



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:05 PM UTC

PDB ID : 8W8P / pdb_00008w8p
Title : Thermus thermophilus initiation transcription complex containing CMPcPP
in the post-translocated state
Authors : Li, L.; Zhang, Y.
Deposited on : 2023-09-04
Resolution : 3.17 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:

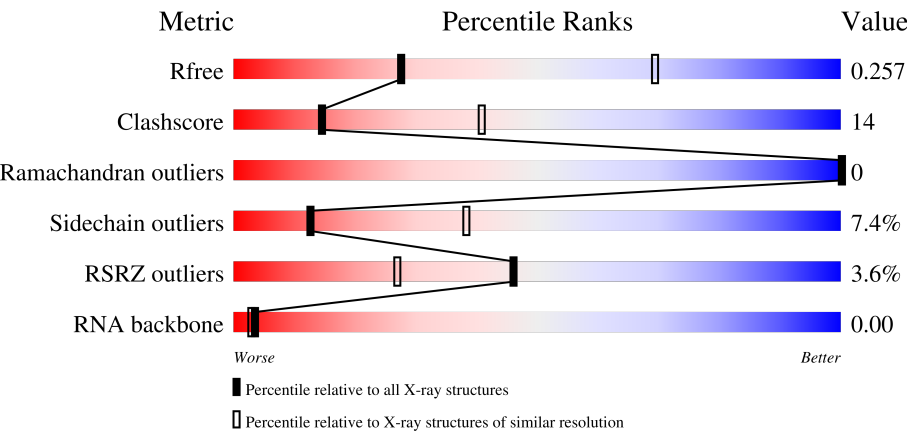
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.17 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)
RNA backbone	3983	1113 (3.42-2.90)

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	A	315	3% 49%22%•27%
1	B	315	3% 46%24%•28%
2	C	1119	3% 63%33%••
3	D	1524	4% 63%33%••

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Mol	Chain	Length	Quality of chain
4	E	99	% 72% 20% • 5%
5	F	443	4% 55% 22% • 22%
6	G	21	5% 43% 33% 19%
7	H	27	4% 15% 41% 33% 11%
8	I	3	33% 67%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28769 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 protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	B	227	Total	C	N	O	S	0	0	0
			1789	1143	310	334	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8771	5547	1565	1635	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1497	Total	C	N	O	S	0	1	0
			11817	7488	2085	2208	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2804	1769	509	522	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called DNA (21-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	17	Total	C	N	O	P	0	0	0
			347	165	66	100	16			

- Molecule 7 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 8 is a RNA chain called RNA (5'-(GTP)GA-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	3	Total	C	N	O	P	0	0	0
			77	30	15	27	5			

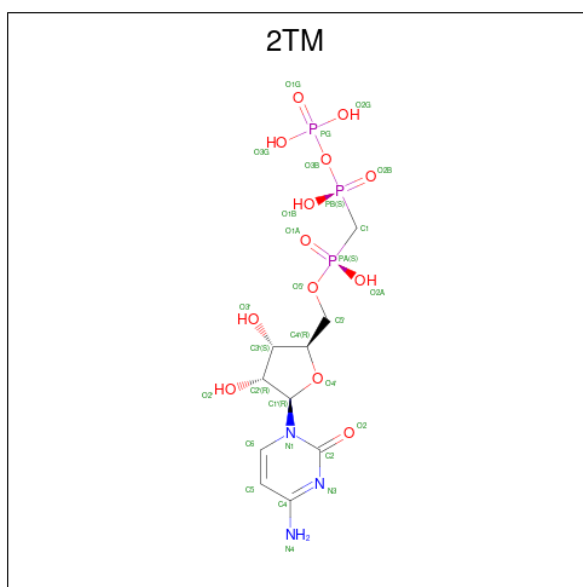
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Mg 2 2	0	0
9	D	3	Total Mg 3 3	0	0
9	F	1	Total Mg 1 1	0	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Zn 2 2	0	0

- Molecule 11 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (CCD ID: 2TM) (formula: C₁₀H₁₈N₃O₁₃P₃).



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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	3	Total O 3 3	0	0
12	B	4	Total O 4 4	0	0

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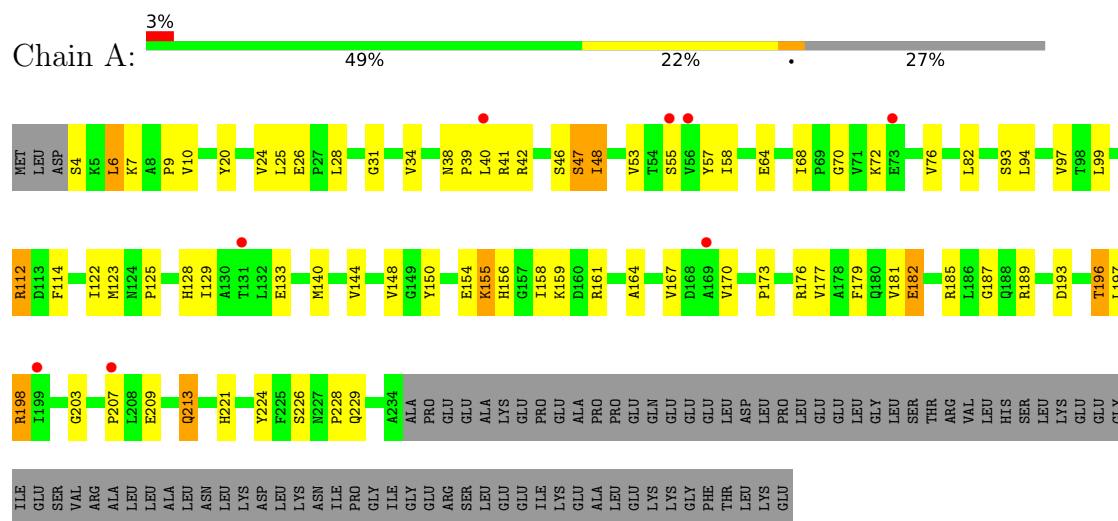
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	19	Total 19	O 19	0	0
12	D	24	Total 24	O 24	0	0
12	E	2	Total 2	O 2	0	0
12	F	1	Total 1	O 1	0	0
12	G	5	Total 5	O 5	0	0
12	H	1	Total 1	O 1	0	0
12	I	3	Total 3	O 3	0	0

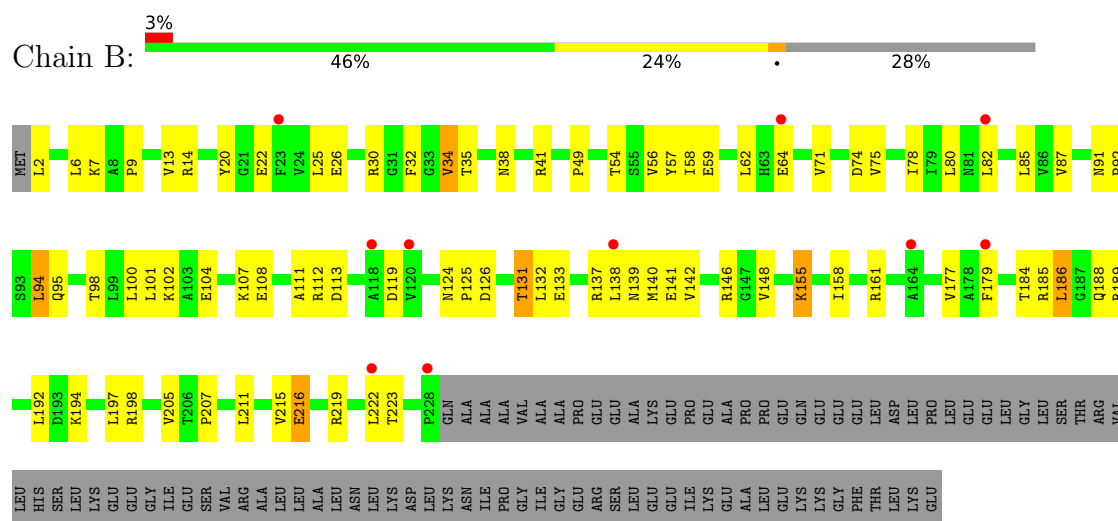
3 Residue-property plots [i](#)

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: DNA-directed RNA polymerase subunit alpha

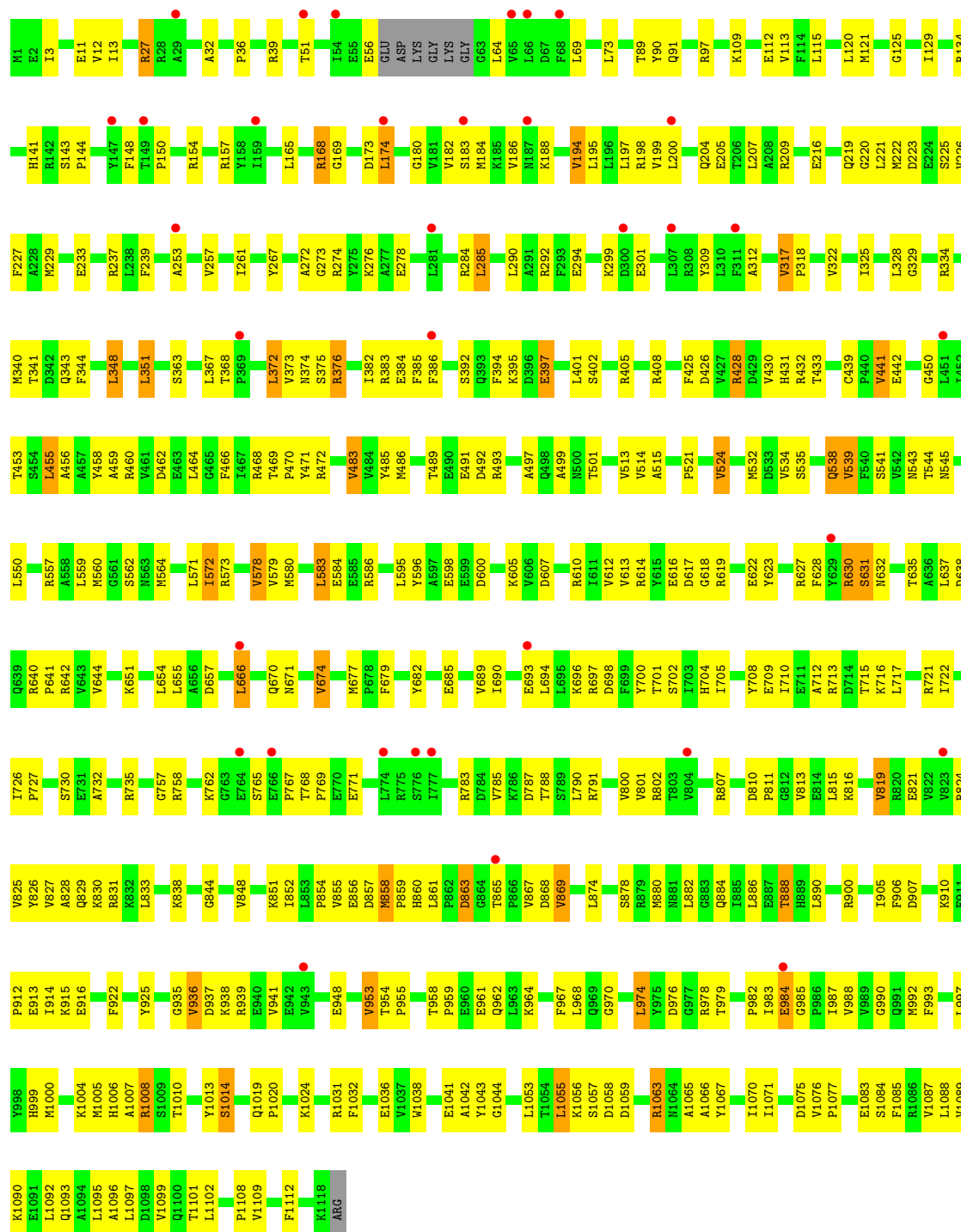


- Molecule 1: DNA-directed RNA polymerase subunit alpha

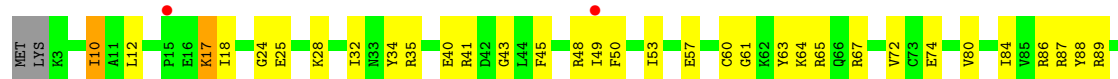


- Molecule 2: DNA-directed RNA polymerase subunit beta

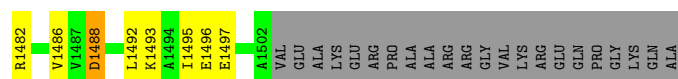




• Molecule 3: DNA-directed RNA polymerase subunit beta'



