



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:04 PM UTC

PDB ID : 7WLD / pdb_00007wld
EMDB ID : EMD-32582
Title : Cryo-EM structure of the human glycosylphosphatidylinositol transamidase complex at 2.53 Angstrom resolution
Authors : Xu, Y.; Li, T.; Luo, Y.; Chao, Y.; Jia, G.; Zhou, Z.; Su, Z.; Qu, Q.; Li, D.
Deposited on : 2022-01-13
Resolution : 2.53 Å(reported)

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:

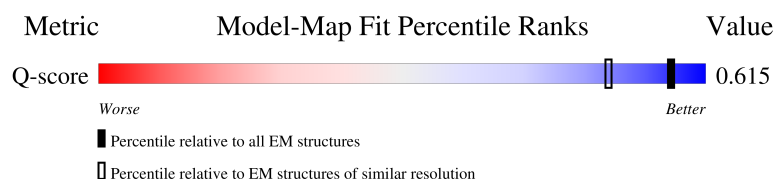
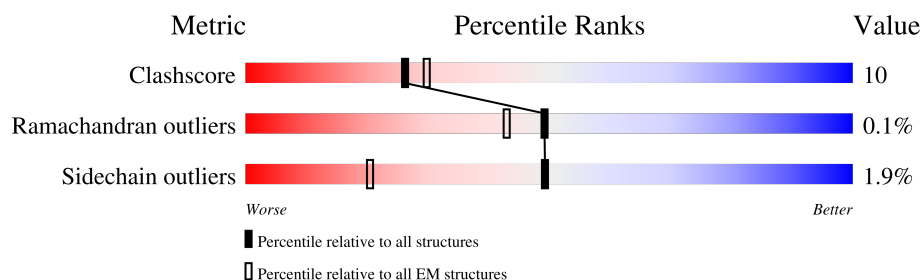
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.53 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	7309 (2.03 - 3.03)

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	G	886	
2	K	647	
3	S	816	
4	T	831	

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Mol	Chain	Length	Quality of chain
5	U	712	 49% 10% 41%
6	A	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLR	S	903	-	-	X	-
7	Y01	U	806	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 19732 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 Glycosylphosphatidylinositol anchor attachment 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	583	Total	C	N	O	S	0	0
			4458	2914	762	763	19		

There are 266 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	MET	-	initiating methionine	UNP O43292
G	0	GLY	-	expression tag	UNP O43292
G	1	SER	-	expression tag	UNP O43292
G	622	GLY	-	expression tag	UNP O43292
G	623	THR	-	expression tag	UNP O43292
G	624	LEU	-	expression tag	UNP O43292
G	625	GLU	-	expression tag	UNP O43292
G	626	VAL	-	expression tag	UNP O43292
G	627	LEU	-	expression tag	UNP O43292
G	628	PHE	-	expression tag	UNP O43292
G	629	GLN	-	expression tag	UNP O43292
G	630	GLY	-	expression tag	UNP O43292
G	631	PRO	-	expression tag	UNP O43292
G	632	GLY	-	expression tag	UNP O43292
G	633	GLY	-	expression tag	UNP O43292
G	634	SER	-	expression tag	UNP O43292
G	635	GLY	-	expression tag	UNP O43292
G	636	GLY	-	expression tag	UNP O43292
G	637	SER	-	expression tag	UNP O43292
G	638	ALA	-	expression tag	UNP O43292
G	639	SER	-	expression tag	UNP O43292
G	640	VAL	-	expression tag	UNP O43292
G	641	ILE	-	expression tag	UNP O43292
G	642	LYS	-	expression tag	UNP O43292
G	643	PRO	-	expression tag	UNP O43292
G	644	GLU	-	expression tag	UNP O43292
G	645	MET	-	expression tag	UNP O43292
G	646	LYS	-	expression tag	UNP O43292

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Chain	Residue	Modelled	Actual	Comment	Reference
G	647	ILE	-	expression tag	UNP O43292
G	648	LYS	-	expression tag	UNP O43292
G	649	LEU	-	expression tag	UNP O43292
G	650	ARG	-	expression tag	UNP O43292
G	651	MET	-	expression tag	UNP O43292
G	652	GLU	-	expression tag	UNP O43292
G	653	GLY	-	expression tag	UNP O43292
G	654	ALA	-	expression tag	UNP O43292
G	655	VAL	-	expression tag	UNP O43292
G	656	ASN	-	expression tag	UNP O43292
G	657	GLY	-	expression tag	UNP O43292
G	658	HIS	-	expression tag	UNP O43292
G	659	LYS	-	expression tag	UNP O43292
G	660	PHE	-	expression tag	UNP O43292
G	661	VAL	-	expression tag	UNP O43292
G	662	ILE	-	expression tag	UNP O43292
G	663	GLU	-	expression tag	UNP O43292
G	664	GLY	-	expression tag	UNP O43292
G	665	GLU	-	expression tag	UNP O43292
G	666	GLY	-	expression tag	UNP O43292
G	667	ILE	-	expression tag	UNP O43292
G	668	GLY	-	expression tag	UNP O43292
G	669	LYS	-	expression tag	UNP O43292
G	670	PRO	-	expression tag	UNP O43292
G	671	TYR	-	expression tag	UNP O43292
G	672	GLU	-	expression tag	UNP O43292
G	673	GLY	-	expression tag	UNP O43292
G	674	THR	-	expression tag	UNP O43292
G	675	GLN	-	expression tag	UNP O43292
G	676	THR	-	expression tag	UNP O43292
G	677	LEU	-	expression tag	UNP O43292
G	678	ASP	-	expression tag	UNP O43292
G	679	LEU	-	expression tag	UNP O43292
G	680	THR	-	expression tag	UNP O43292
G	681	VAL	-	expression tag	UNP O43292
G	682	GLU	-	expression tag	UNP O43292
G	683	GLU	-	expression tag	UNP O43292
G	684	GLY	-	expression tag	UNP O43292
G	685	ALA	-	expression tag	UNP O43292
G	686	PRO	-	expression tag	UNP O43292
G	687	LEU	-	expression tag	UNP O43292
G	688	PRO	-	expression tag	UNP O43292

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Chain	Residue	Modelled	Actual	Comment	Reference
G	689	PHE	-	expression tag	UNP O43292
G	690	SER	-	expression tag	UNP O43292
G	691	TYR	-	expression tag	UNP O43292
G	692	ASP	-	expression tag	UNP O43292
G	693	ILE	-	expression tag	UNP O43292
G	694	LEU	-	expression tag	UNP O43292
G	695	THR	-	expression tag	UNP O43292
G	696	PRO	-	expression tag	UNP O43292
G	697	ALA	-	expression tag	UNP O43292
G	698	PHE	-	expression tag	UNP O43292
G	699	GLN	-	expression tag	UNP O43292
G	700	TYR	-	expression tag	UNP O43292
G	701	GLY	-	expression tag	UNP O43292
G	702	ASN	-	expression tag	UNP O43292
G	703	ARG	-	expression tag	UNP O43292
G	704	ALA	-	expression tag	UNP O43292
G	705	PHE	-	expression tag	UNP O43292
G	706	THR	-	expression tag	UNP O43292
G	707	LYS	-	expression tag	UNP O43292
G	708	TYR	-	expression tag	UNP O43292
G	709	PRO	-	expression tag	UNP O43292
G	710	GLU	-	expression tag	UNP O43292
G	711	ASP	-	expression tag	UNP O43292
G	712	ILE	-	expression tag	UNP O43292
G	713	PRO	-	expression tag	UNP O43292
G	714	ASP	-	expression tag	UNP O43292
G	715	TYR	-	expression tag	UNP O43292
G	716	PHE	-	expression tag	UNP O43292
G	717	LYS	-	expression tag	UNP O43292
G	718	GLN	-	expression tag	UNP O43292
G	719	ALA	-	expression tag	UNP O43292
G	720	PHE	-	expression tag	UNP O43292
G	721	PRO	-	expression tag	UNP O43292
G	722	GLU	-	expression tag	UNP O43292
G	723	GLY	-	expression tag	UNP O43292
G	724	TYR	-	expression tag	UNP O43292
G	725	SER	-	expression tag	UNP O43292
G	726	TRP	-	expression tag	UNP O43292
G	727	GLU	-	expression tag	UNP O43292
G	728	ARG	-	expression tag	UNP O43292
G	729	SER	-	expression tag	UNP O43292
G	730	MET	-	expression tag	UNP O43292

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Chain	Residue	Modelled	Actual	Comment	Reference
G	731	THR	-	expression tag	UNP O43292
G	732	TYR	-	expression tag	UNP O43292
G	733	GLU	-	expression tag	UNP O43292
G	734	ASP	-	expression tag	UNP O43292
G	735	GLN	-	expression tag	UNP O43292
G	736	GLY	-	expression tag	UNP O43292
G	737	ILE	-	expression tag	UNP O43292
G	738	CYS	-	expression tag	UNP O43292
G	739	ILE	-	expression tag	UNP O43292
G	740	ALA	-	expression tag	UNP O43292
G	741	THR	-	expression tag	UNP O43292
G	742	SER	-	expression tag	UNP O43292
G	743	ASP	-	expression tag	UNP O43292
G	744	ILE	-	expression tag	UNP O43292
G	745	THR	-	expression tag	UNP O43292
G	746	MET	-	expression tag	UNP O43292
G	747	GLU	-	expression tag	UNP O43292
G	748	GLY	-	expression tag	UNP O43292
G	749	ASP	-	expression tag	UNP O43292
G	750	CYS	-	expression tag	UNP O43292
G	751	PHE	-	expression tag	UNP O43292
G	752	PHE	-	expression tag	UNP O43292
G	753	TYR	-	expression tag	UNP O43292
G	754	GLU	-	expression tag	UNP O43292
G	755	ILE	-	expression tag	UNP O43292
G	756	ARG	-	expression tag	UNP O43292
G	757	PHE	-	expression tag	UNP O43292
G	758	ASP	-	expression tag	UNP O43292
G	759	GLY	-	expression tag	UNP O43292
G	760	THR	-	expression tag	UNP O43292
G	761	ASN	-	expression tag	UNP O43292
G	762	PHE	-	expression tag	UNP O43292
G	763	PRO	-	expression tag	UNP O43292
G	764	PRO	-	expression tag	UNP O43292
G	765	ASN	-	expression tag	UNP O43292
G	766	GLY	-	expression tag	UNP O43292
G	767	PRO	-	expression tag	UNP O43292
G	768	VAL	-	expression tag	UNP O43292
G	769	MET	-	expression tag	UNP O43292
G	770	GLN	-	expression tag	UNP O43292
G	771	LYS	-	expression tag	UNP O43292
G	772	LYS	-	expression tag	UNP O43292

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Chain	Residue	Modelled	Actual	Comment	Reference
G	773	THR	-	expression tag	UNP O43292
G	774	LEU	-	expression tag	UNP O43292
G	775	LYS	-	expression tag	UNP O43292
G	776	TRP	-	expression tag	UNP O43292
G	777	GLU	-	expression tag	UNP O43292
G	778	PRO	-	expression tag	UNP O43292
G	779	SER	-	expression tag	UNP O43292
G	780	THR	-	expression tag	UNP O43292
G	781	GLU	-	expression tag	UNP O43292
G	782	LYS	-	expression tag	UNP O43292
G	783	MET	-	expression tag	UNP O43292
G	784	TYR	-	expression tag	UNP O43292
G	785	VAL	-	expression tag	UNP O43292
G	786	GLU	-	expression tag	UNP O43292
G	787	ASP	-	expression tag	UNP O43292
G	788	GLY	-	expression tag	UNP O43292
G	789	VAL	-	expression tag	UNP O43292
G	790	LEU	-	expression tag	UNP O43292
G	791	LYS	-	expression tag	UNP O43292
G	792	GLY	-	expression tag	UNP O43292
G	793	ASP	-	expression tag	UNP O43292
G	794	VAL	-	expression tag	UNP O43292
G	795	GLU	-	expression tag	UNP O43292
G	796	MET	-	expression tag	UNP O43292
G	797	ALA	-	expression tag	UNP O43292
G	798	LEU	-	expression tag	UNP O43292
G	799	LEU	-	expression tag	UNP O43292
G	800	LEU	-	expression tag	UNP O43292
G	801	GLU	-	expression tag	UNP O43292
G	802	GLY	-	expression tag	UNP O43292
G	803	GLY	-	expression tag	UNP O43292
G	804	GLY	-	expression tag	UNP O43292
G	805	HIS	-	expression tag	UNP O43292
G	806	TYR	-	expression tag	UNP O43292
G	807	ARG	-	expression tag	UNP O43292
G	808	CYS	-	expression tag	UNP O43292
G	809	ASP	-	expression tag	UNP O43292
G	810	PHE	-	expression tag	UNP O43292
G	811	LYS	-	expression tag	UNP O43292
G	812	THR	-	expression tag	UNP O43292
G	813	THR	-	expression tag	UNP O43292
G	814	TYR	-	expression tag	UNP O43292

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Chain	Residue	Modelled	Actual	Comment	Reference
G	815	LYS	-	expression tag	UNP O43292
G	816	ALA	-	expression tag	UNP O43292
G	817	LYS	-	expression tag	UNP O43292
G	818	LYS	-	expression tag	UNP O43292
G	819	ASP	-	expression tag	UNP O43292
G	820	VAL	-	expression tag	UNP O43292
G	821	ARG	-	expression tag	UNP O43292
G	822	LEU	-	expression tag	UNP O43292
G	823	PRO	-	expression tag	UNP O43292
G	824	ASP	-	expression tag	UNP O43292
G	825	ALA	-	expression tag	UNP O43292
G	826	HIS	-	expression tag	UNP O43292
G	827	GLU	-	expression tag	UNP O43292
G	828	VAL	-	expression tag	UNP O43292
G	829	ASP	-	expression tag	UNP O43292
G	830	HIS	-	expression tag	UNP O43292
G	831	ARG	-	expression tag	UNP O43292
G	832	ILE	-	expression tag	UNP O43292
G	833	GLU	-	expression tag	UNP O43292
G	834	ILE	-	expression tag	UNP O43292
G	835	LEU	-	expression tag	UNP O43292
G	836	SER	-	expression tag	UNP O43292
G	837	HIS	-	expression tag	UNP O43292
G	838	ASP	-	expression tag	UNP O43292
G	839	LYS	-	expression tag	UNP O43292
G	840	ASP	-	expression tag	UNP O43292
G	841	TYR	-	expression tag	UNP O43292
G	842	ASN	-	expression tag	UNP O43292
G	843	LYS	-	expression tag	UNP O43292
G	844	VAL	-	expression tag	UNP O43292
G	845	ARG	-	expression tag	UNP O43292
G	846	LEU	-	expression tag	UNP O43292
G	847	TYR	-	expression tag	UNP O43292
G	848	GLU	-	expression tag	UNP O43292
G	849	HIS	-	expression tag	UNP O43292
G	850	ALA	-	expression tag	UNP O43292
G	851	GLU	-	expression tag	UNP O43292
G	852	ALA	-	expression tag	UNP O43292
G	853	ARG	-	expression tag	UNP O43292
G	854	TYR	-	expression tag	UNP O43292
G	855	SER	-	expression tag	UNP O43292
G	856	GLY	-	expression tag	UNP O43292

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Chain	Residue	Modelled	Actual	Comment	Reference
G	857	GLY	-	expression tag	UNP O43292
G	858	GLY	-	expression tag	UNP O43292
G	859	SER	-	expression tag	UNP O43292
G	860	GLY	-	expression tag	UNP O43292
G	861	GLY	-	expression tag	UNP O43292
G	862	GLY	-	expression tag	UNP O43292
G	863	GLY	-	expression tag	UNP O43292
G	864	SER	-	expression tag	UNP O43292
G	865	GLY	-	expression tag	UNP O43292
G	866	GLY	-	expression tag	UNP O43292
G	867	GLY	-	expression tag	UNP O43292
G	868	GLY	-	expression tag	UNP O43292
G	869	ASP	-	expression tag	UNP O43292
G	870	TYR	-	expression tag	UNP O43292
G	871	LYS	-	expression tag	UNP O43292
G	872	ASP	-	expression tag	UNP O43292
G	873	ASP	-	expression tag	UNP O43292
G	874	ASP	-	expression tag	UNP O43292
G	875	ASP	-	expression tag	UNP O43292
G	876	ALA	-	expression tag	UNP O43292
G	877	ASP	-	expression tag	UNP O43292
G	878	TYR	-	expression tag	UNP O43292
G	879	LYS	-	expression tag	UNP O43292
G	880	ASP	-	expression tag	UNP O43292
G	881	ASP	-	expression tag	UNP O43292
G	882	ASP	-	expression tag	UNP O43292
G	883	ASP	-	expression tag	UNP O43292
G	884	ALA	-	expression tag	UNP O43292

- Molecule 2 is a protein called GPI-anchor transamidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	331	Total	C	N	O	S	0	0
			2644	1691	452	487	14		

There are 253 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	MET	-	initiating methionine	UNP Q92643
K	0	GLY	-	expression tag	UNP Q92643
K	1	SER	-	expression tag	UNP Q92643
K	396	GLY	-	expression tag	UNP Q92643

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Chain	Residue	Modelled	Actual	Comment	Reference
K	397	THR	-	expression tag	UNP Q92643
K	398	LEU	-	expression tag	UNP Q92643
K	399	GLU	-	expression tag	UNP Q92643
K	400	VAL	-	expression tag	UNP Q92643
K	401	LEU	-	expression tag	UNP Q92643
K	402	PHE	-	expression tag	UNP Q92643
K	403	GLN	-	expression tag	UNP Q92643
K	404	GLY	-	expression tag	UNP Q92643
K	405	PRO	-	expression tag	UNP Q92643
K	406	GLY	-	expression tag	UNP Q92643
K	407	GLY	-	expression tag	UNP Q92643
K	408	SER	-	expression tag	UNP Q92643
K	409	GLY	-	expression tag	UNP Q92643
K	410	GLY	-	expression tag	UNP Q92643
K	411	SER	-	expression tag	UNP Q92643
K	412	ALA	-	expression tag	UNP Q92643
K	413	SER	-	expression tag	UNP Q92643
K	414	VAL	-	expression tag	UNP Q92643
K	415	ILE	-	expression tag	UNP Q92643
K	416	LYS	-	expression tag	UNP Q92643
K	417	PRO	-	expression tag	UNP Q92643
K	418	GLU	-	expression tag	UNP Q92643
K	419	MET	-	expression tag	UNP Q92643
K	420	LYS	-	expression tag	UNP Q92643
K	421	ILE	-	expression tag	UNP Q92643
K	422	LYS	-	expression tag	UNP Q92643
K	423	LEU	-	expression tag	UNP Q92643
K	424	ARG	-	expression tag	UNP Q92643
K	425	MET	-	expression tag	UNP Q92643
K	426	GLU	-	expression tag	UNP Q92643
K	427	GLY	-	expression tag	UNP Q92643
K	428	ALA	-	expression tag	UNP Q92643
K	429	VAL	-	expression tag	UNP Q92643
K	430	ASN	-	expression tag	UNP Q92643
K	431	GLY	-	expression tag	UNP Q92643
K	432	HIS	-	expression tag	UNP Q92643
K	433	LYS	-	expression tag	UNP Q92643
K	434	PHE	-	expression tag	UNP Q92643
K	435	VAL	-	expression tag	UNP Q92643
K	436	ILE	-	expression tag	UNP Q92643
K	437	GLU	-	expression tag	UNP Q92643
K	438	GLY	-	expression tag	UNP Q92643

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Chain	Residue	Modelled	Actual	Comment	Reference
K	439	GLU	-	expression tag	UNP Q92643
K	440	GLY	-	expression tag	UNP Q92643
K	441	ILE	-	expression tag	UNP Q92643
K	442	GLY	-	expression tag	UNP Q92643
K	443	LYS	-	expression tag	UNP Q92643
K	444	PRO	-	expression tag	UNP Q92643
K	445	TYR	-	expression tag	UNP Q92643
K	446	GLU	-	expression tag	UNP Q92643
K	447	GLY	-	expression tag	UNP Q92643
K	448	THR	-	expression tag	UNP Q92643
K	449	GLN	-	expression tag	UNP Q92643
K	450	THR	-	expression tag	UNP Q92643
K	451	LEU	-	expression tag	UNP Q92643
K	452	ASP	-	expression tag	UNP Q92643
K	453	LEU	-	expression tag	UNP Q92643
K	454	THR	-	expression tag	UNP Q92643
K	455	VAL	-	expression tag	UNP Q92643
K	456	GLU	-	expression tag	UNP Q92643
K	457	GLU	-	expression tag	UNP Q92643
K	458	GLY	-	expression tag	UNP Q92643
K	459	ALA	-	expression tag	UNP Q92643
K	460	PRO	-	expression tag	UNP Q92643
K	461	LEU	-	expression tag	UNP Q92643
K	462	PRO	-	expression tag	UNP Q92643
K	463	PHE	-	expression tag	UNP Q92643
K	464	SER	-	expression tag	UNP Q92643
K	465	TYR	-	expression tag	UNP Q92643
K	466	ASP	-	expression tag	UNP Q92643
K	467	ILE	-	expression tag	UNP Q92643
K	468	LEU	-	expression tag	UNP Q92643
K	469	THR	-	expression tag	UNP Q92643
K	470	PRO	-	expression tag	UNP Q92643
K	471	ALA	-	expression tag	UNP Q92643
K	472	PHE	-	expression tag	UNP Q92643
K	473	GLN	-	expression tag	UNP Q92643
K	474	TYR	-	expression tag	UNP Q92643
K	475	GLY	-	expression tag	UNP Q92643
K	476	ASN	-	expression tag	UNP Q92643
K	477	ARG	-	expression tag	UNP Q92643
K	478	ALA	-	expression tag	UNP Q92643
K	479	PHE	-	expression tag	UNP Q92643
K	480	THR	-	expression tag	UNP Q92643

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Chain	Residue	Modelled	Actual	Comment	Reference
K	481	LYS	-	expression tag	UNP Q92643
K	482	TYR	-	expression tag	UNP Q92643
K	483	PRO	-	expression tag	UNP Q92643
K	484	GLU	-	expression tag	UNP Q92643
K	485	ASP	-	expression tag	UNP Q92643
K	486	ILE	-	expression tag	UNP Q92643
K	487	PRO	-	expression tag	UNP Q92643
K	488	ASP	-	expression tag	UNP Q92643
K	489	TYR	-	expression tag	UNP Q92643
K	490	PHE	-	expression tag	UNP Q92643
K	491	LYS	-	expression tag	UNP Q92643
K	492	GLN	-	expression tag	UNP Q92643
K	493	ALA	-	expression tag	UNP Q92643
K	494	PHE	-	expression tag	UNP Q92643
K	495	PRO	-	expression tag	UNP Q92643
K	496	GLU	-	expression tag	UNP Q92643
K	497	GLY	-	expression tag	UNP Q92643
K	498	TYR	-	expression tag	UNP Q92643
K	499	SER	-	expression tag	UNP Q92643
K	500	TRP	-	expression tag	UNP Q92643
K	501	GLU	-	expression tag	UNP Q92643
K	502	ARG	-	expression tag	UNP Q92643
K	503	SER	-	expression tag	UNP Q92643
K	504	MET	-	expression tag	UNP Q92643
K	505	THR	-	expression tag	UNP Q92643
K	506	TYR	-	expression tag	UNP Q92643
K	507	GLU	-	expression tag	UNP Q92643
K	508	ASP	-	expression tag	UNP Q92643
K	509	GLN	-	expression tag	UNP Q92643
K	510	GLY	-	expression tag	UNP Q92643
K	511	ILE	-	expression tag	UNP Q92643
K	512	CYS	-	expression tag	UNP Q92643
K	513	ILE	-	expression tag	UNP Q92643
K	514	ALA	-	expression tag	UNP Q92643
K	515	THR	-	expression tag	UNP Q92643
K	516	SER	-	expression tag	UNP Q92643
K	517	ASP	-	expression tag	UNP Q92643
K	518	ILE	-	expression tag	UNP Q92643
K	519	THR	-	expression tag	UNP Q92643
K	520	MET	-	expression tag	UNP Q92643
K	521	GLU	-	expression tag	UNP Q92643
K	522	GLY	-	expression tag	UNP Q92643

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Chain	Residue	Modelled	Actual	Comment	Reference
K	523	ASP	-	expression tag	UNP Q92643
K	524	CYS	-	expression tag	UNP Q92643
K	525	PHE	-	expression tag	UNP Q92643
K	526	PHE	-	expression tag	UNP Q92643
K	527	TYR	-	expression tag	UNP Q92643
K	528	GLU	-	expression tag	UNP Q92643
K	529	ILE	-	expression tag	UNP Q92643
K	530	ARG	-	expression tag	UNP Q92643
K	531	PHE	-	expression tag	UNP Q92643
K	532	ASP	-	expression tag	UNP Q92643
K	533	GLY	-	expression tag	UNP Q92643
K	534	THR	-	expression tag	UNP Q92643
K	535	ASN	-	expression tag	UNP Q92643
K	536	PHE	-	expression tag	UNP Q92643
K	537	PRO	-	expression tag	UNP Q92643
K	538	PRO	-	expression tag	UNP Q92643
K	539	ASN	-	expression tag	UNP Q92643
K	540	GLY	-	expression tag	UNP Q92643
K	541	PRO	-	expression tag	UNP Q92643
K	542	VAL	-	expression tag	UNP Q92643
K	543	MET	-	expression tag	UNP Q92643
K	544	GLN	-	expression tag	UNP Q92643
K	545	LYS	-	expression tag	UNP Q92643
K	546	LYS	-	expression tag	UNP Q92643
K	547	THR	-	expression tag	UNP Q92643
K	548	LEU	-	expression tag	UNP Q92643
K	549	LYS	-	expression tag	UNP Q92643
K	550	TRP	-	expression tag	UNP Q92643
K	551	GLU	-	expression tag	UNP Q92643
K	552	PRO	-	expression tag	UNP Q92643
K	553	SER	-	expression tag	UNP Q92643
K	554	THR	-	expression tag	UNP Q92643
K	555	GLU	-	expression tag	UNP Q92643
K	556	LYS	-	expression tag	UNP Q92643
K	557	MET	-	expression tag	UNP Q92643
K	558	TYR	-	expression tag	UNP Q92643
K	559	VAL	-	expression tag	UNP Q92643
K	560	GLU	-	expression tag	UNP Q92643
K	561	ASP	-	expression tag	UNP Q92643
K	562	GLY	-	expression tag	UNP Q92643
K	563	VAL	-	expression tag	UNP Q92643
K	564	LEU	-	expression tag	UNP Q92643

