



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 10:46 PM UTC

PDB ID : 8XQW / pdb_00008xqw
EMDB ID : EMD-38589
Title : Cryo-EM structure of the Ycf2-FtsHi motor complex from *Chlamydomonas reinhardtii* in AMPPNP bound state
Authors : Liang, K.; Zhan, X.; Wu, J.; Yan, Z.
Deposited on : 2024-01-10
Resolution : 2.90 Å(reported)
Based on initial model : .

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

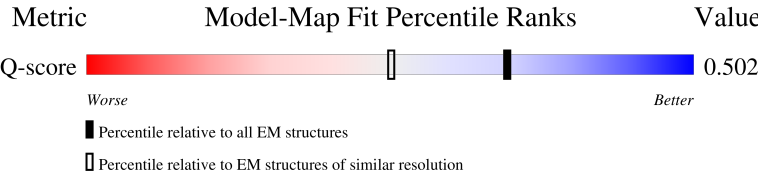
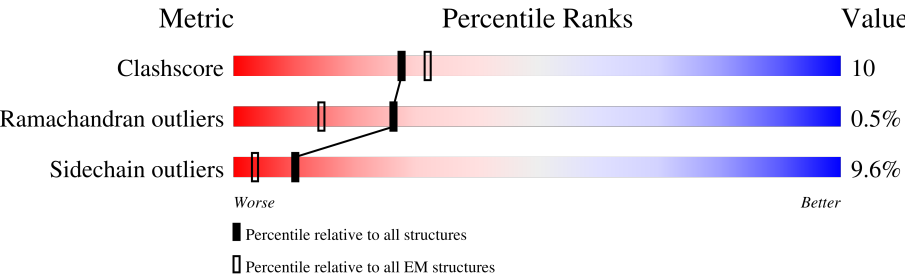
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1182	
2	B	1112	
2	C	1112	
3	D	2971	

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Mol	Chain	Length	Quality of chain
4	E	982	
5	F	1024	
6	G	495	
7	H	555	
8	I	366	
9	J	117	
10	K	255	
11	L	303	
12	M	682	
13	N	137	
14	O	471	
15	P	691	
16	Q	365	
17	R	462	
18	S	324	
19	T	299	
20	V	86	
21	U	156	

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 73643 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Fhl1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	988	Total	C	N	O	S	0	0
			7627	4839	1342	1410	36		

- Molecule 2 is a protein called Fhl3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	751	Total	C	N	O	P	S	0	0
			5844	3675	1037	1094	3	35		
2	C	690	Total	C	N	O	S		0	0
			5324	3359	949	985	31			

- Molecule 3 is a protein called Ycf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1539	Total	C	N	O	S	0	0
			12719	8252	2175	2266	26		

- Molecule 4 is a protein called Ctap1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	868	Total	C	N	O	S	0	0
			6229	3888	1143	1184	14		

- Molecule 5 is a protein called Ctap6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	701	Total	C	N	O	S	0	0
			5333	3344	963	1007	19		

- Molecule 6 is a protein called ARHL.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	394	Total	C	N	O	S	0	0
			2931	1839	539	549	4		

- Molecule 7 is a protein called PcyA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	406	Total	C	N	O	S	0	0
			3246	2061	547	617	21		

- Molecule 8 is a protein called CrTam39.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	272	Total	C	N	O	S	0	0
			2119	1336	394	374	15		

- Molecule 9 is a protein called ACP.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	85	Total	C	N	O	P	S	0	0
			651	404	101	141	1	4		

- Molecule 10 is a protein called CrTam29.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	189	Total	C	N	O	S	0	0
			1567	1032	271	257	7		

- Molecule 11 is a protein called CrTam34.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	151	Total	C	N	O	S	0	0
			1254	844	210	196	4		

- Molecule 12 is a protein called FADL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	390	Total	C	N	O	S	0	0
			3000	1958	510	516	16		

- Molecule 13 is a protein called CrTam15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	115	Total	C	N	O	S	0	0
			921	585	172	161	3		

- Molecule 14 is a protein called CrTam49.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	318	Total	C	N	O	S	0	0
			2040	1317	352	367	4		

- Molecule 15 is a protein called Ctap7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	617	Total	C	N	O	S	0	0
			4510	2802	829	868	11		

- Molecule 16 is a protein called Tic22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	262	Total	C	N	O	S	0	0
			2078	1316	365	388	9		

- Molecule 17 is a protein called DnaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace	
17	R	401	Total	C	N	O	P	S	0	0
			3160	1981	571	585	2	21		

- Molecule 18 is a protein called CrTam35.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	S	117	Total	C	N	O	P	S	0	0
			951	588	169	190	3	1		

- Molecule 19 is a protein called CrTam31.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	T	110	Total	C	N	O	P	S	0	0
			868	535	147	182	2	2		

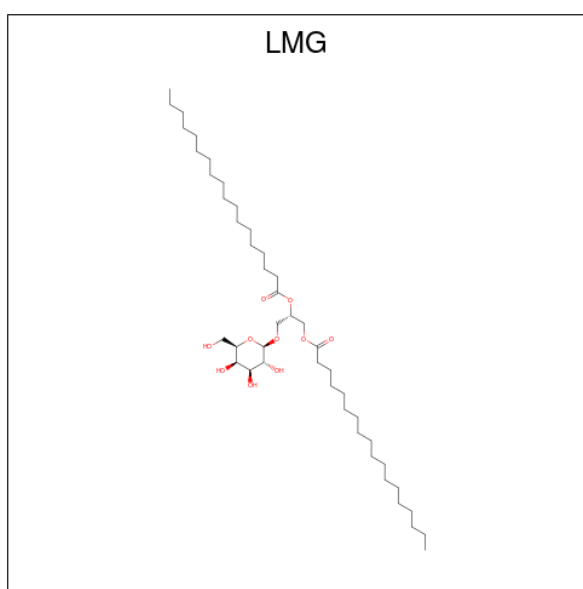
- Molecule 20 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	V	68	Total	C	N	O	0	0
			340	204	68	68		

- Molecule 21 is a protein called UNK.

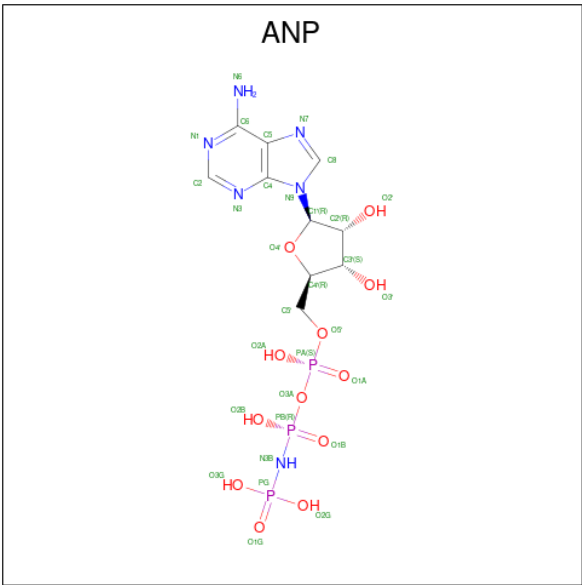
Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	36	Total	C	N	O	1	0
			188	115	36	37		

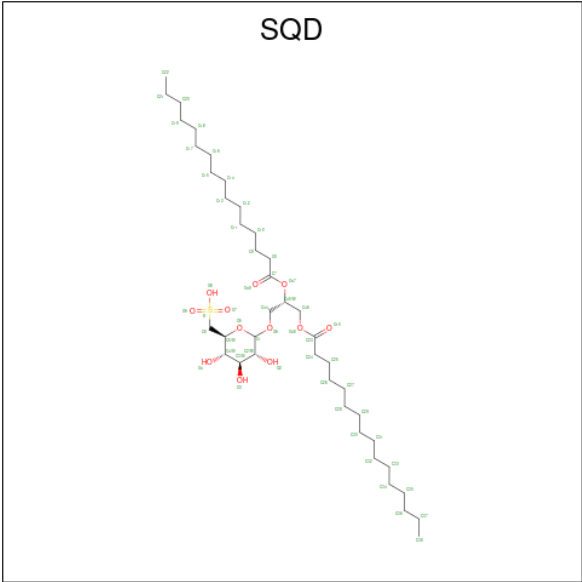
- Molecule 22 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	C	O	0
			46	36	10	
22	C	1	Total	C	O	0
			25	20	5	
22	I	1	Total	C	O	0
			32	22	10	
22	K	1	Total	C	O	0
			41	31	10	
22	M	1	Total	C	O	0
			48	38	10	

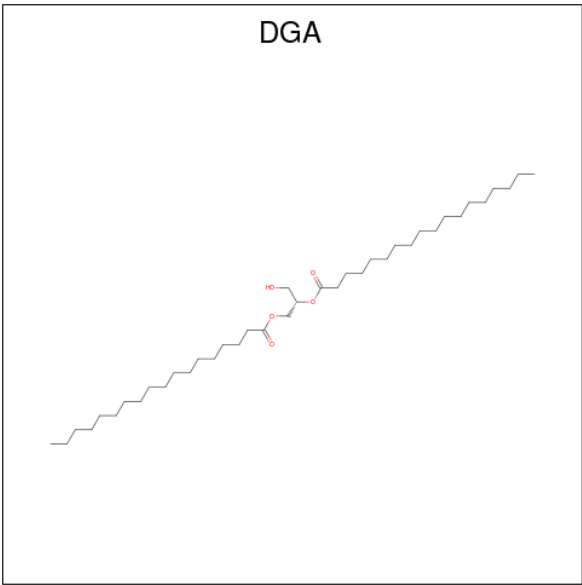
- Molecule 23 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).





Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	S	0
			46	33	12	1	
25	I	1	Total	C	O	S	0
			49	36	12	1	
25	K	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 26 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



Mol	Chain	Residues	Atoms			AltConf
26	D	1	Total	C	O	0
			34	29	5	

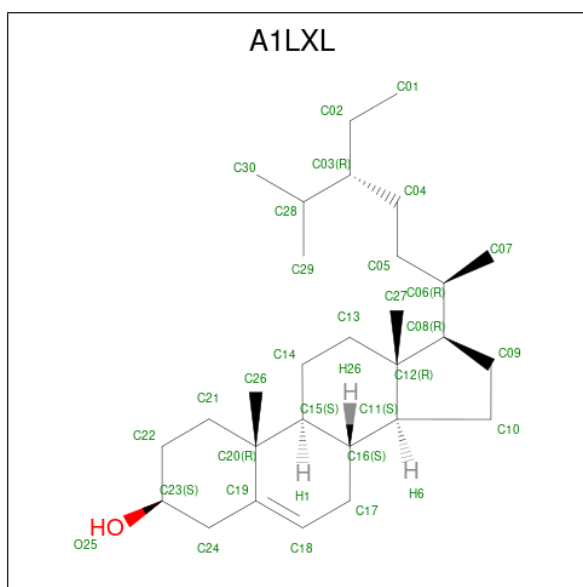
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Mol	Chain	Residues	Atoms	AltConf
26	O	1	Total C O 39 34 5	0

- # Y01

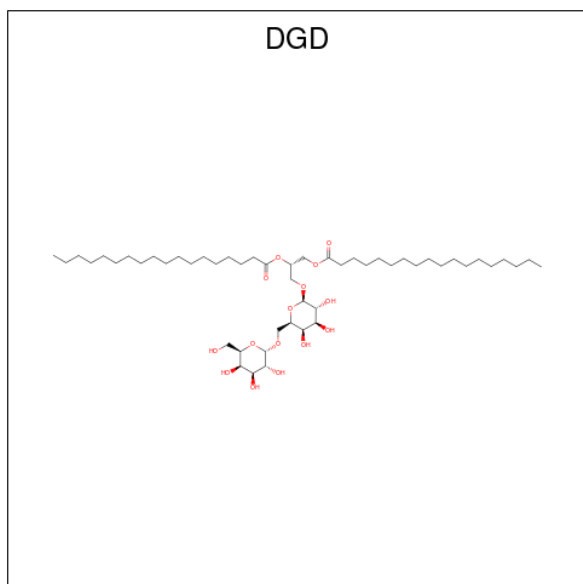
Mol	Chain	Residues	Atoms			AltConf
27	D	1	Total 35	C 31	O 4	0
27	M	1	Total 35	C 31	O 4	0

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Mol	Chain	Residues	Atoms			AltConf
28	D	1	Total	C	O	0
			30	29	1	
28	P	1	Total	C	O	0
			30	29	1	

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
29	I	1	Total	C	O	0
			40	25	15	

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Mol	Chain	Residues	Atoms			AltConf
29	L	1	Total	C	O	0
			41	26	15	

- Molecule 30 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
30	R	2	Total	Zn	0
			2	2	

- Molecule 2: Fhl3



NET	ARG	NET	GLY	MET	ALA	ILE	ARG	CYS	ALA	ALA	SER	GLY	SER	LEU	ALA	SER	PRO	ALA	ALA	SER	ARG	PRO	VAL	LEU	CYS	SER	PRO	ARG	VAL	CYS	THR	PRO	LEU	GLY	GLY	VAL	SER	CYS	ARG	ARG	ARG	CYS	NET	GLN	ARG	ARG	TRP	TRP
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ARG ALA ALA ALA ALA ALA VAL VAL ARG THR THR LEU LEU ALA ALA THR THR SER SER ARG SER GLY GLY GLU GLU GLN GLN PRO PRO GLN GLN ASP ASP SER SER GLY GLY ALA ALA ALA GLU GLU LEU LEU PRO PRO LEU LEU ASP ASP SER SER SER SER ILE ILE GLY GLY LYS LYS LEU LEU ILE ILE SER SER SER SER THR THR THR THR ALA ALA LYS LYS ALA ALA ALA ALA ILE ILE GLY GLY LEU LEU LEU VAL VAL GLY GLY LEU LEU MET MET SER SER LEU LEU SER SER GLY GLY PRO PRO

[illegible]

THR	LEU	GLU	PRO	ALA	THR	SER	THR	THR	SER	LEU	LEU	THR	ASP	ARG																			
1193	1202	1205	1208	1211	1216	1217	1218	1219	1226	1227	1228	1229	1230	1231	1237	1243	1246	1250	1251	1252	1253	1254	1259	1263	1267	1271	1272	1273	1274	1275	1276	1277	1278

[illegible]

340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524	525	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544	545	546	547	548	549	550	551	552	553	554	555	556	557	558	559	560	561	562	563	564	565	566	567	568	569	570	571	572	573	574	575	576	577	578	579	580	581	582	583	584	585	586	587	588	589	590	591	592	593	594	595	596	597	598	599	600	601	602	603	604	605	606	607	608	609	610	611	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632	633	634	635	636	637	638	639	640	641	642	643	644	645	646	647	648	649	650	651	652	653	654	655	656	657	658	659	660	661	662	663	664	665	666	667	668	669	670	671	672	673	674	675	676	677	678	679	680	681	682	683	684	685	686	687	688	689	690	691	692	693	694	695	696	697	698	699	700	701	702	703	704	705	706	707	708	709	710	711	712	713	714	715	716	717	718	719	720	721	722	723	724	725	726	727	728	729	730	731	732	733	734	735	736	737	738	739	740	741	742	743	744	745	746	747	748	749	750	751	752	753	754	755	756	757	758	759	760	761	762	763	764	765	766	767	768	769	770	771	772	773	774	775	776	777	778	779	780	781	782	783	784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850
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Year	2016	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032	2033	2034	2035	2036	2037	2038	2039	2040	2041	2042	2043	2044	2045	2046	2047	2048	2049	2050	2051	2052	2053	2054	2055	2056	2057	2058	2059	2060	2061	2062	2063	2064	2065	2066	2067	2068	2069	2070	2071	2072	2073	2074	2075	2076	2077	2078	2079	2080	2081	2082	2083	2084	2085	2086	2087	2088	2089	2090	2091	2092	2093	2094	2095	2096	2097	2098	2099	2100																																								
Population	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200

Year	0-14	15-24	25-34	35-44	45-54	55-64	65-74	75-84	85-94	95-104
2000	6	7	7	8	8	9	10	10	11	11
2005	5	6	6	7	7	8	8	9	9	10
2010	6	7	7	8	8	9	10	10	11	11
2015	6	7	7	8	8	9	10	10	11	11
2020	6	7	7	8	8	9	10	10	11	11
2025	6	7	7	8	8	9	10	10	11	11
2030	6	7	7	8	8	9	10	10	11	11
2035	6	7	7	8	8	9	10	10	11	11
2040	6	7	7	8	8	9	10	10	11	11
2045	6	7	7	8	8	9	10	10	11	11
2050	6	7	7	8	8	9	10	10	11	11
2055	6	7	7	8	8	9	10	10	11	11
2060	6	7	7	8	8	9	10	10	11	11
2065	6	7	7	8	8	9	10	10	11	11
2070	6	7	7	8	8	9	10	10	11	11
2075	6	7	7	8	8	9	10	10	11	11
2080	6	7	7	8	8	9	10	10	11	11
2085	6	7	7	8	8	9	10	10	11	11
2090	6	7	7	8	8	9	10	10	11	11
2095	6	7	7	8	8	9	10	10	11	11
2100	6	7	7	8	8	9	10	10	11	11

Year	Number of Publications
2000	1
2001	2
2002	3
2003	1
2004	5
2005	3
2006	7
2007	10
2008	10
2009	10
2010	10
2011	10
2012	10
2013	10
2014	10
2015	10
2016	10
2017	10
2018	10
2019	10
2020	2
2021	5
2022	9
2023	9

Age Group	A	B	C	D	E
18-24	7	3	3	4	5
25-34	7	7	1	2	2
35-44	3	3	4	4	5
45-54	6	7	6	7	6
55-64	6	7	9	9	0
65+	1	0	0	0	8

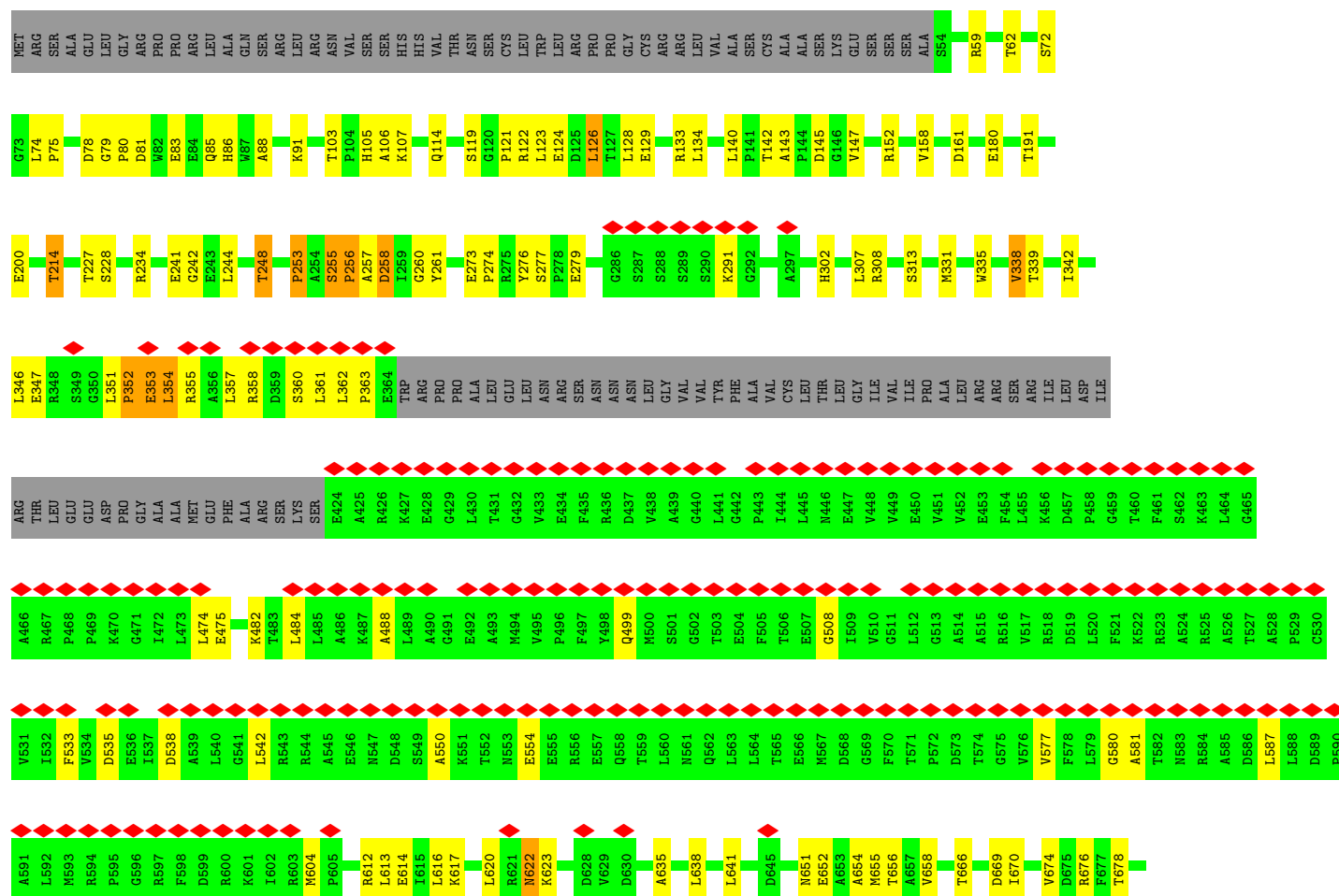
0005
0006
026

HR	HE	FS
1085		
1086		
1091		
1098		
1103		
1104		
1105		
1106		
1107		
1108		
1109		
1110		
1111		
1112		

- Molecule 2: Fhl3





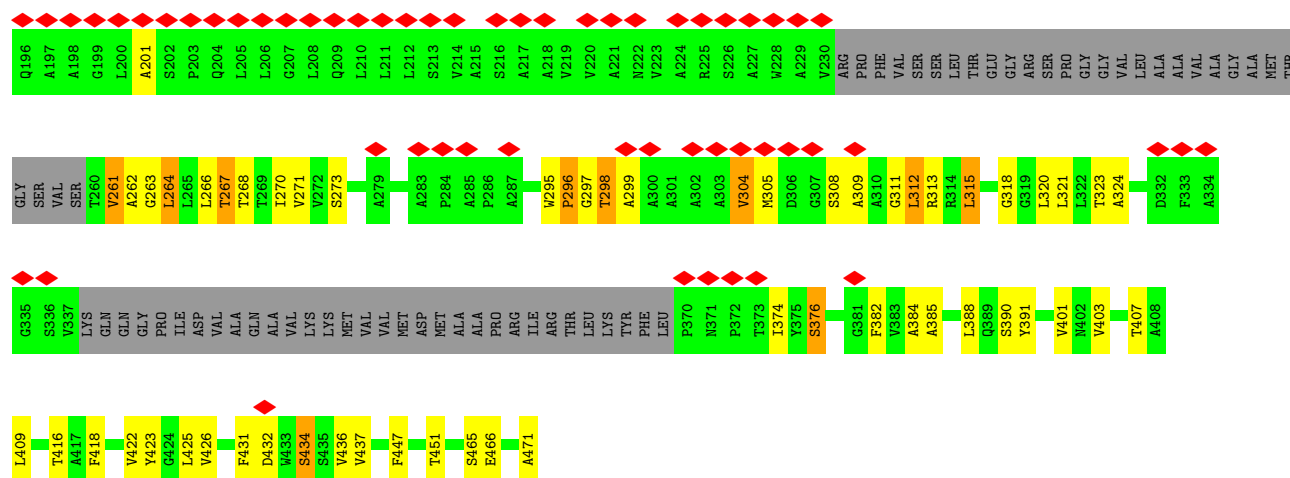




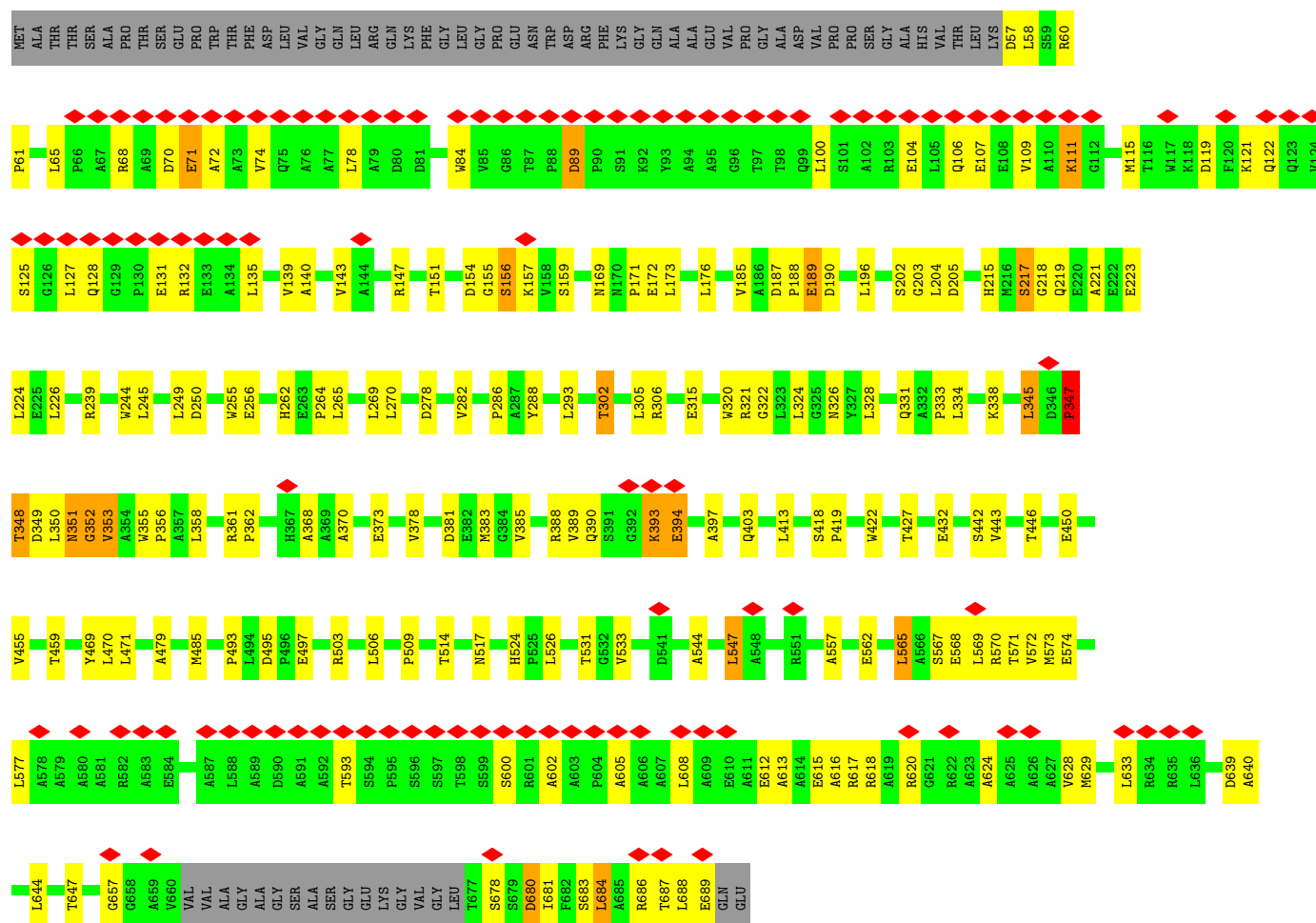
Gln	D543	1336	Ser	Pro	Val	Leu	Met			
	LEU	A337						ALA	GLY	ALA
	THR	P338						THR	VAL	ALA
	ALA	R546						ALA	GLY	THR
	ALA	A547						ALA	GLY	ALA
	GLN	A548						SER	GLY	ALA
	ASP	L344						ALA	SER	ALA
	GLN	T552						SER	GLY	SER
	GLU	Y353						ASP	VAL	ARG
	ALA	L555						PRO	ALA	ARG
ARG	R556	ALA	ASP	THR						
Gln	N569	F368	PRO	SER	SER	HIS				
	GLN	L369	GLU	GLY	SER	LEU				
	VAL	L572	GLU	ASN	ALA	GLY				
	GLU	L383	PRO	GLY	ALA	ARG				
	GLY	V576	ALA	SER	CYS	VAL				
	ARG	S393	ALA	THR	SER	SER				
	GLU	W394	ALA	GLY	SER	CYS				
	GLU	P581	ALA	SER	SER	VAL				
	SER	S584	SER	ASN	GLY	GLY				
	GLY	E602	H416	GLY	GLY	VAL				
Val	L607	L418	ASP	ALA	ILE	THR				
	PRO	T419	L266	ALA	ARG	ARG				
	ALA	R608	P267	ALA	SER	LEU				
	ALA	L609	V421	ALA	VAL	ALA				
	VAL	L610	E268	ALA	CYS	VAL				
	ALA	T611	T269	ALA	THR	LEU				
			Q270	THR	SER	LEU				
		V614	A440	ALA	GLY	ARG				
		Q613	R442	ALA	PRO	ALA				
		E622	V444	ALA	VAL	GLY				
Gln	T626	I449	R282	PRO	ARG	GLN				
	Y627	R450	G284	ASN	GLY	LEU				
	R628	L451	A285	HIS	ARG	ASN				
		F452	D286	PRO	PRO	GLY				
	E632	A453	F287	PRO	LEU	GLN				
	V633	S454	P288	GLY	PRO	ARG				
	G635	V455	P289	SER	SER	ALA				
	E636	G456		SER	ALA	GLY				
	Y637	H457	P293	ASN	LEU	ALA				
		E638	F296	GLY	ARG	GLY				
Gln	A639	D462	ASP	ASP	ARG	ALA				
		D463	G464	ASN	ARG	THR				
	Q643	L300		GLY	ARG	ALA				
	L644	F470	A309	SER	GLY	VAL				
	A645	H471		SER	ALA	ALA				
	A646	S498	V313	ALA	SER	GLN				
	A647		V316	ALA	PRO	VAL				
	A648	S521	Y327	ALA	ILE	THR				
	Q649		Y327	SER	VAL	THR				
	O650	E538	Y332	THR	GLY	TRP				

Category	Color	Relative Frequency (approx.)
MET	Grey	0.05
GLY	Yellow	0.05
GLU	Yellow	0.05
LEU	Yellow	0.05
ALA	Yellow	0.05
ARG	Yellow	0.05
LYS	Yellow	0.05
SER	Yellow	0.05
ALA	Yellow	0.05
SER	Yellow	0.05
ALA	Yellow	0.05
GLY	Yellow	0.05
PRO	Yellow	0.05
ARG	Yellow	0.05
VAL	Yellow	0.05
GLN	Yellow	0.05
MET	Grey	0.05
R23	Orange	0.05
V34	Orange	0.05
K35	Orange	0.05
E36	Orange	0.05
D37	Yellow	0.05
K40	Orange	0.05
T48	Yellow	0.05
K49	Red	0.05
E50	Orange	0.05
K51	Orange	0.05
L52	Orange	0.05
K53	Orange	0.05
E56	Yellow	0.05
S80	Yellow	0.05
L83	Yellow	0.05
E91	Yellow	0.05
D95	Yellow	0.05
I105	Yellow	0.05
Q108	Yellow	0.05
R113	Yellow	0.05
D118	Orange	0.05
Q121	Yellow	0.05
R122	Yellow	0.05
V123	Yellow	0.05
V124	Green	0.05
R130	Green	0.05
S131	Green	0.05
E132	Green	0.05
N137	Green	0.05

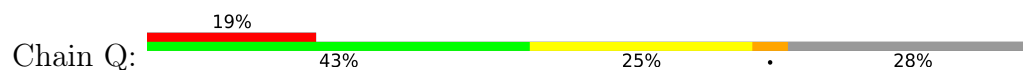
A122	A123	A124	A125	L126	Q127	G128	P129	Q130	L131	L132	L133	A134	S135	P136	A137	A138	A139	D140	P141	W142	L146	L147	V150	Y154	L155	R156	A157	A158	F161	L162	Q163	A166	A167	A170	R177	R180	L181	A182	L183	T184	A185	A186	A187	Y188	G189	M190	V191	A192	V193	L194	T195					
GLN	SER	SER	ALA	ALA	VAL	VAL	PRO	ALA	LEU	VAL	LYS	GLN	VAL	SER	THR	SER	GLY	HIS	ALA	ARG	ASP	ALA	VAL	PRO	ASP	PRO	ASN	ARG	THR	PHE	P93	E94	R95	P96	L97	S98	T99	M100	R101	A102	A103	G104	T105	Q106	Y107	L108	T110	G111	A112	A113	V116	A117	A118	G119	A120	V121
THR	LYS	ASP	ALA	ALA	VAL	VAL	PRO	PRO	ALA	LEU	VAL	LYS	GLN	VAL	VAL	SER	THR	SER	GLY	HIS	ALA	ARG	ASP	ALA	VAL	PRO	ASN	ARG	THR	PHE	P93	E94	R95	P96	L97	S98	T99	M100	R101	A102	A103	G104	T105	Q106	Y107	L108	T110	G111	A112	A113	V116	A117	A118	G119	A120	V121
GLN	SER	SER	ALA	ALA	VAL	VAL	PRO	PRO	ALA	LEU	VAL	LYS	GLN	VAL	VAL	SER	THR	SER	GLY	HIS	ALA	ARG	ASP	ALA	VAL	PRO	ASN	ARG	THR	PHE	P93	E94	R95	P96	L97	S98	T99	M100	R101	A102	A103	G104	T105	Q106	Y107	L108	T110	G111	A112	A113	V116	A117	A118	G119	A120	V121
THR	LYS	ASP	ALA	ALA	VAL	VAL	PRO	PRO	ALA	LEU	VAL	LYS	GLN	VAL	VAL	SER	THR	SER	GLY	HIS	ALA	ARG	ASP	ALA	VAL	PRO	ASN	ARG	THR	PHE	P93	E94	R95	P96	L97	S98	T99	M100	R101	A102	A103	G104	T105	Q106	Y107	L108	T110	G111	A112	A113	V116	A117	A118	G119	A120	V121
GLN	SER	SER	ALA	ALA	VAL	VAL	PRO	PRO	ALA	LEU	VAL	LYS	GLN	VAL	VAL	SER	THR	SER	GLY	HIS	ALA	ARG	ASP	ALA	VAL	PRO	ASN	ARG	THR	PHE	P93	E94	R95	P96	L97	S98	T99	M100	R101	A102	A103	G104	T105	Q106	Y107	L108	T110	G111	A112	A113	V116	A117	A118	G119	A120	V121
THR	LYS	ASP	ALA	ALA	VAL	VAL	PRO	PRO	ALA	LEU	VAL	LYS	GLN	VAL	VAL	SER	THR	SER	GLY	HIS	ALA	ARG	ASP	ALA	VAL	PRO	ASN	ARG	THR	PHE	P93	E94	R95	P96	L97	S98	T99	M100	R101	A102	A103	G104	T105	Q106	Y107	L108	T110	G111	A112	A113	V116	A117	A118	G119	A120	V121
GLN	SER	SER	ALA	ALA	VAL	VAL	PRO	PRO	ALA	LEU	VAL	LYS	GLN	VAL	VAL	SER	THR	SER	GLY	HIS	ALA	ARG	ASP	ALA	VAL	PRO	ASN	ARG	THR	PHE	P93	E94	R95	P96	L97	S98	T99	M100	R101	A102	A103	G104	T105	Q106	Y107	L108	T110	G111	A112	A113	V116	A117	A118	G119	A120	V121
THR	LYS	ASP	ALA	ALA	VAL	VAL	PRO	PRO	ALA	LEU	VAL	LYS	GLN	VAL	VAL	SER	THR	SER	GLY	HIS	ALA	ARG	ASP	ALA	VAL	PRO	ASN	ARG	THR	PHE	P93	E94	R95	P96	L97	S98	T99	M100	R101	A102	A103	G104	T105	Q106	Y107	L108	T110	G111	A112	A113	V116	A117	A118	G119	A120	V121
GLN	SER	SER	ALA	ALA	VAL	VAL	PRO	PRO	ALA	LEU	VAL	LYS	GLN	VAL	VAL	SER	THR	SER	GLY	HIS	ALA	ARG	ASP	ALA	VAL	PRO	ASN	ARG	THR	PHE	P93	E94	R95	P96	L97	S98	T99	M100	R101	A102	A103	G104	T105	Q106	Y107	L108	T110	G111	A112	A113	V116	A117	A118	G119	A120	V121
THR	LYS	ASP	ALA	ALA	VAL	VAL	PRO	PRO	ALA	LEU	VAL	LYS	GL																																											



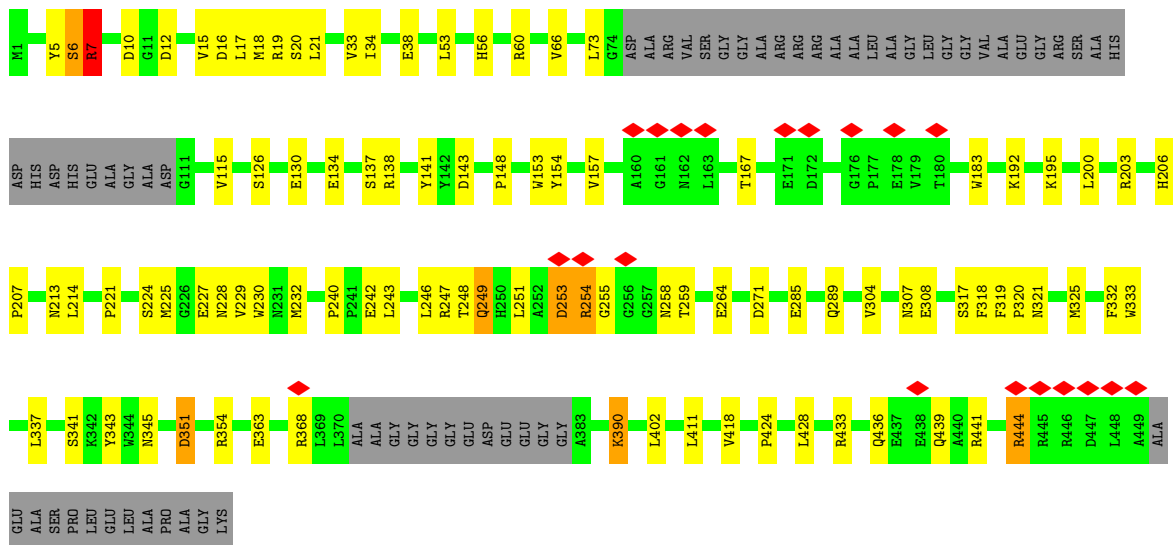
• Molecule 15: Ctap7



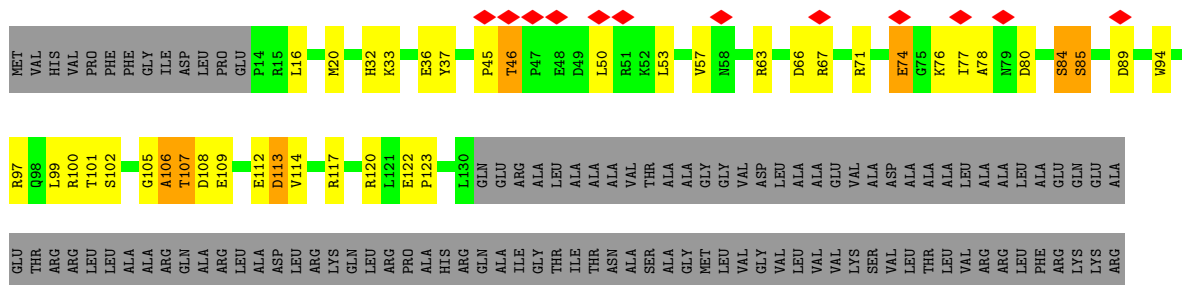
• Molecule 16: Tic22



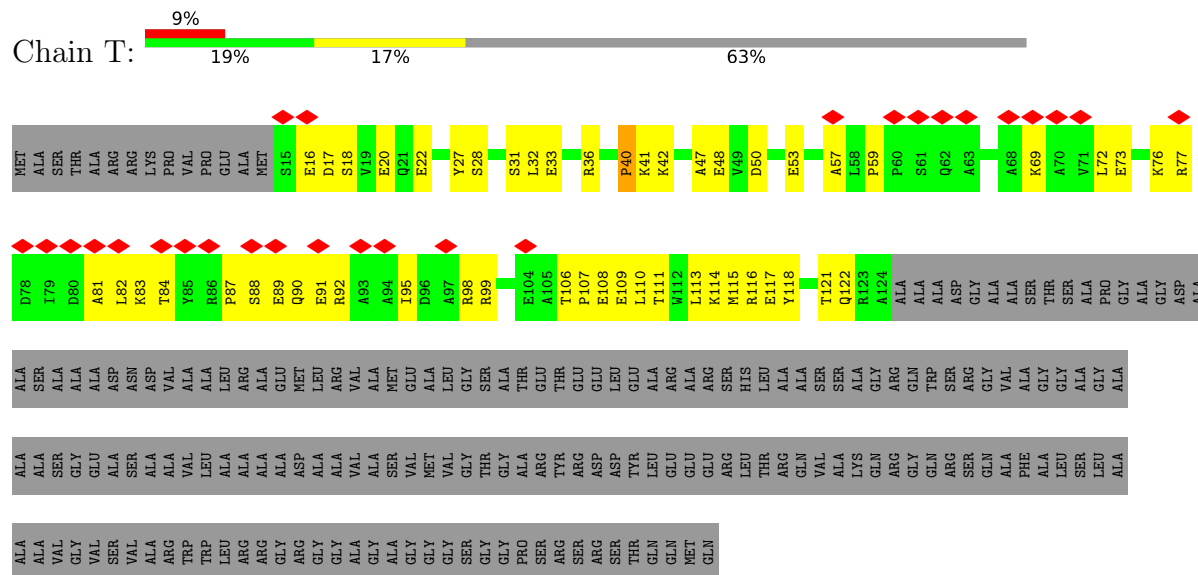
- Molecule 17: DnaJ



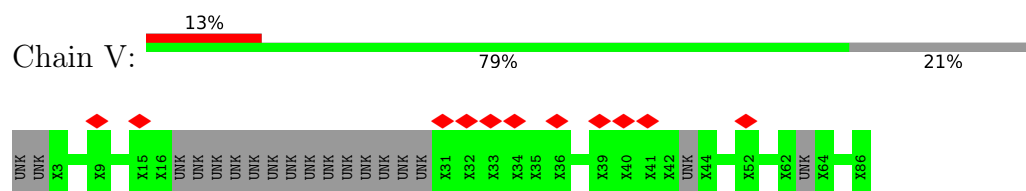
- Molecule 18: CrTam35



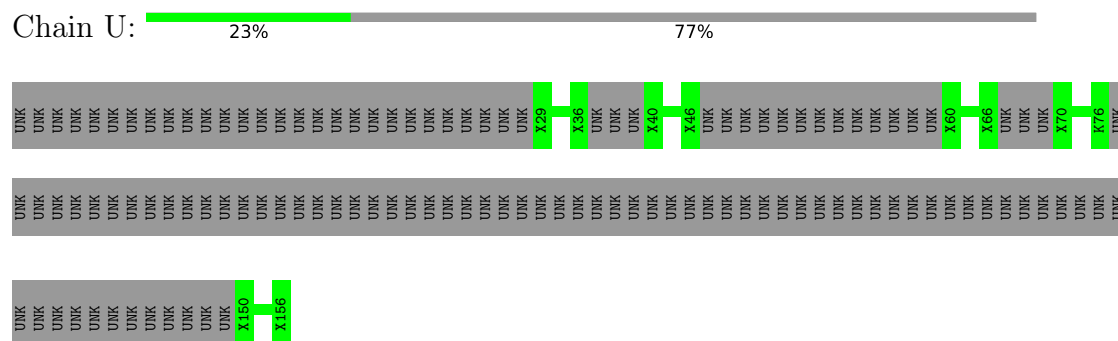
- Molecule 19: CrTam31



- Molecule 20: UNK



- Molecule 21: UNK



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	172550	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.162	Depositor
Minimum map value	-1.990	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.131	Depositor
Recommended contour level	0.45	Depositor
Map size ($\text{\AA}$)	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, TPO, ZN, MG, DGD, Y01, SEP, ANP, 4HH, LMG, DGA, A1LXL