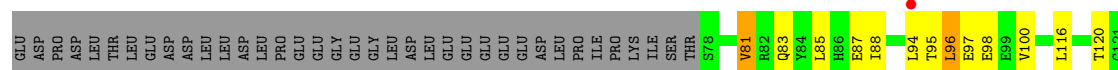
D1365	K1366	H1367	I1368	V1372	R1373	Q1374	M1375	K1376	K1377	Y1378	R1388	E1391	M1398	D1399	V1400	V1424	T1425	L1429	S1430	S1433	V1434	L1435	T1444	L1447	T1448	G1454	K1455	K1456	D1457	I1460	G1461	L1462	K1463	E1464	N1465	V1466	I1467	L1468	G1469	R1470	L1471	I1472	P1473	T1476	D1479			
ALA	ALA	D1251	T1253	Q1254	L1255	L1256	P1257	M1258	V1259	T1260	F1263	I1274	I1283	E1284	E1285	L1290	S1291	S1296	E1297	G1298	F1299	K1304	L1305	A1309	L1312	V1313	K1314	D1315	Q1334	K1339	G1340	P1341	E1342	A1343	V1344	E1345	E1350	Q1353	K1354	R1357	F1241	V1361	K1362	L1363	H1364			
L1156	G1157	V1158	L1166	S1167	M1168	D1169	D1170	V1171	H1172	I1175	E1185	V1188	R1189	L1192	T1193	C1194	R1197	Y1198	G1199	V1200	K1203	C1204	Y1205	D1208	L1209	S1210	M1211	S1216	A1220	V1221	G1222	I1223	V1224	P1232	G1233	T1234	Q1235	L1236	T1237	M1238	R1239	T1240	F1241	H1242	V1246	A1247	GLY	
P846	A849	L850	L851	A852	V853	A854	H855	G856	I857	V858	D859	D862	V863	V864	V670	S771	S774	S782	R783	D784	I785	T786	Y790	Y791	I792	T793	L880	R881	F882	V795	R796	K800	P809	L813	R818	G819	E820	I827	R828	R832	E833	T834	Q906	K908	H909	S910	L911	
V915	Y916	L920	L921	R922	G923	K926	T927	A928	R929	L930	K935	F939	T940	F941	T944	S945	G946	I947	T951	D952	K960	P977	K970	E975	E979	T984	L985	V1003	V1007	E1012	Y1021	V1022	R1029	G1030	N1031	Q1034	I1035	R1036	Q1037	L1038								
C1039	G1040	L1041	R1042	G1043	L1044	M1045	Q1046	K1047	P1048	F1053	P1056	V1057	R1062	V1067	L1068	E1069	I1072	S1073	K1079	G1080	D1083	T1084	A1085	L1086	Y1093	L1094	T1095	V1099	D1100	V1101	T1102	V1107	A1110	D1111	C1112	G1113	T1114	S1119	I1140	L1144	R1147	V1148	L1149					
L1156	G1157	V1158	L1166	S1167	M1168	D1169	D1170	V1171	H1172	I1175	E1185	V1188	R1189	L1192	T1193	C1194	R1197	Y1198	G1199	V1200	K1203	C1204	Y1205	D1208	L1209	S1210	M1211	S1216	A1220	V1221	G1222	I1223	V1224	P1232	G1233	T1234	Q1235	L1236	T1237	M1238	R1239	T1240	F1241	H1242	V1246	A1247	GLY	
H92	I93	E94	L95	A96	T97	A100	F104	D107	T114	L115	L116	D117	L118	E122	L123	E124	L127	Y128	F129	I133	V134	L135	K138	G222	L223	L227	Y236	R237	P238	L242	A243	E244	L245	P248	V258	G262	G267	A268	P269	L270	V175	L178	D181					
G182	E183	V184	E185	V186	K187	L191	A192	P193	S197	R198	L199	G201	D200	L201	Y205	R206	F207	P208	R209	R210	V211	V216	K217	L218	E219	G222	L223	L227	Y236	R237	P238	L242	A243	E244	L245	P248	V258	G262	G267	A268	P269	L270	V175	L178	D181			
D276	L284	P285	V286	G287	K288	T289	V292	V293	S197	R198	L199	G201	D200	L201	Y205	R206	F207	P208	R209	R210	V211	V216	K217	L218	E219	G222	L223	L227	Y236	R237	P238	L242	A243	E244	L245	P248	V258	G262	G267	A268	P269	L270	V175	L178	D181			
E376	V377	I378	A379	V384	V385	H386	L387	H388	E389	P390	A391	S392	L393	L394	V395	V396	K397	Y400	Y401	Y407	E408	V409	S410	T411	G412	V415	D419	V420	L421	A422	K428	S429	D430	V431	Y432	V437	V440	R441	N442	V443	V444	E448	D453	R455	M456	Q463		
L464	L465	L470	A471	A472	L473	E476	L477	L478	E479	F480	M481	K482	H483	P484	A487	R488	K491	D491	A492	R493	K494	R495	E496	E497	R500	L503	I513	P518	V519	L520	P521	P522	D523	L524	R525	P526	M527	V530	D531	R534	T537	N541	D542	L543	Y544	R545	P546	K546
I548	R549	R550	R553	L554	G560	G561	I566	I567	R568	N569	E570	R571	R572	M573	L574	V578	D579	A580	L581	L582	D583	N584	R587	R601	L607	R613	R614	R615	L616	M617	L618	L619	G620	V623	D624	Y625	R628	S629	V630	I631	V632	V633	L639	G643	L644	H645	K646	
K648	A649	L650	E651	K654	P655	F656	L657	L658	H661	K664	V670	S771	S774	S782	R783	D784	I785	T786	Y790	Y791	I792	T793	L880	R881	F882	V795	R796	K800	P809	L813	R818	G819	E820	I827	R828	R832	E833	T834	Q906	K908	H909	S910	L911					
L731	F736	F740	D741	G742	D743	Q744	M745	A746	V747	F754	M763	S771	S774	S782	R783	D784	I785	T786	Y790	Y791	I792	T793	L880	R881	F882	V795	R796	K800	P809	L813	R818	G819	E820	I827	R828	R832	E833	T834	Q906	K908	H909	S910	L911					
P846	A849	L850	L851	A852	V853	A854	H855	G856	I857	V858	D859	D862	V863	V864	V670	S771	S774	S782	R783	D784	I785	T786	Y790	Y791	I792	T793	L880	R881	F882	V795	R796	K800	P809	L813	R818	G819	E820	I827	R828	R832	E833	T834	Q906	K908	H909	S910	L911	
V915	Y916	L920	L921	R922	G923	K926	T927	A928	R929	L930	K935	F939	T940	F941	T944	S945	G946	I947	T951	D952	K960	P977	K970	E975	E979	T984	L985	V1003	V1007	E1012	Y1021	V1022	R1029	G1030	N1031	Q1034	I1035	R1036	Q1037	L1038								
C1039	G1040	L1041	R1042	G1043	L1044	M1045	Q1046	K1047	P1048	F1053	P1056	V1057	R1062	V1067	L1068	E1069	I1072	S1073	K1079	G1080	D1083	T1084	A1085	L1086	Y1093	L1094	T1095	V1099	D1100	V1101	T1102	V1107	A1110	D1111	C1112	G1113	T1114	S1119	I1140	L1144	R1147	V1148	L1149					
L1156	G1157	V1158	L1166	S1167	M1168	D1169	D1170	V1171	H1172	I1175	E1185	V1188	R1189	L1192	T1193	C1194	R1197	Y1198	G1199	V1200	K1203	C1204	Y1205	D1208	L1209	S1210	M1211	S1216	A1220	V1221	G1222	I1223	V1224	P1232	G1233	T1234	Q1235	L1236	T1237	M1238	R1239	T1240	F1241	H1242	V1246	A1247	GLY	



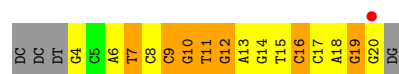
- Molecule 4: DNA-directed RNA polymerase subunit omega



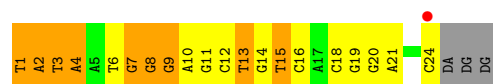
- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 6: DNA (21-MER)



- Molecule 7: DNA (27-MER)



- Molecule 8: RNA (5'-(GTP)GA-3')





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.68Å 103.89Å 294.61Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	39.76 – 3.17 39.76 – 3.17	Depositor EDS
% Data completeness (in resolution range)	94.4 (39.76-3.17) 94.4 (39.76-3.17)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.211 , 0.257 0.211 , 0.257	Depositor DCC
R_{free} test set	2014 reflections (2.26%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.957	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.025 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.025 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28769	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, 2TM, ZN, GTP

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	A	0.42	0/1841	0.65	0/2504
1	B	0.41	0/1821	0.60	0/2476
2	C	0.43	0/8938	0.65	0/12088
3	D	0.44	0/12027	0.65	1/16261 (0.0%)
4	E	0.42	0/775	0.59	0/1045
5	F	0.40	0/2849	0.60	0/3833
6	G	0.48	0/389	1.25	12/599 (2.0%)
7	H	0.51	0/556	1.12	11/858 (1.3%)
8	I	0.54	0/50	1.13	1/76 (1.3%)
All	All	0.43	0/29246	0.67	25/39740 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	3	DT	P-O3'-C3'	-9.80	105.51	120.20
7	H	15	DT	P-O3'-C3'	-9.37	106.15	120.20
6	G	15	DT	P-O3'-C3'	-8.79	107.01	120.20
6	G	14	DG	P-O3'-C3'	-8.35	107.67	120.20
6	G	9	DC	P-O3'-C3'	-8.13	108.01	120.20
6	G	17	DC	P-O3'-C3'	-7.50	108.95	120.20
6	G	16	DC	P-O3'-C3'	-7.49	108.97	120.20
6	G	11	DT	P-O3'-C3'	-7.25	109.33	120.20
6	G	19	DG	P-O3'-C3'	-6.99	109.72	120.20
7	H	13	DT	P-O3'-C3'	-6.97	109.75	120.20
7	H	8	DG	P-O3'-C3'	-6.73	110.10	120.20
8	I	6	G	P-O3'-C3'	-6.62	110.27	120.20
7	H	2	DA	P-O3'-C3'	-6.59	110.32	120.20
7	H	9	DG	P-O3'-C3'	-6.55	110.38	120.20
6	G	8	DC	P-O3'-C3'	-6.44	110.54	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	4	DA	P-O3'-C3'	-6.37	110.65	120.20
6	G	12	DG	P-O3'-C3'	-6.22	110.88	120.20
7	H	6	DT	P-O3'-C3'	-6.14	110.99	120.20
7	H	7	DG	P-O3'-C3'	-5.86	111.41	120.20
7	H	1	DT	P-O3'-C3'	-5.75	111.58	120.20
6	G	18	DA	P-O3'-C3'	-5.67	111.69	120.20
7	H	14	DG	P-O3'-C3'	-5.67	111.70	120.20
6	G	10	DG	P-O3'-C3'	-5.34	112.19	120.20
6	G	7	DT	P-O3'-C3'	-5.33	112.20	120.20
3	D	783	ARG	CB-CA-C	-5.15	110.65	116.63

There are no chirality outliers.

There are no planarity outliers.

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	A	1809	0	1863	53	0
1	B	1789	0	1841	54	0
2	C	8771	0	8868	289	0
3	D	11817	0	12044	368	0
4	E	761	0	778	15	0
5	F	2804	0	2880	68	0
6	G	347	0	192	13	0
7	H	495	0	272	27	0
8	I	77	0	34	1	0
9	B	2	0	0	0	0
9	D	3	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	D	29	0	14	4	0
12	A	3	0	0	0	0
12	B	4	0	0	1	0
12	C	19	0	0	7	0
12	D	24	0	0	2	0
12	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	F	1	0	0	0	0
12	G	5	0	0	0	0
12	H	1	0	0	0	0
12	I	3	0	0	0	0
All	All	28769	0	28786	802	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 14.