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Chain	Residue	Modelled	Actual	Comment	Reference
K	565	LYS	-	expression tag	UNP Q92643
K	566	GLY	-	expression tag	UNP Q92643
K	567	ASP	-	expression tag	UNP Q92643
K	568	VAL	-	expression tag	UNP Q92643
K	569	GLU	-	expression tag	UNP Q92643
K	570	MET	-	expression tag	UNP Q92643
K	571	ALA	-	expression tag	UNP Q92643
K	572	LEU	-	expression tag	UNP Q92643
K	573	LEU	-	expression tag	UNP Q92643
K	574	LEU	-	expression tag	UNP Q92643
K	575	GLU	-	expression tag	UNP Q92643
K	576	GLY	-	expression tag	UNP Q92643
K	577	GLY	-	expression tag	UNP Q92643
K	578	GLY	-	expression tag	UNP Q92643
K	579	HIS	-	expression tag	UNP Q92643
K	580	TYR	-	expression tag	UNP Q92643
K	581	ARG	-	expression tag	UNP Q92643
K	582	CYS	-	expression tag	UNP Q92643
K	583	ASP	-	expression tag	UNP Q92643
K	584	PHE	-	expression tag	UNP Q92643
K	585	LYS	-	expression tag	UNP Q92643
K	586	THR	-	expression tag	UNP Q92643
K	587	THR	-	expression tag	UNP Q92643
K	588	TYR	-	expression tag	UNP Q92643
K	589	LYS	-	expression tag	UNP Q92643
K	590	ALA	-	expression tag	UNP Q92643
K	591	LYS	-	expression tag	UNP Q92643
K	592	LYS	-	expression tag	UNP Q92643
K	593	ASP	-	expression tag	UNP Q92643
K	594	VAL	-	expression tag	UNP Q92643
K	595	ARG	-	expression tag	UNP Q92643
K	596	LEU	-	expression tag	UNP Q92643
K	597	PRO	-	expression tag	UNP Q92643
K	598	ASP	-	expression tag	UNP Q92643
K	599	ALA	-	expression tag	UNP Q92643
K	600	HIS	-	expression tag	UNP Q92643
K	601	GLU	-	expression tag	UNP Q92643
K	602	VAL	-	expression tag	UNP Q92643
K	603	ASP	-	expression tag	UNP Q92643
K	604	HIS	-	expression tag	UNP Q92643
K	605	ARG	-	expression tag	UNP Q92643
K	606	ILE	-	expression tag	UNP Q92643

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Chain	Residue	Modelled	Actual	Comment	Reference
K	607	GLU	-	expression tag	UNP Q92643
K	608	ILE	-	expression tag	UNP Q92643
K	609	LEU	-	expression tag	UNP Q92643
K	610	SER	-	expression tag	UNP Q92643
K	611	HIS	-	expression tag	UNP Q92643
K	612	ASP	-	expression tag	UNP Q92643
K	613	LYS	-	expression tag	UNP Q92643
K	614	ASP	-	expression tag	UNP Q92643
K	615	TYR	-	expression tag	UNP Q92643
K	616	ASN	-	expression tag	UNP Q92643
K	617	LYS	-	expression tag	UNP Q92643
K	618	VAL	-	expression tag	UNP Q92643
K	619	ARG	-	expression tag	UNP Q92643
K	620	LEU	-	expression tag	UNP Q92643
K	621	TYR	-	expression tag	UNP Q92643
K	622	GLU	-	expression tag	UNP Q92643
K	623	HIS	-	expression tag	UNP Q92643
K	624	ALA	-	expression tag	UNP Q92643
K	625	GLU	-	expression tag	UNP Q92643
K	626	ALA	-	expression tag	UNP Q92643
K	627	ARG	-	expression tag	UNP Q92643
K	628	TYR	-	expression tag	UNP Q92643
K	629	SER	-	expression tag	UNP Q92643
K	630	GLY	-	expression tag	UNP Q92643
K	631	GLY	-	expression tag	UNP Q92643
K	632	GLY	-	expression tag	UNP Q92643
K	633	SER	-	expression tag	UNP Q92643
K	634	GLY	-	expression tag	UNP Q92643
K	635	GLY	-	expression tag	UNP Q92643
K	636	GLY	-	expression tag	UNP Q92643
K	637	TYR	-	expression tag	UNP Q92643
K	638	PRO	-	expression tag	UNP Q92643
K	639	TYR	-	expression tag	UNP Q92643
K	640	ASP	-	expression tag	UNP Q92643
K	641	VAL	-	expression tag	UNP Q92643
K	642	PRO	-	expression tag	UNP Q92643
K	643	ASP	-	expression tag	UNP Q92643
K	644	TYR	-	expression tag	UNP Q92643
K	645	ALA	-	expression tag	UNP Q92643

- Molecule 3 is a protein called GPI transamidase component PIG-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	532	Total	C	N	O	S	0	0
			3968	2568	665	721	14		

There are 262 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-1	MET	-	initiating methionine	UNP Q96S52
S	0	GLY	-	expression tag	UNP Q96S52
S	1	SER	-	expression tag	UNP Q96S52
S	556	GLY	-	expression tag	UNP Q96S52
S	557	THR	-	expression tag	UNP Q96S52
S	558	LEU	-	expression tag	UNP Q96S52
S	559	GLU	-	expression tag	UNP Q96S52
S	560	VAL	-	expression tag	UNP Q96S52
S	561	LEU	-	expression tag	UNP Q96S52
S	562	PHE	-	expression tag	UNP Q96S52
S	563	GLN	-	expression tag	UNP Q96S52
S	564	GLY	-	expression tag	UNP Q96S52
S	565	PRO	-	expression tag	UNP Q96S52
S	566	GLY	-	expression tag	UNP Q96S52
S	567	GLY	-	expression tag	UNP Q96S52
S	568	SER	-	expression tag	UNP Q96S52
S	569	GLY	-	expression tag	UNP Q96S52
S	570	GLY	-	expression tag	UNP Q96S52
S	571	SER	-	expression tag	UNP Q96S52
S	572	ALA	-	expression tag	UNP Q96S52
S	573	SER	-	expression tag	UNP Q96S52
S	574	VAL	-	expression tag	UNP Q96S52
S	575	ILE	-	expression tag	UNP Q96S52
S	576	LYS	-	expression tag	UNP Q96S52
S	577	PRO	-	expression tag	UNP Q96S52
S	578	GLU	-	expression tag	UNP Q96S52
S	579	MET	-	expression tag	UNP Q96S52
S	580	LYS	-	expression tag	UNP Q96S52
S	581	ILE	-	expression tag	UNP Q96S52
S	582	LYS	-	expression tag	UNP Q96S52
S	583	LEU	-	expression tag	UNP Q96S52
S	584	ARG	-	expression tag	UNP Q96S52
S	585	MET	-	expression tag	UNP Q96S52
S	586	GLU	-	expression tag	UNP Q96S52
S	587	GLY	-	expression tag	UNP Q96S52
S	588	ALA	-	expression tag	UNP Q96S52
S	589	VAL	-	expression tag	UNP Q96S52

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Chain	Residue	Modelled	Actual	Comment	Reference
S	590	ASN	-	expression tag	UNP Q96S52
S	591	GLY	-	expression tag	UNP Q96S52
S	592	HIS	-	expression tag	UNP Q96S52
S	593	LYS	-	expression tag	UNP Q96S52
S	594	PHE	-	expression tag	UNP Q96S52
S	595	VAL	-	expression tag	UNP Q96S52
S	596	ILE	-	expression tag	UNP Q96S52
S	597	GLU	-	expression tag	UNP Q96S52
S	598	GLY	-	expression tag	UNP Q96S52
S	599	GLU	-	expression tag	UNP Q96S52
S	600	GLY	-	expression tag	UNP Q96S52
S	601	ILE	-	expression tag	UNP Q96S52
S	602	GLY	-	expression tag	UNP Q96S52
S	603	LYS	-	expression tag	UNP Q96S52
S	604	PRO	-	expression tag	UNP Q96S52
S	605	TYR	-	expression tag	UNP Q96S52
S	606	GLU	-	expression tag	UNP Q96S52
S	607	GLY	-	expression tag	UNP Q96S52
S	608	THR	-	expression tag	UNP Q96S52
S	609	GLN	-	expression tag	UNP Q96S52
S	610	THR	-	expression tag	UNP Q96S52
S	611	LEU	-	expression tag	UNP Q96S52
S	612	ASP	-	expression tag	UNP Q96S52
S	613	LEU	-	expression tag	UNP Q96S52
S	614	THR	-	expression tag	UNP Q96S52
S	615	VAL	-	expression tag	UNP Q96S52
S	616	GLU	-	expression tag	UNP Q96S52
S	617	GLU	-	expression tag	UNP Q96S52
S	618	GLY	-	expression tag	UNP Q96S52
S	619	ALA	-	expression tag	UNP Q96S52
S	620	PRO	-	expression tag	UNP Q96S52
S	621	LEU	-	expression tag	UNP Q96S52
S	622	PRO	-	expression tag	UNP Q96S52
S	623	PHE	-	expression tag	UNP Q96S52
S	624	SER	-	expression tag	UNP Q96S52
S	625	TYR	-	expression tag	UNP Q96S52
S	626	ASP	-	expression tag	UNP Q96S52
S	627	ILE	-	expression tag	UNP Q96S52
S	628	LEU	-	expression tag	UNP Q96S52
S	629	THR	-	expression tag	UNP Q96S52
S	630	PRO	-	expression tag	UNP Q96S52
S	631	ALA	-	expression tag	UNP Q96S52

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Chain	Residue	Modelled	Actual	Comment	Reference
S	632	PHE	-	expression tag	UNP Q96S52
S	633	GLN	-	expression tag	UNP Q96S52
S	634	TYR	-	expression tag	UNP Q96S52
S	635	GLY	-	expression tag	UNP Q96S52
S	636	ASN	-	expression tag	UNP Q96S52
S	637	ARG	-	expression tag	UNP Q96S52
S	638	ALA	-	expression tag	UNP Q96S52
S	639	PHE	-	expression tag	UNP Q96S52
S	640	THR	-	expression tag	UNP Q96S52
S	641	LYS	-	expression tag	UNP Q96S52
S	642	TYR	-	expression tag	UNP Q96S52
S	643	PRO	-	expression tag	UNP Q96S52
S	644	GLU	-	expression tag	UNP Q96S52
S	645	ASP	-	expression tag	UNP Q96S52
S	646	ILE	-	expression tag	UNP Q96S52
S	647	PRO	-	expression tag	UNP Q96S52
S	648	ASP	-	expression tag	UNP Q96S52
S	649	TYR	-	expression tag	UNP Q96S52
S	650	PHE	-	expression tag	UNP Q96S52
S	651	LYS	-	expression tag	UNP Q96S52
S	652	GLN	-	expression tag	UNP Q96S52
S	653	ALA	-	expression tag	UNP Q96S52
S	654	PHE	-	expression tag	UNP Q96S52
S	655	PRO	-	expression tag	UNP Q96S52
S	656	GLU	-	expression tag	UNP Q96S52
S	657	GLY	-	expression tag	UNP Q96S52
S	658	TYR	-	expression tag	UNP Q96S52
S	659	SER	-	expression tag	UNP Q96S52
S	660	TRP	-	expression tag	UNP Q96S52
S	661	GLU	-	expression tag	UNP Q96S52
S	662	ARG	-	expression tag	UNP Q96S52
S	663	SER	-	expression tag	UNP Q96S52
S	664	MET	-	expression tag	UNP Q96S52
S	665	THR	-	expression tag	UNP Q96S52
S	666	TYR	-	expression tag	UNP Q96S52
S	667	GLU	-	expression tag	UNP Q96S52
S	668	ASP	-	expression tag	UNP Q96S52
S	669	GLN	-	expression tag	UNP Q96S52
S	670	GLY	-	expression tag	UNP Q96S52
S	671	ILE	-	expression tag	UNP Q96S52
S	672	CYS	-	expression tag	UNP Q96S52
S	673	ILE	-	expression tag	UNP Q96S52

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Chain	Residue	Modelled	Actual	Comment	Reference
S	674	ALA	-	expression tag	UNP Q96S52
S	675	THR	-	expression tag	UNP Q96S52
S	676	SER	-	expression tag	UNP Q96S52
S	677	ASP	-	expression tag	UNP Q96S52
S	678	ILE	-	expression tag	UNP Q96S52
S	679	THR	-	expression tag	UNP Q96S52
S	680	MET	-	expression tag	UNP Q96S52
S	681	GLU	-	expression tag	UNP Q96S52
S	682	GLY	-	expression tag	UNP Q96S52
S	683	ASP	-	expression tag	UNP Q96S52
S	684	CYS	-	expression tag	UNP Q96S52
S	685	PHE	-	expression tag	UNP Q96S52
S	686	PHE	-	expression tag	UNP Q96S52
S	687	TYR	-	expression tag	UNP Q96S52
S	688	GLU	-	expression tag	UNP Q96S52
S	689	ILE	-	expression tag	UNP Q96S52
S	690	ARG	-	expression tag	UNP Q96S52
S	691	PHE	-	expression tag	UNP Q96S52
S	692	ASP	-	expression tag	UNP Q96S52
S	693	GLY	-	expression tag	UNP Q96S52
S	694	THR	-	expression tag	UNP Q96S52
S	695	ASN	-	expression tag	UNP Q96S52
S	696	PHE	-	expression tag	UNP Q96S52
S	697	PRO	-	expression tag	UNP Q96S52
S	698	PRO	-	expression tag	UNP Q96S52
S	699	ASN	-	expression tag	UNP Q96S52
S	700	GLY	-	expression tag	UNP Q96S52
S	701	PRO	-	expression tag	UNP Q96S52
S	702	VAL	-	expression tag	UNP Q96S52
S	703	MET	-	expression tag	UNP Q96S52
S	704	GLN	-	expression tag	UNP Q96S52
S	705	LYS	-	expression tag	UNP Q96S52
S	706	LYS	-	expression tag	UNP Q96S52
S	707	THR	-	expression tag	UNP Q96S52
S	708	LEU	-	expression tag	UNP Q96S52
S	709	LYS	-	expression tag	UNP Q96S52
S	710	TRP	-	expression tag	UNP Q96S52
S	711	GLU	-	expression tag	UNP Q96S52
S	712	PRO	-	expression tag	UNP Q96S52
S	713	SER	-	expression tag	UNP Q96S52
S	714	THR	-	expression tag	UNP Q96S52
S	715	GLU	-	expression tag	UNP Q96S52

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Chain	Residue	Modelled	Actual	Comment	Reference
S	716	LYS	-	expression tag	UNP Q96S52
S	717	MET	-	expression tag	UNP Q96S52
S	718	TYR	-	expression tag	UNP Q96S52
S	719	VAL	-	expression tag	UNP Q96S52
S	720	GLU	-	expression tag	UNP Q96S52
S	721	ASP	-	expression tag	UNP Q96S52
S	722	GLY	-	expression tag	UNP Q96S52
S	723	VAL	-	expression tag	UNP Q96S52
S	724	LEU	-	expression tag	UNP Q96S52
S	725	LYS	-	expression tag	UNP Q96S52
S	726	GLY	-	expression tag	UNP Q96S52
S	727	ASP	-	expression tag	UNP Q96S52
S	728	VAL	-	expression tag	UNP Q96S52
S	729	GLU	-	expression tag	UNP Q96S52
S	730	MET	-	expression tag	UNP Q96S52
S	731	ALA	-	expression tag	UNP Q96S52
S	732	LEU	-	expression tag	UNP Q96S52
S	733	LEU	-	expression tag	UNP Q96S52
S	734	LEU	-	expression tag	UNP Q96S52
S	735	GLU	-	expression tag	UNP Q96S52
S	736	GLY	-	expression tag	UNP Q96S52
S	737	GLY	-	expression tag	UNP Q96S52
S	738	GLY	-	expression tag	UNP Q96S52
S	739	HIS	-	expression tag	UNP Q96S52
S	740	TYR	-	expression tag	UNP Q96S52
S	741	ARG	-	expression tag	UNP Q96S52
S	742	CYS	-	expression tag	UNP Q96S52
S	743	ASP	-	expression tag	UNP Q96S52
S	744	PHE	-	expression tag	UNP Q96S52
S	745	LYS	-	expression tag	UNP Q96S52
S	746	THR	-	expression tag	UNP Q96S52
S	747	THR	-	expression tag	UNP Q96S52
S	748	TYR	-	expression tag	UNP Q96S52
S	749	LYS	-	expression tag	UNP Q96S52
S	750	ALA	-	expression tag	UNP Q96S52
S	751	LYS	-	expression tag	UNP Q96S52
S	752	LYS	-	expression tag	UNP Q96S52
S	753	ASP	-	expression tag	UNP Q96S52
S	754	VAL	-	expression tag	UNP Q96S52
S	755	ARG	-	expression tag	UNP Q96S52
S	756	LEU	-	expression tag	UNP Q96S52
S	757	PRO	-	expression tag	UNP Q96S52

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Chain	Residue	Modelled	Actual	Comment	Reference
S	758	ASP	-	expression tag	UNP Q96S52
S	759	ALA	-	expression tag	UNP Q96S52
S	760	HIS	-	expression tag	UNP Q96S52
S	761	GLU	-	expression tag	UNP Q96S52
S	762	VAL	-	expression tag	UNP Q96S52
S	763	ASP	-	expression tag	UNP Q96S52
S	764	HIS	-	expression tag	UNP Q96S52
S	765	ARG	-	expression tag	UNP Q96S52
S	766	ILE	-	expression tag	UNP Q96S52
S	767	GLU	-	expression tag	UNP Q96S52
S	768	ILE	-	expression tag	UNP Q96S52
S	769	LEU	-	expression tag	UNP Q96S52
S	770	SER	-	expression tag	UNP Q96S52
S	771	HIS	-	expression tag	UNP Q96S52
S	772	ASP	-	expression tag	UNP Q96S52
S	773	LYS	-	expression tag	UNP Q96S52
S	774	ASP	-	expression tag	UNP Q96S52
S	775	TYR	-	expression tag	UNP Q96S52
S	776	ASN	-	expression tag	UNP Q96S52
S	777	LYS	-	expression tag	UNP Q96S52
S	778	VAL	-	expression tag	UNP Q96S52
S	779	ARG	-	expression tag	UNP Q96S52
S	780	LEU	-	expression tag	UNP Q96S52
S	781	TYR	-	expression tag	UNP Q96S52
S	782	GLU	-	expression tag	UNP Q96S52
S	783	HIS	-	expression tag	UNP Q96S52
S	784	ALA	-	expression tag	UNP Q96S52
S	785	GLU	-	expression tag	UNP Q96S52
S	786	ALA	-	expression tag	UNP Q96S52
S	787	ARG	-	expression tag	UNP Q96S52
S	788	TYR	-	expression tag	UNP Q96S52
S	789	SER	-	expression tag	UNP Q96S52
S	790	GLY	-	expression tag	UNP Q96S52
S	791	GLY	-	expression tag	UNP Q96S52
S	792	GLY	-	expression tag	UNP Q96S52
S	793	SER	-	expression tag	UNP Q96S52
S	794	GLY	-	expression tag	UNP Q96S52
S	795	GLY	-	expression tag	UNP Q96S52
S	796	GLY	-	expression tag	UNP Q96S52
S	797	GLY	-	expression tag	UNP Q96S52
S	798	GLY	-	expression tag	UNP Q96S52
S	799	GLY	-	expression tag	UNP Q96S52

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Chain	Residue	Modelled	Actual	Comment	Reference
S	800	GLY	-	expression tag	UNP Q96S52
S	801	GLY	-	expression tag	UNP Q96S52
S	802	GLY	-	expression tag	UNP Q96S52
S	803	GLY	-	expression tag	UNP Q96S52
S	804	GLY	-	expression tag	UNP Q96S52
S	805	GLU	-	expression tag	UNP Q96S52
S	806	GLN	-	expression tag	UNP Q96S52
S	807	LYS	-	expression tag	UNP Q96S52
S	808	LEU	-	expression tag	UNP Q96S52
S	809	ILE	-	expression tag	UNP Q96S52
S	810	SER	-	expression tag	UNP Q96S52
S	811	GLU	-	expression tag	UNP Q96S52
S	812	GLU	-	expression tag	UNP Q96S52
S	813	ASP	-	expression tag	UNP Q96S52
S	814	LEU	-	expression tag	UNP Q96S52

- Molecule 4 is a protein called GPI transamidase component PIG-T.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	528	Total	C	N	O	S	0	0
			4220	2741	707	758	14		

There are 254 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-1	MET	-	initiating methionine	UNP Q969N2
T	0	GLY	-	expression tag	UNP Q969N2
T	1	SER	-	expression tag	UNP Q969N2
T	579	GLY	-	expression tag	UNP Q969N2
T	580	THR	-	expression tag	UNP Q969N2
T	581	LEU	-	expression tag	UNP Q969N2
T	582	GLU	-	expression tag	UNP Q969N2
T	583	VAL	-	expression tag	UNP Q969N2
T	584	LEU	-	expression tag	UNP Q969N2
T	585	PHE	-	expression tag	UNP Q969N2
T	586	GLN	-	expression tag	UNP Q969N2
T	587	GLY	-	expression tag	UNP Q969N2
T	588	PRO	-	expression tag	UNP Q969N2
T	589	GLY	-	expression tag	UNP Q969N2
T	590	GLY	-	expression tag	UNP Q969N2
T	591	SER	-	expression tag	UNP Q969N2
T	592	GLY	-	expression tag	UNP Q969N2

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Chain	Residue	Modelled	Actual	Comment	Reference
T	593	GLY	-	expression tag	UNP Q969N2
T	594	SER	-	expression tag	UNP Q969N2
T	595	ALA	-	expression tag	UNP Q969N2
T	596	SER	-	expression tag	UNP Q969N2
T	597	VAL	-	expression tag	UNP Q969N2
T	598	ILE	-	expression tag	UNP Q969N2
T	599	LYS	-	expression tag	UNP Q969N2
T	600	PRO	-	expression tag	UNP Q969N2
T	601	GLU	-	expression tag	UNP Q969N2
T	602	MET	-	expression tag	UNP Q969N2
T	603	LYS	-	expression tag	UNP Q969N2
T	604	ILE	-	expression tag	UNP Q969N2
T	605	LYS	-	expression tag	UNP Q969N2
T	606	LEU	-	expression tag	UNP Q969N2
T	607	ARG	-	expression tag	UNP Q969N2
T	608	MET	-	expression tag	UNP Q969N2
T	609	GLU	-	expression tag	UNP Q969N2
T	610	GLY	-	expression tag	UNP Q969N2
T	611	ALA	-	expression tag	UNP Q969N2
T	612	VAL	-	expression tag	UNP Q969N2
T	613	ASN	-	expression tag	UNP Q969N2
T	614	GLY	-	expression tag	UNP Q969N2
T	615	HIS	-	expression tag	UNP Q969N2
T	616	LYS	-	expression tag	UNP Q969N2
T	617	PHE	-	expression tag	UNP Q969N2
T	618	VAL	-	expression tag	UNP Q969N2
T	619	ILE	-	expression tag	UNP Q969N2
T	620	GLU	-	expression tag	UNP Q969N2
T	621	GLY	-	expression tag	UNP Q969N2
T	622	GLU	-	expression tag	UNP Q969N2
T	623	GLY	-	expression tag	UNP Q969N2
T	624	ILE	-	expression tag	UNP Q969N2
T	625	GLY	-	expression tag	UNP Q969N2
T	626	LYS	-	expression tag	UNP Q969N2
T	627	PRO	-	expression tag	UNP Q969N2
T	628	TYR	-	expression tag	UNP Q969N2
T	629	GLU	-	expression tag	UNP Q969N2
T	630	GLY	-	expression tag	UNP Q969N2
T	631	THR	-	expression tag	UNP Q969N2
T	632	GLN	-	expression tag	UNP Q969N2
T	633	THR	-	expression tag	UNP Q969N2
T	634	LEU	-	expression tag	UNP Q969N2

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Chain	Residue	Modelled	Actual	Comment	Reference
T	635	ASP	-	expression tag	UNP Q969N2
T	636	LEU	-	expression tag	UNP Q969N2
T	637	THR	-	expression tag	UNP Q969N2
T	638	VAL	-	expression tag	UNP Q969N2
T	639	GLU	-	expression tag	UNP Q969N2
T	640	GLU	-	expression tag	UNP Q969N2
T	641	GLY	-	expression tag	UNP Q969N2
T	642	ALA	-	expression tag	UNP Q969N2
T	643	PRO	-	expression tag	UNP Q969N2
T	644	LEU	-	expression tag	UNP Q969N2
T	645	PRO	-	expression tag	UNP Q969N2
T	646	PHE	-	expression tag	UNP Q969N2
T	647	SER	-	expression tag	UNP Q969N2
T	648	TYR	-	expression tag	UNP Q969N2
T	649	ASP	-	expression tag	UNP Q969N2
T	650	ILE	-	expression tag	UNP Q969N2
T	651	LEU	-	expression tag	UNP Q969N2
T	652	THR	-	expression tag	UNP Q969N2
T	653	PRO	-	expression tag	UNP Q969N2
T	654	ALA	-	expression tag	UNP Q969N2
T	655	PHE	-	expression tag	UNP Q969N2
T	656	GLN	-	expression tag	UNP Q969N2
T	657	TYR	-	expression tag	UNP Q969N2
T	658	GLY	-	expression tag	UNP Q969N2
T	659	ASN	-	expression tag	UNP Q969N2
T	660	ARG	-	expression tag	UNP Q969N2
T	661	ALA	-	expression tag	UNP Q969N2
T	662	PHE	-	expression tag	UNP Q969N2
T	663	THR	-	expression tag	UNP Q969N2
T	664	LYS	-	expression tag	UNP Q969N2
T	665	TYR	-	expression tag	UNP Q969N2
T	666	PRO	-	expression tag	UNP Q969N2
T	667	GLU	-	expression tag	UNP Q969N2
T	668	ASP	-	expression tag	UNP Q969N2
T	669	ILE	-	expression tag	UNP Q969N2
T	670	PRO	-	expression tag	UNP Q969N2
T	671	ASP	-	expression tag	UNP Q969N2
T	672	TYR	-	expression tag	UNP Q969N2
T	673	PHE	-	expression tag	UNP Q969N2
T	674	LYS	-	expression tag	UNP Q969N2
T	675	GLN	-	expression tag	UNP Q969N2
T	676	ALA	-	expression tag	UNP Q969N2