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	0.41	0/7792	0.53	1/10575 (0.0%)
2	B	0.42	0/5925	0.56	2/8024 (0.0%)
2	C	0.41	0/5432	0.56	0/7359
3	D	0.42	0/12978	0.57	5/17507 (0.0%)
4	E	0.38	0/6360	0.52	1/8671 (0.0%)
5	F	0.37	0/5432	0.53	1/7366 (0.0%)
6	G	0.34	0/2999	0.56	2/4087 (0.0%)
7	H	0.45	0/3324	0.49	1/4515 (0.0%)
8	I	0.52	0/2177	0.56	0/2958
9	J	0.41	0/625	0.66	2/839 (0.2%)
10	K	0.54	0/1627	0.62	2/2223 (0.1%)
11	L	0.46	0/1303	0.52	0/1786
12	M	0.41	0/3103	0.56	3/4258 (0.1%)
13	N	0.58	1/945 (0.1%)	0.66	0/1280
14	O	0.33	0/2084	0.54	0/2874
15	P	0.26	0/4601	0.55	1/6273 (0.0%)
16	Q	0.21	0/2115	0.49	0/2857
17	R	0.40	0/3224	0.58	1/4379 (0.0%)
18	S	0.22	0/936	0.44	0/1267
19	T	0.18	0/862	0.45	0/1164
21	U	0.19	0/45	0.31	0/58
All	All	0.40	1/73889 (0.0%)	0.55	22/100320 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
3	D	0	3
5	F	0	1
6	G	0	3
8	I	0	1
13	N	0	2
17	R	0	1
All	All	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	91	GLU	C-O	-9.21	1.12	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2891	PHE	CA-CB-CG	-19.92	93.88	113.80
15	P	347	PRO	N-CA-CB	-13.79	88.77	103.25
9	J	75	THR	N-CA-C	-7.76	103.54	113.16
4	E	253	PRO	N-CA-CB	-6.78	96.13	103.25
5	F	590	PRO	O-C-N	-6.51	118.09	121.15
1	A	1163	PRO	N-CA-CB	6.45	110.13	103.23
12	M	287	PHE	CB-CA-C	6.31	117.45	108.68
3	D	2891	PHE	CB-CA-C	6.23	122.81	110.42
3	D	2891	PHE	N-CA-CB	6.05	120.71	110.49
2	B	443	VAL	N-CA-C	-5.87	106.76	111.81
6	G	253	GLU	N-CA-C	-5.78	105.33	112.38
3	D	2894	ASP	CA-CB-CG	5.75	118.35	112.60
10	K	188	LYS	CB-CA-C	-5.72	101.30	110.79
12	M	288	PRO	N-CA-CB	-5.68	100.01	103.19
12	M	287	PHE	N-CA-CB	-5.67	100.76	110.11
10	K	99	PRO	N-CA-CB	-5.42	96.89	103.45
17	R	7	ARG	N-CA-C	-5.37	106.65	114.12
2	B	454	LEU	N-CA-C	-5.22	107.08	113.50
6	G	251	LEU	N-CA-C	-5.16	106.25	113.37
7	H	243	PRO	N-CA-CB	-5.13	96.96	102.60
3	D	2633	PRO	N-CA-C	5.12	123.02	112.47
9	J	74	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	685	ARG	Sidechain
1	A	686	ARG	Sidechain
2	B	448	ARG	Sidechain
2	B	450	ARG	Sidechain
2	B	496	ARG	Sidechain
2	C	448	ARG	Sidechain
2	C	450	ARG	Sidechain
3	D	966	ARG	Sidechain
3	D	968	ARG	Sidechain
3	D	972	ARG	Sidechain
5	F	706	ARG	Sidechain
6	G	256	ARG	Sidechain
6	G	257	ARG	Sidechain
6	G	265	ARG	Sidechain
8	I	306	ARG	Sidechain
13	N	130	ARG	Sidechain
13	N	49	ARG	Sidechain
17	R	7	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7627	0	7581	131	0
2	B	5844	0	5785	134	0
2	C	5324	0	5301	130	0
3	D	12719	0	13028	296	0
4	E	6229	0	5674	126	0
5	F	5333	0	5318	106	0
6	G	2931	0	2867	68	0
7	H	3246	0	3152	53	0
8	I	2119	0	2069	30	0
9	J	651	0	658	17	0
10	K	1567	0	1558	17	0
11	L	1254	0	1246	17	0
12	M	3000	0	2945	48	0
13	N	921	0	917	12	0
14	O	2040	0	1739	43	0
15	P	4510	0	4451	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Q	2078	0	2090	74	0
17	R	3160	0	3000	73	0
18	S	951	0	924	27	0
19	T	868	0	824	45	0
20	V	340	0	76	0	0
21	U	188	0	63	0	0
22	A	46	0	61	3	0
22	C	25	0	31	0	0
22	I	32	0	33	1	0
22	K	41	0	52	0	0
22	M	48	0	66	2	0
23	A	31	0	13	1	0
23	C	31	0	13	1	0
23	E	31	0	13	2	0
23	F	31	0	13	0	0
24	A	1	0	0	0	0
25	A	46	0	54	0	0
25	I	49	0	64	3	0
25	K	45	0	52	0	0
26	D	34	0	50	1	0
26	O	39	0	63	3	0
27	D	35	0	49	0	0
27	M	35	0	49	1	0
28	D	30	0	0	4	0
28	P	30	0	0	7	0
29	I	40	0	38	0	0
29	L	41	0	40	0	0
30	R	2	0	0	0	0
All	All	73643	0	72020	1413	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 10.