All (802) 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)
2:C:1057:SER:HA	12:C:1202:HOH:O	1.44	1.18
2:C:993:PHE:HB3	12:C:1201:HOH:O	1.46	1.15
3:D:236:TYR:CE2	3:D:322:VAL:HG21	1.95	1.02
2:C:579:VAL:HG23	12:C:1206:HOH:O	1.60	1.01
3:D:1102:THR:HG22	3:D:1222:GLY:CA	1.97	0.92
7:H:8:DG:H2''	7:H:9:DG:H5''	1.52	0.92
3:D:236:TYR:CD2	3:D:322:VAL:HG21	2.06	0.90
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.51	0.90
3:D:1102:THR:CG2	3:D:1222:GLY:CA	2.50	0.90
2:C:693:GLU:OE2	2:C:855:VAL:HG21	1.73	0.89
2:C:628:PHE:H	2:C:638:ASP:HB3	1.39	0.88
3:D:1102:THR:HG22	3:D:1222:GLY:HA3	1.57	0.86
2:C:769:PRO:HG3	3:D:65:ARG:HH12	1.40	0.86
1:B:185:ARG:HH22	3:D:692:GLU:HG3	1.42	0.84
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.60	0.83
2:C:693:GLU:HG2	2:C:696:LYS:HD2	1.59	0.82
5:F:120:THR:HG23	5:F:122:LEU:H	1.42	0.82
5:F:95:THR:HB	5:F:98:GLU:HG3	1.62	0.81
3:D:1216:SER:HB3	4:E:15:SER:HA	1.63	0.80
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.65	0.78
2:C:198:ARG:HE	2:C:227:PHE:HA	1.48	0.78
2:C:395:LYS:HD3	2:C:397:GLU:HG2	1.66	0.78
6:G:4:DG:H1	7:H:24:DC:H42	1.29	0.78
2:C:397:GLU:HG3	2:C:632:ASN:HB2	1.68	0.76
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.66	0.76
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.67	0.75
3:D:244:GLU:HG3	3:D:310:LEU:HD22	1.69	0.74
2:C:144:PRO:HB2	2:C:273:GLY:HA3	1.69	0.74
1:A:64:GLU:OE2	2:C:830:LYS:NZ	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:428:ARG:HB3	2:C:450:GLY:HA3	1.67	0.74
3:D:1102:THR:CG2	3:D:1222:GLY:HA2	2.17	0.74
5:F:316:SER:HB3	5:F:319:THR:HG23	1.69	0.74
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.68	0.74
3:D:187:LYS:HA	12:D:1701:HOH:O	1.88	0.73
2:C:32:ALA:HB2	2:C:73:LEU:HD12	1.71	0.72
5:F:395:GLU:OE2	5:F:398:ARG:NH2	2.23	0.72
2:C:274:ARG:NH2	2:C:285:LEU:O	2.23	0.71
2:C:1019:GLN:NE2	3:D:617:ASN:HB3	2.05	0.71
2:C:1019:GLN:HE22	3:D:617:ASN:HB3	1.55	0.71
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.72	0.71
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.23	0.71
6:G:9:DC:H2'	6:G:10:DG:C8	2.25	0.71
6:G:12:DG:H2'	6:G:13:DA:C8	2.26	0.71
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.73	0.70
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.74	0.70
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.74	0.69
2:C:344:PHE:CD2	2:C:382:ILE:HD11	2.29	0.68
7:H:9:DG:H2''	7:H:10:DA:C8	2.28	0.68
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.75	0.68
2:C:13:ILE:HD13	2:C:483:VAL:HG21	1.75	0.68
2:C:605:LYS:HD3	2:C:610:ARG:HH12	1.59	0.68
2:C:1067:TYR:OH	3:D:674[A]:ARG:NH1	2.27	0.68
5:F:116:LEU:O	5:F:120:THR:HG22	1.94	0.68
3:D:695:ILE:HD12	3:D:718:PRO:HG2	1.75	0.68
3:D:661:MET:HE1	3:D:677:LEU:HD11	1.76	0.67
2:C:674:VAL:HG22	2:C:869:VAL:HG22	1.75	0.67
3:D:243:ALA:HB3	3:D:311:LEU:HD11	1.75	0.67
3:D:677:LEU:HD21	3:D:687:VAL:HG21	1.75	0.67
5:F:172:ARG:O	5:F:176:ILE:HG12	1.95	0.67
3:D:65:ARG:NH1	5:F:378:GLY:O	2.27	0.67
2:C:758:ARG:HH21	2:C:788:THR:HB	1.61	0.66
1:B:132:LEU:HD21	1:B:138:LEU:HB2	1.78	0.66
3:D:1102:THR:HG21	3:D:1222:GLY:O	1.96	0.66
3:D:1144:LEU:O	3:D:1147:ARG:HG3	1.96	0.66
3:D:236:TYR:HE2	3:D:322:VAL:HG21	1.58	0.66
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.78	0.66
3:D:18:ILE:HD13	3:D:518:PRO:HG3	1.76	0.65
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.76	0.65
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.61	0.65
7:H:3:DT:H2'	7:H:4:DA:C8	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:706:PRO:HB2	3:D:708:LEU:HD21	1.78	0.65
2:C:150:PRO:HG3	2:C:322:VAL:HG21	1.77	0.65
2:C:204:GLN:NE2	2:C:222:MET:SD	2.69	0.65
2:C:859:PRO:O	2:C:867:VAL:HG22	1.97	0.65
7:H:12:DC:H1'	7:H:13:DT:C4	2.32	0.65
2:C:545:ASN:HB3	2:C:583:LEU:HD12	1.79	0.64
1:B:20:TYR:C	1:B:207:PRO:HG2	2.22	0.64
2:C:501:THR:HG21	2:C:513:VAL:HG13	1.80	0.64
2:C:612:VAL:HG22	2:C:622:GLU:HG3	1.78	0.64
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.32	0.64
2:C:726:ILE:HD11	2:C:757:GLY:HA3	1.80	0.64
3:D:889:ALA:HB1	3:D:930:LEU:HA	1.80	0.64
3:D:1102:THR:CG2	3:D:1222:GLY:C	2.71	0.63
2:C:999:HIS:HB3	2:C:1004:LYS:NZ	2.13	0.63
2:C:557:ARG:HG3	2:C:844:GLY:HA3	1.79	0.63
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.80	0.63
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.79	0.63
3:D:135:LEU:HD13	3:D:463:GLN:HG2	1.81	0.63
3:D:258:VAL:HG12	3:D:273:ARG:O	1.99	0.63
3:D:542:ASP:OD2	3:D:545:ARG:NH2	2.32	0.63
3:D:1236:LEU:HD12	3:D:1252:ILE:HD13	1.80	0.63
2:C:878:SER:HA	3:D:1034:GLN:OE1	1.99	0.63
3:D:573:MET:SD	5:F:210:LEU:HB3	2.39	0.63
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.81	0.62
3:D:133:ILE:HG13	3:D:152:LEU:HD12	1.80	0.62
3:D:208:PRO:HA	3:D:390:PRO:HA	1.80	0.62
3:D:1094:LEU:HD22	3:D:1260:ILE:HG12	1.80	0.62
3:D:1492:LEU:HD22	4:E:74:VAL:HG21	1.79	0.62
2:C:628:PHE:H	2:C:638:ASP:CB	2.12	0.62
3:D:838:ARG:NH1	3:D:874:GLU:OE1	2.31	0.62
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.82	0.62
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.82	0.62
2:C:1063:ARG:NH1	12:C:1202:HOH:O	2.31	0.61
3:D:645:PRO:HB3	3:D:723:GLY:O	2.00	0.61
3:D:657:LEU:O	3:D:661:MET:HB2	1.99	0.61
3:D:1199:GLY:O	3:D:1373:ARG:NH1	2.25	0.61
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.00	0.61
2:C:468:ARG:HA	2:C:486:MET:O	2.00	0.61
2:C:1071:ILE:HD11	5:F:345:ALA:HB1	1.82	0.61
3:D:683:ILE:HG23	3:D:687:VAL:HG11	1.82	0.61
3:D:828:LYS:HA	3:D:833:GLU:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:915:LYS:NZ	2:C:968:LEU:O	2.25	0.61
3:D:116:LEU:HB2	3:D:118:LEU:HD12	1.83	0.61
3:D:1372:VAL:HA	3:D:1375:MET:HG3	1.83	0.61
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.82	0.60
2:C:197:LEU:HD12	2:C:221:LEU:HD11	1.81	0.60
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.31	0.60
3:D:1211:MET:HE1	4:E:16:LYS:HD2	1.82	0.60
5:F:368:VAL:HG21	5:F:400:ILE:HD11	1.82	0.60
1:B:92:PRO:O	1:B:146:ARG:NH2	2.32	0.60
5:F:85:LEU:HB3	7:H:7:DG:N3	2.17	0.60
3:D:244:GLU:HG3	3:D:310:LEU:CD2	2.32	0.60
3:D:1102:THR:HG22	3:D:1222:GLY:C	2.27	0.60
4:E:45:ARG:NH1	4:E:63:TRP:HH2	2.00	0.60
1:A:31:GLY:N	1:A:193:ASP:OD1	2.35	0.60
3:D:248:PRO:HG3	3:D:308:LYS:HG3	1.83	0.60
2:C:578:VAL:HG12	2:C:671:ASN:OD1	2.01	0.59
3:D:116:LEU:HD21	3:D:465:LEU:HD23	1.83	0.59
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.83	0.59
2:C:910:LYS:O	2:C:914:ILE:HG13	2.02	0.59
3:D:270:LEU:HD12	3:D:284:LEU:HD11	1.83	0.59
1:A:25:LEU:HD23	1:A:28:LEU:HD11	1.85	0.59
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.37	0.59
1:A:185:ARG:NH2	1:A:187:GLY:O	2.35	0.59
2:C:550:LEU:HD23	2:C:906:PHE:HE2	1.66	0.59
3:D:456:MET:HE1	3:D:568:ARG:NE	2.17	0.59
2:C:882:LEU:HD11	3:D:1038:LEU:HD22	1.84	0.59
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.84	0.59
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.85	0.59
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.84	0.59
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.38	0.59
1:B:107:LYS:NZ	1:B:113:ASP:OD1	2.25	0.59
3:D:245:LEU:HD21	3:D:311:LEU:HD21	1.84	0.59
3:D:1240:THR:CG2	12:D:1706:HOH:O	2.51	0.59
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.38	0.58
1:A:154:GLU:CD	1:A:154:GLU:H	2.10	0.58
2:C:922:PHE:CD2	2:C:964:LYS:HG3	2.38	0.58
3:D:142:LEU:HB2	3:D:161:LEU:HD21	1.85	0.58
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.86	0.58
2:C:272:ALA:HA	2:C:464:LEU:HD23	1.85	0.58
2:C:578:VAL:HA	2:C:900:ARG:HG2	1.85	0.58
7:H:10:DA:H2"	7:H:11:DG:OP1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:329:GLY:HA3	2:C:489:THR:HG23	1.85	0.58
3:D:1046:GLN:NE2	3:D:1246:VAL:O	2.37	0.58
3:D:1462:LEU:HD23	3:D:1473:PRO:HD2	1.85	0.58
5:F:237:THR:HG21	7:H:3:DT:H5'	1.86	0.58
1:B:98:THR:CG2	12:B:501:HOH:O	2.52	0.58
2:C:614:ARG:NH2	2:C:618:GLY:O	2.36	0.58
2:C:958:THR:N	2:C:961:GLU:OE1	2.24	0.58
2:C:878:SER:HB2	3:D:1029:ARG:HD2	1.86	0.57
2:C:1056:LYS:HB2	3:D:623:VAL:HG22	1.86	0.57
2:C:816:LYS:O	2:C:819:VAL:HG13	2.04	0.57
2:C:1093:GLN:O	2:C:1096:ALA:N	2.35	0.57
3:D:169:TYR:O	3:D:392:SER:HB2	2.04	0.57
7:H:10:DA:H2'	7:H:11:DG:C8	2.38	0.57
3:D:1479:ASP:OD1	3:D:1482:ARG:NH2	2.35	0.57
1:B:85:LEU:HA	1:B:124:ASN:HD21	1.70	0.57
2:C:700:TYR:CB	2:C:833:LEU:HD22	2.35	0.57
2:C:700:TYR:HB2	2:C:833:LEU:HD22	1.87	0.57
2:C:1059:ASP:O	2:C:1063:ARG:HB3	2.05	0.57
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.24	0.57
3:D:876:SER:OG	3:D:879:ARG:HG3	2.05	0.57
7:H:12:DC:H1'	7:H:13:DT:C5	2.39	0.57
3:D:200:ASP:O	3:D:397:LYS:HG2	2.05	0.57
3:D:353:VAL:HG12	3:D:355:VAL:H	1.69	0.57
7:H:15:DT:H2'	7:H:16:DC:C6	2.39	0.57
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.87	0.57
2:C:115:LEU:O	2:C:375:SER:HB2	2.04	0.57
1:A:6:LEU:HD23	1:A:7:LYS:H	1.68	0.57
3:D:411:THR:O	5:F:178:ARG:NH1	2.33	0.57
6:G:19:DG:H2'	6:G:20:DG:C8	2.39	0.57
2:C:1043:TYR:CD1	3:D:763:MET:HE3	2.40	0.56
3:D:298:VAL:HG12	3:D:302:GLN:NE2	2.20	0.56
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.37	0.56
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.40	0.56
2:C:884:GLN:O	2:C:888:THR:OG1	2.23	0.56
3:D:1444:THR:O	3:D:1448:THR:HG23	2.05	0.56
11:D:1606:2TM:H10	11:D:1606:2TM:C5'	2.35	0.56
1:A:41:ARG:HA	1:A:177:VAL:HG11	1.86	0.56
3:D:534:ARG:NH2	5:F:313:GLU:O	2.38	0.56
3:D:1434:TRP:HB3	3:D:1455:LYS:HD2	1.88	0.56
1:A:72:LYS:HG3	2:C:641:PRO:HG2	1.87	0.56
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.41	0.56
3:D:415:VAL:HG13	3:D:419:ASP:HB2	1.88	0.56
3:D:553:ARG:HD2	3:D:570:GLU:CD	2.30	0.56
1:A:209:GLU:O	1:A:213:GLN:HG2	2.06	0.56
3:D:1102:THR:HG21	3:D:1222:GLY:C	2.31	0.56
1:B:186:LEU:HB2	1:B:192:LEU:HD12	1.86	0.56
3:D:684:LYS:O	3:D:687:VAL:HG12	2.05	0.56
3:D:1296:SER:HB3	3:D:1299:PHE:HB2	1.87	0.55
1:B:59:GLU:CD	1:B:139:ASN:HD22	2.15	0.55
2:C:1092:LEU:HD22	2:C:1097:LEU:HD12	1.89	0.55
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.39	0.55
3:D:1031:ASN:ND2	3:D:1034:GLN:HE21	2.04	0.55
3:D:1111:ASP:OD1	3:D:1189:ARG:NH2	2.40	0.55
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.88	0.55
2:C:690:ILE:HB	2:C:694:LEU:HD12	1.88	0.55
3:D:941:PHE:O	3:D:945:SER:HB3	2.06	0.55
3:D:1101:VAL:O	3:D:1374:GLN:HG3	2.06	0.55
2:C:36:PRO:HA	2:C:39:ARG:HG3	1.88	0.55
2:C:880:MET:SD	3:D:1037:GLN:NE2	2.80	0.55
2:C:1055:LEU:HD13	2:C:1066:ALA:HB2	1.89	0.55
2:C:627:ARG:NH1	2:C:640:ARG:HG2	2.21	0.55
3:D:975:GLU:O	3:D:979:GLU:HG2	2.07	0.55
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.89	0.55
2:C:1087:VAL:HG22	3:D:524:LEU:HD22	1.88	0.54
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.43	0.54
1:B:112:ARG:NH2	1:B:126:ASP:OD2	2.26	0.54
2:C:689:VAL:HG13	2:C:851:LYS:HB3	1.88	0.54
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.90	0.54
2:C:344:PHE:HD2	2:C:382:ILE:HD11	1.70	0.54
2:C:455:LEU:HD22	2:C:459:ALA:HB3	1.90	0.54
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.89	0.54
2:C:27:ARG:NH2	2:C:27:ARG:HB3	2.23	0.54
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.89	0.54
3:D:208:PRO:HG3	3:D:387:LEU:HD22	1.90	0.54
3:D:916:TYR:CZ	3:D:920:LEU:HD11	2.43	0.54
5:F:256:ARG:HD3	5:F:260:ILE:HD12	1.88	0.54
7:H:12:DC:H2"	7:H:13:DT:OP2	2.08	0.54
3:D:869:MET:O	3:D:871:LYS:HG3	2.07	0.54
2:C:226:VAL:HA	2:C:229:MET:HE2	1.89	0.54
3:D:236:TYR:CD2	3:D:322:VAL:CG2	2.86	0.54
3:D:633:VAL:HB	3:D:740:PHE:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:1606:2TM:H10	11:D:1606:2TM:H1	1.90	0.54
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.90	0.54
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.43	0.54
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.08	0.54
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.39	0.54
2:C:1085:PHE:CE2	2:C:1088:LEU:HD23	2.43	0.54
3:D:657:LEU:HG	3:D:661:MET:CE	2.37	0.54
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.90	0.54
2:C:134:ARG:NH1	2:C:392:SER:O	2.39	0.53
1:A:176:ARG:HG3	1:A:177:VAL:N	2.23	0.53
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.89	0.53
2:C:205:GLU:O	2:C:209:ARG:HG2	2.08	0.53
7:H:18:DC:H2'	7:H:19:DG:C8	2.42	0.53
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.08	0.53
1:B:102:LYS:HG2	1:B:139:ASN:OD1	2.07	0.53
2:C:499:ALA:HA	2:C:532:MET:HE3	1.90	0.53
2:C:572:ILE:HG13	2:C:573:ARG:HG3	1.90	0.53
2:C:713:ARG:HA	2:C:819:VAL:HA	1.90	0.53
2:C:984:GLU:HB2	3:D:944:THR:O	2.09	0.53
3:D:487:ALA:O	3:D:491:LYS:HG2	2.08	0.53
1:A:46:SER:O	1:A:47:SER:HB2	2.08	0.53
2:C:890:LEU:HD13	2:C:914:ILE:HG23	1.90	0.53
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.90	0.53
2:C:861:LEU:HD12	2:C:865:THR:HB	1.91	0.53
3:D:629:SER:OG	3:D:630:VAL:N	2.37	0.53
3:D:1046:GLN:NE2	3:D:1247:ALA:HA	2.24	0.53
2:C:598:GLU:O	2:C:651:LYS:NZ	2.41	0.53
2:C:829:GLN:OE1	2:C:831:ARG:NH2	2.42	0.53
2:C:856:GLU:HG2	2:C:857:ASP:OD1	2.08	0.52
2:C:708:TYR:HB3	2:C:790:LEU:HD21	1.91	0.52
2:C:1042:ALA:HB3	3:D:710:ARG:HB2	1.91	0.52
3:D:270:LEU:HD13	3:D:304:LEU:HD13	1.91	0.52
7:H:15:DT:H2''	7:H:16:DC:H5'	1.91	0.52