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Chain	Residue	Modelled	Actual	Comment	Reference
T	677	PHE	-	expression tag	UNP Q969N2
T	678	PRO	-	expression tag	UNP Q969N2
T	679	GLU	-	expression tag	UNP Q969N2
T	680	GLY	-	expression tag	UNP Q969N2
T	681	TYR	-	expression tag	UNP Q969N2
T	682	SER	-	expression tag	UNP Q969N2
T	683	TRP	-	expression tag	UNP Q969N2
T	684	GLU	-	expression tag	UNP Q969N2
T	685	ARG	-	expression tag	UNP Q969N2
T	686	SER	-	expression tag	UNP Q969N2
T	687	MET	-	expression tag	UNP Q969N2
T	688	THR	-	expression tag	UNP Q969N2
T	689	TYR	-	expression tag	UNP Q969N2
T	690	GLU	-	expression tag	UNP Q969N2
T	691	ASP	-	expression tag	UNP Q969N2
T	692	GLN	-	expression tag	UNP Q969N2
T	693	GLY	-	expression tag	UNP Q969N2
T	694	ILE	-	expression tag	UNP Q969N2
T	695	CYS	-	expression tag	UNP Q969N2
T	696	ILE	-	expression tag	UNP Q969N2
T	697	ALA	-	expression tag	UNP Q969N2
T	698	THR	-	expression tag	UNP Q969N2
T	699	SER	-	expression tag	UNP Q969N2
T	700	ASP	-	expression tag	UNP Q969N2
T	701	ILE	-	expression tag	UNP Q969N2
T	702	THR	-	expression tag	UNP Q969N2
T	703	MET	-	expression tag	UNP Q969N2
T	704	GLU	-	expression tag	UNP Q969N2
T	705	GLY	-	expression tag	UNP Q969N2
T	706	ASP	-	expression tag	UNP Q969N2
T	707	CYS	-	expression tag	UNP Q969N2
T	708	PHE	-	expression tag	UNP Q969N2
T	709	PHE	-	expression tag	UNP Q969N2
T	710	TYR	-	expression tag	UNP Q969N2
T	711	GLU	-	expression tag	UNP Q969N2
T	712	ILE	-	expression tag	UNP Q969N2
T	713	ARG	-	expression tag	UNP Q969N2
T	714	PHE	-	expression tag	UNP Q969N2
T	715	ASP	-	expression tag	UNP Q969N2
T	716	GLY	-	expression tag	UNP Q969N2
T	717	THR	-	expression tag	UNP Q969N2
T	718	ASN	-	expression tag	UNP Q969N2

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Chain	Residue	Modelled	Actual	Comment	Reference
T	719	PHE	-	expression tag	UNP Q969N2
T	720	PRO	-	expression tag	UNP Q969N2
T	721	PRO	-	expression tag	UNP Q969N2
T	722	ASN	-	expression tag	UNP Q969N2
T	723	GLY	-	expression tag	UNP Q969N2
T	724	PRO	-	expression tag	UNP Q969N2
T	725	VAL	-	expression tag	UNP Q969N2
T	726	MET	-	expression tag	UNP Q969N2
T	727	GLN	-	expression tag	UNP Q969N2
T	728	LYS	-	expression tag	UNP Q969N2
T	729	LYS	-	expression tag	UNP Q969N2
T	730	THR	-	expression tag	UNP Q969N2
T	731	LEU	-	expression tag	UNP Q969N2
T	732	LYS	-	expression tag	UNP Q969N2
T	733	TRP	-	expression tag	UNP Q969N2
T	734	GLU	-	expression tag	UNP Q969N2
T	735	PRO	-	expression tag	UNP Q969N2
T	736	SER	-	expression tag	UNP Q969N2
T	737	THR	-	expression tag	UNP Q969N2
T	738	GLU	-	expression tag	UNP Q969N2
T	739	LYS	-	expression tag	UNP Q969N2
T	740	MET	-	expression tag	UNP Q969N2
T	741	TYR	-	expression tag	UNP Q969N2
T	742	VAL	-	expression tag	UNP Q969N2
T	743	GLU	-	expression tag	UNP Q969N2
T	744	ASP	-	expression tag	UNP Q969N2
T	745	GLY	-	expression tag	UNP Q969N2
T	746	VAL	-	expression tag	UNP Q969N2
T	747	LEU	-	expression tag	UNP Q969N2
T	748	LYS	-	expression tag	UNP Q969N2
T	749	GLY	-	expression tag	UNP Q969N2
T	750	ASP	-	expression tag	UNP Q969N2
T	751	VAL	-	expression tag	UNP Q969N2
T	752	GLU	-	expression tag	UNP Q969N2
T	753	MET	-	expression tag	UNP Q969N2
T	754	ALA	-	expression tag	UNP Q969N2
T	755	LEU	-	expression tag	UNP Q969N2
T	756	LEU	-	expression tag	UNP Q969N2
T	757	LEU	-	expression tag	UNP Q969N2
T	758	GLU	-	expression tag	UNP Q969N2
T	759	GLY	-	expression tag	UNP Q969N2
T	760	GLY	-	expression tag	UNP Q969N2

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Chain	Residue	Modelled	Actual	Comment	Reference
T	761	GLY	-	expression tag	UNP Q969N2
T	762	HIS	-	expression tag	UNP Q969N2
T	763	TYR	-	expression tag	UNP Q969N2
T	764	ARG	-	expression tag	UNP Q969N2
T	765	CYS	-	expression tag	UNP Q969N2
T	766	ASP	-	expression tag	UNP Q969N2
T	767	PHE	-	expression tag	UNP Q969N2
T	768	LYS	-	expression tag	UNP Q969N2
T	769	THR	-	expression tag	UNP Q969N2
T	770	THR	-	expression tag	UNP Q969N2
T	771	TYR	-	expression tag	UNP Q969N2
T	772	LYS	-	expression tag	UNP Q969N2
T	773	ALA	-	expression tag	UNP Q969N2
T	774	LYS	-	expression tag	UNP Q969N2
T	775	LYS	-	expression tag	UNP Q969N2
T	776	ASP	-	expression tag	UNP Q969N2
T	777	VAL	-	expression tag	UNP Q969N2
T	778	ARG	-	expression tag	UNP Q969N2
T	779	LEU	-	expression tag	UNP Q969N2
T	780	PRO	-	expression tag	UNP Q969N2
T	781	ASP	-	expression tag	UNP Q969N2
T	782	ALA	-	expression tag	UNP Q969N2
T	783	HIS	-	expression tag	UNP Q969N2
T	784	GLU	-	expression tag	UNP Q969N2
T	785	VAL	-	expression tag	UNP Q969N2
T	786	ASP	-	expression tag	UNP Q969N2
T	787	HIS	-	expression tag	UNP Q969N2
T	788	ARG	-	expression tag	UNP Q969N2
T	789	ILE	-	expression tag	UNP Q969N2
T	790	GLU	-	expression tag	UNP Q969N2
T	791	ILE	-	expression tag	UNP Q969N2
T	792	LEU	-	expression tag	UNP Q969N2
T	793	SER	-	expression tag	UNP Q969N2
T	794	HIS	-	expression tag	UNP Q969N2
T	795	ASP	-	expression tag	UNP Q969N2
T	796	LYS	-	expression tag	UNP Q969N2
T	797	ASP	-	expression tag	UNP Q969N2
T	798	TYR	-	expression tag	UNP Q969N2
T	799	ASN	-	expression tag	UNP Q969N2
T	800	LYS	-	expression tag	UNP Q969N2
T	801	VAL	-	expression tag	UNP Q969N2
T	802	ARG	-	expression tag	UNP Q969N2

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Chain	Residue	Modelled	Actual	Comment	Reference
T	803	LEU	-	expression tag	UNP Q969N2
T	804	TYR	-	expression tag	UNP Q969N2
T	805	GLU	-	expression tag	UNP Q969N2
T	806	HIS	-	expression tag	UNP Q969N2
T	807	ALA	-	expression tag	UNP Q969N2
T	808	GLU	-	expression tag	UNP Q969N2
T	809	ALA	-	expression tag	UNP Q969N2
T	810	ARG	-	expression tag	UNP Q969N2
T	811	TYR	-	expression tag	UNP Q969N2
T	812	SER	-	expression tag	UNP Q969N2
T	813	GLY	-	expression tag	UNP Q969N2
T	814	GLY	-	expression tag	UNP Q969N2
T	815	GLY	-	expression tag	UNP Q969N2
T	816	SER	-	expression tag	UNP Q969N2
T	817	GLY	-	expression tag	UNP Q969N2
T	818	GLY	-	expression tag	UNP Q969N2
T	819	GLY	-	expression tag	UNP Q969N2
T	820	HIS	-	expression tag	UNP Q969N2
T	821	HIS	-	expression tag	UNP Q969N2
T	822	HIS	-	expression tag	UNP Q969N2
T	823	HIS	-	expression tag	UNP Q969N2
T	824	HIS	-	expression tag	UNP Q969N2
T	825	HIS	-	expression tag	UNP Q969N2
T	826	HIS	-	expression tag	UNP Q969N2
T	827	HIS	-	expression tag	UNP Q969N2
T	828	HIS	-	expression tag	UNP Q969N2
T	829	HIS	-	expression tag	UNP Q969N2

- Molecule 5 is a protein called Phosphatidylinositol glycan anchor biosynthesis class U protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	419	Total	C	N	O	S	0	0
			3419	2339	506	559	15		

There are 278 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	-1	MET	-	initiating methionine	UNP Q9H490
U	0	GLY	-	expression tag	UNP Q9H490
U	1	SER	-	expression tag	UNP Q9H490
U	436	GLY	-	expression tag	UNP Q9H490
U	437	THR	-	expression tag	UNP Q9H490

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Chain	Residue	Modelled	Actual	Comment	Reference
U	438	LEU	-	expression tag	UNP Q9H490
U	439	GLU	-	expression tag	UNP Q9H490
U	440	VAL	-	expression tag	UNP Q9H490
U	441	LEU	-	expression tag	UNP Q9H490
U	442	PHE	-	expression tag	UNP Q9H490
U	443	GLN	-	expression tag	UNP Q9H490
U	444	GLY	-	expression tag	UNP Q9H490
U	445	PRO	-	expression tag	UNP Q9H490
U	446	GLY	-	expression tag	UNP Q9H490
U	447	GLY	-	expression tag	UNP Q9H490
U	448	SER	-	expression tag	UNP Q9H490
U	449	GLY	-	expression tag	UNP Q9H490
U	450	GLY	-	expression tag	UNP Q9H490
U	451	SER	-	expression tag	UNP Q9H490
U	452	ALA	-	expression tag	UNP Q9H490
U	453	SER	-	expression tag	UNP Q9H490
U	454	VAL	-	expression tag	UNP Q9H490
U	455	ILE	-	expression tag	UNP Q9H490
U	456	LYS	-	expression tag	UNP Q9H490
U	457	PRO	-	expression tag	UNP Q9H490
U	458	GLU	-	expression tag	UNP Q9H490
U	459	MET	-	expression tag	UNP Q9H490
U	460	LYS	-	expression tag	UNP Q9H490
U	461	ILE	-	expression tag	UNP Q9H490
U	462	LYS	-	expression tag	UNP Q9H490
U	463	LEU	-	expression tag	UNP Q9H490
U	464	ARG	-	expression tag	UNP Q9H490
U	465	MET	-	expression tag	UNP Q9H490
U	466	GLU	-	expression tag	UNP Q9H490
U	467	GLY	-	expression tag	UNP Q9H490
U	468	ALA	-	expression tag	UNP Q9H490
U	469	VAL	-	expression tag	UNP Q9H490
U	470	ASN	-	expression tag	UNP Q9H490
U	471	GLY	-	expression tag	UNP Q9H490
U	472	HIS	-	expression tag	UNP Q9H490
U	473	LYS	-	expression tag	UNP Q9H490
U	474	PHE	-	expression tag	UNP Q9H490
U	475	VAL	-	expression tag	UNP Q9H490
U	476	ILE	-	expression tag	UNP Q9H490
U	477	GLU	-	expression tag	UNP Q9H490
U	478	GLY	-	expression tag	UNP Q9H490
U	479	GLU	-	expression tag	UNP Q9H490

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Chain	Residue	Modelled	Actual	Comment	Reference
U	480	GLY	-	expression tag	UNP Q9H490
U	481	ILE	-	expression tag	UNP Q9H490
U	482	GLY	-	expression tag	UNP Q9H490
U	483	LYS	-	expression tag	UNP Q9H490
U	484	PRO	-	expression tag	UNP Q9H490
U	485	TYR	-	expression tag	UNP Q9H490
U	486	GLU	-	expression tag	UNP Q9H490
U	487	GLY	-	expression tag	UNP Q9H490
U	488	THR	-	expression tag	UNP Q9H490
U	489	GLN	-	expression tag	UNP Q9H490
U	490	THR	-	expression tag	UNP Q9H490
U	491	LEU	-	expression tag	UNP Q9H490
U	492	ASP	-	expression tag	UNP Q9H490
U	493	LEU	-	expression tag	UNP Q9H490
U	494	THR	-	expression tag	UNP Q9H490
U	495	VAL	-	expression tag	UNP Q9H490
U	496	GLU	-	expression tag	UNP Q9H490
U	497	GLU	-	expression tag	UNP Q9H490
U	498	GLY	-	expression tag	UNP Q9H490
U	499	ALA	-	expression tag	UNP Q9H490
U	500	PRO	-	expression tag	UNP Q9H490
U	501	LEU	-	expression tag	UNP Q9H490
U	502	PRO	-	expression tag	UNP Q9H490
U	503	PHE	-	expression tag	UNP Q9H490
U	504	SER	-	expression tag	UNP Q9H490
U	505	TYR	-	expression tag	UNP Q9H490
U	506	ASP	-	expression tag	UNP Q9H490
U	507	ILE	-	expression tag	UNP Q9H490
U	508	LEU	-	expression tag	UNP Q9H490
U	509	THR	-	expression tag	UNP Q9H490
U	510	PRO	-	expression tag	UNP Q9H490
U	511	ALA	-	expression tag	UNP Q9H490
U	512	PHE	-	expression tag	UNP Q9H490
U	513	GLN	-	expression tag	UNP Q9H490
U	514	TYR	-	expression tag	UNP Q9H490
U	515	GLY	-	expression tag	UNP Q9H490
U	516	ASN	-	expression tag	UNP Q9H490
U	517	ARG	-	expression tag	UNP Q9H490
U	518	ALA	-	expression tag	UNP Q9H490
U	519	PHE	-	expression tag	UNP Q9H490
U	520	THR	-	expression tag	UNP Q9H490
U	521	LYS	-	expression tag	UNP Q9H490

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Chain	Residue	Modelled	Actual	Comment	Reference
U	522	TYR	-	expression tag	UNP Q9H490
U	523	PRO	-	expression tag	UNP Q9H490
U	524	GLU	-	expression tag	UNP Q9H490
U	525	ASP	-	expression tag	UNP Q9H490
U	526	ILE	-	expression tag	UNP Q9H490
U	527	PRO	-	expression tag	UNP Q9H490
U	528	ASP	-	expression tag	UNP Q9H490
U	529	TYR	-	expression tag	UNP Q9H490
U	530	PHE	-	expression tag	UNP Q9H490
U	531	LYS	-	expression tag	UNP Q9H490
U	532	GLN	-	expression tag	UNP Q9H490
U	533	ALA	-	expression tag	UNP Q9H490
U	534	PHE	-	expression tag	UNP Q9H490
U	535	PRO	-	expression tag	UNP Q9H490
U	536	GLU	-	expression tag	UNP Q9H490
U	537	GLY	-	expression tag	UNP Q9H490
U	538	TYR	-	expression tag	UNP Q9H490
U	539	SER	-	expression tag	UNP Q9H490
U	540	TRP	-	expression tag	UNP Q9H490
U	541	GLU	-	expression tag	UNP Q9H490
U	542	ARG	-	expression tag	UNP Q9H490
U	543	SER	-	expression tag	UNP Q9H490
U	544	MET	-	expression tag	UNP Q9H490
U	545	THR	-	expression tag	UNP Q9H490
U	546	TYR	-	expression tag	UNP Q9H490
U	547	GLU	-	expression tag	UNP Q9H490
U	548	ASP	-	expression tag	UNP Q9H490
U	549	GLN	-	expression tag	UNP Q9H490
U	550	GLY	-	expression tag	UNP Q9H490
U	551	ILE	-	expression tag	UNP Q9H490
U	552	CYS	-	expression tag	UNP Q9H490
U	553	ILE	-	expression tag	UNP Q9H490
U	554	ALA	-	expression tag	UNP Q9H490
U	555	THR	-	expression tag	UNP Q9H490
U	556	SER	-	expression tag	UNP Q9H490
U	557	ASP	-	expression tag	UNP Q9H490
U	558	ILE	-	expression tag	UNP Q9H490
U	559	THR	-	expression tag	UNP Q9H490
U	560	MET	-	expression tag	UNP Q9H490
U	561	GLU	-	expression tag	UNP Q9H490
U	562	GLY	-	expression tag	UNP Q9H490
U	563	ASP	-	expression tag	UNP Q9H490

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Chain	Residue	Modelled	Actual	Comment	Reference
U	564	CYS	-	expression tag	UNP Q9H490
U	565	PHE	-	expression tag	UNP Q9H490
U	566	PHE	-	expression tag	UNP Q9H490
U	567	TYR	-	expression tag	UNP Q9H490
U	568	GLU	-	expression tag	UNP Q9H490
U	569	ILE	-	expression tag	UNP Q9H490
U	570	ARG	-	expression tag	UNP Q9H490
U	571	PHE	-	expression tag	UNP Q9H490
U	572	ASP	-	expression tag	UNP Q9H490
U	573	GLY	-	expression tag	UNP Q9H490
U	574	THR	-	expression tag	UNP Q9H490
U	575	ASN	-	expression tag	UNP Q9H490
U	576	PHE	-	expression tag	UNP Q9H490
U	577	PRO	-	expression tag	UNP Q9H490
U	578	PRO	-	expression tag	UNP Q9H490
U	579	ASN	-	expression tag	UNP Q9H490
U	580	GLY	-	expression tag	UNP Q9H490
U	581	PRO	-	expression tag	UNP Q9H490
U	582	VAL	-	expression tag	UNP Q9H490
U	583	MET	-	expression tag	UNP Q9H490
U	584	GLN	-	expression tag	UNP Q9H490
U	585	LYS	-	expression tag	UNP Q9H490
U	586	LYS	-	expression tag	UNP Q9H490
U	587	THR	-	expression tag	UNP Q9H490
U	588	LEU	-	expression tag	UNP Q9H490
U	589	LYS	-	expression tag	UNP Q9H490
U	590	TRP	-	expression tag	UNP Q9H490
U	591	GLU	-	expression tag	UNP Q9H490
U	592	PRO	-	expression tag	UNP Q9H490
U	593	SER	-	expression tag	UNP Q9H490
U	594	THR	-	expression tag	UNP Q9H490
U	595	GLU	-	expression tag	UNP Q9H490
U	596	LYS	-	expression tag	UNP Q9H490
U	597	MET	-	expression tag	UNP Q9H490
U	598	TYR	-	expression tag	UNP Q9H490
U	599	VAL	-	expression tag	UNP Q9H490
U	600	GLU	-	expression tag	UNP Q9H490
U	601	ASP	-	expression tag	UNP Q9H490
U	602	GLY	-	expression tag	UNP Q9H490
U	603	VAL	-	expression tag	UNP Q9H490
U	604	LEU	-	expression tag	UNP Q9H490
U	605	LYS	-	expression tag	UNP Q9H490

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Chain	Residue	Modelled	Actual	Comment	Reference
U	606	GLY	-	expression tag	UNP Q9H490
U	607	ASP	-	expression tag	UNP Q9H490
U	608	VAL	-	expression tag	UNP Q9H490
U	609	GLU	-	expression tag	UNP Q9H490
U	610	MET	-	expression tag	UNP Q9H490
U	611	ALA	-	expression tag	UNP Q9H490
U	612	LEU	-	expression tag	UNP Q9H490
U	613	LEU	-	expression tag	UNP Q9H490
U	614	LEU	-	expression tag	UNP Q9H490
U	615	GLU	-	expression tag	UNP Q9H490
U	616	GLY	-	expression tag	UNP Q9H490
U	617	GLY	-	expression tag	UNP Q9H490
U	618	GLY	-	expression tag	UNP Q9H490
U	619	HIS	-	expression tag	UNP Q9H490
U	620	TYR	-	expression tag	UNP Q9H490
U	621	ARG	-	expression tag	UNP Q9H490
U	622	CYS	-	expression tag	UNP Q9H490
U	623	ASP	-	expression tag	UNP Q9H490
U	624	PHE	-	expression tag	UNP Q9H490
U	625	LYS	-	expression tag	UNP Q9H490
U	626	THR	-	expression tag	UNP Q9H490
U	627	THR	-	expression tag	UNP Q9H490
U	628	TYR	-	expression tag	UNP Q9H490
U	629	LYS	-	expression tag	UNP Q9H490
U	630	ALA	-	expression tag	UNP Q9H490
U	631	LYS	-	expression tag	UNP Q9H490
U	632	LYS	-	expression tag	UNP Q9H490
U	633	ASP	-	expression tag	UNP Q9H490
U	634	VAL	-	expression tag	UNP Q9H490
U	635	ARG	-	expression tag	UNP Q9H490
U	636	LEU	-	expression tag	UNP Q9H490
U	637	PRO	-	expression tag	UNP Q9H490
U	638	ASP	-	expression tag	UNP Q9H490
U	639	ALA	-	expression tag	UNP Q9H490
U	640	HIS	-	expression tag	UNP Q9H490
U	641	GLU	-	expression tag	UNP Q9H490
U	642	VAL	-	expression tag	UNP Q9H490
U	643	ASP	-	expression tag	UNP Q9H490
U	644	HIS	-	expression tag	UNP Q9H490
U	645	ARG	-	expression tag	UNP Q9H490
U	646	ILE	-	expression tag	UNP Q9H490
U	647	GLU	-	expression tag	UNP Q9H490

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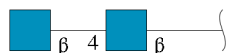
Chain	Residue	Modelled	Actual	Comment	Reference
U	648	ILE	-	expression tag	UNP Q9H490
U	649	LEU	-	expression tag	UNP Q9H490
U	650	SER	-	expression tag	UNP Q9H490
U	651	HIS	-	expression tag	UNP Q9H490
U	652	ASP	-	expression tag	UNP Q9H490
U	653	LYS	-	expression tag	UNP Q9H490
U	654	ASP	-	expression tag	UNP Q9H490
U	655	TYR	-	expression tag	UNP Q9H490
U	656	ASN	-	expression tag	UNP Q9H490
U	657	LYS	-	expression tag	UNP Q9H490
U	658	VAL	-	expression tag	UNP Q9H490
U	659	ARG	-	expression tag	UNP Q9H490
U	660	LEU	-	expression tag	UNP Q9H490
U	661	TYR	-	expression tag	UNP Q9H490
U	662	GLU	-	expression tag	UNP Q9H490
U	663	HIS	-	expression tag	UNP Q9H490
U	664	ALA	-	expression tag	UNP Q9H490
U	665	GLU	-	expression tag	UNP Q9H490
U	666	ALA	-	expression tag	UNP Q9H490
U	667	ARG	-	expression tag	UNP Q9H490
U	668	TYR	-	expression tag	UNP Q9H490
U	669	SER	-	expression tag	UNP Q9H490
U	670	GLY	-	expression tag	UNP Q9H490
U	671	GLY	-	expression tag	UNP Q9H490
U	672	GLY	-	expression tag	UNP Q9H490
U	673	SER	-	expression tag	UNP Q9H490
U	674	GLY	-	expression tag	UNP Q9H490
U	675	GLY	-	expression tag	UNP Q9H490
U	676	GLY	-	expression tag	UNP Q9H490
U	677	LYS	-	expression tag	UNP Q9H490
U	678	LEU	-	expression tag	UNP Q9H490
U	679	GLU	-	expression tag	UNP Q9H490
U	680	PHE	-	expression tag	UNP Q9H490
U	681	SER	-	expression tag	UNP Q9H490
U	682	ALA	-	expression tag	UNP Q9H490
U	683	TRP	-	expression tag	UNP Q9H490
U	684	SER	-	expression tag	UNP Q9H490
U	685	HIS	-	expression tag	UNP Q9H490
U	686	PRO	-	expression tag	UNP Q9H490
U	687	GLN	-	expression tag	UNP Q9H490
U	688	PHE	-	expression tag	UNP Q9H490
U	689	GLU	-	expression tag	UNP Q9H490

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Chain	Residue	Modelled	Actual	Comment	Reference
U	690	LYS	-	expression tag	UNP Q9H490
U	691	GLY	-	expression tag	UNP Q9H490
U	692	GLY	-	expression tag	UNP Q9H490
U	693	GLY	-	expression tag	UNP Q9H490
U	694	SER	-	expression tag	UNP Q9H490
U	695	GLY	-	expression tag	UNP Q9H490
U	696	GLY	-	expression tag	UNP Q9H490
U	697	GLY	-	expression tag	UNP Q9H490
U	698	SER	-	expression tag	UNP Q9H490
U	699	GLY	-	expression tag	UNP Q9H490
U	700	GLY	-	expression tag	UNP Q9H490
U	701	SER	-	expression tag	UNP Q9H490
U	702	ALA	-	expression tag	UNP Q9H490
U	703	TRP	-	expression tag	UNP Q9H490
U	704	SER	-	expression tag	UNP Q9H490
U	705	HIS	-	expression tag	UNP Q9H490
U	706	PRO	-	expression tag	UNP Q9H490
U	707	GLN	-	expression tag	UNP Q9H490
U	708	PHE	-	expression tag	UNP Q9H490
U	709	GLU	-	expression tag	UNP Q9H490
U	710	LYS	-	expression tag	UNP Q9H490

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

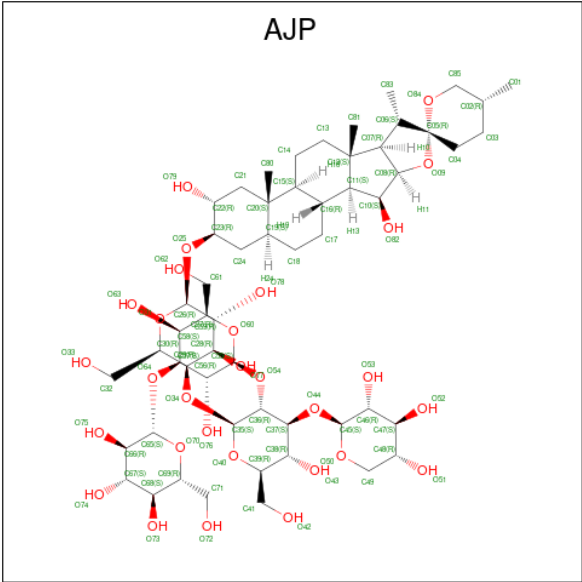


Mol	Chain	Residues	Atoms				AltConf	Trace
6	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).