All (1413) 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)
15:P:68:ARG:NH2	15:P:347:PRO:HB3	1.24	1.43
14:O:201:ALA:HB2	14:O:311:GLY:HA3	1.30	1.14
15:P:68:ARG:HH21	15:P:347:PRO:CB	1.62	1.12
15:P:68:ARG:NH2	15:P:347:PRO:CB	2.20	1.01
5:F:926:TYR:O	5:F:939:THR:HG23	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:68:ARG:HD2	15:P:347:PRO:HB2	1.37	1.00
15:P:320:TRP:CE3	28:P:701:A1LXL:C07	2.44	0.99
15:P:305:LEU:HD21	28:P:701:A1LXL:C29	1.96	0.95
15:P:68:ARG:HD2	15:P:347:PRO:CB	1.97	0.93
15:P:324:LEU:HD22	28:P:701:A1LXL:C01	2.10	0.82
28:D:3003:A1LXL:C01	15:P:443:VAL:HG21	2.11	0.81
11:L:297:VAL:HG23	11:L:298:PRO:HD3	1.64	0.78
2:C:821:GLU:HG2	2:C:842:GLU:HB3	1.68	0.75
2:C:595:ASP:O	2:C:607:ARG:NH2	2.20	0.75
1:A:471:MET:HA	1:A:474:ILE:HG22	1.68	0.74
10:K:161:ARG:NH1	11:L:202:GLU:OE1	2.21	0.74
2:B:906:ARG:NH1	2:C:1094:SER:OG	2.21	0.74
4:E:612:ARG:NH1	4:E:635:ALA:O	2.20	0.74
3:D:1954:THR:OG1	8:I:365:ARG:NH2	2.21	0.74
15:P:388:ARG:NH1	15:P:389:VAL:O	2.20	0.74
5:F:622:TYR:HB3	5:F:625:LEU:HD23	1.69	0.74
2:B:713:VAL:HA	2:B:753:ILE:HG23	1.71	0.73
17:R:5:TYR:HA	17:R:19:ARG:HE	1.53	0.73
1:A:268:ASN:ND2	1:A:277:GLN:O	2.21	0.73
3:D:2827:ILE:HG13	3:D:2828:ASP:H	1.52	0.73
5:F:587:LEU:HG	5:F:714:ILE:HD11	1.69	0.72
17:R:224:SER:O	17:R:228:ASN:ND2	2.20	0.72
17:R:254:ARG:HH11	19:T:59:PRO:HB3	1.53	0.72
2:B:369:THR:O	2:B:373:LEU:HB2	1.89	0.72
6:G:364:LEU:O	6:G:368:ASN:ND2	2.22	0.72
12:M:462:TRP:O	12:M:464:GLY:N	2.23	0.72
15:P:151:THR:H	15:P:351:ASN:HD21	1.35	0.72
14:O:318:GLY:HA2	14:O:321:LEU:HD12	1.72	0.72
3:D:2679:LYS:O	3:D:2681:LEU:N	2.22	0.72
4:E:727:GLN:O	4:E:735:ARG:NH2	2.22	0.71
17:R:411:LEU:HD13	17:R:428:LEU:HD11	1.72	0.71
6:G:263:SER:HA	6:G:268:ARG:HD3	1.72	0.71
15:P:320:TRP:CZ3	28:P:701:A1LXL:C07	2.73	0.71
16:Q:108:VAL:HG13	16:Q:166:MET:HE3	1.71	0.71
2:C:559:ARG:NH2	2:C:659:GLU:OE1	2.24	0.71
15:P:128:GLN:HA	15:P:132:ARG:HG2	1.72	0.71
1:A:911:ARG:NH1	1:A:949:GLU:OE1	2.23	0.71
12:M:361:HIS:HD2	12:M:394:TRP:HE1	1.38	0.70
3:D:965:LYS:NZ	18:S:85:SEP:O3P	2.24	0.70
14:O:201:ALA:CB	14:O:311:GLY:HA3	2.15	0.70
2:B:610:GLU:OE1	13:N:113:ARG:NH1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:241:GLU:HB2	4:E:261:TYR:CZ	2.27	0.70
7:H:266:LEU:HD23	7:H:272:GLN:HG2	1.72	0.70
6:G:346:SER:O	6:G:350:ASN:ND2	2.23	0.70
5:F:643:CYS:SG	5:F:644:ILE:N	2.64	0.70
1:A:775:THR:HA	1:A:778:MET:HE3	1.74	0.69
2:B:267:GLN:OE1	3:D:1251:ARG:NH1	2.23	0.69
2:C:822:GLU:HG3	2:C:841:VAL:HG13	1.72	0.69
17:R:341:SER:O	17:R:345:ASN:ND2	2.25	0.69
18:S:100:ARG:NH2	18:S:107:TPO:O2P	2.25	0.69
2:C:946:THR:HG21	2:C:948:MET:HE2	1.72	0.69
14:O:142:TRP:CZ2	14:O:309:ALA:HA	2.26	0.69
1:A:548:ARG:NH2	1:A:589:GLN:OE1	2.26	0.69
5:F:622:TYR:HD1	5:F:623:MET:H	1.41	0.69
4:E:346:LEU:O	4:E:351:LEU:N	2.26	0.69
14:O:142:TRP:HZ2	14:O:309:ALA:HA	1.58	0.69
2:C:645:ALA:O	2:C:649:ASN:ND2	2.25	0.69
2:B:346:TPO:O1P	3:D:899:LYS:NZ	2.26	0.69
2:B:615:LEU:HD11	2:B:623:LEU:HB2	1.73	0.69
3:D:904:LYS:NZ	18:S:106:ALA:O	2.26	0.69
15:P:115:MET:HE2	15:P:119:ASP:HB3	1.74	0.69
2:B:679:ALA:O	2:B:685:ARG:NH1	2.26	0.68
3:D:1262:ASN:O	3:D:1266:ASN:HB2	1.94	0.68
3:D:2250:ILE:HG13	3:D:2715:ARG:HD3	1.74	0.68
1:A:422:LYS:HA	1:A:425:LYS:HE2	1.75	0.68
15:P:68:ARG:CZ	15:P:347:PRO:HB3	2.20	0.68
1:A:566:ALA:HA	1:A:613:ASP:HB2	1.76	0.67
2:C:546:LEU:HD12	2:C:586:VAL:HG21	1.76	0.67
4:E:484:LEU:O	4:E:488:ALA:N	2.27	0.67
3:D:2366:ASN:HB2	3:D:2369:LYS:HG3	1.76	0.67
15:P:320:TRP:HE3	28:P:701:A1LXL:C07	2.04	0.67
15:P:345:LEU:C	15:P:347:PRO:HD2	2.19	0.67
2:C:565:LEU:HD12	2:C:669:ALA:HB2	1.75	0.67
3:D:1946:ARG:NH1	3:D:1952:PHE:O	2.26	0.67
16:Q:353:GLU:OE1	16:Q:356:ARG:NH1	2.24	0.67
15:P:239:ARG:NH2	15:P:250:ASP:OD2	2.27	0.67
15:P:547:LEU:HB2	16:Q:250:ALA:HB1	1.77	0.67
3:D:1696:LEU:HD23	13:N:83:LEU:HD21	1.75	0.67
5:F:668:ASP:O	5:F:672:ASN:ND2	2.28	0.67
7:H:212:TRP:O	7:H:249:ASN:ND2	2.28	0.66
2:C:787:GLY:HA2	2:C:793:ASP:OD1	1.96	0.66
1:A:322:ASP:OD1	2:B:231:ARG:NH2	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:405:ALA:HB3	6:G:408:GLU:HG3	1.77	0.66
1:A:905:ARG:NH1	1:A:961:GLU:OE1	2.28	0.66
1:A:782:THR:O	1:A:793:ASP:N	2.29	0.66
2:B:740:ARG:HD3	2:B:764:ASN:HD21	1.61	0.66
3:D:881:LEU:HD11	3:D:986:THR:HG23	1.77	0.66
2:C:430:ASP:OD1	2:C:430:ASP:N	2.17	0.66
15:P:107:GLU:O	15:P:111:LYS:HB2	1.95	0.66
12:M:332:TYR:HD1	12:M:333:MET:HG3	1.60	0.66
15:P:427:THR:HG1	15:P:469:TYR:HH	1.44	0.66
2:B:345:PHE:O	3:D:952:LYS:NZ	2.29	0.66
15:P:305:LEU:CD2	28:P:701:A1LXL:C29	2.72	0.65
6:G:263:SER:HB3	6:G:268:ARG:HG2	1.77	0.65
1:A:147:ASP:OD2	2:B:394:ARG:NH2	2.22	0.65
1:A:576:SER:O	1:A:580:GLU:HG3	1.96	0.65
2:C:640:SER:HB3	3:D:2063:PHE:HE1	1.62	0.65
5:F:572:GLU:HB2	5:F:573:LYS:HE2	1.79	0.65
14:O:426:VAL:HG23	14:O:431:PHE:HB2	1.77	0.65
2:B:740:ARG:NH2	2:B:764:ASN:OD1	2.30	0.65
3:D:2874:ASN:HD22	3:D:2874:ASN:H	1.45	0.65
3:D:2892:ASN:O	3:D:2893:PHE:C	2.39	0.65
5:F:82:PRO:O	5:F:84:LYS:NZ	2.30	0.65
5:F:615:ALA:HB3	5:F:649:GLU:HB3	1.77	0.65
2:B:457:MET:HB2	26:O:3101:DGA:HA92	1.78	0.64
4:E:59:ARG:HH22	19:T:122:GLN:HE22	1.43	0.64
5:F:991:ARG:NH1	5:F:998:GLU:OE1	2.30	0.64
17:R:224:SER:HB2	17:R:227:GLU:HG3	1.78	0.64
17:R:213:ASN:OD1	17:R:214:LEU:N	2.31	0.64
3:D:1325:PHE:O	3:D:1327:ASN:N	2.30	0.64
11:L:242:VAL:HG13	11:L:248:TRP:HB3	1.79	0.64
16:Q:192:ASP:OD1	16:Q:192:ASP:N	2.31	0.64
14:O:305:MET:HE2	14:O:309:ALA:HB1	1.79	0.64
18:S:101:THR:HG22	18:S:106:ALA:HA	1.78	0.64
2:B:541:GLU:OE1	2:B:688:ARG:NH1	2.30	0.64
2:C:1062:ALA:HA	2:C:1065:LYS:HE3	1.80	0.64
3:D:2031:ASP:N	3:D:2031:ASP:OD1	2.31	0.64
1:A:164:GLU:OE1	1:A:188:ARG:NH2	2.29	0.64
3:D:2744:SER:O	3:D:2747:GLN:HG3	1.97	0.64
3:D:2747:GLN:O	3:D:2748:LEU:C	2.39	0.64
5:F:225:GLY:N	5:F:236:VAL:O	2.22	0.64
16:Q:200:LEU:HD21	16:Q:213:PHE:HB2	1.80	0.63
13:N:121:GLN:O	13:N:124:TYR:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:652:LEU:O	2:C:656:ASP:N	2.31	0.63
3:D:1126:ASN:HD22	3:D:1128:ARG:H	1.46	0.63
2:C:779:GLY:HA2	3:D:2562:LEU:HD23	1.81	0.63
4:E:273:GLU:OE2	5:F:186:ARG:NH1	2.30	0.63
4:E:80:PRO:HG2	4:E:85:GLN:HG2	1.81	0.62
7:H:198:ASP:OD1	7:H:198:ASP:N	2.30	0.62
15:P:602:ALA:HB1	15:P:605:ALA:HB3	1.81	0.62
18:S:63:ARG:NH2	18:S:107:TPO:O3P	2.28	0.62
4:E:474:LEU:N	4:E:580:GLY:O	2.30	0.62
7:H:313:ASP:HB2	7:H:315:LYS:HG2	1.81	0.62
8:I:241:VAL:HB	12:M:498:SER:HB2	1.81	0.62
16:Q:166:MET:HA	16:Q:169:VAL:HG13	1.81	0.62
5:F:913:HIS:HB3	5:F:916:TYR:HB2	1.82	0.62
6:G:124:ASN:ND2	6:G:167:ASP:OD1	2.32	0.62
2:B:259:ASN:HB3	2:B:263:GLN:HB2	1.82	0.62
2:C:733:ASP:OD1	3:D:2330:ARG:NH2	2.32	0.62
14:O:323:THR:HG1	14:O:382:PHE:HE1	1.45	0.62
16:Q:312:SER:HA	16:Q:315:ARG:HB2	1.82	0.62
19:T:33:GLU:OE2	19:T:36:ARG:NH1	2.30	0.62
1:A:1067:HIS:ND1	1:A:1069:GLU:OE1	2.32	0.62
2:C:819:ASP:OD1	6:G:134:ARG:NH1	2.32	0.62
3:D:2800:ARG:O	3:D:2802:GLY:N	2.33	0.62
4:E:78:ASP:OD1	4:E:79:GLY:N	2.33	0.62
16:Q:191:PRO:HB3	16:Q:216:VAL:HG13	1.82	0.62
15:P:533:VAL:HG21	16:Q:345:SER:HB3	1.81	0.62
3:D:2152:ASP:O	3:D:2154:SER:N	2.32	0.61
3:D:2366:ASN:ND2	3:D:2366:ASN:O	2.32	0.61
3:D:2504:SER:OG	3:D:2508:LYS:NZ	2.33	0.61
7:H:149:THR:OG1	7:H:150:GLY:N	2.27	0.61
6:G:273:PRO:HB3	6:G:310:PRO:HD2	1.81	0.61
15:P:455:VAL:HG23	15:P:471:LEU:HB2	1.81	0.61
3:D:977:ARG:HD3	17:R:153:TRP:CG	2.34	0.61
5:F:571:PRO:HB2	5:F:575:LYS:HE2	1.83	0.61
19:T:88:SER:OG	19:T:89:GLU:N	2.33	0.61
6:G:371:GLN:NE2	6:G:418:LEU:O	2.33	0.61
3:D:1363:ILE:HG21	17:R:317:SER:HB2	1.83	0.61
15:P:331:GLN:HE22	15:P:479:ALA:HA	1.65	0.61
12:M:556:ARG:NH1	12:M:602:GLU:OE2	2.31	0.61
1:A:650:GLU:HG2	1:A:690:ALA:HB3	1.83	0.61
2:B:629:ASP:N	2:B:629:ASP:OD1	2.32	0.61
3:D:1162:ARG:HG3	17:R:230:TRP:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:296:PRO:HG2	15:P:286:PRO:HA	1.83	0.60
2:C:793:ASP:HB2	2:C:794:PRO:HD3	1.83	0.60
3:D:2650:ASN:HB3	3:D:2653:ASN:HD22	1.66	0.60
5:F:555:LYS:H	5:F:555:LYS:HD2	1.66	0.60
6:G:206:VAL:HG21	6:G:214:SER:HB2	1.83	0.60
2:B:536:LYS:O	2:B:540:ASN:ND2	2.35	0.60
5:F:685:GLN:HG2	5:F:686:GLN:H	1.67	0.60
3:D:957:ARG:HB2	3:D:959:GLU:HG3	1.84	0.60
3:D:1360:SER:N	3:D:1361:GLU:OE1	2.35	0.60
15:P:322:GLY:O	15:P:326:ASN:ND2	2.34	0.60
17:R:441:ARG:HH11	17:R:444:ARG:HH11	1.49	0.60
1:A:542:SER:O	1:A:546:ASN:ND2	2.33	0.60
2:B:883:MET:HG3	3:D:2784:GLN:HG3	1.83	0.60
4:E:722:GLU:OE1	4:E:723:ARG:NH1	2.34	0.60
15:P:68:ARG:CD	15:P:347:PRO:CB	2.76	0.60
1:A:512:ILE:O	1:A:516:ALA:HB2	2.01	0.60
4:E:847:ASP:OD1	4:E:847:ASP:N	2.34	0.60
12:M:614:VAL:O	12:M:618:GLN:NE2	2.24	0.60
2:B:475:HIS:HB3	17:R:34:ILE:HG21	1.84	0.60
2:B:807:GLU:OE2	2:B:838:THR:OG1	2.20	0.60
3:D:2966:ASN:ND2	7:H:460:GLU:OE2	2.35	0.60
2:B:254:GLU:OE1	18:S:120:ARG:NE	2.35	0.60
3:D:1769:GLN:O	3:D:1773:THR:HG23	2.02	0.60
3:D:2097:ARG:NH2	3:D:2294:ASP:OD2	2.34	0.60
12:M:266:LEU:HD13	12:M:270:GLN:HB3	1.83	0.60
1:A:530:GLU:HG3	1:A:535:VAL:HG21	1.82	0.59
2:C:1080:ASP:OD1	2:C:1080:ASP:N	2.34	0.59
15:P:345:LEU:O	15:P:347:PRO:HD2	2.02	0.59
2:B:274:GLN:O	3:D:1258:GLN:NE2	2.34	0.59
16:Q:312:SER:O	16:Q:316:ALA:N	2.35	0.59
5:F:270:ASP:HB3	19:T:83:LYS:HZ1	1.67	0.59
5:F:644:ILE:HD13	5:F:689:VAL:HB	1.85	0.59
2:B:526:TRP:CH2	2:B:539:ILE:HD11	2.37	0.59
15:P:514:THR:O	15:P:524:HIS:NE2	2.30	0.59
15:P:557:ALA:HB3	16:Q:325:SER:H	1.68	0.59
15:P:629:MET:HE2	15:P:633:LEU:HD12	1.83	0.59
10:K:71:PHE:HB2	10:K:72:ILE:HG12	1.85	0.59
17:R:12:ASP:HB3	17:R:15:VAL:HG12	1.84	0.59
17:R:240:PRO:HD2	17:R:243:LEU:HD12	1.83	0.59
12:M:453:ALA:HB1	22:M:801:LMG:H112	1.85	0.59
15:P:334:LEU:H	15:P:390:GLN:HE21	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:276:ILE:HD11	16:Q:295:ARG:HD2	1.85	0.59
3:D:1179:GLN:HA	3:D:1182:TRP:HD1	1.68	0.59
5:F:701:ASP:OD1	5:F:702:ALA:N	2.36	0.59
16:Q:279:GLN:CD	16:Q:292:LEU:HG	2.28	0.59
2:C:374:ARG:HH12	2:C:376:LEU:HD21	1.68	0.58
3:D:2770:LYS:HA	3:D:2773:THR:HG22	1.85	0.58
1:A:162:ASP:OD2	1:A:188:ARG:NH1	2.36	0.58
3:D:549:SER:OG	3:D:572:LYS:NZ	2.36	0.58
3:D:2777:LEU:O	3:D:2779:THR:N	2.36	0.58
4:E:351:LEU:O	4:E:354:LEU:HG	2.02	0.58
4:E:482:LYS:NZ	23:E:1001:ANP:O1G	2.30	0.58
4:E:977:GLN:HA	4:E:980:ALA:HB3	1.84	0.58
5:F:745:SER:O	5:F:749:LEU:HB2	2.04	0.58
1:A:530:GLU:HG2	1:A:539:ARG:NH2	2.19	0.58
5:F:234:THR:HG23	19:T:99:ARG:HG3	1.84	0.58
5:F:638:ARG:NH2	5:F:677:GLU:OE1	2.31	0.58
14:O:374:ILE:H	14:O:374:ILE:HD12	1.69	0.58
4:E:242:GLY:H	4:E:260:GLY:HA3	1.68	0.58
5:F:121:ARG:NH2	17:R:363:GLU:OE1	2.35	0.58
5:F:251:THR:OG1	5:F:254:GLU:OE1	2.20	0.58
5:F:666:GLU:O	5:F:669:ASN:HB3	2.03	0.58
2:B:996:THR:OG1	2:B:999:GLU:OE2	2.20	0.58
3:D:555:HIS:NE2	15:P:450:GLU:OE2	2.37	0.58
1:A:656:LEU:O	1:A:660:THR:HG22	2.04	0.58
5:F:280:VAL:HG11	19:T:72:LEU:HD22	1.86	0.58
15:P:262:HIS:HD2	15:P:265:LEU:H	1.51	0.58
3:D:911:TRP:CE2	3:D:921:LYS:HB2	2.39	0.58
14:O:263:GLY:O	14:O:267:THR:OG1	2.20	0.58
2:C:393:VAL:HG13	2:C:403:VAL:HG13	1.85	0.57
6:G:101:TRP:CZ2	6:G:104:PRO:HD2	2.39	0.57
1:A:364:GLY:O	1:A:367:GLU:HG3	2.04	0.57
3:D:1810:ASN:OD1	3:D:1811:ILE:N	2.37	0.57
7:H:311:ARG:NH2	7:H:317:GLN:HE22	2.02	0.57
1:A:881:GLY:O	1:A:885:GLU:HG3	2.04	0.57
2:C:646:SER:HA	2:C:649:ASN:HD21	1.70	0.57
2:C:655:MET:HA	2:C:658:PHE:HB2	1.85	0.57
3:D:450:ILE:H	3:D:450:ILE:HD12	1.69	0.57
4:E:86:HIS:HD2	4:E:161:ASP:HB3	1.69	0.57
4:E:960:PRO:HB3	5:F:954:ASP:OD1	2.05	0.57
6:G:477:GLU:HA	6:G:480:VAL:HG12	1.85	0.57
3:D:467:THR:O	3:D:471:THR:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:287:PHE:HZ	12:M:296:PHE:HZ	1.52	0.57
15:P:557:ALA:HB2	16:Q:329:VAL:HG23	1.86	0.57
17:R:424:PRO:O	17:R:433:ARG:NH2	2.37	0.57
19:T:73:GLU:O	19:T:77:ARG:HG3	2.05	0.57
2:B:503:SER:OG	2:B:504:LYS:NZ	2.36	0.57
2:C:707:HIS:CE1	2:C:735:MET:HB3	2.40	0.57
3:D:1241:ASN:ND2	17:R:143:ASP:OD1	2.37	0.57
15:P:57:ASP:OD2	15:P:60:ARG:NH2	2.37	0.57
3:D:551:PHE:HB3	3:D:635:TYR:CZ	2.39	0.57
3:D:2891:PHE:O	3:D:2892:ASN:HB2	2.03	0.57
23:E:1001:ANP:O1B	23:E:1001:ANP:O3G	2.22	0.57
17:R:16:ASP:OD1	17:R:17:LEU:N	2.37	0.57
1:A:572:GLY:HA2	2:B:638:GLN:HE22	1.69	0.57
3:D:1261:ARG:NE	18:S:84:SEP:O1P	2.33	0.57
4:E:920:ARG:O	4:E:925:ARG:NH1	2.38	0.57
16:Q:244:ASP:HA	16:Q:247:VAL:HG12	1.86	0.57
1:A:421:SER:OG	1:A:422:LYS:N	2.24	0.57
2:C:482:LEU:HB2	2:C:488:ARG:NH2	2.20	0.57
4:E:638:LEU:HB3	4:E:641:LEU:HD13	1.86	0.57
5:F:284:LEU:O	5:F:288:GLU:HG2	2.05	0.57
15:P:533:VAL:HG12	16:Q:231:MET:HE1	1.87	0.57
4:E:83:GLU:OE1	4:E:83:GLU:N	2.33	0.57
16:Q:262:TYR:CZ	16:Q:307:ARG:HB2	2.39	0.57
2:B:251:ALA:HB3	2:B:254:GLU:HG2	1.85	0.56
3:D:2865:ASP:OD1	3:D:2865:ASP:N	2.35	0.56
4:E:362:LEU:HB3	4:E:363:PRO:HD3	1.86	0.56
4:E:743:ASP:OD1	4:E:747:GLN:NE2	2.38	0.56
14:O:315:LEU:O	14:O:318:GLY:N	2.37	0.56
15:P:569:LEU:O	15:P:573:MET:HG2	2.04	0.56
16:Q:262:TYR:OH	16:Q:307:ARG:HB2	2.04	0.56
16:Q:311:GLU:O	16:Q:315:ARG:N	2.37	0.56
15:P:68:ARG:HH21	15:P:347:PRO:HB3	0.75	0.56
2:C:587:ARG:HH21	2:C:589:PHE:HZ	1.54	0.56
3:D:1386:SER:O	3:D:1386:SER:OG	2.21	0.56
5:F:995:SER:N	5:F:998:GLU:OE2	2.24	0.56
15:P:151:THR:OG1	15:P:157:LYS:NZ	2.35	0.56
2:B:513:GLU:OE1	2:B:515:ARG:NH1	2.39	0.56
3:D:2097:ARG:HH22	3:D:2297:THR:HG23	1.71	0.56
4:E:872:LYS:HD2	4:E:935:MET:HB3	1.88	0.56
9:J:84:GLU:OE1	10:K:98:ARG:NH1	2.38	0.56
12:M:552:THR:HG21	12:M:572:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:307:ASN:OD1	17:R:307:ASN:N	2.38	0.56
19:T:117:GLU:O	19:T:121:THR:HG22	2.06	0.56
2:B:579:ALA:O	2:B:583:GLU:HG2	2.06	0.56
3:D:1781:ASP:OD1	3:D:1781:ASP:N	2.39	0.56
4:E:62:THR:HG22	4:E:147:VAL:HG12	1.88	0.56
4:E:81:ASP:OD1	5:F:207:TYR:OH	2.23	0.56
17:R:253:ASP:N	17:R:253:ASP:OD1	2.35	0.56
1:A:875:ARG:HB3	3:D:2185:ASN:HD21	1.71	0.56
2:C:511:ALA:O	2:C:614:ARG:NH1	2.38	0.56
3:D:2735:LYS:O	3:D:2739:HIS:HD2	1.89	0.56
9:J:71:ASP:O	9:J:72:4HH:C	2.53	0.56
17:R:15:VAL:HA	17:R:18:MET:HE2	1.86	0.56
3:D:2296:ILE:O	3:D:2300:LEU:HB2	2.06	0.55
12:M:538:GLU:OE2	12:M:539:GLY:N	2.37	0.55
3:D:1414:SER:HB2	3:D:1763:THR:HG23	1.88	0.55
3:D:2878:ARG:NH1	4:E:855:PRO:O	2.39	0.55
3:D:2970:ARG:NH2	7:H:196:ASP:O	2.38	0.55
4:E:129:GLU:HG2	4:E:152:ARG:HG2	1.87	0.55
4:E:277:SER:OG	4:E:279:GLU:OE2	2.22	0.55
12:M:607:LEU:O	12:M:611:THR:HG23	2.05	0.55
15:P:217:SER:O	15:P:217:SER:OG	2.21	0.55
3:D:1308:ASN:HB2	3:D:1316:VAL:HG21	1.87	0.55
3:D:2182:GLU:OE1	3:D:2687:ASN:ND2	2.39	0.55
1:A:477:MET:HA	1:A:481:ASP:HB3	1.87	0.55
3:D:2298:ASP:HA	3:D:2301:VAL:HG12	1.89	0.55
1:A:146:MET:O	1:A:149:THR:OG1	2.24	0.55
5:F:621:MET:HE1	5:F:663:SER:HA	1.88	0.55
5:F:635:ASN:HA	5:F:638:ARG:HD2	1.88	0.55
2:B:545:TYR:HB2	2:B:552:LEU:HD22	1.89	0.55
2:B:806:TYR:OH	2:B:887:ASP:OD2	2.22	0.55
3:D:961:ARG:HG2	3:D:962:ARG:CZ	2.37	0.55
16:Q:193:MET:HA	16:Q:196:VAL:HB	1.89	0.55
16:Q:254:ARG:O	16:Q:258:GLN:HG2	2.06	0.55
1:A:481:ASP:OD1	1:A:481:ASP:N	2.37	0.55
1:A:1047:ASP:OD1	1:A:1048:LEU:N	2.40	0.55
2:B:526:TRP:HB2	2:B:583:GLU:HG3	1.89	0.55
3:D:1364:ASN:ND2	17:R:317:SER:OG	2.40	0.55
2:B:826:VAL:HG22	2:B:838:THR:HG23	1.89	0.55
3:D:1130:ILE:HD13	17:R:246:LEU:HD13	1.89	0.55
5:F:237:GLU:OE2	5:F:249:GLY:N	2.33	0.55
12:M:409:TRP:H	12:M:416:HIS:HE1	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:754:THR:OG1	2:B:755:GLU:N	2.38	0.54
2:C:872:LYS:HD3	2:C:877:GLU:HG3	1.90	0.54
23:C:1202:ANP:O1A	23:C:1202:ANP:N3B	2.39	0.54
3:D:1670:ASP:HB3	3:D:1673:THR:HG22	1.89	0.54
2:B:1106:GLU:OE2	2:B:1109:ARG:NH1	2.40	0.54
3:D:753:THR:OG1	3:D:754:LEU:N	2.40	0.54
4:E:128:LEU:HD21	5:F:104:LEU:HD21	1.89	0.54
6:G:328:CYS:HB3	6:G:452:LEU:HB2	1.89	0.54
16:Q:99:ASP:OD1	16:Q:99:ASP:N	2.40	0.54
2:C:843:ASP:OD1	2:C:843:ASP:N	2.38	0.54
3:D:632:TYR:O	3:D:636:LYS:HB2	2.07	0.54
5:F:828:PRO:HG2	5:F:848:LYS:HD2	1.89	0.54
1:A:617:LEU:HD12	3:D:2236:VAL:HG11	1.90	0.54
2:B:208:GLU:HA	2:B:211:LEU:HG	1.90	0.54
7:H:421:LYS:O	7:H:424:ARG:HG3	2.07	0.54
1:A:509:ALA:O	1:A:512:ILE:HG13	2.08	0.54
1:A:823:ASP:OD1	1:A:823:ASP:N	2.40	0.54
3:D:2874:ASN:HD22	3:D:2874:ASN:N	2.04	0.54
15:P:172:GLU:HG2	15:P:173:LEU:N	2.23	0.54
2:B:697:ALA:HB1	2:B:724:ARG:HE	1.72	0.54
3:D:1811:ILE:HD12	3:D:1812:SER:N	2.23	0.54
4:E:538:ASP:O	4:E:542:LEU:N	2.40	0.54
4:E:666:THR:OG1	4:E:669:ASP:OD1	2.26	0.54
2:C:634:ALA:O	2:C:638:GLN:NE2	2.35	0.54
6:G:106:GLU:OE2	6:G:332:GLN:HB3	2.08	0.54
15:P:616:ALA:O	15:P:620:ARG:HG2	2.08	0.54
19:T:106:THR:N	19:T:109:GLU:OE2	2.39	0.54
3:D:2178:LEU:O	3:D:2877:ARG:NH1	2.37	0.54
8:I:265:ARG:HH11	10:K:79:VAL:HG23	1.73	0.54
12:M:441:ALA:HA	12:M:444:VAL:HG12	1.88	0.54
2:C:524:ILE:HG12	2:C:575:LEU:HD22	1.89	0.53
2:C:622:ILE:HG23	2:C:665:VAL:HG23	1.89	0.53
3:D:2631:LEU:O	3:D:2632:LEU:C	2.50	0.53
6:G:355:THR:HG22	6:G:356:ALA:H	1.73	0.53
9:J:72:4HH:C	9:J:74:ASP:H	2.21	0.53
1:A:774:GLU:HG2	1:A:778:MET:HE2	1.90	0.53
4:E:354:LEU:HD13	4:E:355:ARG:HH21	1.73	0.53
18:S:16:LEU:O	18:S:20:MET:HG3	2.08	0.53
2:C:429:LEU:HB2	4:E:256:PRO:HG3	1.90	0.53
3:D:736:ASN:O	28:D:3003:A1LXL:C26	2.56	0.53
2:B:508:ARG:HD2	3:D:1776:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:444:VAL:HA	12:M:449:ILE:HD11	1.89	0.53
16:Q:198:HIS:O	16:Q:201:GLN:HG3	2.08	0.53
2:B:642:ASP:OD1	2:B:642:ASP:N	2.41	0.53
4:E:214:THR:O	4:E:214:THR:OG1	2.26	0.53
14:O:323:THR:OG1	14:O:382:PHE:HE1	1.91	0.53
15:P:633:LEU:HD11	15:P:644:LEU:HD13	1.90	0.53
2:C:821:GLU:OE2	2:C:860:ARG:NH2	2.42	0.53
3:D:2269:ARG:NH1	3:D:2272:TYR:OH	2.41	0.53
8:I:198:TRP:HE1	8:I:200:ARG:HE	1.55	0.53
15:P:368:ALA:HB2	15:P:608:LEU:HD11	1.90	0.53
2:C:515:ARG:HH12	2:C:588:MET:H	1.56	0.53
2:C:525:LYS:N	2:C:528:ASP:OD2	2.37	0.53
4:E:200:GLU:OE2	4:E:200:GLU:N	2.38	0.53
5:F:269:LEU:HD11	19:T:82:LEU:HD12	1.89	0.53
5:F:926:TYR:O	5:F:939:THR:CG2	2.45	0.53
12:M:440:ALA:O	12:M:443:LEU:HD23	2.07	0.53
16:Q:237:PHE:HA	16:Q:350:VAL:HG22	1.90	0.53
2:B:511:ALA:HB2	2:B:611:THR:HG23	1.91	0.53
6:G:113:ALA:HB1	6:G:486:LEU:HD23	1.91	0.53
14:O:142:TRP:HH2	14:O:313:ARG:HG3	1.74	0.53
4:E:358:ARG:HD3	4:E:361:LEU:HD12	1.91	0.53
2:B:216:GLN:HG2	2:B:217:MET:H	1.73	0.53
3:D:554:ASP:OD2	15:P:353:VAL:HG12	2.08	0.53
3:D:1243:ASN:HA	3:D:1325:PHE:HD2	1.73	0.53
15:P:334:LEU:O	15:P:390:GLN:N	2.37	0.53
3:D:2694:SER:HB3	3:D:2695:PRO:HD2	1.90	0.52
7:H:345:TRP:O	7:H:348:LYS:NZ	2.39	0.52
17:R:130:GLU:N	17:R:130:GLU:OE1	2.42	0.52
2:B:533:ASP:O	2:B:536:LYS:HB3	2.10	0.52
5:F:234:THR:OG1	19:T:99:ARG:NH1	2.42	0.52
6:G:387:TRP:O	6:G:391:THR:OG1	2.26	0.52
12:M:270:GLN:HA	12:M:273:VAL:HG12	1.90	0.52
17:R:195:LYS:HB2	19:T:27:TYR:HE2	1.73	0.52
6:G:134:ARG:HH21	6:G:400:HIS:HB3	1.75	0.52
12:M:632:GLU:HA	12:M:635:ASP:OD2	2.09	0.52
1:A:746:MET:HB3	1:A:927:GLU:HB3	1.90	0.52
2:C:997:GLY:O	6:G:261:SER:HB2	2.08	0.52
3:D:983:ASN:O	3:D:987:GLU:HG2	2.10	0.52
3:D:2160:ASN:O	3:D:2164:THR:HG23	2.10	0.52
6:G:134:ARG:NH2	6:G:400:HIS:HB3	2.25	0.52
15:P:262:HIS:CD2	15:P:265:LEU:H	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:525:LYS:N	2:B:528:ASP:OD2	2.42	0.52
3:D:2344:HIS:ND1	3:D:2345:THR:HG23	2.25	0.52
3:D:2958:SER:O	3:D:2962:ILE:HG12	2.10	0.52
4:E:106:ALA:HB1	19:T:116:ARG:HB2	1.90	0.52
4:E:740:ARG:NH2	4:E:831:SER:HA	2.24	0.52
9:J:72:4HH:C	9:J:74:ASP:N	2.71	0.52
14:O:267:THR:O	14:O:270:ILE:HG13	2.09	0.52
17:R:225:MET:O	17:R:229:VAL:HG22	2.10	0.52
1:A:285:GLU:OE1	1:A:290:LYS:NZ	2.42	0.52
3:D:563:LYS:HD2	3:D:564:THR:N	2.23	0.52
4:E:335:TRP:O	4:E:339:THR:HG23	2.10	0.52
7:H:345:TRP:CD1	7:H:345:TRP:H	2.26	0.52
9:J:72:4HH:O	9:J:74:ASP:N	2.43	0.52
12:M:338:PRO:HG2	12:M:340:TRP:CD1	2.45	0.52
16:Q:230:ASP:O	17:R:354:ARG:NH1	2.38	0.52
17:R:53:LEU:O	17:R:321:ASN:HB3	2.08	0.52
19:T:27:TYR:HB3	19:T:31:SER:HB2	1.91	0.52
1:A:458:PHE:HA	1:A:461:ILE:HD11	1.91	0.52
2:C:552:LEU:HA	2:C:555:ARG:HB2	1.92	0.52
2:C:698:LEU:O	2:C:702:LYS:HG2	2.10	0.52
3:D:973:PRO:HB3	3:D:975:TRP:NE1	2.25	0.52
3:D:2065:ILE:HD12	3:D:2066:GLY:N	2.24	0.52
6:G:190:LEU:O	6:G:194:THR:HG22	2.10	0.52
6:G:269:GLU:OE1	6:G:402:LEU:HB3	2.10	0.52
16:Q:276:ILE:HG21	16:Q:296:LEU:HD13	1.90	0.52
2:B:526:TRP:HE1	2:B:536:LYS:HZ2	1.58	0.52
2:C:614:ARG:HA	2:C:617:ASN:HD21	1.74	0.52
8:I:82:GLU:OE1	8:I:82:GLU:N	2.42	0.52
12:M:289:PRO:HB3	12:M:546:ARG:HH21	1.74	0.52
14:O:142:TRP:CH2	14:O:313:ARG:HG3	2.45	0.52
18:S:46:THR:O	18:S:50:LEU:HD23	2.10	0.52
2:B:526:TRP:HE1	2:B:536:LYS:NZ	2.07	0.52
16:Q:269:TYR:HA	16:Q:272:ASP:HB2	1.92	0.52
18:S:113:ASP:OD1	18:S:113:ASP:N	2.42	0.52
1:A:574:PRO:O	1:A:578:GLU:HG2	2.10	0.52
3:D:1182:TRP:HE3	3:D:1230:LEU:HD22	1.75	0.52
5:F:245:GLY:HA3	19:T:114:LYS:HD3	1.92	0.52
7:H:173:LYS:O	7:H:174:ASP:HB2	2.09	0.52
2:C:373:LEU:HD23	2:C:417:LEU:HB3	1.91	0.51
2:C:586:VAL:HB	2:C:621:ALA:HA	1.92	0.51
3:D:271:GLN:NE2	12:M:471:HIS:H	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:808:ARG:HH22	5:F:886:GLU:HB3	1.74	0.51
7:H:437:ALA:O	7:H:441:GLN:HG2	2.10	0.51
1:A:530:GLU:HG2	1:A:539:ARG:HH22	1.75	0.51
2:C:896:ARG:HH11	2:C:944:HIS:HD2	1.58	0.51
3:D:2336:GLU:H	3:D:2336:GLU:CD	2.18	0.51
4:E:126:LEU:HD22	4:E:158:VAL:HG11	1.92	0.51
6:G:359:CYS:SG	6:G:363:ARG:NH1	2.78	0.51
11:L:175:PRO:O	11:L:179:VAL:HG23	2.10	0.51
2:B:533:ASP:HA	2:B:536:LYS:HB3	1.93	0.51
2:C:621:ALA:O	2:C:664:ILE:HA	2.11	0.51
3:D:988:ARG:NH1	17:R:141:TYR:HB2	2.26	0.51
15:P:68:ARG:CD	15:P:347:PRO:HB2	2.25	0.51
15:P:572:VAL:HG23	15:P:629:MET:HE1	1.91	0.51
5:F:617:GLU:O	5:F:629:ARG:NH1	2.44	0.51
15:P:84:TRP:HE1	15:P:100:LEU:HB2	1.75	0.51
16:Q:182:LEU:HD12	16:Q:185:ILE:HB	1.91	0.51
3:D:1761:PRO:HD3	14:O:471:ALA:HB3	1.93	0.51
5:F:911:SER:OG	5:F:912:SER:N	2.42	0.51
8:I:155:ARG:HH21	8:I:156:ARG:HH12	1.59	0.51
1:A:493:LYS:N	1:A:623:GLU:OE1	2.38	0.51
2:B:1002:HIS:O	2:B:1006:SER:OG	2.28	0.51
15:P:140:ALA:HA	15:P:143:VAL:HG12	1.92	0.51
6:G:250:TYR:C	6:G:252:ALA:H	2.18	0.51
6:G:275:ASP:OD1	6:G:309:HIS:NE2	2.35	0.51
6:G:441:THR:O	6:G:445:VAL:HG23	2.11	0.51
12:M:462:TRP:HB2	27:M:802:Y01:HAD2	1.91	0.51
2:B:563:VAL:HG13	2:B:688:ARG:HB2	1.92	0.51
2:C:571:THR:HB	2:C:573:LYS:HE3	1.93	0.51
4:E:652:GLU:O	4:E:656:THR:HG23	2.11	0.51
8:I:198:TRP:NE1	8:I:200:ARG:HE	2.09	0.51
8:I:235:SER:HB3	8:I:244:VAL:HB	1.93	0.51
9:J:38:ALA:O	9:J:42:GLU:HG2	2.11	0.51
15:P:288:TYR:OH	15:P:503:ARG:O	2.29	0.51
15:P:351:ASN:O	15:P:352:GLY:C	2.53	0.51
15:P:547:LEU:HD13	16:Q:254:ARG:HD3	1.92	0.51
3:D:810:LEU:O	3:D:814:LEU:HG	2.11	0.51
5:F:232:VAL:O	19:T:99:ARG:NH2	2.39	0.51
12:M:419:THR:OG1	12:M:422:GLU:OE1	2.29	0.51
16:Q:242:ASP:HB3	16:Q:355:LEU:HD23	1.92	0.51
16:Q:257:ALA:HA	16:Q:260:LYS:NZ	2.26	0.51
2:B:713:VAL:HA	2:B:753:ILE:CG2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:741:ILE:HD11	5:F:778:ASN:HA	1.93	0.51
5:F:946:ASN:OD1	5:F:946:ASN:N	2.41	0.51
9:J:55:GLU:H	9:J:58:LYS:NZ	2.09	0.51
11:L:160:ALA:O	11:L:164:VAL:HG23	2.11	0.51
15:P:278:ASP:O	15:P:282:VAL:HG23	2.11	0.51
15:P:615:GLU:OE1	15:P:618:ARG:NH1	2.44	0.51
19:T:42:LYS:HG2	19:T:48:GLU:HG3	1.92	0.51
3:D:65:GLN:HB3	7:H:454:TYR:HE1	1.75	0.50
3:D:2458:GLU:HG3	7:H:480:MET:HE2	1.93	0.50
3:D:2632:LEU:O	3:D:2634:LYS:N	2.44	0.50
12:M:309:ALA:O	12:M:313:VAL:HG22	2.10	0.50
18:S:114:VAL:HG22	18:S:117:ARG:HH21	1.76	0.50
2:C:380:GLN:H	2:C:380:GLN:CD	2.16	0.50
2:C:458:LEU:O	2:C:461:THR:HG22	2.10	0.50
3:D:1418:CYS:SG	3:D:1762:ASP:HB2	2.52	0.50
4:E:274:PRO:HD3	5:F:121:ARG:NH2	2.26	0.50
6:G:473:GLU:OE1	6:G:476:ARG:NH2	2.44	0.50
15:P:70:ASP:O	15:P:72:ALA:N	2.44	0.50
18:S:71:ARG:HH21	18:S:77:ILE:HA	1.75	0.50
1:A:176:ASN:HB2	18:S:32:HIS:CD2	2.47	0.50
4:E:499:GLN:HA	4:E:533:PHE:O	2.11	0.50
4:E:670:ILE:O	4:E:674:VAL:HG23	2.12	0.50
8:I:337:ASN:HB3	8:I:339:GLY:H	1.76	0.50
1:A:256:ASP:OD1	1:A:257:SER:N	2.44	0.50
1:A:786:THR:HG23	1:A:787:ASN:H	1.76	0.50
3:D:1361:GLU:O	3:D:1365:SER:OG	2.26	0.50
7:H:122:LEU:HD12	7:H:327:LEU:HD21	1.93	0.50
1:A:740:PRO:HD2	1:A:760:ILE:HD11	1.93	0.50
2:B:598:ASP:HB2	2:B:600:TYR:CE1	2.46	0.50
2:B:699:GLY:O	2:B:703:ILE:HG13	2.11	0.50
2:C:641:GLY:O	2:C:645:ALA:CB	2.60	0.50
2:C:691:TYR:HB2	4:E:681:GLU:HG3	1.93	0.50
4:E:74:LEU:O	5:F:244:ARG:NH2	2.37	0.50
12:M:264:ASP:HA	12:M:286:ASP:OD1	2.11	0.50
12:M:353:TYR:OH	12:M:383:LEU:O	2.21	0.50
15:P:680:ASP:OD1	15:P:680:ASP:N	2.45	0.50
1:A:692:SER:OG	1:A:694:PRO:HD2	2.12	0.50
4:E:976:LYS:HE3	4:E:977:GLN:HE21	1.76	0.50
5:F:635:ASN:OD1	5:F:636:THR:N	2.45	0.50
3:D:2892:ASN:O	3:D:2894:ASP:N	2.44	0.50
4:E:342:ILE:O	4:E:346:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:150:TRP:NE1	6:G:152:TYR:O	2.45	0.50
15:P:393:LYS:HG3	15:P:394:GLU:H	1.77	0.50
2:B:441:THR:HG22	2:B:442:GLY:H	1.77	0.50
2:B:751:HIS:CD2	2:B:751:HIS:H	2.30	0.50
15:P:333:PRO:HA	15:P:390:GLN:HE21	1.76	0.50
16:Q:201:GLN:HA	16:Q:204:LYS:HG2	1.93	0.50
16:Q:204:LYS:NZ	16:Q:205:ASP:OD1	2.38	0.50
18:S:109:GLU:HB2	18:S:113:ASP:HB2	1.93	0.50
2:C:774:SER:O	3:D:2168:LEU:HD21	2.12	0.50
16:Q:113:VAL:HG21	16:Q:145:ILE:HG22	1.94	0.50
3:D:2124:ARG:HE	4:E:823:GLN:HE21	1.60	0.49
14:O:150:VAL:HG22	14:O:315:LEU:HG	1.94	0.49
3:D:449:LEU:O	3:D:453:LYS:HG2	2.12	0.49
3:D:750:PRO:HG3	15:P:215:HIS:CE1	2.47	0.49
14:O:295:TRP:O	14:O:297:GLY:N	2.46	0.49
15:P:338:LYS:HE2	15:P:388:ARG:HB2	1.94	0.49
3:D:1127:LEU:HD12	19:T:47:ALA:HB1	1.93	0.49
3:D:2059:VAL:HG21	3:D:2293:LEU:HD12	1.94	0.49
4:E:351:LEU:C	4:E:353:GLU:N	2.70	0.49
3:D:1947:TRP:HB2	13:N:108:GLN:HE22	1.77	0.49
4:E:622:ASN:OD1	4:E:622:ASN:N	2.44	0.49
18:S:74:GLU:O	18:S:76:LYS:N	2.42	0.49
1:A:300:ASP:OD1	1:A:300:ASP:N	2.37	0.49
1:A:556:PHE:HE2	1:A:558:ASP:HB2	1.76	0.49
2:B:231:ARG:NH1	15:P:190:ASP:HA	2.27	0.49
3:D:901:PHE:HD1	3:D:941:LEU:HD13	1.77	0.49
3:D:1369:LYS:HE3	3:D:1373:ASN:ND2	2.26	0.49
4:E:701:GLU:OE2	4:E:736:THR:OG1	2.25	0.49
7:H:254:SER:OG	7:H:255:LYS:N	2.43	0.49
15:P:71:GLU:HA	15:P:74:VAL:HG23	1.95	0.49
15:P:657:GLY:O	15:P:686:ARG:NH2	2.45	0.49
16:Q:225:THR:OG1	16:Q:233:TYR:O	2.21	0.49
2:B:517:ASP:HB3	2:B:520:SER:HB2	1.95	0.49
2:C:598:ASP:N	2:C:643:GLU:OE2	2.36	0.49
4:E:88:ALA:HA	4:E:91:LYS:HE2	1.94	0.49
4:E:124:GLU:N	4:E:124:GLU:OE1	2.44	0.49
11:L:217:ARG:NH2	13:N:96:ASP:OD1	2.44	0.49
1:A:254:TYR:OH	1:A:287:ASP:OD2	2.21	0.49
1:A:692:SER:OG	1:A:693:LEU:N	2.45	0.49
2:B:632:GLY:O	2:B:676:ILE:HA	2.12	0.49
12:M:313:VAL:HA	12:M:316:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:632:GLU:OE2	12:M:633:VAL:HG23	2.12	0.49
15:P:68:ARG:H	15:P:348:THR:HG23	1.78	0.49
19:T:17:ASP:N	19:T:17:ASP:OD1	2.46	0.49
1:A:714:ASP:N	1:A:714:ASP:OD1	2.45	0.49
2:B:1103:TYR:O	2:B:1107:VAL:HG13	2.12	0.49
6:G:251:LEU:C	6:G:253:GLU:H	2.21	0.49
6:G:398:SER:OG	6:G:399:PHE:N	2.44	0.49
12:M:361:HIS:CD2	12:M:394:TRP:HE1	2.23	0.49
15:P:393:LYS:HZ3	15:P:397:ALA:H	1.60	0.49
1:A:321:TRP:HD1	15:P:185:VAL:HG23	1.78	0.49
1:A:471:MET:HE1	1:A:508:LEU:HD21	1.95	0.49
2:C:525:LYS:HD3	2:C:527:ASP:H	1.77	0.49
2:C:635:ARG:HH22	2:C:645:ALA:HB1	1.77	0.49
11:L:246:LEU:HD13	11:L:284:VAL:HG11	1.95	0.49
16:Q:139:GLU:OE1	16:Q:139:GLU:N	2.30	0.49
1:A:575:GLY:HA3	1:A:579:ARG:HH21	1.78	0.49
2:B:227:ALA:HA	2:B:230:VAL:HG12	1.95	0.49
2:B:593:GLY:HA2	2:B:631:MET:SD	2.53	0.49
3:D:1249:SER:OG	3:D:1250:LYS:N	2.45	0.49
4:E:276:TYR:CE1	4:E:302:HIS:HB3	2.48	0.49
9:J:55:GLU:H	9:J:58:LYS:HZ3	1.60	0.49
15:P:256:GLU:OE2	15:P:306:ARG:NH1	2.46	0.49
15:P:293:LEU:HD12	15:P:485:MET:HG3	1.94	0.49
15:P:678:SER:HA	15:P:681:ILE:HG22	1.95	0.49
17:R:258:ASN:OD1	17:R:258:ASN:N	2.46	0.49
1:A:258:ALA:O	1:A:260:ASN:N	2.44	0.48
1:A:1088:PRO:C	1:A:1090:PHE:H	2.21	0.48
2:B:340:MET:HE2	3:D:953:ALA:HA	1.93	0.48
2:C:1058:ASP:OD1	2:C:1058:ASP:N	2.46	0.48
3:D:1918:LYS:N	3:D:1919:PRO:HD2	2.28	0.48
3:D:2255:PRO:C	3:D:2257:THR:H	2.21	0.48
3:D:2883:ASN:O	3:D:2883:ASN:ND2	2.42	0.48
6:G:287:LEU:O	6:G:290:ARG:NH1	2.43	0.48
7:H:344:GLU:H	7:H:344:GLU:CD	2.21	0.48
7:H:478:GLU:O	7:H:481:GLU:HG3	2.13	0.48
12:M:273:VAL:O	12:M:277:GLU:HB2	2.13	0.48
15:P:393:LYS:NZ	15:P:397:ALA:H	2.11	0.48
16:Q:263:LYS:HD3	16:Q:263:LYS:HA	1.52	0.48
2:B:580:ILE:HG13	2:B:581:ALA:N	2.29	0.48
2:C:597:TYR:OH	2:C:630:ALA:O	2.21	0.48
3:D:2249:LYS:HB3	3:D:2249:LYS:HE2	1.68	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:105:HIS:ND1	4:E:107:LYS:HG2	2.28	0.48
6:G:147:THR:O	6:G:147:THR:OG1	2.26	0.48
8:I:60:SER:OG	8:I:61:ASN:N	2.45	0.48
15:P:565:LEU:HD11	15:P:640:ALA:HA	1.95	0.48
16:Q:137:ARG:HH12	16:Q:194:LYS:HE3	1.77	0.48
19:T:81:ALA:O	19:T:84:THR:OG1	2.31	0.48
1:A:195:LEU:O	1:A:197:GLN:HG3	2.13	0.48
1:A:479:LYS:HD3	1:A:518:VAL:HG11	1.95	0.48
3:D:1811:ILE:O	3:D:1815:PHE:HB2	2.12	0.48
5:F:949:ARG:O	5:F:949:ARG:HG2	2.12	0.48
14:O:447:PHE:O	14:O:451:THR:HG23	2.12	0.48
1:A:693:LEU:HB3	1:A:694:PRO:HD3	1.95	0.48
2:C:602:GLY:HA3	4:E:508:GLY:H	1.78	0.48
15:P:61:PRO:HB3	15:P:156:SER:HB2	1.96	0.48
2:C:475:HIS:HA	2:C:479:LEU:HG	1.94	0.48
2:C:488:ARG:NH1	13:N:132:GLU:OE1	2.47	0.48
3:D:1750:LEU:HA	3:D:1753:THR:HG22	1.94	0.48
3:D:2275:ARG:NH1	5:F:929:GLY:O	2.46	0.48
14:O:135:SER:CB	14:O:308:SER:HB3	2.43	0.48
15:P:419:PRO:HA	15:P:422:TRP:CE2	2.48	0.48
17:R:253:ASP:OD2	17:R:254:ARG:NH2	2.46	0.48
1:A:435:SER:OG	1:A:436:SER:N	2.46	0.48
2:B:272:LEU:HD22	17:R:148:PRO:HB2	1.95	0.48
3:D:67:PHE:HB3	7:H:453:PRO:HB2	1.96	0.48
3:D:2177:ASN:OD1	3:D:2892:ASN:ND2	2.46	0.48
4:E:475:GLU:O	4:E:604:MET:HG2	2.13	0.48
10:K:230:LEU:HD21	10:K:236:VAL:HG23	1.95	0.48
12:M:454:SER:O	12:M:457:HIS:HB3	2.14	0.48
15:P:219:GLN:O	15:P:223:GLU:HG2	2.13	0.48
1:A:658:LEU:HD21	3:D:2749:ASN:HD22	1.77	0.48
1:A:744:VAL:HB	1:A:929:ILE:HG22	1.94	0.48
1:A:1028:ASP:OD1	1:A:1028:ASP:N	2.46	0.48
2:B:730:THR:O	2:B:734:VAL:HG23	2.13	0.48
2:C:700:ARG:O	2:C:704:MET:HG2	2.13	0.48
3:D:336:LEU:HD11	26:O:3101:DGA:HBH1	1.95	0.48
17:R:436:GLN:O	17:R:439:GLN:HG3	2.14	0.48
1:A:556:PHE:CE2	1:A:558:ASP:HB2	2.49	0.48
2:B:532:ILE:O	2:B:536:LYS:N	2.43	0.48
2:B:822:GLU:O	2:B:841:VAL:HG12	2.14	0.48
3:D:62:LYS:O	3:D:62:LYS:HG2	2.13	0.48
3:D:907:LYS:NZ	18:S:108:ASP:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1250:LYS:HG3	3:D:1319:GLU:CD	2.38	0.48
3:D:1762:ASP:OD1	3:D:1762:ASP:N	2.41	0.48
6:G:320:VAL:HG13	6:G:348:LEU:HD21	1.95	0.48
1:A:782:THR:HB	1:A:793:ASP:HA	1.96	0.48
2:B:877:GLU:OE1	2:B:877:GLU:N	2.41	0.48
2:C:822:GLU:HA	6:G:262:SER:HB3	1.96	0.48
3:D:318:SER:O	3:D:318:SER:OG	2.32	0.48
5:F:232:VAL:HB	19:T:99:ARG:HH12	1.79	0.48
5:F:551:ILE:HD12	5:F:597:LEU:HD12	1.95	0.48
6:G:254:THR:O	6:G:255:THR:C	2.57	0.48
15:P:612:GLU:HA	15:P:615:GLU:HB2	1.96	0.48
15:P:684:LEU:O	15:P:687:THR:OG1	2.29	0.48
16:Q:144:LEU:O	16:Q:148:ILE:HG12	2.14	0.48
19:T:91:GLU:O	19:T:95:ILE:HG12	2.14	0.48
1:A:442:MET:SD	1:A:442:MET:N	2.87	0.48
3:D:2733:LEU:HD23	3:D:2733:LEU:HA	1.66	0.48
4:E:616:LEU:O	4:E:620:LEU:HG	2.13	0.48
5:F:227:VAL:HG12	5:F:236:VAL:HB	1.95	0.48
5:F:720:ASP:OD1	5:F:721:PHE:N	2.38	0.48
6:G:261:SER:O	6:G:262:SER:C	2.57	0.48
15:P:185:VAL:HG13	15:P:196:LEU:HD12	1.95	0.48
1:A:148:TRP:CD1	1:A:148:TRP:H	2.30	0.47
2:B:647:ILE:HG13	2:B:648:ILE:N	2.28	0.47
2:C:477:TRP:CD2	2:C:478:ILE:HG23	2.49	0.47
3:D:342:LEU:HD13	17:R:325:MET:HE1	1.95	0.47
3:D:2870:ASP:OD1	3:D:2870:ASP:N	2.44	0.47
5:F:569:ARG:HG3	5:F:570:THR:HG23	1.96	0.47
11:L:292:LEU:HD22	11:L:296:VAL:HG11	1.95	0.47
14:O:268:THR:HA	14:O:271:VAL:HG12	1.95	0.47
16:Q:257:ALA:HA	16:Q:260:LYS:HD3	1.96	0.47
2:B:644:SER:HA	2:B:647:ILE:HG12	1.95	0.47
3:D:1227:GLN:NE2	3:D:1334:ASN:O	2.47	0.47
3:D:2065:ILE:HA	3:D:2068:LYS:HE2	1.96	0.47
3:D:2934:LEU:HD11	3:D:2963:ILE:HD12	1.96	0.47
4:E:255:SER:C	4:E:257:ALA:H	2.22	0.47
4:E:307:LEU:HD11	5:F:118:GLU:HG3	1.96	0.47
5:F:565:VAL:HG23	5:F:602:VAL:HG23	1.96	0.47
8:I:78:ALA:O	8:I:80:ALA:N	2.45	0.47
16:Q:171:GLU:O	16:Q:175:THR:HG23	2.14	0.47
18:S:94:TRP:CD1	18:S:97:ARG:HH21	2.32	0.47
2:B:711:LYS:HD2	2:B:711:LYS:HA	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:145:ASP:N	4:E:145:ASP:OD1	2.47	0.47
3:D:271:GLN:HE22	12:M:470:PHE:HB3	1.78	0.47
3:D:1137:ASN:HD21	3:D:1162:ARG:HD2	1.79	0.47
3:D:2016:ASN:HD21	3:D:2306:VAL:HG23	1.79	0.47
3:D:2777:LEU:C	3:D:2779:THR:H	2.22	0.47
4:E:121:PRO:O	4:E:122:ARG:NH1	2.47	0.47
12:M:580:LEU:HD12	12:M:581:PRO:HD2	1.96	0.47
15:P:147:ARG:HA	15:P:147:ARG:HD3	1.68	0.47
2:B:226:VAL:HA	2:B:229:VAL:HG12	1.96	0.47
2:C:774:SER:OG	2:C:775:THR:N	2.47	0.47
3:D:334:TYR:O	3:D:338:PRO:HD2	2.14	0.47
3:D:348:THR:HG23	3:D:1374:LYS:HB3	1.96	0.47
3:D:554:ASP:OD1	15:P:355:TRP:HB3	2.14	0.47
15:P:121:LYS:O	15:P:125:SER:OG	2.24	0.47
16:Q:260:LYS:HA	16:Q:263:LYS:HB2	1.96	0.47
19:T:109:GLU:O	19:T:113:LEU:HD12	2.14	0.47