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.27	0.52
2:C:888:THR:HG22	2:C:990:GLY:HA3	1.90	0.52
3:D:34:TYR:CE2	5:F:261:PRO:HD2	2.44	0.52
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.28	0.52
1:A:4:SER:HA	1:A:189:ARG:HH22	1.75	0.52
2:C:607:ASP:HB3	2:C:610:ARG:HG2	1.92	0.52
1:A:133:GLU:OE2	2:C:605:LYS:HB3	2.09	0.52
3:D:646:LYS:HB3	3:D:688:TRP:CZ3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.91	0.52
3:D:795:VAL:HG12	3:D:876:SER:HB3	1.91	0.52
3:D:945:SER:OG	3:D:947:ILE:HG12	2.10	0.52
3:D:1080:GLY:O	3:D:1084:THR:HG23	2.09	0.52
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.45	0.52
2:C:705:ILE:HG12	2:C:828:ALA:HB2	1.92	0.52
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.92	0.52
2:C:1053:LEU:CD1	3:D:1466:VAL:HG13	2.40	0.52
3:D:28:LYS:O	3:D:43:GLY:HA2	2.10	0.52
3:D:236:TYR:CE1	3:D:242:LEU:HD12	2.44	0.52
3:D:654:LYS:O	3:D:658:LEU:HG	2.10	0.52
3:D:828:LYS:HZ3	3:D:833:GLU:HB3	1.75	0.52
3:D:1197:ARG:HD2	3:D:1398:TRP:CE2	2.45	0.52
2:C:173:ASP:O	2:C:184:MET:HA	2.09	0.51
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.92	0.51
3:D:771:SER:HB2	3:D:778:LEU:HD22	1.92	0.51
4:E:9:LEU:HD13	4:E:65:MET:HE2	1.92	0.51
2:C:27:ARG:HB3	2:C:27:ARG:HH21	1.74	0.51
3:D:373:PRO:HA	3:D:376:GLU:HG3	1.93	0.51
3:D:785:ILE:HD13	3:D:935:LYS:HA	1.92	0.51
3:D:222:GLY:HA2	3:D:333:LEU:O	2.11	0.51
1:A:156:HIS:NE2	1:A:167:VAL:O	2.36	0.51
1:B:58:ILE:HG12	1:B:140:MET:HE2	1.92	0.51
1:B:64:GLU:O	1:B:75:VAL:HB	2.10	0.51
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.92	0.51
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.91	0.51
3:D:243:ALA:HB3	3:D:311:LEU:CD1	2.41	0.51
3:D:397:LYS:O	3:D:448:GLU:HG2	2.11	0.51
2:C:682:TYR:CZ	2:C:851:LYS:HE2	2.46	0.51
2:C:722:ILE:HD12	2:C:821:GLU:HG3	1.93	0.51
2:C:1085:PHE:HE2	2:C:1088:LEU:HD23	1.74	0.51
3:D:911:LEU:O	3:D:915:VAL:HG23	2.11	0.51
4:E:52:GLU:OE1	4:E:52:GLU:N	2.39	0.51
5:F:195:VAL:HG13	5:F:216:GLY:HA3	1.93	0.51
7:H:19:DG:H2"	7:H:20:DG:C8	2.46	0.51
2:C:1008:ARG:NH1	3:D:624:ASP:OD1	2.40	0.51
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.92	0.51
3:D:657:LEU:HG	3:D:661:MET:HE2	1.92	0.51
3:D:1149:LEU:HG	3:D:1166:LEU:HD21	1.92	0.51
2:C:948:GLU:HG3	2:C:953:VAL:HG23	1.91	0.50
5:F:383:LEU:HD12	5:F:394:ARG:NH2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:686:GLU:CD	3:D:686:GLU:H	2.18	0.50
3:D:696:HIS:ND1	4:E:57:ASP:OD1	2.44	0.50
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.27	0.50
3:D:1156:LEU:O	3:D:1158:VAL:HG23	2.11	0.50
5:F:392:VAL:HG13	5:F:396:ARG:HB3	1.92	0.50
1:A:9:PRO:HB3	1:A:26:GLU:C	2.36	0.50
1:B:38:ASN:ND2	2:C:979:THR:HA	2.26	0.50
2:C:441:VAL:HG11	2:C:544:THR:HG21	1.93	0.50
3:D:1168:MET:HE3	3:D:1171:VAL:HB	1.93	0.50
2:C:539:VAL:HG21	3:D:1067:VAL:HG11	1.94	0.50
2:C:223:ASP:OD1	2:C:225:SER:OG	2.26	0.50
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.46	0.50
3:D:530:VAL:HG12	3:D:531:ASP:H	1.76	0.50
3:D:882:PHE:O	3:D:886:VAL:HG23	2.12	0.50
5:F:181:GLU:O	5:F:185:GLN:HG2	2.12	0.50
2:C:401:LEU:HD21	2:C:543:ASN:ND2	2.27	0.50
3:D:472:ALA:O	3:D:476:GLU:HG2	2.11	0.50
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.93	0.50
2:C:712:ALA:HB3	2:C:821:GLU:HG2	1.93	0.50
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.11	0.50
3:D:1220:ALA:O	3:D:1224:VAL:HG23	2.11	0.50
1:B:108:GLU:HG2	1:B:131:THR:HB	1.93	0.50
1:A:82:LEU:HD21	1:A:140:MET:HE1	1.94	0.49
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.93	0.49
3:D:45:PHE:HZ	3:D:541:ASN:HD21	1.60	0.49
3:D:631:ILE:HD11	3:D:743:ASP:HB2	1.94	0.49
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.47	0.49
3:D:1110:ALA:O	3:D:1203:LYS:HG2	2.11	0.49
4:E:37:ASN:OD1	4:E:37:ASN:N	2.44	0.49
5:F:81:VAL:O	5:F:85:LEU:HG	2.12	0.49
2:C:807:ARG:HB2	2:C:810:ASP:OD2	2.11	0.49
3:D:41:ARG:HE	3:D:48:ARG:CZ	2.25	0.49
3:D:493:ARG:O	3:D:497:GLU:HG3	2.11	0.49
3:D:851:LEU:O	3:D:855:HIS:HD2	1.95	0.49
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.94	0.49
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.26	0.49
2:C:521:PRO:HG2	3:D:1072:ILE:HD11	1.94	0.49
3:D:970:LYS:HD3	3:D:995:LEU:HD13	1.94	0.49
2:C:278:GLU:HG2	2:C:284:ARG:HA	1.94	0.49
2:C:571:LEU:HD22	2:C:700:TYR:HA	1.93	0.49
7:H:12:DC:OP2	7:H:12:DC:H3'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TYR:CE1	1:A:161:ARG:HD2	2.47	0.49
3:D:288:MET:SD	3:D:307:ALA:HB2	2.52	0.49
3:D:1200:VAL:HG23	3:D:1373:ARG:NH1	2.27	0.49
5:F:135:ILE:HG13	5:F:181:GLU:HB2	1.94	0.49
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.95	0.49
1:A:155:LYS:O	1:A:155:LYS:HE3	2.12	0.49
2:C:829:GLN:OE1	2:C:831:ARG:NE	2.46	0.49
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.48	0.49
3:D:800:LYS:HE3	3:D:819:GLY:O	2.13	0.49
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.94	0.48
3:D:926:LYS:HG2	3:D:929:ARG:NH2	2.28	0.48
4:E:12:MET:HE1	4:E:69:LEU:HA	1.95	0.48
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.47	0.48
3:D:481:MET:HE1	3:D:1391:GLU:HB3	1.94	0.48
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.47	0.48
6:G:6:DA:H2''	6:G:7:DT:C5'	2.43	0.48
1:A:181:VAL:HG12	2:C:938:LYS:HD2	1.96	0.48
2:C:564:MET:SD	2:C:997:LEU:HD11	2.54	0.48
2:C:580:MET:HB3	2:C:584:GLU:CD	2.38	0.48
2:C:704:HIS:CE1	2:C:1000:MET:HE1	2.48	0.48
2:C:1053:LEU:HD13	3:D:1466:VAL:HG13	1.94	0.48
2:C:469:THR:OG1	2:C:538:GLN:NE2	2.46	0.48
1:A:97:VAL:HG12	1:A:99:LEU:HD12	1.95	0.48
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.49	0.48
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.14	0.48
5:F:95:THR:O	5:F:98:GLU:N	2.47	0.48
1:B:41:ARG:HG3	1:B:177:VAL:HG12	1.94	0.48
3:D:209:ARG:HG2	3:D:389:GLU:O	2.14	0.48
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.47	0.48
3:D:818:ARG:HE	3:D:820:GLU:CD	2.21	0.48
5:F:271:LEU:HA	5:F:295:MET:HE1	1.94	0.48
7:H:3:DT:H2''	7:H:4:DA:H5'	1.95	0.48
2:C:11:GLU:HG2	2:C:535:SER:HB2	1.94	0.48
3:D:1232:PRO:HB3	3:D:1361:VAL:HG11	1.95	0.48
3:D:1263:PHE:HA	3:D:1375:MET:HE1	1.96	0.48
1:B:85:LEU:HG	1:B:87:VAL:HG23	1.96	0.48
2:C:937:ASP:OD1	2:C:938:LYS:N	2.47	0.48
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.94	0.48
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.95	0.48
3:D:45:PHE:O	3:D:86:ARG:NH2	2.47	0.48
5:F:237:THR:HG21	7:H:3:DT:C5'	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:560:MET:O	2:C:564:MET:HG3	2.14	0.48
2:C:600:ASP:O	2:C:616:GLU:HG2	2.14	0.48
2:C:1010:THR:HA	3:D:624:ASP:OD1	2.14	0.48
3:D:367:ILE:HD11	3:D:379:ALA:HB2	1.96	0.48
3:D:846:PRO:HB3	3:D:880:ILE:CG2	2.43	0.48
3:D:882:PHE:CE1	3:D:906:GLN:HG3	2.49	0.48
3:D:1493:LYS:HZ2	3:D:1496:GLU:HG2	1.79	0.48
5:F:192:LEU:HD23	5:F:220:LEU:HD23	1.96	0.48
6:G:6:DA:H2'	6:G:7:DT:C6	2.49	0.48
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.46	0.47
3:D:227:LEU:HD13	3:D:331:VAL:CG2	2.44	0.47
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.49	0.47
3:D:1255:GLY:O	3:D:1259:VAL:HG23	2.13	0.47
1:A:193:ASP:OD2	2:C:938:LYS:NZ	2.42	0.47
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.47	0.47
5:F:184:ARG:O	5:F:188:ILE:HG13	2.14	0.47
2:C:471:TYR:OH	2:C:491:GLU:OE1	2.30	0.47
3:D:1012:GLU:HB2	3:D:1021:TYR:OH	2.15	0.47
3:D:1205:TYR:O	3:D:1366:LYS:HD3	2.13	0.47
2:C:1031:ARG:NE	6:G:16:DC:OP1	2.44	0.47
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.95	0.47
2:C:408:ARG:NH1	2:C:456:ALA:O	2.47	0.47
7:H:9:DG:H2''	7:H:10:DA:N7	2.29	0.47
2:C:693:GLU:CD	2:C:855:VAL:HG21	2.37	0.47
2:C:726:ILE:HD11	2:C:757:GLY:CA	2.45	0.47
2:C:913:GLU:HA	2:C:916:GLU:CD	2.40	0.47
3:D:371:ILE:HG21	5:F:232:ARG:NH1	2.29	0.47
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.50	0.47
3:D:782:SER:HA	3:D:786:ILE:HD12	1.97	0.47
1:A:41:ARG:NE	1:A:177:VAL:O	2.34	0.47
1:B:94:LEU:HD23	1:B:95:GLN:H	1.79	0.47
2:C:351:LEU:HD12	2:C:374:ASN:O	2.15	0.47
2:C:838:LYS:HE3	3:D:741:ASP:O	2.15	0.47
2:C:999:HIS:HB3	2:C:1004:LYS:HZ1	1.76	0.47
3:D:223:LEU:HD11	3:D:288:MET:HE1	1.96	0.47
3:D:479:GLU:HA	3:D:482:LYS:HE2	1.97	0.47
3:D:648:MET:HE1	3:D:726:ILE:HD11	1.97	0.47
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.97	0.47
3:D:1167:SER:O	3:D:1171:VAL:HG23	2.15	0.47
5:F:96:LEU:O	5:F:100:VAL:HG23	2.14	0.47
5:F:367:MET:HB3	5:F:390:PHE:HZ	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.96	0.47
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	1.96	0.47
2:C:351:LEU:HD11	2:C:373:VAL:HG13	1.97	0.47
2:C:811:PRO:O	2:C:813:VAL:HG23	2.15	0.47
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.25	0.47
3:D:1205:TYR:CE1	3:D:1366:LYS:HD2	2.49	0.47
6:G:19:DG:O5'	6:G:19:DG:H8	1.97	0.47
2:C:513:VAL:HB	2:C:524:VAL:O	2.15	0.47
3:D:581:LEU:HG	3:D:582:LEU:HD23	1.96	0.47
3:D:706:PRO:HB2	3:D:708:LEU:CD2	2.44	0.47
3:D:138:LYS:NZ	3:D:453:ASP:HB2	2.30	0.46
3:D:1291:SER:OG	3:D:1304:LYS:HG2	2.15	0.46
3:D:1341:PRO:HB3	3:D:1376:MET:HE2	1.98	0.46
4:E:14:ASP:OD2	4:E:18:ARG:NH1	2.42	0.46
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.97	0.46
2:C:642:ARG:HG3	2:C:654:LEU:HD21	1.98	0.46
2:C:1008:ARG:CZ	2:C:1020:PRO:HB3	2.45	0.46
3:D:100:ALA:HA	3:D:513:ILE:HD13	1.97	0.46
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.22	0.46
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.15	0.46
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.51	0.46
2:C:382:ILE:O	2:C:383:ARG:C	2.58	0.46
1:A:99:LEU:HD21	1:A:122:ILE:HD11	1.96	0.46
1:B:6:LEU:HD12	1:B:7:LYS:H	1.80	0.46
2:C:144:PRO:HB2	2:C:273:GLY:CA	2.43	0.46
2:C:974:LEU:HD12	2:C:974:LEU:HA	1.79	0.46
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.96	0.46
2:C:583:LEU:HA	2:C:583:LEU:HD23	1.66	0.46
2:C:595:LEU:HD11	2:C:623:TYR:HB3	1.97	0.46
2:C:1032:PHE:CZ	2:C:1036:GLU:HB3	2.49	0.46
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.96	0.46
1:A:70:GLY:N	2:C:607:ASP:OD1	2.48	0.46
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.97	0.46
3:D:57:GLU:HA	3:D:64:LYS:HA	1.97	0.46
1:B:223:THR:HG22	1:B:223:THR:O	2.16	0.46
3:D:1234:THR:HG22	3:D:1238:MET:HE2	1.97	0.46
2:C:888:THR:HG22	2:C:990:GLY:CA	2.45	0.46
3:D:1463:LYS:HE2	3:D:1463:LYS:HB3	1.56	0.46
2:C:180:GLY:O	2:C:220:GLY:HA3	2.15	0.46
2:C:372:LEU:HD12	2:C:372:LEU:HA	1.69	0.46
2:C:497:ALA:HA	2:C:515:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:THR:OG1	2:C:348:LEU:HB3	2.16	0.46
2:C:276:LYS:HD2	2:C:466:PHE:HZ	1.81	0.46
2:C:1067:TYR:O	2:C:1071:ILE:HG12	2.15	0.46
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.51	0.46
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.98	0.46
2:C:97:ARG:HG3	2:C:112:GLU:HG3	1.98	0.45
2:C:1042:ALA:HB1	3:D:1224:VAL:HG22	1.98	0.45
3:D:134:VAL:HG22	3:D:151:GLN:O	2.16	0.45
3:D:708:LEU:N	3:D:708:LEU:HD23	2.29	0.45
1:A:228:PRO:HB3	1:B:13:VAL:HG21	1.96	0.45
2:C:294:GLU:HB3	2:C:299:LYS:HE2	1.97	0.45
3:D:154:THR:OG1	3:D:157:GLU:HG3	2.15	0.45
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.98	0.45
3:D:1263:PHE:HD2	3:D:1375:MET:HE2	1.81	0.45
1:A:20:TYR:C	1:A:207:PRO:HG2	2.41	0.45
2:C:148:PHE:CZ	2:C:309:TYR:HB3	2.51	0.45
2:C:453:THR:HG22	12:C:1205:HOH:O	2.16	0.45
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.17	0.45
5:F:83:GLN:O	5:F:87:GLU:HG3	2.17	0.45
2:C:223:ASP:OD1	2:C:226:VAL:HG23	2.17	0.45
2:C:405:ARG:HD2	2:C:442:GLU:CD	2.42	0.45
2:C:596:TYR:O	2:C:655:LEU:HD12	2.16	0.45
3:D:178:LEU:HG	3:D:193:PRO:HD3	1.98	0.45
3:D:242:LEU:HB3	3:D:311:LEU:O	2.17	0.45
3:D:643:GLY:HA3	3:D:727:GLN:HG3	1.98	0.45
3:D:790:TYR:CD1	3:D:1022:VAL:HG13	2.52	0.45
3:D:813:LEU:HD21	3:D:840:LYS:HA	1.97	0.45
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	1.98	0.45
3:D:349:PRO:HB3	5:F:97:GLU:HG3	1.99	0.45
5:F:158:GLU:O	5:F:162:LYS:HG3	2.16	0.45
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.97	0.45
1:A:41:ARG:NH1	2:C:860:HIS:CE1	2.83	0.45
1:A:159:LYS:HG2	1:A:164:ALA:O	2.17	0.45
2:C:385:PHE:HD2	2:C:386:PHE:CD1	2.34	0.45
2:C:1014:SER:N	2:C:1019:GLN:O	2.50	0.45
3:D:916:TYR:CE1	3:D:920:LEU:HD11	2.52	0.45
3:D:1172:HIS:HA	3:D:1175:ILE:HD12	1.99	0.45
4:E:50:THR:HG22	4:E:51:LEU:H	1.81	0.45
1:A:112:ARG:HG2	1:A:125:PRO:O	2.17	0.45
2:C:432:ARG:HH22	2:C:492:ASP:CG	2.25	0.45
2:C:584:GLU:HB3	2:C:666:LEU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:219:GLU:HB2	3:D:339:TRP:CZ3	2.52	0.45
3:D:554:LEU:HD13	3:D:570:GLU:HB3	1.99	0.45
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.52	0.45
2:C:825:VAL:HG12	2:C:827:VAL:HG23	1.99	0.45
3:D:1457:ASP:OD1	3:D:1464:GLU:HG2	2.16	0.45
5:F:386:VAL:HG12	5:F:397:ILE:HG12	1.99	0.45
2:C:290:LEU:O	2:C:301:GLU:HB2	2.17	0.45
2:C:685:GLU:HA	2:C:685:GLU:OE1	2.17	0.45
3:D:527:MET:HE2	3:D:527:MET:HB2	1.82	0.45
3:D:867:ARG:HA	3:D:871:LYS:O	2.17	0.45
1:B:32:PHE:HA	1:B:35:THR:HB	1.99	0.44
2:C:121:MET:SD	2:C:125:GLY:HA2	2.57	0.44
2:C:1007:ALA:O	3:D:651:GLU:HG2	2.17	0.44
3:D:10:ILE:O	3:D:1454:GLY:HA2	2.17	0.44
1:A:182:GLU:OE1	2:C:935:GLY:N	2.49	0.44
1:B:74:ASP:O	1:B:78:ILE:HG13	2.17	0.44
2:C:677:MET:HE2	2:C:679:PHE:HD1	1.82	0.44
