



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2026 – 12:13 PM EDT

PDB ID : 9PVV / pdb_00009pvv
Title : RNA polymerase II elongation complex with dC at +1 site, 8-oxo-GTP bound in A-site.
Authors : Hou, P.; Oh, J.; Wang, D.
Deposited on : 2025-08-03
Resolution : 3.48 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

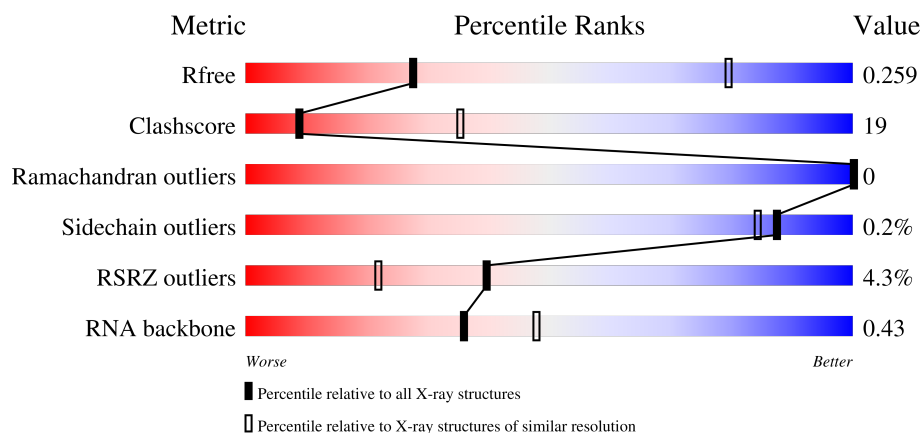
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)
RNA backbone	3983	1001 (3.94-3.02)

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

Mol	Chain	Length	Quality of chain
1	R	9	<div> <div>5%</div> <div>33% 56% 11%</div> </div>
2	T	29	<div> <div>48% 38% 14%</div> </div>
3	N	18	<div> <div>17% 61% 22%</div> </div>
4	A	1733	<div> <div>5% 47% 34% 20%</div> </div>

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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 29102 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			193	88	40	57	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	25	Total	C	N	O	P	0	0	0
			497	239	76	157	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	14	Total	C	N	O	P	0	0	0
			296	138	66	78	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1393	Total	C	N	O	S	0	0	0
			10894	6875	1908	2051	60			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

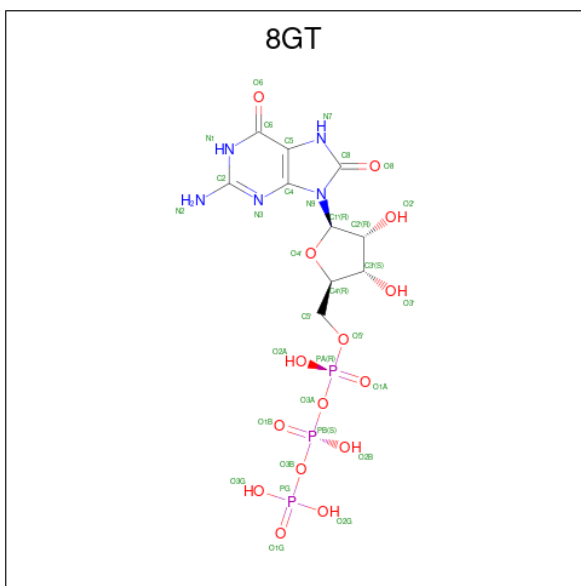
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

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

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

- Molecule 14 is 8-OXO-GUANOSINE-5'-TRIPHOSPHATE (CCD ID: 8GT) (formula:

C₁₀H₁₆N₅O₁₅P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	T	1	Total	C	N	O	P	0	0
			33	10	5	15	3		

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

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

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

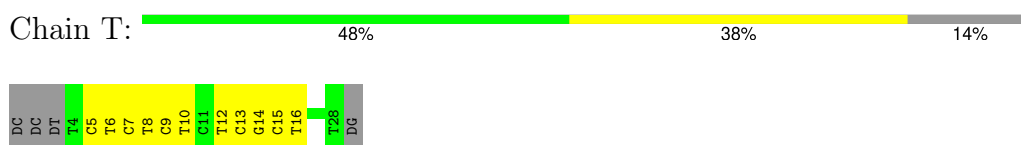
3 Residue-property plots

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

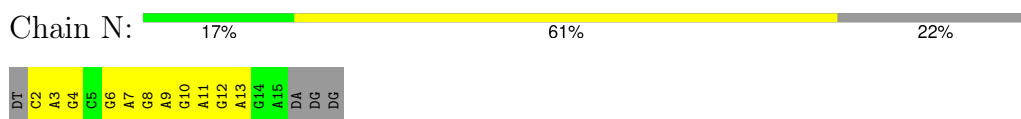
- Molecule 1: RNA



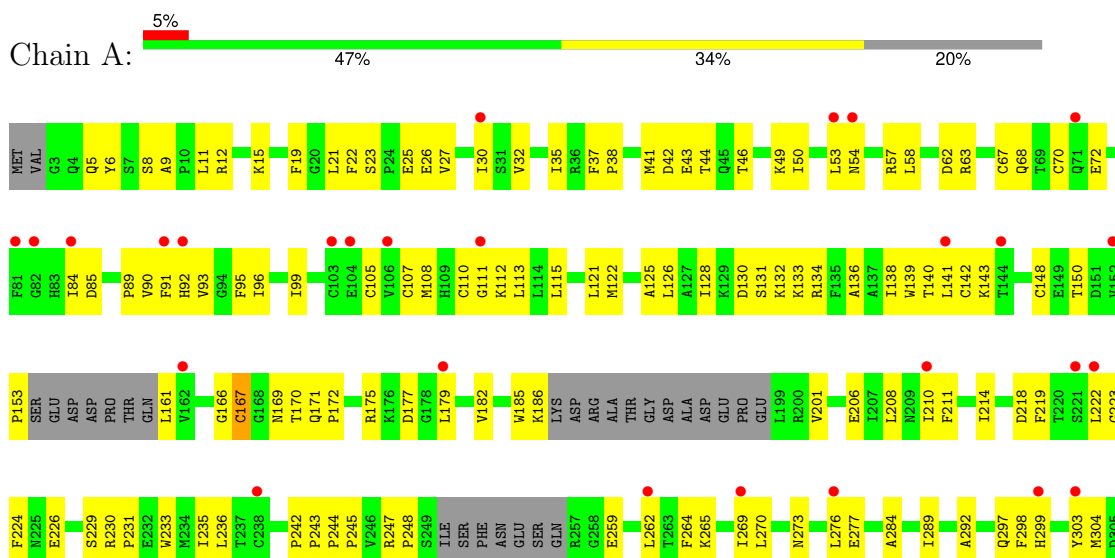
- Molecule 2: Template strand DNA



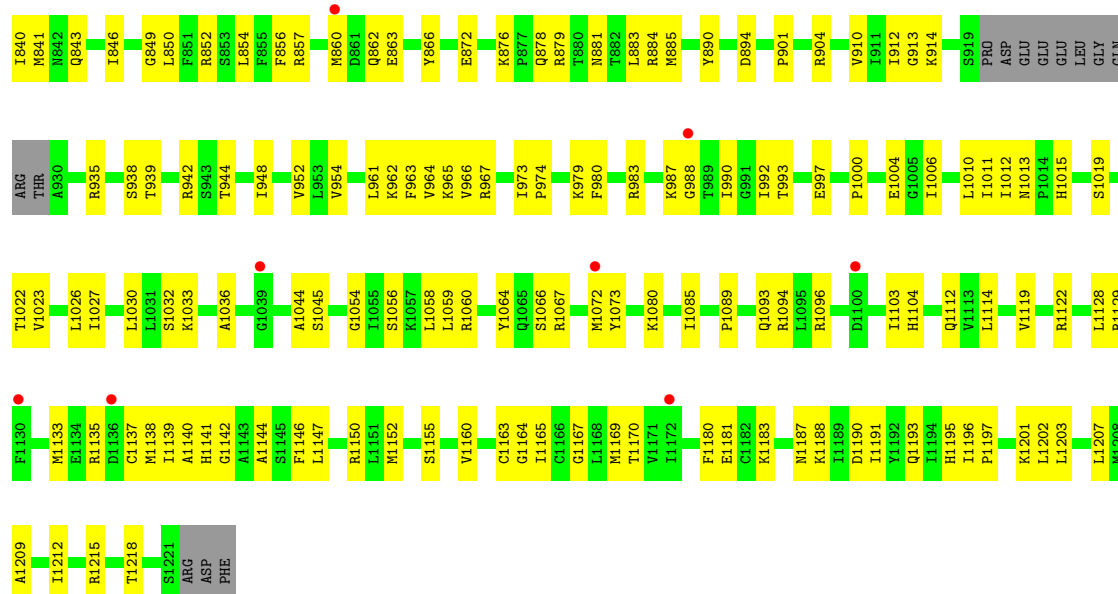
- Molecule 3: Non-template strand DNA



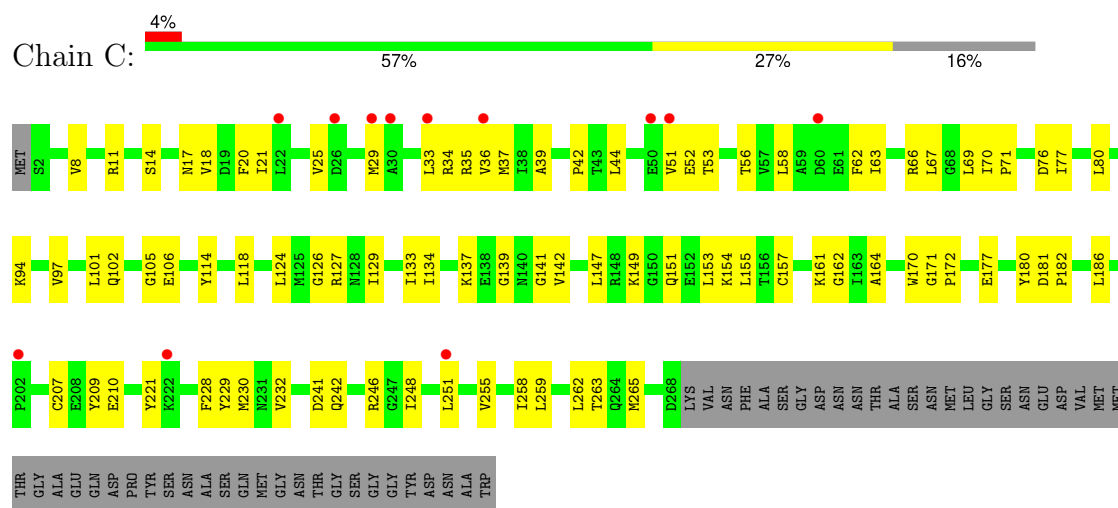
- Molecule 4: DNA-directed RNA polymerase II subunit RPB1



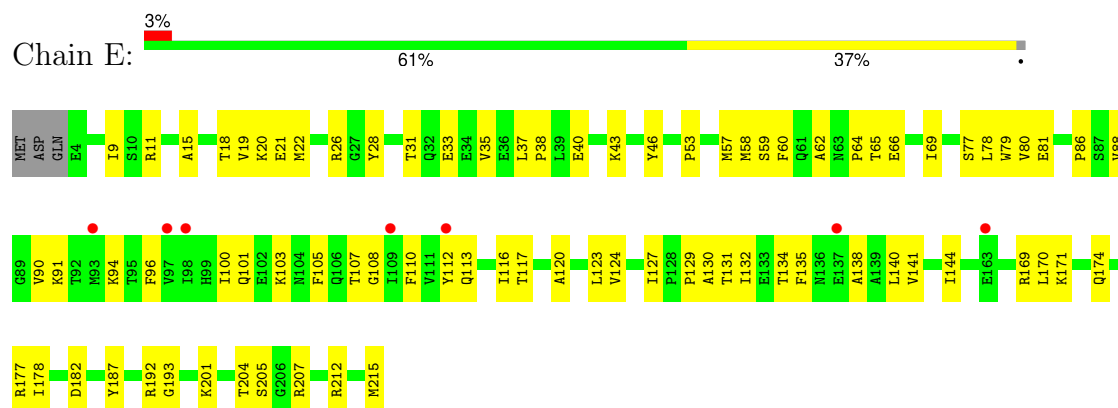
VAL	L1348	L1193	V1107	V948	V863	D781	I683	F591	L501	R407	N306
LYS	N1270	R1194	A1108	D949	T867	R782	K687	D592	L501	R407	P312
TYR	I1271	E1195	N1109	G950	T868	T783	K687	E593	V507	I413	L315
MET	L1272	E1196	N1110	E951	G869	P785	D692	G594	L511	D414	L315
PRO	L1273	D1198	M1111	N952	G870	H786	L702	T596	V512	L415	P321
GLU	R1274	R1199	S1115	N954	D871	F787	L702	L597	S513	R420	V322
GLN	G1275	R1199	L1116	P955	G872	S788	L702	L598	P519	R420	V322
LYS	V1276	M1202	T1117	L956	H873	K789	K705	L598	C520	R420	K323
ILE	G1360	N1203	V1119	P957	D874	S796	K705	D602	N603	I424	S324
THR	S1361	D1206	Y1118	N958	H877	S796	H706	D602	N603	I424	I325
GLU	R1366	L1207	Y1119	N959	H878	K797	H706	D602	N603	I424	R328
ILE	R1366	L1207	Y1119	N959	H878	K797	H706	D602	N603	I424	R336
ASP	V1283	T1208	E1121	I960	E879	G798	M708	G504	N521	Q427	R336
GLY	M1284	G1210	P1122	R961	E880	F799	L710	G605	N521	Q427	R336
GLN	K1286	Q1211	E1127	R962	D881	V800	R711	G605	N521	Q427	R336
ASP	K1286	Q1211	E1127	R962	D881	V800	R711	G605	N521	Q427	R336
GLY	Y1287	G1213	E1127	R962	D881	V800	R711	G605	N521	Q427	R336
GLY	D1288	E1214	E1127	R962	D881	V800	R711	G605	N521	Q427	R336
VAL	R1289	E1214	E1127	R962	D881	V800	R711	G605	N521	Q427	R336
THR	K1290	E1214	E1127	R962	D881	V800	R711	G605	N521	Q427	R336
PRO	N1393	I1216	E1127	R962	D881	V800	R711	G605	N521	Q427	R336
TYR	P1292	I1216	E1127	R962	D881	V800	R711	G605	N521	Q427	R336
SER	G1395	T1219	A1137	H975	K895	F815	R726	V622	D538	P446	R336
ASN	T1296	F1220	I1138	V1088	R896	H816	R726	V622	D538	P446	R336
GLU	L1397	K1221	E1139	V1088	R896	H816	R726	V622	D538	P446	R336
SER	Y1298	L1224	E1140	M1063	T897	A817	R726	V622	D538	P446	R336
GLY	P1302	L1224	E1140	M1063	T897	A817	R726	V622	D538	P446	R336
LEU	E1303	F1225	T1141	V1064	R898	M818	R726	V622	D538	P446	R336
VAL	V1304	G1226	R1135	G1065	V899	G819	R726	V622	D538	P446	R336
ASN	V1305	I1227	K1144	N982	D900	G820	R726	V622	D538	P446	R336
ALA	L1306	I1227	K1144	N982	D900	G820	R726	V622	D538	P446	R336
ASP	L1306	I1227	K1144	N982	D900	G820	R726	V622	D538	P446	R336
LEU	L1306	I1227	K1144	N982	D900	G820	R726	V622	D538	P446	R336
ASP	L1306	I1227	K1144	N982	D900	G820	R726	V622	D538	P446	R336
VAL	L1306	I1227	K1144	N982	D900	G820	R726	V622	D538	P446	R336
LYS	L1306	I1227	K1144	N982	D900	G820	R726	V622	D538	P446	R336
ASP	L1306	I1227	K1144	N982	D900	G820	R726	V622	D538	P446	R336
LEU	L1306	I1227	K1144	N982	D900	G820	R726	V622	D538	P446	R336
MET	S1314	V1242	D1166	N996	E915	B833	S761	Q650	P563	I463	T375
PHE	V1428	ARG	D1166	N996	E915	B833	S761	Q650	P563	I463	T375
SER	V1316	LYS	I1170	L1000	N998	T836	F755	W656	W666	Y465	V376
PRO	V1316	SER	I1170	L1000	N998	T836	F755	W656	W666	Y465	V376
LEU	V1319	LEU	L1176	F1084	N1001	R840	Q760	L658	P569	Y465	V376
VAL	A1434	ASP	L1176	F1084	N1001	R840	Q760	L658	P569	Y465	V376
ASP	P1435	ALA	ASP	V1089	N1004	L841	C764	I666	S573	Y474	L388
SER	I1436	GLU	GLU	A1090	E1006	V842	C764	I666	S573	Y474	L388
GLY	G1437	THR	GLU	S1091	I1007	K843	V765	G667	S573	Y474	L388
SER	T1438	ALA	ALA	K1092	Q1008	A844	G766	G667	S573	Y474	L388
ASN	I1327	GLU	GLN	K1093	Q1008	L845	Q767	G667	S573	Y474	L388
ASP	Y1328	ALA	GLN	V1098	D1013	T848	Q768	G673	Q576	Y478	V392
ALA	T1329	GLU	GLN	V1098	D1013	T848	Q768	G673	Q576	Y478	V392
MET	S1331	GLU	SER	F1018	F1018	H851	V770	M676	L578	F482	G395
GLY	F1441	D1257	PHE	C1019	F942	H851	V770	M676	L578	F482	G395
ALA	V1443	L1260	ASP	C1020	F942	H851	V770	M676	L578	F482	G395
GLY	D1446	L1260	GLN	C1020	F942	H851	V770	M676	L578	F482	G395
GLY	GLU	L1266	GLN	L1101	R944	R857	F777	L678	P583	F486	P400
PHE	M1336	T1266	GLU	K1102	R944	R857	F777	L678	P583	F486	P400
THR	S1341	M1267	W1191	L1105	E945	L860	G778	T680	L588	H487	G401
ALA	L1268	L1268	L1192	L1105	V946	G861	G778	T680	L588	H487	G401
				L1106	F947	N862	V780	T682	L590	H488	A402
											K403
											Y404