3:D:1779:TRP:CE3	3:D:1779:TRP:HA	2.49	0.47
3:D:2679:LYS:HA	3:D:2679:LYS:HD3	1.60	0.47
6:G:340:THR:HG23	6:G:343:ALA:H	1.78	0.47
11:L:157:ALA:O	11:L:161:VAL:HG23	2.15	0.47
11:L:259:TRP:NE1	14:O:466:GLU:OE2	2.42	0.47
3:D:570:GLN:O	3:D:573:LEU:HD23	2.15	0.47
3:D:735:GLN:NE2	3:D:737:ILE:O	2.47	0.47
3:D:2126:GLU:OE1	4:E:831:SER:N	2.43	0.47
15:P:288:TYR:HE1	15:P:503:ARG:HB3	1.80	0.47
2:C:407:THR:HG22	2:C:408:ARG:H	1.80	0.47
2:C:1033:LYS:HE3	2:C:1033:LYS:HB3	1.69	0.47
3:D:2883:ASN:HA	3:D:2886:SER:O	2.14	0.47
15:P:239:ARG:HH21	15:P:250:ASP:HB2	1.79	0.47
16:Q:182:LEU:HG	16:Q:184:GLY:H	1.79	0.47
1:A:682:LEU:O	1:A:683:THR:C	2.58	0.47
2:B:600:TYR:HE2	2:B:603:VAL:HG11	1.79	0.47
2:B:677:ASP:OD1	2:B:679:ALA:N	2.34	0.47
2:C:919:THR:HG22	2:C:920:SER:H	1.80	0.47
5:F:239:PRO:HB2	5:F:241:ASP:OD1	2.14	0.47
7:H:422:THR:HA	7:H:425:VAL:HG22	1.97	0.47
15:P:351:ASN:ND2	15:P:351:ASN:H	2.12	0.47
17:R:390:LYS:HB3	17:R:390:LYS:HE2	1.38	0.47
1:A:165:LEU:HB3	22:A:1201:LMG:H132	1.97	0.47
2:C:370:GLN:O	2:C:372:VAL:HG13	2.15	0.47
2:C:902:MET:HG2	4:E:780:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1127:LEU:HD11	17:R:247:ARG:HB2	1.96	0.47
3:D:2022:PRO:HG2	3:D:2342:ASN:HB2	1.96	0.47
17:R:192:LYS:HB3	17:R:195:LYS:HE3	1.96	0.47
1:A:323:PRO:HG2	15:P:188:PRO:HG3	1.96	0.46
2:B:576:LEU:HD23	2:B:576:LEU:H	1.80	0.46
3:D:1243:ASN:HA	3:D:1325:PHE:CD2	2.50	0.46
4:E:241:GLU:OE2	4:E:244:LEU:HD13	2.15	0.46
9:J:100:THR:HG23	9:J:103:ASP:OD2	2.15	0.46
1:A:785:LYS:HD3	1:A:790:VAL:HG13	1.96	0.46
2:B:497:GLU:HG3	17:R:21:LEU:HD11	1.97	0.46
3:D:914:ASP:OD2	3:D:920:ARG:NE	2.47	0.46
3:D:1418:CYS:SG	3:D:1763:THR:OG1	2.73	0.46
11:L:244:ASN:N	11:L:244:ASN:OD1	2.48	0.46
15:P:89:ASP:OD1	15:P:89:ASP:N	2.47	0.46
16:Q:330:VAL:O	16:Q:334:THR:HG23	2.15	0.46
19:T:118:TYR:OH	19:T:122:GLN:NE2	2.45	0.46
2:C:445:GLU:HG3	2:C:449:LEU:HG	1.96	0.46
3:D:1172:THR:O	3:D:1178:ASN:HB2	2.15	0.46
7:H:237:LYS:HE3	7:H:237:LYS:HB3	1.71	0.46
12:M:287:PHE:HZ	12:M:296:PHE:CZ	2.32	0.46
12:M:637:ILE:HD12	12:M:637:ILE:HA	1.82	0.46
14:O:273:SER:HB2	14:O:324:ALA:HB2	1.96	0.46
15:P:135:LEU:O	15:P:139:VAL:HG13	2.15	0.46
15:P:154:ASP:OD1	15:P:155:GLY:N	2.49	0.46
2:C:381:LEU:HD22	2:C:420:VAL:HG11	1.97	0.46
4:E:140:LEU:HG	4:E:143:ALA:HB3	1.97	0.46
4:E:654:ALA:O	4:E:658:VAL:HG13	2.15	0.46
6:G:116:CYS:SG	6:G:117:LEU:N	2.88	0.46
8:I:151:ARG:O	8:I:154:GLN:HG3	2.16	0.46
15:P:302:THR:HG23	15:P:446:THR:HB	1.97	0.46
16:Q:254:ARG:NH1	16:Q:255:ASN:OD1	2.48	0.46
1:A:933:ARG:O	1:A:937:ILE:HG13	2.16	0.46
2:C:397:GLY:H	3:D:1374:LYS:NZ	2.13	0.46
2:C:614:ARG:HA	2:C:617:ASN:ND2	2.31	0.46
2:C:872:LYS:HB2	2:C:872:LYS:HE3	1.56	0.46
3:D:960:THR:HG22	3:D:961:ARG:H	1.81	0.46
3:D:1239:LYS:HD2	3:D:1239:LYS:HA	1.75	0.46
3:D:2596:LYS:HD2	7:H:174:ASP:OD1	2.15	0.46
4:E:613:LEU:O	4:E:617:LYS:HG2	2.15	0.46
14:O:266:LEU:O	14:O:270:ILE:HG23	2.16	0.46
18:S:53:LEU:O	18:S:57:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ILE:HD11	1:A:491:CYS:HB2	1.98	0.46
2:B:704:MET:HE2	2:B:704:MET:HB3	1.80	0.46
2:C:619:ALA:HB1	2:C:662:ARG:HB2	1.97	0.46
3:D:1990:ASN:OD1	3:D:1993:LEU:HD13	2.16	0.46
17:R:251:LEU:HD12	17:R:251:LEU:O	2.15	0.46
19:T:88:SER:O	19:T:92:ARG:NH2	2.48	0.46
1:A:486:ARG:HD2	2:B:751:HIS:HB3	1.97	0.46
1:A:552:PRO:HB3	1:A:599:GLN:HB2	1.96	0.46
1:A:797:GLY:C	1:A:799:PHE:H	2.23	0.46
3:D:2049:ILE:HD12	3:D:2077:ILE:HD12	1.98	0.46
3:D:2134:VAL:O	3:D:2138:THR:HG23	2.16	0.46
5:F:809:PHE:O	5:F:813:GLU:HG2	2.15	0.46
7:H:117:ASP:OD1	7:H:118:ASP:N	2.49	0.46
8:I:206:TRP:CG	8:I:207:PRO:HD3	2.51	0.46
8:I:286:LYS:NZ	8:I:291:GLY:O	2.49	0.46
15:P:202:SER:O	15:P:205:ASP:N	2.47	0.46
19:T:89:GLU:H	19:T:89:GLU:CD	2.24	0.46
1:A:584:LEU:O	1:A:588:VAL:HG12	2.16	0.46
2:B:252:PRO:O	2:B:374:ARG:NE	2.42	0.46
2:B:536:LYS:CE	2:B:540:ASN:HD21	2.29	0.46
2:B:949:SER:OG	3:D:2899:GLU:OE1	2.33	0.46
2:C:391:ALA:HB2	2:C:408:ARG:HB3	1.98	0.46
2:C:883:MET:HE2	2:C:883:MET:HB3	1.69	0.46
3:D:469:LEU:HD21	16:Q:332:ARG:HG2	1.97	0.46
3:D:750:PRO:CD	15:P:217:SER:HA	2.45	0.46
3:D:1805:ASN:OD1	3:D:1805:ASN:N	2.49	0.46
15:P:169:ASN:O	15:P:171:PRO:HD3	2.16	0.46
4:E:119:SER:O	4:E:119:SER:OG	2.30	0.46
4:E:652:GLU:HG3	4:E:676:ARG:HD2	1.98	0.46
7:H:433:GLU:OE1	7:H:433:GLU:N	2.44	0.46
15:P:262:HIS:CD2	15:P:264:PRO:HD2	2.51	0.46
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.70	0.46
1:A:351:GLN:NE2	22:A:1201:LMG:O2	2.49	0.46
1:A:760:ILE:HB	1:A:764:ASP:HB2	1.98	0.46
3:D:455:CYS:SG	15:P:526:LEU:HG	2.56	0.46
5:F:682:GLU:C	5:F:684:GLU:H	2.24	0.46
6:G:226:TYR:HE2	6:G:309:HIS:CE1	2.34	0.46
8:I:306:ARG:HE	8:I:306:ARG:HB3	1.45	0.46
11:L:238:TRP:NE1	11:L:253:PRO:HG3	2.31	0.46
17:R:368:ARG:O	17:R:368:ARG:NH2	2.49	0.46
1:A:380:ARG:NH1	2:B:478:ILE:O	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:GLU:OE2	18:S:123:PRO:HG3	2.16	0.45
2:C:856:GLU:OE2	2:C:860:ARG:NH1	2.50	0.45
3:D:1443:ASN:O	3:D:1446:GLN:HG3	2.16	0.45
3:D:2073:VAL:O	3:D:2077:ILE:HG12	2.16	0.45
5:F:673:GLN:O	5:F:677:GLU:HG2	2.16	0.45
8:I:303:SER:O	8:I:303:SER:OG	2.28	0.45
17:R:253:ASP:O	17:R:255:GLY:N	2.50	0.45
17:R:351:ASP:OD1	17:R:351:ASP:N	2.49	0.45
1:A:536:ALA:O	1:A:540:VAL:HG22	2.15	0.45
1:A:660:THR:O	1:A:664:THR:OG1	2.23	0.45
2:B:613:ASP:OD1	2:B:614:ARG:N	2.50	0.45
2:B:815:TYR:OH	2:B:1005:GLU:OE1	2.23	0.45
3:D:2507:LYS:HB3	3:D:2507:LYS:HE3	1.66	0.45
15:P:419:PRO:HA	15:P:422:TRP:CD2	2.51	0.45
19:T:87:PRO:O	19:T:92:ARG:NH2	2.37	0.45
1:A:473:GLU:OE2	2:B:747:ARG:NE	2.46	0.45
3:D:963:GLN:O	3:D:964:LYS:HE2	2.16	0.45
4:E:248:THR:O	4:E:248:THR:OG1	2.32	0.45
7:H:433:GLU:H	7:H:433:GLU:CD	2.24	0.45
1:A:229:MET:HB3	1:A:302:TRP:HE1	1.81	0.45
2:B:202:TYR:HA	2:B:205:ARG:NH2	2.31	0.45
2:B:243:GLU:OE2	2:B:246:ARG:HD2	2.16	0.45
2:B:1091:MET:HB3	2:B:1091:MET:HE2	1.53	0.45
4:E:134:LEU:HB2	4:E:147:VAL:HG23	1.99	0.45
4:E:740:ARG:NE	4:E:835:MET:HE1	2.31	0.45
12:M:293:PRO:HG3	12:M:548:ALA:HB3	1.98	0.45
17:R:154:TYR:HB2	17:R:206:HIS:CE1	2.52	0.45
17:R:337:LEU:HD23	17:R:337:LEU:HA	1.76	0.45
2:B:591:CYS:SG	2:B:592:SER:N	2.89	0.45
2:B:670:THR:OG1	2:B:671:ASN:N	2.50	0.45
2:B:700:ARG:HG3	2:B:723:ALA:HB1	1.97	0.45
2:C:381:LEU:HD22	2:C:420:VAL:HG21	1.96	0.45
2:C:382:TRP:CE2	2:C:431:HIS:HD2	2.34	0.45
2:C:478:ILE:HG13	2:C:479:LEU:N	2.32	0.45
3:D:51:THR:O	3:D:55:GLU:HG3	2.15	0.45
3:D:1915:ASN:ND2	3:D:1918:LYS:HD2	2.31	0.45
4:E:242:GLY:N	4:E:260:GLY:HA3	2.30	0.45
11:L:159:LEU:O	11:L:162:VAL:HG12	2.16	0.45
15:P:506:LEU:O	15:P:509:PRO:HD2	2.17	0.45
15:P:544:ALA:O	16:Q:226:VAL:HA	2.17	0.45
16:Q:251:TYR:OH	16:Q:313:VAL:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:276:ILE:HD13	16:Q:276:ILE:HA	1.82	0.45
19:T:16:GLU:OE1	19:T:20:GLU:HB3	2.17	0.45
2:B:461:THR:HG22	26:O:3101:DGA:HB21	1.99	0.45
2:B:528:ASP:OD1	2:B:529:ILE:N	2.49	0.45
3:D:2274:VAL:HG13	3:D:2708:GLU:HG3	1.99	0.45
4:E:81:ASP:O	4:E:85:GLN:HG3	2.16	0.45
4:E:347:GLU:HA	4:E:351:LEU:HG	1.97	0.45
10:K:238:LEU:HD23	10:K:238:LEU:HA	1.77	0.45
12:M:543:ASP:HB3	12:M:546:ARG:HB3	1.98	0.45
16:Q:288:GLU:O	16:Q:292:LEU:HD22	2.16	0.45
18:S:112:GLU:OE1	18:S:112:GLU:N	2.41	0.45
3:D:2122:SER:OG	3:D:2123:GLN:N	2.50	0.45
3:D:2678:PRO:HG3	3:D:2891:PHE:CE1	2.51	0.45
5:F:229:THR:OG1	5:F:232:VAL:HG22	2.16	0.45
6:G:250:TYR:C	6:G:252:ALA:N	2.75	0.45
7:H:421:LYS:O	7:H:425:VAL:HG13	2.17	0.45
15:P:315:GLU:OE1	15:P:315:GLU:N	2.50	0.45
18:S:45:PRO:HB2	18:S:50:LEU:HD21	1.98	0.45
1:A:764:ASP:N	1:A:764:ASP:OD1	2.49	0.45
2:B:800:ARG:O	2:B:804:SER:OG	2.25	0.45
2:C:455:VAL:HG22	3:D:1368:ILE:HD12	1.98	0.45
3:D:822:LYS:HB2	3:D:822:LYS:HE3	1.65	0.45
3:D:1790:TYR:OH	3:D:1817:ASN:ND2	2.49	0.45
3:D:2019:LEU:HD23	3:D:2338:ILE:HB	1.98	0.45
4:E:674:VAL:O	4:E:678:THR:HG23	2.17	0.45
4:E:701:GLU:OE1	4:E:734:SER:OG	2.31	0.45
15:P:361:ARG:HB3	15:P:362:PRO:HD3	1.99	0.45
15:P:393:LYS:HA	15:P:393:LYS:HD2	1.75	0.45
1:A:785:LYS:HD3	1:A:790:VAL:CG1	2.47	0.45
2:B:430:ASP:N	2:B:430:ASP:OD1	2.50	0.45
3:D:993:LEU:HD23	3:D:993:LEU:HA	1.83	0.45
5:F:742:ASP:OD1	5:F:742:ASP:N	2.50	0.45
15:P:613:ALA:O	15:P:617:ARG:HG3	2.17	0.45
17:R:138:ARG:NH1	17:R:243:LEU:HD11	2.32	0.45
17:R:246:LEU:HA	17:R:249:GLN:HG3	1.99	0.45
17:R:441:ARG:HA	17:R:444:ARG:NE	2.32	0.45
1:A:595:ASN:HB2	1:A:598:GLU:HG3	1.99	0.45
2:C:431:HIS:CE1	2:C:435:ASN:HD21	2.35	0.45
2:C:530:ASN:O	2:C:532:ILE:HG23	2.17	0.45
4:E:255:SER:O	4:E:257:ALA:N	2.50	0.45
7:H:406:GLN:HE21	7:H:406:GLN:HB3	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:132:PRO:C	10:K:134:ALA:H	2.24	0.45
14:O:388:LEU:HD23	14:O:388:LEU:HA	1.79	0.45
19:T:110:LEU:HD12	19:T:111:THR:N	2.32	0.45
1:A:450:LYS:NZ	1:A:452:ARG:HG2	2.32	0.44
1:A:500:PRO:HD2	1:A:503:THR:HG21	2.00	0.44
2:C:513:GLU:HB3	2:C:589:PHE:CD2	2.52	0.44
3:D:782:ASN:OD1	3:D:783:GLY:N	2.50	0.44
3:D:2129:GLU:OE1	3:D:2129:GLU:N	2.50	0.44
5:F:704:LEU:HD23	5:F:704:LEU:HA	1.78	0.44
7:H:292:ASP:HB2	7:H:304:VAL:HG13	1.97	0.44
18:S:33:LYS:HA	18:S:33:LYS:HD3	1.57	0.44
2:C:812:LEU:HD23	2:C:975:LEU:HD23	1.99	0.44
3:D:1922:GLU:O	3:D:1926:SER:HB3	2.17	0.44
4:E:550:ALA:O	4:E:554:GLU:N	2.43	0.44
4:E:802:ALA:HB2	4:E:866:GLU:HG3	1.98	0.44
5:F:273:TYR:CZ	19:T:76:LYS:HE3	2.51	0.44
6:G:202:SER:OG	6:G:203:SER:N	2.51	0.44
6:G:420:SER:HB3	6:G:426:GLN:HE21	1.82	0.44
7:H:311:ARG:HH22	7:H:317:GLN:HE22	1.65	0.44
2:B:508:ARG:HD2	3:D:1776:TRP:HD1	1.83	0.44
3:D:2137:LEU:HD23	3:D:2137:LEU:HA	1.77	0.44
3:D:2359:LYS:HA	3:D:2359:LYS:HD2	1.81	0.44
5:F:600:ARG:HG2	5:F:610:PHE:CE2	2.52	0.44
7:H:172:LEU:HD13	7:H:266:LEU:HD12	1.98	0.44
14:O:298:THR:HG22	14:O:299:ALA:H	1.83	0.44
15:P:639:ASP:OD1	15:P:639:ASP:N	2.50	0.44
16:Q:236:LEU:HD13	16:Q:347:VAL:HG13	1.99	0.44
1:A:1143:ASP:OD1	1:A:1161:PRO:HD3	2.17	0.44
2:C:770:THR:OG1	2:C:771:LEU:N	2.51	0.44
3:D:2903:THR:O	3:D:2907:LEU:HG	2.17	0.44
4:E:953:LEU:HD12	4:E:953:LEU:HA	1.86	0.44
6:G:106:GLU:OE2	6:G:334:GLY:N	2.51	0.44
6:G:185:GLU:OE2	6:G:187:ALA:N	2.51	0.44
6:G:253:GLU:H	6:G:253:GLU:HG3	1.66	0.44
6:G:345:LEU:HD12	6:G:345:LEU:HA	1.81	0.44
10:K:101:SER:O	10:K:103:TRP:N	2.50	0.44
15:P:255:TRP:CE3	15:P:305:LEU:HB3	2.51	0.44
15:P:328:LEU:HD23	15:P:403:GLN:HG3	1.99	0.44
16:Q:254:ARG:HB3	16:Q:254:ARG:HH11	1.82	0.44
18:S:77:ILE:HG23	18:S:78:ALA:N	2.32	0.44
2:B:1105:LYS:O	2:B:1108:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:398:PRO:N	3:D:1374:LYS:HE2	2.32	0.44
2:C:807:GLU:OE2	2:C:838:THR:OG1	2.36	0.44
3:D:1424:LEU:HD23	3:D:1424:LEU:HA	1.77	0.44
3:D:2124:ARG:NE	4:E:823:GLN:HE21	2.15	0.44
3:D:2259:LEU:HD12	3:D:2264:LEU:HD12	2.00	0.44
4:E:128:LEU:HD11	5:F:104:LEU:HD11	1.99	0.44
7:H:99:HIS:O	7:H:102:VAL:HG12	2.18	0.44
7:H:187:LEU:HD12	7:H:276:VAL:HG21	1.99	0.44
8:I:213:ASP:OD1	8:I:213:ASP:N	2.47	0.44
1:A:450:LYS:HZ3	1:A:452:ARG:HG2	1.82	0.44
1:A:659:LYS:HB3	1:A:659:LYS:HE3	1.76	0.44
6:G:118:LEU:HD12	6:G:118:LEU:HA	1.85	0.44
7:H:306:ASP:N	7:H:306:ASP:OD1	2.50	0.44
7:H:401:ARG:O	7:H:405:ILE:HG12	2.16	0.44
7:H:449:LYS:H	7:H:449:LYS:HD3	1.82	0.44
8:I:242:GLU:N	8:I:243:PRO:HD2	2.32	0.44
12:M:266:LEU:CD1	12:M:270:GLN:HB3	2.48	0.44
15:P:202:SER:O	15:P:204:LEU:N	2.50	0.44
3:D:1915:ASN:HD21	3:D:1918:LYS:HD2	1.82	0.44
4:E:331:MET:SD	13:N:66:GLU:HB3	2.58	0.44
5:F:232:VAL:HB	19:T:99:ARG:NH1	2.33	0.44
5:F:896:GLN:HE21	5:F:899:ARG:HH21	1.66	0.44
5:F:982:ASP:HA	5:F:985:THR:HG22	1.99	0.44
6:G:111:ASP:OD1	6:G:111:ASP:N	2.50	0.44
7:H:267:ARG:NH2	7:H:269:ASP:OD2	2.39	0.44
16:Q:145:ILE:HG13	16:Q:146:GLU:N	2.33	0.44
16:Q:276:ILE:O	16:Q:280:LEU:HG	2.18	0.44
1:A:422:LYS:HG3	1:A:423:GLN:NE2	2.32	0.44
2:B:530:ASN:ND2	2:B:702:LYS:HE3	2.33	0.44
2:C:444:THR:O	2:C:445:GLU:C	2.57	0.44
3:D:2502:LYS:HB2	3:D:2503:LYS:HZ3	1.83	0.44
3:D:2929:ASN:O	3:D:2933:THR:HG22	2.18	0.44
4:E:351:LEU:N	4:E:352:PRO:HD2	2.32	0.44
4:E:969:GLU:O	4:E:972:GLU:HG3	2.17	0.44
5:F:889:SER:O	5:F:889:SER:OG	2.31	0.44
12:M:451:LEU:O	12:M:521:SER:OG	2.34	0.44
13:N:53:LYS:HB3	13:N:53:LYS:HE2	1.49	0.44
2:B:497:GLU:O	2:B:498:MET:C	2.61	0.44
2:C:681:ILE:HD12	2:C:681:ILE:HA	1.82	0.44
3:D:2116:LYS:HD3	4:E:820:VAL:HG11	1.99	0.44
4:E:651:ASN:O	4:E:655:MET:HE3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:408:GLU:O	6:G:412:VAL:HG12	2.17	0.44
8:I:216:MET:HB3	8:I:216:MET:HE3	1.60	0.44
15:P:683:SER:O	15:P:687:THR:HG23	2.17	0.44
17:R:56:HIS:CE1	17:R:321:ASN:HB2	2.53	0.44
1:A:244:VAL:HG12	1:A:244:VAL:O	2.18	0.43
1:A:868:ASP:OD1	1:A:868:ASP:N	2.38	0.43
2:C:456:GLN:HE22	2:C:459:ARG:HH21	1.66	0.43
3:D:2212:ASN:OD1	3:D:2212:ASN:N	2.49	0.43
5:F:1010:GLU:N	5:F:1010:GLU:OE1	2.51	0.43
7:H:218:MET:HE3	7:H:218:MET:HB3	1.86	0.43
7:H:271:LEU:HD12	7:H:296:VAL:HG22	1.99	0.43
25:I:401:SQD:H272	25:I:401:SQD:H301	1.89	0.43
9:J:92:GLU:HB3	10:K:208:THR:HG23	2.00	0.43
14:O:374:ILE:C	14:O:376:SER:N	2.75	0.43
1:A:1119:TRP:CE2	3:D:2640:ALA:HB3	2.53	0.43
1:A:1125:ASP:N	1:A:1125:ASP:OD1	2.51	0.43
2:C:590:THR:HG23	2:C:624:PHE:HD2	1.83	0.43
2:C:645:ALA:O	2:C:648:ILE:HG13	2.18	0.43
3:D:735:GLN:HE21	3:D:735:GLN:HB3	1.68	0.43
3:D:2704:ALA:O	3:D:2708:GLU:HG2	2.18	0.43
3:D:2748:LEU:O	3:D:2749:ASN:C	2.61	0.43
5:F:228:ASP:HA	5:F:233:ALA:HA	2.01	0.43
10:K:191:ALA:HB2	10:K:205:PHE:HB3	2.00	0.43
14:O:418:PHE:O	14:O:422:VAL:HG12	2.18	0.43
16:Q:230:ASP:OD1	16:Q:230:ASP:N	2.51	0.43
17:R:203:ARG:NH2	19:T:41:LYS:HA	2.32	0.43
19:T:108:GLU:H	19:T:108:GLU:CD	2.26	0.43
1:A:656:LEU:HD23	1:A:657:LEU:HD23	2.01	0.43
1:A:778:MET:HG2	1:A:784:PHE:CE2	2.53	0.43
2:C:998:LYS:H	6:G:259:ALA:HA	1.84	0.43
3:D:2685:ASP:O	3:D:2878:ARG:HG2	2.18	0.43
3:D:2876:LYS:HE3	5:F:947:GLN:HB3	2.00	0.43
5:F:999:VAL:O	5:F:1003:VAL:HG13	2.17	0.43
6:G:172:LEU:O	6:G:176:THR:HG22	2.19	0.43
15:P:74:VAL:O	15:P:78:LEU:HG	2.17	0.43
15:P:570:ARG:O	15:P:574:GLU:HG2	2.18	0.43
16:Q:210:THR:HG22	16:Q:212:GLN:H	1.82	0.43
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.83	0.43
2:C:1084:LYS:HD2	2:C:1084:LYS:HA	1.79	0.43
3:D:911:TRP:HE1	18:S:122:GLU:CD	2.26	0.43
3:D:1303:LYS:HD3	3:D:1303:LYS:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1785:THR:HA	3:D:1788:ASP:OD2	2.18	0.43
3:D:2502:LYS:HB2	3:D:2503:LYS:NZ	2.33	0.43
3:D:2689:LEU:HD12	3:D:2689:LEU:HA	1.74	0.43
6:G:109:ASP:OD1	6:G:290:ARG:NH2	2.51	0.43
14:O:423:TYR:HA	14:O:426:VAL:HG12	2.00	0.43
16:Q:176:PRO:O	16:Q:179:GLN:HB3	2.18	0.43
1:A:815:ALA:HA	1:A:907:VAL:HG11	2.00	0.43
2:B:673:PRO:HA	2:B:676:ILE:CD1	2.49	0.43
3:D:793:LEU:O	3:D:795:THR:N	2.49	0.43
3:D:937:GLU:HG3	17:R:183:TRP:CE2	2.53	0.43
3:D:969:PHE:O	3:D:970:PHE:C	2.61	0.43
3:D:1242:ILE:HB	17:R:221:PRO:HB3	2.01	0.43
3:D:2632:LEU:HD13	3:D:2632:LEU:HA	1.82	0.43
4:E:75:PRO:HD2	19:T:115:MET:HE1	1.99	0.43
5:F:766:CYS:SG	5:F:767:PHE:N	2.92	0.43
6:G:112:LYS:NZ	6:G:329:GLY:O	2.49	0.43
6:G:229:LEU:HA	6:G:232:ASP:OD2	2.19	0.43
10:K:107:TRP:CD1	10:K:107:TRP:H	2.35	0.43
15:P:370:ALA:O	15:P:373:GLU:HG3	2.18	0.43
17:R:60:ARG:HD3	17:R:308:GLU:HG3	2.00	0.43
17:R:317:SER:O	17:R:318:PHE:HB3	2.18	0.43
17:R:319:PHE:HA	17:R:320:PRO:HD3	1.87	0.43
1:A:1123:ARG:NH1	1:A:1135:ILE:O	2.52	0.43
22:A:1201:LMG:H302	22:A:1201:LMG:H331	1.25	0.43
2:B:735:MET:O	2:B:738:MET:HG3	2.19	0.43
3:D:547:LEU:HA	3:D:634:GLN:HE22	1.84	0.43
3:D:793:LEU:O	3:D:795:THR:HG22	2.19	0.43
3:D:1779:TRP:O	3:D:1783:LEU:HD23	2.18	0.43
3:D:2404:ARG:HA	3:D:2404:ARG:NH1	2.33	0.43
3:D:2600:LYS:HE3	3:D:2600:LYS:HB3	1.83	0.43
25:I:401:SQD:H111	22:I:402:LMG:H132	2.01	0.43
15:P:324:LEU:HB2	28:P:701:A1LXL:C01	2.48	0.43
15:P:557:ALA:HB3	16:Q:325:SER:N	2.32	0.43
2:C:580:ILE:O	2:C:584:GLY:N	2.51	0.43
2:C:766:THR:O	2:C:770:THR:HG23	2.18	0.43
2:C:997:GLY:C	6:G:261:SER:HB2	2.44	0.43
3:D:2046:MET:HB3	3:D:2046:MET:HE3	1.78	0.43
3:D:2251:VAL:HG11	3:D:2712:ARG:HH21	1.83	0.43
3:D:2252:GLU:HG3	3:D:2253:GLU:N	2.33	0.43
5:F:580:ARG:HE	5:F:580:ARG:HB3	1.65	0.43
5:F:1006:LEU:HD23	5:F:1006:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:37:ASP:HB3	13:N:40:LYS:NZ	2.33	0.43
14:O:264:LEU:HD22	14:O:264:LEU:HA	1.91	0.43
17:R:130:GLU:O	17:R:134:GLU:HG3	2.19	0.43
17:R:433:ARG:O	17:R:436:GLN:HG3	2.19	0.43
19:T:107:PRO:HA	19:T:110:LEU:HG	2.00	0.43
1:A:649:LEU:HD23	1:A:653:GLY:HA3	2.01	0.43
2:B:595:ASP:OD1	2:B:595:ASP:N	2.52	0.43
2:C:606:ARG:HD2	2:C:606:ARG:HA	1.76	0.43
2:C:606:ARG:O	2:C:606:ARG:NH1	2.48	0.43
3:D:545:SER:OG	15:P:226:LEU:HA	2.19	0.43
3:D:574:ASN:O	3:D:577:PRO:HD2	2.18	0.43
3:D:1401:LEU:HD12	26:D:3001:DGA:HBW2	2.00	0.43
3:D:2255:PRO:O	3:D:2256:TRP:HB2	2.19	0.43
5:F:885:ASP:OD1	5:F:885:ASP:N	2.45	0.43
7:H:297:ASP:N	7:H:297:ASP:OD1	2.52	0.43
7:H:304:VAL:HA	7:H:355:LEU:O	2.19	0.43
2:C:594:THR:HG21	3:D:2298:ASP:OD1	2.18	0.43
3:D:2070:LEU:HD12	3:D:2070:LEU:HA	1.83	0.43
3:D:2234:PHE:O	3:D:2238:LEU:HD13	2.19	0.43
3:D:2318:THR:OG1	3:D:2319:ASP:N	2.52	0.43
3:D:2695:PRO:HD3	3:D:2700:LEU:O	2.18	0.43
4:E:291:LYS:HD2	4:E:291:LYS:HA	1.74	0.43
7:H:85:SER:N	7:H:86:PRO:HD2	2.34	0.43
8:I:284:VAL:HG23	8:I:314:ALA:HB3	2.01	0.43
9:J:36:ASP:N	9:J:36:ASP:OD1	2.50	0.43
15:P:143:VAL:O	15:P:147:ARG:HB2	2.19	0.43
17:R:444:ARG:HE	17:R:444:ARG:HB3	1.67	0.43
19:T:69:LYS:HD2	19:T:69:LYS:HA	1.80	0.43
2:B:680:LEU:O	2:B:686:PHE:HB2	2.18	0.43
2:B:831:LEU:HD21	3:D:2770:LYS:HG3	2.01	0.43
2:C:454:LEU:HD23	3:D:1368:ILE:HD13	2.00	0.43
2:C:532:ILE:HB	2:C:535:VAL:CG2	2.48	0.43
2:C:947:ASP:OD1	2:C:947:ASP:N	2.50	0.43
3:D:636:LYS:HB3	3:D:636:LYS:HE3	1.87	0.43
3:D:750:PRO:HD3	15:P:217:SER:HA	2.01	0.43
6:G:182:ARG:HB3	6:G:491:LEU:HB3	2.01	0.43
6:G:194:THR:OG1	6:G:235:LEU:HG	2.18	0.43
10:K:131:ILE:HA	10:K:132:PRO:HD3	1.77	0.43
14:O:261:VAL:HG13	14:O:262:ALA:H	1.83	0.43
14:O:388:LEU:O	14:O:391:TYR:HB3	2.19	0.43
2:C:525:LYS:NZ	2:C:527:ASP:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:594:THR:HA	2:C:597:TYR:HD1	1.84	0.42
4:E:760:LEU:HD23	4:E:760:LEU:HA	1.77	0.42
4:E:906:GLU:HA	4:E:909:ASP:OD2	2.19	0.42
5:F:640:VAL:HG12	5:F:640:VAL:O	2.17	0.42
5:F:998:GLU:H	5:F:998:GLU:HG3	1.51	0.42
9:J:73:LEU:HA	9:J:73:LEU:HD23	1.80	0.42
12:M:416:HIS:HD2	12:M:417:PRO:O	2.02	0.42
15:P:187:ASP:OD1	15:P:189:GLU:HG3	2.19	0.42
1:A:446:GLU:HA	1:A:449:GLY:H	1.83	0.42
2:C:568:ALA:O	2:C:569:PRO:C	2.61	0.42
3:D:975:TRP:H	3:D:975:TRP:CD1	2.37	0.42
3:D:2016:ASN:HB3	3:D:2334:LEU:HD23	1.99	0.42
4:E:347:GLU:HA	4:E:351:LEU:CG	2.49	0.42
5:F:760:GLY:O	5:F:764:THR:HG23	2.18	0.42
11:L:287:ASP:OD1	11:L:288:ALA:N	2.52	0.42
14:O:312:LEU:O	14:O:315:LEU:HB3	2.19	0.42
16:Q:141:ALA:O	16:Q:145:ILE:HG23	2.18	0.42
2:B:762:MET:O	2:B:766:THR:OG1	2.37	0.42
2:B:831:LEU:HD11	3:D:2770:LYS:HG3	2.01	0.42
2:C:660:ASP:O	2:C:662:ARG:NE	2.49	0.42
2:C:813:LEU:HD13	2:C:813:LEU:HA	1.80	0.42
2:C:992:ARG:NH1	2:C:999:GLU:OE1	2.52	0.42
5:F:908:SER:OG	5:F:910:MET:SD	2.77	0.42
5:F:987:LEU:O	5:F:990:GLU:HG3	2.19	0.42
7:H:95:LEU:HD23	7:H:95:LEU:HA	1.89	0.42
25:I:401:SQD:H91	25:I:401:SQD:H122	1.64	0.42
15:P:495:ASP:OD1	15:P:497:GLU:HG2	2.19	0.42
16:Q:170:TYR:O	16:Q:174:THR:HG22	2.19	0.42
17:R:195:LYS:HB2	19:T:27:TYR:CE2	2.52	0.42
17:R:203:ARG:NH2	19:T:40:PRO:O	2.52	0.42
17:R:248:THR:HG21	17:R:259:THR:HG22	2.01	0.42
1:A:506:THR:O	1:A:507:TYR:C	2.63	0.42
3:D:1773:THR:O	3:D:1777:ASP:HB2	2.19	0.42
4:E:244:LEU:HG	17:R:343:TYR:CE1	2.55	0.42
8:I:136:TRP:CG	10:K:71:PHE:HZ	2.36	0.42
9:J:39:LYS:HE2	9:J:39:LYS:HB3	1.84	0.42
13:N:118:ASP:N	17:R:10:ASP:O	2.48	0.42
1:A:645:LYS:HE3	1:A:645:LYS:HB2	1.68	0.42
2:B:1098:GLU:N	2:B:1098:GLU:OE1	2.52	0.42
3:D:1328:SER:O	3:D:1330:TRP:N	2.50	0.42
15:P:156:SER:OG	15:P:157:LYS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:351:ALA:HB3	16:Q:354:LEU:HB2	2.01	0.42
1:A:805:LEU:HD23	1:A:805:LEU:HA	1.85	0.42
2:B:399:GLU:HB2	17:R:332:PHE:HA	2.02	0.42
3:D:1293:SER:HA	3:D:1296:ILE:HG12	2.01	0.42
3:D:2027:ASN:N	3:D:2027:ASN:OD1	2.52	0.42
28:D:3003:A1LXL:C27	15:P:471:LEU:HB3	2.50	0.42
4:E:655:MET:HE2	4:E:655:MET:HB3	1.86	0.42
7:H:170:TRP:CZ3	7:H:248:GLU:HG2	2.54	0.42
12:M:628:ARG:HB3	12:M:632:GLU:OE2	2.20	0.42
16:Q:299:ALA:O	16:Q:302:LYS:HG3	2.19	0.42
17:R:73:LEU:HD23	17:R:73:LEU:HA	1.87	0.42
2:B:505:LEU:HD13	3:D:1783:LEU:HD11	2.02	0.42
2:C:703:ILE:O	2:C:706:VAL:HG22	2.19	0.42
3:D:338:PRO:HD3	3:D:1401:LEU:HD13	2.02	0.42
3:D:903:LYS:HG3	3:D:904:LYS:H	1.84	0.42
3:D:1703:LEU:HD23	3:D:1703:LEU:HA	1.89	0.42
3:D:1787:ALA:O	3:D:1791:ASN:N	2.50	0.42
3:D:2022:PRO:CG	3:D:2342:ASN:HB2	2.50	0.42
3:D:2670:LEU:O	3:D:2671:TYR:HB2	2.20	0.42
7:H:475:MET:HE1	8:I:349:TYR:HA	2.02	0.42
9:J:75:THR:O	9:J:79:MET:HG2	2.20	0.42
15:P:624:ALA:O	15:P:628:VAL:HG12	2.20	0.42
16:Q:310:VAL:HA	16:Q:313:VAL:HG12	2.01	0.42
16:Q:311:GLU:HA	16:Q:314:GLU:HB2	2.01	0.42
17:R:289:GLN:H	17:R:289:GLN:HG3	1.55	0.42
2:C:732:ALA:O	2:C:735:MET:HG3	2.20	0.42
4:E:977:GLN:N	4:E:978:PRO:HD2	2.35	0.42
14:O:146:LEU:O	14:O:150:VAL:HG23	2.20	0.42
4:E:360:SER:O	4:E:363:PRO:HD2	2.20	0.42
4:E:956:ALA:O	5:F:949:ARG:NH1	2.53	0.42
4:E:976:LYS:NZ	4:E:977:GLN:HG3	2.35	0.42
5:F:561:LEU:HA	5:F:564:VAL:HG12	2.02	0.42
5:F:768:LEU:HD22	5:F:768:LEU:HA	1.94	0.42
12:M:368:PHE:CD2	12:M:369:ILE:HG13	2.55	0.42
15:P:381:ASP:OD2	15:P:383:MET:HE3	2.20	0.42
2:B:696:ASP:O	2:B:700:ARG:HG2	2.20	0.42
2:B:995:ILE:HG23	2:B:999:GLU:HB2	2.01	0.42
2:C:1088:HIS:C	2:C:1090:ASN:H	2.26	0.42
3:D:2298:ASP:O	3:D:2302:ILE:HG23	2.20	0.42
4:E:123:LEU:HA	4:E:126:LEU:HD12	2.01	0.42
9:J:67:ASP:OD1	9:J:67:ASP:N	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:97:ALA:O	16:Q:101:VAL:HG23	2.19	0.42
16:Q:175:THR:HB	16:Q:176:PRO:HD2	2.01	0.42
16:Q:262:TYR:CE2	16:Q:307:ARG:HD3	2.54	0.42
17:R:251:LEU:HD13	19:T:57:ALA:HB2	2.00	0.42
17:R:317:SER:C	17:R:319:PHE:H	2.28	0.42
19:T:107:PRO:O	19:T:110:LEU:HG	2.20	0.42
2:C:601:SER:O	4:E:508:GLY:HA3	2.19	0.41
2:C:610:GLU:HA	2:C:613:ASP:OD2	2.20	0.41
3:D:2023:LYS:HD2	3:D:2023:LYS:C	2.45	0.41
3:D:2124:ARG:O	4:E:827:ARG:NH2	2.53	0.41
3:D:2232:SER:O	3:D:2236:VAL:HG12	2.18	0.41
3:D:2774:LEU:HD23	3:D:2774:LEU:HA	1.78	0.41
4:E:72:SER:HB3	4:E:133:ARG:HH21	1.85	0.41
4:E:927:GLU:OE1	6:G:379:ARG:NH1	2.49	0.41
7:H:92:ILE:HB	12:M:288:PRO:HG3	2.02	0.41
9:J:55:GLU:HB2	9:J:57:GLU:OE1	2.20	0.41
9:J:65:PHE:O	9:J:70:ALA:HB3	2.19	0.41
10:K:90:SER:HB2	10:K:91:ILE:H	1.63	0.41
14:O:432:ASP:C	14:O:434:SER:H	2.28	0.41
16:Q:238:LEU:HB2	16:Q:352:PRO:HG3	2.01	0.41
1:A:624:VAL:HG13	3:D:2231:THR:HG21	2.01	0.41
2:B:598:ASP:N	2:B:598:ASP:OD1	2.52	0.41
3:D:1165:TRP:CE2	3:D:1185:LEU:HD21	2.55	0.41
3:D:1415:GLN:NE2	17:R:38:GLU:OE2	2.51	0.41
4:E:62:THR:O	4:E:62:THR:OG1	2.36	0.41
4:E:945:ARG:HA	4:E:945:ARG:HD2	1.76	0.41
5:F:812:MET:HG3	5:F:813:GLU:N	2.35	0.41
7:H:360:SER:OG	7:H:361:GLY:N	2.53	0.41
14:O:384:ALA:O	14:O:385:ALA:C	2.63	0.41
15:P:355:TRP:CG	15:P:356:PRO:HD3	2.55	0.41
2:B:748:GLN:NE2	2:B:750:ARG:HD3	2.35	0.41
2:C:368:ARG:HD2	8:I:290:VAL:O	2.20	0.41
4:E:976:LYS:C	4:E:976:LYS:HD2	2.45	0.41
5:F:258:ALA:HA	19:T:87:PRO:HG2	2.01	0.41
11:L:162:VAL:HA	11:L:165:ARG:HG2	2.02	0.41
12:M:626:THR:OG1	12:M:627:TYR:N	2.52	0.41
1:A:778:MET:HG2	1:A:784:PHE:CZ	2.55	0.41
2:B:534:GLU:CD	2:B:534:GLU:H	2.28	0.41
2:C:370:GLN:H	8:I:290:VAL:HG13	1.84	0.41
3:D:1232:ARG:HD3	17:R:271:ASP:OD1	2.21	0.41
3:D:1679:VAL:O	3:D:1683:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2183:ASN:HD22	3:D:2184:HIS:H	1.67	0.41
3:D:2686:GLY:O	3:D:2687:ASN:ND2	2.54	0.41
3:D:2727:LYS:HG3	3:D:2728:SER:O	2.19	0.41
3:D:2827:ILE:HG22	5:F:757:GLN:HE22	1.85	0.41
5:F:570:THR:O	5:F:572:GLU:HG3	2.19	0.41
5:F:821:THR:HG21	5:F:1003:VAL:HG21	2.02	0.41
6:G:357:GLU:OE2	6:G:357:GLU:N	2.54	0.41
15:P:218:GLY:O	15:P:221:ALA:N	2.53	0.41
2:B:907:ARG:HB2	2:B:959:GLU:OE2	2.20	0.41
2:C:423:PRO:O	2:C:424:PRO:C	2.63	0.41
2:C:652:LEU:O	2:C:656:ASP:HB2	2.21	0.41
3:D:2683:PHE:O	3:D:2879:ARG:NH2	2.47	0.41
4:E:335:TRP:O	4:E:338:VAL:HG22	2.21	0.41
6:G:297:LEU:O	6:G:301:VAL:HG13	2.20	0.41
7:H:104:ALA:O	7:H:107:GLU:HG3	2.21	0.41
8:I:85:ASN:OD1	8:I:85:ASN:N	2.53	0.41
1:A:445:ASP:H	1:A:451:MET:HA	1.84	0.41
2:C:734:VAL:O	2:C:738:MET:HG2	2.20	0.41
3:D:1296:ILE:O	3:D:1300:VAL:HG13	2.21	0.41
3:D:1315:ASN:O	3:D:1316:VAL:HG13	2.20	0.41
3:D:2069:LEU:O	3:D:2073:VAL:HG23	2.20	0.41
4:E:258:ASP:OD1	4:E:258:ASP:N	2.52	0.41
5:F:135:ARG:HD2	5:F:157:PRO:O	2.21	0.41
5:F:881:VAL:HG12	5:F:882:LEU:HD23	2.03	0.41
14:O:142:TRP:CE3	14:O:146:LEU:HG	2.55	0.41
14:O:146:LEU:HD21	14:O:409:LEU:HD21	2.03	0.41
14:O:426:VAL:CG2	14:O:431:PHE:HB2	2.47	0.41
15:P:68:ARG:HB2	15:P:348:THR:HG23	2.03	0.41
15:P:127:LEU:HD23	15:P:131:GLU:HG2	2.03	0.41
1:A:1147:GLN:HE21	1:A:1147:GLN:HB3	1.72	0.41
2:B:246:ARG:HE	2:B:246:ARG:HB2	1.51	0.41
2:B:526:TRP:HB2	2:B:583:GLU:CG	2.50	0.41
3:D:912:HIS:HD1	3:D:914:ASP:HB3	1.85	0.41
3:D:2306:VAL:HG23	3:D:2306:VAL:O	2.20	0.41
4:E:535:ASP:HA	4:E:581:ALA:HB3	2.02	0.41
6:G:264:ASP:O	6:G:265:ARG:C	2.63	0.41
10:K:106:GLN:HE21	10:K:106:GLN:HB2	1.70	0.41
16:Q:227:THR:HB	16:Q:232:GLN:HG2	2.03	0.41
18:S:66:ASP:OD1	18:S:67:ARG:N	2.54	0.41
2:B:847:ASN:OD1	2:B:847:ASN:N	2.44	0.41
2:C:535:VAL:HG11	2:C:690:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:564:LEU:HA	2:C:668:GLY:O	2.21	0.41
2:C:571:THR:HG21	2:C:692:MET:HB3	2.03	0.41
4:E:180:GLU:OE2	4:E:234:ARG:NH2	2.54	0.41
4:E:720:LEU:HD23	4:E:720:LEU:HA	1.93	0.41
5:F:626:GLY:O	5:F:630:VAL:HG23	2.21	0.41
5:F:703:ALA:O	5:F:706:ARG:HG2	2.21	0.41
5:F:749:LEU:O	5:F:749:LEU:HD23	2.21	0.41
5:F:891:ASN:O	5:F:895:LEU:HG	2.21	0.41
6:G:273:PRO:HB2	6:G:311:THR:HG23	2.01	0.41
7:H:254:SER:O	7:H:281:ARG:NH2	2.43	0.41
16:Q:166:MET:HA	16:Q:169:VAL:CG1	2.49	0.41
16:Q:194:LYS:HB2	16:Q:194:LYS:HE2	1.85	0.41
1:A:370:GLU:HG2	18:S:16:LEU:HG	2.03	0.41
1:A:471:MET:HE2	1:A:471:MET:HB2	1.70	0.41
1:A:473:GLU:OE1	2:B:747:ARG:NH2	2.51	0.41
1:A:575:GLY:CA	1:A:579:ARG:HH21	2.33	0.41
1:A:618:ARG:HG2	1:A:619:PRO:HD2	2.01	0.41
1:A:876:ASP:OD2	2:B:896:ARG:NH2	2.52	0.41
2:B:610:GLU:HA	2:B:613:ASP:OD2	2.20	0.41
2:B:982:LEU:O	2:B:986:THR:HG22	2.21	0.41
2:B:1085:HIS:HB3	2:B:1086:GLY:H	1.55	0.41
3:D:906:LEU:H	3:D:906:LEU:HG	1.65	0.41
3:D:1337:ASN:H	3:D:1337:ASN:ND2	2.19	0.41
3:D:1664:LEU:O	3:D:1668:SER:OG	2.31	0.41
3:D:1804:GLN:O	3:D:1807:LEU:HB2	2.21	0.41
3:D:2421:GLN:OE1	7:H:145:GLN:NE2	2.54	0.41
28:D:3003:A1LXL:C08	15:P:413:LEU:HD11	2.51	0.41
4:E:482:LYS:HG2	4:E:604:MET:SD	2.61	0.41
5:F:236:VAL:HA	5:F:250:PRO:HG2	2.02	0.41
5:F:769:ALA:HA	5:F:774:ARG:NE	2.36	0.41
5:F:947:GLN:O	5:F:948:THR:HG22	2.20	0.41
6:G:127:ALA:HB1	6:G:438:ALA:HB1	2.03	0.41
6:G:184:VAL:HB	6:G:303:ARG:HH21	1.85	0.41
7:H:111:LEU:HD23	7:H:111:LEU:HA	1.66	0.41
7:H:401:ARG:HD3	7:H:401:ARG:HA	1.81	0.41
8:I:144:LEU:HD22	8:I:144:LEU:HA	1.91	0.41
12:M:327:TYR:HD1	12:M:327:TYR:HA	1.79	0.41
14:O:142:TRP:HZ2	14:O:309:ALA:CA	2.30	0.41
14:O:146:LEU:HD22	14:O:146:LEU:HA	1.79	0.41
16:Q:240:LYS:O	16:Q:243:LEU:HB3	2.21	0.41
2:B:577:ALA:HA	2:B:580:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1111:SER:O	2:B:1111:SER:OG	2.32	0.41
3:D:561:THR:HG21	15:P:373:GLU:HG2	2.02	0.41
3:D:1696:LEU:HA	3:D:1696:LEU:HD12	1.83	0.41
3:D:2378:ASN:OD1	3:D:2378:ASN:N	2.53	0.41
3:D:2534:GLN:HE21	8:I:155:ARG:NH1	2.19	0.41
3:D:2688:ILE:CG2	3:D:2691:GLU:HG3	2.51	0.41
4:E:542:LEU:HA	4:E:587:LEU:O	2.21	0.41
4:E:623:LYS:H	4:E:623:LYS:HG2	1.61	0.41
5:F:248:VAL:O	19:T:98:ARG:HD3	2.21	0.41
6:G:301:VAL:O	6:G:305:LEU:HG	2.21	0.41
12:M:609:LEU:HD12	12:M:609:LEU:HA	1.89	0.41
16:Q:346:GLN:HE21	16:Q:346:GLN:HB2	1.69	0.41
17:R:206:HIS:CG	17:R:207:PRO:HD2	2.56	0.41
1:A:168:ARG:HG3	1:A:184:LYS:HG3	2.02	0.40
1:A:937:ILE:O	1:A:941:THR:HG22	2.22	0.40
2:B:604:GLY:HA3	2:B:647:ILE:HG22	2.03	0.40
2:B:636:GLY:HA3	3:D:2058:LEU:HD22	2.03	0.40
2:B:761:ALA:HA	2:B:764:ASN:ND2	2.37	0.40
2:C:793:ASP:H	8:I:93:GLY:HA3	1.87	0.40
2:C:1077:ARG:NH2	2:C:1081:GLY:O	2.54	0.40
3:D:35:THR:HG23	3:D:36:LEU:HD22	2.02	0.40
3:D:57:LEU:HD23	3:D:57:LEU:HA	1.83	0.40
3:D:977:ARG:HE	3:D:977:ARG:HB2	1.72	0.40
3:D:2320:ILE:O	3:D:2323:VAL:HG22	2.20	0.40
4:E:351:LEU:HA	4:E:351:LEU:HD23	1.67	0.40
4:E:474:LEU:O	4:E:581:ALA:HA	2.21	0.40
4:E:856:SER:C	4:E:858:VAL:H	2.29	0.40
4:E:862:ARG:H	4:E:862:ARG:HG3	1.71	0.40
5:F:95:PRO:O	13:N:34:VAL:HG13	2.21	0.40
5:F:681:PHE:C	5:F:683:ALA:H	2.29	0.40
6:G:448:LEU:HA	6:G:451:THR:HG22	2.03	0.40
10:K:252:PHE:C	10:K:254:LEU:N	2.79	0.40
12:M:456:GLY:HA3	22:M:801:LMG:H131	2.02	0.40
12:M:649:GLN:HG3	12:M:650:GLN:N	2.36	0.40
14:O:407:THR:HB	15:P:244:TRP:HH2	1.85	0.40
1:A:505:LYS:H	23:A:1202:ANP:PB	2.43	0.40
2:B:495:ARG:O	2:B:496:ARG:C	2.63	0.40
2:C:543:ILE:HG12	2:C:580:ILE:HG23	2.03	0.40
3:D:1951:GLN:H	3:D:1951:GLN:HG2	1.61	0.40
3:D:2729:GLN:HG2	3:D:2788:ASN:HD21	1.86	0.40
6:G:296:ARG:NH2	6:G:492:ALA:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:49:ARG:O	13:N:50:GLU:C	2.64	0.40
15:P:119:ASP:HA	15:P:122:GLN:HE21	1.85	0.40
15:P:224:LEU:HD12	15:P:224:LEU:HA	1.84	0.40
15:P:269:LEU:HB3	15:P:270:LEU:HD12	2.03	0.40
15:P:358:LEU:HD22	15:P:361:ARG:NH1	2.36	0.40
19:T:89:GLU:HG2	19:T:90:GLN:H	1.86	0.40
1:A:192:LYS:HD3	17:R:285:GLU:OE2	2.21	0.40
1:A:444:LYS:HE2	1:A:444:LYS:N	2.37	0.40
1:A:467:LEU:HD23	1:A:497:PHE:HE1	1.87	0.40
1:A:1140:ARG:HD2	1:A:1140:ARG:HA	1.83	0.40
1:A:1161:PRO:HA	1:A:1162:PRO:HD3	1.92	0.40
2:B:342:ASP:OD1	2:B:342:ASP:N	2.54	0.40
2:B:660:ASP:OD1	2:B:660:ASP:N	2.54	0.40
2:B:989:LEU:HD23	2:B:989:LEU:HA	1.85	0.40
2:C:680:LEU:HB3	2:C:686:PHE:HD2	1.86	0.40
2:C:873:LEU:HD12	2:C:873:LEU:HA	1.88	0.40
3:D:912:HIS:CE1	3:D:914:ASP:HB3	2.57	0.40
3:D:1170:ASN:HD21	17:R:224:SER:HB3	1.87	0.40
3:D:1694:ILE:N	3:D:1695:PRO:HD2	2.36	0.40
3:D:2191:LYS:N	3:D:2191:LYS:HD2	2.37	0.40
3:D:2444:SER:OG	3:D:2445:LEU:N	2.54	0.40
8:I:109:GLN:NE2	8:I:141:GLU:O	2.52	0.40
15:P:245:LEU:HD23	15:P:245:LEU:HA	1.87	0.40
18:S:101:THR:HA	18:S:105:GLY:O	2.21	0.40
19:T:50:ASP:HB2	19:T:53:GLU:HB2	2.03	0.40
1:A:192:LYS:HB2	1:A:192:LYS:HE3	1.86	0.40
1:A:667:TRP:CZ2	1:A:700:VAL:HG23	2.56	0.40
2:C:467:ILE:HG13	2:C:468:SER:N	2.37	0.40
3:D:2124:ARG:HB2	4:E:827:ARG:HH21	1.86	0.40
4:E:871:LEU:HD23	4:E:871:LEU:HA	1.81	0.40
5:F:613:SER:OG	5:F:617:GLU:OE1	2.25	0.40
7:H:219:ASP:OD2	7:H:228:SER:OG	2.39	0.40
8:I:337:ASN:HD22	8:I:337:ASN:HA	1.62	0.40
11:L:159:LEU:HA	11:L:162:VAL:HG12	2.03	0.40
11:L:274:MET:HE3	11:L:274:MET:HB3	1.93	0.40
1:A:251:HIS:HA	1:A:252:PRO:HD3	1.95	0.40
1:A:465:GLU:O	1:A:468:VAL:HG22	2.21	0.40
1:A:908:ALA:O	1:A:911:ARG:NH2	2.54	0.40
1:A:920:GLU:OE1	1:A:933:ARG:NH2	2.50	0.40
2:B:730:THR:HG22	2:B:731:GLY:H	1.87	0.40
2:B:738:MET:HE3	2:B:739:ALA:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:545:TYR:HA	2:C:552:LEU:HD11	2.03	0.40
2:C:620:PRO:HB3	2:C:662:ARG:O	2.22	0.40
3:D:477:PHE:HE2	15:P:647:THR:HG21	1.86	0.40
3:D:880:SER:H	3:D:882:ARG:NH1	2.20	0.40
3:D:910:LYS:HE2	3:D:910:LYS:HB2	1.76	0.40
3:D:912:HIS:ND1	3:D:914:ASP:HB3	2.37	0.40
3:D:1363:ILE:HD12	17:R:56:HIS:HB2	2.02	0.40
3:D:1389:GLU:N	3:D:1389:GLU:OE2	2.55	0.40
3:D:2010:ASN:OD1	3:D:2010:ASN:N	2.55	0.40
4:E:75:PRO:HD3	5:F:245:GLY:HA2	2.02	0.40
4:E:898:ASP:N	4:E:898:ASP:OD1	2.53	0.40
6:G:257:ARG:HB3	6:G:268:ARG:NH2	2.36	0.40
10:K:94:THR:OG1	10:K:95:GLY:N	2.54	0.40
16:Q:134:PHE:HE2	16:Q:187:PHE:HB3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	982/1182 (83%)	895 (91%)	87 (9%)	0	100	100
2	B	736/1112 (66%)	670 (91%)	62 (8%)	4 (0%)	24	54
2	C	682/1112 (61%)	620 (91%)	60 (9%)	2 (0%)	36	65
3	D	1471/2971 (50%)	1319 (90%)	135 (9%)	17 (1%)	10	34
4	E	864/982 (88%)	803 (93%)	59 (7%)	2 (0%)	43	72
5	F	695/1024 (68%)	637 (92%)	57 (8%)	1 (0%)	48	77
6	G	392/495 (79%)	360 (92%)	31 (8%)	1 (0%)	36	65
7	H	404/555 (73%)	380 (94%)	23 (6%)	1 (0%)	43	72
8	I	268/366 (73%)	238 (89%)	30 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	82/117 (70%)	78 (95%)	3 (4%)	1 (1%)	10	34
10	K	187/255 (73%)	165 (88%)	17 (9%)	5 (3%)	4	16
11	L	149/303 (49%)	137 (92%)	12 (8%)	0	100	100
12	M	388/682 (57%)	366 (94%)	21 (5%)	1 (0%)	36	65
13	N	113/137 (82%)	103 (91%)	10 (9%)	0	100	100
14	O	312/471 (66%)	285 (91%)	25 (8%)	2 (1%)	21	51
15	P	613/691 (89%)	544 (89%)	63 (10%)	6 (1%)	12	39
16	Q	260/365 (71%)	251 (96%)	9 (4%)	0	100	100
17	R	393/462 (85%)	349 (89%)	42 (11%)	2 (0%)	24	54
18	S	112/324 (35%)	97 (87%)	14 (12%)	1 (1%)	14	41
19	T	106/299 (36%)	96 (91%)	9 (8%)	1 (1%)	14	41
21	U	6/156 (4%)	5 (83%)	1 (17%)	0	100	100
All	All	9215/14061 (66%)	8398 (91%)	770 (8%)	47 (0%)	26	54