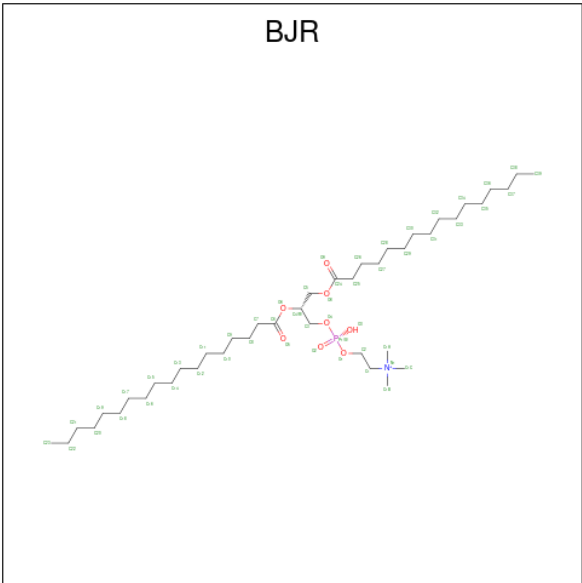


- Molecule 8 is Digitonin (CCD ID: AJP) (formula: $C_{56}H_{92}O_{29}$).



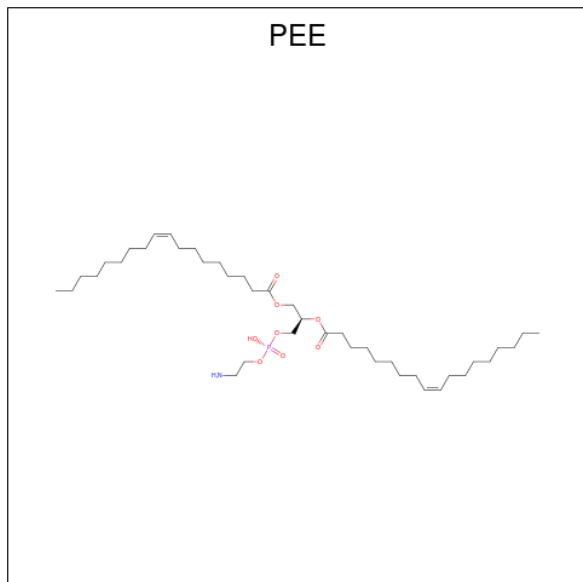
Mol	Chain	Residues	Atoms			AltConf
8	G	1	Total	C	O	0
			85	56	29	

- Molecule 9 is (4S,7R)-7-[(hexadecanoyloxy)methyl]-4-hydroxy-N,N,N-trimethyl-4,9-dioxo-3,5,8-trioxa-4lambda 5 -phosphahehexacosan-1-aminium (CCD ID: BJR) (formula: C₄₂H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
9	G	1	Total	C	N	O	P	0
			44	34	1	8	1	
9	G	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 10 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).

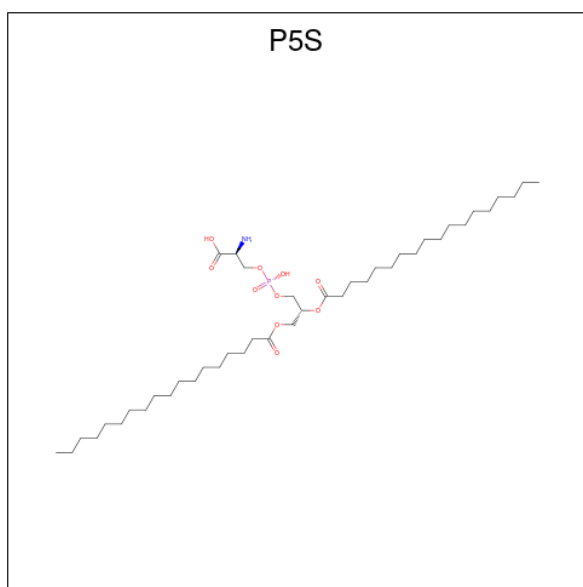


Mol	Chain	Residues	Atoms					AltConf
10	G	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

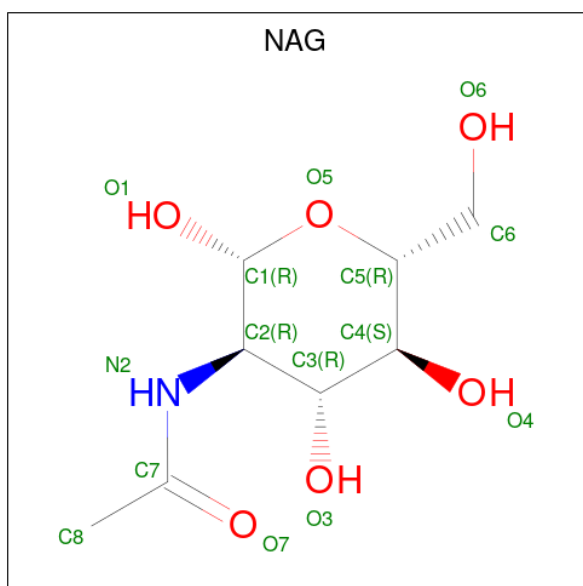
Mol	Chain	Residues	Atoms		AltConf
11	K	1	Total	Ca	0
			1	1	

- Molecule 12 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: $C_{42}H_{82}NO_{10}P$).



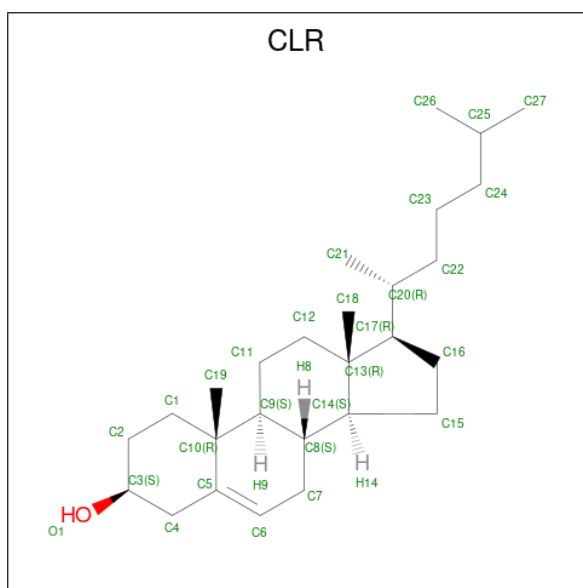
Mol	Chain	Residues	Atoms					AltConf
12	K	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



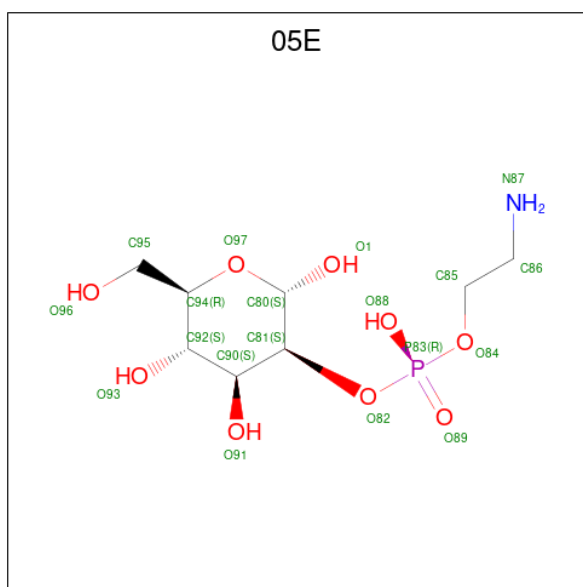
Mol	Chain	Residues	Atoms				AltConf
13	S	1	Total	C	N	O	0
			14	8	1	5	
13	T	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 14 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



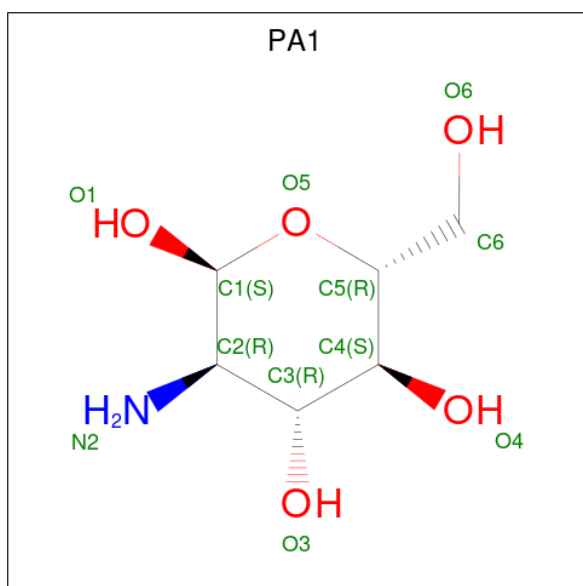
Mol	Chain	Residues	Atoms			AltConf
14	S	1	Total	C	O	0
			28	27	1	
14	S	1	Total	C	O	0
			28	27	1	
14	S	1	Total	C	O	0
			28	27	1	
14	U	1	Total	C	O	0
			28	27	1	
14	U	1	Total	C	O	0
			28	27	1	

- Molecule 15 is 2-azanylethyl [(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-2,4,5-tris(oxidanyl)oxan-3-yl] hydrogen phosphate (CCD ID: 05E) (formula: $C_8H_{18}NO_9P$) (labeled as "Ligand of Interest" by depositor).



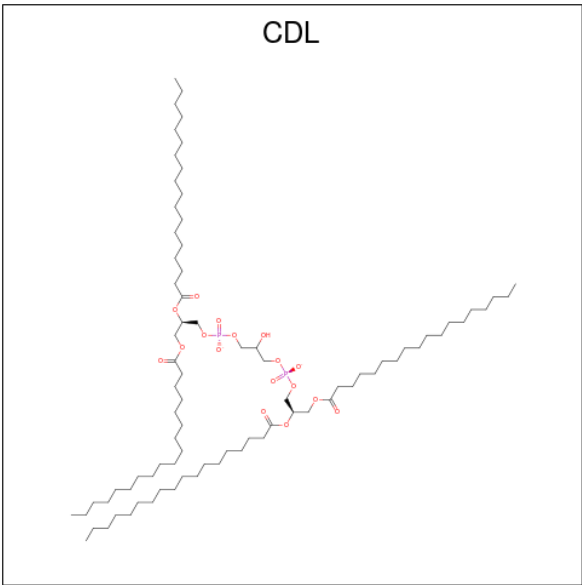
Mol	Chain	Residues	Atoms					AltConf
15	T	1	Total	C	N	O	P	0
			18	8	1	8	1	

- Molecule 16 is 2-amino-2-deoxy- α -D-glucopyranose (CCD ID: PA1) (formula: C₆H₁₃NO₅) (labeled as "Ligand of Interest" by depositor).



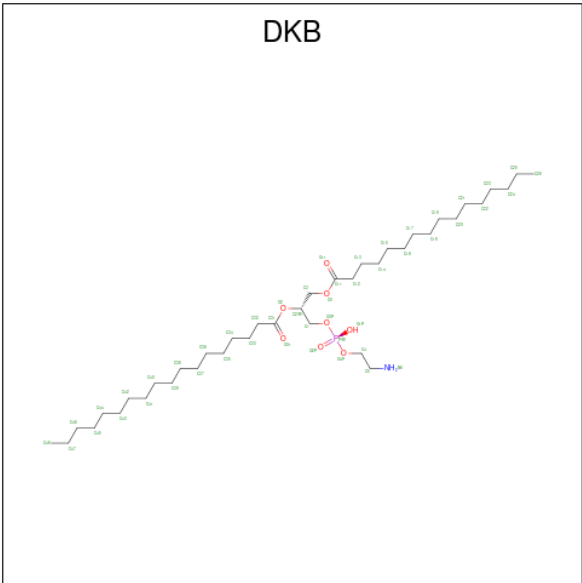
Mol	Chain	Residues	Atoms				AltConf
16	T	1	Total	C	N	O	0
			11	6	1	4	

- Molecule 17 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	U	1	86	67	17	2	0

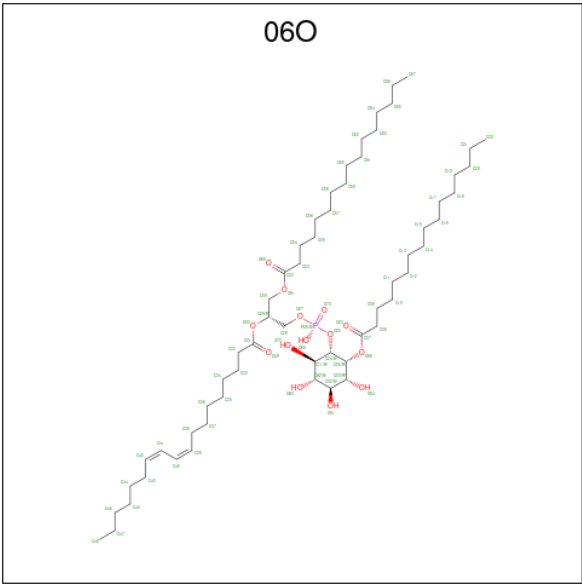
- Molecule 18 is [(2R)-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propan-2-yl] octadecanoate (CCD ID: DKB) (formula: C₃₉H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	U	1	49	39	1	8	1	0

- Molecule 19 is [(2 {R})-1-hexadecanoyloxy-3-[(1 {S},2 {R},3 {R},4 {S},5 {S},6 {R})-2-hexadecanoyloxy-3,4,5,6-tetrakis(oxidanyl)cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-propan-2-yl

] (9 {Z},11 {Z})-octadeca-9,11-dienoate (CCD ID: 06O) (formula: C₅₉H₁₀₉O₁₄P) (labeled as "Ligand of Interest" by depositor).

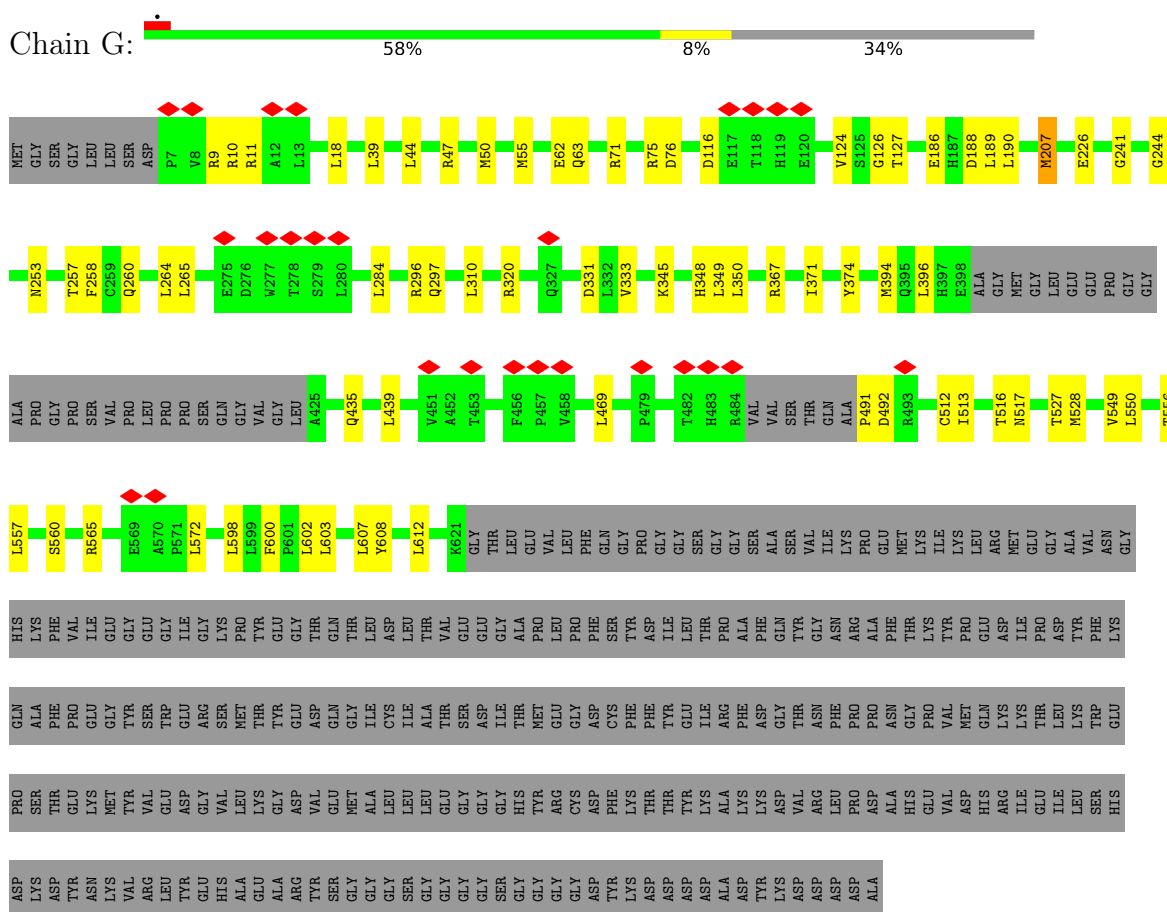


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	U	1	74	59	14	1	0

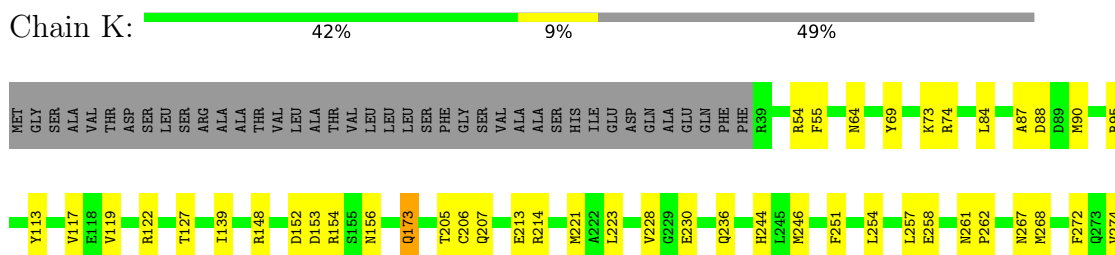
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

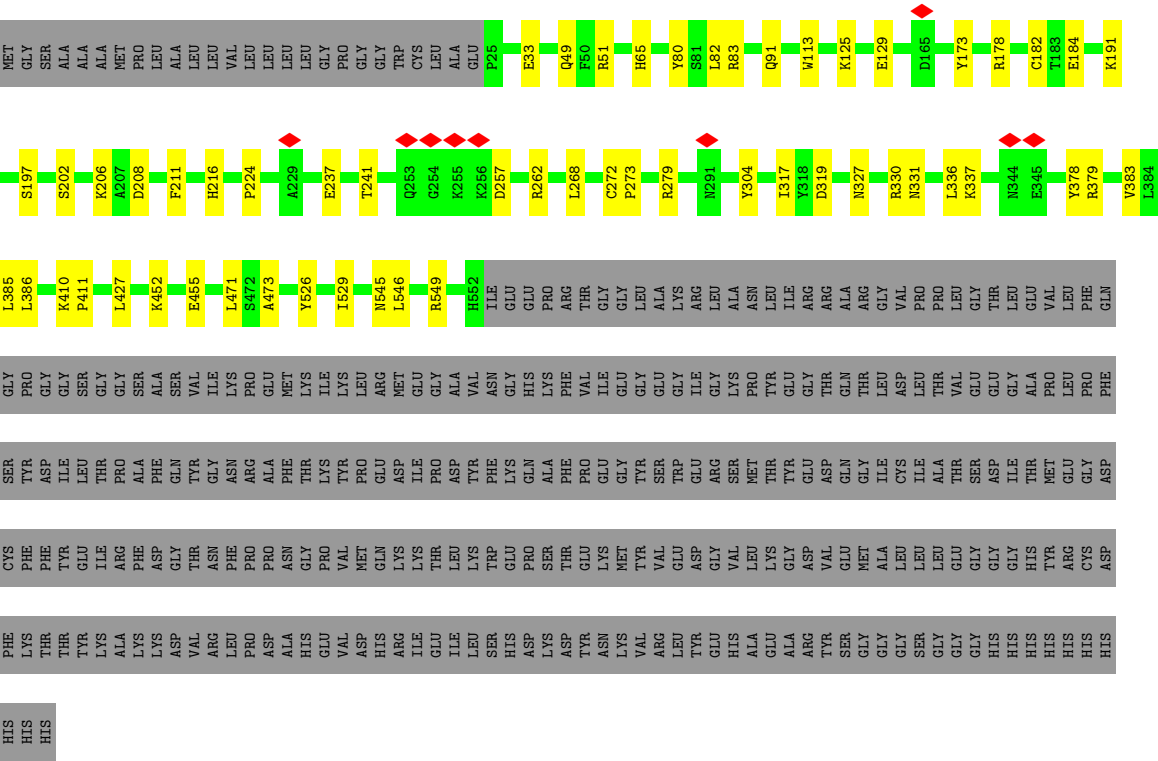
• Molecule 1: Glycosylphosphatidylinositol anchor attachment 1 protein



• Molecule 2: GPI-anchor transamidase

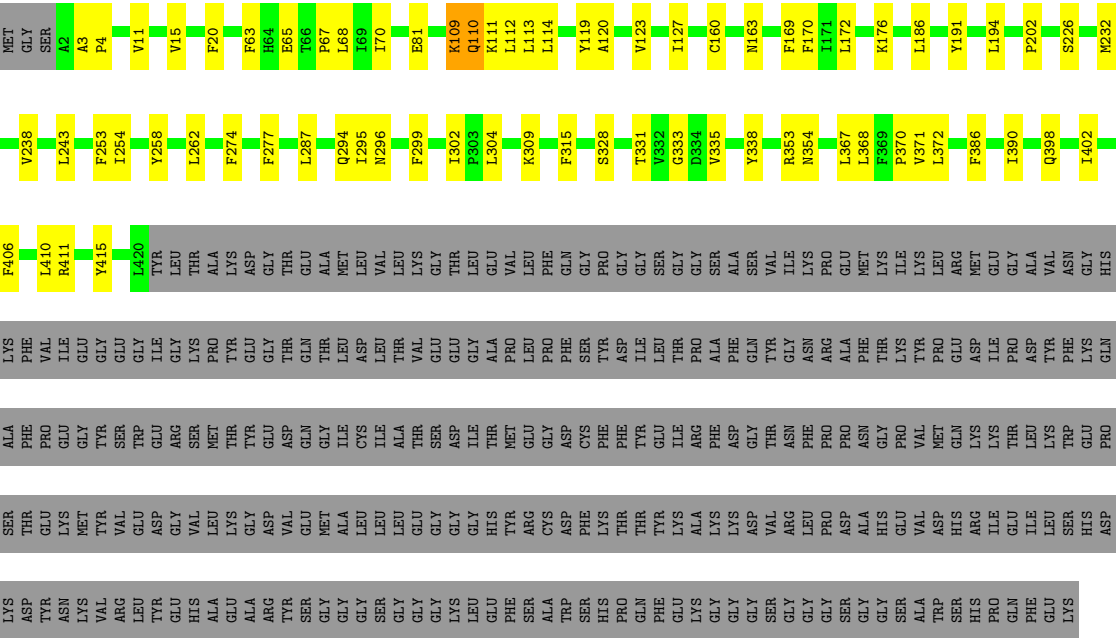






● Molecule 5: Phosphatidylinositol glycan anchor biosynthesis class U protein

Chain U: 49% 10% 41%



● Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 100%

MAG
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	151590	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.015	Depositor
Minimum map value	-3.089	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.182	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	238.0, 238.0, 238.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BJR, PEE, CLR, AJP, NAG, 06O, P5S, DKB, PA1, 05E, Y01, CA, CDL