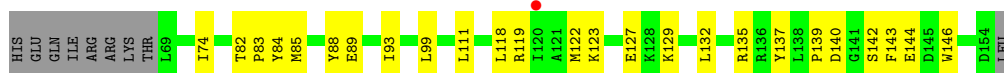
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3



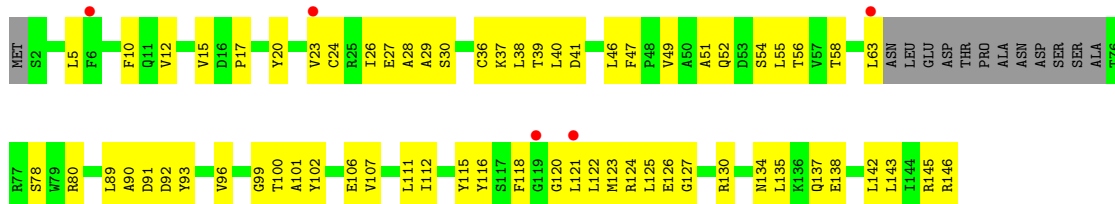
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



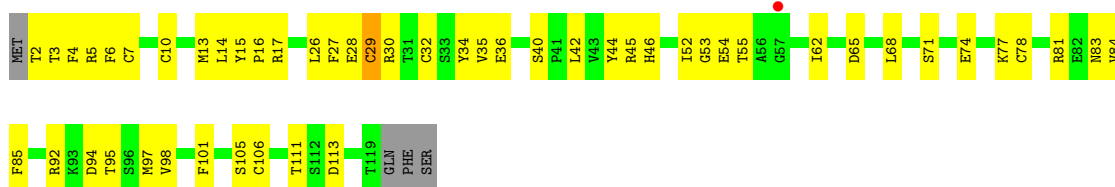
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



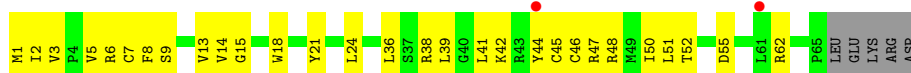
- Chain H: 



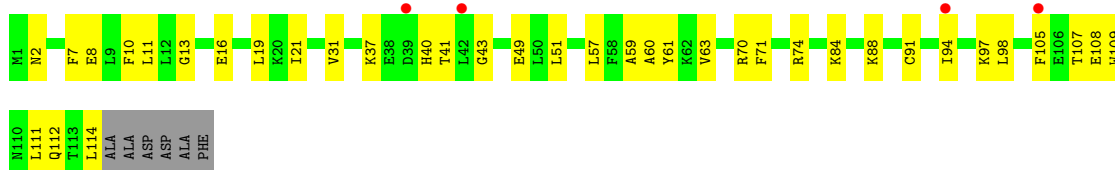
- Chain I:  %



- Chain J: 



- Chain K: 



- Chain L: 

MET	SER	ARG	GLU	GLY	PHE	GLN	ILE	PRO	THR	ASN	LEU	ASP	ALA	ALA	ALA	GLY	THR	SER	GLN	ALA	ARG	THR	ALA	THR	LEU	K28	Y29	I30	C31	C34	K37	L38	S39	L40	V46	R47	C48	C51	L56	A59	L64	F70
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.52Å 222.70Å 191.19Å 90.00° 97.82° 90.00°	Depositor
Resolution (Å)	38.52 – 3.48 38.52 – 3.48	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.52-3.48) 98.7 (38.52-3.48)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.218 , 0.258 0.218 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å ²)	89.4	Xtriage
Anisotropy	0.842	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 116.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29102	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 8GT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	R	0.16	0/217	0.32	0/337
2	T	0.22	0/551	0.44	0/845
3	N	0.21	0/335	0.36	0/516
4	A	0.18	0/11089	0.40	0/15001
5	B	0.17	0/9030	0.37	0/12186
6	C	0.16	0/2139	0.34	0/2899
7	E	0.17	0/1767	0.36	0/2378
8	F	0.16	0/696	0.33	0/943
9	H	0.18	0/1082	0.43	0/1466
10	I	0.16	0/970	0.41	0/1308
11	J	0.16	0/541	0.36	0/727
12	K	0.17	0/937	0.37	0/1265
13	L	0.21	0/339	0.43	0/450
All	All	0.17	0/29693	0.38	0/40321

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	193	0	98	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	497	0	285	10	0
3	N	296	0	155	16	0
4	A	10894	0	10937	491	0
5	B	8859	0	8816	340	0
6	C	2101	0	2056	68	0
7	E	1731	0	1758	70	0
8	F	684	0	692	22	0
9	H	1064	0	1029	58	0
10	I	952	0	897	43	0
11	J	532	0	542	24	0
12	K	919	0	929	34	0
13	L	337	0	352	9	0
14	T	33	0	11	6	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	2	0	0	0	0
All	All	29102	0	28557	1075	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 19.