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	2680	LEU
3	D	2749	ASN
3	D	2801	HIS
3	D	2891	PHE
3	D	2894	ASP
15	P	347	PRO
3	D	969	PHE
3	D	2631	LEU
3	D	2633	PRO
10	K	90	SER
10	K	100	ALA
2	B	595	ASP
2	C	424	PRO
3	D	1326	HIS
3	D	2153	TYR
3	D	2251	VAL
3	D	2679	LYS
3	D	2778	SER
3	D	2893	PHE
10	K	241	PRO
12	M	285	ALA

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Mol	Chain	Res	Type
15	P	71	GLU
15	P	203	GLY
15	P	352	GLY
19	T	40	PRO
2	B	250	PRO
3	D	2748	LEU
6	G	261	SER
9	J	73	LEU
2	B	444	THR
3	D	2250	ILE
4	E	256	PRO
5	F	154	PRO
15	P	517	ASN
17	R	6	SER
17	R	333	TRP
2	B	453	LEU
7	H	150	GLY
10	K	91	ILE
18	S	106	ALA
14	O	304	VAL
4	E	352	PRO
2	C	779	GLY
3	D	971	PRO
10	K	242	VAL
14	O	296	PRO
15	P	493	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	774/936 (83%)	701 (91%)	73 (9%)	8	26
2	B	599/858 (70%)	542 (90%)	57 (10%)	8	26
2	C	548/858 (64%)	496 (90%)	52 (10%)	8	26
3	D	1443/2762 (52%)	1283 (89%)	160 (11%)	6	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	540/774 (70%)	497 (92%)	43 (8%)	11	34
5	F	542/773 (70%)	492 (91%)	50 (9%)	8	27
6	G	283/358 (79%)	244 (86%)	39 (14%)	3	12
7	H	346/451 (77%)	324 (94%)	22 (6%)	16	44
8	I	204/263 (78%)	184 (90%)	20 (10%)	7	25
9	J	64/87 (74%)	56 (88%)	8 (12%)	4	15
10	K	163/215 (76%)	145 (89%)	18 (11%)	6	20
11	L	124/243 (51%)	115 (93%)	9 (7%)	13	38
12	M	298/492 (61%)	282 (95%)	16 (5%)	20	51
13	N	92/107 (86%)	81 (88%)	11 (12%)	5	16
14	O	129/340 (38%)	110 (85%)	19 (15%)	3	10
15	P	431/485 (89%)	386 (90%)	45 (10%)	7	23
16	Q	218/296 (74%)	193 (88%)	25 (12%)	5	18
17	R	312/345 (90%)	291 (93%)	21 (7%)	15	43
18	S	97/226 (43%)	88 (91%)	9 (9%)	8	27
19	T	83/198 (42%)	81 (98%)	2 (2%)	43	75
21	U	1/7 (14%)	1 (100%)	0	100	100
All	All	7291/11074 (66%)	6592 (90%)	699 (10%)	10	26

All (699) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	THR
1	A	152	SER
1	A	225	VAL
1	A	262	VAL
1	A	275	VAL
1	A	306	VAL
1	A	314	GLN
1	A	353	SER
1	A	381	VAL
1	A	388	ILE
1	A	422	LYS
1	A	435	SER
1	A	450	LYS
1	A	461	ILE

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Mol	Chain	Res	Type
1	A	464	MET
1	A	465	GLU
1	A	467	LEU
1	A	471	MET
1	A	481	ASP
1	A	503	THR
1	A	523	SER
1	A	526	SER
1	A	557	ILE
1	A	560	ILE
1	A	568	SER
1	A	570	LEU
1	A	579	ARG
1	A	597	THR
1	A	616	LEU
1	A	625	VAL
1	A	649	LEU
1	A	658	LEU
1	A	664	THR
1	A	675	LEU
1	A	678	GLU
1	A	683	THR
1	A	686	ARG
1	A	688	VAL
1	A	695	MET
1	A	697	LEU
1	A	699	LEU
1	A	730	VAL
1	A	738	LEU
1	A	739	GLU
1	A	745	THR
1	A	773	GLU
1	A	774	GLU
1	A	775	THR
1	A	781	ARG
1	A	782	THR
1	A	791	VAL
1	A	796	LEU
1	A	819	LEU
1	A	823	ASP
1	A	826	SER
1	A	827	LEU

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Mol	Chain	Res	Type
1	A	833	LEU
1	A	883	ASP
1	A	940	SER
1	A	941	THR
1	A	968	LEU
1	A	973	GLU
1	A	1031	THR
1	A	1036	SER
1	A	1043	LEU
1	A	1055	VAL
1	A	1093	SER
1	A	1096	SER
1	A	1098	GLU
1	A	1104	SER
1	A	1136	LEU
1	A	1147	GLN
1	A	1152	THR
2	B	208	GLU
2	B	237	THR
2	B	246	ARG
2	B	271	ILE
2	B	356	LEU
2	B	363	VAL
2	B	372	VAL
2	B	381	LEU
2	B	416	ARG
2	B	417	LEU
2	B	418	CYS
2	B	439	VAL
2	B	441	THR
2	B	446	ASP
2	B	448	ARG
2	B	458	LEU
2	B	470	LEU
2	B	479	LEU
2	B	495	ARG
2	B	524	ILE
2	B	551	LEU
2	B	552	LEU
2	B	554	SER
2	B	576	LEU
2	B	592	SER

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Mol	Chain	Res	Type
2	B	595	ASP
2	B	603	VAL
2	B	611	THR
2	B	622	ILE
2	B	625	ILE
2	B	660	ASP
2	B	670	THR
2	B	681	ILE
2	B	711	LYS
2	B	713	VAL
2	B	716	ASN
2	B	719	TRP
2	B	722	VAL
2	B	730	THR
2	B	753	ILE
2	B	754	THR
2	B	755	GLU
2	B	763	GLU
2	B	795	ILE
2	B	804	SER
2	B	813	LEU
2	B	817	THR
2	B	845	ASP
2	B	853	THR
2	B	855	SER
2	B	881	THR
2	B	885	SER
2	B	919	THR
2	B	921	GLU
2	B	961	VAL
2	B	1006	SER
2	B	1091	MET
2	C	377	SER
2	C	406	THR
2	C	407	THR
2	C	418	CYS
2	C	420	VAL
2	C	424	PRO
2	C	430	ASP
2	C	440	ASP
2	C	443	VAL
2	C	446	ASP

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Mol	Chain	Res	Type
2	C	452	SER
2	C	467	ILE
2	C	474	ILE
2	C	487	ARG
2	C	499	LEU
2	C	522	ASP
2	C	529	ILE
2	C	546	LEU
2	C	548	ASN
2	C	552	LEU
2	C	557	VAL
2	C	592	SER
2	C	612	PHE
2	C	623	LEU
2	C	626	ASP
2	C	665	VAL
2	C	680	LEU
2	C	705	GLN
2	C	707	HIS
2	C	722	VAL
2	C	730	THR
2	C	754	THR
2	C	768	GLU
2	C	771	LEU
2	C	774	SER
2	C	783	VAL
2	C	813	LEU
2	C	817	THR
2	C	827	SER
2	C	841	VAL
2	C	845	ASP
2	C	848	VAL
2	C	873	LEU
2	C	919	THR
2	C	946	THR
2	C	949	SER
2	C	998	LYS
2	C	1056	THR
2	C	1058	ASP
2	C	1071	THR
2	C	1095	VAL
2	C	1099	LEU

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Mol	Chain	Res	Type
3	D	35	THR
3	D	58	ILE
3	D	62	LYS
3	D	273	LEU
3	D	318	SER
3	D	319	LEU
3	D	324	THR
3	D	326	LEU
3	D	332	LEU
3	D	333	SER
3	D	350	LEU
3	D	353	THR
3	D	355	GLN
3	D	474	LEU
3	D	475	PHE
3	D	476	LEU
3	D	549	SER
3	D	553	ILE
3	D	554	ASP
3	D	557	LEU
3	D	560	ILE
3	D	563	LYS
3	D	576	SER
3	D	616	SER
3	D	735	GLN
3	D	740	LEU
3	D	745	THR
3	D	753	THR
3	D	755	ILE
3	D	784	HIS
3	D	786	SER
3	D	793	LEU
3	D	795	THR
3	D	810	LEU
3	D	879	THR
3	D	887	PHE
3	D	888	LEU
3	D	890	SER
3	D	905	THR
3	D	906	LEU
3	D	915	THR
3	D	939	SER

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Mol	Chain	Res	Type
3	D	940	SER
3	D	952	LYS
3	D	960	THR
3	D	963	GLN
3	D	982	LEU
3	D	988	ARG
3	D	1125	GLN
3	D	1126	ASN
3	D	1133	LYS
3	D	1222	THR
3	D	1248	TYR
3	D	1249	SER
3	D	1314	LEU
3	D	1315	ASN
3	D	1316	VAL
3	D	1319	GLU
3	D	1324	ILE
3	D	1329	TRP
3	D	1333	LEU
3	D	1365	SER
3	D	1370	SER
3	D	1374	LYS
3	D	1375	THR
3	D	1411	VAL
3	D	1412	SER
3	D	1426	LEU
3	D	1431	SER
3	D	1435	ASN
3	D	1688	SER
3	D	1694	ILE
3	D	1763	THR
3	D	1770	GLU
3	D	1776	TRP
3	D	1783	LEU
3	D	1805	ASN
3	D	1818	LEU
3	D	1944	LEU
3	D	1951	GLN
3	D	1957	SER
3	D	1958	TRP
3	D	1984	ILE
3	D	2020	VAL

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Mol	Chain	Res	Type
3	D	2023	LYS
3	D	2026	SER
3	D	2027	ASN
3	D	2031	ASP
3	D	2046	MET
3	D	2058	LEU
3	D	2088	GLU
3	D	2128	HIS
3	D	2143	THR
3	D	2153	TYR
3	D	2165	ASP
3	D	2183	ASN
3	D	2212	ASN
3	D	2232	SER
3	D	2239	LEU
3	D	2249	LYS
3	D	2251	VAL
3	D	2283	GLU
3	D	2287	SER
3	D	2293	LEU
3	D	2294	ASP
3	D	2295	MET
3	D	2297	THR
3	D	2300	LEU
3	D	2303	ILE
3	D	2320	ILE
3	D	2335	ASP
3	D	2340	LEU
3	D	2366	ASN
3	D	2445	LEU
3	D	2446	ASN
3	D	2451	SER
3	D	2459	LEU
3	D	2524	LEU
3	D	2532	LEU
3	D	2554	ILE
3	D	2558	ASP
3	D	2560	LEU
3	D	2577	ILE
3	D	2600	LYS
3	D	2601	SER
3	D	2630	HIS

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Mol	Chain	Res	Type
3	D	2632	LEU
3	D	2633	PRO
3	D	2634	LYS
3	D	2680	LEU
3	D	2688	ILE
3	D	2689	LEU
3	D	2714	PHE
3	D	2719	THR
3	D	2721	ASP
3	D	2730	ILE
3	D	2731	THR
3	D	2733	LEU
3	D	2734	GLU
3	D	2748	LEU
3	D	2767	THR
3	D	2778	SER
3	D	2806	THR
3	D	2808	GLN
3	D	2810	TRP
3	D	2815	SER
3	D	2831	SER
3	D	2860	LEU
3	D	2861	ASP
3	D	2863	LEU
3	D	2868	ASP
3	D	2870	ASP
3	D	2874	ASN
3	D	2878	ARG
3	D	2891	PHE
3	D	2896	LEU
3	D	2900	GLU
3	D	2911	ILE
3	D	2929	ASN
3	D	2964	LEU
4	E	103	THR
4	E	114	GLN
4	E	126	LEU
4	E	142	THR
4	E	191	THR
4	E	214	THR
4	E	227	THR
4	E	228	SER

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Mol	Chain	Res	Type
4	E	248	THR
4	E	253	PRO
4	E	255	SER
4	E	258	ASP
4	E	308	ARG
4	E	313	SER
4	E	338	VAL
4	E	353	GLU
4	E	354	LEU
4	E	357	LEU
4	E	577	VAL
4	E	614	GLU
4	E	622	ASN
4	E	682	VAL
4	E	692	LEU
4	E	694	VAL
4	E	707	VAL
4	E	718	VAL
4	E	721	VAL
4	E	725	SER
4	E	742	THR
4	E	748	LEU
4	E	769	ARG
4	E	807	ILE
4	E	816	SER
4	E	818	ASP
4	E	820	VAL
4	E	843	THR
4	E	847	ASP
4	E	901	GLU
4	E	919	SER
4	E	936	THR
4	E	944	SER
4	E	945	ARG
4	E	977	GLN
5	F	78	VAL
5	F	129	LEU
5	F	138	THR
5	F	223	VAL
5	F	224	LEU
5	F	263	GLU
5	F	265	LEU

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Mol	Chain	Res	Type
5	F	290	TRP
5	F	544	GLU
5	F	556	GLN
5	F	561	LEU
5	F	562	MET
5	F	565	VAL
5	F	595	LYS
5	F	597	LEU
5	F	619	ILE
5	F	622	TYR
5	F	633	LEU
5	F	644	ILE
5	F	645	ILE
5	F	647	ILE
5	F	672	ASN
5	F	674	LEU
5	F	690	VAL
5	F	748	SER
5	F	761	VAL
5	F	767	PHE
5	F	768	LEU
5	F	782	LEU
5	F	783	THR
5	F	784	LEU
5	F	787	GLU
5	F	788	GLN
5	F	829	VAL
5	F	833	THR
5	F	837	SER
5	F	866	GLU
5	F	884	ARG
5	F	885	ASP
5	F	889	SER
5	F	892	GLN
5	F	920	ARG
5	F	932	GLU
5	F	939	THR
5	F	946	ASN
5	F	947	GLN
5	F	949	ARG
5	F	950	SER
5	F	988	LEU

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Mol	Chain	Res	Type
5	F	1001	GLN
6	G	102	ARG
6	G	116	CYS
6	G	117	LEU
6	G	147	THR
6	G	165	THR
6	G	172	LEU
6	G	174	VAL
6	G	181	SER
6	G	203	SER
6	G	204	VAL
6	G	213	SER
6	G	218	LEU
6	G	238	THR
6	G	241	LEU
6	G	243	VAL
6	G	245	GLU
6	G	253	GLU
6	G	256	ARG
6	G	257	ARG
6	G	260	SER
6	G	265	ARG
6	G	274	SER
6	G	305	LEU
6	G	345	LEU
6	G	348	LEU
6	G	362	LEU
6	G	369	LEU
6	G	376	THR
6	G	391	THR
6	G	402	LEU
6	G	408	GLU
6	G	411	SER
6	G	414	LEU
6	G	419	SER
6	G	428	VAL
6	G	443	GLN
6	G	460	GLU
6	G	466	LEU
6	G	490	GLU
7	H	98	GLN
7	H	107	GLU

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Mol	Chain	Res	Type
7	H	108	SER
7	H	114	GLN
7	H	137	VAL
7	H	184	VAL
7	H	198	ASP
7	H	217	SER
7	H	243	PRO
7	H	259	LYS
7	H	271	LEU
7	H	273	VAL
7	H	283	SER
7	H	292	ASP
7	H	304	VAL
7	H	310	VAL
7	H	313	ASP
7	H	323	THR
7	H	351	SER
7	H	357	ILE
7	H	383	SER
7	H	458	SER
8	I	61	ASN
8	I	84	THR
8	I	92	ILE
8	I	99	ARG
8	I	122	ARG
8	I	125	SER
8	I	139	GLN
8	I	144	LEU
8	I	153	GLU
8	I	210	ASP
8	I	232	LEU
8	I	241	VAL
8	I	266	CYS
8	I	289	SER
8	I	300	LEU
8	I	303	SER
8	I	306	ARG
8	I	309	LEU
8	I	329	MET
8	I	352	SER
9	J	36	ASP
9	J	46	SER

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Mol	Chain	Res	Type
9	J	54	THR
9	J	67	ASP
9	J	74	ASP
9	J	76	VAL
9	J	88	ILE
9	J	100	THR
10	K	67	THR
10	K	76	THR
10	K	82	GLU
10	K	87	THR
10	K	90	SER
10	K	94	THR
10	K	101	SER
10	K	114	GLU
10	K	143	THR
10	K	150	GLN
10	K	152	ARG
10	K	193	LEU
10	K	202	THR
10	K	206	SER
10	K	219	SER
10	K	233	THR
10	K	236	VAL
10	K	250	THR
11	L	183	VAL
11	L	234	VAL
11	L	241	LEU
11	L	244	ASN
11	L	245	HIS
11	L	263	ARG
11	L	296	VAL
11	L	297	VAL
11	L	299	LEU
12	M	282	ARG
12	M	283	VAL
12	M	286	ASP
12	M	300	LEU
12	M	336	ILE
12	M	344	LEU
12	M	393	SER
12	M	421	VAL
12	M	443	LEU

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Mol	Chain	Res	Type
12	M	445	LEU
12	M	555	LEU
12	M	569	ASN
12	M	576	VAL
12	M	584	SER
12	M	622	GLU
12	M	643	GLN
13	N	34	VAL
13	N	35	LYS
13	N	48	THR
13	N	49	ARG
13	N	52	LEU
13	N	53	LYS
13	N	80	SER
13	N	105	ILE
13	N	122	ARG
13	N	130	ARG
13	N	132	GLU
14	O	146	LEU
14	O	261	VAL
14	O	264	LEU
14	O	267	THR
14	O	298	THR
14	O	304	VAL
14	O	312	LEU
14	O	315	LEU
14	O	320	LEU
14	O	376	SER
14	O	390	SER
14	O	401	VAL
14	O	403	VAL
14	O	416	THR
14	O	425	LEU
14	O	434	SER
14	O	436	VAL
14	O	437	VAL
14	O	465	SER
15	P	58	LEU
15	P	65	LEU
15	P	89	ASP
15	P	104	GLU
15	P	106	GLN

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Mol	Chain	Res	Type
15	P	109	VAL
15	P	111	LYS
15	P	156	SER
15	P	159	SER
15	P	176	LEU
15	P	189	GLU
15	P	217	SER
15	P	249	LEU
15	P	302	THR
15	P	321	ARG
15	P	345	LEU
15	P	347	PRO
15	P	348	THR
15	P	349	ASP
15	P	350	LEU
15	P	351	ASN
15	P	353	VAL
15	P	378	VAL
15	P	385	VAL
15	P	393	LYS
15	P	394	GLU
15	P	418	SER
15	P	432	GLU
15	P	442	SER
15	P	459	THR
15	P	470	LEU
15	P	531	THR
15	P	547	LEU
15	P	562	GLU
15	P	565	LEU
15	P	567	SER
15	P	568	GLU
15	P	571	THR
15	P	577	LEU
15	P	593	THR
15	P	600	SER
15	P	680	ASP
15	P	684	LEU
15	P	688	LEU
15	P	689	GLU
16	Q	99	ASP
16	Q	121	VAL

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Mol	Chain	Res	Type
16	Q	131	LEU
16	Q	133	PHE
16	Q	140	ASP
16	Q	144	LEU
16	Q	166	MET
16	Q	169	VAL
16	Q	174	THR
16	Q	192	ASP
16	Q	196	VAL
16	Q	226	VAL
16	Q	243	LEU
16	Q	247	VAL
16	Q	261	LEU
16	Q	263	LYS
16	Q	276	ILE
16	Q	292	LEU
16	Q	293	GLU
16	Q	300	ARG
16	Q	302	LYS
16	Q	303	LEU
16	Q	314	GLU
16	Q	323	VAL
16	Q	350	VAL
17	R	6	SER
17	R	7	ARG
17	R	20	SER
17	R	33	VAL
17	R	66	VAL
17	R	115	VAL
17	R	137	SER
17	R	157	VAL
17	R	200	LEU
17	R	232	MET
17	R	242	GLU
17	R	249	GLN
17	R	253	ASP
17	R	254	ARG
17	R	264	GLU
17	R	304	VAL
17	R	351	ASP
17	R	390	LYS
17	R	402	LEU

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Mol	Chain	Res	Type
17	R	418	VAL
17	R	444	ARG
18	S	36	GLU
18	S	37	TYR
18	S	46	THR
18	S	74	GLU
18	S	80	ASP
18	S	89	ASP
18	S	99	LEU
18	S	102	SER
18	S	113	ASP
19	T	22	GLU
19	T	32	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (184) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	308	GLN
1	A	340	GLN
1	A	351	GLN
1	A	423	GLN
1	A	541	ASN
1	A	665	GLN
1	A	677	ASN
1	A	783	ASN
1	A	801	HIS
1	A	1147	GLN
2	B	274	GLN
2	B	530	ASN
2	B	638	GLN
2	B	748	GLN
2	B	751	HIS
2	B	892	ASN
2	B	952	GLN
2	B	1088	HIS
2	C	431	HIS
2	C	435	ASN
2	C	456	GLN
2	C	617	ASN
2	C	649	ASN
2	C	654	GLN

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Mol	Chain	Res	Type
2	C	707	HIS
2	C	890	HIS
2	C	944	HIS
2	C	952	GLN
3	D	37	GLN
3	D	38	ASN
3	D	44	GLN
3	D	65	GLN
3	D	271	GLN
3	D	325	GLN
3	D	355	GLN
3	D	461	ASN
3	D	465	ASN
3	D	574	ASN
3	D	634	GLN
3	D	637	ASN
3	D	743	ASN
3	D	818	ASN
3	D	819	GLN
3	D	897	HIS
3	D	909	HIS
3	D	1126	ASN
3	D	1137	ASN
3	D	1138	ASN
3	D	1178	ASN
3	D	1226	ASN
3	D	1227	GLN
3	D	1315	ASN
3	D	1317	GLN
3	D	1337	ASN
3	D	1364	ASN
3	D	1678	ASN
3	D	1728	GLN
3	D	1741	HIS
3	D	1760	GLN
3	D	1817	ASN
3	D	1915	ASN
3	D	1951	GLN
3	D	1959	HIS
3	D	1961	HIS
3	D	1976	HIS
3	D	1994	GLN

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Mol	Chain	Res	Type
3	D	2012	GLN
3	D	2016	ASN
3	D	2028	ASN
3	D	2136	GLN
3	D	2140	HIS
3	D	2183	ASN
3	D	2184	HIS
3	D	2185	ASN
3	D	2212	ASN
3	D	2263	GLN
3	D	2374	ASN
3	D	2377	GLN
3	D	2416	ASN
3	D	2446	ASN
3	D	2531	GLN
3	D	2572	ASN
3	D	2652	GLN
3	D	2687	ASN
3	D	2729	GLN
3	D	2739	HIS
3	D	2749	ASN
3	D	2763	ASN
3	D	2780	ASN
3	D	2874	ASN
3	D	2884	ASN
3	D	2929	ASN
3	D	2953	GLN
4	E	68	ASN
4	E	86	HIS
4	E	114	GLN
4	E	194	HIS
4	E	250	GLN
4	E	263	HIS
4	E	270	GLN
4	E	651	ASN
4	E	679	GLN
4	E	727	GLN
4	E	823	GLN
4	E	886	GLN
4	E	964	GLN
4	E	977	GLN
5	F	153	GLN

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Mol	Chain	Res	Type
5	F	272	ASN
5	F	664	ASN
5	F	672	ASN
5	F	695	ASN
5	F	763	ASN
5	F	779	GLN
5	F	867	GLN
5	F	891	ASN
5	F	892	GLN
5	F	896	GLN
5	F	913	HIS
5	F	1001	GLN
5	F	1008	HIS
5	F	1017	GLN
6	G	157	GLN
6	G	258	HIS
6	G	400	HIS
6	G	426	GLN
6	G	437	HIS
6	G	443	GLN
6	G	481	GLN
7	H	98	GLN
7	H	110	GLN
7	H	114	GLN
7	H	145	GLN
7	H	210	GLN
7	H	261	HIS
7	H	317	GLN
7	H	406	GLN
8	I	61	ASN
8	I	160	GLN
8	I	337	ASN
8	I	355	GLN
10	K	106	GLN
10	K	150	GLN
10	K	186	GLN
11	L	293	GLN
12	M	298	GLN
12	M	361	HIS
12	M	400	HIS
12	M	404	HIS
12	M	416	HIS

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Mol	Chain	Res	Type
12	M	457	HIS
13	N	56	GLN
13	N	60	ASN
13	N	108	GLN
15	P	123	GLN
15	P	262	HIS
15	P	267	ASN
15	P	268	GLN
15	P	326	ASN
15	P	331	GLN
15	P	351	ASN
15	P	390	GLN
15	P	403	GLN
15	P	466	GLN
16	Q	168	ASN
16	Q	195	GLN
16	Q	220	GLN
16	Q	253	GLN
16	Q	285	ASN
16	Q	346	GLN
17	R	45	HIS
17	R	191	HIS
17	R	237	ASN
17	R	260	GLN
17	R	321	ASN
17	R	443	GLN
18	S	32	HIS
18	S	55	GLN
18	S	58	ASN
18	S	82	GLN
19	T	21	GLN
19	T	54	GLN
19	T	122	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	TPO	R	167	17	8,10,11	1.62	1 (12%)	10,14,16	2.32	2 (20%)
18	SEP	S	85	18	8,9,10	1.60	1 (12%)	7,12,14	0.83	0
2	TPO	B	346	2	8,10,11	1.64	1 (12%)	10,14,16	2.03	1 (10%)
18	SEP	S	84	18	8,9,10	1.56	1 (12%)	7,12,14	1.25	1 (14%)
19	SEP	T	28	19	8,9,10	1.58	1 (12%)	7,12,14	1.15	1 (14%)
2	TPO	B	337	2	8,10,11	1.61	1 (12%)	10,14,16	2.02	1 (10%)
17	SEP	R	126	17	8,9,10	1.58	1 (12%)	7,12,14	0.97	0
18	TPO	S	107	18	8,10,11	1.64	1 (12%)	10,14,16	2.11	1 (10%)
2	TPO	B	347	2	8,10,11	1.60	1 (12%)	10,14,16	2.37	2 (20%)
19	SEP	T	18	19	8,9,10	1.59	1 (12%)	7,12,14	1.15	1 (14%)
9	4HH	J	72	9	22,26,27	0.38	0	27,35,37	0.69	0

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
17	TPO	R	167	17	-	3/9/11/13	-
18	SEP	S	85	18	-	1/6/8/10	-
2	TPO	B	346	2	-	0/9/11/13	-
18	SEP	S	84	18	-	2/6/8/10	-
19	SEP	T	28	19	-	2/6/8/10	-
2	TPO	B	337	2	-	4/9/11/13	-
17	SEP	R	126	17	-	0/6/8/10	-
18	TPO	S	107	18	-	4/9/11/13	-
2	TPO	B	347	2	-	2/9/11/13	-
19	SEP	T	18	19	-	0/6/8/10	-
9	4HH	J	72	9	-	14/33/35/37	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	S	85	SEP	P-O1P	3.53	1.61	1.50
18	S	107	TPO	P-O1P	3.52	1.61	1.50
2	B	337	TPO	P-O1P	3.50	1.61	1.50
2	B	346	TPO	P-O1P	3.47	1.61	1.50
19	T	18	SEP	P-O1P	3.47	1.61	1.50
19	T	28	SEP	P-O1P	3.44	1.61	1.50
2	B	347	TPO	P-O1P	3.43	1.61	1.50
17	R	126	SEP	P-O1P	3.43	1.61	1.50
17	R	167	TPO	P-O1P	3.42	1.61	1.50
18	S	84	SEP	P-O1P	3.38	1.61	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	347	TPO	P-OG1-CB	-6.75	104.98	123.33
17	R	167	TPO	P-OG1-CB	-6.58	105.44	123.33
18	S	107	TPO	P-OG1-CB	-6.25	106.34	123.33
2	B	346	TPO	P-OG1-CB	-5.70	107.84	123.33
2	B	337	TPO	P-OG1-CB	-5.68	107.91	123.33
18	S	84	SEP	OG-CB-CA	2.63	110.71	108.14
19	T	28	SEP	OG-CB-CA	2.41	110.49	108.14
2	B	347	TPO	CG2-CB-CA	-2.26	108.86	113.26
19	T	18	SEP	OG-CB-CA	2.26	110.34	108.14
17	R	167	TPO	CG2-CB-CA	-2.08	109.20	113.26

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	72	4HH	C-CA-CB-OG
9	J	72	4HH	N-CA-CB-OG
9	J	72	4HH	CB-OG-P-O1P
9	J	72	4HH	CB-OG-P-O2P
9	J	72	4HH	CB-OG-P-O3P
9	J	72	4HH	CJ-O3P-P-O1P
9	J	72	4HH	NN-CO-CP-CQ
9	J	72	4HH	CP-CQ-NR-CS
9	J	72	4HH	OR-CQ-NR-CS
18	S	84	SEP	N-CA-CB-OG
18	S	84	SEP	C-CA-CB-OG
18	S	107	TPO	N-CA-CB-CG2
18	S	107	TPO	N-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
18	S	107	TPO	C-CA-CB-CG2
18	S	107	TPO	O-C-CA-CB
2	B	337	TPO	N-CA-CB-OG1
2	B	337	TPO	C-CA-CB-CG2
2	B	337	TPO	N-CA-CB-CG2
19	T	28	SEP	CA-CB-OG-P
9	J	72	4HH	O3P-CJ-CK-CL2
9	J	72	4HH	NR-CS-CT-SU
9	J	72	4HH	CJ-O3P-P-OG
9	J	72	4HH	CJ-O3P-P-O2P
19	T	28	SEP	CB-OG-P-O1P
18	S	85	SEP	N-CA-CB-OG
17	R	167	TPO	CB-OG1-P-O3P
9	J	72	4HH	O3P-CJ-CK-CL1
17	R	167	TPO	O-C-CA-CB
2	B	337	TPO	O-C-CA-CB
2	B	347	TPO	O-C-CA-CB
17	R	167	TPO	N-CA-CB-CG2
2	B	347	TPO	N-CA-CB-CG2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	S	85	SEP	1	0
2	B	346	TPO	1	0
18	S	84	SEP	1	0
18	S	107	TPO	2	0
9	J	72	4HH	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 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
22	LMG	C	1201	-	24,24,55	0.75	0	26,26,63	1.15	1 (3%)
27	Y01	M	802	-	38,38,38	0.51	0	57,57,57	0.76	1 (1%)
29	DGD	L	401	-	42,42,67	1.06	2 (4%)	56,56,81	1.42	9 (16%)
23	ANP	F	1101	-	33,33,33	0.93	4 (12%)	45,52,52	0.64	0
23	ANP	E	1001	-	33,33,33	0.92	4 (12%)	45,52,52	0.60	0
25	SQD	I	401	-	47,49,54	1.09	6 (12%)	57,60,65	1.65	12 (21%)
28	A1LXL	P	701	-	33,33,33	4.71	12 (36%)	51,51,51	2.75	21 (41%)
22	LMG	A	1201	-	46,46,55	1.03	4 (8%)	54,54,63	1.41	7 (12%)
25	SQD	K	302	-	43,45,54	1.16	6 (13%)	53,56,65	1.72	10 (18%)
23	ANP	A	1202	24	33,33,33	1.10	5 (15%)	45,52,52	0.93	2 (4%)
22	LMG	M	801	-	48,48,55	0.91	3 (6%)	56,56,63	1.46	9 (16%)
22	LMG	K	301	-	41,41,55	0.91	4 (9%)	49,49,63	1.45	7 (14%)
27	Y01	D	3002	-	38,38,38	0.48	0	57,57,57	0.66	0
23	ANP	C	1202	-	33,33,33	0.94	4 (12%)	45,52,52	0.62	0
26	DGA	D	3001	-	33,33,43	1.22	3 (9%)	35,35,45	1.71	3 (8%)
25	SQD	A	1204	-	44,46,54	1.14	6 (13%)	54,57,65	1.70	11 (20%)
28	A1LXL	D	3003	-	33,33,33	4.62	12 (36%)	51,51,51	2.51	14 (27%)
29	DGD	I	403	-	41,41,67	1.51	11 (26%)	55,55,81	1.54	8 (14%)
26	DGA	O	3101	-	38,38,43	1.12	3 (7%)	40,40,45	1.81	5 (12%)
22	LMG	I	402	-	32,32,55	1.17	3 (9%)	40,40,63	1.39	8 (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
22	LMG	C	1201	-	-	12/26/26/70	-
27	Y01	M	802	-	-	3/19/77/77	0/4/4/4
29	DGD	L	401	-	-	11/30/70/95	0/2/2/2
23	ANP	F	1101	-	-	5/18/38/38	0/3/3/3
23	ANP	E	1001	-	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SQD	I	401	-	-	18/44/64/69	0/1/1/1
28	A1LXL	P	701	-	-	10/15/73/73	0/4/4/4
22	LMG	A	1201	-	-	19/41/61/70	0/1/1/1
25	SQD	K	302	-	-	18/40/60/69	0/1/1/1
23	ANP	A	1202	24	-	4/18/38/38	0/3/3/3
22	LMG	M	801	-	-	23/43/63/70	0/1/1/1
22	LMG	K	301	-	-	13/36/56/70	0/1/1/1
27	Y01	D	3002	-	-	13/19/77/77	0/4/4/4
23	ANP	C	1202	-	-	5/18/38/38	0/3/3/3
26	DGA	D	3001	-	-	17/35/35/45	-
25	SQD	A	1204	-	-	19/41/61/69	0/1/1/1
28	A1LXL	D	3003	-	-	8/15/73/73	0/4/4/4
29	DGD	I	403	-	-	12/29/69/95	0/2/2/2
26	DGA	O	3101	-	-	25/40/40/45	-
22	LMG	I	402	-	-	16/27/47/70	0/1/1/1