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	G	0.36	0/4564	0.54	0/6220
2	K	0.51	2/2712 (0.1%)	0.72	5/3688 (0.1%)
3	S	0.36	0/4061	0.56	4/5556 (0.1%)
4	T	0.20	0/4353	0.38	0/5965
5	U	0.25	0/3530	0.45	0/4822
All	All	0.34	2/19220 (0.0%)	0.53	9/26251 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	152	ASP	C-O	-5.76	1.18	1.24
2	K	156	ASN	C-O	-5.07	1.17	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	279	LEU	N-CA-C	-7.26	104.04	113.12
3	S	153	LEU	N-CA-C	-7.08	104.77	113.41
2	K	281	VAL	N-CA-C	-6.89	106.41	113.10
3	S	160	SER	N-CA-C	5.55	118.61	109.72
3	S	284	PRO	N-CA-C	5.49	119.84	111.11
3	S	179	PHE	N-CA-C	-5.41	106.26	112.92
2	K	153	ASP	CA-CB-CG	5.36	117.96	112.60
2	K	284	PRO	N-CA-CB	-5.34	98.71	103.35
2	K	230	GLU	CB-CG-CD	5.32	121.65	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4458	0	4548	75	0
2	K	2644	0	2562	47	0
3	S	3968	0	3908	82	0
4	T	4220	0	4134	49	0
5	U	3419	0	3480	84	0
6	A	28	0	25	0	0
7	G	175	0	245	45	0
7	U	140	0	196	50	0
8	G	85	0	0	0	0
9	G	96	0	0	6	0
10	G	51	0	82	9	0
11	K	1	0	0	0	0
12	K	41	0	51	11	0
13	S	14	0	13	0	0
13	T	14	0	13	0	0
14	S	84	0	138	55	0
14	U	56	0	92	19	0
15	T	18	0	0	0	0
16	T	11	0	10	0	0
17	U	86	0	125	10	0
18	U	49	0	0	1	0
19	U	74	0	0	0	0
All	All	19732	0	19622	397	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 (397) 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)
3:S:247:ILE:HD12	4:T:65:HIS:ND1	1.52	1.25
14:S:903:CLR:H221	7:U:806:Y01:CAC	1.66	1.23
1:G:253:ASN:O	1:G:257:THR:HG23	1.42	1.16
7:G:1602:Y01:HAA1	7:G:1602:Y01:HAC3	1.20	1.16
3:S:247:ILE:HD11	4:T:65:HIS:CG	1.84	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1601:Y01:HAC1	7:G:1601:Y01:HAE2	1.29	1.11
3:S:119:LEU:HD11	3:S:131:LEU:HD11	1.15	1.09
14:S:903:CLR:H213	7:U:806:Y01:HBE	1.11	1.07
3:S:522:TYR:HB2	14:S:902:CLR:H41	1.13	1.07
1:G:516:THR:HG21	9:G:1604:BJR:C7	1.84	1.06
14:S:903:CLR:H213	7:U:806:Y01:CBE	1.85	1.05
5:U:254:ILE:HG23	7:U:802:Y01:HAK1	1.38	1.05
5:U:176:LYS:HE3	14:U:804:CLR:H41	1.37	1.05
7:U:802:Y01:HAR2	7:U:802:Y01:HAM2	1.35	1.05
3:S:119:LEU:CD1	3:S:131:LEU:HD11	1.86	1.04
14:S:902:CLR:H273	5:U:296:ASN:HA	1.39	1.04
5:U:262:LEU:HD13	7:U:806:Y01:HAK1	1.33	1.04
3:S:247:ILE:CD1	4:T:65:HIS:ND1	2.20	1.02
5:U:176:LYS:CE	14:U:804:CLR:H41	1.88	1.02
3:S:119:LEU:HD11	3:S:131:LEU:CD1	1.91	0.99
1:G:550:LEU:HD23	7:G:1607:Y01:CAB	1.92	0.99
7:G:1608:Y01:HAA2	7:G:1608:Y01:HAO1	1.43	0.98
5:U:254:ILE:CG2	7:U:802:Y01:HAK1	1.94	0.97
14:S:903:CLR:H221	7:U:806:Y01:HAC2	1.43	0.97
14:S:903:CLR:H221	7:U:806:Y01:HAC1	1.43	0.97
3:S:247:ILE:CD1	4:T:65:HIS:CG	2.46	0.96
14:S:903:CLR:C21	7:U:806:Y01:HBE	1.98	0.94
4:T:49:GLN:HG2	4:T:241:THR:HG22	1.50	0.94
5:U:176:LYS:NZ	14:U:804:CLR:H41	1.84	0.92
3:S:247:ILE:HD11	4:T:65:HIS:CB	2.00	0.90
1:G:550:LEU:HD23	7:G:1607:Y01:HAB3	1.52	0.87
3:S:31:GLY:HA3	14:S:902:CLR:H121	1.54	0.87
7:G:1608:Y01:CAB	7:G:1608:Y01:HAC3	2.05	0.86
2:K:221:MET:HG3	2:K:288:THR:HG22	1.57	0.86
5:U:238:VAL:HG22	7:U:807:Y01:HAB3	1.58	0.86
7:G:1608:Y01:CAE	7:G:1608:Y01:HAO2	2.06	0.86
3:S:247:ILE:HD11	4:T:65:HIS:HB3	1.57	0.84
5:U:194:LEU:HD21	5:U:258:TYR:CD1	2.13	0.83
3:S:522:TYR:CB	14:S:902:CLR:H41	2.04	0.83
14:S:903:CLR:H25	7:U:806:Y01:HAN2	1.62	0.81
1:G:350:LEU:HD21	2:K:95:ARG:NH1	1.96	0.81
2:K:64:ASN:OD1	2:K:246:MET:HG3	1.79	0.81
3:S:519:PHE:HA	3:S:522:TYR:CE1	2.17	0.80
5:U:254:ILE:CG2	7:U:802:Y01:CAK	2.59	0.80
1:G:253:ASN:O	1:G:257:THR:CG2	2.29	0.80
7:G:1602:Y01:HAC3	7:G:1602:Y01:CAA	2.09	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:903:CLR:C27	7:U:806:Y01:HAN2	2.11	0.79
1:G:516:THR:HG21	9:G:1604:BJR:C8	2.13	0.79
1:G:527:THR:HG23	1:G:528:MET:HG3	1.65	0.78
5:U:110:GLN:OE1	5:U:127:ILE:HG23	1.84	0.78
5:U:176:LYS:HE3	14:U:804:CLR:H6	1.66	0.78
1:G:350:LEU:CD1	2:K:55:PHE:HB3	2.14	0.77
5:U:176:LYS:HZ1	14:U:804:CLR:H41	1.49	0.77
3:S:247:ILE:HD12	4:T:65:HIS:CE1	2.20	0.77
2:K:55:PHE:O	2:K:90:MET:HE1	1.86	0.76
1:G:550:LEU:HD23	7:G:1607:Y01:HAB1	1.67	0.76
7:G:1607:Y01:HAJ1	7:G:1607:Y01:HAP1	1.68	0.76
5:U:232:MET:HG2	14:U:803:CLR:H21	1.68	0.76
3:S:154:LEU:HB3	3:S:171:ARG:NH2	2.01	0.75
7:G:1602:Y01:HAA1	7:G:1602:Y01:CAC	2.10	0.74
7:G:1608:Y01:HAC3	7:G:1608:Y01:HAB1	1.68	0.74
7:G:1608:Y01:HAO2	7:G:1608:Y01:HAE2	1.69	0.74
14:S:902:CLR:H273	5:U:296:ASN:CA	2.18	0.73
14:S:903:CLR:C25	7:U:806:Y01:HAN2	2.19	0.73
7:G:1601:Y01:HAC1	7:G:1601:Y01:CAE	2.15	0.72
14:U:803:CLR:H183	14:U:803:CLR:H212	1.71	0.72
1:G:349:LEU:O	2:K:95:ARG:NH2	2.22	0.72
14:S:903:CLR:C22	7:U:806:Y01:HAC2	2.19	0.72
5:U:202:PRO:HB3	5:U:315:PHE:HD2	1.52	0.72
4:T:182:CYS:HB3	4:T:184:GLU:OE1	1.89	0.72
4:T:83:ARG:CZ	4:T:224:PRO:HG3	2.19	0.72
7:U:802:Y01:HAR2	7:U:802:Y01:CAM	2.16	0.72
3:S:31:GLY:HA3	14:S:902:CLR:C12	2.20	0.71
3:S:154:LEU:HB3	3:S:171:ARG:HH21	1.54	0.71
14:S:903:CLR:H213	7:U:806:Y01:CAC	2.21	0.71
7:U:806:Y01:HAP2	7:U:806:Y01:HAN1	1.73	0.71
14:S:903:CLR:C22	7:U:806:Y01:CAC	2.59	0.71
1:G:516:THR:CG2	9:G:1604:BJR:C7	2.67	0.71
7:G:1608:Y01:HAO1	7:G:1608:Y01:HAB3	1.71	0.70
4:T:257:ASP:HB3	4:T:337:LYS:HD2	1.72	0.70
12:K:702:P5S:H49A	14:U:804:CLR:H25	1.74	0.70
1:G:284:LEU:HD21	7:G:1602:Y01:HAR2	1.76	0.68
7:G:1608:Y01:HAC3	7:G:1608:Y01:HAB3	1.76	0.68
7:U:808:Y01:HAC3	7:U:808:Y01:HAB3	1.75	0.68
5:U:254:ILE:HG22	7:U:802:Y01:HAI	1.76	0.68
1:G:350:LEU:HD21	2:K:95:ARG:HH12	1.58	0.68
7:G:1608:Y01:HAO1	7:G:1608:Y01:CAA	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:808:Y01:HAB3	7:U:808:Y01:CAC	2.23	0.68
7:G:1608:Y01:HAA2	7:G:1608:Y01:CAO	2.21	0.68
7:U:802:Y01:HAM2	7:U:802:Y01:CAR	2.20	0.67
7:U:808:Y01:HAE2	7:U:808:Y01:HAC1	1.75	0.67
14:S:903:CLR:H41	5:U:287:LEU:HD21	1.76	0.67
5:U:176:LYS:HE3	14:U:804:CLR:C4	2.21	0.67
5:U:274:PHE:CE2	5:U:328:SER:HA	2.30	0.67
4:T:546:LEU:HB3	5:U:406:PHE:HE2	1.59	0.67
7:G:1608:Y01:HAJ2	7:G:1608:Y01:HAP1	1.77	0.67
2:K:139:ILE:HD11	2:K:148:ARG:CZ	2.25	0.67
1:G:348:HIS:HA	2:K:95:ARG:HE	1.59	0.66
14:S:903:CLR:H241	7:U:806:Y01:HAC2	1.77	0.66
2:K:69:TYR:CZ	2:K:73:LYS:HD2	2.31	0.66
7:G:1608:Y01:HAB3	7:G:1608:Y01:CAO	2.26	0.65
4:T:546:LEU:HB3	5:U:406:PHE:CE2	2.31	0.65
14:S:903:CLR:C22	7:U:806:Y01:HAC1	2.24	0.65
7:G:1601:Y01:HAE2	7:G:1601:Y01:CAC	2.16	0.64
5:U:172:LEU:HD21	14:U:804:CLR:H151	1.79	0.64
3:S:519:PHE:HA	3:S:522:TYR:CD1	2.32	0.64
1:G:549:VAL:HG12	7:G:1607:Y01:HBA	1.80	0.64
3:S:87:VAL:HG13	3:S:103:ARG:HD2	1.80	0.64
1:G:350:LEU:CD2	2:K:95:ARG:HH12	2.11	0.64
5:U:238:VAL:HG22	7:U:807:Y01:CAB	2.27	0.63
5:U:274:PHE:CD2	5:U:328:SER:HA	2.32	0.63
1:G:350:LEU:HD23	2:K:95:ARG:HH22	1.63	0.63
1:G:350:LEU:HD12	2:K:55:PHE:HB3	1.79	0.63
14:S:903:CLR:H272	7:U:806:Y01:HAN2	1.78	0.63
2:K:84:LEU:HD23	2:K:119:VAL:HG22	1.81	0.63
7:U:808:Y01:HAC3	7:U:808:Y01:HAA2	1.79	0.63
3:S:522:TYR:HB2	14:S:902:CLR:C4	2.08	0.63
14:S:902:CLR:C27	5:U:296:ASN:HA	2.22	0.63
1:G:549:VAL:CG1	7:G:1607:Y01:HBA	2.28	0.62
2:K:64:ASN:OD1	2:K:246:MET:CG	2.46	0.62
5:U:304:LEU:HB3	5:U:315:PHE:HE1	1.64	0.62
1:G:550:LEU:CD2	7:G:1607:Y01:HAB1	2.29	0.62
4:T:49:GLN:CG	4:T:241:THR:HG22	2.27	0.62
3:S:21:LEU:HB3	14:S:904:CLR:H191	1.80	0.62
3:S:154:LEU:O	3:S:155:PRO:C	2.38	0.62
14:S:903:CLR:C21	7:U:806:Y01:HAC2	2.30	0.62
1:G:50:MET:CE	1:G:55:MET:HE3	2.30	0.62
3:S:154:LEU:HD12	3:S:155:PRO:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:GLY:HA3	1:G:186:GLU:HG2	1.82	0.61
7:G:1607:Y01:HAP1	7:G:1607:Y01:CAJ	2.23	0.61
2:K:268:MET:O	2:K:268:MET:HG3	2.00	0.61
5:U:172:LEU:CD2	14:U:804:CLR:H151	2.31	0.61
4:T:182:CYS:HB3	4:T:184:GLU:CD	2.26	0.61
7:G:1608:Y01:HAB3	7:G:1608:Y01:CBB	2.31	0.61
7:G:1608:Y01:HAO2	7:G:1608:Y01:HAE3	1.82	0.61
1:G:71:ARG:O	1:G:75:ARG:HD2	2.01	0.60
2:K:113:TYR:OH	4:T:184:GLU:OE1	2.20	0.60
1:G:550:LEU:CD2	7:G:1607:Y01:CAB	2.75	0.60
1:G:297:GLN:HG2	1:G:517:ASN:HD21	1.66	0.60
5:U:304:LEU:HB3	5:U:315:PHE:CE1	2.37	0.60
1:G:396:LEU:HD21	7:G:1609:Y01:HAQ2	1.84	0.60
1:G:557:LEU:HD11	10:G:1606:PEE:H19	1.83	0.59
14:S:902:CLR:H272	5:U:299:PHE:CG	2.36	0.59
7:U:806:Y01:HAN1	7:U:806:Y01:CAP	2.32	0.59
17:U:801:CDL:CB6	17:U:801:CDL:H511	2.32	0.59
5:U:202:PRO:HD3	5:U:315:PHE:HE2	1.67	0.59
4:T:545:ASN:OD1	4:T:549:ARG:HD3	2.03	0.58
3:S:149:GLU:CD	3:S:174:MET:H	2.12	0.58
7:U:802:Y01:HAN2	7:U:802:Y01:CAC	2.33	0.58
5:U:176:LYS:HZ1	14:U:804:CLR:C4	2.15	0.58
1:G:11:ARG:HD2	1:G:11:ARG:O	2.04	0.58
2:K:386:TYR:HE1	12:K:702:P5S:H21A	1.69	0.58
12:K:702:P5S:H44A	12:K:702:P5S:C20	2.34	0.58
14:S:903:CLR:H213	7:U:806:Y01:HAC2	1.85	0.57
5:U:254:ILE:HG22	7:U:802:Y01:CAI	2.34	0.57
4:T:546:LEU:HD13	5:U:406:PHE:HD2	1.70	0.57
5:U:113:LEU:HD13	5:U:119:TYR:CE1	2.38	0.57
1:G:241:GLY:HA3	1:G:310:LEU:HD12	1.86	0.57
2:K:223:LEU:HD11	2:K:272:PHE:HE1	1.70	0.57
3:S:116:GLU:O	3:S:120:SER:HB3	2.04	0.57
5:U:68:LEU:HD13	5:U:191:TYR:CE2	2.40	0.57
7:G:1608:Y01:HAP1	7:G:1608:Y01:CAJ	2.34	0.56
4:T:113:TRP:HB3	4:T:173:TYR:HD1	1.69	0.56
1:G:47:ARG:NH2	1:G:367:ARG:NH2	2.53	0.56
3:S:182:ILE:O	3:S:186:ILE:HG12	2.04	0.56
4:T:378:TYR:CD1	4:T:379:ARG:HG2	2.40	0.56
5:U:172:LEU:HD21	14:U:804:CLR:C7	2.35	0.56
4:T:385:LEU:HD13	4:T:471:LEU:HD13	1.87	0.56
14:S:902:CLR:H272	5:U:299:PHE:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:904:CLR:C21	14:S:904:CLR:H25	2.36	0.55
5:U:226:SER:HB3	17:U:801:CDL:H202	1.86	0.55
12:K:702:P5S:O18	12:K:702:P5S:H3A	2.06	0.55
1:G:350:LEU:CD2	2:K:95:ARG:NH1	2.66	0.55
5:U:238:VAL:CG2	7:U:807:Y01:HAB3	2.34	0.55
5:U:172:LEU:HD21	14:U:804:CLR:H72	1.88	0.55
7:U:808:Y01:OAG	7:U:808:Y01:HAV2	2.06	0.55
7:G:1608:Y01:HAB3	7:G:1608:Y01:CAC	2.37	0.55
5:U:338:TYR:OH	5:U:398:GLN:OE1	2.25	0.55
12:K:702:P5S:H44A	12:K:702:P5S:H20	1.89	0.54
2:K:374:LEU:HD23	5:U:243:LEU:HD21	1.89	0.54
3:S:247:ILE:CD1	4:T:65:HIS:HB3	2.33	0.54
1:G:18:LEU:HB2	1:G:394:MET:HE1	1.90	0.54
2:K:261:ASN:HB2	2:K:262:PRO:HD2	1.89	0.54
4:T:529:ILE:HA	5:U:277:PHE:HE1	1.73	0.54
3:S:163:GLY:HA2	3:S:411:SER:HB3	1.88	0.54
2:K:315:GLU:OE1	3:S:401:GLN:NE2	2.33	0.54
7:U:802:Y01:HAN2	7:U:802:Y01:HAC3	1.89	0.54
14:S:903:CLR:H213	7:U:806:Y01:CBB	2.37	0.53
12:K:702:P5S:C49	14:U:804:CLR:H25	2.39	0.53
14:S:904:CLR:C25	14:S:904:CLR:H213	2.39	0.53
7:G:1607:Y01:CAJ	7:G:1607:Y01:CAP	2.86	0.53
3:S:8:ALA:O	3:S:12:GLU:OE1	2.27	0.53
2:K:317:ILE:O	3:S:387:GLU:HG2	2.09	0.53
3:S:31:GLY:CA	14:S:902:CLR:C12	2.87	0.53
5:U:202:PRO:HB3	5:U:315:PHE:CD2	2.41	0.52
14:S:904:CLR:H25	14:S:904:CLR:H211	1.92	0.52
5:U:67:PRO:HA	5:U:70:ILE:HD12	1.90	0.52
2:K:88:ASP:HB3	2:K:90:MET:HE2	1.89	0.52
1:G:39:LEU:HD23	1:G:44:LEU:HD13	1.91	0.52
2:K:213:GLU:HG3	2:K:214:ARG:HG2	1.91	0.52
3:S:239:LYS:HD3	4:T:273:PRO:HG3	1.91	0.52
5:U:176:LYS:HE3	14:U:804:CLR:C6	2.37	0.52
4:T:327:ASN:OD1	4:T:330:ARG:N	2.43	0.51
3:S:18:ARG:HH22	17:U:801:CDL:HA21	1.76	0.51
1:G:284:LEU:HD11	7:G:1602:Y01:HAR2	1.92	0.51
3:S:173:ILE:HG21	3:S:181:ILE:HD11	1.93	0.51
7:G:1608:Y01:HAE2	7:G:1608:Y01:CAO	2.39	0.51
5:U:170:PHE:CE1	5:U:186:LEU:HB2	2.45	0.51
2:K:313:THR:HG21	3:S:392:GLN:HE21	1.74	0.50
1:G:608:TYR:CE2	1:G:612:LEU:HD11	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:181:ILE:HG22	3:S:184:ARG:HH21	1.77	0.50
14:S:902:CLR:H221	14:S:902:CLR:H263	1.93	0.50
17:U:801:CDL:H372	7:U:808:Y01:HAN2	1.92	0.50
1:G:603:LEU:HD23	1:G:607:LEU:HD12	1.93	0.50
5:U:372:LEU:HD12	5:U:390:ILE:HG13	1.92	0.50
3:S:54:LEU:HD11	3:S:469:VAL:HG13	1.93	0.50
3:S:144:VAL:HG11	3:S:186:ILE:HD12	1.93	0.50
14:S:903:CLR:C21	7:U:806:Y01:CAC	2.89	0.50
4:T:91:GLN:HE22	4:T:211:PHE:HD1	1.59	0.50
4:T:51:ARG:HE	4:T:237:GLU:CD	2.20	0.50
1:G:516:THR:CG2	9:G:1604:BJR:C8	2.87	0.49
1:G:284:LEU:HD11	7:G:1602:Y01:CAD	2.42	0.49
1:G:435:GLN:O	1:G:439:LEU:HD23	2.12	0.49
3:S:198:ASP:OD1	3:S:199:VAL:N	2.45	0.49
4:T:304:TYR:HB2	4:T:317:ILE:HD11	1.92	0.49
1:G:10:ARG:HH22	5:U:353:ARG:HD2	1.77	0.49
2:K:87:ALA:HB1	2:K:173:GLN:NE2	2.27	0.49
5:U:194:LEU:CD2	5:U:258:TYR:CD1	2.92	0.49
1:G:47:ARG:NH2	1:G:367:ARG:CZ	2.76	0.49
3:S:35:TRP:CD2	14:S:902:CLR:H3	2.48	0.49
3:S:219:ARG:N	3:S:220:PRO:HD2	2.28	0.49
3:S:22:PHE:HD1	14:S:904:CLR:H212	1.76	0.49
12:K:702:P5S:H51	5:U:169:PHE:CE2	2.47	0.49
3:S:465:VAL:O	3:S:469:VAL:HG23	2.13	0.49
4:T:257:ASP:O	4:T:262:ARG:NH1	2.46	0.49
14:S:903:CLR:H241	7:U:806:Y01:HAJ1	1.94	0.48
1:G:600:PHE:CD1	10:G:1606:PEE:H29	2.48	0.48
3:S:119:LEU:CD1	3:S:131:LEU:CD1	2.67	0.48
14:S:903:CLR:H272	7:U:806:Y01:CAN	2.43	0.48
2:K:258:GLU:HA	2:K:258:GLU:OE1	2.13	0.48
1:G:350:LEU:HD23	2:K:95:ARG:NH2	2.29	0.48
1:G:600:PHE:HD1	10:G:1606:PEE:H29	1.77	0.48
14:S:904:CLR:H213	14:S:904:CLR:C24	2.44	0.48
7:G:1607:Y01:HAJ1	7:G:1607:Y01:CAP	2.40	0.48
1:G:50:MET:HE1	1:G:55:MET:HE3	1.94	0.48
2:K:386:TYR:CE1	12:K:702:P5S:H21A	2.48	0.48
17:U:801:CDL:H511	17:U:801:CDL:HB62	1.96	0.48
2:K:261:ASN:HB2	2:K:262:PRO:CD	2.44	0.48
5:U:411:ARG:HE	5:U:415:TYR:HE2	1.62	0.48
12:K:702:P5S:H44A	12:K:702:P5S:H20A	1.96	0.47
14:S:904:CLR:H12	17:U:801:CDL:H512	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:348:HIS:HA	2:K:95:ARG:NE	2.27	0.47
4:T:206:LYS:HG2	4:T:208:ASP:OD1	2.15	0.47
5:U:367:LEU:O	5:U:370:PRO:HD2	2.14	0.47
5:U:160:CYS:HA	5:U:163:ASN:HD22	1.78	0.47
1:G:512:CYS:HB3	9:G:1604:BJR:C10	2.43	0.47
2:K:69:TYR:CE2	2:K:73:LYS:HD2	2.50	0.47
3:S:28:ILE:HG13	3:S:29:VAL:N	2.29	0.47
5:U:176:LYS:NZ	14:U:804:CLR:C4	2.68	0.47
7:G:1609:Y01:HAC3	18:U:805:DKB:O11	2.15	0.47
3:S:31:GLY:CA	14:S:902:CLR:H121	2.35	0.47
5:U:274:PHE:CE2	5:U:294:GLN:NE2	2.83	0.47
3:S:69:PHE:CZ	3:S:179:PHE:HE1	2.33	0.47
4:T:268:LEU:O	4:T:331:ASN:HB2	2.15	0.47
1:G:124:VAL:HG21	1:G:190:LEU:HD13	1.96	0.47
5:U:110:GLN:HE21	5:U:110:GLN:HB3	1.54	0.47
3:S:63:VAL:CG2	3:S:104:PHE:CD1	2.98	0.46
5:U:353:ARG:O	5:U:354:ASN:OD1	2.32	0.46
3:S:402:PRO:HB3	3:S:421:TRP:HH2	1.80	0.46
14:S:903:CLR:H222	14:S:903:CLR:H162	1.58	0.46
4:T:182:CYS:HB3	4:T:184:GLU:OE2	2.16	0.46
3:S:35:TRP:CE2	14:S:902:CLR:H3	2.50	0.46
3:S:161:TYR:HB3	3:S:169:VAL:HB	1.98	0.46
4:T:257:ASP:HB2	4:T:336:LEU:O	2.16	0.46
1:G:297:GLN:HG2	1:G:517:ASN:ND2	2.30	0.46
3:S:22:PHE:HA	14:S:904:CLR:C18	2.46	0.46
14:S:903:CLR:H241	7:U:806:Y01:CAC	2.44	0.46
4:T:546:LEU:HD13	5:U:406:PHE:CD2	2.49	0.46
17:U:801:CDL:H391	17:U:801:CDL:H362	1.74	0.46
1:G:71:ARG:O	1:G:75:ARG:CD	2.64	0.46
2:K:74:ARG:NH2	2:K:257:LEU:O	2.48	0.46
14:S:904:CLR:C21	14:S:904:CLR:C24	2.94	0.46
1:G:226:GLU:HB2	1:G:320:ARG:HG2	1.98	0.46
2:K:207:GLN:NE2	2:K:228:VAL:O	2.34	0.46
2:K:246:MET:CE	2:K:251:PHE:HA	2.46	0.46
14:S:902:CLR:H241	5:U:295:ILE:HG22	1.98	0.46
4:T:197:SER:HA	4:T:202:SER:HB3	1.98	0.46
2:K:236:GLN:HG3	2:K:244:HIS:CE1	2.51	0.45
3:S:69:PHE:CD1	3:S:82:LEU:HD11	2.51	0.45
3:S:334:SER:HB3	3:S:335:PRO:HD3	1.98	0.45
3:S:520:ALA:HB1	4:T:526:TYR:OH	2.16	0.45
1:G:188:ASP:OD1	1:G:189:LEU:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1601:Y01:HAA2	7:G:1601:Y01:HAJ1	1.84	0.45
3:S:87:VAL:CG1	3:S:103:ARG:HD2	2.46	0.45
3:S:233:LEU:C	3:S:233:LEU:HD23	2.42	0.45
5:U:372:LEU:HD13	5:U:386:PHE:HB3	1.99	0.45
1:G:244:GLY:HA3	1:G:517:ASN:HD22	1.82	0.45
1:G:565:ARG:HG3	1:G:572:LEU:HD22	1.97	0.45
3:S:164:PRO:HB3	3:S:419:MET:HG2	1.99	0.45
10:G:1606:PEE:H48	10:G:1606:PEE:H7	1.53	0.45
3:S:62:MET:HE3	3:S:62:MET:HB3	1.85	0.45
3:S:151:SER:H	3:S:171:ARG:HH12	1.65	0.45
12:K:702:P5S:C48	14:U:804:CLR:H25	2.47	0.45
1:G:396:LEU:CD2	7:G:1609:Y01:HAQ2	2.45	0.44
7:U:806:Y01:HAO2	7:U:806:Y01:HAP1	1.35	0.44
4:T:452:LYS:HB2	4:T:455:GLU:HG3	1.99	0.44
4:T:410:LYS:HD2	4:T:411:PRO:HD2	1.97	0.44
1:G:331:ASP:OD2	1:G:333:VAL:HG23	2.18	0.44
1:G:469:LEU:HD23	10:G:1606:PEE:H45	2.00	0.44
1:G:556:THR:HG23	7:G:1601:Y01:HAB2	1.99	0.44
10:G:1606:PEE:H67	10:G:1606:PEE:H61	1.51	0.44
3:S:22:PHE:HA	14:S:904:CLR:H183	1.99	0.44
1:G:560:SER:HB3	10:G:1606:PEE:H66	1.98	0.44
4:T:91:GLN:HG2	4:T:216:HIS:HB3	1.99	0.44
5:U:398:GLN:O	5:U:402:ILE:HG12	2.18	0.44
5:U:254:ILE:CG2	7:U:802:Y01:CAI	2.95	0.44
1:G:350:LEU:HD13	2:K:55:PHE:HD1	1.82	0.44
4:T:33:GLU:CD	4:T:33:GLU:C	2.86	0.44
1:G:527:THR:CG2	1:G:528:MET:HG3	2.42	0.44
3:S:520:ALA:HB1	4:T:526:TYR:CZ	2.53	0.44
4:T:378:TYR:CE1	4:T:379:ARG:HG2	2.53	0.44
1:G:350:LEU:CD1	2:K:55:PHE:CB	2.93	0.43
14:S:902:CLR:H221	14:S:902:CLR:H162	1.66	0.43
1:G:116:ASP:C	1:G:116:ASP:OD1	2.60	0.43
2:K:87:ALA:HB1	2:K:173:GLN:HE22	1.83	0.43
5:U:63:PHE:CZ	5:U:65:GLU:HB2	2.52	0.43
1:G:371:ILE:HA	1:G:374:TYR:CZ	2.53	0.43
4:T:125:LYS:O	4:T:129:GLU:HG3	2.19	0.43
14:S:903:CLR:O1	14:S:903:CLR:H192	2.18	0.43
3:S:216:GLU:HA	3:S:219:ARG:HG3	2.01	0.43
1:G:258:PHE:HZ	1:G:345:LYS:HG3	1.83	0.43
3:S:89:GLU:OE2	3:S:101:LYS:HB2	2.18	0.43
4:T:80:TYR:O	4:T:82:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:120:ALA:O	5:U:123:VAL:HG22	2.18	0.43
2:K:205:THR:HG22	2:K:206:CYS:N	2.34	0.43
2:K:236:GLN:HG3	2:K:244:HIS:HE1	1.84	0.43
3:S:63:VAL:HG21	3:S:104:PHE:CE1	2.54	0.43
5:U:262:LEU:HD13	7:U:806:Y01:CAK	2.24	0.43
5:U:309:LYS:NZ	17:U:801:CDL:OA4	2.46	0.43
1:G:598:LEU:HD11	9:G:1604:BJR:O2	2.18	0.42
3:S:247:ILE:HD13	3:S:272:SER:OG	2.19	0.42
7:U:802:Y01:CAM	7:U:802:Y01:CAR	2.86	0.42
10:G:1606:PEE:H32	10:G:1606:PEE:H25	1.65	0.42
3:S:151:SER:HB2	3:S:171:ARG:HH12	1.83	0.42
1:G:491:PRO:HB2	1:G:492:ASP:H	1.64	0.42
5:U:67:PRO:HD2	5:U:191:TYR:OH	2.19	0.42
1:G:598:LEU:O	1:G:602:LEU:HG	2.19	0.42
4:T:386:LEU:HD11	4:T:427:LEU:HD11	2.02	0.42
5:U:302:ILE:HG23	17:U:801:CDL:H741	2.01	0.42
3:S:461:VAL:O	3:S:465:VAL:HG23	2.19	0.42
1:G:244:GLY:HA3	1:G:517:ASN:ND2	2.35	0.42
3:S:160:SER:HB2	3:S:408:CYS:SG	2.60	0.42
3:S:233:LEU:HD11	3:S:243:VAL:HG11	2.01	0.42
4:T:383:VAL:HG12	4:T:473:ALA:HB2	2.02	0.42
3:S:333:HIS:CE1	3:S:336:LEU:HD22	2.55	0.42
5:U:123:VAL:HG23	5:U:123:VAL:O	2.20	0.42
3:S:228:GLU:OE2	3:S:317:SER:OG	2.35	0.41
3:S:340:ASP:OD1	3:S:344:ALA:N	2.53	0.41
14:S:902:CLR:H273	5:U:296:ASN:CB	2.50	0.41
4:T:178:ARG:O	4:T:178:ARG:HG2	2.20	0.41
3:S:394:ARG:HH11	3:S:418:LEU:HD23	1.85	0.41
1:G:207:MET:HE2	1:G:207:MET:HB2	1.82	0.41
2:K:370:PHE:CE2	2:K:374:LEU:HD11	2.55	0.41
5:U:274:PHE:HE2	5:U:294:GLN:HE22	1.68	0.41
5:U:331:THR:HG22	5:U:333:GLY:H	1.85	0.41
3:S:75:PRO:HG3	3:S:174:MET:O	2.20	0.41
3:S:280:LEU:HG	3:S:303:VAL:HG13	2.01	0.41
5:U:68:LEU:HD13	5:U:191:TYR:CZ	2.55	0.41
1:G:127:THR:O	1:G:186:GLU:HB2	2.21	0.41
4:T:191:LYS:HE3	4:T:191:LYS:HB2	1.95	0.41
2:K:267:ASN:O	2:K:300:ILE:HD11	2.21	0.41
1:G:560:SER:OG	7:G:1601:Y01:HAA3	2.21	0.41
3:S:74:VAL:HG21	3:S:179:PHE:CZ	2.56	0.41
5:U:335:VAL:HA	5:U:338:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1608:Y01:CAB	7:G:1608:Y01:CAO	2.92	0.41
2:K:236:GLN:CD	2:K:236:GLN:O	2.64	0.41
3:S:149:GLU:HG3	3:S:172:GLY:O	2.21	0.41
3:S:181:ILE:HA	3:S:184:ARG:HE	1.85	0.41
14:S:902:CLR:C27	5:U:296:ASN:OD1	2.69	0.41
4:T:279:ARG:NH2	4:T:319:ASP:OD1	2.46	0.41
7:U:808:Y01:HAB3	7:U:808:Y01:HAC2	2.03	0.41
1:G:284:LEU:HD11	7:G:1602:Y01:HAD1	2.02	0.40
7:G:1607:Y01:HAC2	7:G:1607:Y01:HAJ2	1.84	0.40
12:K:702:P5S:H49A	14:U:804:CLR:C25	2.46	0.40
5:U:3:ALA:N	5:U:4:PRO:HD2	2.36	0.40
5:U:11:VAL:O	5:U:15:VAL:HG23	2.22	0.40
5:U:109:LYS:HB3	5:U:109:LYS:HE2	1.64	0.40
5:U:253:PHE:CE2	5:U:254:ILE:HG13	2.56	0.40
1:G:296:ARG:HG2	10:G:1606:PEE:H55	2.03	0.40
3:S:74:VAL:HG21	3:S:179:PHE:CE2	2.57	0.40
5:U:368:LEU:HD23	5:U:368:LEU:HA	1.75	0.40
5:U:406:PHE:CE2	5:U:410:LEU:HD11	2.57	0.40
3:S:451:LYS:HB2	3:S:451:LYS:HE2	1.83	0.40
5:U:20:PHE:CE1	5:U:81:GLU:HG2	2.57	0.40
14:S:904:CLR:H25	14:S:904:CLR:H213	2.02	0.40
2:K:69:TYR:CE2	2:K:117:VAL:HG23	2.56	0.40
17:U:801:CDL:H272	7:U:808:Y01:HAP2	2.04	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	G	577/886 (65%)	559 (97%)	18 (3%)	0	100	100
2	K	327/647 (50%)	314 (96%)	11 (3%)	2 (1%)	21	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S	530/816 (65%)	520 (98%)	10 (2%)	0	100	100
4	T	526/831 (63%)	519 (99%)	7 (1%)	0	100	100
5	U	417/712 (59%)	411 (99%)	6 (1%)	0	100	100
All	All	2377/3892 (61%)	2323 (98%)	52 (2%)	2 (0%)	49	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	278	SER
2	K	277	LYS