All (1075) 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)
9:H:89:LEU:HD13	9:H:91:ASP:C	1.47	1.39
9:H:89:LEU:HD13	9:H:91:ASP:O	1.28	1.31
7:E:94:LYS:HG2	7:E:123:LEU:HD13	1.30	1.08
9:H:89:LEU:CD1	9:H:91:ASP:C	2.36	0.98
4:A:705:LYS:HE3	4:A:708:MET:SD	2.06	0.95
7:E:94:LYS:HE2	7:E:123:LEU:HD22	1.45	0.95
7:E:28:TYR:HA	7:E:64:PRO:HA	1.51	0.92
4:A:1224:LEU:HD21	4:A:1240:CYS:HB3	1.52	0.91
4:A:57:ARG:H	4:A:68:GLN:HB2	1.37	0.90
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.54	0.90
4:A:150:THR:HA	4:A:166:GLY:HA3	1.54	0.89
9:H:89:LEU:CD1	9:H:91:ASP:O	2.20	0.89
4:A:666:ILE:HG22	5:B:1026:LEU:HB3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:463:ILE:HD13	4:A:469:ARG:HG2	1.57	0.85
5:B:486:TYR:HE1	5:B:778:MET:HG2	1.41	0.85
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.59	0.85
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.56	0.85
4:A:226:GLU:HB2	4:A:230:ARG:HH21	1.43	0.83
5:B:832:GLY:HA2	5:B:835:GLN:HE21	1.44	0.83
5:B:703:ILE:HG22	5:B:740:HIS:HB2	1.62	0.81
4:A:247:ARG:HG2	4:A:262:LEU:HD11	1.61	0.81
4:A:1281:ARG:HG3	4:A:1309:ASP:HB2	1.62	0.81
4:A:1155:ASP:HB2	4:A:1192:LEU:HD23	1.61	0.81
5:B:345:LYS:HA	5:B:348:ARG:HH11	1.45	0.81
5:B:904:ARG:HG3	5:B:948:ILE:HG12	1.62	0.81
4:A:575:LYS:HE3	9:H:120:GLY:HA3	1.63	0.81
4:A:208:LEU:HB2	4:A:235:ILE:HD13	1.62	0.80
8:F:74:ILE:HG13	8:F:144:GLU:HG2	1.66	0.78
4:A:873:MET:HE2	4:A:957:PRO:HB3	1.66	0.78
4:A:91:PHE:HB2	4:A:179:LEU:HD21	1.65	0.78
5:B:465:ASN:HB3	5:B:474:SER:HB2	1.65	0.78
4:A:471:ASN:O	4:A:474:VAL:HG12	1.84	0.78
8:F:74:ILE:HD11	8:F:142:SER:HB2	1.66	0.76
4:A:54:ASN:HA	4:A:58:LEU:HD12	1.66	0.76
7:E:124:VAL:HG13	7:E:132:ILE:HB	1.67	0.76
7:E:94:LYS:CE	7:E:123:LEU:HD22	2.13	0.76
4:A:1138:ILE:HG23	4:A:1282:VAL:HG21	1.66	0.76
4:A:1329:THR:H	4:A:1335:ILE:HD11	1.51	0.76
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.69	0.75
5:B:852:ARG:HD2	5:B:973:ILE:HG12	1.67	0.75
4:A:1144:LYS:HB3	4:A:1268:LEU:HB3	1.67	0.75
6:C:124:LEU:HG	6:C:126:GLY:H	1.50	0.75
4:A:526:ASP:HB2	5:B:835:GLN:HE22	1.53	0.74
5:B:1104:HIS:HB2	5:B:1122:ARG:HG3	1.69	0.74
4:A:392:VAL:HG11	4:A:424:ILE:HD11	1.69	0.74
4:A:1089:VAL:HG22	4:A:1091:SER:H	1.52	0.74
7:E:94:LYS:HE2	7:E:123:LEU:CD2	2.18	0.74
4:A:1136:SER:HB3	4:A:1206:ASP:HB2	1.69	0.74
10:I:5:ARG:HH22	10:I:40:SER:HB3	1.53	0.73
9:H:38:LEU:HB3	9:H:125:LEU:HD13	1.70	0.73
4:A:573:SER:HB3	4:A:576:GLN:HG3	1.69	0.72
7:E:144:ILE:HD11	7:E:187:TYR:HB2	1.70	0.72
4:A:170:THR:HG23	4:A:185:TRP:HE1	1.54	0.71
5:B:400:HIS:HB3	5:B:403:LYS:HG2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:954:VAL:HG12	5:B:964:VAL:HG22	1.72	0.71
4:A:919:ILE:HG12	4:A:983:ILE:HD12	1.71	0.71
4:A:466:SER:HB2	5:B:1103:ILE:HD11	1.71	0.71
4:A:1288:ASP:HA	4:A:1302:PRO:HA	1.70	0.71
4:A:381:THR:H	4:A:384:ASN:HB3	1.55	0.71
5:B:789:MET:HE3	5:B:967:ARG:HB2	1.70	0.71
7:E:62:ALA:HB3	7:E:78:LEU:HB3	1.72	0.71
5:B:486:TYR:CE1	5:B:778:MET:HG2	2.24	0.70
4:A:483:ASP:HB2	5:B:987:LYS:HG3	1.73	0.70
4:A:908:LEU:HD21	4:A:983:ILE:HD11	1.73	0.70
11:J:36:LEU:HD13	11:J:47:ARG:HG2	1.72	0.70
6:C:262:LEU:HD13	12:K:88:LYS:HG2	1.74	0.69
7:E:11:ARG:HD2	7:E:141:VAL:HG21	1.74	0.69
4:A:598:LEU:HD21	9:H:124:ARG:HB2	1.73	0.69
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.74	0.69
4:A:396:PRO:HD3	4:A:415:LEU:HB3	1.73	0.69
4:A:1127:ASP:HB3	4:A:1130:GLN:OE1	1.93	0.69
6:C:142:VAL:HG23	11:J:15:GLY:HA3	1.74	0.69
4:A:961:ARG:H	4:A:961:ARG:HD3	1.58	0.69
5:B:637:LEU:HD12	5:B:693:ILE:HG13	1.72	0.69
4:A:590:ARG:HD3	4:A:621:THR:HG22	1.73	0.69
4:A:981:LEU:HD13	4:A:986:ILE:HG12	1.74	0.69
4:A:439:ASN:HA	4:A:459:ARG:HG2	1.72	0.69
5:B:102:VAL:HG22	5:B:112:LEU:HB2	1.75	0.69
4:A:513:SER:HB3	4:A:520:CYS:HB3	1.74	0.68
5:B:619:ILE:HD12	10:I:65:ASP:HB2	1.75	0.68
5:B:860:MET:HB2	5:B:963:PHE:HE1	1.59	0.68
4:A:1329:THR:HB	4:A:1335:ILE:HG13	1.74	0.68
6:C:52:GLU:HA	13:L:64:LEU:HD11	1.75	0.68
3:N:7:DA:H3'	4:A:139:TRP:HH2	1.59	0.67
4:A:592:ASP:HB2	4:A:603:ASN:HB2	1.75	0.67
4:A:569:LYS:HE2	6:C:221:TYR:HB2	1.76	0.67
7:E:20:LYS:HD2	7:E:35:VAL:HA	1.77	0.67
4:A:833:GLU:HB3	4:A:1098:VAL:HG11	1.76	0.67
4:A:1035:TYR:CD1	4:A:1037:LEU:HG	2.30	0.67
4:A:737:LEU:HD13	4:A:741:ASN:HD21	1.60	0.67
5:B:680:THR:HG23	5:B:683:SER:H	1.60	0.67
9:H:135:LEU:HB3	9:H:137:GLN:HG2	1.77	0.67
4:A:916:GLY:O	4:A:919:ILE:HG22	1.94	0.66
4:A:121:LEU:HB3	4:A:141:LEU:HD13	1.76	0.66
4:A:488:ASN:HD22	5:B:1128:LEU:HD13	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:452:LYS:HD2	5:B:1140:ALA:HB1	1.78	0.66
5:B:104:GLU:HG2	5:B:110:HIS:CE1	2.31	0.66
5:B:706:GLN:HG3	5:B:708:GLU:H	1.59	0.66
4:A:1072:ILE:HG23	4:A:1356:ILE:HD11	1.78	0.66
14:T:101:8GT:C4	4:A:1081:LEU:HD11	2.27	0.65
5:B:520:GLY:HA3	5:B:635:ARG:HE	1.61	0.65
4:A:128:ILE:HG23	4:A:134:ARG:HB2	1.78	0.65
4:A:886:ILE:HG13	4:A:944:ARG:HG2	1.79	0.65
5:B:277:LYS:H	5:B:277:LYS:HD2	1.60	0.65
5:B:866:TYR:HE1	5:B:872:GLU:HG3	1.62	0.65
6:C:29:MET:HE1	12:K:97:LYS:HD2	1.78	0.65
4:A:899:VAL:HG13	4:A:929:LEU:HD13	1.79	0.65
12:K:61:TYR:HB2	12:K:71:PHE:CE1	2.31	0.65
5:B:802:PRO:HG2	5:B:805:THR:HG22	1.79	0.65
5:B:806:THR:HG22	5:B:808:ALA:H	1.61	0.65
4:A:445:ASN:HB2	4:A:455:MET:HG3	1.79	0.65
6:C:25:VAL:HG23	6:C:228:PHE:CE2	2.32	0.65
10:I:78:CYS:HB3	10:I:106:CYS:HB3	1.79	0.65
5:B:292:ILE:HD11	5:B:327:ARG:HG2	1.79	0.65
4:A:247:ARG:CG	4:A:262:LEU:HD11	2.27	0.64
4:A:779:PHE:HB2	4:A:782:ARG:HG3	1.78	0.64
5:B:827:ILE:HG23	5:B:1012:ILE:HG13	1.79	0.64
4:A:1225:PHE:HE1	4:A:1241:ARG:HB2	1.63	0.64
14:T:101:8GT:H3'	4:A:1081:LEU:HD12	1.80	0.64
5:B:1181:GLU:HG3	5:B:1188:LYS:HB3	1.78	0.64
11:J:21:TYR:HB2	11:J:39:LEU:HD11	1.80	0.64
4:A:914:GLU:HG3	4:A:978:PRO:HB2	1.80	0.64
5:B:803:LEU:HD13	5:B:1032:SER:HB3	1.79	0.64
4:A:391:LEU:HD22	4:A:400:PRO:HB2	1.79	0.64
5:B:834:ASN:HD22	5:B:1013:ASN:HA	1.62	0.64
6:C:76:ASP:HB2	6:C:129:ILE:HG12	1.78	0.64
14:T:101:8GT:C5	4:A:1081:LEU:HD11	2.27	0.64
5:B:597:MET:HE3	5:B:601:ARG:HH21	1.61	0.64
8:F:127:GLU:HB2	8:F:129:LYS:HG2	1.78	0.64
10:I:28:GLU:HB2	10:I:35:VAL:HG22	1.80	0.64
4:A:53:LEU:HD22	4:A:54:ASN:OD1	1.98	0.63
4:A:752:LYS:HD2	5:B:1019:SER:HB2	1.80	0.63
4:A:583:PRO:HD3	4:A:645:LEU:HD12	1.80	0.63
5:B:884:ARG:HH11	5:B:935:ARG:HD3	1.63	0.63
6:C:8:VAL:HG11	12:K:105:PHE:HD1	1.64	0.63
5:B:365:THR:HG22	5:B:367:LEU:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:640:VAL:HG11	5:B:710:LEU:HD22	1.81	0.63
4:A:37:PHE:HB2	4:A:50:ILE:CD1	2.28	0.63
6:C:33:LEU:HG	6:C:37:MET:HE2	1.79	0.63
4:A:1207:LEU:HG	4:A:1274:ARG:HH12	1.64	0.62
4:A:1063:MET:HG3	5:B:1139:ILE:HG22	1.82	0.62
4:A:464:PRO:O	12:K:2:ASN:HB3	1.99	0.62
4:A:878:ILE:HD12	4:A:957:PRO:HA	1.82	0.62
9:H:15:VAL:HG22	9:H:51:ALA:HB2	1.81	0.62
4:A:67:CYS:SG	4:A:70:CYS:HB3	2.40	0.62
4:A:182:VAL:HB	4:A:201:VAL:HG12	1.81	0.62
4:A:269:ILE:HG12	4:A:299:HIS:HB3	1.82	0.62
4:A:885:THR:HG23	4:A:1024:SER:HB3	1.82	0.62
4:A:1207:LEU:HA	4:A:1274:ARG:HH22	1.64	0.62
4:A:388:LEU:HD13	4:A:432:VAL:HB	1.82	0.61
4:A:1433:MET:HE3	5:B:1144:ALA:HB3	1.82	0.61
4:A:711:ARG:CZ	10:I:97:MET:HB3	2.30	0.61
4:A:1152:ILE:HB	10:I:44:TYR:HB3	1.82	0.61
6:C:25:VAL:HG23	6:C:228:PHE:HE2	1.65	0.61
4:A:37:PHE:CB	4:A:50:ILE:HD12	2.29	0.61
7:E:46:TYR:HD1	7:E:57:MET:HG3	1.64	0.61
8:F:123:LYS:O	8:F:127:GLU:HG2	2.00	0.61
5:B:796:LEU:HD23	5:B:799:PRO:HA	1.82	0.61
9:H:5:LEU:HD23	9:H:134:ASN:HA	1.81	0.61
6:C:56:THR:HG22	6:C:147:LEU:HD21	1.82	0.61
4:A:12:ARG:HB2	5:B:1218:THR:HB	1.82	0.61
4:A:37:PHE:HB2	4:A:50:ILE:HD12	1.82	0.61
4:A:877:HIS:CE1	4:A:1056:SER:HA	2.35	0.61
5:B:683:SER:O	5:B:687:GLU:HG2	2.01	0.61
4:A:131:SER:HB3	4:A:223:GLY:HA3	1.83	0.61
4:A:956:LEU:HD13	4:A:1021:LEU:HD22	1.83	0.61
4:A:1107:VAL:HG22	4:A:1383:SER:HB2	1.83	0.61
13:L:31:CYS:HB3	13:L:34:CYS:SG	2.40	0.61
5:B:809:MET:HE1	5:B:983:ARG:NH1	2.16	0.60
5:B:863:GLU:O	5:B:961:LEU:HB2	2.02	0.60
4:A:605:MET:HE3	4:A:621:THR:HG21	1.82	0.60
4:A:1035:TYR:HD1	4:A:1037:LEU:HG	1.66	0.60
5:B:883:LEU:HG	5:B:884:ARG:HG3	1.82	0.60
4:A:21:LEU:HB2	4:A:229:SER:HA	1.83	0.60
4:A:1134:ILE:O	4:A:1138:ILE:HG22	2.02	0.60
5:B:199:MET:HE2	5:B:492:LEU:HD23	1.83	0.60
4:A:341:MET:HE1	4:A:1425:SER:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:98:VAL:HG11	10:I:111:THR:HG23	1.83	0.60
4:A:1031:VAL:HG13	4:A:1037:LEU:HD12	1.81	0.60
5:B:243:ALA:HB1	5:B:249:ARG:HG3	1.81	0.60
4:A:596:THR:HG22	4:A:598:LEU:H	1.66	0.60
6:C:242:GLN:HB3	6:C:246:ARG:HE	1.67	0.59
9:H:106:GLU:HA	9:H:112:ILE:HA	1.83	0.59
4:A:105:CYS:CB	4:A:142:CYS:HB3	2.32	0.59
4:A:810:PRO:HD3	5:B:730:ARG:HH21	1.65	0.59
5:B:104:GLU:HG2	5:B:110:HIS:HE1	1.66	0.59
7:E:169:ARG:HB3	8:F:140:ASP:HB3	1.84	0.59
4:A:877:HIS:HE1	4:A:1056:SER:HA	1.67	0.59
6:C:14:SER:HA	12:K:114:LEU:HD22	1.84	0.59
6:C:101:LEU:HB2	6:C:118:LEU:HG	1.82	0.59
13:L:30:ILE:HG13	13:L:37:LYS:HA	1.83	0.59
5:B:293:PRO:HB2	5:B:296:GLU:HB2	1.83	0.59
4:A:840:ARG:HE	4:A:1384:VAL:HG23	1.67	0.59
7:E:94:LYS:HE2	7:E:123:LEU:HB3	1.84	0.59
4:A:560:ILE:HD12	9:H:78:SER:HB2	1.85	0.59
4:A:1206:ASP:HB3	4:A:1274:ARG:CZ	2.32	0.59
4:A:779:PHE:HE2	4:A:785:PRO:HD3	1.67	0.59
4:A:42:ASP:HB3	4:A:46:THR:HB	1.84	0.59
4:A:1267:MET:HA	4:A:1271:ILE:HG12	1.85	0.59
5:B:228:LYS:HE3	5:B:234:ILE:HD11	1.84	0.59
5:B:597:MET:HE2	5:B:617:ARG:HB2	1.85	0.59
4:A:630:ILE:HD12	4:A:630:ILE:H	1.68	0.59
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.84	0.59
9:H:101:ALA:HA	9:H:116:TYR:HA	1.83	0.59
12:K:61:TYR:HB2	12:K:71:PHE:HE1	1.67	0.59
4:A:1078:GLN:C	4:A:1080:THR:H	2.10	0.58
5:B:1004:GLU:OE2	5:B:1064:TYR:CE2	2.56	0.58
5:B:1112:GLN:HG3	5:B:1119:VAL:HG12	1.83	0.58
5:B:58:THR:O	5:B:62:ILE:HG12	2.03	0.58
4:A:666:ILE:HG13	4:A:667:GLY:N	2.18	0.58
10:I:92:ARG:HE	10:I:95:THR:HA	1.69	0.58
4:A:981:LEU:HG	4:A:1039:LYS:HA	1.84	0.58
5:B:424:LEU:HD11	5:B:448:ILE:HG13	1.84	0.58
10:I:85:PHE:HB3	10:I:101:PHE:CD2	2.39	0.58
9:H:12:VAL:HA	9:H:28:ALA:HA	1.85	0.58
12:K:49:GLU:HG3	12:K:94:ILE:HG13	1.85	0.58
4:A:107:CYS:HB2	4:A:167:CYS:SG	2.43	0.58
4:A:175:ARG:HH12	4:A:177:ASP:HB2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:948:VAL:HG11	4:A:1289:ARG:HH21	1.69	0.58
5:B:581:PHE:HE1	5:B:623:GLU:HG2	1.69	0.58
7:E:108:GLY:O	7:E:132:ILE:HA	2.03	0.58
13:L:38:LEU:HD11	13:L:48:CYS:HB3	1.85	0.58
4:A:1025:ARG:HA	4:A:1030:ARG:HH11	1.68	0.58
6:C:11:ARG:HG3	6:C:21:ILE:HD11	1.85	0.58
8:F:85:MET:HG3	8:F:89:GLU:HG3	1.86	0.58
5:B:361:LEU:HD21	5:B:377:PHE:HB3	1.84	0.58
5:B:879:ARG:HA	5:B:885:MET:HE2	1.85	0.58
6:C:180:TYR:HB3	6:C:228:PHE:HD1	1.69	0.58
5:B:1167:GLY:H	5:B:1215:ARG:HG2	1.69	0.57
7:E:46:TYR:CD1	7:E:57:MET:HG3	2.38	0.57
4:A:871:ASP:HB3	7:E:204:THR:HB	1.86	0.57
4:A:53:LEU:HD22	4:A:54:ASN:CG	2.29	0.57
4:A:545:GLN:HG2	4:A:549:MET:HE3	1.86	0.57
4:A:706:HIS:NE2	4:A:1281:ARG:HB2	2.19	0.57
4:A:68:GLN:H	4:A:68:GLN:CD	2.12	0.57
4:A:210:ILE:O	4:A:214:ILE:HG13	2.04	0.57
4:A:273:ASN:O	4:A:277:GLU:HG2	2.03	0.57
4:A:813:PHE:HZ	5:B:767:ASN:HD22	1.52	0.57
5:B:261:ARG:HG3	5:B:263:GLY:H	1.69	0.57
9:H:17:PRO:HA	9:H:24:CYS:SG	2.44	0.57
4:A:563:PRO:HG2	4:A:566:ILE:HG12	1.87	0.57
10:I:78:CYS:SG	10:I:105:SER:HB3	2.44	0.57
4:A:451:HIS:HB3	4:A:453:MET:HE2	1.87	0.57
4:A:1209:MET:SD	4:A:1236:LEU:HG	2.44	0.57
5:B:281:PRO:HD2	5:B:284:ILE:HD12	1.87	0.57
5:B:770:GLN:HE22	5:B:1093:GLN:HE22	1.53	0.57
5:B:878:GLN:HG3	5:B:881:ASN:H	1.69	0.57
6:C:44:LEU:HB2	6:C:77:ILE:HD13	1.85	0.57
4:A:898:ARG:HB2	4:A:933:TYR:CE1	2.40	0.57
4:A:774:ARG:HB3	4:A:797:LYS:HB3	1.86	0.56
4:A:1282:VAL:HG12	4:A:1306:LEU:HD22	1.85	0.56
9:H:101:ALA:HB2	9:H:116:TYR:CE2	2.40	0.56
4:A:276:LEU:HD13	4:A:292:ALA:HB3	1.86	0.56
4:A:304:MET:HA	4:A:325:ILE:HG22	1.87	0.56
4:A:961:ARG:HD2	4:A:1025:ARG:NH1	2.20	0.56
5:B:282:ILE:HA	5:B:285:ILE:HD12	1.87	0.56
4:A:112:LYS:HD3	4:A:113:LEU:HD23	1.87	0.56
4:A:550:LEU:HB3	4:A:556:TRP:CE2	2.40	0.56
4:A:880:LYS:HA	4:A:955:PRO:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1148:ILE:HD12	4:A:1196:GLU:HG3	1.87	0.56
6:C:76:ASP:C	6:C:129:ILE:HD11	2.29	0.56
4:A:37:PHE:CD2	4:A:50:ILE:HD12	2.40	0.56
4:A:598:LEU:O	9:H:122:LEU:HD12	2.04	0.56
4:A:1284:MET:HG2	4:A:1306:LEU:HD21	1.87	0.56
5:B:1072:MET:HG3	5:B:1085:ILE:HB	1.88	0.56
4:A:449:SER:HB2	5:B:1133:MET:HG2	1.88	0.56
4:A:1329:THR:HG22	4:A:1331:SER:N	2.21	0.56
4:A:733:ALA:O	4:A:737:LEU:HG	2.06	0.56
4:A:1116:LEU:HB3	4:A:1308:THR:OG1	2.05	0.56
4:A:265:LYS:HE3	4:A:322:VAL:HG11	1.88	0.56
5:B:62:ILE:HG23	5:B:418:LYS:HG2	1.86	0.56
5:B:276:ILE:HG23	5:B:335:GLY:HA2	1.88	0.56
6:C:8:VAL:O	12:K:108:GLU:HG3	2.06	0.56
4:A:340:LEU:HD13	4:A:1429:ILE:HG13	1.88	0.55
4:A:567:LYS:HB2	9:H:96:VAL:HB	1.87	0.55
4:A:1152:ILE:HD12	4:A:1260:LEU:HD21	1.88	0.55
11:J:6:ARG:HG2	11:J:13:VAL:HG22	1.88	0.55
4:A:1329:THR:HG22	4:A:1331:SER:H	1.70	0.55
5:B:345:LYS:N	5:B:347:LYS:HG2	2.21	0.55
5:B:658:ILE:HG22	5:B:662:MET:HE2	1.88	0.55
9:H:12:VAL:HG13	9:H:52:GLN:H	1.71	0.55
9:H:15:VAL:HG12	9:H:26:ILE:HD12	1.87	0.55
4:A:315:LEU:HA	4:A:321:PRO:HA	1.87	0.55
5:B:872:GLU:HB3	5:B:914:LYS:HD2	1.89	0.55
2:T:15:DC:H4'	2:T:16:DT:OP1	2.05	0.55
4:A:729:ALA:HA	4:A:732:LEU:HD12	1.89	0.55
5:B:21:GLU:O	5:B:654:ARG:HB3	2.07	0.55
5:B:566:LEU:HD13	5:B:588:GLY:HA2	1.87	0.55
4:A:528:LEU:O	4:A:531:ILE:HG22	2.07	0.55
4:A:814:PHE:O	4:A:818:MET:HG3	2.07	0.55
5:B:283:VAL:HG21	5:B:321:GLY:CA	2.37	0.55
5:B:857:ARG:CZ	5:B:942:ARG:HE	2.20	0.55
4:A:407:ARG:HH11	4:A:413:ILE:HD11	1.71	0.55
9:H:91:ASP:HB3	9:H:143:LEU:HD23	1.89	0.55
4:A:349:ALA:HB1	4:A:370:ILE:HD12	1.89	0.54
4:A:482:PHE:CD2	5:B:836:GLU:HB2	2.42	0.54
4:A:11:LEU:HG	5:B:1193:GLN:HB3	1.89	0.54
7:E:81:GLU:HG3	7:E:110:PHE:HE1	1.71	0.54
4:A:662:PHE:CZ	4:A:742:ASN:HB3	2.43	0.54
5:B:310:MET:O	5:B:314:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:600:LEU:HD22	5:B:609:ILE:HD11	1.90	0.54
2:T:14:DG:C6	3:N:4:DG:C6	2.96	0.54
5:B:424:LEU:HB2	5:B:453:ILE:HD11	1.90	0.54
5:B:429:PHE:HA	5:B:432:MET:HE2	1.90	0.54
5:B:952:VAL:HG22	5:B:966:VAL:HG22	1.89	0.54
5:B:36:ALA:HA	5:B:39:ARG:HD3	1.89	0.54
10:I:92:ARG:HB2	10:I:94:ASP:O	2.07	0.54
4:A:920:LEU:HD23	4:A:921:GLY:N	2.23	0.54
4:A:1111:MET:HE2	4:A:1331:SER:HA	1.89	0.54
8:F:137:TYR:CE1	8:F:143:PHE:HB3	2.43	0.54
9:H:102:TYR:CZ	9:H:115:TYR:HB3	2.43	0.54
9:H:100:THR:HG23	9:H:138:GLU:HA	1.88	0.54
4:A:265:LYS:HG3	4:A:303:TYR:HB2	1.90	0.54
5:B:1152:MET:HE1	5:B:1195:HIS:HB3	1.88	0.54
7:E:117:THR:HG23	7:E:120:ALA:H	1.73	0.54
9:H:89:LEU:HD13	9:H:92:ASP:N	2.15	0.54
4:A:1348:LEU:HD23	4:A:1372:VAL:HG13	1.90	0.54
5:B:615:MET:HB3	5:B:626:ILE:HG12	1.90	0.54
5:B:1196:ILE:HD11	5:B:1201:LYS:HB2	1.89	0.54
2:T:5:DC:H2"	2:T:6:DT:H2'	1.90	0.53
5:B:259:TYR:O	5:B:267:ARG:HB2	2.07	0.53
4:A:140:THR:HA	4:A:143:LYS:HE3	1.89	0.53
4:A:1000:LEU:HD22	4:A:1007:ILE:HD12	1.89	0.53
4:A:1005:GLU:HA	4:A:1008:GLN:OE1	2.08	0.53
4:A:1093:LYS:O	4:A:1097:GLY:HA3	2.08	0.53
6:C:180:TYR:HB3	6:C:228:PHE:CD1	2.43	0.53
4:A:941:LYS:O	4:A:945:GLU:HG2	2.09	0.53
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.43	0.53
4:A:679:ILE:HG21	4:A:763:ALA:HB1	1.90	0.53
4:A:1093:LYS:HD2	4:A:1358:SER:C	2.34	0.53
8:F:119:ARG:HA	8:F:122:MET:HE2	1.88	0.53
4:A:862:ASN:OD1	7:E:174:GLN:HA	2.08	0.53
6:C:11:ARG:HD3	6:C:209:TYR:CZ	2.44	0.53
4:A:702:LEU:HD21	4:A:710:LEU:HD12	1.90	0.53
7:E:94:LYS:HE2	7:E:123:LEU:CG	2.39	0.53
11:J:36:LEU:HD11	11:J:51:LEU:HD22	1.90	0.53
4:A:779:PHE:HA	5:B:699:GLU:OE2	2.09	0.53
4:A:1210:GLY:O	4:A:1214:GLU:HG2	2.08	0.53
5:B:980:PHE:CE1	5:B:990:ILE:HD11	2.43	0.53
6:C:71:PRO:HB2	6:C:133:ILE:HD12	1.91	0.53
5:B:298:LEU:HD22	5:B:314:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:7:DA:C6	3:N:8:DG:C6	2.97	0.52
5:B:884:ARG:NH1	5:B:935:ARG:HD3	2.24	0.52
4:A:1436:ILE:HG22	4:A:1437:GLY:N	2.24	0.52
7:E:79:TRP:HB2	7:E:105:PHE:CD2	2.44	0.52
4:A:534:LEU:HA	4:A:539:THR:HG21	1.91	0.52
4:A:172:PRO:HB3	4:A:185:TRP:HB2	1.91	0.52
5:B:745:PRO:O	5:B:748:ILE:HG12	2.09	0.52
11:J:41:LEU:HD23	11:J:46:CYS:HB3	1.91	0.52
5:B:839:MET:HE3	5:B:988:GLY:HA3	1.90	0.52
5:B:44:VAL:HG11	5:B:495:LEU:HD13	1.91	0.52
5:B:980:PHE:CE2	5:B:1094:ARG:HG3	2.45	0.52
4:A:1004:ASN:HD21	4:A:1007:ILE:HG12	1.74	0.52
5:B:41:LYS:O	5:B:45:SER:HB3	2.10	0.52
4:A:420:ARG:O	4:A:424:ILE:HG23	2.09	0.52
4:A:679:ILE:HG12	4:A:729:ALA:HB1	1.92	0.52
5:B:62:ILE:HG21	5:B:417:PHE:HD1	1.75	0.52
5:B:69:LEU:HB2	5:B:90:ILE:HB	1.92	0.52
5:B:545:ILE:HG12	5:B:633:VAL:HG22	1.92	0.52
9:H:27:GLU:HG3	9:H:39:THR:HG23	1.91	0.52
4:A:834:THR:HG22	4:A:1098:VAL:HG21	1.91	0.52
5:B:565:PRO:HG2	5:B:568:ASP:HB2	1.91	0.52
11:J:14:VAL:HB	11:J:50:ILE:HD11	1.91	0.52