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	P	701	A1LXL	C18-C19	16.92	1.67	1.33
28	D	3003	A1LXL	C18-C19	16.58	1.67	1.33
28	P	701	A1LXL	C06-C08	-11.35	1.35	1.54
28	D	3003	A1LXL	C06-C08	-10.78	1.35	1.54
28	D	3003	A1LXL	C17-C16	8.98	1.67	1.53
28	P	701	A1LXL	C17-C16	8.85	1.67	1.53
28	P	701	A1LXL	C09-C08	7.50	1.69	1.54
28	D	3003	A1LXL	C09-C08	7.34	1.69	1.54
28	P	701	A1LXL	C13-C14	6.57	1.66	1.53
28	D	3003	A1LXL	C13-C14	6.04	1.65	1.53
28	D	3003	A1LXL	C12-C08	6.01	1.66	1.55
28	D	3003	A1LXL	C13-C12	-5.97	1.43	1.54
28	P	701	A1LXL	C13-C12	-5.89	1.43	1.54
28	P	701	A1LXL	C12-C08	5.85	1.65	1.55
28	P	701	A1LXL	C20-C15	3.85	1.62	1.56
28	D	3003	A1LXL	C20-C15	3.79	1.62	1.56
28	P	701	A1LXL	C10-C11	3.51	1.61	1.54
28	D	3003	A1LXL	C10-C11	3.40	1.61	1.54
26	D	3001	DGA	OG2-CB1	3.35	1.43	1.34
26	D	3001	DGA	OG1-CA1	3.34	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O	3101	DGA	OG2-CB1	3.34	1.43	1.34
29	I	403	DGD	O2G-C2G	-3.33	1.38	1.46
28	D	3003	A1LXL	C07-C06	3.29	1.61	1.53
28	P	701	A1LXL	C07-C06	3.24	1.61	1.53
29	I	403	DGD	O1G-C1G	-3.21	1.38	1.45
22	M	801	LMG	O1-C7	-3.06	1.38	1.43
22	I	402	LMG	O7-C8	-3.04	1.39	1.46
28	D	3003	A1LXL	C05-C06	3.04	1.61	1.54
26	O	3101	DGA	OG1-CA1	3.01	1.42	1.33
23	A	1202	ANP	PG-O1G	2.96	1.50	1.46
29	I	403	DGD	O3G-C3G	-2.94	1.38	1.43
25	I	401	SQD	O48-C23	2.91	1.41	1.33
22	A	1201	LMG	O4-C4	-2.85	1.35	1.43
22	A	1201	LMG	O6-C5	-2.84	1.37	1.44
25	A	1204	SQD	O48-C23	2.81	1.41	1.33
23	A	1202	ANP	PB-O1B	2.79	1.50	1.46
25	K	302	SQD	O47-C7	2.76	1.42	1.34
25	K	302	SQD	O48-C23	2.75	1.41	1.33
25	I	401	SQD	O47-C7	2.71	1.41	1.34
22	M	801	LMG	O8-C9	-2.69	1.39	1.45
29	I	403	DGD	O6D-C5D	-2.68	1.37	1.44
28	P	701	A1LXL	C24-C19	2.68	1.57	1.51
22	A	1201	LMG	O7-C8	-2.67	1.40	1.46
29	I	403	DGD	O3G-C1D	-2.62	1.35	1.40
22	A	1201	LMG	O1-C7	-2.61	1.39	1.43
23	A	1202	ANP	PG-O2G	-2.59	1.49	1.56
22	M	801	LMG	O7-C8	-2.58	1.40	1.46
25	K	302	SQD	O2-C2	-2.55	1.36	1.43
25	A	1204	SQD	O47-C7	2.55	1.41	1.34
25	A	1204	SQD	O2-C2	-2.53	1.36	1.43
23	E	1001	ANP	PB-O3A	-2.53	1.55	1.59
23	A	1202	ANP	PG-O3G	-2.53	1.50	1.56
23	C	1202	ANP	PB-O3A	-2.53	1.55	1.59
29	I	403	DGD	O5D-C6D	-2.52	1.39	1.43
28	D	3003	A1LXL	C24-C19	2.50	1.56	1.51
22	I	402	LMG	O4-C4	-2.50	1.36	1.43
23	F	1101	ANP	PG-N3B	2.50	1.69	1.63
23	F	1101	ANP	PB-O1B	2.48	1.49	1.46
25	K	302	SQD	O4-C4	-2.45	1.36	1.43
29	I	403	DGD	O4D-C4D	-2.45	1.36	1.43
23	F	1101	ANP	PG-O1G	2.44	1.49	1.46
23	E	1001	ANP	PG-O1G	2.42	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	301	LMG	O1-C7	-2.42	1.39	1.43
25	I	401	SQD	O2-C2	-2.41	1.37	1.43
29	L	401	DGD	O2G-C2G	-2.40	1.41	1.46
25	A	1204	SQD	O47-C45	-2.38	1.41	1.46
23	A	1202	ANP	PB-O2B	-2.38	1.50	1.56
23	C	1202	ANP	PG-O1G	2.38	1.49	1.46
23	E	1001	ANP	PB-O1B	2.37	1.49	1.46
25	K	302	SQD	O47-C45	-2.36	1.41	1.46
29	I	403	DGD	O2D-C2D	-2.34	1.37	1.43
26	D	3001	DGA	OG2-CG2	-2.34	1.41	1.46
23	C	1202	ANP	PB-O1B	2.31	1.49	1.46
23	E	1001	ANP	PG-N3B	2.30	1.69	1.63
23	C	1202	ANP	PG-N3B	2.26	1.69	1.63
22	K	301	LMG	O7-C8	-2.26	1.41	1.46
25	A	1204	SQD	O3-C3	-2.26	1.37	1.43
22	I	402	LMG	O8-C9	-2.25	1.40	1.45
25	K	302	SQD	O3-C3	-2.24	1.37	1.43
25	I	401	SQD	O47-C45	-2.24	1.41	1.46
28	P	701	A1LXL	C05-C06	2.23	1.59	1.54
29	I	403	DGD	O2E-C2E	-2.22	1.37	1.43
25	I	401	SQD	O3-C3	-2.21	1.37	1.43
23	F	1101	ANP	PB-O3A	-2.21	1.56	1.59
29	I	403	DGD	O6E-C5E	-2.21	1.39	1.44
25	I	401	SQD	O4-C4	-2.21	1.37	1.43
22	K	301	LMG	O6-C5	-2.19	1.39	1.44
26	O	3101	DGA	OG2-CG2	-2.18	1.41	1.46
25	A	1204	SQD	O4-C4	-2.18	1.37	1.43
29	L	401	DGD	O1G-C1G	-2.13	1.40	1.45
22	K	301	LMG	O8-C9	-2.12	1.40	1.45
29	I	403	DGD	O4E-C4E	-2.01	1.38	1.43

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	3003	A1LXL	C24-C19-C20	-8.04	106.12	116.42
28	D	3003	A1LXL	C17-C18-C19	-6.90	113.37	125.02
26	O	3101	DGA	CDB-CCB-CBB	-6.79	80.05	114.37
26	D	3001	DGA	CDB-CCB-CBB	-6.71	80.47	114.37
28	P	701	A1LXL	C24-C19-C20	-6.67	107.89	116.42
28	P	701	A1LXL	C17-C18-C19	-6.44	114.14	125.02
28	P	701	A1LXL	C12-C11-C16	-5.72	106.30	114.41
25	I	401	SQD	O6-C1-C2	5.45	116.56	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1204	SQD	O6-C1-C2	5.41	116.49	108.27
26	O	3101	DGA	OG2-CB1-CB2	5.40	123.17	111.48
28	P	701	A1LXL	C27-C12-C11	-5.34	101.99	111.68
28	P	701	A1LXL	C04-C05-C06	-5.24	101.91	115.37
28	D	3003	A1LXL	C27-C12-C11	-4.98	102.64	111.68
28	P	701	A1LXL	C13-C12-C08	4.81	123.68	116.60
25	K	302	SQD	O6-C1-C2	4.79	115.55	108.27
28	D	3003	A1LXL	C20-C19-C18	-4.77	115.97	122.93
28	P	701	A1LXL	C10-C11-C16	4.64	126.51	119.10
25	K	302	SQD	O9-S-O7	-4.53	99.10	113.82
29	I	403	DGD	O3G-C3G-C2G	-4.52	99.81	110.82
28	D	3003	A1LXL	C26-C20-C15	-4.50	106.61	111.66
28	P	701	A1LXL	C20-C19-C18	-4.49	116.38	122.93
28	D	3003	A1LXL	C12-C08-C06	-4.44	112.63	119.50
28	P	701	A1LXL	C16-C17-C18	-4.38	106.69	112.76
29	L	401	DGD	O3G-C3G-C2G	-4.30	100.35	110.82
28	P	701	A1LXL	C12-C08-C06	-4.21	112.99	119.50
28	D	3003	A1LXL	C13-C12-C08	4.16	122.72	116.60
25	K	302	SQD	O47-C7-C8	4.15	120.45	111.48
23	A	1202	ANP	O2B-PB-O1B	4.07	118.61	109.87
26	D	3001	DGA	OG2-CB1-CB2	4.06	120.26	111.48
25	I	401	SQD	O9-S-O7	-3.93	101.04	113.82
25	A	1204	SQD	O9-S-O7	-3.87	101.25	113.82
28	D	3003	A1LXL	C13-C12-C11	3.81	112.95	107.25
28	P	701	A1LXL	C26-C20-C15	-3.72	107.49	111.66
22	K	301	LMG	O1-C1-C2	-3.61	102.79	108.27
29	L	401	DGD	O6D-C1D-O3G	-3.55	101.64	110.04
29	I	403	DGD	O6D-C1D-O3G	-3.55	101.65	110.04
28	P	701	A1LXL	C21-C22-C23	3.55	115.18	110.48
25	A	1204	SQD	O47-C7-C8	3.55	119.15	111.48
28	D	3003	A1LXL	C08-C12-C11	3.48	104.10	100.10
28	D	3003	A1LXL	C21-C22-C23	3.48	115.09	110.48
22	K	301	LMG	O6-C1-O1	-3.39	102.03	110.04
25	K	302	SQD	C1-C2-C3	-3.36	102.95	110.01
25	A	1204	SQD	O8-S-C6	3.33	112.40	105.97
25	A	1204	SQD	C1-C2-C3	-3.31	103.05	110.01
25	I	401	SQD	O7-S-C6	3.25	111.60	106.76
28	P	701	A1LXL	C08-C12-C11	3.24	103.81	100.10
25	K	302	SQD	O7-S-C6	3.14	111.44	106.76
25	I	401	SQD	O47-C7-C8	3.11	118.20	111.48
25	K	302	SQD	O9-S-C6	3.10	111.39	106.76
22	A	1201	LMG	O6-C1-O1	-3.07	102.79	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	3003	A1LXL	C27-C12-C08	-3.07	106.12	111.68
25	A	1204	SQD	O9-S-C6	3.04	111.29	106.76
25	I	401	SQD	O9-S-C6	3.03	111.28	106.76
25	I	401	SQD	O5-C5-C4	3.00	115.10	109.70
25	I	401	SQD	C1-C2-C3	-2.90	103.90	110.01
25	K	302	SQD	O5-C5-C4	2.90	114.92	109.70
29	I	403	DGD	C1D-C2D-C3D	-2.88	103.94	110.01
25	A	1204	SQD	O7-S-C6	2.88	111.06	106.76
28	D	3003	A1LXL	C27-C12-C13	-2.85	106.41	110.61
28	P	701	A1LXL	C27-C12-C13	-2.83	106.43	110.61
28	P	701	A1LXL	C17-C16-C11	2.79	114.89	110.93
22	I	402	LMG	O3-C3-C2	-2.79	103.80	110.38
25	I	401	SQD	O48-C23-C24	2.78	120.31	111.83
22	A	1201	LMG	C1-C2-C3	-2.78	104.17	110.01
28	P	701	A1LXL	C13-C12-C11	2.74	111.34	107.25
26	O	3101	DGA	OG1-CA1-CA2	2.73	120.15	111.83
26	D	3001	DGA	OG1-CA1-CA2	2.72	120.12	111.83
22	M	801	LMG	O1-C7-C8	-2.71	104.24	110.82
29	L	401	DGD	C3G-C2G-C1G	-2.69	105.52	111.78
28	D	3003	A1LXL	C11-C16-C15	2.63	112.52	109.09
22	K	301	LMG	O3-C3-C2	-2.62	104.21	110.38
22	M	801	LMG	C1-C2-C3	-2.60	104.53	110.01
22	A	1201	LMG	O3-C3-C2	-2.59	104.28	110.38
25	K	302	SQD	O48-C23-C24	2.58	119.69	111.83
25	A	1204	SQD	O48-C23-O10	-2.57	117.19	123.63
22	I	402	LMG	O6-C1-C2	-2.55	105.14	110.37
22	I	402	LMG	C1-C2-C3	-2.54	104.66	110.01
22	K	301	LMG	O1-C7-C8	-2.53	104.67	110.82
25	A	1204	SQD	O5-C5-C4	2.52	114.24	109.70
22	K	301	LMG	O2-C2-C1	-2.51	104.10	110.08
26	O	3101	DGA	CB3-CB2-CB1	-2.50	104.52	113.69
29	I	403	DGD	O2D-C2D-C1D	-2.50	104.12	110.08
22	M	801	LMG	O1-C1-C2	-2.48	104.50	108.27
22	I	402	LMG	O2-C2-C1	-2.48	104.17	110.08
22	C	1201	LMG	O1-C7-C8	-2.48	105.41	111.77
22	K	301	LMG	O7-C10-O9	-2.47	117.94	123.70
29	I	403	DGD	O3E-C3E-C2E	-2.46	104.57	110.38
22	M	801	LMG	C40-C39-C38	-2.44	102.04	114.37
22	M	801	LMG	O6-C1-O1	-2.43	104.29	110.04
22	M	801	LMG	C38-C37-C36	-2.42	102.13	114.37
22	M	801	LMG	O3-C3-C2	-2.38	104.76	110.38
22	A	1201	LMG	O2-C2-C1	-2.36	104.46	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1201	LMG	C38-C37-C36	-2.34	102.52	114.37
25	I	401	SQD	C3-C4-C5	2.34	114.48	110.23
23	A	1202	ANP	O2G-PG-O1G	-2.34	107.59	113.45
27	M	802	Y01	CAP-CAQ-CBG	-2.32	100.60	105.14
28	P	701	A1LXL	C22-C23-C24	2.31	113.54	110.29
26	O	3101	DGA	CG1-CG2-CG3	-2.30	106.48	111.80
28	P	701	A1LXL	C27-C12-C08	-2.29	107.52	111.68
22	I	402	LMG	O7-C10-O9	-2.29	118.36	123.70
29	I	403	DGD	C3G-C2G-C1G	-2.29	106.46	111.78
29	L	401	DGD	C3D-C4D-C5D	-2.28	106.09	110.23
25	K	302	SQD	O8-S-C6	2.26	110.34	105.97
29	L	401	DGD	O2D-C2D-C1D	-2.25	104.71	110.08
22	I	402	LMG	O6-C1-O1	-2.25	104.73	110.04
28	D	3003	A1LXL	C14-C15-C20	-2.24	110.33	113.08
22	I	402	LMG	O8-C28-O10	-2.21	118.10	123.63
22	A	1201	LMG	C1-O6-C5	-2.21	109.41	113.72
25	K	302	SQD	O48-C23-O10	-2.20	118.13	123.63
29	L	401	DGD	O3G-C1D-C2D	-2.16	104.99	108.27
22	M	801	LMG	O2-C2-C1	-2.16	104.93	110.08
29	I	403	DGD	O4D-C4D-C5D	-2.14	104.05	109.32
25	A	1204	SQD	O48-C23-C24	2.13	118.34	111.83
28	P	701	A1LXL	C09-C08-C06	-2.13	108.96	112.18
28	P	701	A1LXL	C07-C06-C05	-2.12	107.06	110.34
22	K	301	LMG	C6-C5-C4	-2.10	107.86	113.02
25	I	401	SQD	O8-S-C6	2.09	110.02	105.97
29	I	403	DGD	O6D-C5D-C6D	-2.09	102.55	106.69
29	L	401	DGD	O4D-C4D-C5D	-2.09	104.19	109.32
25	A	1204	SQD	C45-O47-C7	2.07	122.75	117.80
28	P	701	A1LXL	C20-C15-C16	-2.06	109.70	112.71
22	I	402	LMG	C1-O6-C5	-2.04	109.73	113.72
22	A	1201	LMG	O1-C7-C8	-2.04	105.85	110.82
29	L	401	DGD	C4E-C3E-C2E	-2.04	107.25	110.83
29	L	401	DGD	O5E-C6E-C5E	-2.03	104.44	111.33
25	I	401	SQD	O47-C7-O49	-2.02	118.98	123.70
22	M	801	LMG	C9-C8-C7	-2.02	107.08	111.78
25	I	401	SQD	O48-C23-O10	-2.01	118.60	123.63

There are no chirality outliers.

All (254) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	C	1201	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	C	1201	LMG	O1-C7-C8-O7
22	I	402	LMG	O6-C1-O1-C7
22	I	402	LMG	C11-C10-O7-C8
22	K	301	LMG	O7-C8-C9-O8
23	A	1202	ANP	PB-N3B-PG-O1G
23	A	1202	ANP	PG-N3B-PB-O1B
23	A	1202	ANP	C5'-O5'-PA-O3A
23	C	1202	ANP	PG-N3B-PB-O1B
23	C	1202	ANP	PG-N3B-PB-O3A
23	C	1202	ANP	C5'-O5'-PA-O1A
23	C	1202	ANP	C5'-O5'-PA-O3A
23	E	1001	ANP	C5'-O5'-PA-O2A
23	E	1001	ANP	C5'-O5'-PA-O3A
23	F	1101	ANP	PB-N3B-PG-O1G
23	F	1101	ANP	PA-O3A-PB-O2B
25	I	401	SQD	C5-C6-S-O7
25	I	401	SQD	C5-C6-S-O8
25	I	401	SQD	C5-C6-S-O9
25	K	302	SQD	O49-C7-O47-C45
25	K	302	SQD	C8-C7-O47-C45
25	K	302	SQD	C5-C6-S-O7
26	D	3001	DGA	CB2-CB1-OG2-CG2
26	O	3101	DGA	CG1-CG2-CG3-OXT
26	O	3101	DGA	OG2-CG2-CG3-OXT
28	D	3003	A1LXL	C03-C04-C05-C06
28	P	701	A1LXL	C01-C02-C03-C04
27	D	3002	Y01	CAJ-CAO-CBB-CAC
25	A	1204	SQD	O10-C23-O48-C46
25	I	401	SQD	O49-C7-O47-C45
26	D	3001	DGA	OB1-CB1-OG2-CG2
22	M	801	LMG	C4-C5-C6-O5
28	P	701	A1LXL	C04-C05-C06-C07
22	A	1201	LMG	O10-C28-O8-C9
22	I	402	LMG	O9-C10-O7-C8
27	D	3002	Y01	OAG-CAY-OAW-CBC
25	A	1204	SQD	C24-C23-O48-C46
22	A	1201	LMG	C4-C5-C6-O5
27	D	3002	Y01	CAM-CAY-OAW-CBC
22	I	402	LMG	O6-C5-C6-O5
22	M	801	LMG	O10-C28-O8-C9
22	M	801	LMG	O6-C1-O1-C7
22	M	801	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
26	D	3001	DGA	CA2-CA1-OG1-CG1
22	A	1201	LMG	O6-C5-C6-O5
22	A	1201	LMG	C29-C28-O8-C9
22	M	801	LMG	C29-C28-O8-C9
26	O	3101	DGA	CA2-CA1-OG1-CG1
28	P	701	A1LXL	C04-C05-C06-C08
29	L	401	DGD	C1B-C2B-C3B-C4B
22	M	801	LMG	O9-C10-O7-C8
29	I	403	DGD	C1B-C2B-C3B-C4B
29	I	403	DGD	O6D-C1D-O3G-C3G
22	A	1201	LMG	C30-C31-C32-C33
26	O	3101	DGA	OA1-CA1-OG1-CG1
26	O	3101	DGA	CB1-CB2-CB3-CB4
22	M	801	LMG	C11-C10-O7-C8
26	D	3001	DGA	OA1-CA1-OG1-CG1
22	C	1201	LMG	C10-C11-C12-C13
26	O	3101	DGA	CA6-CA7-CA8-CA9
26	O	3101	DGA	CA1-CA2-CA3-CA4
22	I	402	LMG	C29-C28-O8-C9
27	D	3002	Y01	CAX-CAL-CAM-CAY
29	L	401	DGD	C2B-C1B-O2G-C2G
28	D	3003	A1LXL	C01-C02-C03-C04
25	I	401	SQD	C8-C7-O47-C45
29	I	403	DGD	O1A-C1A-O1G-C1G
25	K	302	SQD	C24-C25-C26-C27
26	O	3101	DGA	CB5-CB6-CB7-CB8
22	C	1201	LMG	C13-C14-C15-C16
22	K	301	LMG	C31-C32-C33-C34
25	K	302	SQD	C11-C10-C9-C8
26	O	3101	DGA	CB2-CB1-OG2-CG2
26	D	3001	DGA	CA4-CA5-CA6-CA7
22	C	1201	LMG	C32-C33-C34-C35
25	K	302	SQD	C26-C27-C28-C29
25	I	401	SQD	C30-C31-C32-C33
22	M	801	LMG	C13-C14-C15-C16
28	D	3003	A1LXL	C01-C02-C03-C28
28	P	701	A1LXL	C01-C02-C03-C28
25	K	302	SQD	C10-C11-C12-C13
22	C	1201	LMG	C28-C29-C30-C31
25	K	302	SQD	C32-C33-C34-C35
22	K	301	LMG	C15-C16-C17-C18
26	D	3001	DGA	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
26	D	3001	DGA	CA2-CA3-CA4-CA5
22	K	301	LMG	C18-C19-C20-C21
22	M	801	LMG	C12-C13-C14-C15
26	O	3101	DGA	CB6-CB7-CB8-CB9
22	M	801	LMG	C17-C18-C19-C20
22	M	801	LMG	C33-C34-C35-C36
25	K	302	SQD	C30-C31-C32-C33
26	D	3001	DGA	CBB-CCB-CDB-CEB
26	O	3101	DGA	CB4-CB5-CB6-CB7
26	O	3101	DGA	OB1-CB1-OG2-CG2
25	A	1204	SQD	C13-C14-C15-C16
22	I	402	LMG	C2-C1-O1-C7
22	M	801	LMG	C38-C39-C40-C41
29	I	403	DGD	C2B-C1B-O2G-C2G
22	I	402	LMG	C13-C14-C15-C16
26	D	3001	DGA	CB2-CB3-CB4-CB5
22	A	1201	LMG	C29-C30-C31-C32
22	A	1201	LMG	C32-C33-C34-C35
26	O	3101	DGA	CDB-CEB-CFB-CGB
29	I	403	DGD	C2B-C3B-C4B-C5B
22	A	1201	LMG	C35-C36-C37-C38
22	M	801	LMG	C11-C12-C13-C14
22	C	1201	LMG	C11-C10-O7-C8
25	A	1204	SQD	C10-C11-C12-C13
25	K	302	SQD	C7-C8-C9-C10
25	A	1204	SQD	O47-C45-C46-O48
22	I	402	LMG	C4-C5-C6-O5
25	I	401	SQD	C9-C10-C11-C12
25	A	1204	SQD	C9-C10-C11-C12
22	K	301	LMG	C16-C17-C18-C19
26	O	3101	DGA	CAB-CBB-CCB-CDB
25	A	1204	SQD	C8-C7-O47-C45
25	I	401	SQD	C11-C12-C13-C14
26	D	3001	DGA	CB6-CB7-CB8-CB9
26	D	3001	DGA	CBB-CAB-CB9-CB8
28	P	701	A1LXL	C02-C03-C28-C29
28	P	701	A1LXL	C04-C03-C28-C29
29	L	401	DGD	O1B-C1B-O2G-C2G
22	M	801	LMG	C37-C38-C39-C40
29	I	403	DGD	C2D-C1D-O3G-C3G
22	K	301	LMG	C7-C8-C9-O8
25	I	401	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
29	L	401	DGD	O1G-C1G-C2G-C3G
22	M	801	LMG	C32-C33-C34-C35
22	A	1201	LMG	C33-C34-C35-C36
25	I	401	SQD	C12-C13-C14-C15
26	O	3101	DGA	CBB-CCB-CDB-CEB
22	M	801	LMG	C14-C15-C16-C17
26	D	3001	DGA	CB4-CB5-CB6-CB7
25	A	1204	SQD	C26-C27-C28-C29
29	I	403	DGD	C3B-C4B-C5B-C6B
22	K	301	LMG	C30-C31-C32-C33
22	A	1201	LMG	O7-C8-C9-O8
22	A	1201	LMG	C16-C17-C18-C19
26	O	3101	DGA	CA8-CA9-CAA-CBA
22	A	1201	LMG	C31-C32-C33-C34
29	I	403	DGD	C2A-C1A-O1G-C1G
26	D	3001	DGA	CA6-CA7-CA8-CA9
28	P	701	A1LXL	C02-C03-C28-C30
26	D	3001	DGA	CB3-CB4-CB5-CB6
29	I	403	DGD	O6E-C5E-C6E-O5E
25	A	1204	SQD	C25-C26-C27-C28
22	K	301	LMG	C32-C33-C34-C35
26	O	3101	DGA	CA5-CA6-CA7-CA8
22	M	801	LMG	O1-C7-C8-C9
25	A	1204	SQD	C44-C45-C46-O48
25	K	302	SQD	C44-C45-C46-O48
22	I	402	LMG	C28-C29-C30-C31
27	D	3002	Y01	CAO-CAJ-CAN-CBA
26	O	3101	DGA	CBB-CAB-CB9-CB8
22	K	301	LMG	C13-C14-C15-C16
22	K	301	LMG	C17-C18-C19-C20
23	F	1101	ANP	O4'-C4'-C5'-O5'
22	C	1201	LMG	C30-C31-C32-C33
25	A	1204	SQD	C12-C13-C14-C15
22	M	801	LMG	C18-C19-C20-C21
29	L	401	DGD	O6D-C1D-O3G-C3G
26	D	3001	DGA	CCB-CDB-CEB-CFB
28	P	701	A1LXL	C02-C03-C04-C05
22	A	1201	LMG	C19-C20-C21-C22
28	P	701	A1LXL	C04-C03-C28-C30
25	K	302	SQD	C25-C26-C27-C28
23	F	1101	ANP	C3'-C4'-C5'-O5'
29	L	401	DGD	O1G-C1A-C2A-C3A

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Mol	Chain	Res	Type	Atoms
22	A	1201	LMG	C7-C8-C9-O8
22	C	1201	LMG	C33-C34-C35-C36
22	C	1201	LMG	C29-C30-C31-C32
25	K	302	SQD	C31-C32-C33-C34
25	K	302	SQD	O47-C45-C46-O48
29	L	401	DGD	C2B-C3B-C4B-C5B
25	K	302	SQD	C12-C13-C14-C15
22	M	801	LMG	C35-C36-C37-C38
22	M	801	LMG	C34-C35-C36-C37
22	A	1201	LMG	C15-C16-C17-C18
27	D	3002	Y01	CAJ-CAO-CBB-CBE
28	D	3003	A1LXL	C07-C06-C08-C12
22	M	801	LMG	O1-C7-C8-O7
25	I	401	SQD	O6-C44-C45-O47
25	I	401	SQD	O47-C45-C46-O48
29	L	401	DGD	O1G-C1G-C2G-O2G
22	I	402	LMG	O1-C7-C8-C9
25	I	401	SQD	C7-C8-C9-C10
25	A	1204	SQD	C11-C12-C13-C14
23	A	1202	ANP	C5'-O5'-PA-O1A
23	C	1202	ANP	C5'-O5'-PA-O2A
23	E	1001	ANP	C5'-O5'-PA-O1A
26	O	3101	DGA	CB7-CB8-CB9-CAB
22	I	402	LMG	O10-C28-O8-C9
22	M	801	LMG	C7-C8-O7-C10
22	A	1201	LMG	C37-C38-C39-C40
27	D	3002	Y01	CAC-CBB-CBE-CBI
26	O	3101	DGA	CA9-CAA-CBA-CCA
27	D	3002	Y01	CAO-CBB-CBE-CAP
25	I	401	SQD	C10-C11-C12-C13
27	D	3002	Y01	CAO-CBB-CBE-CBI
26	O	3101	DGA	CB9-CAB-CBB-CCB
28	P	701	A1LXL	C28-C03-C04-C05
22	A	1201	LMG	C11-C12-C13-C14
26	D	3001	DGA	CA8-CA9-CAA-CBA
26	O	3101	DGA	CB2-CB3-CB4-CB5
25	A	1204	SQD	O5-C1-O6-C44
25	K	302	SQD	C29-C30-C31-C32
25	I	401	SQD	C25-C26-C27-C28
25	A	1204	SQD	C28-C29-C30-C31
29	L	401	DGD	C2A-C3A-C4A-C5A
22	I	402	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
27	D	3002	Y01	CAC-CBB-CBE-CAP
27	D	3002	Y01	CAJ-CAN-CBA-CAA
27	M	802	Y01	CAO-CAJ-CAN-CBA
22	K	301	LMG	C20-C21-C22-C23
22	I	402	LMG	C7-C8-C9-O8
29	I	403	DGD	C4E-C5E-C6E-O5E
25	A	1204	SQD	C30-C31-C32-C33
28	D	3003	A1LXL	C04-C03-C28-C30
27	D	3002	Y01	CAM-CAL-CAX-OAH
25	I	401	SQD	C27-C28-C29-C30
22	K	301	LMG	O6-C1-O1-C7
25	K	302	SQD	C45-C44-O6-C1
25	K	302	SQD	C5-C6-S-O8
22	A	1201	LMG	C17-C18-C19-C20
29	L	401	DGD	C2D-C1D-O3G-C3G
25	I	401	SQD	C34-C35-C36-C37
27	D	3002	Y01	CAM-CAL-CAX-OAF
25	A	1204	SQD	C14-C15-C16-C17
22	K	301	LMG	O1-C7-C8-C9
25	I	401	SQD	O6-C44-C45-C46
28	D	3003	A1LXL	C02-C03-C28-C29
22	I	402	LMG	O1-C7-C8-O7
26	O	3101	DGA	OG1-CA1-CA2-CA3
25	A	1204	SQD	C24-C25-C26-C27
22	M	801	LMG	C28-C29-C30-C31
22	I	402	LMG	C11-C12-C13-C14
22	C	1201	LMG	C14-C15-C16-C17
25	A	1204	SQD	O48-C23-C24-C25
22	I	402	LMG	O8-C28-C29-C30
25	A	1204	SQD	O47-C7-C8-C9
29	I	403	DGD	O2G-C1B-C2B-C3B
26	O	3101	DGA	CA3-CA4-CA5-CA6
27	M	802	Y01	CAM-CAL-CAX-OAH
28	D	3003	A1LXL	C02-C03-C04-C05
27	M	802	Y01	CAJ-CAN-CBA-CAB
22	A	1201	LMG	C34-C35-C36-C37
26	O	3101	DGA	OA1-CA1-CA2-CA3
23	F	1101	ANP	PG-N3B-PB-O3A
28	D	3003	A1LXL	C05-C06-C08-C12
29	L	401	DGD	O2G-C1B-C2B-C3B
22	C	1201	LMG	O9-C10-O7-C8
29	I	403	DGD	O1B-C1B-C2B-C3B

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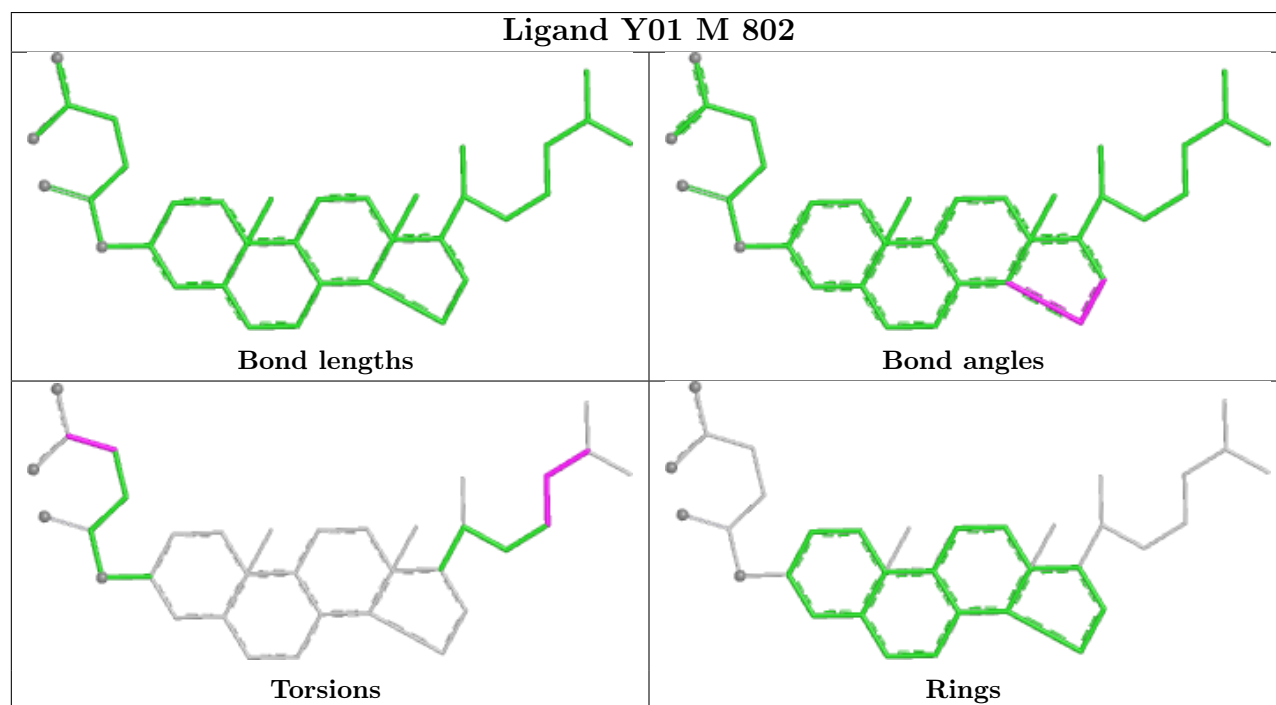
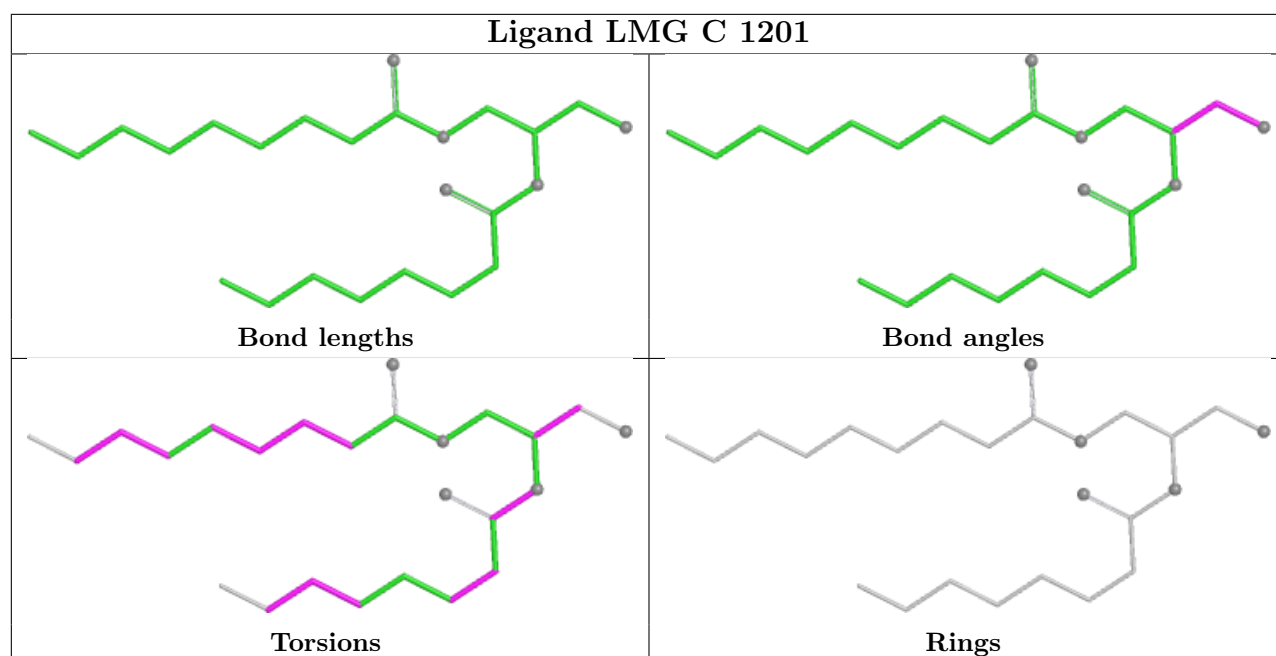
Mol	Chain	Res	Type	Atoms
26	D	3001	DGA	OG1-CA1-CA2-CA3

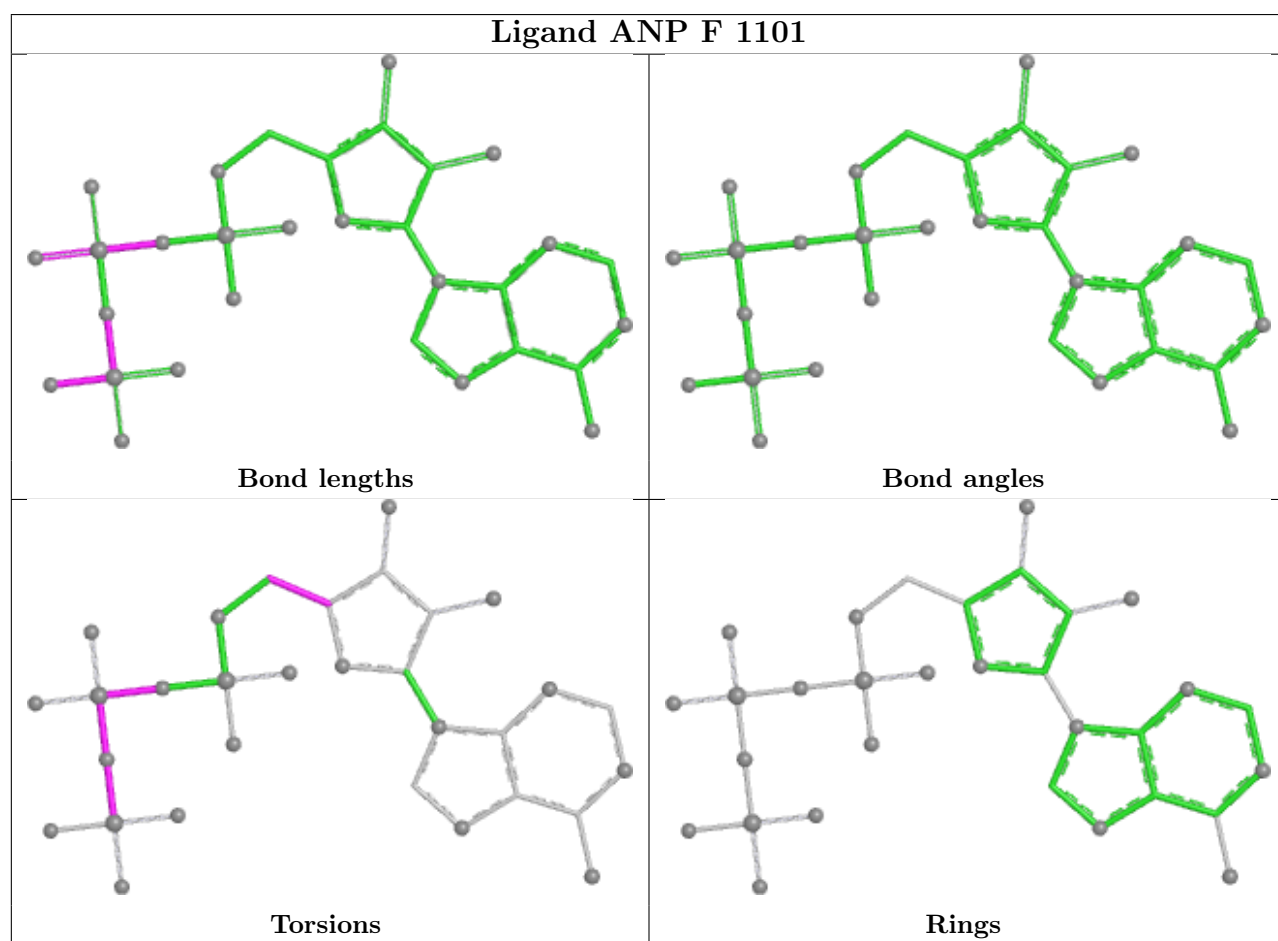
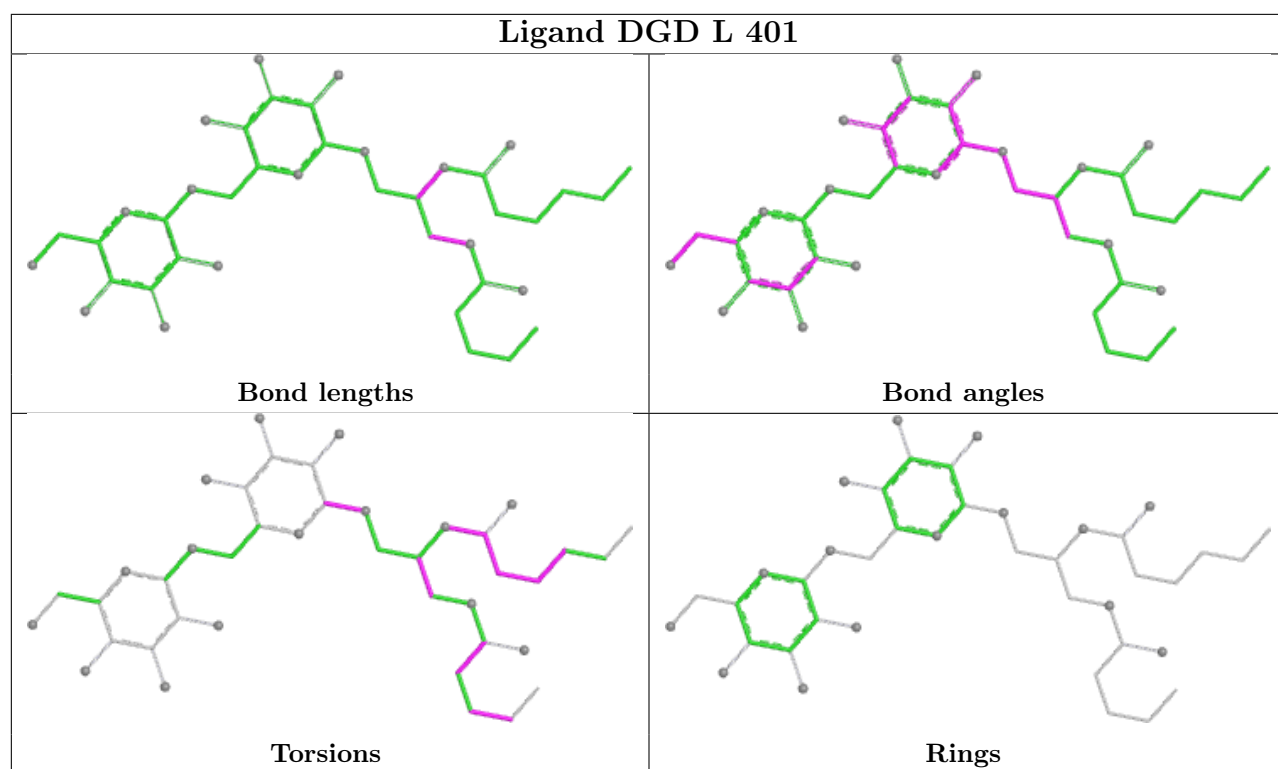
There are no ring outliers.