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	G	455/714 (64%)	446 (98%)	9 (2%)	48	73
2	K	290/563 (52%)	280 (97%)	10 (3%)	32	57
3	S	403/681 (59%)	392 (97%)	11 (3%)	39	65
4	T	466/728 (64%)	465 (100%)	1 (0%)	87	95
5	U	369/609 (61%)	363 (98%)	6 (2%)	55	78
All	All	1983/3295 (60%)	1946 (98%)	37 (2%)	49	74

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	9	ARG
1	G	62	GLU
1	G	63	GLN
1	G	76	ASP
1	G	207	MET
1	G	260	GLN
1	G	264	LEU
1	G	265	LEU

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Mol	Chain	Res	Type
1	G	513	ILE
2	K	54	ARG
2	K	122	ARG
2	K	127	THR
2	K	154	ARG
2	K	173	GLN
2	K	254	LEU
2	K	274	VAL
2	K	278	SER
2	K	283	THR
2	K	344	LYS
3	S	147	ILE
3	S	148	SER
3	S	149	GLU
3	S	151	SER
3	S	153	LEU
3	S	154	LEU
3	S	160	SER
3	S	179	PHE
3	S	272	SER
3	S	279	MET
3	S	280	LEU
4	T	272	CYS
5	U	109	LYS
5	U	110	GLN
5	U	111	LYS
5	U	112	LEU
5	U	114	LEU
5	U	371	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	63	GLN
1	G	248	ASN
1	G	297	GLN
1	G	449	GLN
1	G	593	HIS
2	K	44	ASN
2	K	61	HIS
2	K	81	HIS
2	K	156	ASN

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Mol	Chain	Res	Type
2	K	197	ASN
2	K	219	ASN
2	K	227	GLN
3	S	88	HIS
3	S	256	GLN
3	S	305	ASN
3	S	352	HIS
3	S	392	GLN
4	T	49	GLN
4	T	132	ASN
4	T	185	ASN
4	T	228	ASN
4	T	426	HIS
4	T	552	HIS
5	U	110	GLN
5	U	163	ASN
5	U	418	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides 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	$\# Z > 2$
6	NAG	A	1	1,6	14,14,15	0.37	0	17,19,21	0.53	0
6	NAG	A	2	6	14,14,15	0.52	0	17,19,21	0.58	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
6	NAG	A	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

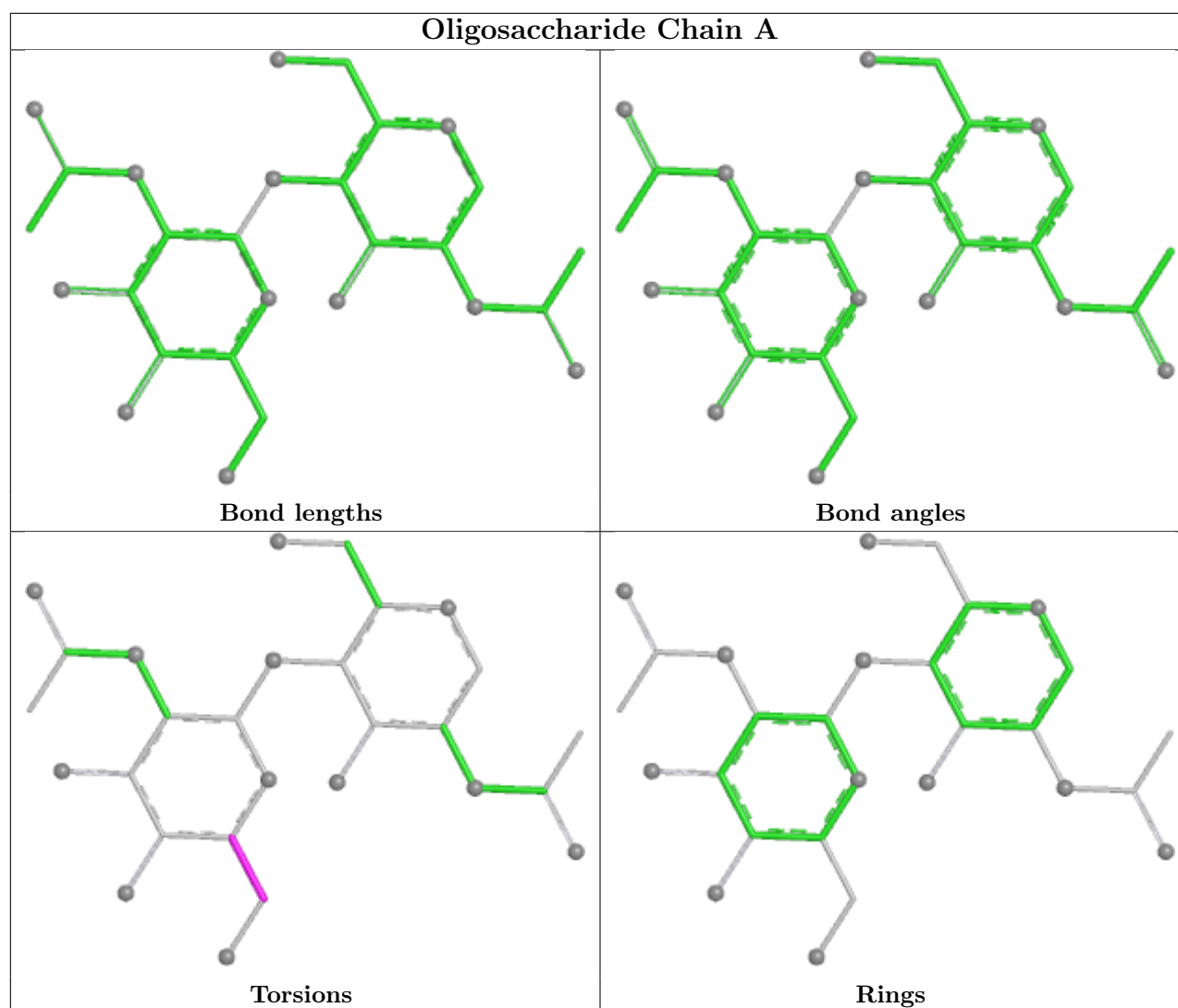
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2	NAG	O5-C5-C6-O6
6	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 1 is monoatomic - leaving 26 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	$\# Z > 2$
18	DKB	U	805	-	48,48,48	0.27	0	51,53,53	0.31	0
9	BJR	G	1604	-	43,43,51	0.29	0	49,51,59	0.32	0
14	CLR	S	904	-	31,31,31	0.29	0	48,48,48	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	Y01	U	807	-	38,38,38	0.45	0	57,57,57	0.44	0
7	Y01	U	802	-	38,38,38	0.45	0	57,57,57	0.44	0
7	Y01	G	1608	-	38,38,38	0.45	0	57,57,57	0.43	0
15	05E	T	901	16	18,18,19	2.12	6 (33%)	21,25,27	1.58	5 (23%)
14	CLR	S	903	-	31,31,31	0.29	0	48,48,48	0.33	0
10	PEE	G	1606	-	50,50,50	0.75	2 (4%)	53,55,55	0.50	0
17	CDL	U	801	-	85,85,99	0.28	0	91,97,111	0.33	0
8	AJP	G	1603	-	95,95,95	0.12	0	144,149,149	0.29	0
14	CLR	U	804	-	31,31,31	0.29	0	48,48,48	0.33	0
16	PA1	T	903	15,19	11,11,12	2.77	5 (45%)	13,15,17	2.13	3 (23%)
13	NAG	S	901	3	14,14,15	0.34	0	17,19,21	0.36	0
13	NAG	T	902	4	14,14,15	0.26	0	17,19,21	0.66	0
12	P5S	K	702	-	40,40,53	0.30	0	43,45,60	0.35	0
7	Y01	G	1602	-	38,38,38	0.45	0	57,57,57	0.43	0
7	Y01	G	1609	-	38,38,38	0.45	0	57,57,57	0.44	0
14	CLR	S	902	-	31,31,31	0.29	0	48,48,48	0.33	0
9	BJR	G	1605	-	51,51,51	0.32	0	57,59,59	0.41	0
7	Y01	U	806	-	38,38,38	0.45	0	57,57,57	0.43	0
7	Y01	G	1607	-	38,38,38	0.45	0	57,57,57	0.44	0
19	06O	U	809	16	74,74,74	1.55	11 (14%)	84,87,87	1.51	13 (15%)
7	Y01	U	808	-	38,38,38	0.45	0	57,57,57	0.44	0
14	CLR	U	803	-	31,31,31	0.29	0	48,48,48	0.33	0
7	Y01	G	1601	-	38,38,38	0.45	0	57,57,57	0.44	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
18	DKB	U	805	-	-	23/52/52/52	-
9	BJR	G	1604	-	-	20/47/47/55	-
14	CLR	S	904	-	-	6/10/68/68	0/4/4/4
7	Y01	U	807	-	-	15/19/77/77	0/4/4/4
7	Y01	U	802	-	-	13/19/77/77	0/4/4/4
7	Y01	G	1608	-	-	12/19/77/77	0/4/4/4
15	05E	T	901	16	-	10/12/29/32	0/1/1/1
14	CLR	S	903	-	-	6/10/68/68	0/4/4/4
10	PEE	G	1606	-	-	33/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CDL	U	801	-	-	37/96/96/110	-
8	AJP	G	1603	-	-	12/28/220/220	0/11/11/11
14	CLR	U	804	-	-	6/10/68/68	0/4/4/4
16	PA1	T	903	15,19	-	0/2/19/22	0/1/1/1
13	NAG	S	901	3	-	1/6/23/26	0/1/1/1
13	NAG	T	902	4	-	3/6/23/26	0/1/1/1
12	P5S	K	702	-	-	31/44/44/59	-
7	Y01	G	1602	-	-	10/19/77/77	0/4/4/4
7	Y01	G	1609	-	-	6/19/77/77	0/4/4/4
14	CLR	S	902	-	-	7/10/68/68	0/4/4/4
9	BJR	G	1605	-	-	31/55/55/55	-
7	Y01	U	806	-	-	12/19/77/77	0/4/4/4
7	Y01	G	1607	-	-	13/19/77/77	0/4/4/4
19	06O	U	809	16	-	46/71/95/95	0/1/1/1
7	Y01	U	808	-	-	14/19/77/77	0/4/4/4
14	CLR	U	803	-	-	7/10/68/68	0/4/4/4
7	Y01	G	1601	-	-	14/19/77/77	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	U	809	06O	C41-C42	6.49	1.55	1.33
16	T	903	PA1	O5-C5	5.98	1.55	1.43
15	T	901	05E	O97-C94	5.67	1.54	1.43
19	U	809	06O	O06-C07	3.62	1.44	1.34
16	T	903	PA1	C1-C2	-3.55	1.47	1.52
10	G	1606	PEE	C39-C38	3.46	1.51	1.31
19	U	809	06O	C41-C40	3.46	1.55	1.44
10	G	1606	PEE	C18-C19	3.45	1.51	1.31
15	T	901	05E	C90-C81	-3.35	1.45	1.53
19	U	809	06O	P26-O27	3.28	1.72	1.59
15	T	901	05E	P83-O82	3.17	1.68	1.59
16	T	903	PA1	C3-C2	-3.15	1.47	1.53
19	U	809	06O	O30-C31	3.09	1.43	1.34
16	T	903	PA1	C6-C5	-3.08	1.41	1.51
19	U	809	06O	O51-C52	2.93	1.41	1.33
15	T	901	05E	C95-C94	-2.89	1.42	1.51
19	U	809	06O	O30-C29	-2.67	1.40	1.46
19	U	809	06O	P26-O25	2.59	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	U	809	06O	O51-C50	-2.51	1.39	1.45
19	U	809	06O	C08-C07	2.40	1.57	1.50
16	T	903	PA1	O5-C1	2.38	1.47	1.43
15	T	901	05E	O91-C90	2.21	1.48	1.43
19	U	809	06O	C32-C31	2.11	1.56	1.50
15	T	901	05E	C92-C90	-2.03	1.47	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	903	PA1	C1-O5-C5	5.73	119.87	112.19
19	U	809	06O	O30-C31-C32	5.02	122.34	111.48
19	U	809	06O	C05-O06-C07	-4.90	109.61	117.59
19	U	809	06O	O06-C07-C08	4.14	120.44	111.48
15	T	901	05E	O82-C81-C80	4.13	116.39	108.58
19	U	809	06O	C03-C05-C24	3.98	120.68	111.72
19	U	809	06O	CA2-C71-C24	-3.77	101.12	109.68
19	U	809	06O	CA2-C02-C03	-3.61	104.50	110.83
19	U	809	06O	O51-C52-C53	3.23	121.67	111.83
16	T	903	PA1	C3-C4-C5	2.82	115.34	110.23
15	T	901	05E	O97-C80-C81	2.77	115.12	109.51
15	T	901	05E	C90-C92-C94	2.61	114.96	110.23
19	U	809	06O	O06-C05-C24	2.42	113.06	108.25
19	U	809	06O	C02-C03-C05	2.40	115.12	109.68
19	U	809	06O	O30-C31-O49	-2.39	118.12	123.70
19	U	809	06O	C71-CA2-C02	-2.26	106.86	110.83
15	T	901	05E	C92-C90-C81	2.26	114.32	110.23
19	U	809	06O	O25-C24-C71	2.23	113.44	108.73
19	U	809	06O	C43-C42-C41	-2.15	115.09	125.66
16	T	903	PA1	O3-C3-C2	-2.12	105.94	109.90
15	T	901	05E	C95-C94-C92	-2.01	108.08	113.02

There are no chirality outliers.

All (388) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	1601	Y01	CAO-CBB-CBE-CAP
7	G	1601	Y01	CAM-CAY-OAW-CBC
7	G	1607	Y01	CAM-CAY-OAW-CBC
7	G	1608	Y01	CAM-CAY-OAW-CBC
7	G	1609	Y01	OAG-CAY-OAW-CBC
7	G	1609	Y01	CAM-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
7	U	802	Y01	OAG-CAY-OAW-CBC
7	U	806	Y01	CAC-CBB-CBE-CAP
7	U	806	Y01	CAC-CBB-CBE-CBI
7	U	807	Y01	OAG-CAY-OAW-CBC
7	U	807	Y01	CAM-CAY-OAW-CBC
8	G	1603	AJP	C46-C45-O44-C37
9	G	1604	BJR	C4-C3-O4-P1
9	G	1604	BJR	C2-O1-P1-O2
9	G	1604	BJR	N1-C1-C2-O1
9	G	1605	BJR	C3-O4-P1-O1
9	G	1605	BJR	C3-O4-P1-O2
9	G	1605	BJR	C3-O4-P1-O3
9	G	1605	BJR	N1-C1-C2-O1
10	G	1606	PEE	C1-O3P-P-O2P
10	G	1606	PEE	C1-O3P-P-O1P
10	G	1606	PEE	C1-O3P-P-O4P
10	G	1606	PEE	C4-O4P-P-O3P
10	G	1606	PEE	C4-O4P-P-O2P
10	G	1606	PEE	C4-O4P-P-O1P
10	G	1606	PEE	C31-C30-O3-C3
12	K	702	P5S	N-CA-CB-OG
12	K	702	P5S	CB-OG-P12-O13
12	K	702	P5S	C3-O16-P12-OG
12	K	702	P5S	C3-O16-P12-O13
12	K	702	P5S	C39-C38-O37-C2
13	T	902	NAG	C3-C2-N2-C7
13	T	902	NAG	C8-C7-N2-C2
13	T	902	NAG	O7-C7-N2-C2
15	T	901	05E	C80-C81-O82-P83
15	T	901	05E	O84-C85-C86-N87
15	T	901	05E	C81-O82-P83-O84
15	T	901	05E	C85-O84-P83-O82
15	T	901	05E	C85-O84-P83-O88
15	T	901	05E	C85-O84-P83-O89
17	U	801	CDL	CA3-OA5-PA1-OA2
17	U	801	CDL	CA3-OA5-PA1-OA3
17	U	801	CDL	CA3-OA5-PA1-OA4
17	U	801	CDL	C11-CA5-OA6-CA4
17	U	801	CDL	CB2-OB2-PB2-OB5
17	U	801	CDL	OB7-CB5-OB6-CB4
17	U	801	CDL	C51-CB5-OB6-CB4
18	U	805	DKB	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
18	U	805	DKB	C4-O4P-P-O1P
18	U	805	DKB	C4-O4P-P-O2P
18	U	805	DKB	O4P-C4-C5-N6
19	U	809	06O	C32-C31-O30-C29
19	U	809	06O	C24-O25-P26-O27
19	U	809	06O	C24-O25-P26-O69
19	U	809	06O	C28-O27-P26-O25
19	U	809	06O	C28-O27-P26-O69
19	U	809	06O	C28-O27-P26-O70
8	G	1603	AJP	O50-C45-O44-C37
10	G	1606	PEE	O5-C30-O3-C3
14	S	902	CLR	C22-C23-C24-C25
7	G	1607	Y01	CAV-CBC-OAW-CAY
7	U	802	Y01	CAV-CBC-OAW-CAY
7	U	808	Y01	CAV-CBC-OAW-CAY
9	G	1605	BJR	O9-C24-O8-C5
7	G	1601	Y01	CAC-CBB-CBE-CBI
7	U	807	Y01	CAC-CBB-CBE-CBI
7	U	806	Y01	CAO-CBB-CBE-CAP
7	G	1601	Y01	CAO-CBB-CBE-CBI
7	U	806	Y01	CAO-CBB-CBE-CBI
7	G	1608	Y01	CAO-CAJ-CAN-CBA
7	G	1601	Y01	OAG-CAY-OAW-CBC
7	G	1607	Y01	OAG-CAY-OAW-CBC
7	G	1608	Y01	OAG-CAY-OAW-CBC
12	K	702	P5S	O47-C38-O37-C2
17	U	801	CDL	OA7-CA5-OA6-CA4
19	U	809	06O	O49-C31-O30-C29
7	U	802	Y01	CAM-CAY-OAW-CBC
7	G	1602	Y01	CAJ-CAO-CBB-CAC
7	G	1601	Y01	CAC-CBB-CBE-CAP
7	U	807	Y01	CAC-CBB-CBE-CAP
14	S	903	CLR	C16-C17-C20-C21
14	S	903	CLR	C13-C17-C20-C21
7	U	807	Y01	CAO-CBB-CBE-CBI
14	S	903	CLR	C13-C17-C20-C22
12	K	702	P5S	C2-C1-O19-C17
9	G	1605	BJR	C25-C24-O8-C5
7	U	806	Y01	CAJ-CAO-CBB-CAC
14	S	904	CLR	C21-C20-C22-C23
15	T	901	05E	O97-C94-C95-O96
7	U	807	Y01	CAJ-CAO-CBB-CBE