4:A:1438:THR:HA	4:A:1441:PHE:CZ	2.45	0.51
4:A:336:ILE:HG13	4:A:1405:THR:HG21	1.90	0.51
4:A:613:ILE:HG12	9:H:102:TYR:HB3	1.92	0.51
4:A:666:ILE:HD11	5:B:1067:ARG:HA	1.92	0.51
4:A:782:ARG:NH2	4:A:785:PRO:HA	2.26	0.51
4:A:730:GLY:C	4:A:755:PHE:HE1	2.17	0.51
4:A:57:ARG:N	4:A:68:GLN:HB2	2.15	0.51
4:A:946:VAL:HG22	7:E:201:LYS:HD2	1.93	0.51
4:A:1227:ILE:HD11	4:A:1239:ARG:HB2	1.91	0.51
4:A:913:LEU:HG	4:A:1032:LEU:HD13	1.92	0.51
4:A:1225:PHE:HZ	4:A:1241:ARG:HH11	1.59	0.51
5:B:309:GLN:HE22	10:I:52:ILE:HG21	1.76	0.51
5:B:593:PRO:HB2	5:B:617:ARG:HH21	1.76	0.51
3:N:9:DA:H2''	3:N:10:DG:H5'	1.93	0.51
4:A:92:HIS:HB2	4:A:236:LEU:HD11	1.93	0.51
4:A:243:PRO:HB2	4:A:245:PRO:HG2	1.93	0.51
4:A:800:VAL:HG13	4:A:812:GLU:CD	2.34	0.51
6:C:162:GLY:HA3	6:C:170:TRP:CE2	2.45	0.51
4:A:1117:THR:O	4:A:1327:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:167:ILE:HG22	5:B:448:ILE:HD11	1.92	0.51
5:B:576:ASP:HA	5:B:622:LYS:HE3	1.92	0.51
4:A:511:ILE:HA	4:A:521:MET:HE3	1.93	0.51
5:B:846:ILE:HD13	5:B:974:PRO:HB2	1.91	0.51
5:B:1207:LEU:HB3	5:B:1212:ILE:O	2.10	0.51
4:A:105:CYS:SG	4:A:142:CYS:HB3	2.51	0.51
4:A:806:ARG:HH12	5:B:729:ILE:HG13	1.76	0.51
5:B:116:GLU:HG3	5:B:120:ARG:HG3	1.92	0.51
5:B:351:TYR:CZ	5:B:355:ILE:HD11	2.46	0.51
5:B:813:LYS:HD2	5:B:816:GLU:OE2	2.11	0.51
7:E:90:VAL:HG23	7:E:123:LEU:HD11	1.92	0.51
2:T:5:DC:H2''	2:T:6:DT:H5'	1.91	0.51
4:A:42:ASP:HA	4:A:50:ILE:HG23	1.92	0.51
4:A:214:ILE:HB	4:A:219:PHE:CE1	2.45	0.51
7:E:112:TYR:HE2	7:E:134:THR:HA	1.75	0.51
4:A:111:GLY:O	4:A:214:ILE:HA	2.11	0.50
5:B:579:ARG:HH11	5:B:623:GLU:HG3	1.76	0.50
2:T:7:DC:H1'	2:T:8:DT:O4'	2.10	0.50
5:B:789:MET:HG2	5:B:967:ARG:HH11	1.76	0.50
6:C:101:LEU:HB3	6:C:155:LEU:HD11	1.93	0.50
1:R:3:C:H2'	1:R:4:G:O4'	2.11	0.50
4:A:781:ASP:HB2	4:A:789:LYS:HG2	1.93	0.50
4:A:845:LEU:HD12	4:A:1069:ALA:HB2	1.91	0.50
9:H:41:ASP:HB2	9:H:121:LEU:HB3	1.94	0.50
4:A:452:LYS:HB2	5:B:1141:HIS:CE1	2.47	0.50
5:B:755:ILE:HA	5:B:809:MET:HE2	1.93	0.50
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.94	0.50
6:C:62:PHE:O	6:C:66:ARG:HG3	2.11	0.50
4:A:248:PRO:HD3	5:B:1114:LEU:HD13	1.94	0.50
4:A:848:ILE:HG22	4:A:1064:VAL:HG23	1.93	0.50
5:B:223:VAL:HG21	5:B:381:MET:HG2	1.93	0.50
5:B:286:PHE:HD1	5:B:291:ILE:HB	1.76	0.50
5:B:728:ARG:HD2	5:B:730:ARG:CZ	2.42	0.50
9:H:127:GLY:HA3	9:H:130:ARG:NH2	2.26	0.50
4:A:107:CYS:SG	4:A:169:ASN:HB2	2.52	0.50
4:A:1138:ILE:HG13	4:A:1276:VAL:HB	1.94	0.50
4:A:1443:VAL:HG11	8:F:132:LEU:HD13	1.94	0.50
5:B:577:ALA:HB1	5:B:589:VAL:HB	1.92	0.50
5:B:890:TYR:CE1	5:B:910:VAL:HG21	2.46	0.50
4:A:1316:VAL:O	4:A:1322:ILE:HD11	2.11	0.50
4:A:1341:ILE:HD12	7:E:178:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:121:ASN:HA	5:B:207:GLY:HA3	1.93	0.50
11:J:41:LEU:O	11:J:47:ARG:HG3	2.12	0.50
4:A:30:ILE:O	5:B:1183:LYS:HD3	2.12	0.50
4:A:527:THR:HG21	4:A:650:GLN:HG2	1.93	0.50
4:A:528:LEU:HD23	4:A:751:SER:HA	1.93	0.50
5:B:579:ARG:NH1	5:B:623:GLU:HG3	2.26	0.50
5:B:1073:TYR:CE2	5:B:1080:LYS:HG3	2.47	0.50
4:A:549:MET:HE2	4:A:656:TRP:HB2	1.93	0.50
6:C:258:ILE:HG23	12:K:19:LEU:HD11	1.93	0.49
8:F:82:THR:HG22	8:F:84:TYR:H	1.77	0.49
4:A:323:LYS:HD3	4:A:328:ARG:HB3	1.95	0.49
4:A:602:ASP:OD2	4:A:616:VAL:HG23	2.12	0.49
4:A:1101:LEU:HD13	4:A:1355:VAL:HG21	1.93	0.49
5:B:322:PHE:CE2	10:I:30:ARG:HB2	2.47	0.49
5:B:345:LYS:N	5:B:347:LYS:HZ3	2.09	0.49
5:B:762:ASN:OD1	5:B:1022:THR:HA	2.12	0.49
7:E:127:ILE:HG22	7:E:129:PRO:HD2	1.94	0.49
9:H:56:THR:HB	9:H:145:ARG:HB3	1.94	0.49
12:K:61:TYR:CG	12:K:71:PHE:HE1	2.30	0.49
5:B:825:VAL:HG22	5:B:1010:LEU:HB3	1.93	0.49
4:A:5:GLN:CD	4:A:6:TYR:H	2.21	0.49
4:A:998:LEU:HD11	4:A:1001:ARG:HD3	1.95	0.49
4:A:107:CYS:HB3	4:A:110:CYS:O	2.13	0.49
9:H:63:LEU:HB3	9:H:90:ALA:HB2	1.95	0.49
9:H:80:ARG:HH11	12:K:57:LEU:HD22	1.77	0.49
4:A:35:ILE:O	4:A:84:ILE:HD12	2.13	0.49
4:A:43:GLU:HG2	4:A:44:THR:HG23	1.94	0.49
4:A:1102:LYS:HG3	4:A:1106:ASN:OD1	2.12	0.49
5:B:91:SER:HB3	5:B:133:LYS:HB2	1.94	0.49
5:B:205:ILE:HG13	5:B:461:LEU:HB3	1.94	0.49
5:B:234:ILE:HG21	5:B:257:LYS:HB3	1.95	0.49
5:B:290:GLY:HA2	5:B:327:ARG:HD2	1.93	0.49
12:K:51:LEU:HD22	12:K:59:ALA:HB3	1.95	0.49
4:A:89:PRO:HB2	4:A:235:ILE:HD11	1.94	0.49
4:A:131:SER:CB	4:A:223:GLY:HA3	2.42	0.49
4:A:1101:LEU:O	4:A:1105:LEU:HG	2.13	0.49
4:A:1130:GLN:O	4:A:1134:ILE:HG12	2.13	0.49
4:A:1225:PHE:CE1	4:A:1241:ARG:HB2	2.46	0.49
12:K:21:ILE:HG21	12:K:84:LYS:HE2	1.94	0.49
4:A:90:VAL:HB	4:A:297:GLN:NE2	2.28	0.49
4:A:376:TYR:CZ	4:A:498:ARG:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:667:GLY:CA	5:B:1067:ARG:HD2	2.43	0.49
4:A:779:PHE:CB	4:A:782:ARG:HG3	2.43	0.49
4:A:940:ARG:O	4:A:944:ARG:HG3	2.12	0.49
5:B:599:THR:O	5:B:603:LEU:HG	2.12	0.49
9:H:40:LEU:HB2	9:H:123:MET:HG3	1.94	0.49
9:H:107:VAL:HB	9:H:111:LEU:HB3	1.94	0.49
4:A:306:ASN:N	4:A:324:SER:HB3	2.28	0.49
7:E:60:PHE:CE1	7:E:80:VAL:HG11	2.48	0.49
4:A:375:THR:HB	4:A:433:GLU:HB3	1.94	0.49
5:B:579:ARG:HA	5:B:589:VAL:HG12	1.95	0.49
6:C:97:VAL:HG21	6:C:129:ILE:HG22	1.94	0.49
10:I:2:THR:OG1	10:I:45:ARG:HB3	2.13	0.49
4:A:108:MET:O	4:A:210:ILE:HG12	2.14	0.48
4:A:874:ASP:HB2	4:A:1058:VAL:HA	1.94	0.48
4:A:1311:VAL:HG11	4:A:1329:THR:HG23	1.95	0.48
5:B:620:ARG:HH12	10:I:68:LEU:HD21	1.78	0.48
4:A:1219:THR:HG21	4:A:1271:ILE:HD12	1.94	0.48
4:A:23:SER:HB2	4:A:233:TRP:CH2	2.49	0.48
4:A:218:ASP:O	4:A:222:LEU:HG	2.13	0.48
4:A:383:TYR:OH	8:F:111:LEU:HD21	2.14	0.48
4:A:968:GLN:HE21	4:A:1035:TYR:HB3	1.77	0.48
4:A:1140:HIS:HA	4:A:1275:GLY:HA3	1.94	0.48
4:A:1166:ASP:OD2	4:A:1237:ILE:HG21	2.12	0.48
4:A:1395:GLY:O	4:A:1399:ARG:HD3	2.12	0.48
11:J:2:ILE:HA	11:J:55:ASP:OD1	2.13	0.48
4:A:863:VAL:HG23	7:E:170:LEU:HD21	1.95	0.48
4:A:1000:LEU:HB2	4:A:1007:ILE:HG23	1.95	0.48
5:B:667:GLN:HG3	5:B:676:VAL:HG21	1.94	0.48
5:B:177:LYS:HE3	5:B:177:LYS:HB2	1.56	0.48
5:B:510:LYS:HE3	5:B:513:GLN:OE1	2.13	0.48
5:B:1146:PHE:O	5:B:1150:ARG:HG2	2.14	0.48
7:E:94:LYS:CE	7:E:123:LEU:HB3	2.43	0.48
7:E:107:THR:HG22	7:E:131:THR:HB	1.94	0.48
10:I:14:LEU:HD23	10:I:29:CYS:N	2.28	0.48
12:K:43:GLY:HA2	12:K:71:PHE:CZ	2.49	0.48
4:A:23:SER:HB3	4:A:26:GLU:HB2	1.95	0.48
4:A:752:LYS:HG2	5:B:1015:HIS:O	2.14	0.48
4:A:1138:ILE:HA	4:A:1276:VAL:HG23	1.95	0.48
4:A:1289:ARG:HD2	4:A:1303:GLU:OE1	2.14	0.48
4:A:1316:VAL:O	4:A:1322:ILE:CD1	2.62	0.48
7:E:31:THR:HG22	7:E:33:GLU:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:593:GLU:CD	4:A:594:GLY:H	2.21	0.48
4:A:683:ILE:O	4:A:687:LYS:HG3	2.13	0.48
4:A:896:ARG:NH1	4:A:1030:ARG:HH21	2.12	0.48
5:B:234:ILE:HD12	5:B:237:VAL:HG22	1.96	0.48
5:B:840:ILE:HG12	5:B:992:ILE:HG22	1.94	0.48
5:B:1036:ALA:O	11:J:47:ARG:HD3	2.13	0.48
9:H:127:GLY:HA3	9:H:130:ARG:HH21	1.78	0.48
3:N:12:DG:OP2	3:N:12:DG:H2'	2.13	0.48
4:A:107:CYS:HA	4:A:171:GLN:CD	2.39	0.48
4:A:122:MET:O	4:A:126:LEU:HG	2.13	0.48
4:A:336:ILE:HD12	5:B:1203:LEU:HD11	1.95	0.48
5:B:218:SER:HA	5:B:404:LYS:HA	1.94	0.48
5:B:234:ILE:HG22	5:B:259:TYR:HA	1.94	0.48
4:A:57:ARG:O	4:A:58:LEU:HD23	2.14	0.48
4:A:997:LEU:HB2	4:A:1053:PHE:CD1	2.48	0.48
5:B:100:PRO:HG3	5:B:172:ILE:HG13	1.95	0.48
11:J:9:SER:HB2	11:J:45:CYS:HB2	1.95	0.48
4:A:679:ILE:O	4:A:683:ILE:HG12	2.14	0.48
4:A:1116:LEU:HB2	4:A:1311:VAL:HG13	1.96	0.48
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.96	0.48
4:A:1239:ARG:HH12	4:A:1241:ARG:HH22	1.61	0.47
5:B:944:THR:HB	5:B:1122:ARG:HH12	1.78	0.47
7:E:65:THR:O	7:E:69:ILE:HG23	2.14	0.47
3:N:10:DG:H2''	3:N:11:DA:C8	2.50	0.47
4:A:787:PHE:CE2	4:A:796:SER:HA	2.49	0.47
4:A:1312:ASN:CG	4:A:1315:GLU:HG2	2.40	0.47
5:B:190:TYR:CD2	11:J:62:ARG:HG2	2.49	0.47
5:B:606:LYS:HE2	5:B:608:ASP:OD1	2.14	0.47
5:B:850:LEU:HB2	11:J:8:PHE:CG	2.49	0.47
5:B:1033:LYS:HD3	5:B:1059:LEU:HD11	1.95	0.47
3:N:9:DA:C2'	3:N:10:DG:H5'	2.44	0.47
4:A:99:ILE:HG23	4:A:211:PHE:HZ	1.78	0.47
4:A:339:ASN:O	4:A:343:LYS:HG3	2.13	0.47
4:A:380:VAL:HA	4:A:384:ASN:OD1	2.15	0.47
5:B:370:PHE:CD2	5:B:373:ARG:HD2	2.49	0.47
5:B:380:TYR:O	5:B:384:ARG:HG2	2.15	0.47
5:B:806:THR:H	5:B:809:MET:HE3	1.79	0.47
6:C:259:LEU:HD11	12:K:91:CYS:CB	2.44	0.47
9:H:116:TYR:HB2	9:H:123:MET:HE2	1.95	0.47
4:A:42:ASP:HA	4:A:50:ILE:CG2	2.45	0.47
4:A:579:SER:OG	4:A:612:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:867:ILE:HD12	4:A:1000:LEU:HD11	1.96	0.47
4:A:963:ILE:HD12	4:A:1049:ILE:HG12	1.97	0.47
5:B:261:ARG:NE	5:B:262:GLU:H	2.11	0.47
5:B:1164:GLY:HA3	5:B:1190:ASP:OD2	2.14	0.47
1:R:9:G:H2'	14:T:101:8GT:H1'	1.96	0.47
4:A:244:PRO:N	4:A:245:PRO:HD2	2.30	0.47
4:A:464:PRO:HG2	4:A:465:TYR:HD1	1.78	0.47
4:A:658:LEU:HD12	5:B:831:SER:HA	1.97	0.47
5:B:486:TYR:HE2	5:B:1096:ARG:HD2	1.80	0.47
6:C:17:ASN:HA	6:C:232:VAL:O	2.14	0.47
7:E:94:LYS:HG2	7:E:123:LEU:CD1	2.23	0.47
4:A:38:PRO:HA	4:A:270:LEU:HD13	1.95	0.47
4:A:93:VAL:O	4:A:96:ILE:HG12	2.14	0.47
4:A:538:ASP:CG	9:H:20:TYR:HB3	2.40	0.47
4:A:666:ILE:HD11	5:B:1067:ARG:HD3	1.97	0.47
5:B:69:LEU:HD21	5:B:425:THR:HG22	1.97	0.47
5:B:299:GLU:HG3	5:B:571:PRO:HG2	1.96	0.47
5:B:862:GLN:HG2	5:B:963:PHE:HD1	1.79	0.47
7:E:79:TRP:HB2	7:E:105:PHE:HD2	1.79	0.47
4:A:348:SER:HB2	5:B:1128:LEU:HD12	1.96	0.47
4:A:380:VAL:HG23	4:A:428:TYR:HA	1.96	0.47
4:A:388:LEU:HD23	4:A:388:LEU:HA	1.80	0.47
4:A:631:HIS:O	4:A:635:ARG:HG2	2.14	0.47
4:A:727:ASP:O	4:A:755:PHE:HZ	1.97	0.47
4:A:816:HIS:CD2	5:B:764:SER:HB3	2.49	0.47
4:A:851:HIS:ND1	8:F:139:PRO:HG3	2.29	0.47
4:A:881:GLN:HB2	4:A:956:LEU:HD12	1.96	0.47
4:A:965:GLN:O	4:A:969:GLN:HG2	2.14	0.47
4:A:973:ILE:HB	4:A:975:HIS:CD2	2.50	0.47
4:A:1021:LEU:O	4:A:1025:ARG:HG2	2.15	0.47
4:A:1138:ILE:HD11	4:A:1279:ILE:HG12	1.97	0.47
4:A:1141:THR:HG21	4:A:1207:LEU:HD12	1.97	0.47
5:B:212:LEU:HD22	5:B:479:VAL:HG12	1.96	0.47
6:C:181:ASP:OD2	6:C:186:LEU:HB2	2.14	0.47
7:E:15:ALA:O	7:E:19:VAL:HG23	2.14	0.47
8:F:135:ARG:HD3	8:F:137:TYR:CZ	2.50	0.47
10:I:4:PHE:CZ	10:I:13:MET:HB3	2.49	0.47
10:I:16:PRO:HB3	10:I:27:PHE:CZ	2.50	0.47
4:A:32:VAL:HB	5:B:1183:LYS:HZ2	1.80	0.47
4:A:344:ARG:HA	5:B:1129:ARG:HA	1.96	0.47
4:A:1121:GLU:HG3	4:A:1122:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1306:LEU:HD23	4:A:1306:LEU:HA	1.81	0.47
5:B:114:PRO:HG3	5:B:181:LEU:HD11	1.97	0.47
3:N:11:DA:H2"	3:N:12:DG:C8	2.50	0.47
4:A:351:THR:OG1	5:B:1103:ILE:HG12	2.15	0.47
4:A:1013:ASP:O	7:E:205:SER:HB2	2.15	0.47
9:H:55:LEU:HD22	9:H:146:ARG:HA	1.97	0.47
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.50	0.47
4:A:15:LYS:HG2	5:B:1218:THR:O	2.15	0.47
4:A:53:LEU:CD2	4:A:54:ASN:OD1	2.63	0.47
4:A:860:LEU:HG	4:A:1394:THR:HB	1.97	0.47
4:A:1031:VAL:HA	4:A:1035:TYR:CE1	2.50	0.47
4:A:1212:VAL:O	4:A:1216:ILE:HG13	2.15	0.47
5:B:215:GLN:HB3	5:B:476:ARG:HH22	1.80	0.47
1:R:5:A:H2'	1:R:6:G:C8	2.50	0.46
4:A:41:MET:HA	4:A:49:LYS:HA	1.96	0.46
4:A:259:GLU:HB3	4:A:264:PHE:CE1	2.50	0.46
5:B:660:LYS:HB3	5:B:660:LYS:HE2	1.73	0.46
5:B:912:ILE:HB	5:B:939:THR:OG1	2.15	0.46
5:B:1165:ILE:HG12	5:B:1187:ASN:HB3	1.97	0.46
7:E:101:GLN:HB2	7:E:127:ILE:HD12	1.97	0.46
4:A:1166:ASP:O	4:A:1170:ILE:HG12	2.15	0.46
5:B:639:ILE:HD12	5:B:688:GLY:O	2.16	0.46
5:B:654:ARG:HA	5:B:654:ARG:HD3	1.72	0.46
5:B:832:GLY:HA2	5:B:835:GLN:NE2	2.23	0.46
7:E:94:LYS:HE2	7:E:123:LEU:CB	2.46	0.46
4:A:1037:LEU:HD13	4:A:1042:PHE:HB2	1.98	0.46
7:E:9:ILE:HG12	7:E:53:PRO:HD3	1.97	0.46
7:E:37:LEU:HD12	7:E:38:PRO:HD2	1.96	0.46
4:A:214:ILE:HG22	4:A:218:ASP:HB2	1.96	0.46
4:A:353:ILE:HB	4:A:470:LEU:HD21	1.98	0.46
4:A:351:THR:HG22	4:A:468:PHE:CD2	2.51	0.46
4:A:380:VAL:HG21	4:A:427:GLN:O	2.15	0.46
5:B:188:ASP:O	5:B:192:LEU:HG	2.15	0.46
5:B:770:GLN:NE2	5:B:1093:GLN:HE22	2.12	0.46
9:H:58:THR:OG1	9:H:143:LEU:HB2	2.15	0.46
4:A:869:GLY:HA3	4:A:1366:ARG:NH1	2.30	0.46
4:A:1132:LYS:HG2	4:A:1135:ARG:NH2	2.30	0.46
5:B:101:MET:HG2	5:B:111:ALA:HA	1.98	0.46
5:B:277:LYS:NZ	5:B:336:ARG:H	2.13	0.46
5:B:554:ILE:O	5:B:558:LEU:HG	2.16	0.46
5:B:1023:VAL:O	5:B:1027:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:251:LEU:O	6:C:255:VAL:HG23	2.15	0.46
7:E:22:MET:O	7:E:26:ARG:HG2	2.16	0.46
4:A:242:PRO:HG3	5:B:1209:ALA:HB2	1.98	0.46
4:A:340:LEU:HB3	4:A:1429:ILE:HG13	1.98	0.46
4:A:673:GLY:O	4:A:677:ARG:HG2	2.15	0.46
4:A:890:ASP:HB2	4:A:1295:THR:O	2.15	0.46
5:B:601:ARG:O	5:B:605:ARG:HG2	2.16	0.46
4:A:1428:VAL:HG22	5:B:1147:LEU:HD21	1.97	0.46
5:B:129:PHE:HB3	5:B:164:LYS:HE3	1.97	0.46
5:B:1142:GLY:HA3	8:F:88:TYR:HE2	1.80	0.46
13:L:64:LEU:HD23	13:L:64:LEU:HA	1.65	0.46
4:A:1282:VAL:HA	4:A:1307:GLU:O	2.16	0.46
5:B:212:LEU:HD21	5:B:466:TRP:CH2	2.51	0.46
5:B:418:LYS:HE2	5:B:418:LYS:HB3	1.85	0.46
5:B:797:TYR:HB3	5:B:798:TYR:CD2	2.51	0.46
9:H:89:LEU:CD1	9:H:92:ASP:N	2.76	0.46
4:A:185:TRP:O	4:A:186:LYS:HG2	2.15	0.46
4:A:1202:MET:HE1	4:A:1207:LEU:HB3	1.98	0.46
4:A:153:PRO:HA	4:A:161:LEU:N	2.30	0.45
4:A:886:ILE:HD11	4:A:950:GLY:HA2	1.98	0.45
4:A:1115:SER:HB3	4:A:1330:ASN:ND2	2.31	0.45
5:B:470:LYS:HG3	5:B:473:MET:H	1.81	0.45
5:B:640:VAL:HA	5:B:651:LEU:HA	1.98	0.45
5:B:846:ILE:HG23	5:B:974:PRO:HD2	1.97	0.45
9:H:47:PHE:CZ	9:H:146:ARG:HD3	2.51	0.45
11:J:42:LYS:HA	11:J:47:ARG:NH1	2.31	0.45
4:A:901:LEU:HD13	4:A:919:ILE:HG13	1.98	0.45
5:B:569:TYR:CD1	5:B:589:VAL:HG21	2.51	0.45
5:B:860:MET:HB2	5:B:963:PHE:CE1	2.47	0.45
5:B:1054:GLY:O	5:B:1058:LEU:HG	2.16	0.45
7:E:177:ARG:C	7:E:212:ARG:HG2	2.41	0.45
9:H:29:ALA:HA	9:H:37:LYS:HA	1.99	0.45
12:K:7:PHE:HB2	12:K:11:LEU:HD22	1.98	0.45
4:A:25:GLU:CD	4:A:25:GLU:H	2.25	0.45
4:A:567:LYS:HB3	4:A:568:PRO:HD3	1.96	0.45
4:A:913:LEU:HD23	4:A:913:LEU:HA	1.73	0.45
5:B:755:ILE:HD13	5:B:809:MET:HG2	1.98	0.45
5:B:834:ASN:O	5:B:1013:ASN:HB2	2.16	0.45
7:E:79:TRP:HE1	7:E:96:PHE:HE1	1.63	0.45
4:A:630:ILE:HG23	4:A:642:CYS:SG	2.56	0.45
4:A:981:LEU:HD11	4:A:1042:PHE:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.52	0.45
5:B:610:ASN:HB3	5:B:613:VAL:HG23	1.98	0.45
5:B:806:THR:HG23	5:B:1045:SER:HA	1.98	0.45
10:I:34:TYR:OH	10:I:36:GLU:HB3	2.15	0.45
4:A:836:TYR:O	4:A:840:ARG:HG3	2.17	0.45
7:E:59:SER:HB3	7:E:81:GLU:HA	1.97	0.45
4:A:37:PHE:HB2	4:A:50:ILE:HD11	1.99	0.45
5:B:27:ALA:O	5:B:30:SER:HB3	2.17	0.45
5:B:901:PRO:HD2	13:L:59:ALA:O	2.17	0.45
10:I:14:LEU:HB3	10:I:27:PHE:HB3	1.99	0.45
10:I:111:THR:HG22	10:I:113:ASP:H	1.80	0.45
2:T:10:DT:H3	3:N:9:DA:H61	1.65	0.45
4:A:1050:GLU:O	4:A:1054:LEU:HG	2.17	0.45
5:B:597:MET:SD	5:B:624:LEU:HD11	2.57	0.45
10:I:4:PHE:CZ	10:I:13:MET:CB	3.00	0.45
2:T:12:DT:H2''	2:T:13:DC:C6	2.52	0.45
14:T:101:8GT:O2'	4:A:448:PRO:HG3	2.16	0.45
4:A:298:PHE:HE1	4:A:312:PRO:HB3	1.81	0.45
4:A:825:ILE:O	4:A:829:VAL:HG22	2.17	0.45
5:B:620:ARG:HG2	10:I:62:ILE:HD11	1.99	0.45
5:B:884:ARG:HH11	5:B:935:ARG:CD	2.28	0.45
6:C:67:LEU:HD13	6:C:157:CYS:SG	2.57	0.45
6:C:164:ALA:HB2	6:C:171:GLY:CA	2.47	0.45
7:E:91:LYS:HB3	7:E:91:LYS:HE2	1.76	0.45
8:F:119:ARG:O	8:F:123:LYS:HG2	2.16	0.45
9:H:125:LEU:HD12	9:H:126:GLU:H	1.82	0.45
11:J:24:LEU:HD22	11:J:38:ARG:NH1	2.31	0.45
4:A:1119:TYR:CD2	4:A:1326:ARG:HB3	2.51	0.45
5:B:983:ARG:HG2	5:B:1093:GLN:HE21	1.82	0.45
5:B:1060:ARG:HG2	5:B:1066:SER:HB3	1.98	0.45
12:K:7:PHE:O	12:K:11:LEU:HB2	2.17	0.45
2:T:14:DG:H2''	2:T:15:DC:C5	2.52	0.45
4:A:30:ILE:HG23	5:B:1170:THR:HB	1.99	0.45
4:A:813:PHE:HZ	5:B:767:ASN:ND2	2.15	0.45
4:A:883:LEU:HD13	4:A:954:TRP:HD1	1.80	0.45
5:B:486:TYR:CE2	5:B:1096:ARG:HD2	2.52	0.45
7:E:88:VAL:HG12	7:E:116:ILE:HA	1.98	0.45
4:A:122:MET:HE1	4:A:138:ILE:HG23	2.00	0.44
6:C:177:GLU:O	6:C:230:MET:HA	2.17	0.44
7:E:135:PHE:HB3	7:E:140:LEU:HD11	1.99	0.44
9:H:10:PHE:O	9:H:54:SER:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:9:ALA:HB2	5:B:1191:ILE:HB	1.98	0.44
4:A:92:HIS:O	4:A:96:ILE:HG23	2.17	0.44
4:A:590:ARG:NH2	4:A:620:LYS:HD3	2.32	0.44
4:A:986:ILE:HD11	4:A:1032:LEU:HD21	1.98	0.44
4:A:1290:LYS:HE2	4:A:1298:TYR:HB3	1.99	0.44
5:B:270:LYS:HG3	5:B:281:PRO:HA	1.98	0.44
5:B:579:ARG:HB3	5:B:586:TRP:CE2	2.53	0.44
7:E:43:LYS:HB2	7:E:43:LYS:HE2	1.81	0.44
7:E:171:LYS:HB3	7:E:174:GLN:HG3	1.98	0.44
12:K:7:PHE:HA	12:K:10:PHE:CE1	2.52	0.44
4:A:148:CYS:HB3	4:A:167:CYS:SG	2.58	0.44
4:A:206:GLU:O	4:A:210:ILE:HG13	2.17	0.44
4:A:662:PHE:O	5:B:828:ALA:HA	2.18	0.44
4:A:716:ASP:O	4:A:720:ARG:HG3	2.17	0.44
4:A:1287:TYR:CG	4:A:1305:VAL:HG21	2.52	0.44
5:B:578:THR:HA	5:B:622:LYS:O	2.18	0.44
6:C:154:LYS:HB3	6:C:154:LYS:HE2	1.70	0.44
10:I:68:LEU:HB3	10:I:84:VAL:CG2	2.46	0.44
4:A:115:LEU:HD23	4:A:142:CYS:HA	2.00	0.44
4:A:540:PHE:CD1	4:A:573:SER:HA	2.52	0.44
5:B:614:SER:HB3	5:B:632:ARG:HH21	1.82	0.44
5:B:693:ILE:HG21	5:B:701:ILE:HD13	1.99	0.44
6:C:80:LEU:HG	6:C:94:LYS:O	2.17	0.44
6:C:114:TYR:HB3	6:C:141:GLY:H	1.82	0.44
9:H:30:SER:HB2	9:H:36:CYS:SG	2.57	0.44