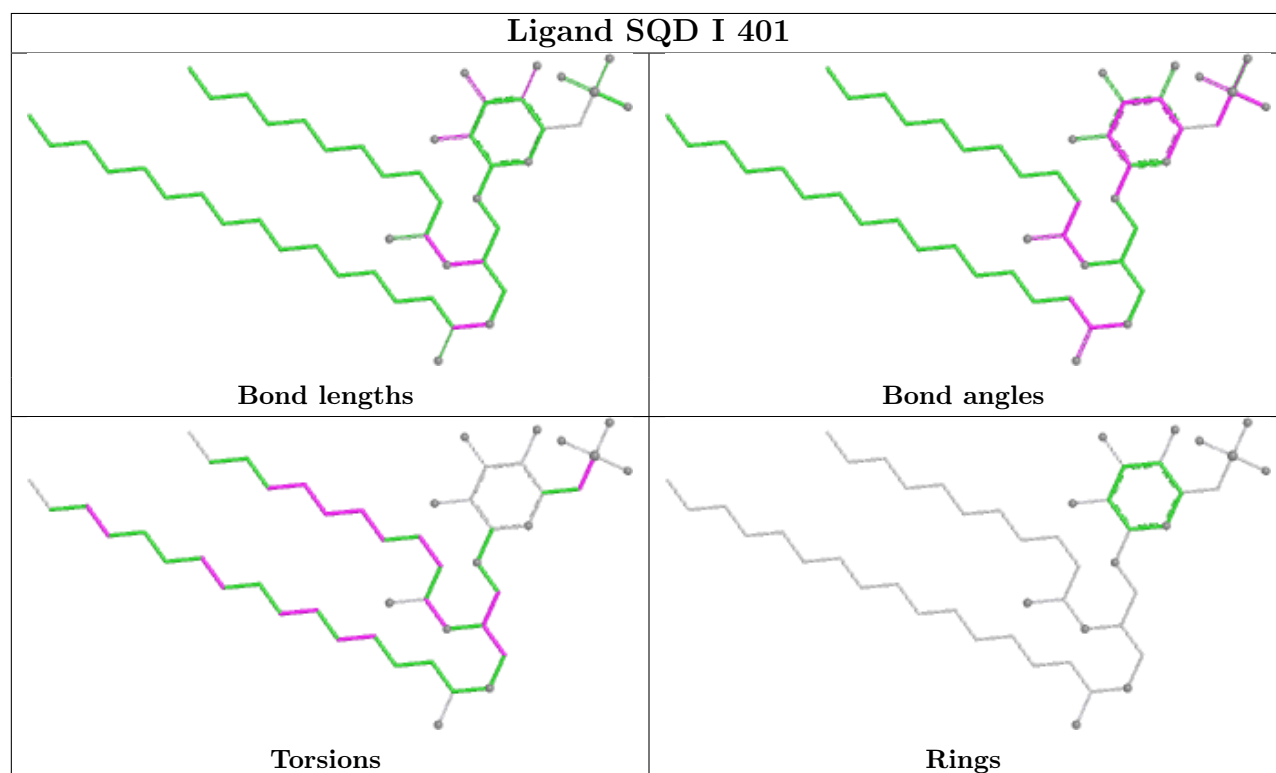
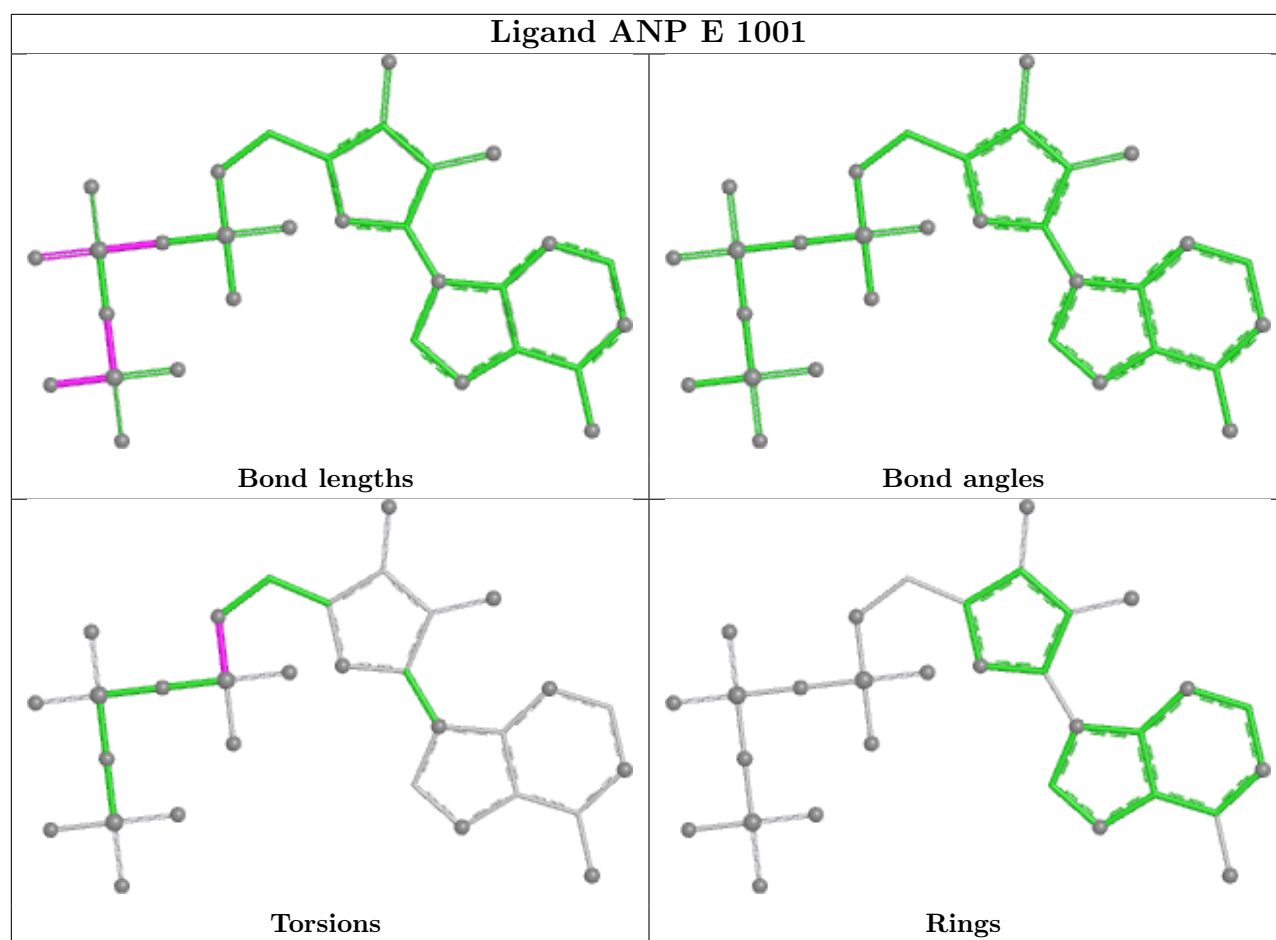
12 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	M	802	Y01	1	0
23	E	1001	ANP	2	0
25	I	401	SQD	3	0
28	P	701	A1LXL	7	0
22	A	1201	LMG	3	0
23	A	1202	ANP	1	0
22	M	801	LMG	2	0
23	C	1202	ANP	1	0
26	D	3001	DGA	1	0
28	D	3003	A1LXL	4	0
26	O	3101	DGA	3	0
22	I	402	LMG	1	0

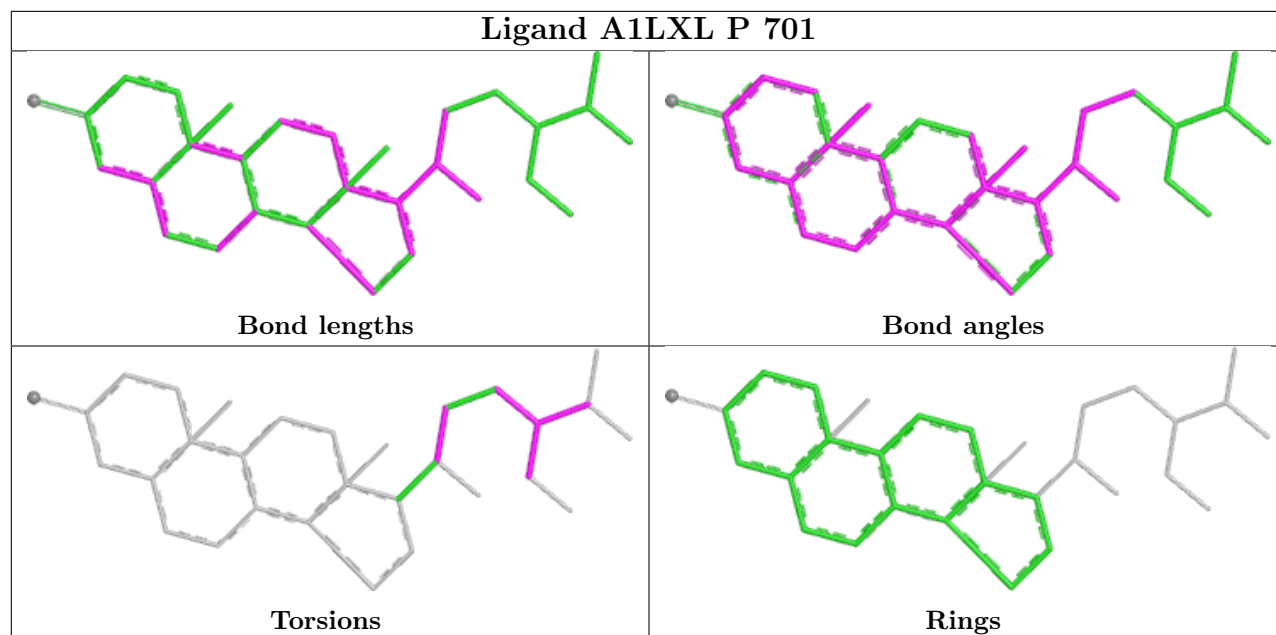
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



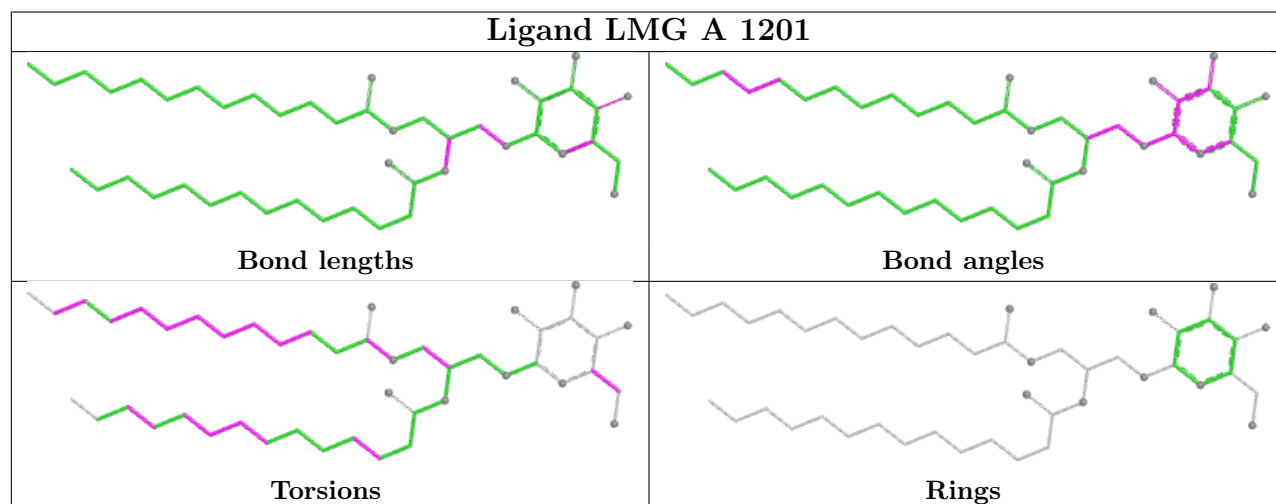


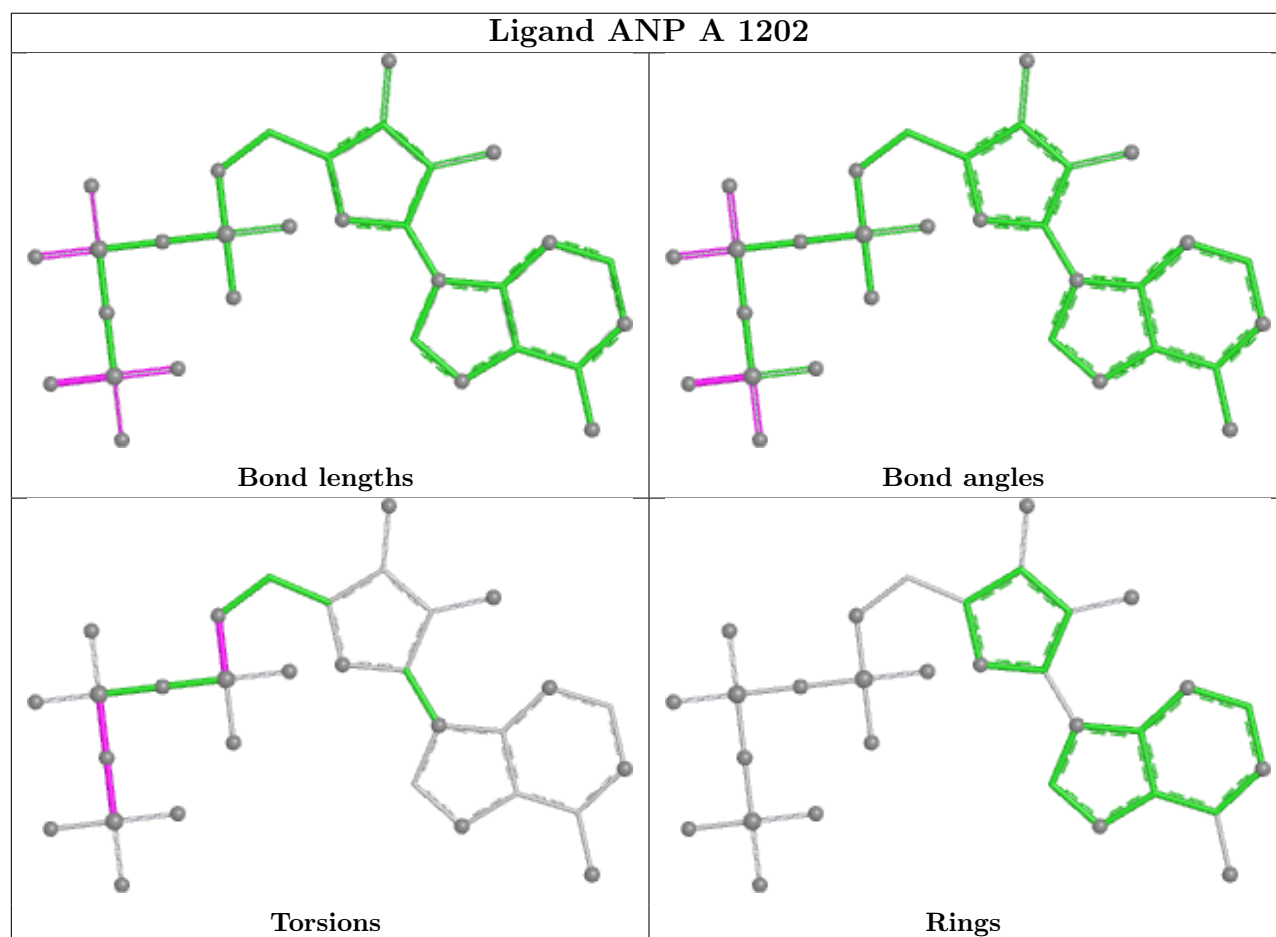
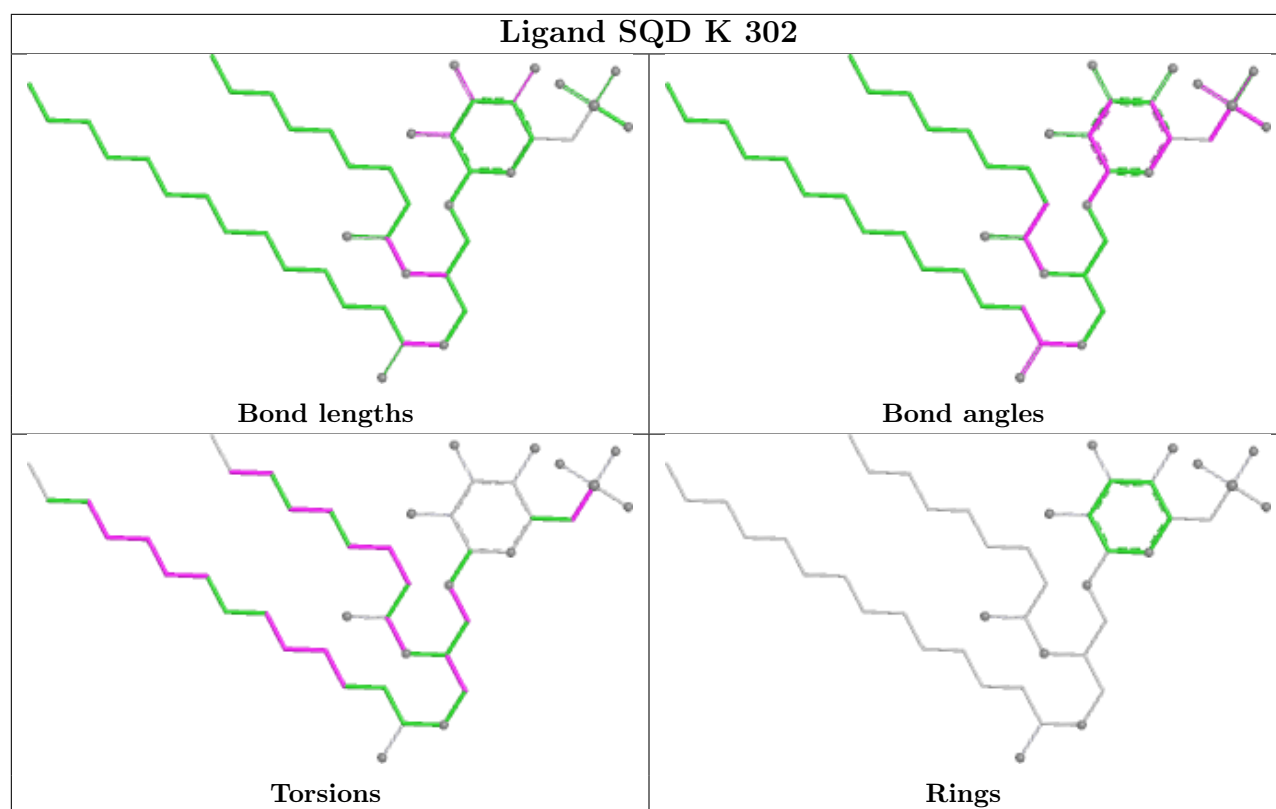


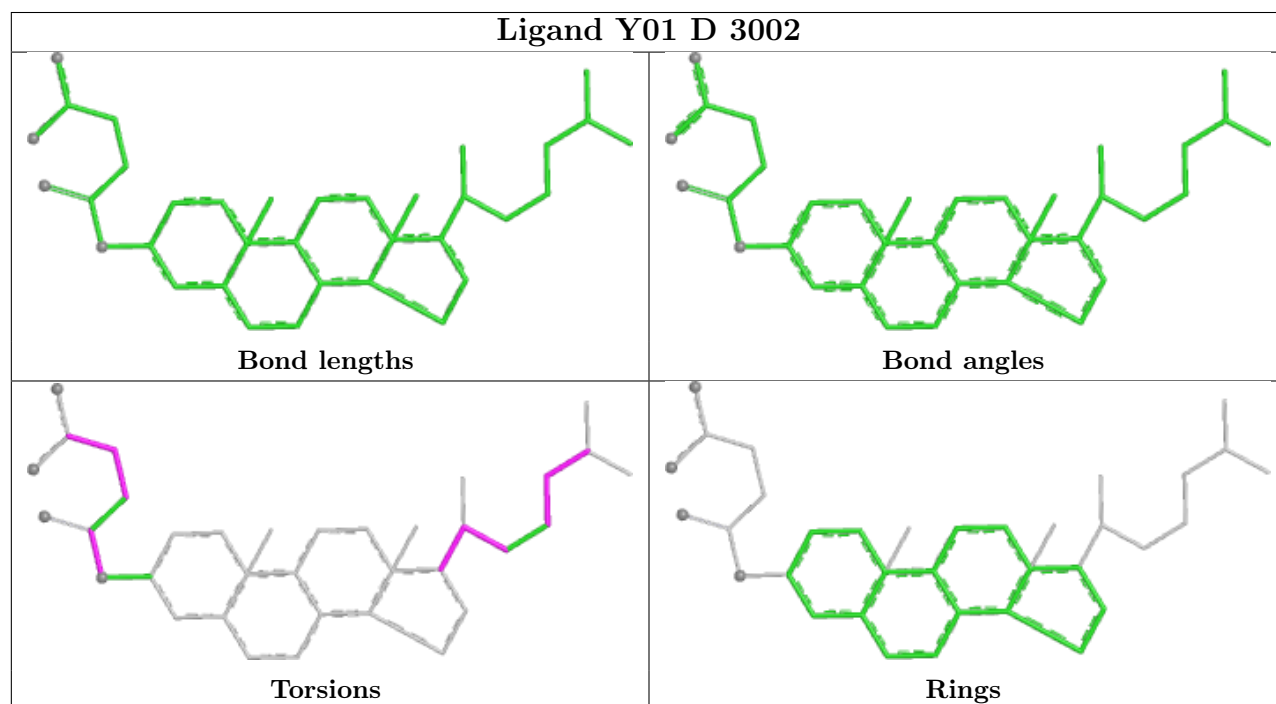
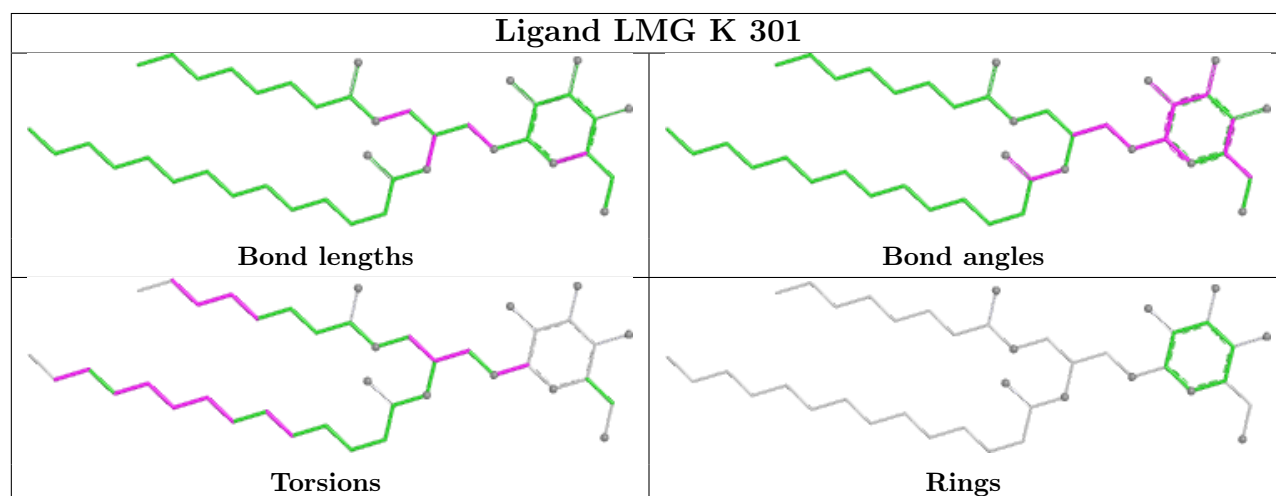
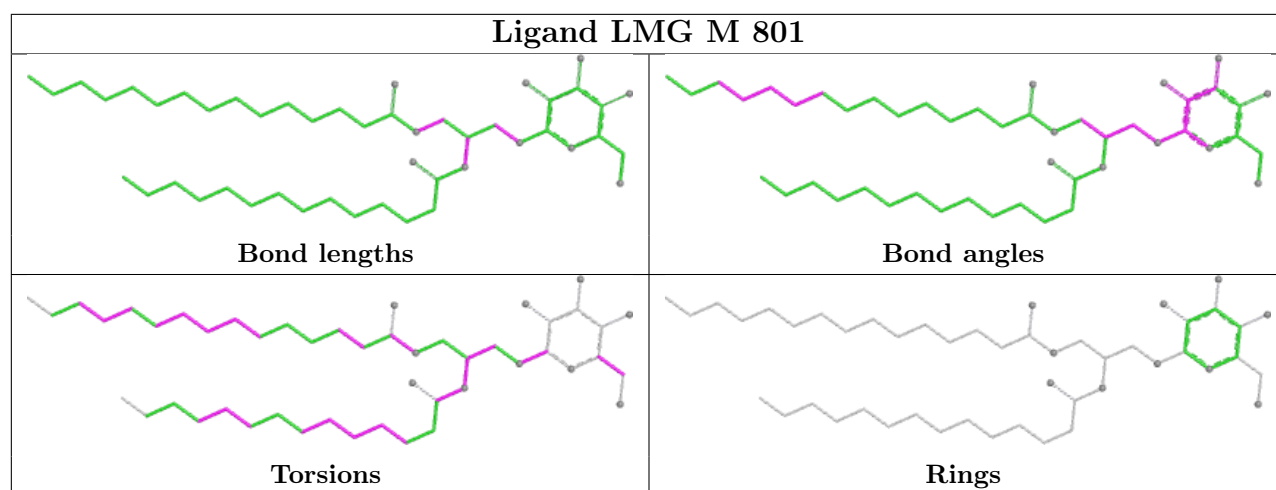
Ligand A1LXL P 701

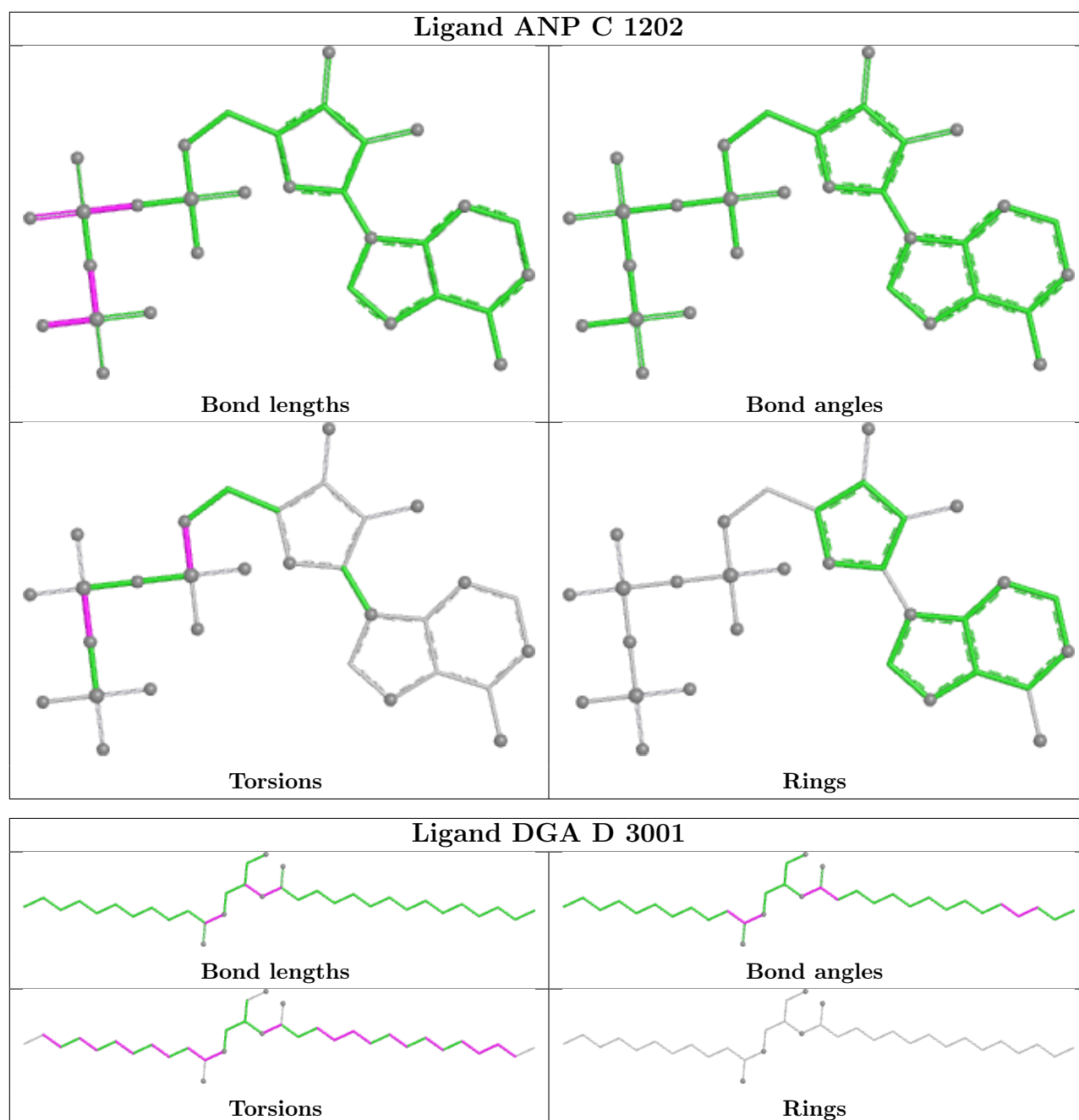


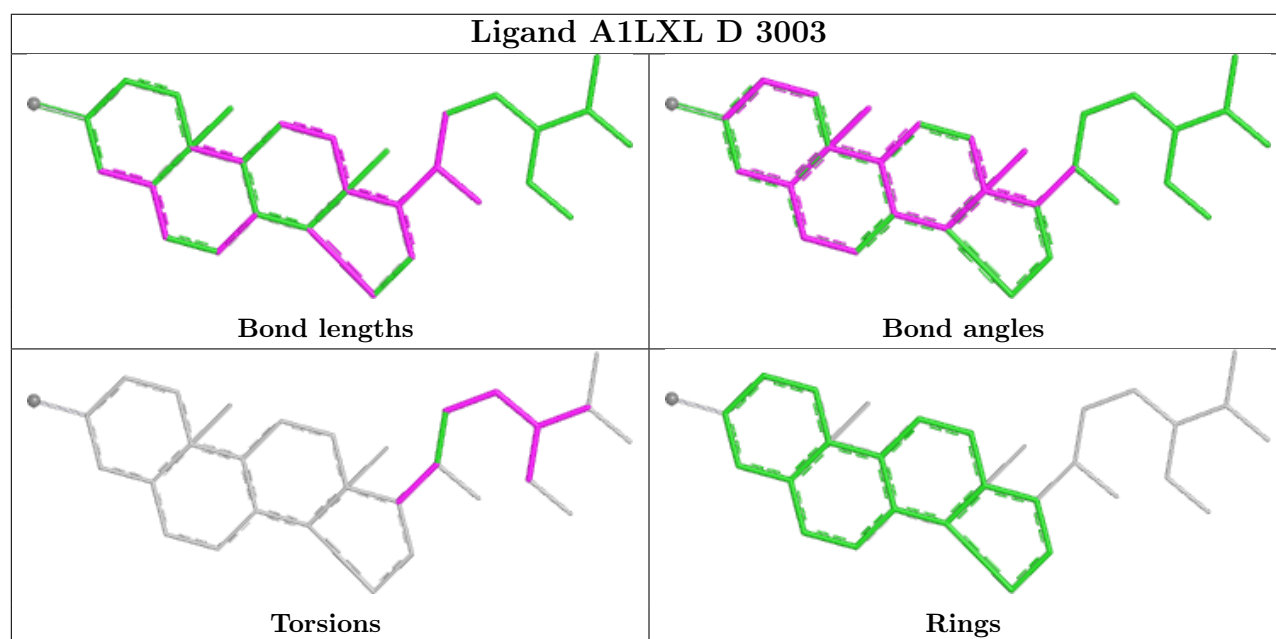
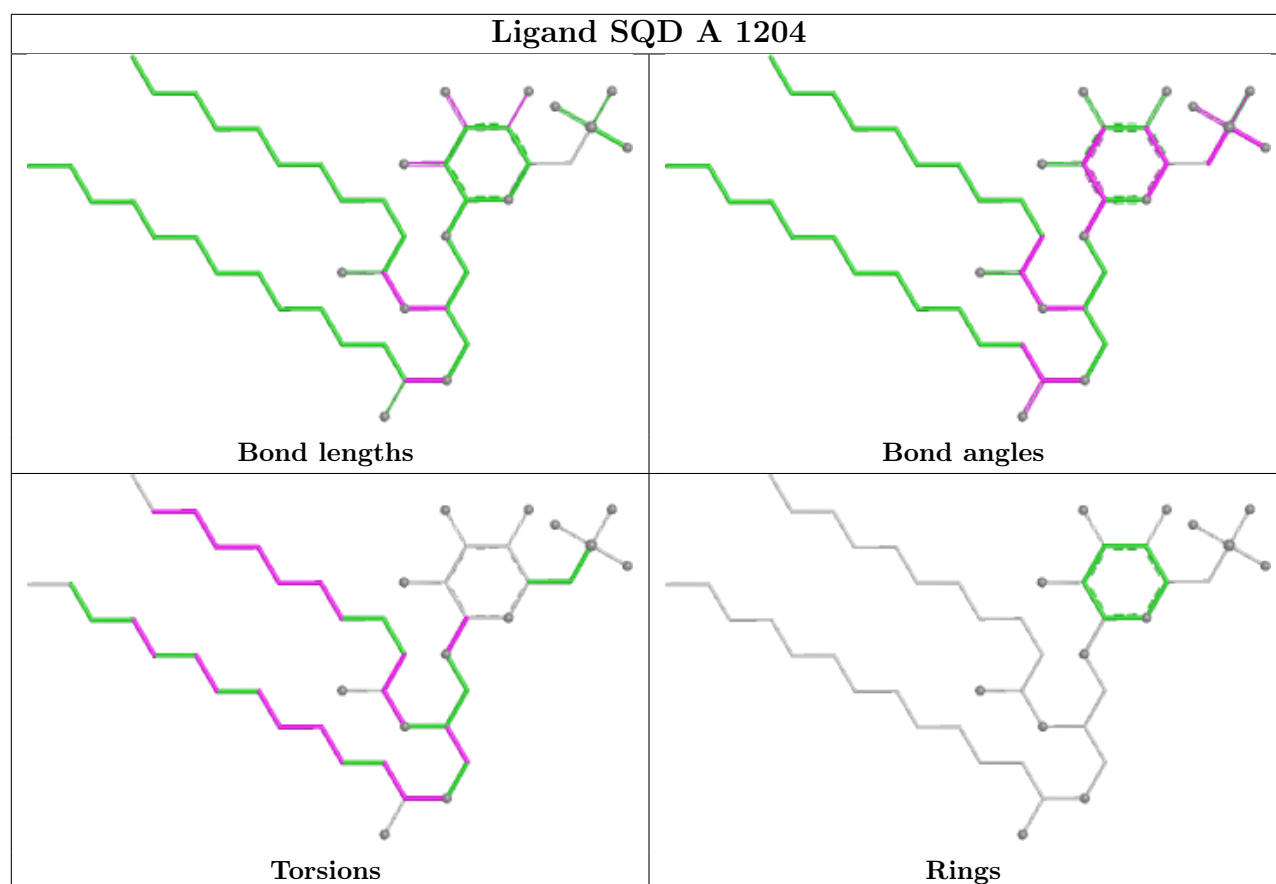
Ligand LMG A 1201

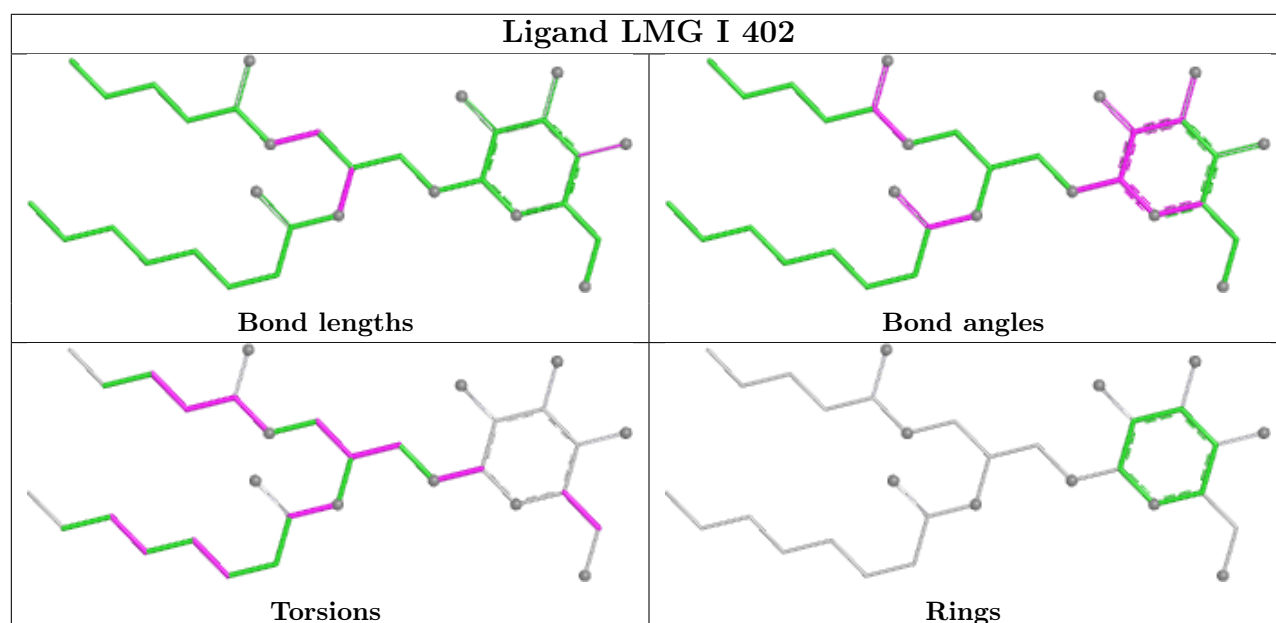
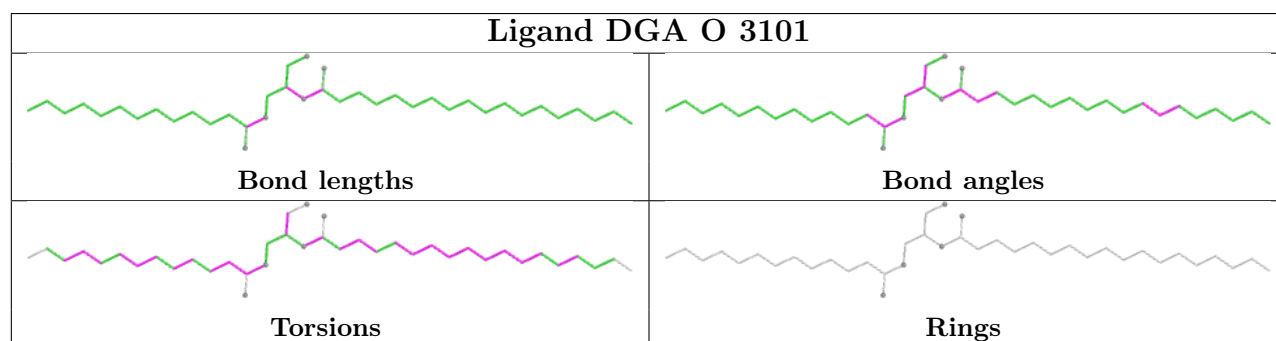
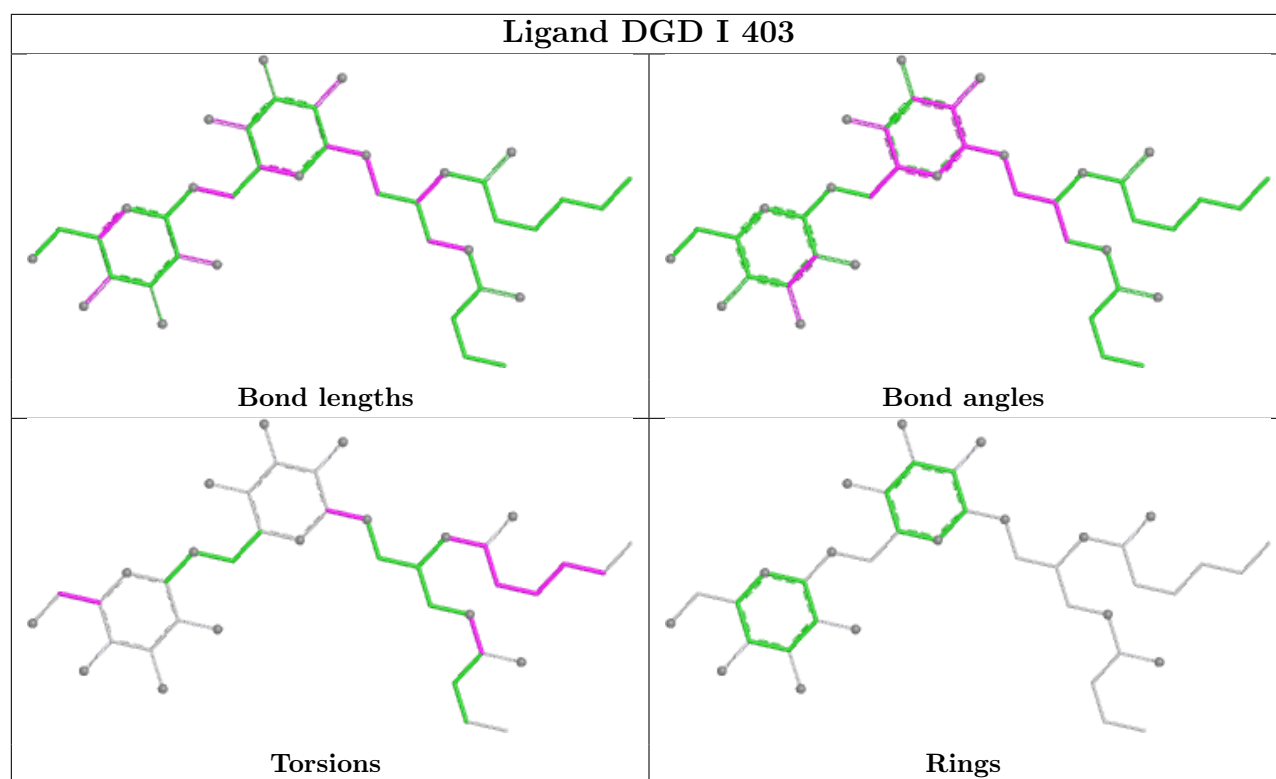












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

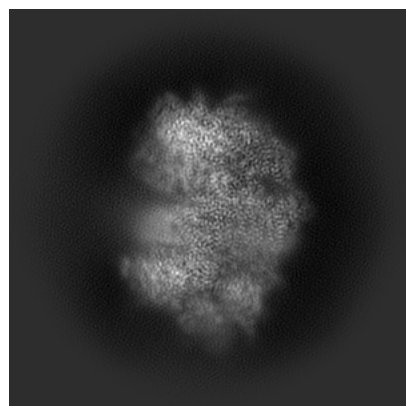
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38589. These allow visual inspection of the internal detail of the map and identification of artifacts.