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Mol	Chain	Res	Type	Atoms
19	U	809	06O	C62-C63-C64-C65
14	U	803	CLR	C13-C17-C20-C21
7	G	1608	Y01	CAJ-CAO-CBB-CBE
15	T	901	05E	C92-C94-C95-O96
19	U	809	06O	C39-C40-C41-C42
18	U	805	DKB	C12-C11-O3-C3
18	U	805	DKB	C41-C42-C43-C44
19	U	809	06O	C43-C44-C45-C46
7	U	802	Y01	CAO-CBB-CBE-CBI
7	G	1609	Y01	CAJ-CAO-CBB-CBE
18	U	805	DKB	C35-C36-C37-C38
18	U	805	DKB	C33-C34-C35-C36
7	G	1609	Y01	CAJ-CAO-CBB-CAC
7	U	807	Y01	CAJ-CAO-CBB-CAC
18	U	805	DKB	O11-C11-O3-C3
19	U	809	06O	C13-C14-C15-C16
19	U	809	06O	C60-C61-C62-C63
9	G	1605	BJR	C34-C35-C36-C37
10	G	1606	PEE	C33-C34-C35-C36
14	S	902	CLR	C13-C17-C20-C22
14	S	902	CLR	C17-C20-C22-C23
7	G	1607	Y01	CAX-CAL-CAM-CAY
9	G	1604	BJR	C12-C13-C14-C15
7	G	1607	Y01	CAC-CBB-CBE-CAP
18	U	805	DKB	C31-C32-C33-C34
19	U	809	06O	C52-C53-C54-C55
19	U	809	06O	C53-C54-C55-C56
7	U	807	Y01	CAO-CBB-CBE-CAP
14	S	903	CLR	C16-C17-C20-C22
14	U	804	CLR	C17-C20-C22-C23
7	G	1602	Y01	CAM-CAY-OAW-CBC
19	U	809	06O	C08-C09-C10-C11
7	G	1602	Y01	CAN-CAJ-CAO-CBB
7	G	1607	Y01	CAO-CAJ-CAN-CBA
7	G	1607	Y01	CAO-CBB-CBE-CBI
7	G	1602	Y01	CAJ-CAO-CBB-CBE
7	U	806	Y01	CAJ-CAO-CBB-CBE
7	G	1601	Y01	CAX-CAL-CAM-CAY
7	G	1609	Y01	CAX-CAL-CAM-CAY
7	U	802	Y01	CAX-CAL-CAM-CAY
7	U	807	Y01	CAX-CAL-CAM-CAY
18	U	805	DKB	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	U	809	06O	C32-C33-C34-C35
7	G	1607	Y01	CAC-CBB-CBE-CBI
7	U	802	Y01	CAC-CBB-CBE-CBI
14	S	902	CLR	C13-C17-C20-C21
9	G	1604	BJR	C24-C25-C26-C27
7	U	808	Y01	CAN-CAJ-CAO-CBB
19	U	809	06O	C07-C08-C09-C10
7	G	1601	Y01	CAO-CAJ-CAN-CBA
14	S	904	CLR	C22-C23-C24-C25
7	G	1608	Y01	CAC-CBB-CBE-CAP
7	G	1602	Y01	CAX-CAL-CAM-CAY
9	G	1604	BJR	C6-C7-C8-C9
14	S	904	CLR	C17-C20-C22-C23
7	G	1602	Y01	OAG-CAY-OAW-CBC
9	G	1605	BJR	C12-C13-C14-C15
14	S	903	CLR	C22-C23-C24-C25
14	S	903	CLR	C20-C22-C23-C24
7	G	1608	Y01	CAJ-CAO-CBB-CAC
14	U	803	CLR	C17-C20-C22-C23
7	U	802	Y01	CAC-CBB-CBE-CAP
7	G	1607	Y01	CAO-CBB-CBE-CAP
14	S	902	CLR	C16-C17-C20-C21
10	G	1606	PEE	C22-C23-C24-C25
17	U	801	CDL	C36-C37-C38-C39
7	U	808	Y01	CAC-CBB-CBE-CBI
17	U	801	CDL	CB7-C71-C72-C73
14	U	803	CLR	C16-C17-C20-C22
17	U	801	CDL	C41-C42-C43-C44
18	U	805	DKB	C44-C45-C46-C47
9	G	1604	BJR	C11-C10-C9-C8
12	K	702	P5S	C42-C43-C44-C45
17	U	801	CDL	C42-C43-C44-C45
18	U	805	DKB	C37-C38-C39-C40
12	K	702	P5S	C24-C25-C26-C27
19	U	809	06O	C10-C11-C12-C13
19	U	809	06O	C56-C57-C58-C59
9	G	1605	BJR	C9-C10-C11-C12
18	U	805	DKB	C20-C21-C22-C23
7	U	807	Y01	CAJ-CAN-CBA-CAA
7	G	1608	Y01	CAO-CBB-CBE-CBI
19	U	809	06O	C08-C07-O06-C05
8	G	1603	AJP	C68-C69-C71-O72

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Mol	Chain	Res	Type	Atoms
8	G	1603	AJP	O31-C26-O25-C23
9	G	1605	BJR	C7-C8-C9-C10
10	G	1606	PEE	C21-C22-C23-C24
10	G	1606	PEE	C32-C33-C34-C35
10	G	1606	PEE	C40-C41-C42-C43
19	U	809	06O	C54-C55-C56-C57
17	U	801	CDL	CB5-C51-C52-C53
7	G	1601	Y01	CAJ-CAN-CBA-CAB
19	U	809	06O	C11-C12-C13-C14
9	G	1605	BJR	C29-C30-C31-C32
19	U	809	06O	C35-C36-C37-C38
14	U	803	CLR	C21-C20-C22-C23
17	U	801	CDL	C11-C12-C13-C14
17	U	801	CDL	C77-C78-C79-C80
7	U	802	Y01	CAO-CBB-CBE-CAP
14	S	902	CLR	C16-C17-C20-C22
18	U	805	DKB	C40-C41-C42-C43
18	U	805	DKB	C14-C15-C16-C17
10	G	1606	PEE	C11-C12-C13-C14
10	G	1606	PEE	C12-C13-C14-C15
7	G	1608	Y01	CAC-CBB-CBE-CBI
9	G	1605	BJR	C19-C20-C21-C22
17	U	801	CDL	C38-C39-C40-C41
9	G	1604	BJR	C10-C11-C12-C13
12	K	702	P5S	C23-C24-C25-C26
12	K	702	P5S	C44-C45-C46-C48
17	U	801	CDL	C14-C15-C16-C17
12	K	702	P5S	C43-C44-C45-C46
9	G	1605	BJR	C7-C6-O6-C4
7	U	807	Y01	CAN-CAJ-CAO-CBB
14	S	902	CLR	C21-C20-C22-C23
9	G	1605	BJR	O5-C6-O6-C4
19	U	809	06O	O23-C07-O06-C05
9	G	1604	BJR	O4-C3-C4-O6
7	U	807	Y01	CAJ-CAN-CBA-CAB
9	G	1604	BJR	C16-C17-C18-C19
9	G	1605	BJR	C24-C25-C26-C27
9	G	1605	BJR	C18-C19-C20-C21
9	G	1604	BJR	C18-C19-C20-C21
17	U	801	CDL	C78-C79-C80-C81
10	G	1606	PEE	C13-C14-C15-C16
17	U	801	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
9	G	1605	BJR	C30-C31-C32-C33
7	G	1602	Y01	CAO-CAJ-CAN-CBA
12	K	702	P5S	C20-C21-C22-C23
7	U	808	Y01	CAR-CBC-OAW-CAY
7	U	808	Y01	CAO-CBB-CBE-CAP
17	U	801	CDL	C33-C34-C35-C36
10	G	1606	PEE	C19-C20-C21-C22
19	U	809	06O	C42-C43-C44-C45
9	G	1605	BJR	O4-C3-C4-C5
9	G	1605	BJR	C32-C33-C34-C35
19	U	809	06O	C57-C58-C59-C60
12	K	702	P5S	O19-C1-C2-C3
8	G	1603	AJP	O31-C30-C32-O33
9	G	1605	BJR	C27-C28-C29-C30
10	G	1606	PEE	C44-C45-C46-C47
17	U	801	CDL	C82-C83-C84-C85
9	G	1604	BJR	C13-C14-C15-C16
12	K	702	P5S	C40-C41-C42-C43
18	U	805	DKB	C43-C44-C45-C46
12	K	702	P5S	C25-C26-C27-C28
14	U	803	CLR	C16-C17-C20-C21
10	G	1606	PEE	C15-C16-C17-C18
10	G	1606	PEE	C17-C18-C19-C20
10	G	1606	PEE	C37-C38-C39-C40
19	U	809	06O	C59-C60-C61-C62
10	G	1606	PEE	O3P-C1-C2-O2
12	K	702	P5S	C27-C28-C29-C30
19	U	809	06O	C12-C13-C14-C15
17	U	801	CDL	C79-C80-C81-C82
12	K	702	P5S	C49-C50-C51-C52
18	U	805	DKB	C23-C24-C25-C26
17	U	801	CDL	C31-C32-C33-C34
19	U	809	06O	C64-C65-C66-C67
7	G	1602	Y01	CAL-CAM-CAY-OAW
7	G	1607	Y01	CAJ-CAO-CBB-CBE
7	U	806	Y01	CAN-CAJ-CAO-CBB
12	K	702	P5S	C2-C3-O16-P12
9	G	1605	BJR	C11-C10-C9-C8
12	K	702	P5S	C39-C40-C41-C42
10	G	1606	PEE	C30-C31-C32-C33
9	G	1604	BJR	C20-C21-C22-C23
7	U	806	Y01	CAO-CAJ-CAN-CBA

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Mol	Chain	Res	Type	Atoms
7	U	808	Y01	CAX-CAL-CAM-CAY
12	K	702	P5S	C48-C49-C50-C51
8	G	1603	AJP	O70-C69-C71-O72
9	G	1604	BJR	C9-C10-C11-C12
17	U	801	CDL	CB3-CB4-CB6-OB8
7	G	1608	Y01	CAN-CAJ-CAO-CBB
7	G	1601	Y01	CAN-CAJ-CAO-CBB
17	U	801	CDL	C81-C82-C83-C84
9	G	1605	BJR	O4-C3-C4-O6
18	U	805	DKB	C39-C40-C41-C42
7	G	1607	Y01	CAN-CAJ-CAO-CBB
12	K	702	P5S	C38-C39-C40-C41
10	G	1606	PEE	C42-C43-C44-C45
7	G	1601	Y01	CAJ-CAN-CBA-CAA
9	G	1604	BJR	C14-C15-C16-C17
12	K	702	P5S	C46-C48-C49-C50
19	U	809	06O	C15-C16-C17-C18
17	U	801	CDL	O1-C1-CA2-OA2
14	S	904	CLR	C23-C24-C25-C26
7	U	808	Y01	CAJ-CAO-CBB-CBE
10	G	1606	PEE	C41-C42-C43-C44
19	U	809	06O	C53-C52-O51-C50
19	U	809	06O	C33-C34-C35-C36
9	G	1604	BJR	C5-C4-O6-C6
19	U	809	06O	C36-C37-C38-C39
14	U	804	CLR	C13-C17-C20-C22
19	U	809	06O	C34-C35-C36-C37
12	K	702	P5S	CA-CB-OG-P12
18	U	805	DKB	C16-C17-C18-C19
9	G	1605	BJR	O6-C4-C5-O8
7	U	802	Y01	CAJ-CAN-CBA-CAB
17	U	801	CDL	C34-C35-C36-C37
17	U	801	CDL	C12-C13-C14-C15
19	U	809	06O	O68-C52-O51-C50
10	G	1606	PEE	C23-C24-C25-C26
14	U	804	CLR	C13-C17-C20-C21
15	T	901	05E	C81-O82-P83-O88
15	T	901	05E	C81-O82-P83-O89
10	G	1606	PEE	C35-C36-C37-C38
7	U	808	Y01	CAC-CBB-CBE-CAP
19	U	809	06O	C19-C20-C21-C22
9	G	1605	BJR	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
19	U	809	06O	C31-C32-C33-C34
19	U	809	06O	C63-C64-C65-C66
9	G	1604	BJR	O4-C3-C4-C5
14	U	804	CLR	C16-C17-C20-C22
17	U	801	CDL	OB6-CB4-CB6-OB8
12	K	702	P5S	CB-OG-P12-O15
12	K	702	P5S	CB-OG-P12-O16
12	K	702	P5S	C3-O16-P12-O15
17	U	801	CDL	CB2-OB2-PB2-OB3
7	G	1609	Y01	CAN-CAJ-CAO-CBB
9	G	1605	BJR	C17-C18-C19-C20
14	S	904	CLR	C23-C24-C25-C27
12	K	702	P5S	C45-C46-C48-C49
10	G	1606	PEE	O3P-C1-C2-C3
17	U	801	CDL	C16-C17-C18-C19
7	U	808	Y01	CAJ-CAO-CBB-CAC
14	U	804	CLR	C21-C20-C22-C23
12	K	702	P5S	O19-C1-C2-O37
19	U	809	06O	O30-C29-C50-O51
14	U	804	CLR	C16-C17-C20-C21
14	U	803	CLR	C13-C17-C20-C22
7	U	807	Y01	CAO-CAJ-CAN-CBA
7	U	802	Y01	CAN-CAJ-CAO-CBB
9	G	1605	BJR	O6-C6-C7-C8
19	U	809	06O	C28-C29-C50-O51
9	G	1605	BJR	C35-C36-C37-C38
9	G	1604	BJR	C7-C8-C9-C10
10	G	1606	PEE	C31-C32-C33-C34
9	G	1605	BJR	C15-C16-C17-C18
7	U	808	Y01	CAJ-CAN-CBA-CAA
18	U	805	DKB	C13-C14-C15-C16
19	U	809	06O	C55-C56-C57-C58
10	G	1606	PEE	O4-C10-O2-C2
9	G	1605	BJR	C11-C12-C13-C14
17	U	801	CDL	C18-C19-C20-C21
10	G	1606	PEE	C11-C10-O2-C2
7	G	1601	Y01	CAJ-CAO-CBB-CAC
13	S	901	NAG	C4-C5-C6-O6
7	G	1602	Y01	CAL-CAM-CAY-OAG
7	U	807	Y01	CAM-CAL-CAX-OAF
7	G	1601	Y01	CAM-CAL-CAX-OAF
7	U	806	Y01	CAM-CAL-CAX-OAF

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Mol	Chain	Res	Type	Atoms
7	U	806	Y01	CAM-CAL-CAX-OAH
7	G	1601	Y01	CAM-CAL-CAX-OAH
9	G	1605	BJR	C36-C37-C38-C39
7	U	808	Y01	CAJ-CAN-CBA-CAB
17	U	801	CDL	C35-C36-C37-C38
9	G	1605	BJR	C3-C4-C5-O8
7	U	807	Y01	CAM-CAL-CAX-OAH
8	G	1603	AJP	C36-C37-O44-C45
7	U	802	Y01	CAM-CAL-CAX-OAF
17	U	801	CDL	C37-C38-C39-C40
19	U	809	06O	O27-C28-C29-C50
7	U	808	Y01	CAM-CAL-CAX-OAH
12	K	702	P5S	C41-C42-C43-C44
8	G	1603	AJP	O60-C55-O54-C36
14	U	803	CLR	C23-C24-C25-C27
7	G	1607	Y01	CAM-CAL-CAX-OAH
17	U	801	CDL	O1-C1-CB2-OB2
17	U	801	CDL	OA9-CA7-OA8-CA6
7	U	808	Y01	CAM-CAL-CAX-OAF
17	U	801	CDL	C31-CA7-OA8-CA6
19	U	809	06O	C37-C38-C39-C40
7	G	1607	Y01	CAM-CAL-CAX-OAF
18	U	805	DKB	C32-C33-C34-C35
8	G	1603	AJP	C58-C57-O64-C65
10	G	1606	PEE	C16-C17-C18-C19
8	G	1603	AJP	C56-C55-O54-C36
19	U	809	06O	C24-O25-P26-O70
8	G	1603	AJP	C38-C37-O44-C45
18	U	805	DKB	C12-C13-C14-C15
7	G	1608	Y01	CAM-CAL-CAX-OAH
7	U	802	Y01	CAM-CAL-CAX-OAH
9	G	1604	BJR	O6-C6-C7-C8
7	U	808	Y01	CAO-CAJ-CAN-CBA
7	U	806	Y01	CAL-CAM-CAY-OAW
8	G	1603	AJP	C27-C26-O25-C23
7	G	1602	Y01	CAM-CAL-CAX-OAH
7	G	1608	Y01	CAM-CAL-CAX-OAF
19	U	809	06O	C16-C17-C18-C19
14	S	904	CLR	C20-C22-C23-C24
7	U	802	Y01	CAJ-CAN-CBA-CAA
9	G	1604	BJR	O5-C6-C7-C8
10	G	1606	PEE	C20-C21-C22-C23

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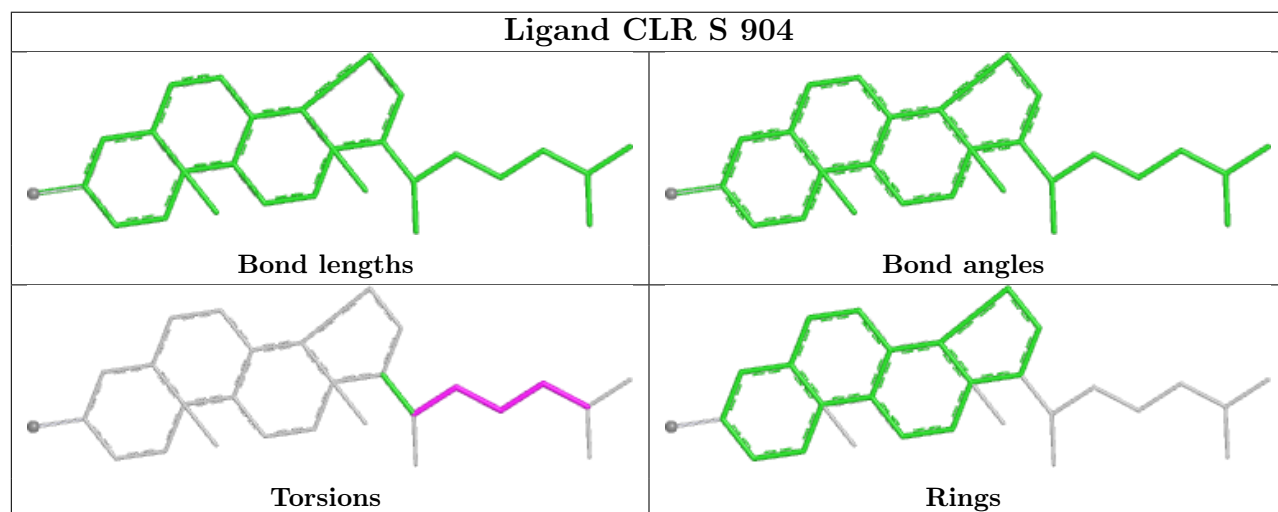
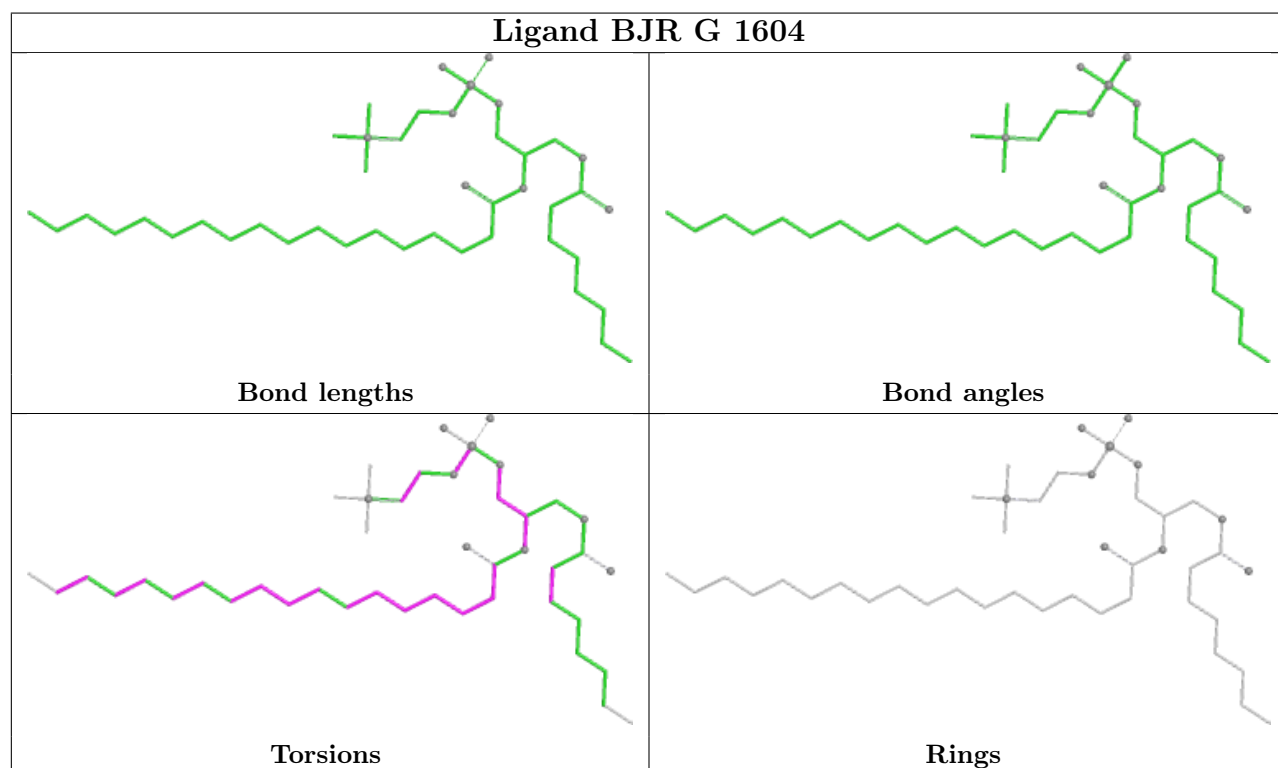
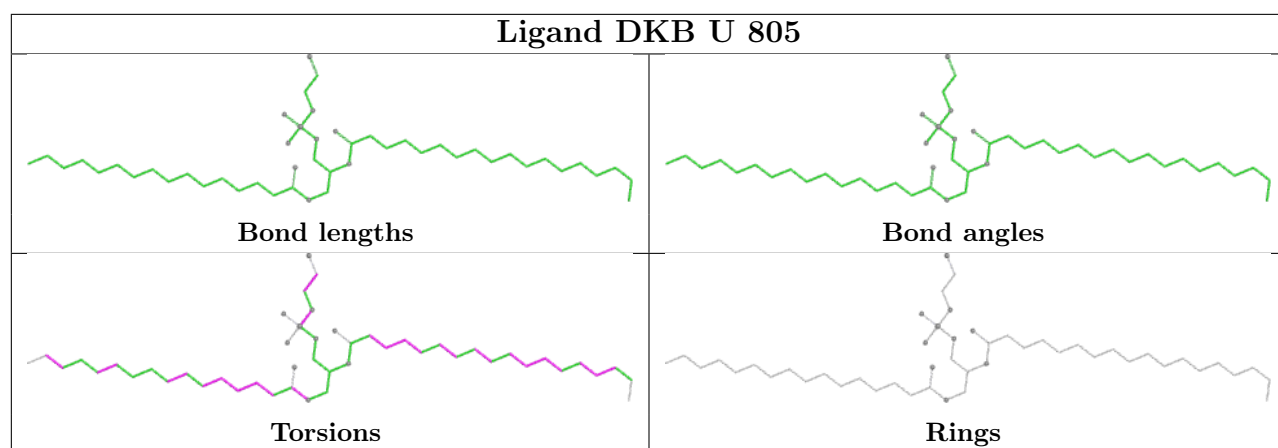
Mol	Chain	Res	Type	Atoms
7	U	806	Y01	CAL-CAM-CAY-OAG
12	K	702	P5S	C17-C20-C21-C22
19	U	809	06O	O06-C07-C08-C09
7	G	1608	Y01	CAL-CAM-CAY-OAW