9:H:39:THR:O	9:H:123:MET:HA	2.16	0.44
9:H:93:TYR:HA	9:H:145:ARG:HD3	1.98	0.44
4:A:1316:VAL:O	4:A:1319:VAL:HB	2.18	0.44
5:B:313:MET:O	5:B:316:PRO:HD2	2.18	0.44
6:C:134:ILE:HG21	6:C:139:GLY:C	2.43	0.44
7:E:192:ARG:CZ	7:E:215:MET:HG2	2.48	0.44
4:A:130:ASP:HB3	4:A:133:LYS:HD2	2.00	0.44
4:A:1239:ARG:NH1	4:A:1241:ARG:HH12	2.15	0.44
6:C:66:ARG:O	6:C:70:ILE:HG13	2.17	0.44
7:E:46:TYR:CD2	7:E:58:MET:HG2	2.52	0.44
4:A:38:PRO:HB3	4:A:270:LEU:HD22	2.00	0.44
4:A:452:LYS:HA	5:B:1137:CYS:HB3	1.99	0.44
4:A:809:THR:HA	5:B:730:ARG:HH21	1.81	0.44
4:A:942:PHE:O	4:A:946:VAL:HG23	2.17	0.44
4:A:975:HIS:CE1	4:A:1036:ARG:H	2.35	0.44
4:A:1080:THR:C	4:A:1082:ASN:H	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1239:ARG:HH12	4:A:1241:ARG:HH12	1.65	0.44
7:E:11:ARG:HH12	7:E:138:ALA:HA	1.83	0.44
7:E:40:GLU:HA	7:E:43:LYS:HD3	1.99	0.44
7:E:81:GLU:HG3	7:E:110:PHE:CE1	2.51	0.44
10:I:17:ARG:HB2	10:I:28:GLU:OE1	2.18	0.44
3:N:9:DA:H2'	3:N:10:DG:O4'	2.18	0.44
4:A:359:LEU:HA	4:A:359:LEU:HD23	1.81	0.44
4:A:380:VAL:HG22	4:A:430:TRP:O	2.17	0.44
4:A:388:LEU:O	4:A:392:VAL:HG23	2.17	0.44
4:A:457:ALA:O	4:A:507:VAL:HG23	2.18	0.44
5:B:173:MET:O	5:B:176:SER:HB3	2.18	0.44
5:B:550:ASP:OD2	5:B:553:PRO:HD3	2.18	0.44
5:B:857:ARG:NH1	5:B:942:ARG:HE	2.16	0.44
6:C:18:VAL:HG12	6:C:20:PHE:HD1	1.83	0.44
6:C:105:GLY:O	6:C:149:LYS:HA	2.18	0.44
1:R:8:G:H2'	1:R:9:G:C8	2.53	0.44
3:N:3:DA:H2''	3:N:4:DG:C8	2.52	0.44
4:A:535:THR:HG21	4:A:617:VAL:HG23	2.00	0.44
4:A:984:LYS:HG3	4:A:988:LEU:HD23	1.99	0.44
4:A:1392:SER:O	4:A:1399:ARG:HD2	2.17	0.44
5:B:59:LEU:O	5:B:63:ILE:HG12	2.18	0.44
5:B:769:TYR:O	5:B:773:MET:HG3	2.18	0.44
6:C:77:ILE:N	6:C:129:ILE:HD11	2.33	0.44
7:E:116:ILE:H	7:E:116:ILE:HG13	1.66	0.44
4:A:19:PHE:O	4:A:1416:ALA:HA	2.18	0.43
4:A:214:ILE:HB	4:A:219:PHE:HE1	1.83	0.43
5:B:67:SER:HB2	5:B:92:PHE:HB2	1.99	0.43
5:B:841:MET:HG2	5:B:846:ILE:HD11	2.00	0.43
10:I:97:MET:HB2	10:I:97:MET:HE3	1.73	0.43
3:N:8:DG:C5	3:N:9:DA:C5	3.06	0.43
4:A:356:ASP:HB3	4:A:359:LEU:HB2	2.00	0.43
4:A:588:LEU:HB3	4:A:607:ILE:HD12	2.00	0.43
5:B:52:ASN:ND2	5:B:177:LYS:HG3	2.33	0.43
5:B:520:GLY:HA3	5:B:635:ARG:NE	2.32	0.43
5:B:963:PHE:HZ	5:B:965:LYS:HE3	1.83	0.43
6:C:36:VAL:HG23	12:K:41:THR:HG21	1.99	0.43
10:I:78:CYS:HB3	10:I:106:CYS:SG	2.58	0.43
12:K:8:GLU:O	12:K:37:LYS:HE3	2.18	0.43
4:A:41:MET:O	4:A:50:ILE:HG23	2.18	0.43
4:A:224:PHE:CE2	4:A:231:PRO:HG3	2.54	0.43
4:A:392:VAL:HG12	4:A:415:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:569:LYS:HG3	4:A:570:PRO:HD2	1.99	0.43
5:B:272:THR:HB	5:B:279:ASP:HB3	2.00	0.43
6:C:102:GLN:HB3	6:C:154:LYS:HG2	2.00	0.43
6:C:124:LEU:O	6:C:127:ARG:HG2	2.18	0.43
10:I:54:GLU:HG3	10:I:55:THR:HG23	1.98	0.43
10:I:78:CYS:HB3	10:I:106:CYS:CB	2.48	0.43
4:A:678:GLU:O	4:A:681:GLU:HG2	2.17	0.43
4:A:1412:ALA:HA	4:A:1417:GLU:CD	2.43	0.43
4:A:1415:SER:HB2	4:A:1417:GLU:HG3	2.01	0.43
5:B:174:LEU:HD22	5:B:202:TYR:CE2	2.52	0.43
5:B:640:VAL:HG13	5:B:650:GLU:C	2.43	0.43
5:B:801:LYS:HG2	11:J:52:THR:HA	1.98	0.43
5:B:1004:GLU:OE2	5:B:1064:TYR:HE2	1.99	0.43
5:B:1135:ARG:O	5:B:1139:ILE:HG12	2.19	0.43
6:C:182:PRO:HB2	6:C:207:CYS:SG	2.58	0.43
10:I:32:CYS:SG	10:I:34:TYR:HB3	2.58	0.43
5:B:175:ARG:HG3	5:B:200:GLY:HA3	2.01	0.43
5:B:758:PHE:CE1	5:B:1044:ALA:HA	2.54	0.43
3:N:6:DG:C2	3:N:7:DA:C2	3.07	0.43
4:A:345:VAL:HA	5:B:1155:SER:OG	2.19	0.43
4:A:474:VAL:HG22	4:A:478:TYR:CE2	2.54	0.43
4:A:548:ASN:HA	12:K:60:ALA:HB1	2.00	0.43
4:A:666:ILE:HG21	5:B:1030:LEU:HD13	2.01	0.43
4:A:881:GLN:CD	4:A:959:ASN:HA	2.44	0.43
4:A:1013:ASP:HB3	7:E:207:ARG:O	2.18	0.43
5:B:510:LYS:HB3	5:B:513:GLN:OE1	2.18	0.43
6:C:210:GLU:HG3	6:C:229:TYR:OH	2.18	0.43
7:E:79:TRP:CE2	7:E:81:GLU:HB2	2.53	0.43
10:I:3:THR:HG21	10:I:40:SER:HB2	2.01	0.43
2:T:8:DT:H2''	2:T:9:DC:O4'	2.19	0.43
4:A:54:ASN:O	4:A:58:LEU:HB2	2.19	0.43
4:A:182:VAL:HA	4:A:201:VAL:HA	2.01	0.43
4:A:895:LYS:HB2	4:A:895:LYS:HE3	1.81	0.43
4:A:1398:MET:HE3	4:A:1398:MET:HB2	1.94	0.43
5:B:1004:GLU:HB2	5:B:1006:ILE:HD12	2.00	0.43
5:B:1033:LYS:HB2	5:B:1089:PRO:HD3	2.00	0.43
6:C:147:LEU:HD22	6:C:151:GLN:HB3	2.00	0.43
7:E:66:GLU:O	7:E:69:ILE:HG12	2.18	0.43
12:K:61:TYR:CB	12:K:71:PHE:HE1	2.29	0.43
12:K:107:THR:O	12:K:111:LEU:HG	2.19	0.43
4:A:230:ARG:HB2	4:A:233:TRP:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:501:LEU:HD21	5:B:1146:PHE:CD2	2.53	0.43
4:A:843:LYS:HG3	4:A:1402:PHE:HB2	2.00	0.43
4:A:1291:VAL:HG22	4:A:1292:PRO:HD2	2.00	0.43
4:A:1311:VAL:HG11	4:A:1329:THR:CG2	2.49	0.43
5:B:170:LEU:HD12	5:B:171:PRO:HD2	2.00	0.43
5:B:876:LYS:HB2	5:B:894:ASP:O	2.19	0.43
5:B:1138:MET:HE3	5:B:1138:MET:HA	2.00	0.43
6:C:58:LEU:HD22	11:J:1:MET:HE3	2.00	0.43
4:A:340:LEU:HD12	5:B:1203:LEU:HD12	2.00	0.43
4:A:523:ILE:HD12	4:A:622:VAL:HG22	2.00	0.43
4:A:540:PHE:HB3	4:A:571:LEU:HD12	2.00	0.43
4:A:705:LYS:HB2	4:A:713:SER:OG	2.18	0.43
5:B:800:GLN:HB3	11:J:52:THR:HB	2.00	0.43
6:C:52:GLU:HG2	6:C:53:THR:HG23	2.01	0.43
7:E:78:LEU:HA	7:E:107:THR:OG1	2.18	0.43
10:I:77:LYS:HA	10:I:77:LYS:HD3	1.89	0.43
13:L:38:LEU:HD22	13:L:56:LEU:HD21	2.01	0.43
4:A:125:ALA:O	4:A:134:ARG:HD3	2.18	0.43
4:A:837:ILE:O	4:A:841:LEU:HG	2.19	0.43
4:A:961:ARG:HD2	4:A:1025:ARG:HH12	1.84	0.43
4:A:1109:LYS:HD2	4:A:1109:LYS:N	2.34	0.43
5:B:167:ILE:O	5:B:450:ALA:HA	2.19	0.43
5:B:270:LYS:HD2	5:B:279:ASP:OD2	2.19	0.43
5:B:291:ILE:HG23	5:B:296:GLU:HB3	2.01	0.43
5:B:365:THR:HG21	5:B:370:PHE:CD1	2.54	0.43
5:B:528:PRO:HG2	5:B:536:VAL:HB	2.01	0.43
5:B:843:GLN:HB2	5:B:993:THR:HG22	2.01	0.43
10:I:15:TYR:CD1	10:I:30:ARG:HG2	2.54	0.43
11:J:3:VAL:HG11	11:J:18:TRP:HB2	2.01	0.43
11:J:24:LEU:HD22	11:J:38:ARG:HH12	1.83	0.43
12:K:94:ILE:O	12:K:98:LEU:HG	2.19	0.43
4:A:32:VAL:HG11	4:A:57:ARG:CB	2.49	0.42
4:A:132:LYS:HE2	4:A:1417:GLU:OE2	2.18	0.42
4:A:208:LEU:HD12	4:A:235:ILE:HG23	2.01	0.42
4:A:628:GLY:O	4:A:632:VAL:HG23	2.19	0.42
4:A:760:GLN:HA	4:A:765:VAL:HA	2.01	0.42
6:C:265:MET:HE3	6:C:265:MET:HB3	1.90	0.42
8:F:89:GLU:O	8:F:93:ILE:HG12	2.19	0.42
10:I:26:LEU:HD22	10:I:35:VAL:HG11	2.00	0.42
4:A:179:LEU:HD22	4:A:297:GLN:HG2	2.01	0.42
4:A:820:GLY:O	4:A:824:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1025:ARG:O	4:A:1026:LEU:HD23	2.20	0.42
5:B:979:LYS:HB2	5:B:979:LYS:HE3	1.78	0.42
4:A:62:ASP:O	4:A:63:ARG:HB3	2.18	0.42
4:A:1148:ILE:HG12	4:A:1198:ASP:HB2	2.00	0.42
5:B:283:VAL:HG21	5:B:321:GLY:HA3	2.01	0.42
7:E:127:ILE:HB	7:E:130:ALA:HB3	2.00	0.42
12:K:108:GLU:O	12:K:112:GLN:HG2	2.20	0.42
4:A:980:ASP:HB3	4:A:1039:LYS:H	1.84	0.42
4:A:1092:LYS:O	4:A:1093:LYS:HB2	2.19	0.42
5:B:331:LEU:HD13	5:B:349:ILE:HG23	2.01	0.42
5:B:564:GLU:O	5:B:588:GLY:HA3	2.20	0.42
6:C:58:LEU:HB2	6:C:63:ILE:HD11	2.02	0.42
11:J:44:TYR:O	11:J:48:ARG:HG2	2.19	0.42
12:K:84:LYS:O	12:K:88:LYS:HG3	2.20	0.42
4:A:23:SER:HB2	4:A:233:TRP:CZ2	2.55	0.42
4:A:403:LYS:HB2	4:A:404:TYR:HD1	1.85	0.42
4:A:550:LEU:HD13	4:A:556:TRP:CZ2	2.54	0.42
4:A:901:LEU:HD22	4:A:919:ILE:HG13	2.00	0.42
6:C:34:ARG:HA	6:C:37:MET:HE3	2.00	0.42
6:C:137:LYS:H	6:C:137:LYS:HG2	1.58	0.42
7:E:103:LYS:HB3	7:E:105:PHE:CD1	2.54	0.42
9:H:96:VAL:HA	9:H:142:LEU:O	2.18	0.42
10:I:42:LEU:HD11	10:I:45:ARG:HB2	2.02	0.42
4:A:23:SER:O	4:A:27:VAL:HG23	2.18	0.42
4:A:325:ILE:HA	4:A:328:ARG:HD3	2.01	0.42
4:A:1194:ARG:HG2	4:A:1237:ILE:HG23	2.02	0.42
5:B:89:GLU:OE2	5:B:91:SER:HB2	2.19	0.42
9:H:99:GLY:HA3	9:H:118:PHE:HD1	1.84	0.42
10:I:71:SER:HB2	10:I:85:PHE:CE1	2.54	0.42
4:A:22:PHE:CD2	4:A:27:VAL:HG22	2.55	0.42
4:A:70:CYS:O	4:A:72:GLU:HG2	2.19	0.42
4:A:556:TRP:HZ3	12:K:74:ARG:NH1	2.18	0.42
4:A:568:PRO:HB2	9:H:46:LEU:HD22	2.01	0.42
4:A:777:PHE:CD1	4:A:783:THR:HG23	2.54	0.42
5:B:22:SER:O	5:B:654:ARG:HD2	2.20	0.42
5:B:551:PRO:O	5:B:555:ILE:HG12	2.19	0.42
6:C:171:GLY:HA2	6:C:172:PRO:HD3	1.83	0.42
8:F:83:PRO:HA	8:F:146:TRP:CZ3	2.55	0.42
4:A:848:ILE:HG21	4:A:1370:LEU:HD11	2.01	0.42
4:A:973:ILE:HG21	4:A:1036:ARG:O	2.20	0.42
5:B:780:VAL:HG12	5:B:795:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:241:ASP:HB3	12:K:109:TRP:NE1	2.35	0.42
10:I:16:PRO:HA	10:I:27:PHE:HA	2.02	0.42
2:T:13:DC:N3	2:T:14:DG:C6	2.88	0.42
4:A:767:GLN:HA	4:A:799:PHE:HA	2.01	0.42
4:A:830:LYS:O	4:A:834:THR:HG23	2.20	0.42
4:A:1341:ILE:HG13	7:E:182:ASP:OD1	2.20	0.42
5:B:377:PHE:CD2	5:B:381:MET:HE2	2.54	0.42
5:B:541:LEU:HD21	5:B:751:VAL:HA	2.01	0.42
5:B:566:LEU:HD12	5:B:566:LEU:HA	1.85	0.42
5:B:828:ALA:HB2	5:B:1085:ILE:HG12	2.01	0.42
5:B:849:GLY:O	5:B:852:ARG:HG3	2.20	0.42
7:E:192:ARG:HH11	7:E:193:GLY:H	1.68	0.42
9:H:12:VAL:HG13	9:H:52:GLN:N	2.33	0.42
9:H:23:VAL:HG21	9:H:121:LEU:HD22	2.01	0.42
9:H:40:LEU:HD13	9:H:123:MET:HB2	2.02	0.42
4:A:455:MET:HE2	5:B:1137:CYS:HB2	2.00	0.42
4:A:779:PHE:CE1	5:B:517:THR:HG22	2.55	0.42
4:A:919:ILE:CG1	4:A:983:ILE:HD12	2.47	0.42
4:A:1313:LEU:HD23	4:A:1313:LEU:HA	1.87	0.42
5:B:377:PHE:HD2	5:B:381:MET:HE2	1.85	0.42
5:B:487:THR:HG22	5:B:488:TYR:N	2.35	0.42
5:B:839:MET:HE2	5:B:839:MET:HB3	1.92	0.42
5:B:1152:MET:HE2	5:B:1152:MET:HB3	1.85	0.42
6:C:106:GLU:CD	6:C:106:GLU:H	2.28	0.42
6:C:248:ILE:HG23	12:K:98:LEU:HB3	2.02	0.42
4:A:900:ASP:H	4:A:906:HIS:HB3	1.85	0.41
4:A:1029:ARG:O	4:A:1033:GLN:HB2	2.19	0.41
4:A:1166:ASP:HA	4:A:1169:ILE:HD12	2.02	0.41
5:B:236:HIS:CD2	5:B:388:CYS:HB3	2.54	0.41
5:B:791:THR:O	5:B:857:ARG:HA	2.20	0.41
5:B:800:GLN:HG3	5:B:821:GLN:HG2	2.01	0.41
8:F:99:LEU:HD23	8:F:99:LEU:HA	1.84	0.41
8:F:135:ARG:HD3	8:F:137:TYR:OH	2.20	0.41
10:I:71:SER:HB3	10:I:83:ASN:OD1	2.19	0.41
4:A:136:ALA:O	4:A:140:THR:HG23	2.20	0.41
4:A:810:PRO:HD3	5:B:730:ARG:NH2	2.32	0.41
4:A:818:MET:HG2	5:B:514:LEU:HD23	2.02	0.41
5:B:311:LEU:O	5:B:315:LYS:HG3	2.20	0.41
5:B:546:SER:HB2	5:B:612:GLU:CD	2.44	0.41
5:B:1196:ILE:HG13	5:B:1197:PRO:O	2.19	0.41
8:F:118:LEU:O	8:F:122:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:190:TYR:CZ	5:B:196:PRO:HG2	2.55	0.41
5:B:345:LYS:HA	5:B:348:ARG:NH1	2.25	0.41
5:B:635:ARG:NH1	5:B:637:LEU:HD11	2.35	0.41
6:C:259:LEU:O	6:C:263:THR:HG23	2.20	0.41
10:I:74:GLU:HA	10:I:81:ARG:HA	2.02	0.41
4:A:265:LYS:CG	4:A:303:TYR:HB2	2.51	0.41
4:A:597:LEU:HB3	9:H:102:TYR:HE2	1.85	0.41
4:A:679:ILE:HD13	4:A:763:ALA:HB2	2.02	0.41
4:A:1078:GLN:C	4:A:1080:THR:N	2.77	0.41
4:A:1116:LEU:HD12	4:A:1328:TYR:O	2.20	0.41
5:B:701:ILE:HB	5:B:739:THR:OG1	2.20	0.41
5:B:866:TYR:CE1	5:B:872:GLU:HG3	2.49	0.41
13:L:34:CYS:HB3	13:L:51:CYS:SG	2.60	0.41
4:A:395:GLY:O	4:A:401:GLY:HA3	2.20	0.41
4:A:396:PRO:HB3	4:A:403:LYS:HA	2.01	0.41
4:A:569:LYS:HE3	4:A:571:LEU:HD21	2.02	0.41
4:A:674:PRO:O	4:A:678:GLU:HG3	2.21	0.41
4:A:986:ILE:HD12	4:A:1028:THR:HG23	2.02	0.41
4:A:1141:THR:HB	4:A:1273:LEU:O	2.20	0.41
5:B:115:GLN:O	5:B:119:LEU:HG	2.20	0.41
5:B:392:ARG:HH11	10:I:53:GLY:HA3	1.85	0.41
7:E:86:PRO:HB3	7:E:113:GLN:NE2	2.36	0.41
4:A:70:CYS:SG	4:A:72:GLU:HB2	2.61	0.41
4:A:920:LEU:HD23	4:A:921:GLY:H	1.85	0.41
4:A:1084:PHE:O	5:B:765:PRO:HG2	2.21	0.41
5:B:661:LEU:O	5:B:665:GLU:HG3	2.20	0.41
5:B:854:LEU:HD12	5:B:854:LEU:H	1.85	0.41
6:C:69:LEU:HD12	11:J:5:VAL:HB	2.03	0.41
6:C:102:GLN:HA	6:C:153:LEU:O	2.21	0.41
10:I:4:PHE:CD2	10:I:6:PHE:CZ	3.07	0.41
1:R:5:A:H2'	1:R:6:G:H8	1.86	0.41
4:A:112:LYS:HD3	4:A:113:LEU:N	2.36	0.41
4:A:676:MET:HE2	4:A:806:ARG:HE	1.86	0.41
4:A:784:LEU:HA	4:A:784:LEU:HD23	1.80	0.41
4:A:1025:ARG:O	4:A:1030:ARG:HD3	2.20	0.41
4:A:1221:LYS:HE3	4:A:1221:LYS:HB3	1.92	0.41
4:A:1227:ILE:HD11	4:A:1239:ARG:HH11	1.85	0.41
5:B:523:CYS:HB2	5:B:750:GLY:HA3	2.03	0.41
6:C:62:PHE:CE1	6:C:66:ARG:HD2	2.56	0.41
7:E:90:VAL:CG2	7:E:123:LEU:HD11	2.50	0.41
7:E:124:VAL:O	7:E:132:ILE:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:63:LEU:HB3	9:H:90:ALA:CB	2.50	0.41
3:N:12:DG:H1'	3:N:13:DA:C4	2.56	0.41
4:A:8:SER:HB2	5:B:1180:PHE:HE2	1.86	0.41
4:A:247:ARG:CD	4:A:262:LEU:HD11	2.51	0.41
4:A:838:GLN:O	4:A:842:VAL:HG23	2.21	0.41
4:A:1154:TYR:HB2	4:A:1191:TRP:CH2	2.55	0.41
7:E:18:THR:HA	7:E:21:GLU:OE1	2.21	0.41
12:K:31:VAL:O	12:K:74:ARG:HA	2.21	0.41
4:A:284:ALA:HB3	4:A:289:ILE:HG12	2.03	0.41
4:A:335:ARG:NH2	5:B:1202:LEU:HD13	2.35	0.41
4:A:898:ARG:HD3	4:A:933:TYR:CG	2.56	0.41
4:A:960:ILE:HG23	4:A:964:ILE:HD13	2.03	0.41
4:A:1213:GLY:HA2	4:A:1216:ILE:HD12	2.03	0.41
5:B:459:TYR:CE1	5:B:463:THR:HG21	2.56	0.41
5:B:580:VAL:HG12	5:B:624:LEU:HB3	2.03	0.41
5:B:637:LEU:CD2	5:B:742:GLU:HA	2.51	0.41
5:B:1160:VAL:HG11	5:B:1169:MET:SD	2.61	0.41
6:C:51:VAL:HA	6:C:155:LEU:HA	2.03	0.41
7:E:77:SER:HB3	7:E:105:PHE:CG	2.56	0.41
10:I:44:TYR:OH	10:I:46:HIS:HB2	2.21	0.41
12:K:40:HIS:HE2	12:K:63:VAL:CG2	2.34	0.41
4:A:96:ILE:HA	4:A:99:ILE:HB	2.02	0.41
4:A:511:ILE:O	4:A:519:PRO:HA	2.21	0.41
4:A:1266:THR:O	4:A:1270:ASN:HB2	2.20	0.41
5:B:212:LEU:HD23	5:B:212:LEU:HA	1.79	0.41
5:B:308:TRP:O	5:B:312:GLU:HG2	2.21	0.41
5:B:361:LEU:HD23	5:B:364:ILE:HD12	2.03	0.41
5:B:698:GLU:O	5:B:701:ILE:HG12	2.21	0.41
5:B:1114:LEU:HD12	5:B:1114:LEU:HA	1.88	0.41
7:E:79:TRP:HD1	7:E:100:ILE:HD11	1.86	0.41
7:E:112:TYR:CG	7:E:116:ILE:HG12	2.56	0.41
10:I:68:LEU:HB3	10:I:84:VAL:HG23	2.02	0.41
4:A:21:LEU:HD11	4:A:95:PHE:CE2	2.56	0.40
4:A:32:VAL:HB	5:B:1183:LYS:NZ	2.36	0.40
4:A:540:PHE:HD1	4:A:573:SER:HA	1.87	0.40
4:A:605:MET:SD	4:A:612:ILE:HD11	2.60	0.40
4:A:997:LEU:HB2	4:A:1053:PHE:CE1	2.55	0.40
4:A:1286:LYS:HD3	4:A:1304:TRP:CD2	2.56	0.40
4:A:1356:ILE:HD13	4:A:1356:ILE:HA	1.92	0.40
5:B:31:TRP:CE3	5:B:34:ILE:HD12	2.56	0.40
5:B:69:LEU:HB3	5:B:429:PHE:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:221:ASN:OD1	5:B:242:SER:HA	2.21	0.40
5:B:549:THR:HB	5:B:628:THR:HB	2.02	0.40
5:B:639:ILE:HA	5:B:740:HIS:HD2	1.86	0.40
5:B:706:GLN:HG3	5:B:708:GLU:N	2.32	0.40
3:N:7:DA:C2	3:N:8:DG:C4	3.09	0.40
4:A:857:ARG:HD3	4:A:861:GLY:O	2.21	0.40
4:A:1211:GLN:H	4:A:1211:GLN:HG3	1.75	0.40
8:F:93:ILE:HD13	8:F:93:ILE:HA	1.87	0.40
9:H:36:CYS:HB2	9:H:125:LEU:HD11	2.02	0.40
9:H:49:VAL:HA	9:H:146:ARG:HH12	1.86	0.40
12:K:70:ARG:HE	12:K:70:ARG:HB3	1.43	0.40
14:T:101:8GT:C4	4:A:1081:LEU:CD1	2.99	0.40
3:N:2:DC:H2''	3:N:3:DA:O5'	2.20	0.40
4:A:1199:ARG:HG3	4:A:1203:ASN:HD21	1.87	0.40
4:A:1315:GLU:O	4:A:1319:VAL:HG23	2.22	0.40
4:A:1436:ILE:CG2	4:A:1437:GLY:N	2.84	0.40
5:B:112:LEU:HD21	5:B:117:ALA:HB2	2.03	0.40
5:B:173:MET:HE3	5:B:173:MET:HB2	1.93	0.40
5:B:483:LEU:HD23	5:B:483:LEU:HA	1.94	0.40
5:B:574:SER:HB3	5:B:591:ARG:NH2	2.36	0.40
5:B:997:GLU:HB2	6:C:35:ARG:HG2	2.03	0.40
6:C:42:PRO:HB3	6:C:161:LYS:HE2	2.03	0.40
9:H:93:TYR:CG	9:H:143:LEU:HB3	2.57	0.40
4:A:99:ILE:HG12	4:A:211:PHE:HE2	1.86	0.40
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.61	0.40
5:B:62:ILE:HG21	5:B:417:PHE:CD1	2.55	0.40
5:B:962:LYS:NZ	13:L:46:VAL:HG21	2.37	0.40
5:B:1139:ILE:HD11	5:B:1147:LEU:HD13	2.02	0.40
12:K:13:GLY:O	12:K:16:GLU:HB2	2.22	0.40
4:A:335:ARG:CZ	5:B:1202:LEU:HD22	2.52	0.40
4:A:1336:MET:HE3	4:A:1336:MET:HB3	1.90	0.40
4:A:1357:ALA:HA	4:A:1361:SER:O	2.21	0.40
5:B:792:MET:HA	5:B:856:PHE:O	2.21	0.40
5:B:913:GLY:HA2	5:B:938:SER:OG	2.21	0.40
5:B:1183:LYS:H	5:B:1183:LYS:HG2	1.70	0.40
6:C:77:ILE:HD12	6:C:77:ILE:HA	1.99	0.40
9:H:111:LEU:HD23	9:H:111:LEU:HA	1.90	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	1379/1733 (80%)	1344 (98%)	35 (2%)	0	100	100
5	B	1103/1224 (90%)	1086 (98%)	17 (2%)	0	100	100
6	C	265/318 (83%)	264 (100%)	1 (0%)	0	100	100
7	E	210/215 (98%)	207 (99%)	3 (1%)	0	100	100
8	F	84/155 (54%)	82 (98%)	2 (2%)	0	100	100
9	H	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
10	I	116/122 (95%)	115 (99%)	1 (1%)	0	100	100
11	J	63/70 (90%)	63 (100%)	0	0	100	100
12	K	112/120 (93%)	111 (99%)	1 (1%)	0	100	100
13	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
All	All	3502/4173 (84%)	3439 (98%)	63 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1200/1520 (79%)	1198 (100%)	2 (0%)	87	84
5	B	955/1061 (90%)	954 (100%)	1 (0%)	88	87
6	C	235/274 (86%)	235 (100%)	0	100	100
7	E	193/197 (98%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	116/128 (91%)	116 (100%)	0	100	100
10	I	110/116 (95%)	107 (97%)	3 (3%)	39	62
11	J	60/65 (92%)	59 (98%)	1 (2%)	53	69
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	37/57 (65%)	37 (100%)	0	100	100
All	All	3078/3657 (84%)	3071 (100%)	7 (0%)	87	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	85	ASP
4	A	167	CYS
5	B	1163	CYS
10	I	7	CYS
10	I	10	CYS
10	I	29	CYS
11	J	7	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	18	GLN
4	A	83	HIS
4	A	169	ASN
4	A	287	HIS
4	A	313	GLN
4	A	445	ASN
4	A	447	GLN
4	A	877	HIS
4	A	975	HIS
4	A	1004	ASN
4	A	1106	ASN
4	A	1110	ASN
4	A	1378	GLN
5	B	115	GLN
5	B	206	ASN
5	B	350	GLN
5	B	433	GLN

