11	J	64	ASN
12	K	1	MET
12	K	5	ASP
12	K	6	ARG
12	K	18	LYS
12	K	20	LYS
12	K	31	VAL
12	K	32	VAL
12	K	33	ILE
12	K	41	THR
12	K	42	LEU
12	K	47	ARG
12	K	56	VAL
12	K	64	GLU
12	K	78	THR
12	K	93	SER
12	K	101	LEU
12	K	113	THR
13	L	27	LEU
13	L	46	VAL
13	L	48	CYS
13	L	61	THR
13	L	62	LYS
13	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	18	GLN
4	A	80	HIS
4	A	83	HIS
4	A	109	HIS
4	A	118	HIS
4	A	160	GLN
4	A	169	ASN
4	A	171	GLN
4	A	273	ASN
4	A	297	GLN

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Mol	Chain	Res	Type
4	A	299	HIS
4	A	313	GLN
4	A	435	HIS
4	A	503	GLN
4	A	515	GLN
4	A	517	ASN
4	A	548	ASN
4	A	640	GLN
4	A	659	HIS
4	A	660	ASN
4	A	736	ASN
4	A	741	ASN
4	A	745	GLN
4	A	757	ASN
4	A	858	ASN
4	A	877	HIS
4	A	926	GLN
4	A	953	ASN
4	A	965	GLN
4	A	968	GLN
4	A	996	ASN
4	A	1048	ASN
4	A	1124	HIS
4	A	1278	ASN
4	A	1312	ASN
4	A	1364	ASN
4	A	1393	ASN
4	A	1432	GLN
5	B	73	GLN
5	B	121	ASN
5	B	325	GLN
5	B	350	GLN
5	B	366	GLN
5	B	415	GLN
5	B	433	GLN
5	B	465	ASN
5	B	484	ASN
5	B	513	GLN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	657	HIS

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Mol	Chain	Res	Type
5	B	734	HIS
5	B	744	HIS
5	B	770	GLN
5	B	794	ASN
5	B	822	ASN
5	B	842	ASN
5	B	878	GLN
5	B	975	GLN
5	B	984	HIS
5	B	986	GLN
5	B	1013	ASN
5	B	1062	HIS
5	B	1076	HIS
5	B	1097	HIS
5	B	1195	HIS
6	C	73	GLN
6	C	91	HIS
6	C	102	GLN
6	C	112	ASN
6	C	140	ASN
6	C	188	HIS
6	C	242	GLN
7	E	146	HIS
7	E	147	HIS
9	H	11	GLN
9	H	35	GLN
9	H	128	ASN
9	H	137	GLN
9	H	139	ASN
10	I	12	ASN
10	I	46	HIS
12	K	65	HIS
12	K	76	GLN
12	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	9/10 (90%)	5 (55%)	1 (11%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	3	C
1	R	7	A
1	R	8	G
1	R	9	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	1	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	DGT	B	1308[A]	-	32,33,33	1.71	7 (21%)	48,52,52	1.69	9 (18%)
16	DGT	B	1308[B]	-	32,33,33	1.49	5 (15%)	48,52,52	1.66	6 (12%)