3:D:286:VAL:O	3:D:311:LEU:HA	2.17	0.44
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.99	0.44
2:C:769:PRO:HG3	3:D:65:ARG:NH1	2.20	0.44
2:C:1057:SER:O	2:C:1058:ASP:HB2	2.16	0.44
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.50	0.44
3:D:1083:ASP:HB3	3:D:1253:THR:HG21	1.99	0.44
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	2.00	0.44
3:D:86:ARG:HB3	3:D:522:PRO:HG2	1.98	0.44
3:D:566:ILE:HG23	5:F:214:GLN:HE22	1.83	0.44
3:D:285:PRO:HD2	3:D:288:MET:HE2	1.99	0.44
3:D:572:ARG:HH12	5:F:83:GLN:HB3	1.83	0.44
3:D:709:HIS:HD2	3:D:711:LEU:H	1.64	0.44
6:G:6:DA:H2''	6:G:7:DT:O5'	2.18	0.44
1:A:226:SER:O	1:A:228:PRO:HD3	2.18	0.44
1:B:155:LYS:HA	1:B:155:LYS:HD3	1.77	0.44
2:C:863:ASP:OD2	2:C:925:TYR:HE2	1.99	0.44
3:D:50:PHE:O	3:D:89:ARG:HD2	2.18	0.44
3:D:394:LEU:HG	3:D:396:VAL:HG23	1.99	0.44
3:D:566:ILE:HG12	5:F:217:ASN:ND2	2.33	0.44
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.33	0.44
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.99	0.44
2:C:1041:GLU:O	2:C:1044:GLY:N	2.44	0.44
3:D:432:TYR:O	3:D:448:GLU:HA	2.18	0.44
3:D:862:ASP:O	3:D:877:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1194:CYS:HB2	3:D:1204:CYS:SG	2.56	0.44
3:D:1364:HIS:CD2	3:D:1366:LYS:HE2	2.52	0.44
1:A:48:ILE:HD13	1:A:48:ILE:HA	1.69	0.44
1:A:123:MET:HE2	1:A:203:GLY:HA3	2.00	0.44
2:C:3:ILE:CD1	2:C:900:ARG:HB2	2.48	0.44
2:C:627:ARG:CZ	2:C:640:ARG:HG2	2.47	0.44
2:C:765:SER:O	2:C:767:PRO:HD3	2.17	0.44
3:D:285:PRO:HD2	3:D:288:MET:CE	2.47	0.44
5:F:229:TYR:CZ	5:F:230:LYS:HD3	2.53	0.44
2:C:207:LEU:HD13	2:C:221:LEU:HD21	1.99	0.44
2:C:987:ILE:HD11	3:D:946:GLY:HA2	2.00	0.44
2:C:1043:TYR:CE2	3:D:710:ARG:HG3	2.53	0.44
3:D:523:ASP:O	3:D:526:PRO:HG3	2.18	0.44
3:D:790:TYR:CE1	3:D:1022:VAL:HG13	2.52	0.44
3:D:960:LYS:NZ	3:D:1040:GLY:O	2.38	0.44
3:D:1208:ASP:C	3:D:1210:SER:H	2.26	0.44
3:D:1238:MET:SD	11:D:1606:2TM:H6	2.58	0.44
3:D:1447:LEU:HD23	3:D:1447:LEU:HA	1.90	0.44
5:F:189:GLU:HA	5:F:192:LEU:HG	2.00	0.44
2:C:499:ALA:HA	2:C:532:MET:CE	2.48	0.43
2:C:697:ARG:NH2	2:C:868:ASP:OD1	2.50	0.43
3:D:17:LYS:HB2	3:D:17:LYS:HE2	1.73	0.43
3:D:828:LYS:NZ	3:D:833:GLU:HB3	2.32	0.43
5:F:127:ILE:O	5:F:131:VAL:HG23	2.19	0.43
5:F:154:LYS:O	5:F:158:GLU:HG3	2.18	0.43
5:F:262:VAL:O	5:F:266:GLU:HG3	2.18	0.43
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.87	0.43
2:C:693:GLU:O	2:C:697:ARG:HG2	2.17	0.43
3:D:67:ARG:HE	5:F:379:ARG:HG2	1.83	0.43
3:D:784:ASP:HB2	3:D:939:PHE:CD2	2.54	0.43
3:D:832:ARG:NH1	3:D:833:GLU:HG2	2.33	0.43
5:F:271:LEU:HD12	5:F:295:MET:HE3	1.99	0.43
2:C:13:ILE:O	2:C:458:TYR:OH	2.35	0.43
2:C:858:MET:HG2	2:C:867:VAL:O	2.19	0.43
3:D:709:HIS:C	3:D:711:LEU:H	2.25	0.43
3:D:1285:GLU:HB2	3:D:1290:LEU:HD13	2.00	0.43
7:H:18:DC:H2''	7:H:19:DG:H5'	1.99	0.43
2:C:188:LYS:HB2	2:C:188:LYS:HE2	1.83	0.43
2:C:730:SER:OG	2:C:732:ALA:HB3	2.19	0.43
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.70	0.43
3:D:185:VAL:HG11	3:D:203:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:439:CYS:HB2	2:C:541:SER:N	2.34	0.43
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.53	0.43
3:D:197:SER:OG	3:D:395:VAL:HG21	2.19	0.43
3:D:520:LEU:HD11	3:D:524:LEU:HD12	1.99	0.43
3:D:792:ILE:HD13	3:D:941:PHE:CD1	2.53	0.43
3:D:853:VAL:HG22	3:D:858:VAL:HG23	1.99	0.43
5:F:163:LEU:HD13	5:F:174:LEU:CD1	2.49	0.43
1:A:10:VAL:HG12	1:A:26:GLU:O	2.19	0.43
2:C:886:LEU:HD21	3:D:951:ILE:HG12	2.01	0.43
3:D:114:THR:HG23	3:D:495:ARG:HG2	2.00	0.43
3:D:704:ARG:HD3	3:D:736:PHE:O	2.19	0.43
4:E:12:MET:HE1	4:E:68:LEU:O	2.19	0.43
5:F:304:VAL:O	5:F:308:LEU:HG	2.18	0.43
2:C:363:SER:O	2:C:367:LEU:HG	2.18	0.43
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.54	0.43
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.19	0.43
3:D:1057:VAL:HG13	3:D:1069:GLU:CD	2.43	0.43
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.38	0.43
2:C:312:ALA:O	2:C:317:VAL:HG13	2.19	0.43
2:C:1058:ASP:N	12:C:1202:HOH:O	2.51	0.43
3:D:796:ARG:NH2	3:D:859:ASP:OD2	2.46	0.43
4:E:46:PRO:HG3	4:E:66:LYS:HD2	2.01	0.43
1:B:34:VAL:HG21	2:C:978:ARG:HB3	2.00	0.43
1:B:185:ARG:HG3	1:B:189:ARG:O	2.18	0.43
2:C:983:ILE:C	2:C:985:GLY:N	2.76	0.43
2:C:1032:PHE:CE2	2:C:1036:GLU:HB3	2.54	0.43
3:D:123:LEU:O	3:D:127:LEU:HB2	2.19	0.43
3:D:478:LEU:HD21	3:D:500:ARG:NH2	2.34	0.43
3:D:704:ARG:HH22	11:D:1606:2TM:C1'	2.32	0.43
3:D:1084:THR:HB	3:D:1237:THR:O	2.19	0.43
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.19	0.42
3:D:923:GLY:O	3:D:927:THR:OG1	2.32	0.42
2:C:195:LEU:O	2:C:199:VAL:HG23	2.19	0.42
2:C:631:SER:HB3	2:C:635:THR:O	2.19	0.42
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.52	0.42
3:D:25:GLU:OE2	3:D:94:GLU:HB3	2.19	0.42
5:F:227:PHE:CE1	7:H:2:DA:H2	2.37	0.42
5:F:369:LEU:HD12	5:F:401:GLU:HG3	2.02	0.42
1:A:53:VAL:HG22	1:A:144:VAL:HG22	2.00	0.42
2:C:195:LEU:HD21	2:C:237:ARG:HG3	2.01	0.42
2:C:441:VAL:HG23	2:C:559:LEU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:938:LYS:O	2:C:941:VAL:HB	2.20	0.42
2:C:953:VAL:HG11	2:C:962:GLN:HB3	2.01	0.42
2:C:1056:LYS:HD3	3:D:625:TYR:HD1	1.83	0.42
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.54	0.42
2:C:762:LYS:HD2	2:C:783:ARG:O	2.18	0.42
3:D:204:LEU:HD22	3:D:441:ARG:CZ	2.49	0.42
3:D:702:LEU:HD23	3:D:702:LEU:HA	1.85	0.42
3:D:1140:ILE:O	3:D:1144:LEU:HB2	2.19	0.42
5:F:193:ARG:HB3	7:H:7:DG:H5"	2.01	0.42
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.54	0.42
2:C:109:LYS:HG2	2:C:368:THR:HG22	2.00	0.42
2:C:174:LEU:HA	2:C:183:SER:O	2.19	0.42
3:D:236:TYR:CE2	3:D:322:VAL:CG2	2.84	0.42
1:B:138:LEU:HD11	1:B:140:MET:HE3	2.01	0.42
2:C:3:ILE:HD12	2:C:900:ARG:HB2	2.02	0.42
2:C:1008:ARG:NH1	2:C:1020:PRO:HB3	2.35	0.42
3:D:679:ARG:NH2	3:D:681:ARG:HD2	2.34	0.42
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.20	0.42
1:B:7:LYS:HA	1:B:7:LYS:HD3	1.88	0.42
2:C:431:HIS:ND1	2:C:433:THR:HG23	2.35	0.42
2:C:584:GLU:OE2	2:C:584:GLU:N	2.34	0.42
2:C:912:PRO:O	2:C:916:GLU:HG3	2.20	0.42
2:C:983:ILE:O	2:C:984:GLU:C	2.63	0.42
3:D:613:ARG:HG3	3:D:618:LEU:HD11	2.02	0.42
3:D:774:SER:HB3	3:D:1362:LYS:O	2.19	0.42
3:D:869:MET:HE2	3:D:869:MET:HB3	1.90	0.42
3:D:999:THR:O	3:D:1003:VAL:HG13	2.20	0.42
3:D:1167:SER:O	3:D:1170:ASP:HB2	2.20	0.42
3:D:1256:LEU:HB3	3:D:1257:PRO:HD3	2.00	0.42
6:G:7:DT:H3	7:H:21:DA:H61	1.68	0.42
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.55	0.42
3:D:553:ARG:HD3	5:F:214:GLN:HB3	2.02	0.42
3:D:864:VAL:HG13	3:D:865:THR:N	2.34	0.42
3:D:1048:PRO:O	3:D:1079:LYS:NZ	2.52	0.42
2:C:344:PHE:CE2	2:C:382:ILE:HD11	2.54	0.42
2:C:721:ARG:HH12	2:C:785:VAL:HG11	1.85	0.42
3:D:84:ILE:HD12	3:D:87:ARG:HD2	2.02	0.42
3:D:155:ASP:OD1	3:D:159:ARG:NH2	2.52	0.42
3:D:242:LEU:HB3	3:D:311:LEU:HD12	2.02	0.42
3:D:547:LEU:HA	3:D:547:LEU:HD12	1.71	0.42
3:D:868:TYR:HB3	3:D:873:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1031:ASN:HD21	3:D:1034:GLN:HE21	1.65	0.42
3:D:1353:GLN:HG2	3:D:1368:ILE:CD1	2.49	0.42
1:A:41:ARG:HD2	1:A:177:VAL:HG12	2.00	0.42
1:A:221:HIS:HA	1:A:224:TYR:CE2	2.55	0.42
2:C:90:TYR:CD2	2:C:120:LEU:HB2	2.55	0.42
2:C:425:PHE:O	2:C:428:ARG:N	2.52	0.42
2:C:1065:ALA:CB	2:C:1077:PRO:HG3	2.50	0.42
3:D:951:ILE:HD11	3:D:1062:ARG:HG3	2.01	0.42
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.55	0.41
2:C:557:ARG:CG	2:C:844:GLY:HA3	2.49	0.41
2:C:1013:TYR:HE1	2:C:1020:PRO:HG3	1.85	0.41
3:D:1192:LEU:HD13	3:D:1345:GLU:HB3	2.02	0.41
3:D:1223:ILE:HD12	3:D:1223:ILE:HG23	1.71	0.41
1:B:9:PRO:HG2	1:B:25:LEU:HD11	2.02	0.41
1:B:91:ASN:HB2	1:B:119:ASP:CG	2.45	0.41
2:C:154:ARG:HH21	2:C:157:ARG:HG3	1.85	0.41
2:C:216:GLU:HG2	2:C:219:GLN:HB2	2.01	0.41
2:C:630:ARG:HD2	2:C:705:ILE:O	2.20	0.41
2:C:690:ILE:HG12	2:C:852:ILE:HG12	2.02	0.41
3:D:550:ARG:CZ	3:D:573:MET:HE3	2.50	0.41
7:H:18:DC:H4'	7:H:19:DG:OP1	2.20	0.41
1:B:132:LEU:HD21	1:B:138:LEU:CB	2.50	0.41
2:C:165:LEU:HB2	2:C:168:ARG:HG3	2.02	0.41
2:C:905:ILE:C	2:C:907:ASP:H	2.28	0.41
3:D:288:MET:HG2	3:D:305:ALA:HB1	2.02	0.41
3:D:319:ALA:HA	3:D:337:LEU:HD23	2.01	0.41
3:D:428:LYS:HE2	3:D:428:LYS:HB3	1.83	0.41
3:D:1312:LEU:HD12	3:D:1312:LEU:HA	1.94	0.41
6:G:11:DT:H2''	6:G:12:DG:C8	2.55	0.41
2:C:631:SER:HB2	2:C:637:LEU:HD11	2.02	0.41
2:C:800:VAL:HG22	2:C:827:VAL:HG22	2.02	0.41
3:D:60:CYS:SG	3:D:61:GLY:N	2.93	0.41
1:B:179:PHE:HB3	1:B:197:LEU:HD13	2.01	0.41
2:C:154:ARG:NH2	2:C:157:ARG:HG3	2.35	0.41
3:D:142:LEU:HD13	3:D:161:LEU:HD21	2.01	0.41
3:D:580:ALA:HA	3:D:584:ASN:HA	2.03	0.41
1:A:4:SER:C	1:A:189:ARG:HH22	2.28	0.41
1:B:54:THR:OG1	1:B:158:ILE:HD11	2.20	0.41
2:C:89:THR:O	2:C:91:GLN:HG2	2.19	0.41
3:D:827:ILE:HG12	3:D:834:THR:O	2.20	0.41
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:HIS:CD2	1:A:129:ILE:N	2.88	0.41
1:B:177:VAL:HG13	1:B:197:LEU:HD11	2.02	0.41
1:B:216:GLU:CD	1:B:219:ARG:HE	2.28	0.41
2:C:586:ARG:HD2	2:C:586:ARG:HA	1.84	0.41
2:C:735:ARG:HH11	3:D:681:ARG:NH1	2.19	0.41
2:C:970:GLY:O	2:C:988:VAL:HA	2.21	0.41
2:C:1043:TYR:HD1	3:D:763:MET:HE3	1.82	0.41
3:D:115:LEU:HD23	3:D:115:LEU:HA	1.92	0.41
2:C:1005:MET:SD	3:D:648:MET:HG3	2.60	0.41
3:D:24:GLY:HA3	3:D:49:ILE:HG23	2.02	0.41
3:D:366:LYS:HD3	3:D:369:ALA:HB2	2.03	0.41
3:D:729:HIS:CE1	3:D:731:LEU:HB2	2.56	0.41
3:D:849:ALA:O	3:D:853:VAL:HG23	2.21	0.41
3:D:1034:GLN:HA	3:D:1037:GLN:HE21	1.86	0.41
3:D:1093:TYR:CE2	6:G:13:DA:H5'	2.56	0.41
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.60	0.41
2:C:13:ILE:HG21	2:C:483:VAL:HG11	2.02	0.41
2:C:129:ILE:HG13	2:C:386:PHE:HB3	2.03	0.41
2:C:317:VAL:HA	2:C:318:PRO:HD3	1.93	0.41
2:C:340:MET:HE3	2:C:341:THR:N	2.36	0.41
2:C:939:ARG:HG2	2:C:982:PRO:HD3	2.03	0.41
2:C:999:HIS:HB3	2:C:1004:LYS:HZ2	1.84	0.41
2:C:1071:ILE:HB	3:D:670:VAL:HG21	2.02	0.41
2:C:1101:THR:O	2:C:1109:VAL:N	2.53	0.41
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.53	0.41
3:D:871:LYS:NZ	3:D:897:TRP:HE1	2.18	0.41
3:D:882:PHE:HE2	3:D:900:ILE:HG23	1.86	0.41
3:D:1194:CYS:HB2	3:D:1204:CYS:CB	2.51	0.41
5:F:85:LEU:HD23	5:F:85:LEU:HA	1.82	0.41
5:F:383:LEU:HD13	5:F:398:ARG:HB2	2.02	0.41
7:H:10:DA:H3'	7:H:11:DG:N7	2.36	0.41
7:H:12:DC:H4'	7:H:13:DT:O5'	2.20	0.41
1:B:14:ARG:NH2	1:B:22:GLU:OE1	2.54	0.41
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.85	0.41
2:C:954:THR:HA	2:C:955:PRO:HD3	1.91	0.41
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.75	0.41
3:D:544:TYR:O	3:D:548:ILE:HG13	2.21	0.41
3:D:1208:ASP:O	3:D:1209:LEU:HB2	2.21	0.41
3:D:1296:SER:OG	3:D:1297:GLU:N	2.54	0.41
1:B:211:LEU:O	1:B:215:VAL:HG13	2.21	0.40
2:C:292:ARG:HE	2:C:292:ARG:HB2	1.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:394:PHE:CE2	6:G:20:DG:H5''	2.56	0.40
2:C:1066:ALA:O	2:C:1070:ILE:HG13	2.20	0.40
3:D:360:ARG:HG2	3:D:384:VAL:HG12	2.02	0.40
3:D:483:HIS:CD2	3:D:484:PRO:HD2	2.56	0.40
7:H:1:DT:O2	7:H:1:DT:O4'	2.37	0.40
1:A:42:ARG:NH2	1:B:34:VAL:HG22	2.35	0.40
2:C:1089:VAL:HG11	2:C:1112:PHE:CZ	2.57	0.40
3:D:129:PHE:CD1	3:D:456:MET:HB3	2.56	0.40
3:D:601:ARG:CD	5:F:318:GLU:HG2	2.51	0.40
3:D:1283:ILE:HG12	3:D:1315:ASP:HB2	2.02	0.40
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.21	0.40
5:F:286:PRO:HA	5:F:290:GLU:OE1	2.21	0.40
1:A:55:SER:HB2	1:A:158:ILE:HG22	2.03	0.40
2:C:276:LYS:HD2	2:C:466:PHE:CZ	2.56	0.40
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.57	0.40
3:D:709:HIS:O	3:D:711:LEU:N	2.55	0.40
3:D:908:LYS:HB3	3:D:908:LYS:HE2	1.97	0.40
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.51	0.40
4:E:47:LYS:NZ	4:E:56:ASP:OD1	2.52	0.40
5:F:271:LEU:CD1	5:F:295:MET:HE3	2.51	0.40
2:C:141:HIS:CD2	2:C:334:ARG:HD2	2.57	0.40
2:C:169:GLY:HA3	2:C:267:TYR:CD1	2.56	0.40
3:D:123:LEU:HG	3:D:127:LEU:HD12	2.03	0.40
3:D:1468:LEU:HD12	3:D:1470:ARG:HD2	2.04	0.40
5:F:123:ASP:O	5:F:127:ILE:HG13	2.22	0.40
5:F:228:GLU:OE2	5:F:231:ARG:NE	2.40	0.40
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.89	0.40
2:C:376:ARG:HH11	2:C:376:ARG:HD2	1.78	0.40
2:C:671:ASN:HA	2:C:992:MET:O	2.21	0.40
2:C:701:THR:HA	2:C:831:ARG:O	2.22	0.40
2:C:993:PHE:CB	12:C:1201:HOH:O	2.28	0.40
3:D:25:GLU:HB2	3:D:92:HIS:CE1	2.56	0.40
3:D:421:LEU:HD11	3:D:429:SER:HB2	2.02	0.40
3:D:852:ALA:HB1	3:D:857:ILE:HB	2.02	0.40
8:I:6:G:C2'	8:I:7:A:H5'	2.51	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	
1	A	229/315 (73%)	216 (94%)	13 (6%)	0	100	100
1	B	225/315 (71%)	212 (94%)	13 (6%)	0	100	100
2	C	1108/1119 (99%)	1050 (95%)	58 (5%)	0	100	100
3	D	1494/1524 (98%)	1411 (94%)	83 (6%)	0	100	100
4	E	92/99 (93%)	84 (91%)	8 (9%)	0	100	100
5	F	344/443 (78%)	334 (97%)	10 (3%)	0	100	100
All	All	3492/3815 (92%)	3307 (95%)	185 (5%)	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	
1	A	200/273 (73%)	184 (92%)	16 (8%)	11	35
1	B	200/273 (73%)	189 (94%)	11 (6%)	19	47
2	C	935/941 (99%)	860 (92%)	75 (8%)	11	35
3	D	1259/1279 (98%)	1168 (93%)	91 (7%)	13	39
4	E	83/88 (94%)	79 (95%)	4 (5%)	23	52
5	F	300/388 (77%)	277 (92%)	23 (8%)	12	37
All	All	2977/3242 (92%)	2757 (93%)	220 (7%)	13	38