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Mol	Chain	Res	Type
5	B	465	ASN
5	B	481	GLN
5	B	573	GLN
5	B	686	ASN
5	B	767	ASN
5	B	794	ASN
5	B	835	GLN
5	B	932	HIS
5	B	1093	GLN
5	B	1117	GLN
5	B	1178	ASN
5	B	1193	GLN
5	B	1211	ASN
6	C	54	ASN
6	C	195	GLN
6	C	267	GLN
11	J	23	ASN
12	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	7/9 (77%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	5	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	8GT	T	101	16	34,35,35	4.96	21 (61%)	48,56,56	1.96	10 (20%)

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
14	8GT	T	101	16	-	8/22/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	101	8GT	C4-N3	10.02	1.57	1.34
14	T	101	8GT	C6-N1	9.55	1.56	1.38
14	T	101	8GT	C3'-C4'	-9.39	1.29	1.53
14	T	101	8GT	C2'-C1'	-9.08	1.24	1.53
14	T	101	8GT	O4'-C1'	8.69	1.62	1.42
14	T	101	8GT	C5-C4	7.67	1.47	1.37
14	T	101	8GT	C2-N3	6.80	1.49	1.33
14	T	101	8GT	C2'-C3'	6.02	1.69	1.53
14	T	101	8GT	PB-O3A	5.72	1.65	1.59
14	T	101	8GT	C5-N7	5.69	1.46	1.37
14	T	101	8GT	PA-O3A	5.61	1.65	1.59
14	T	101	8GT	C8-N7	5.51	1.48	1.38
14	T	101	8GT	PB-O3B	5.09	1.65	1.59
14	T	101	8GT	C2-N2	4.50	1.44	1.34
14	T	101	8GT	C4-N9	4.09	1.46	1.39
14	T	101	8GT	C8-N9	4.08	1.47	1.40
14	T	101	8GT	O4'-C4'	4.06	1.54	1.45
14	T	101	8GT	O8-C8	-2.58	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	101	8GT	C5'-C4'	2.27	1.58	1.51
14	T	101	8GT	C5-C6	-2.02	1.36	1.41
14	T	101	8GT	O6-C6	-2.00	1.19	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	101	8GT	O6-C6-C5	-5.63	113.68	127.26
14	T	101	8GT	N9-C4-N3	5.49	132.99	126.13
14	T	101	8GT	C5-C6-N1	4.71	125.08	112.13
14	T	101	8GT	C2-N3-C4	4.20	119.54	112.30
14	T	101	8GT	C2'-C1'-N9	-3.76	110.86	115.90
14	T	101	8GT	C3'-C2'-C1'	3.08	107.29	101.46
14	T	101	8GT	C2-N1-C6	-2.78	120.06	125.11
14	T	101	8GT	C2'-C3'-C4'	2.77	107.96	102.61
14	T	101	8GT	N2-C2-N1	2.42	121.88	116.76
14	T	101	8GT	N1-C2-N3	-2.21	119.28	123.32