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	DGT	B	1308[A]	-	-	6/22/34/34	0/3/3/3
16	DGT	B	1308[B]	-	-	6/22/34/34	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1308[A]	DGT	PA-O3A	4.68	1.64	1.59
16	B	1308[A]	DGT	PB-O3B	4.16	1.64	1.59
16	B	1308[A]	DGT	PB-O3A	3.76	1.63	1.59
16	B	1308[B]	DGT	PB-O3B	3.70	1.63	1.59
16	B	1308[B]	DGT	PB-O3A	3.45	1.63	1.59
16	B	1308[B]	DGT	PA-O3A	3.31	1.63	1.59
16	B	1308[A]	DGT	C5-C4	3.26	1.47	1.38
16	B	1308[B]	DGT	C5-C4	3.20	1.47	1.38
16	B	1308[B]	DGT	C6-N1	-2.24	1.34	1.38
16	B	1308[A]	DGT	C4-N9	-2.23	1.32	1.38
16	B	1308[A]	DGT	C5-N7	-2.20	1.34	1.39
16	B	1308[A]	DGT	C6-N1	-2.08	1.35	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1308[B]	DGT	C5-C4-N3	-5.22	120.09	128.39
16	B	1308[A]	DGT	C5-C4-N3	-5.16	120.18	128.39
16	B	1308[B]	DGT	C2-N3-C4	4.61	120.24	112.30
16	B	1308[A]	DGT	C2-N3-C4	4.60	120.23	112.30
16	B	1308[A]	DGT	N9-C4-N3	4.14	134.23	125.95
16	B	1308[B]	DGT	N9-C4-N3	4.05	134.05	125.95
16	B	1308[B]	DGT	C6-C5-N7	3.64	136.91	130.29
16	B	1308[A]	DGT	C6-C5-N7	3.20	136.11	130.29
16	B	1308[A]	DGT	O6-C6-C5	-2.60	119.68	126.53
16	B	1308[A]	DGT	C2'-C3'-C4'	2.48	107.83	102.80
16	B	1308[B]	DGT	C4-C5-N7	-2.28	107.05	110.67
16	B	1308[B]	DGT	O6-C6-C5	-2.25	120.58	126.53
16	B	1308[A]	DGT	O5'-C5'-C4'	2.21	116.50	108.99
16	B	1308[A]	DGT	C2'-C1'-N9	-2.10	108.56	113.81
16	B	1308[A]	DGT	O4'-C1'-C2'	2.03	110.04	106.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	1308[A]	DGT	C5'-O5'-PA-O3A
16	B	1308[A]	DGT	C5'-O5'-PA-O2A
16	B	1308[A]	DGT	C4'-C5'-O5'-PA
16	B	1308[B]	DGT	C5'-O5'-PA-O1A
16	B	1308[B]	DGT	C3'-C4'-C5'-O5'
16	B	1308[B]	DGT	O4'-C4'-C5'-O5'
16	B	1308[A]	DGT	O4'-C4'-C5'-O5'
16	B	1308[B]	DGT	C4'-C5'-O5'-PA
16	B	1308[A]	DGT	C5'-O5'-PA-O1A
16	B	1308[B]	DGT	C5'-O5'-PA-O3A
16	B	1308[B]	DGT	C5'-O5'-PA-O2A
16	B	1308[A]	DGT	PA-O3A-PB-O1B

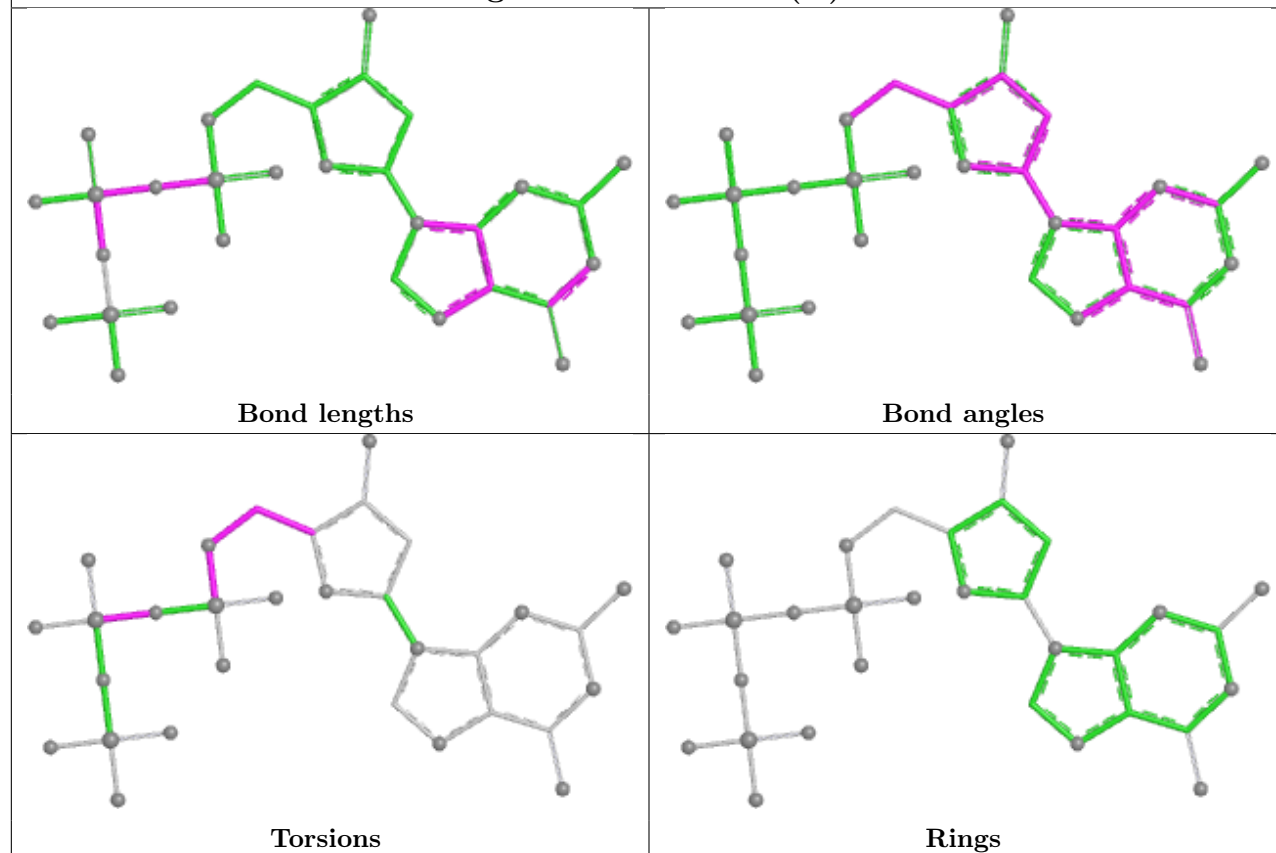
There are no ring outliers.