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	34	VAL
1	A	47	SER
1	A	48	ILE
1	A	76	VAL
1	A	93	SER
1	A	94	LEU
1	A	112	ARG
1	A	148	VAL
1	A	155	LYS
1	A	170	VAL
1	A	182	GLU
1	A	196	THR
1	A	198	ARG
1	A	213	GLN
1	A	229	GLN
1	B	2	LEU
1	B	34	VAL
1	B	94	LEU
1	B	131	THR
1	B	133	GLU
1	B	155	LYS
1	B	184	THR
1	B	186	LEU
1	B	188	GLN
1	B	205	VAL
1	B	216	GLU
2	C	27	ARG
2	C	56	GLU
2	C	64	LEU
2	C	69	LEU
2	C	113	VAL
2	C	143	SER
2	C	168	ARG
2	C	174	LEU
2	C	182	VAL
2	C	186	VAL
2	C	194	VAL
2	C	200	LEU
2	C	257	VAL
2	C	285	LEU
2	C	317	VAL

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Mol	Chain	Res	Type
2	C	325	ILE
2	C	328	LEU
2	C	348	LEU
2	C	351	LEU
2	C	372	LEU
2	C	376	ARG
2	C	384	GLU
2	C	397	GLU
2	C	402	SER
2	C	426	ASP
2	C	428	ARG
2	C	430	VAL
2	C	441	VAL
2	C	455	LEU
2	C	460	ARG
2	C	483	VAL
2	C	493	ARG
2	C	514	VAL
2	C	524	VAL
2	C	534	VAL
2	C	538	GLN
2	C	539	VAL
2	C	562	SER
2	C	572	ILE
2	C	578	VAL
2	C	583	LEU
2	C	613	VAL
2	C	630	ARG
2	C	631	SER
2	C	644	VAL
2	C	657	ASP
2	C	666	LEU
2	C	670	GLN
2	C	674	VAL
2	C	698	ASP
2	C	702	SER
2	C	715	THR
2	C	716	LYS
2	C	717	LEU
2	C	801	VAL
2	C	815	LEU
2	C	819	VAL