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	101	8GT	C5'-O5'-PA-O3A
14	T	101	8GT	C5'-O5'-PA-O2A
14	T	101	8GT	C4'-C5'-O5'-PA
14	T	101	8GT	O4'-C1'-N9-C8
14	T	101	8GT	O4'-C1'-N9-C4
14	T	101	8GT	C3'-C4'-C5'-O5'
14	T	101	8GT	PG-O3B-PB-O3A
14	T	101	8GT	PG-O3B-PB-O2B

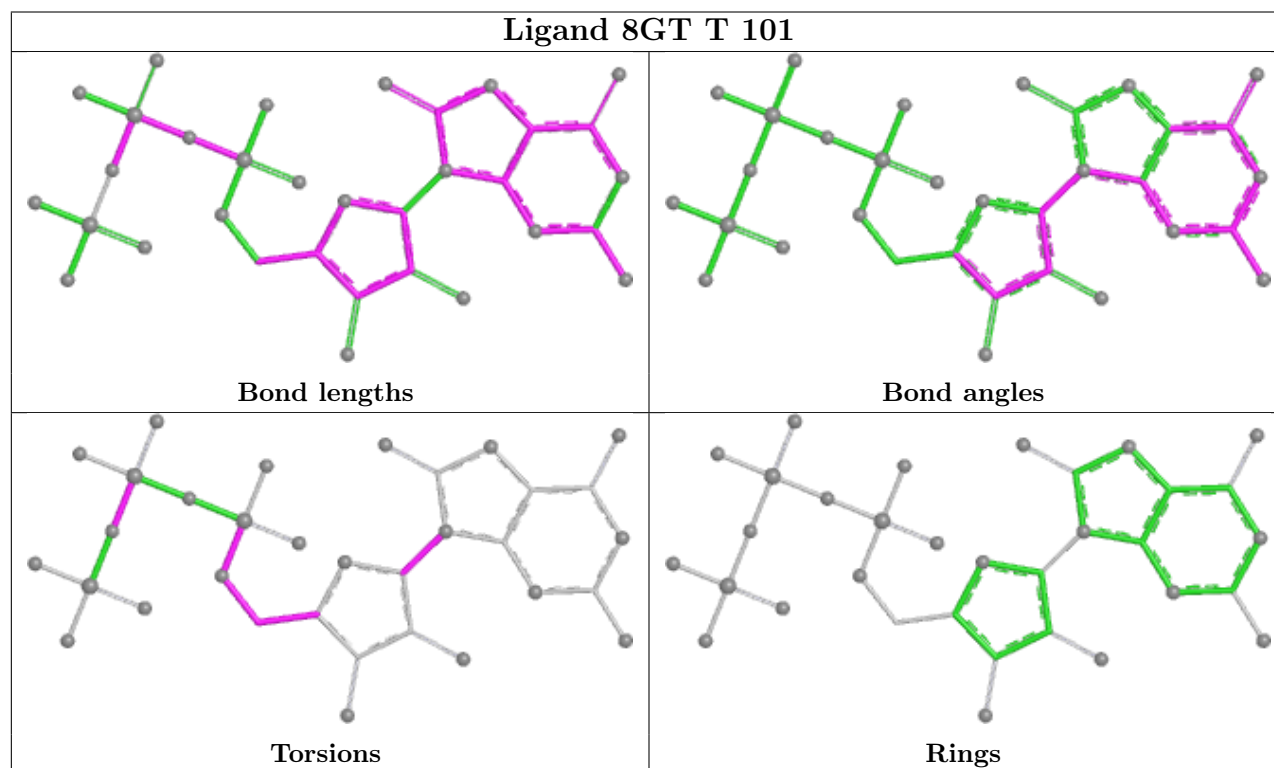
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	101	8GT	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	R	9/9 (100%)	-0.27	0	100	100	78, 84, 138, 140	0
2	T	25/29 (86%)	0.31	0	100	100	78, 121, 257, 265	0
3	N	14/18 (77%)	0.48	0	100	100	144, 231, 286, 286	0
4	A	1393/1733 (80%)	0.45	87 (6%)	26	17	52, 117, 202, 273	0
5	B	1123/1224 (91%)	0.37	34 (3%)	52	31	50, 96, 167, 297	0
6	C	267/318 (83%)	0.42	12 (4%)	38	21	45, 87, 136, 218	0
7	E	212/215 (98%)	0.36	7 (3%)	49	28	98, 149, 214, 243	0
8	F	86/155 (55%)	0.28	1 (1%)	76	53	84, 117, 166, 205	0
9	H	133/146 (91%)	0.37	5 (3%)	44	25	87, 129, 178, 267	0
10	I	118/122 (96%)	0.40	1 (0%)	82	61	80, 142, 199, 225	0
11	J	65/70 (92%)	0.52	2 (3%)	51	30	56, 78, 130, 153	0
12	K	114/120 (95%)	0.28	4 (3%)	47	27	58, 92, 134, 181	0
13	L	43/70 (61%)	0.67	3 (6%)	22	15	81, 146, 219, 305	0
All	All	3602/4229 (85%)	0.41	156 (4%)	40	22	45, 109, 193, 305	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	1136	ASP	5.6
7	E	97	VAL	5.1
4	A	1282	VAL	5.1
7	E	93	MET	4.5
4	A	1098	VAL	4.3
13	L	46	VAL	4.1
4	A	103	CYS	4.0
5	B	424	LEU	4.0
4	A	111	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
5	B	533	CYS	3.8
5	B	988	GLY	3.7
5	B	386	LEU	3.7
4	A	1081	LEU	3.7
4	A	486	GLU	3.6
4	A	1332	PHE	3.6
5	B	534	GLY	3.6
5	B	420	LEU	3.6
4	A	873	MET	3.5
4	A	448	PRO	3.5
4	A	1078	GLN	3.4
4	A	1018	PHE	3.4
5	B	681	TRP	3.4
5	B	775	LYS	3.4
4	A	1020	CYS	3.4
4	A	1026	LEU	3.4
4	A	830	LYS	3.4
5	B	1172	ILE	3.4
4	A	833	GLU	3.3
4	A	751	SER	3.3
4	A	1084	PHE	3.2
5	B	446	LEU	3.2
12	K	42	LEU	3.2
4	A	30	ILE	3.2
9	H	63	LEU	3.1
4	A	815	PHE	3.1
7	E	109	ILE	3.1
4	A	299	HIS	3.1
4	A	1434	ALA	3.0
6	C	251	LEU	3.0
4	A	82	GLY	3.0
5	B	822	ASN	3.0
9	H	119	GLY	3.0
4	A	1066	VAL	3.0
4	A	162	VAL	3.0
4	A	92	HIS	2.9
5	B	524	PRO	2.9
4	A	179	LEU	2.9
6	C	22	LEU	2.9
4	A	54	ASN	2.9
4	A	91	PHE	2.9
4	A	872	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
5	B	381	MET	2.8
4	A	1077	THR	2.8
6	C	50	GLU	2.8
5	B	75	ALA	2.8
4	A	1007	ILE	2.8
4	A	152	VAL	2.7
4	A	53	LEU	2.7
5	B	638	PHE	2.7
4	A	238	CYS	2.7
4	A	106	VAL	2.7
4	A	642	CYS	2.7
4	A	144	THR	2.7
4	A	1358	SER	2.7
6	C	60	ASP	2.7
4	A	336	ILE	2.7
4	A	1306	LEU	2.6
5	B	1072	MET	2.6
6	C	29	MET	2.6
12	K	94	ILE	2.6
4	A	443	LEU	2.6
4	A	84	ILE	2.6
7	E	112	TYR	2.5
6	C	51	VAL	2.5
5	B	468	GLU	2.5
4	A	269	ILE	2.5
4	A	770	VAL	2.5
4	A	1176	LEU	2.4
4	A	1271	ILE	2.4
7	E	137	GLU	2.4
4	A	328	ARG	2.4
5	B	1100	ASP	2.4
4	A	915	SER	2.4
4	A	764	CYS	2.4
4	A	960	ILE	2.4
4	A	1396	ALA	2.4
4	A	303	TYR	2.4
5	B	529	GLU	2.4
10	I	57	GLY	2.3
4	A	577	ILE	2.3
4	A	1328	TYR	2.3
5	B	334	ILE	2.3
5	B	823	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
4	A	997	LEU	2.3
4	A	221	SER	2.3
4	A	952	ALA	2.3
4	A	983	ILE	2.3
8	F	120	ILE	2.3
5	B	647	GLY	2.3
4	A	1267	MET	2.3
4	A	262	LEU	2.3
4	A	81	PHE	2.3
4	A	939	ASP	2.3
4	A	141	LEU	2.3
7	E	98	ILE	2.3
4	A	646	PHE	2.3
6	C	26	ASP	2.3
6	C	33	LEU	2.2
4	A	957	PRO	2.2
4	A	883	LEU	2.2
5	B	1039	GLY	2.2
4	A	726	ARG	2.2
11	J	44	TYR	2.2
4	A	1079	MET	2.2
5	B	1130	PHE	2.2
4	A	210	ILE	2.2
5	B	787	VAL	2.1
4	A	908	LEU	2.1
9	H	121	LEU	2.1
5	B	778	MET	2.1
4	A	104	GLU	2.1
5	B	816	GLU	2.1
4	A	835	GLY	2.1
13	L	64	LEU	2.1
4	A	768	GLN	2.1
4	A	932	GLU	2.1
5	B	543	SER	2.1
12	K	105	PHE	2.1
6	C	36	VAL	2.1
11	J	61	LEU	2.1
5	B	860	MET	2.1
4	A	999	VAL	2.1
4	A	222	LEU	2.1
4	A	276	LEU	2.1
5	B	743	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
5	B	752	ALA	2.1
7	E	163	GLU	2.1
4	A	928	LEU	2.0
13	L	40	LEU	2.0
4	A	692	ASP	2.0
12	K	39	ASP	2.0
4	A	707	GLY	2.0
9	H	6	PHE	2.0
6	C	222	LYS	2.0
5	B	493	SER	2.0
4	A	996	ASN	2.0
4	A	706	HIS	2.0
5	B	806	THR	2.0
6	C	30	ALA	2.0
4	A	1073	GLY	2.0
4	A	71	GLN	2.0
6	C	202	PRO	2.0
9	H	23	VAL	2.0
4	A	722	LEU	2.0
4	A	666	ILE	2.0
4	A	1138	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