1 monomer is involved in 2 short contacts:

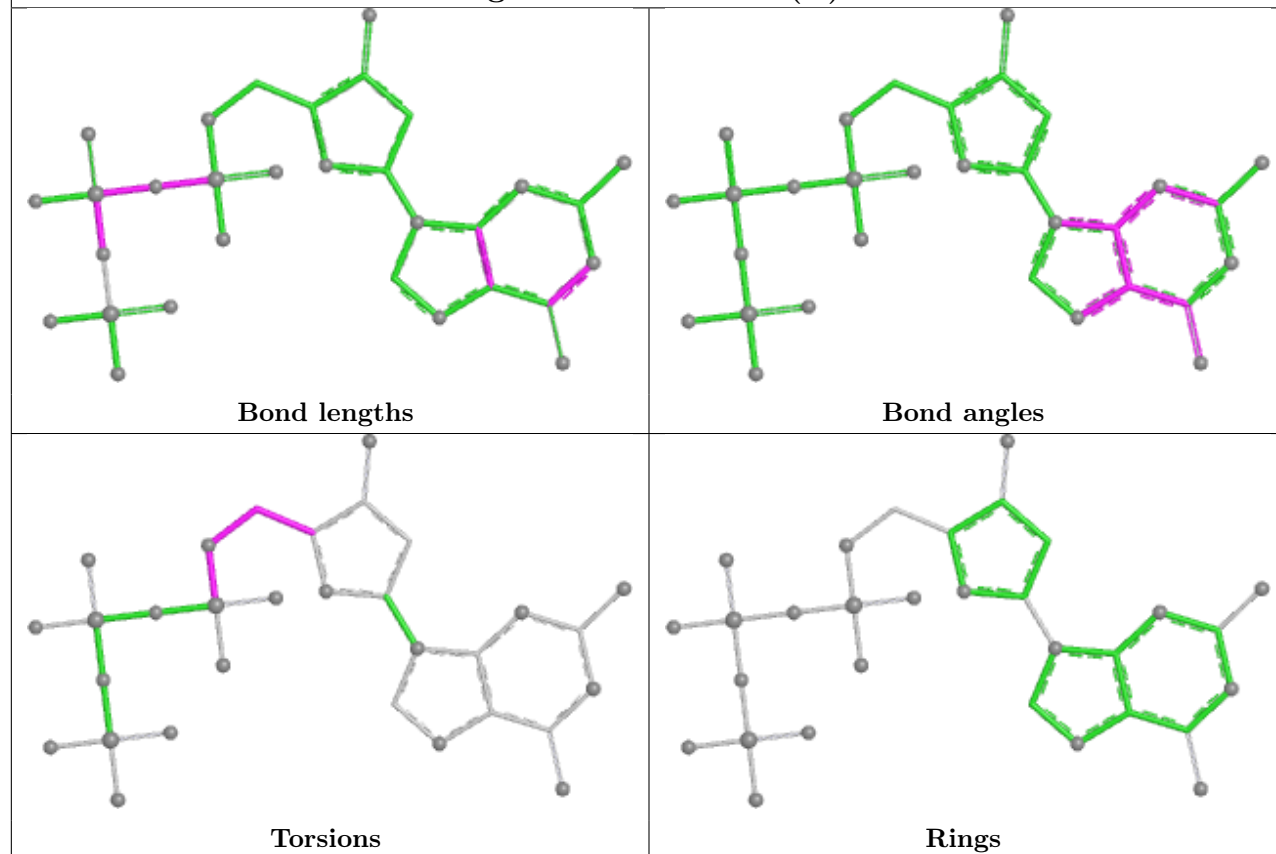
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1308[A]	DGT	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DGT B 1308 (A)