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Mol	Chain	Res	Type
2	C	848	VAL
2	C	858	MET
2	C	863	ASP
2	C	869	VAL
2	C	888	THR
2	C	936	VAL
2	C	953	VAL
2	C	974	LEU
2	C	984	GLU
2	C	1008	ARG
2	C	1014	SER
2	C	1055	LEU
2	C	1063	ARG
2	C	1075	ASP
2	C	1076	VAL
2	C	1084	SER
2	C	1095	LEU
2	C	1099	VAL
3	D	10	ILE
3	D	17	LYS
3	D	32	ILE
3	D	40	GLU
3	D	53	ILE
3	D	72	VAL
3	D	80	VAL
3	D	97	THR
3	D	133	ILE
3	D	138	LYS
3	D	145	VAL
3	D	150	ARG
3	D	175	VAL
3	D	183	GLU
3	D	185	VAL
3	D	191	LEU
3	D	206	ARG
3	D	216	VAL
3	D	245	LEU
3	D	273	ARG
3	D	274	ARG
3	D	275	GLU
3	D	276	ASP
3	D	293	VAL

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Mol	Chain	Res	Type
3	D	310	LEU
3	D	311	LEU
3	D	317	VAL
3	D	335	LEU
3	D	354	VAL
3	D	415	VAL
3	D	420	VAL
3	D	429	SER
3	D	431	VAL
3	D	440	VAL
3	D	443	VAL
3	D	503	LEU
3	D	530	VAL
3	D	537	THR
3	D	574	LEU
3	D	578	VAL
3	D	607	LEU
3	D	615	ARG
3	D	618	LEU
3	D	623	VAL
3	D	628	ARG
3	D	650	LEU
3	D	710	ARG
3	D	724	GLN
3	D	725	SER
3	D	747	VAL
3	D	754	PHE
3	D	784	ASP
3	D	785	ILE
3	D	827	ILE
3	D	828	LYS
3	D	832	ARG
3	D	833	GLU
3	D	864	VAL
3	D	899	LEU
3	D	910	SER
3	D	922	LEU
3	D	984	THR
3	D	1035	ILE
3	D	1041	LEU
3	D	1086	LEU
3	D	1100	ASP

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Mol	Chain	Res	Type
3	D	1101	VAL
3	D	1119	SER
3	D	1185	GLU
3	D	1188	VAL
3	D	1200	VAL
3	D	1209	LEU
3	D	1216	SER
3	D	1237	THR
3	D	1297	GLU
3	D	1312	LEU
3	D	1313	VAL
3	D	1344	VAL
3	D	1361	VAL
3	D	1400	VAL
3	D	1424	VAL
3	D	1425	THR
3	D	1430	SER
3	D	1433	SER
3	D	1435	LEU
3	D	1460	ILE
3	D	1468	LEU
3	D	1472	ILE
3	D	1476	THR
3	D	1486	VAL
3	D	1488	ASP
4	E	50	THR
4	E	51	LEU
4	E	74	VAL
4	E	93	TYR
5	F	81	VAL
5	F	88	ILE
5	F	94	LEU
5	F	96	LEU
5	F	122	LEU
5	F	135	ILE
5	F	136	LEU
5	F	141	VAL
5	F	171	LYS
5	F	226	LYS
5	F	234	LYS
5	F	267	THR
5	F	310	ILE

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Mol	Chain	Res	Type
5	F	319	THR
5	F	321	ILE
5	F	338	LEU
5	F	347	GLN
5	F	349	LEU
5	F	358	LEU
5	F	369	LEU
5	F	375	LEU
5	F	392	VAL
5	F	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	163	ASN
2	C	187	ASN
2	C	434	HIS
2	C	663	ASN
2	C	962	GLN
2	C	991	GLN
2	C	1019	GLN
2	C	1026	GLN
3	D	294	HIS
3	D	442	ASN
3	D	569	ASN
3	D	593	ASN
3	D	709	HIS
3	D	1025	GLN
3	D	1034	GLN
3	D	1037	GLN
3	D	1046	GLN
3	D	1172	HIS
3	D	1227	GLN
3	D	1242	HIS
3	D	1465	ASN
5	F	214	GLN
5	F	245	GLN
5	F	411	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/3 (33%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	7	A

There are no RNA pucker outliers to report.