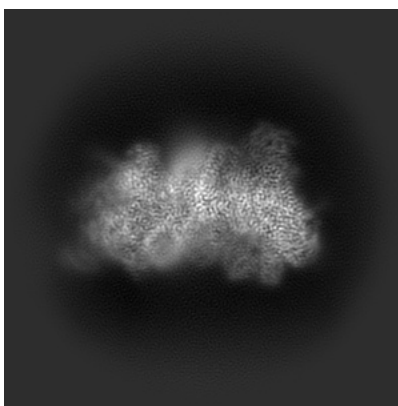
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

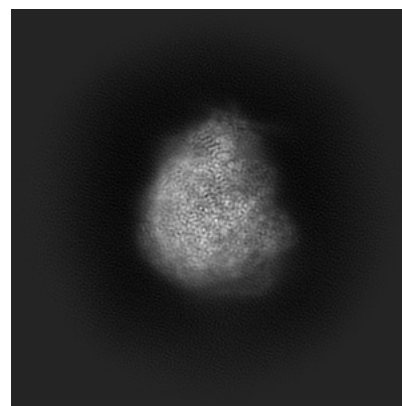
6.1.1 Primary map



X

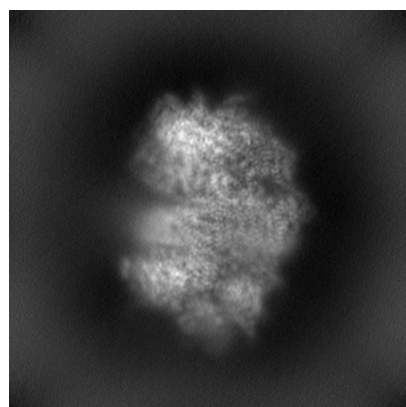


Y

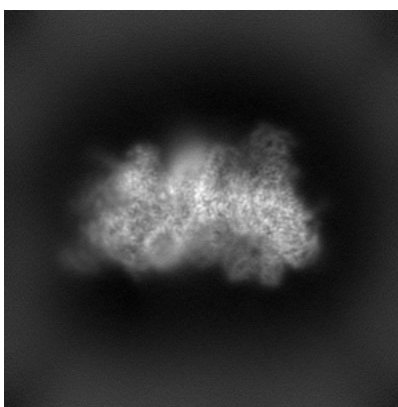


Z

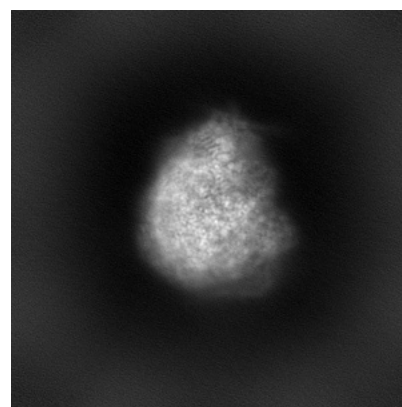
6.1.2 Raw map



X



Y

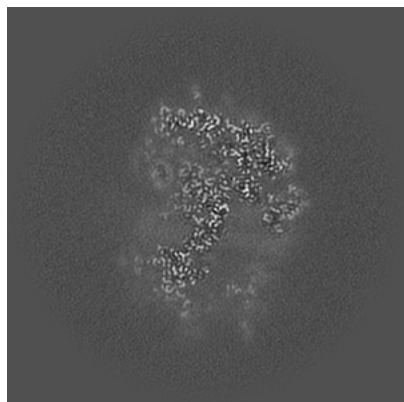


Z

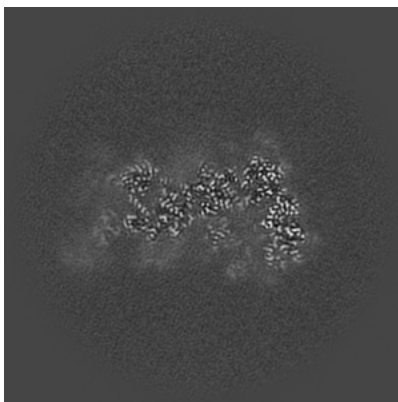
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

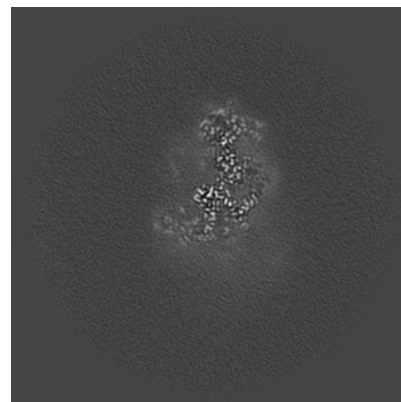
6.2.1 Primary map



X Index: 180

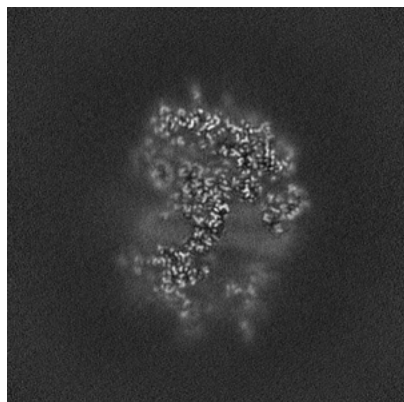


Y Index: 180

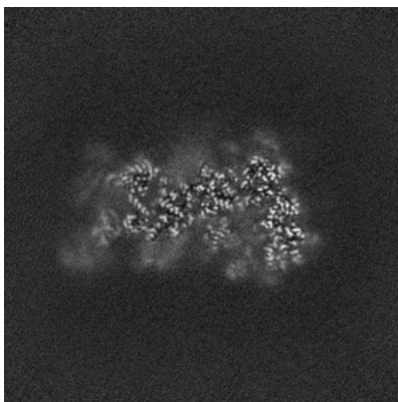


Z Index: 180

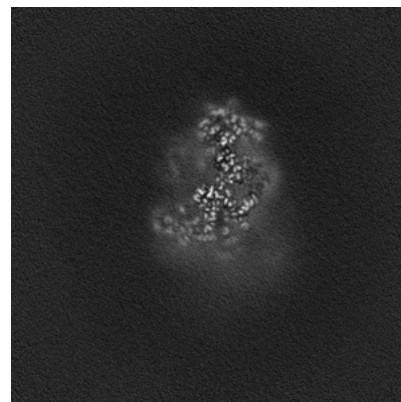
6.2.2 Raw map



X Index: 180



Y Index: 180

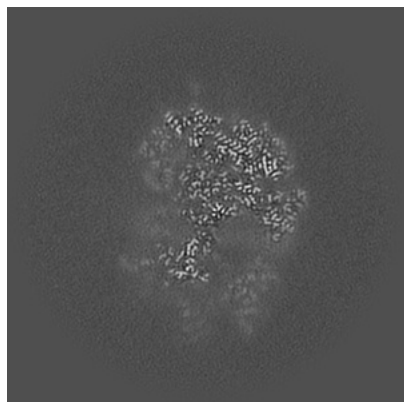


Z Index: 180

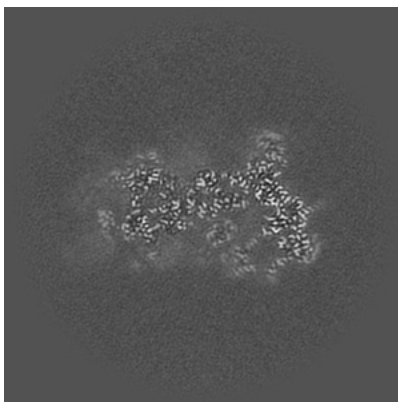
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

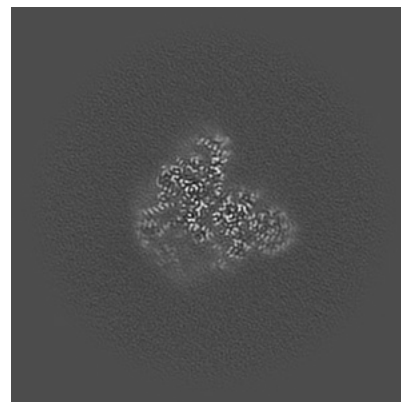
6.3.1 Primary map



X Index: 185

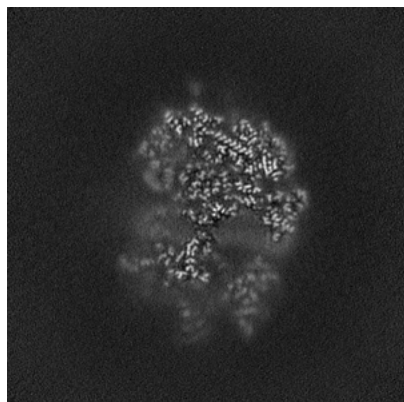


Y Index: 173

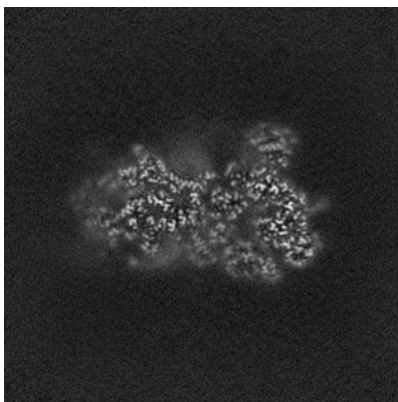


Z Index: 241

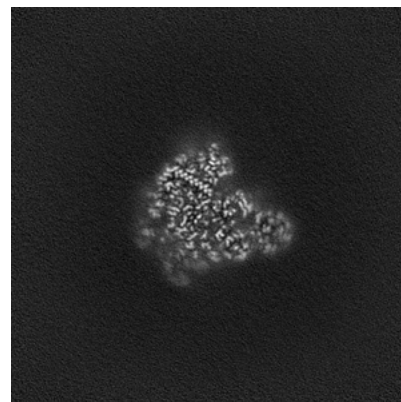
6.3.2 Raw map



X Index: 185



Y Index: 167

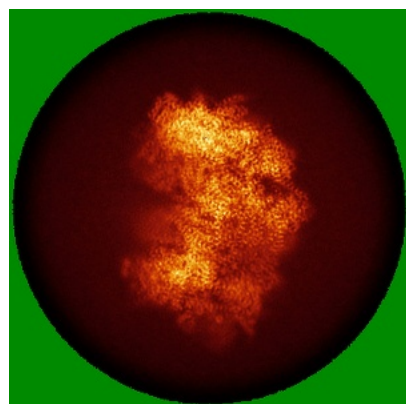


Z Index: 248

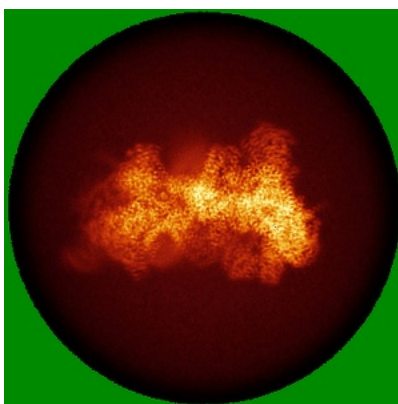
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

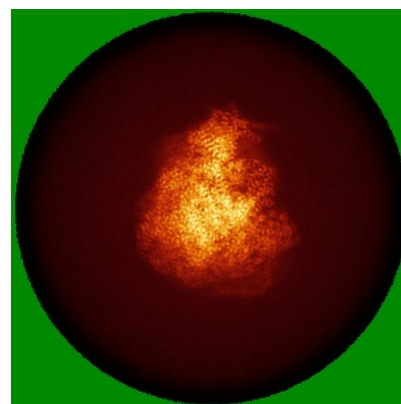
6.4.1 Primary map



X

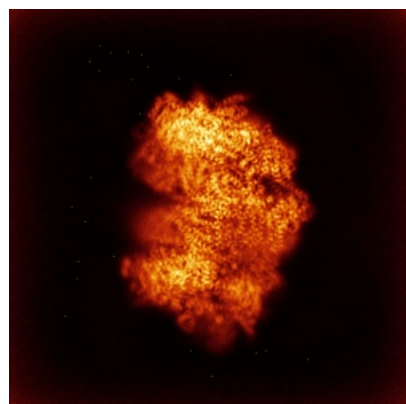


Y

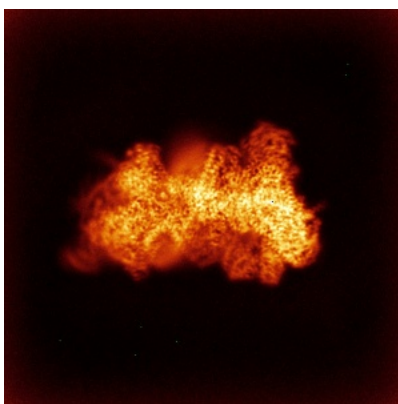


Z

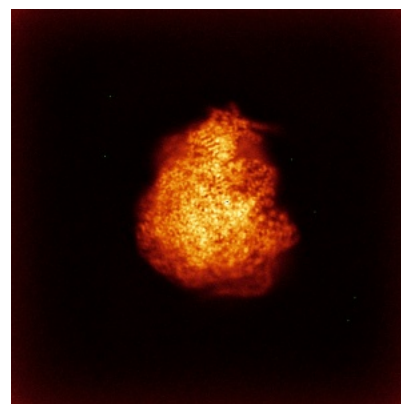
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

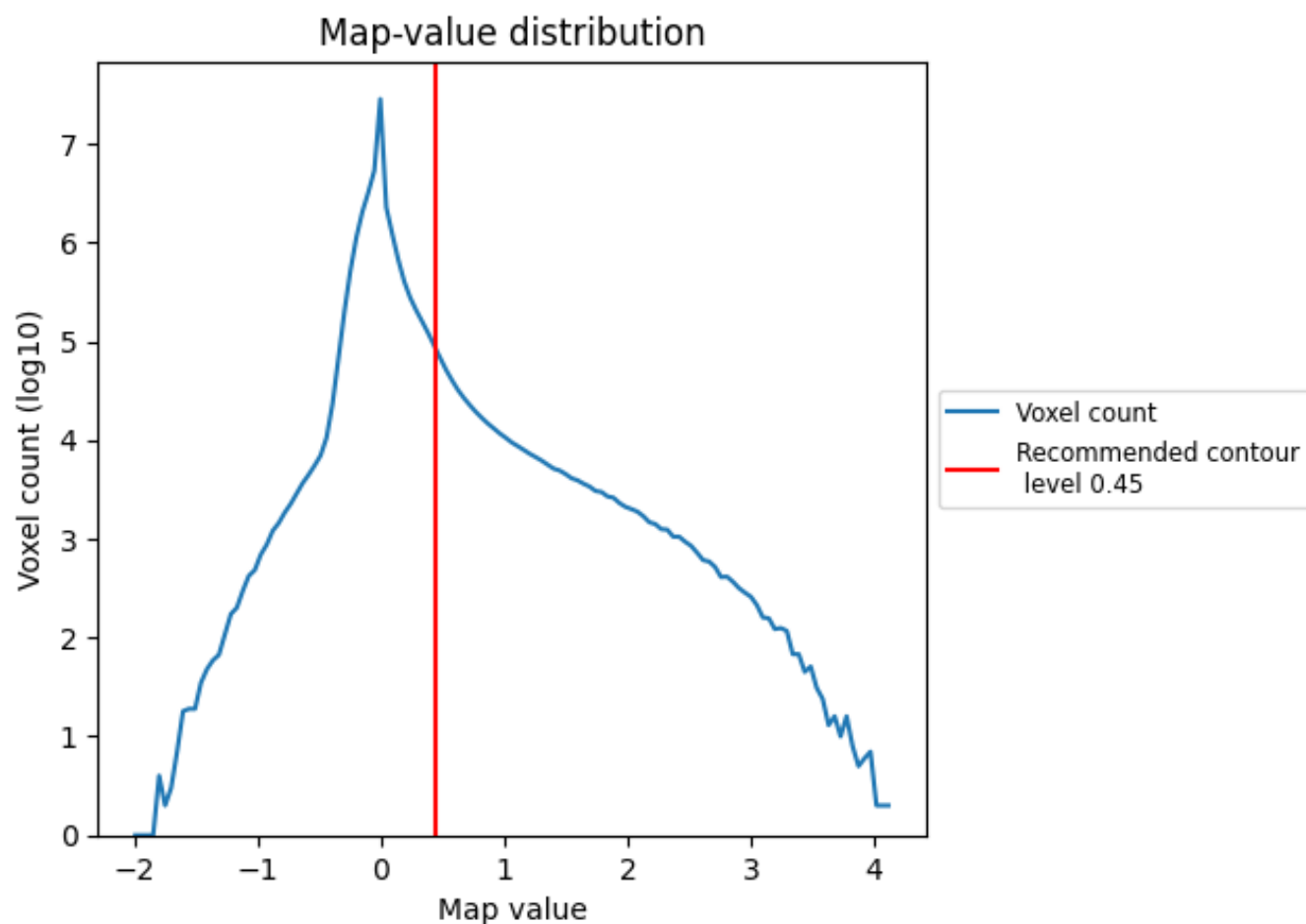
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

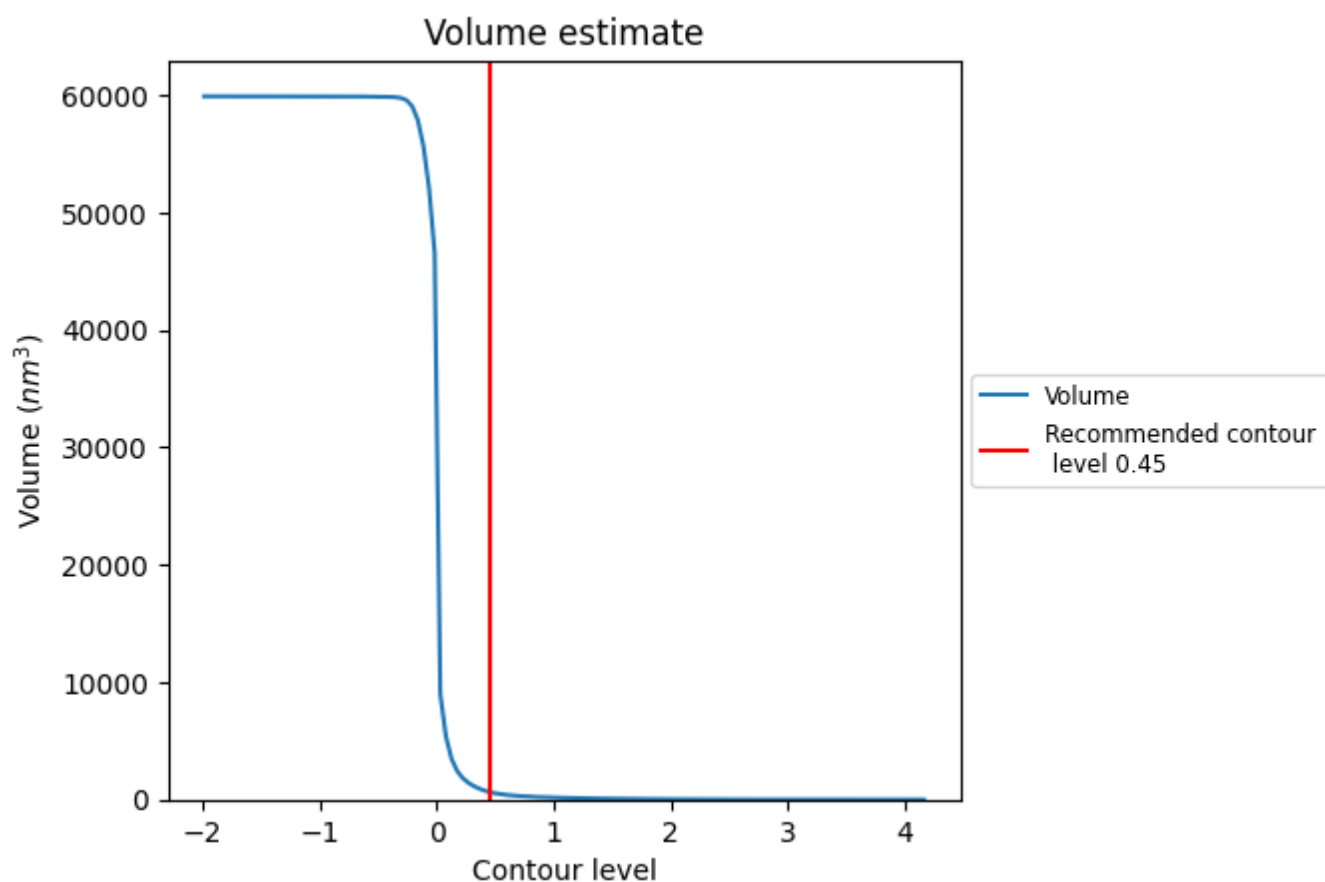
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

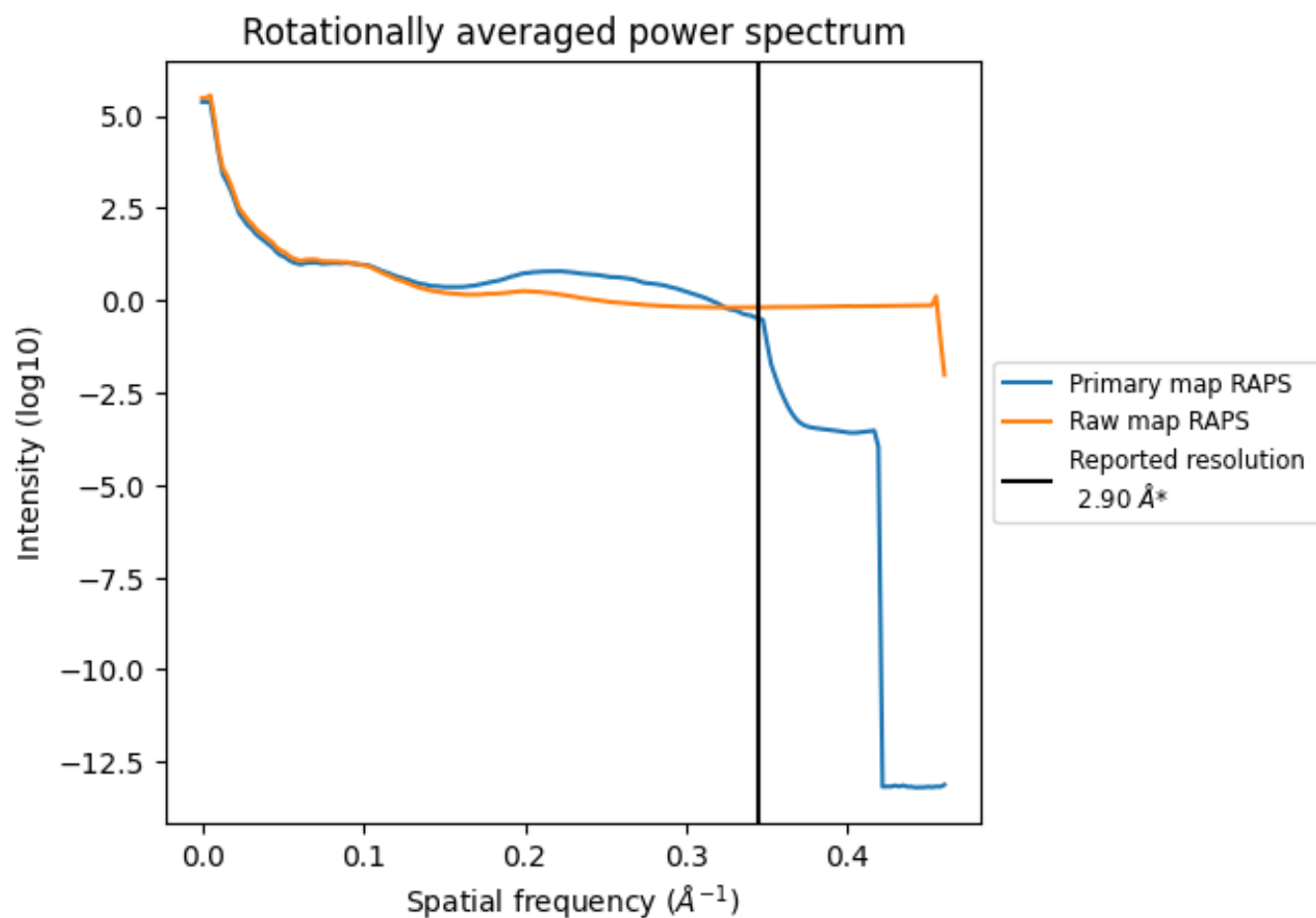
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 643 nm³; this corresponds to an approximate mass of 581 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

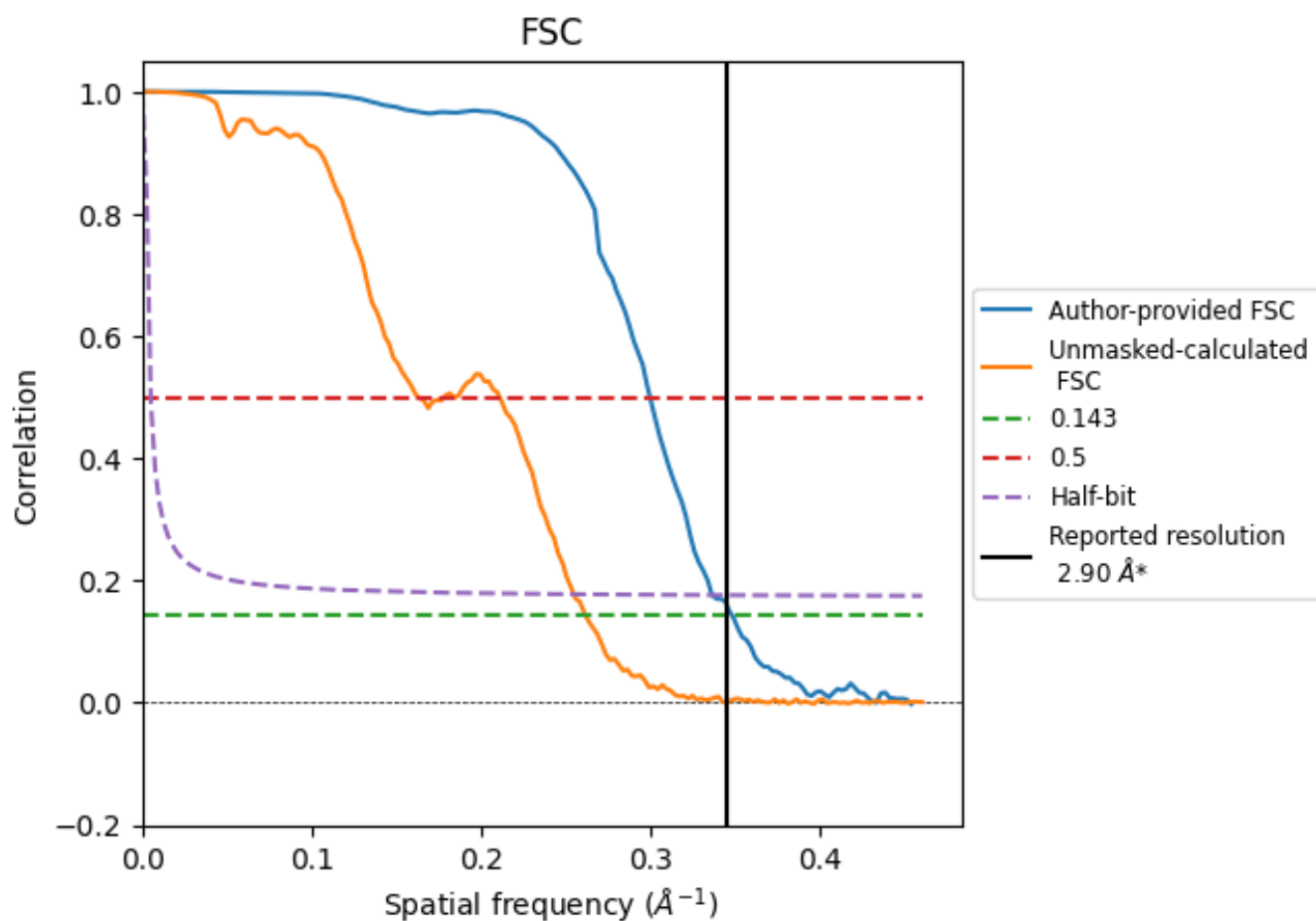


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

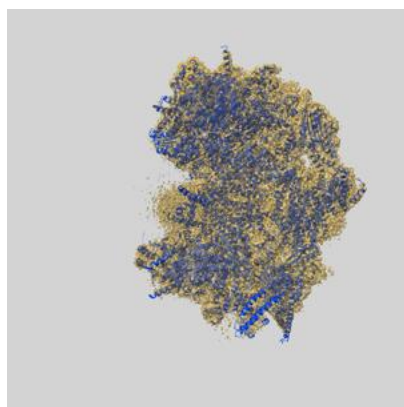
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.88	3.34	2.97
Unmasked-calculated*	3.83	6.14	3.93

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 2.9 by more than 10 %

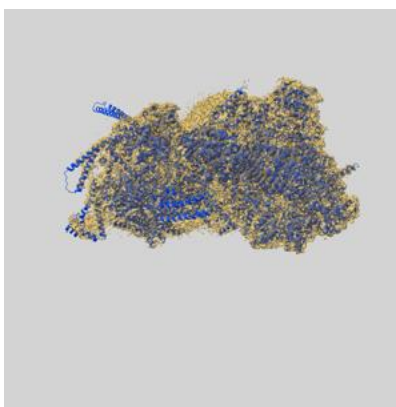
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38589 and PDB model 8XQW. Per-residue inclusion information can be found in section [3](#) on page [13](#).

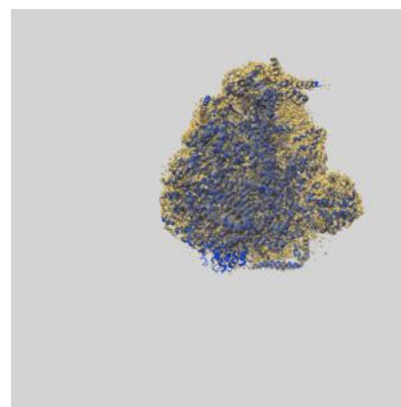
9.1 Map-model overlay [i](#)



X



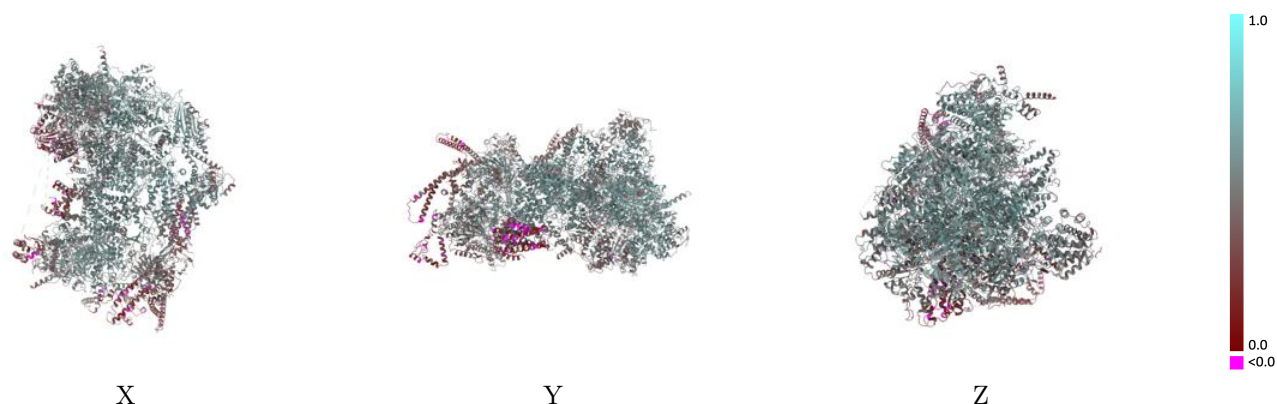
Y



Z

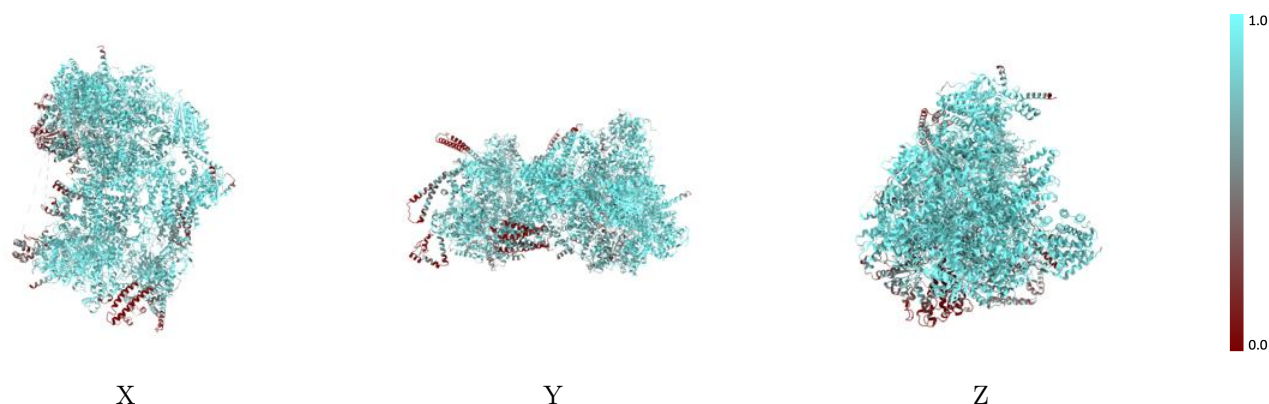
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



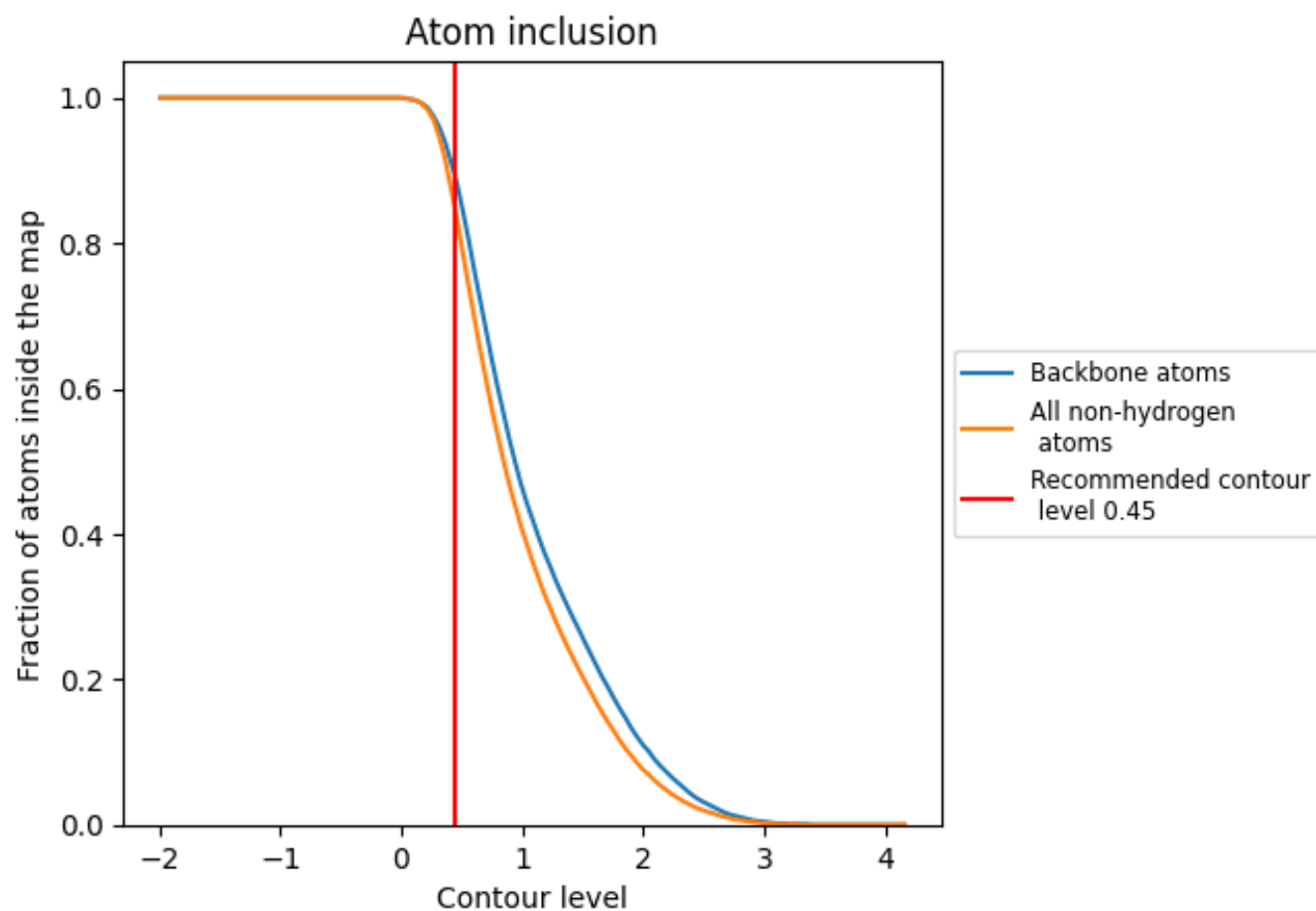
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8430	 0.5020
A	 0.8970	 0.5340
B	 0.8780	 0.5240
C	 0.8810	 0.5130
D	 0.9010	 0.5380
E	 0.7800	 0.4730
F	 0.7390	 0.4900
G	 0.8360	 0.4830
H	 0.9390	 0.5520
I	 0.9530	 0.5790
J	 0.9010	 0.5370
K	 0.9660	 0.5890
L	 0.8560	 0.5360
M	 0.9240	 0.5450
N	 0.8930	 0.5420
O	 0.6210	 0.3320
P	 0.6970	 0.3820
Q	 0.6270	 0.3780
R	 0.8860	 0.5280
S	 0.7510	 0.4620
T	 0.6370	 0.3630
U	 0.9190	 0.4750
V	 0.7530	 0.3300