Ligand DGT B 1308 (B)



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	10/10 (100%)	0.50	1 (10%) 12 12	72, 93, 202, 234	0
2	T	28/28 (100%)	1.97	15 (53%) 0 0	118, 195, 427, 447	0
3	N	14/14 (100%)	2.53	9 (64%) 0 0	270, 338, 424, 426	0
4	A	1411/1733 (81%)	0.45	74 (5%) 33 24	56, 105, 206, 247	0
5	B	1143/1224 (93%)	0.24	31 (2%) 56 41	27, 88, 156, 185	0
6	C	266/318 (83%)	0.06	1 (0%) 88 81	59, 91, 135, 151	0
7	E	213/215 (99%)	0.79	13 (6%) 27 21	96, 142, 228, 233	0
8	F	86/155 (55%)	0.42	2 (2%) 61 46	83, 117, 137, 141	0
9	H	134/146 (91%)	0.89	14 (10%) 11 12	35, 140, 171, 175	0
10	I	119/122 (97%)	0.52	3 (2%) 58 43	85, 121, 156, 165	0
11	J	65/70 (92%)	-0.04	1 (1%) 72 58	60, 82, 110, 117	0
12	K	114/120 (95%)	0.05	1 (0%) 81 69	77, 102, 119, 122	0
13	L	46/70 (65%)	1.08	6 (13%) 7 8	87, 165, 176, 179	0
All	All	3649/4225 (86%)	0.40	171 (4%) 36 27	27, 103, 198, 447	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	L	26	THR	5.1
4	A	72	GLU	4.7
5	B	89	GLU	4.3
4	A	320	ARG	4.2
9	H	1	MET	4.2
9	H	139	ASN	4.2
2	T	21	DC	4.2
4	A	97	ALA	4.2
4	A	94	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
9	H	63	LEU	4.0
2	T	20	DC	4.0
2	T	22	DT	3.9
5	B	869	SER	3.9
13	L	28	LYS	3.8
5	B	882	THR	3.8
4	A	1176	LEU	3.8
4	A	756	ILE	3.7
7	E	70	SER	3.7
5	B	474	SER	3.6
13	L	27	LEU	3.6
3	N	10	DG	3.6
9	H	134	ASN	3.6
4	A	151	ASP	3.6
3	N	13	DA	3.5
10	I	13	MET	3.5
9	H	137	GLN	3.5
7	E	7	ARG	3.5
4	A	98	LYS	3.4
4	A	96	ILE	3.3
4	A	321	PRO	3.3
3	N	1	DC	3.3
5	B	1173	ALA	3.2
3	N	11	DG	3.2
5	B	477	ALA	3.2
3	N	9	DC	3.1
4	A	265	LYS	3.1
4	A	144	THR	3.1
7	E	211	TYR	3.1
5	B	708	GLU	3.1
4	A	152	VAL	3.0
13	L	25	ALA	3.0
5	B	1169	MET	2.9
2	T	7	DA	2.9
5	B	883	LEU	2.9
4	A	78	PRO	2.9
3	N	8	DT	2.9
4	A	53	LEU	2.9
4	A	145	LYS	2.9
4	A	181	LEU	2.8
4	A	399	HIS	2.8
7	E	16	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
4	A	255	SER	2.8
9	H	90	ALA	2.8
5	B	88	TYR	2.8
3	N	7	DA	2.7
4	A	50	ILE	2.7
5	B	90	ILE	2.7
9	H	86	ASP	2.7