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 9 ligands modelled in this entry, 8 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	$\# Z > 2$
11	2TM	D	1606	9	26,30,30	4.03	15 (57%)	39,47,47	1.17	3 (7%)

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
11	2TM	D	1606	9	-	2/19/38/38	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	1606	2TM	PB-O3B	8.24	1.67	1.58
11	D	1606	2TM	O4'-C1'	7.57	1.59	1.42
11	D	1606	2TM	O4'-C4'	-7.01	1.29	1.45
11	D	1606	2TM	C2-N3	6.56	1.49	1.36
11	D	1606	2TM	C2'-C1'	-5.91	1.34	1.53
11	D	1606	2TM	C4-N4	5.75	1.47	1.33
11	D	1606	2TM	C6-C5	5.70	1.48	1.35
11	D	1606	2TM	C4-N3	5.52	1.45	1.34
11	D	1606	2TM	C2-N1	4.17	1.48	1.40
11	D	1606	2TM	C6-N1	3.53	1.46	1.38
11	D	1606	2TM	O2-C2	-3.14	1.17	1.23
11	D	1606	2TM	O2'-C2'	2.91	1.50	1.43
11	D	1606	2TM	O3'-C3'	-2.38	1.37	1.43
11	D	1606	2TM	C5-C4	2.33	1.48	1.42
11	D	1606	2TM	C3'-C4'	2.32	1.58	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	1606	2TM	PB-O3B-PG	-3.15	121.15	132.45
11	D	1606	2TM	O2G-PG-O3B	3.06	114.91	104.64
11	D	1606	2TM	N4-C4-N3	2.36	122.13	117.91

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	1606	2TM	O4'-C4'-C5'-O5'
11	D	1606	2TM	C3'-C4'-C5'-O5'

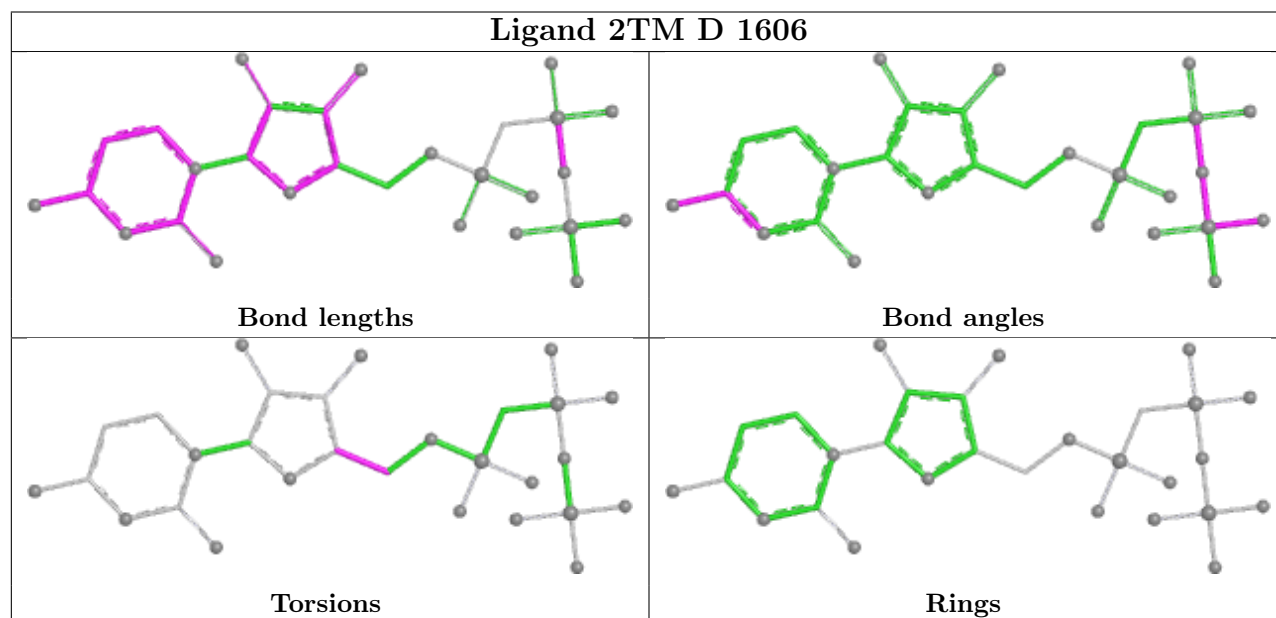
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	1606	2TM	4	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	A	231/315 (73%)	0.43	8 (3%)	47	28	36, 54, 76, 122	0
1	B	227/315 (72%)	0.60	10 (4%)	39	22	37, 68, 91, 126	0
2	C	1112/1119 (99%)	0.46	34 (3%)	51	31	21, 54, 99, 121	0
3	D	1497/1524 (98%)	0.47	58 (3%)	43	25	20, 56, 108, 167	2 (0%)
4	E	94/99 (94%)	0.41	1 (1%)	78	60	36, 59, 90, 96	0
5	F	346/443 (78%)	0.53	16 (4%)	37	21	33, 65, 107, 125	0
6	G	17/21 (80%)	0.58	1 (5%)	28	16	36, 67, 142, 143	0
7	H	24/27 (88%)	0.65	1 (4%)	40	23	53, 84, 122, 154	0
8	I	2/3 (66%)	0.04	0	100	100	38, 38, 38, 39	0
All	All	3550/3866 (91%)	0.48	129 (3%)	46	27	20, 57, 105, 167	2 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	203	ALA	7.1
3	D	412	GLY	4.8
3	D	368	VAL	4.5
2	C	764	GLU	4.3
3	D	1246	VAL	4.1
3	D	409	VAL	4.0
2	C	183	SER	3.9
5	F	377	ASP	3.7
3	D	305	ALA	3.7
3	D	303	PRO	3.6
3	D	322	VAL	3.6
3	D	377	VAL	3.5
6	G	20	DG	3.4
3	D	560	GLN	3.4
1	B	120	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	C	66	LEU	3.3
2	C	307	LEU	3.3
3	D	311	LEU	3.2
3	D	202	VAL	3.2
2	C	68	PHE	3.2
3	D	444	VAL	3.2
3	D	267	GLY	3.1
5	F	219	GLY	3.1
1	A	40	LEU	3.0
2	C	774	LEU	3.0
3	D	875	THR	3.0
1	A	73	GLU	3.0
2	C	281	LEU	3.0
2	C	823	VAL	3.0
1	B	222	LEU	3.0
3	D	269	PHE	2.9
3	D	791	TYR	2.9
2	C	29	ALA	2.9
3	D	289	THR	2.9
2	C	65	VAL	2.8
1	A	55	SER	2.8
3	D	1429	LEU	2.8
2	C	300	ASP	2.8
1	B	23	PHE	2.8
5	F	400	ILE	2.8
3	D	422	ALA	2.8
3	D	211	VAL	2.8
1	A	169	ALA	2.7
3	D	367	ILE	2.7
3	D	470	LEU	2.7
5	F	421	PHE	2.7
3	D	410	SER	2.7
3	D	415	VAL	2.7
2	C	174	LEU	2.6
3	D	152	LEU	2.6
3	D	1073	SER	2.6
5	F	145	PRO	2.6
5	F	94	LEU	2.6
2	C	984	GLU	2.5
2	C	865	THR	2.5
3	D	531	ASP	2.5
3	D	443	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	199	ILE	2.5
2	C	693	GLU	2.5
2	C	777	ILE	2.4
2	C	666	LEU	2.4
2	C	451	LEU	2.4
1	A	131	THR	2.4
3	D	353	VAL	2.4
3	D	355	VAL	2.4
2	C	159	ILE	2.4
3	D	566	ILE	2.4
2	C	776	SER	2.4
3	D	400	VAL	2.4
2	C	311	PHE	2.4
3	D	407	VAL	2.4
3	D	431	VAL	2.4
4	E	38	THR	2.3
3	D	1252	ILE	2.3
5	F	149	GLU	2.3
3	D	694	VAL	2.3
2	C	149	THR	2.3
5	F	139	ALA	2.3
2	C	386	PHE	2.3
3	D	624	ASP	2.3
2	C	804	VAL	2.3
5	F	156	VAL	2.3
3	D	809	PRO	2.2
1	B	138	LEU	2.2
2	C	187	ASN	2.2
3	D	1107	VAL	2.2
5	F	195	VAL	2.2
5	F	125	ASP	2.2
3	D	15	PRO	2.2
5	F	404	ALA	2.2
3	D	316	GLN	2.2
2	C	54	ILE	2.2
3	D	161	LEU	2.2
1	A	56	VAL	2.2
1	B	228	PRO	2.2
2	C	766	GLU	2.2
3	D	378	ILE	2.1
3	D	620	GLY	2.1
3	D	401	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	82	LEU	2.1
5	F	405	LEU	2.1
2	C	369	PRO	2.1
2	C	200	LEU	2.1
3	D	421	LEU	2.1
2	C	253	ALA	2.1
3	D	1247	ALA	2.1
3	D	141	ILE	2.1
3	D	223	LEU	2.1
3	D	1192	LEU	2.1
1	B	164	ALA	2.1
1	B	64	GLU	2.1
5	F	395	GLU	2.1
3	D	1242	HIS	2.1
7	H	24	DC	2.1
1	A	207	PRO	2.1
2	C	51	THR	2.0
5	F	146	GLY	2.0
3	D	262	LYS	2.0
5	F	134	LYS	2.0
3	D	49	ILE	2.0
1	B	118	ALA	2.0
2	C	147	TYR	2.0
2	C	629	TYR	2.0
3	D	107	ASP	2.0
1	B	179	PHE	2.0
2	C	943	VAL	2.0
3	D	122	GLU	2.0
3	D	292	VAL	2.0
3	D	1313	VAL	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 ⓘ

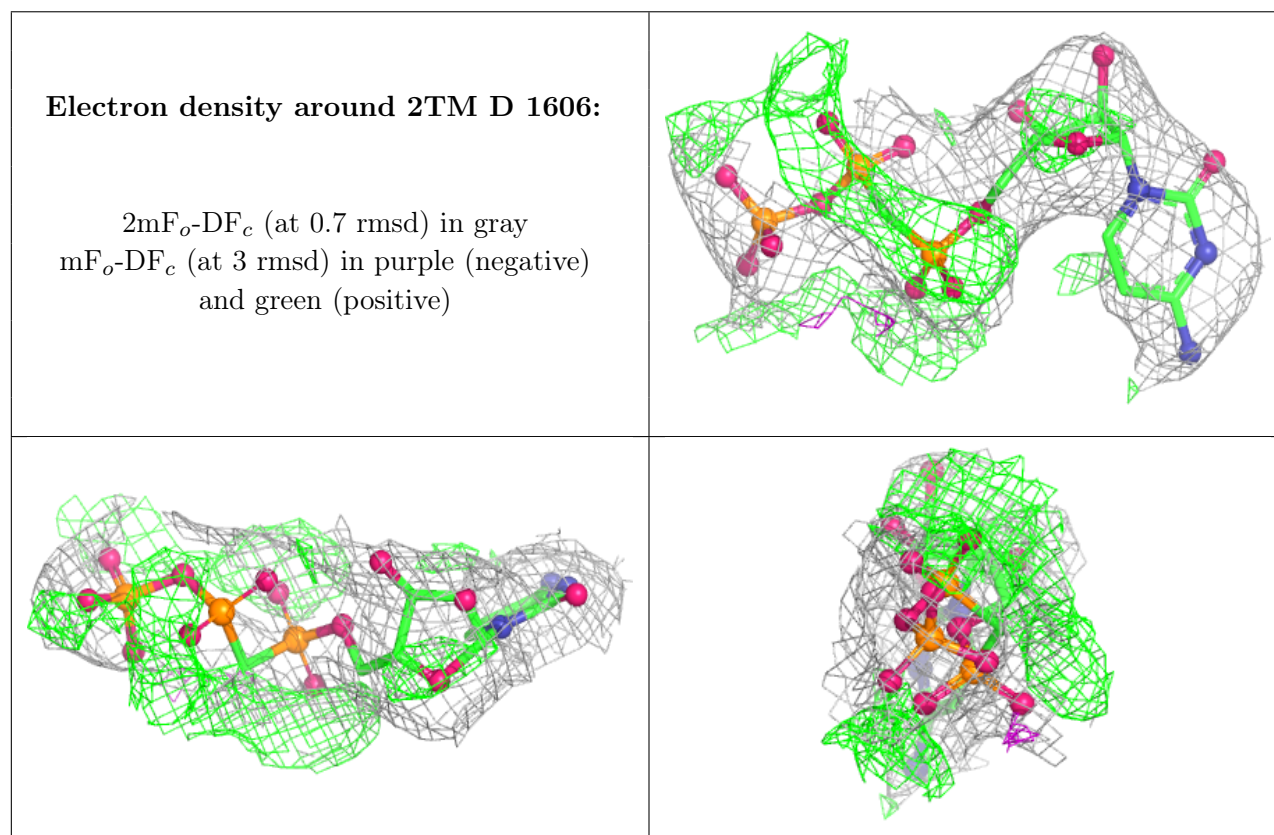
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	2TM	D	1606	29/29	0.81	0.15	26,37,62,75	29
9	MG	D	1605	1/1	0.86	0.15	59,59,59,59	0
9	MG	B	402	1/1	0.87	0.24	44,44,44,44	0
9	MG	B	401	1/1	0.89	0.07	73,73,73,73	0
9	MG	D	1604	1/1	0.92	0.24	42,42,42,42	0
9	MG	F	501	1/1	0.94	0.06	65,65,65,65	0
9	MG	D	1603	1/1	0.96	0.07	27,27,27,27	0
10	ZN	D	1602	1/1	0.99	0.02	57,57,57,57	0
10	ZN	D	1601	1/1	0.99	0.05	46,46,46,46	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.