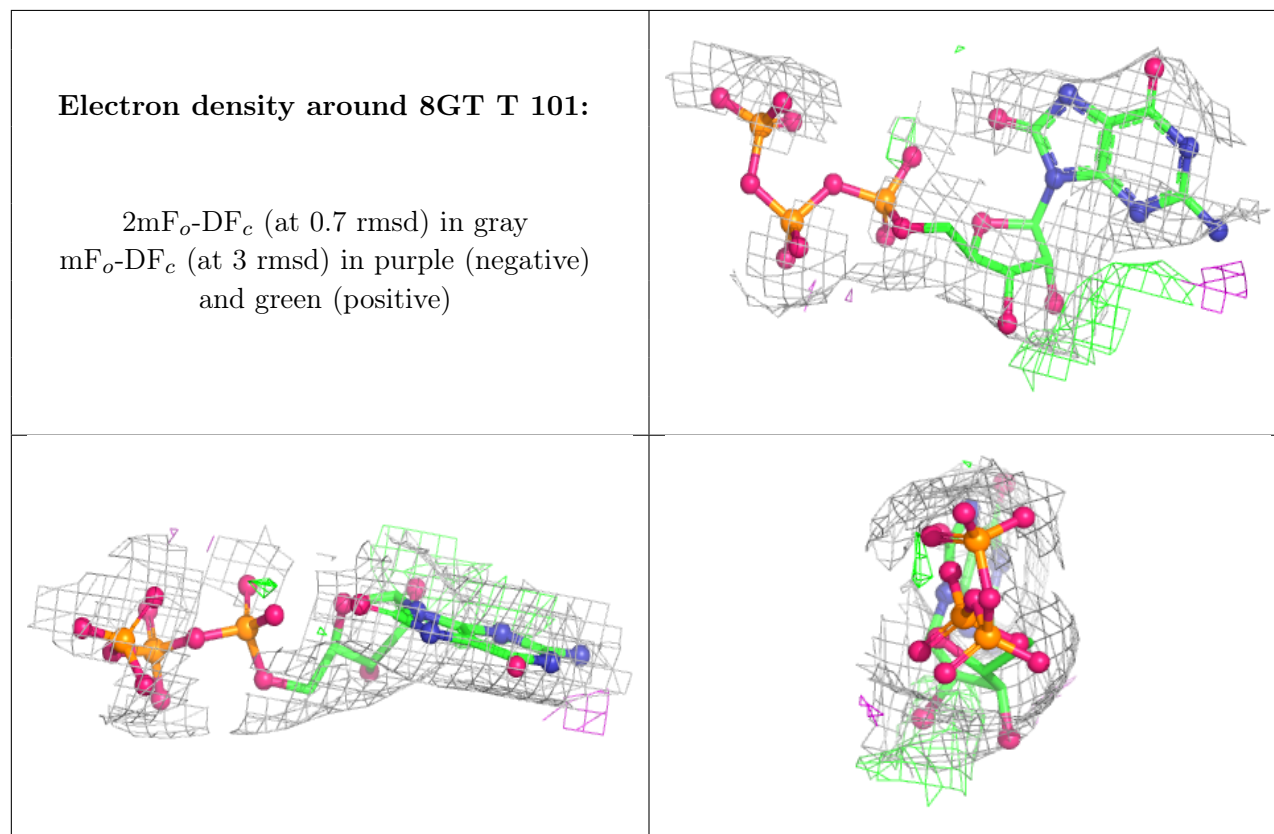
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	MG	A	1803	1/1	0.72	0.15	123,123,123,123	0
15	ZN	L	101	1/1	0.88	0.09	297,297,297,297	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	ZN	A	1801	1/1	0.88	0.08	272,272,272,272	0
14	8GT	T	101	33/33	0.93	0.09	46,68,125,132	0
15	ZN	I	202	1/1	0.93	0.09	245,245,245,245	0
16	MG	A	1804	1/1	0.97	0.05	103,103,103,103	0
15	ZN	A	1802	1/1	0.98	0.03	169,169,169,169	0
15	ZN	I	201	1/1	0.98	0.15	204,204,204,204	0
15	ZN	B	1301	1/1	0.99	0.03	191,191,191,191	0
15	ZN	C	401	1/1	0.99	0.14	154,154,154,154	0
15	ZN	J	101	1/1	0.99	0.10	104,104,104,104	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.