3	N	12	DT	2.7
4	A	314	ALA	2.7
4	A	1260	LEU	2.7
12	K	114	LEU	2.7
2	T	19	DT	2.7
8	F	93	ILE	2.6
4	A	115	LEU	2.6
4	A	567	LYS	2.6
4	A	973	ILE	2.6
8	F	74	ILE	2.6
4	A	587	HIS	2.6
3	N	14	DG	2.6
4	A	980	ASP	2.6
2	T	23	DC	2.6
4	A	132	LYS	2.6
4	A	920	LEU	2.5
5	B	1151	LEU	2.5
7	E	133	GLU	2.5
5	B	92	PHE	2.5
5	B	335	GLY	2.5
10	I	52	ILE	2.5
11	J	2	ILE	2.5
4	A	1410	PHE	2.5
5	B	866	TYR	2.5
5	B	643	ASP	2.5
7	E	121	MET	2.5
7	E	131	THR	2.5
1	R	1	A	2.5
5	B	501	PRO	2.5
5	B	1180	PHE	2.4
7	E	76	GLY	2.4
4	A	885	THR	2.4
13	L	32	ALA	2.4
4	A	975	HIS	2.4
4	A	308	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
4	A	114	LEU	2.4
5	B	710	LEU	2.4
4	A	69	THR	2.4
4	A	140	THR	2.4
4	A	312	PRO	2.4
4	A	1225	PHE	2.4
2	T	10	DA	2.4
4	A	323	LYS	2.3
9	H	2	SER	2.3
2	T	8	DT	2.3
7	E	68	SER	2.3
7	E	108	GLY	2.3
5	B	1217	TYR	2.3
5	B	1172	ILE	2.3
9	H	79	TRP	2.3
4	A	76	GLU	2.3
4	A	289	ILE	2.3
9	H	140	ALA	2.3
4	A	315	LEU	2.3
5	B	356	LEU	2.3
2	T	1	DC	2.3
5	B	106	ASP	2.3
5	B	359	GLU	2.2
4	A	73	GLY	2.2
2	T	13	DA	2.2
4	A	113	LEU	2.2
9	H	7	ASP	2.2
4	A	1238	ILE	2.2
4	A	136	ALA	2.2
4	A	1267	MET	2.2
9	H	132	LEU	2.2
4	A	135	PHE	2.2
4	A	1237	ILE	2.2
4	A	141	LEU	2.2
4	A	51	GLY	2.2
4	A	727	ASP	2.2
5	B	475	SER	2.2
4	A	902	LEU	2.2
7	E	20	LYS	2.2
9	H	130	ARG	2.2
2	T	6	DG	2.1
4	A	65	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
5	B	865	LYS	2.1
4	A	1194	ARG	2.1
4	A	365	GLY	2.1
4	A	1002	GLY	2.1
4	A	496	GLU	2.1
5	B	933	SER	2.1
4	A	61	ILE	2.1
4	A	1062	GLU	2.1
10	I	6	PHE	2.1
5	B	870	ILE	2.1
13	L	57	LEU	2.1
2	T	4	DC	2.1
6	C	16	ASP	2.1
4	A	755	PHE	2.1
9	H	82	PRO	2.1
4	A	93	VAL	2.0
2	T	9	DA	2.0
4	A	276	LEU	2.0
4	A	1081	LEU	2.0
4	A	1200	ALA	2.0
4	A	1446	ASP	2.0
7	E	107	THR	2.0
4	A	91	PHE	2.0
4	A	176	LYS	2.0
5	B	69	LEU	2.0
5	B	502	ILE	2.0
5	B	918	ILE	2.0
7	E	69	ILE	2.0
2	T	2	DT	2.0
2	T	3	DA	2.0
4	A	1126	ALA	2.0
4	A	319	GLY	2.0
4	A	1220	PHE	2.0
4	A	1240	CYS	2.0
4	A	106	VAL	2.0
4	A	250	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

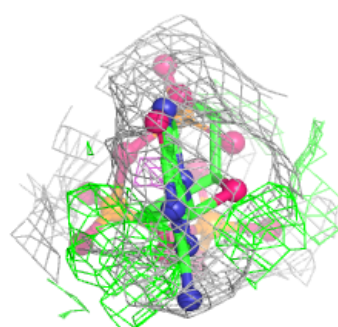
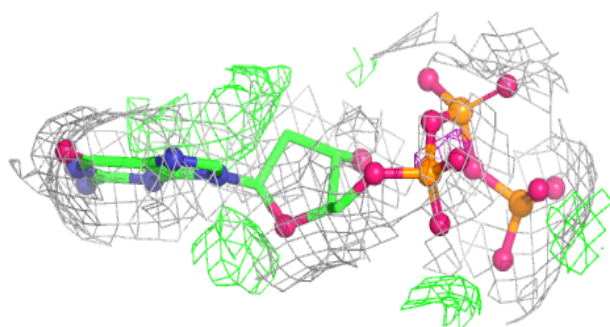
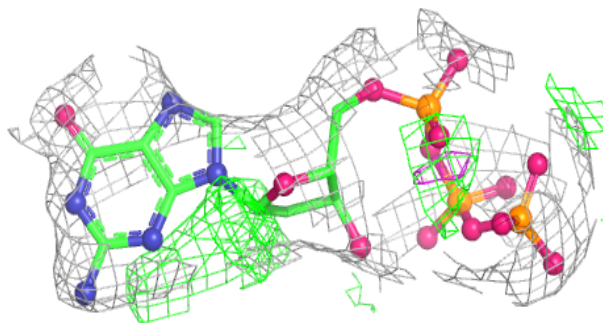
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	DGT	B	1308[A]	31/31	0.74	0.18	126,132,152,153	31
16	DGT	B	1308[B]	31/31	0.74	0.18	80,86,113,113	31
15	MG	A	2001	1/1	0.76	0.25	116,116,116,116	0
14	ZN	B	1307	1/1	0.96	0.06	143,143,143,143	0
14	ZN	A	1734	1/1	0.97	0.04	226,226,226,226	0
14	ZN	L	105	1/1	0.98	0.04	190,190,190,190	0
14	ZN	A	1735	1/1	0.98	0.04	139,139,139,139	0
14	ZN	I	204	1/1	0.99	0.02	106,106,106,106	0
14	ZN	J	101	1/1	0.99	0.04	105,105,105,105	0
14	ZN	I	203	1/1	0.99	0.07	131,131,131,131	0
14	ZN	C	319	1/1	1.00	0.01	95,95,95,95	0

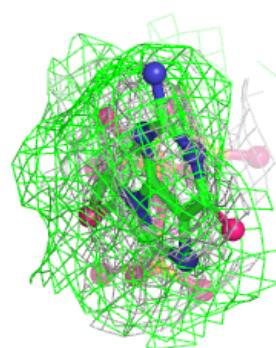
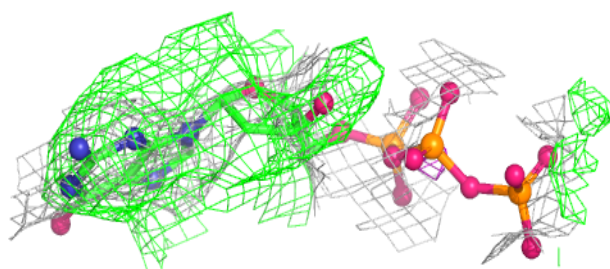
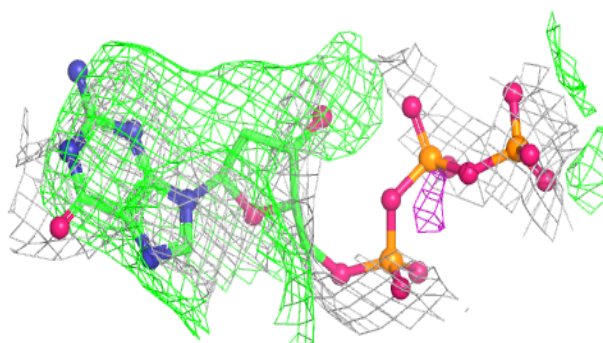
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGT B 1308 (A):

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

**Electron density around DGT B 1308 (B):**

$2mF_o-DF_c$ (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.