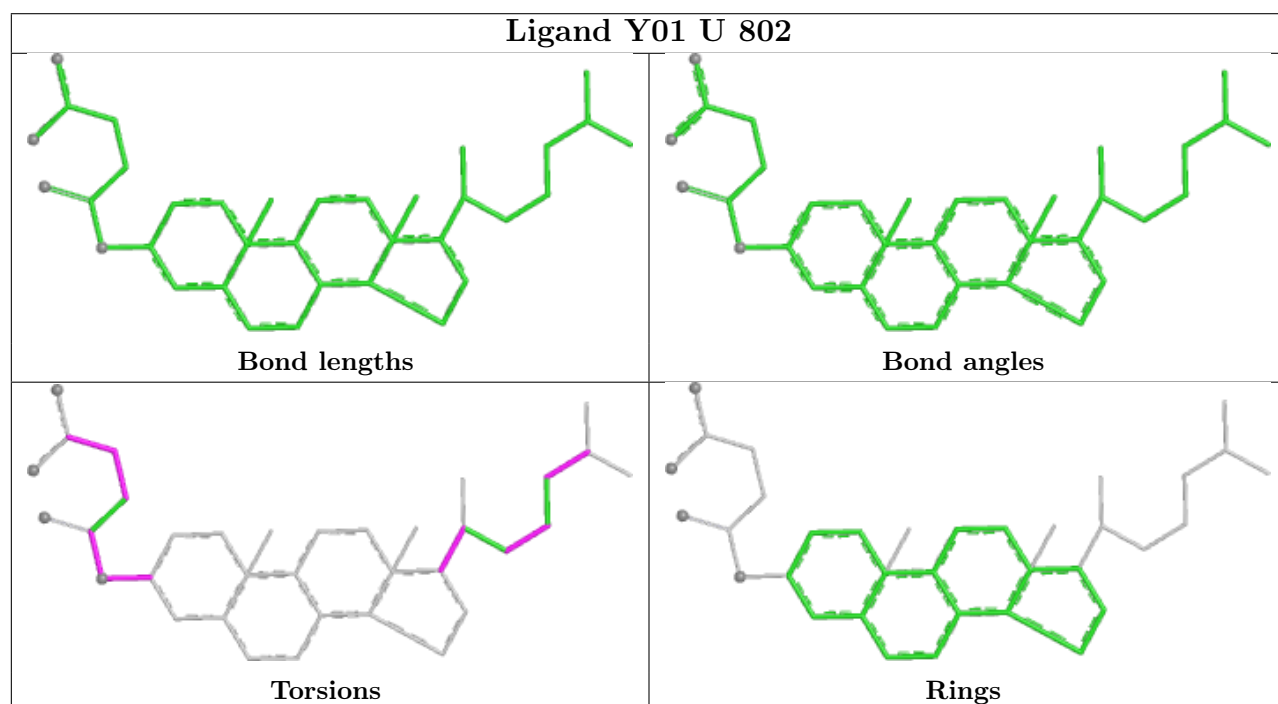
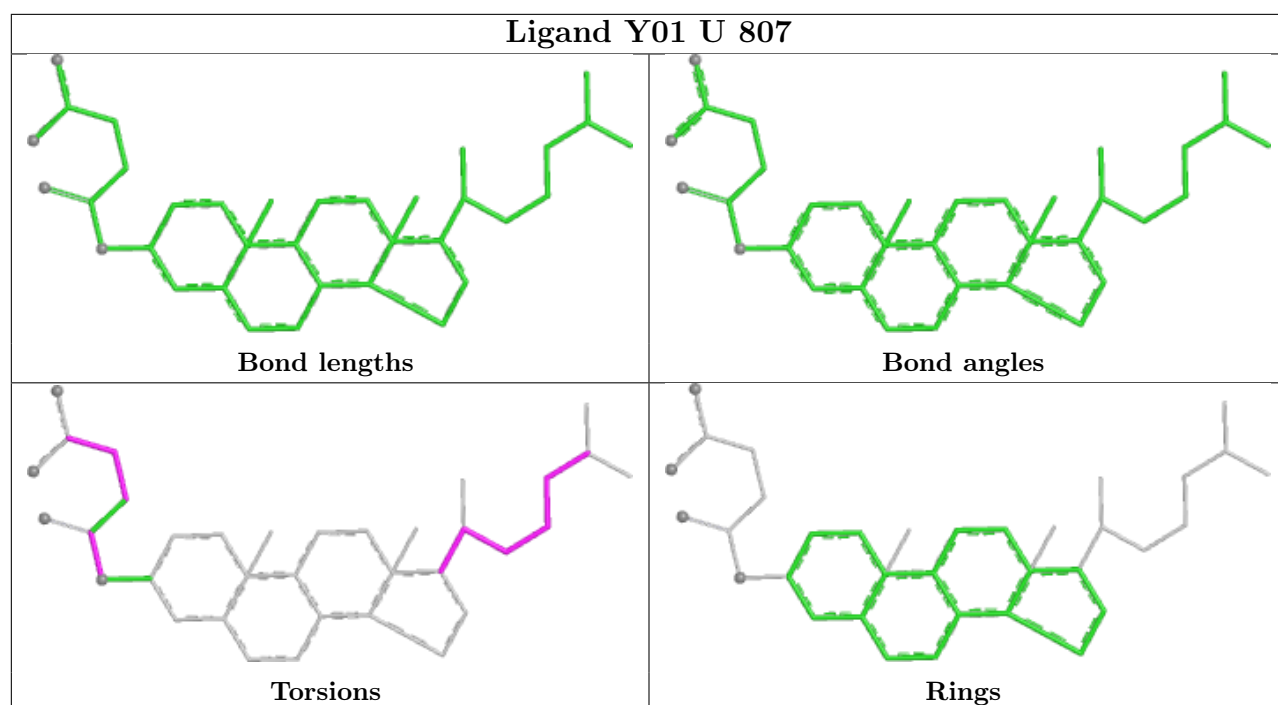
There are no ring outliers.

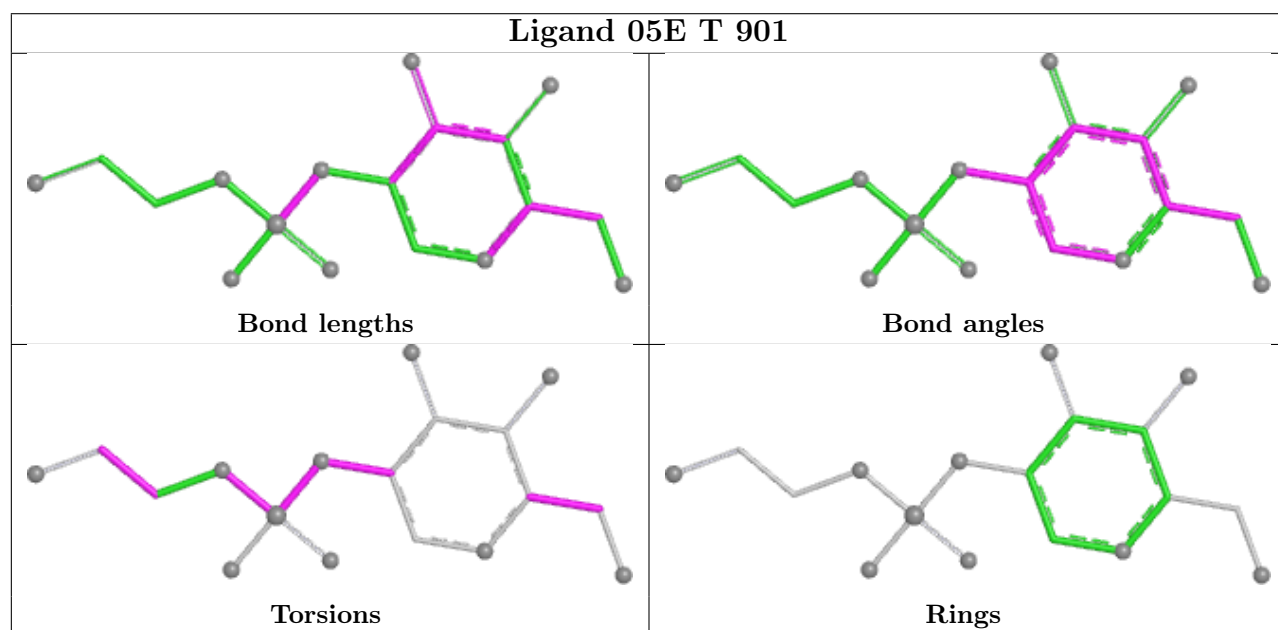
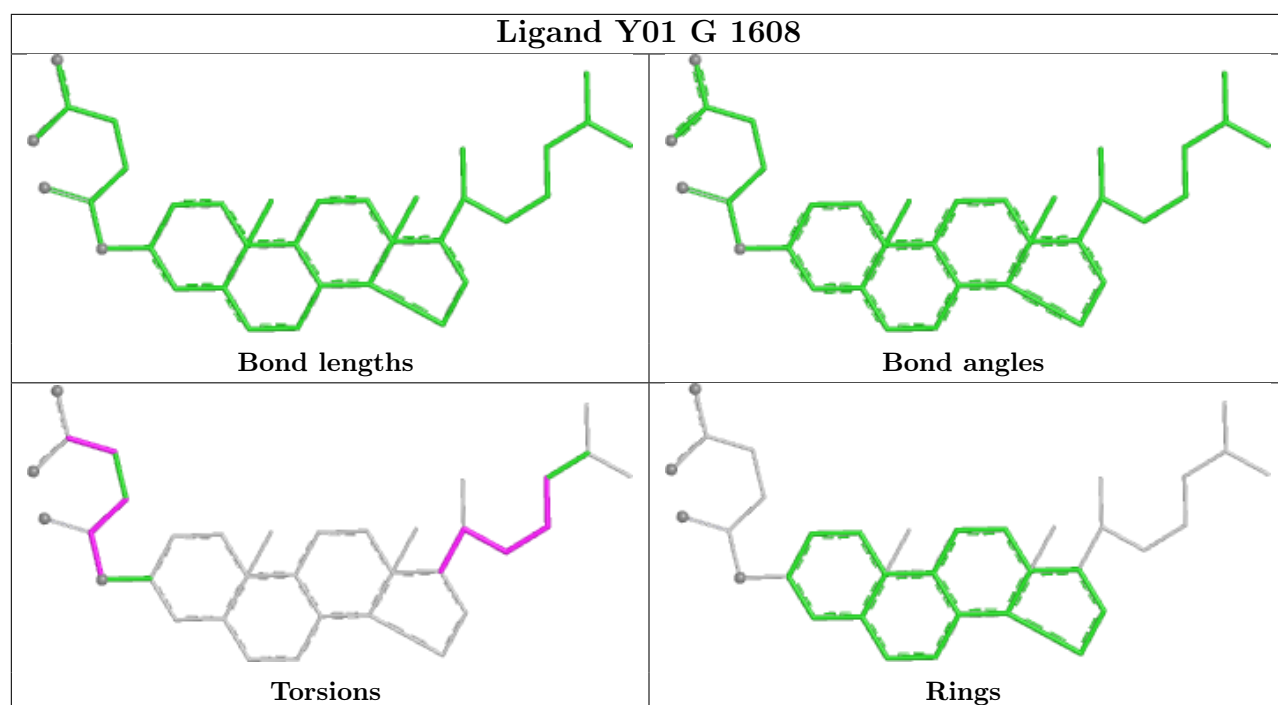
19 monomers are involved in 176 short contacts:

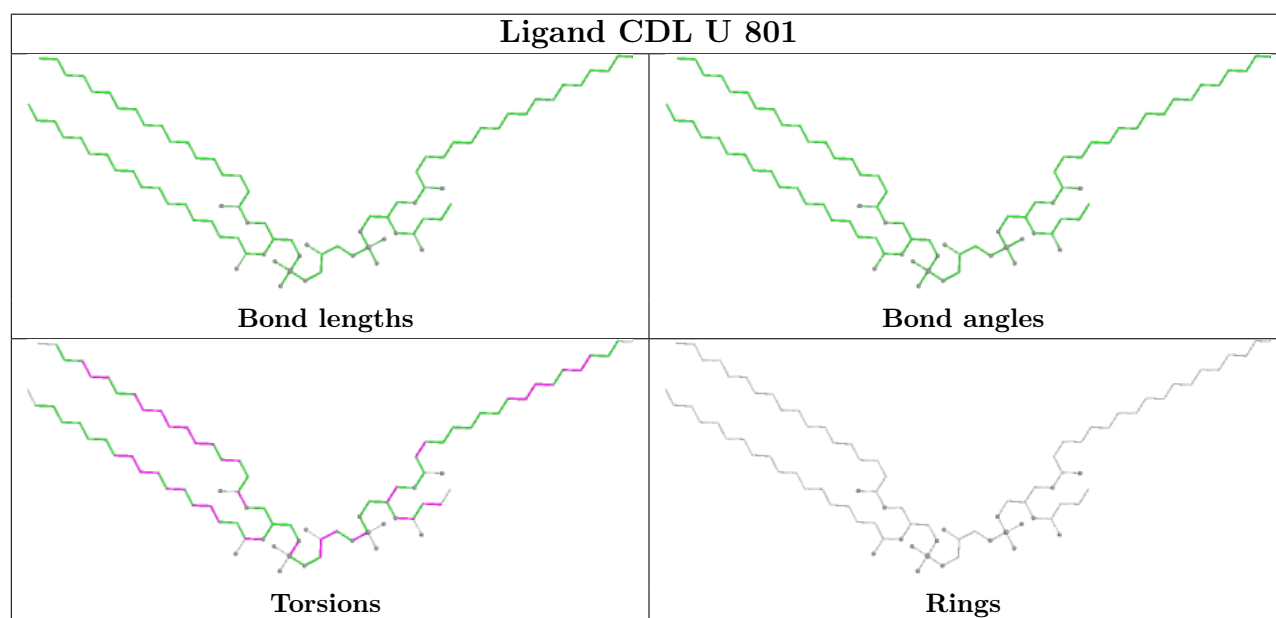
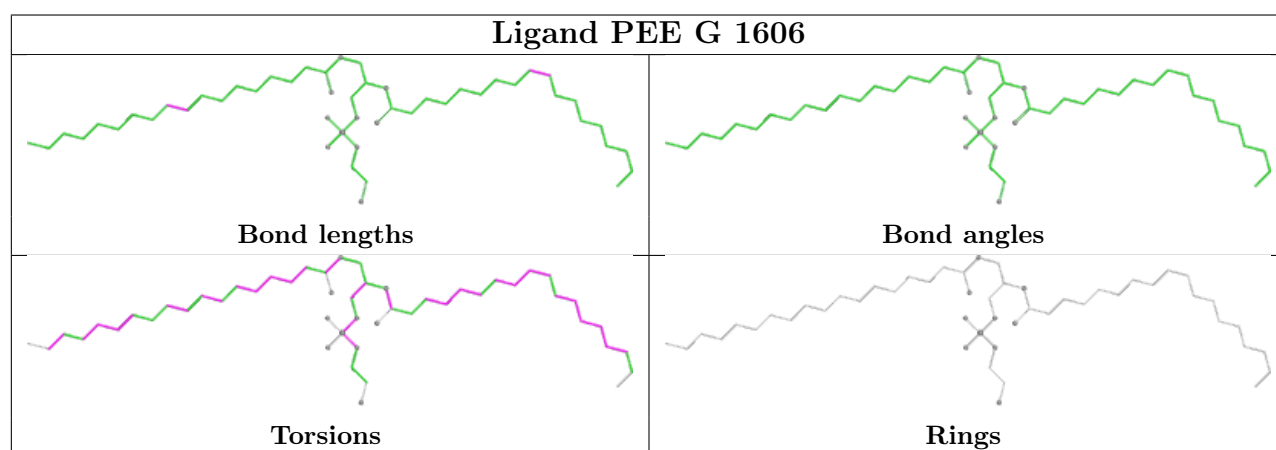
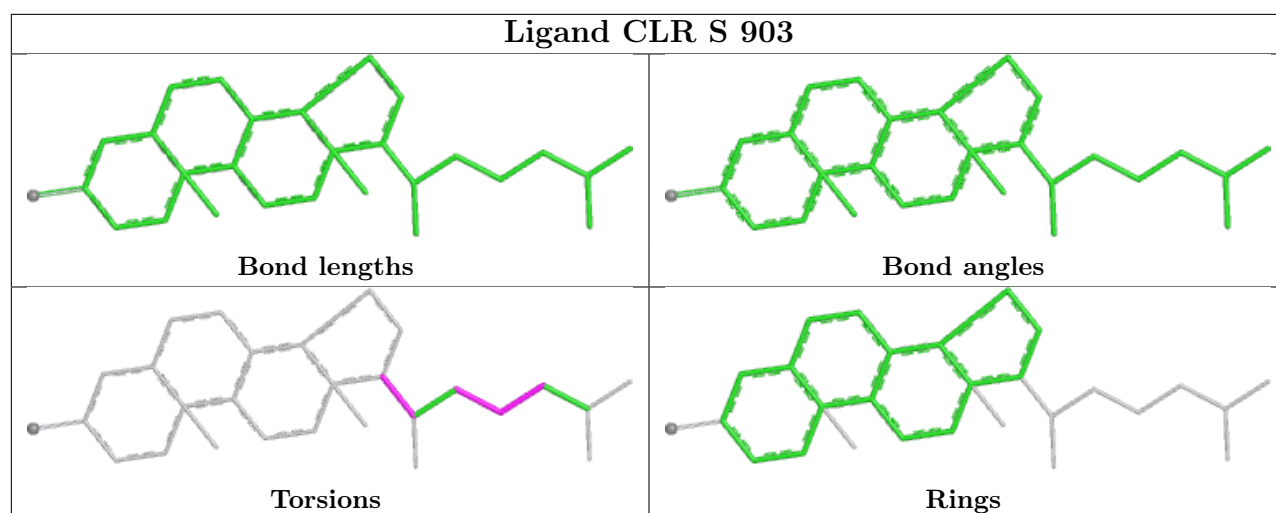
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	U	805	DKB	1	0
9	G	1604	BJR	6	0
14	S	904	CLR	11	0
7	U	807	Y01	3	0
7	U	802	Y01	12	0
7	G	1608	Y01	17	0
14	S	903	CLR	25	0
10	G	1606	PEE	9	0
17	U	801	CDL	10	0
14	U	804	CLR	17	0
12	K	702	P5S	11	0
7	G	1602	Y01	7	0
7	G	1609	Y01	3	0
14	S	902	CLR	19	0
7	U	806	Y01	27	0
7	G	1607	Y01	12	0
7	U	808	Y01	8	0
14	U	803	CLR	2	0
7	G	1601	Y01	6	0

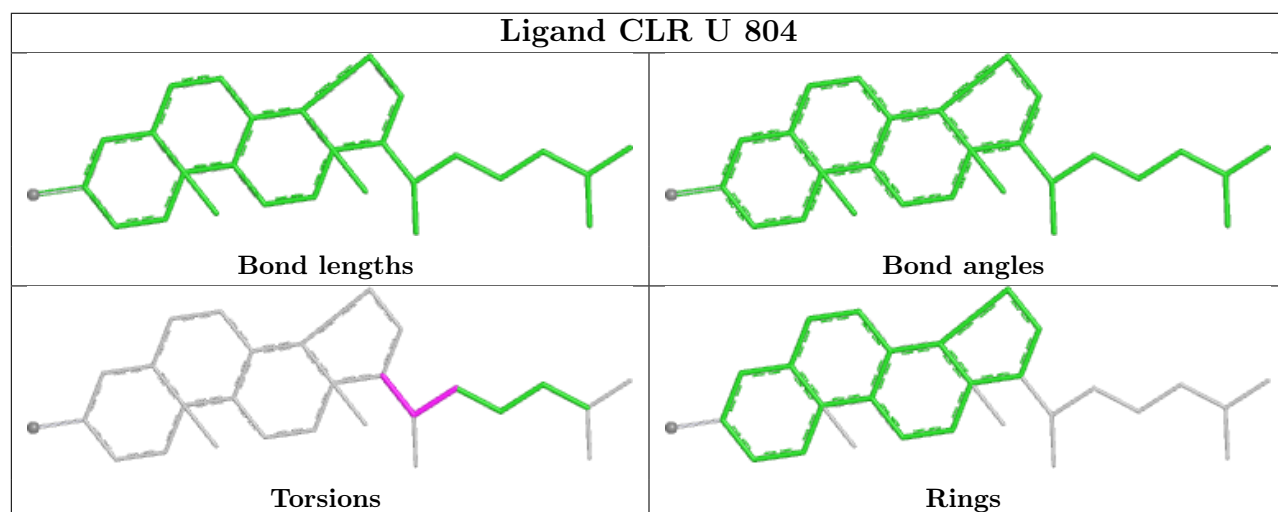
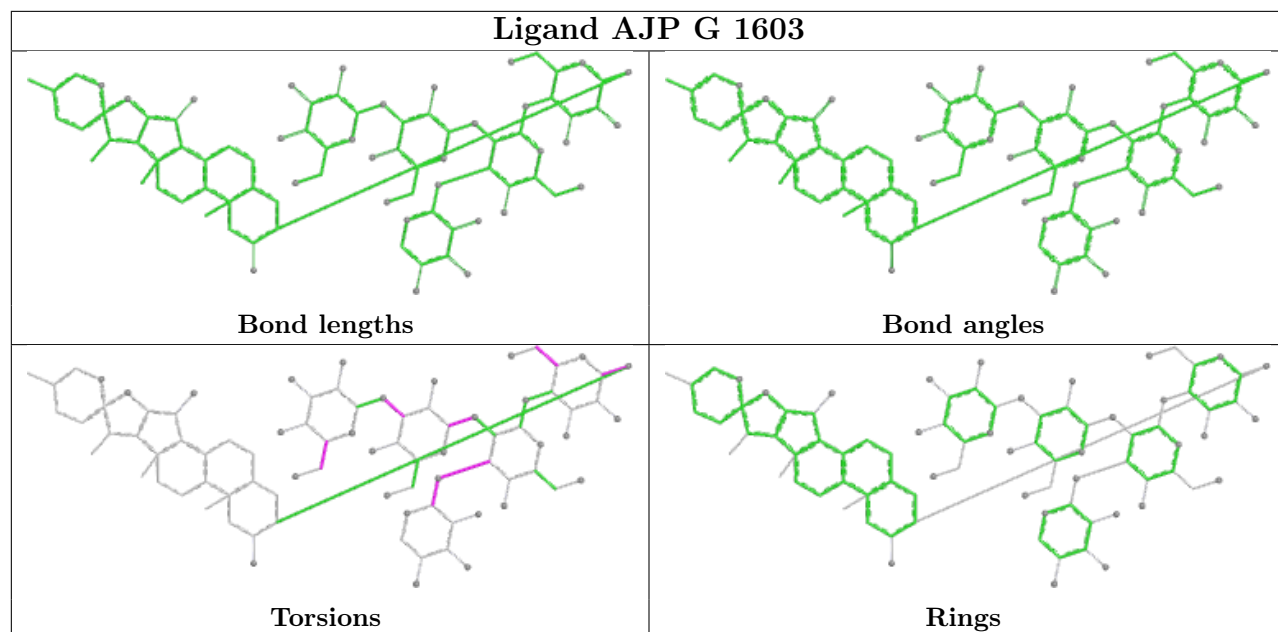
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

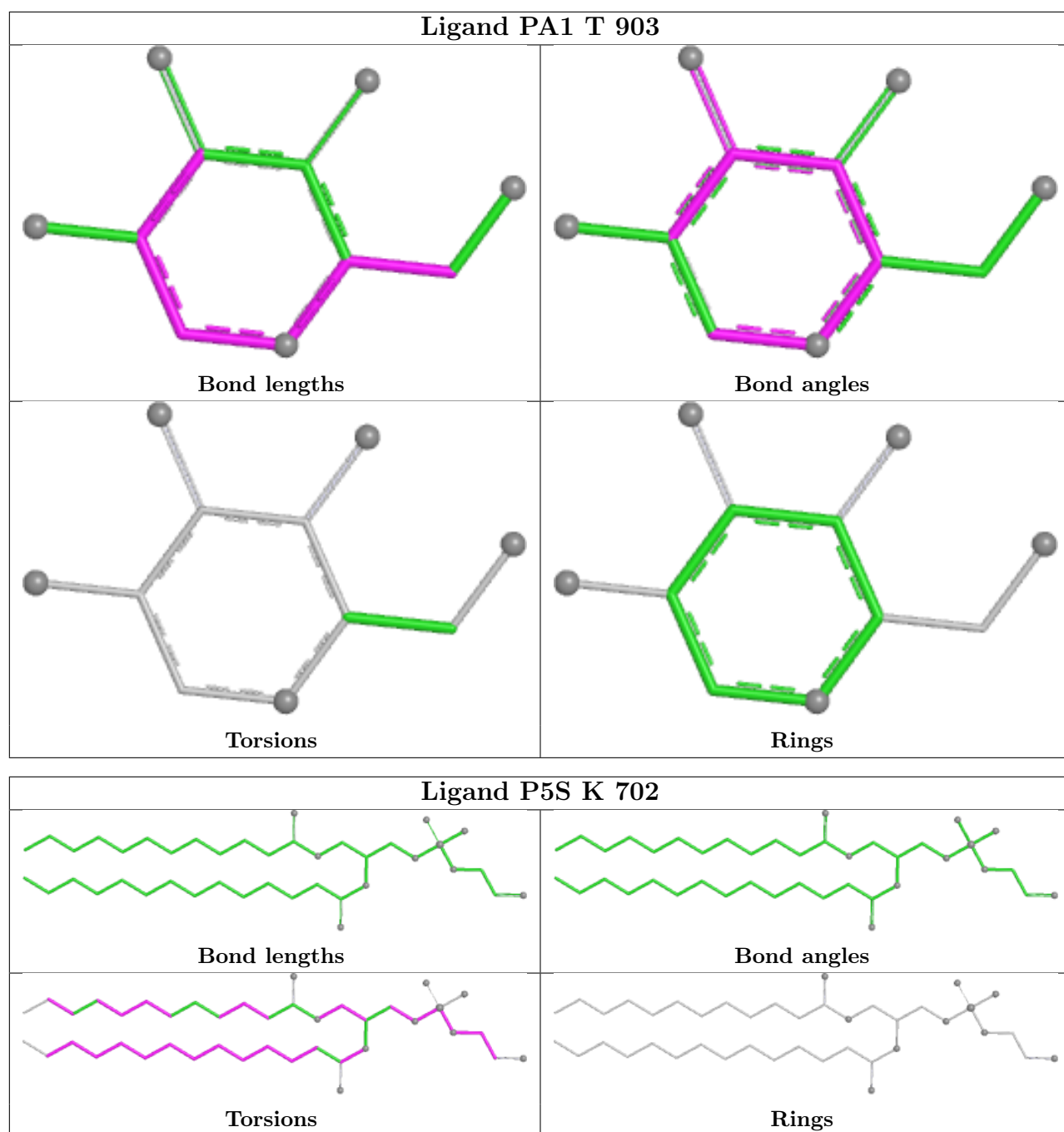


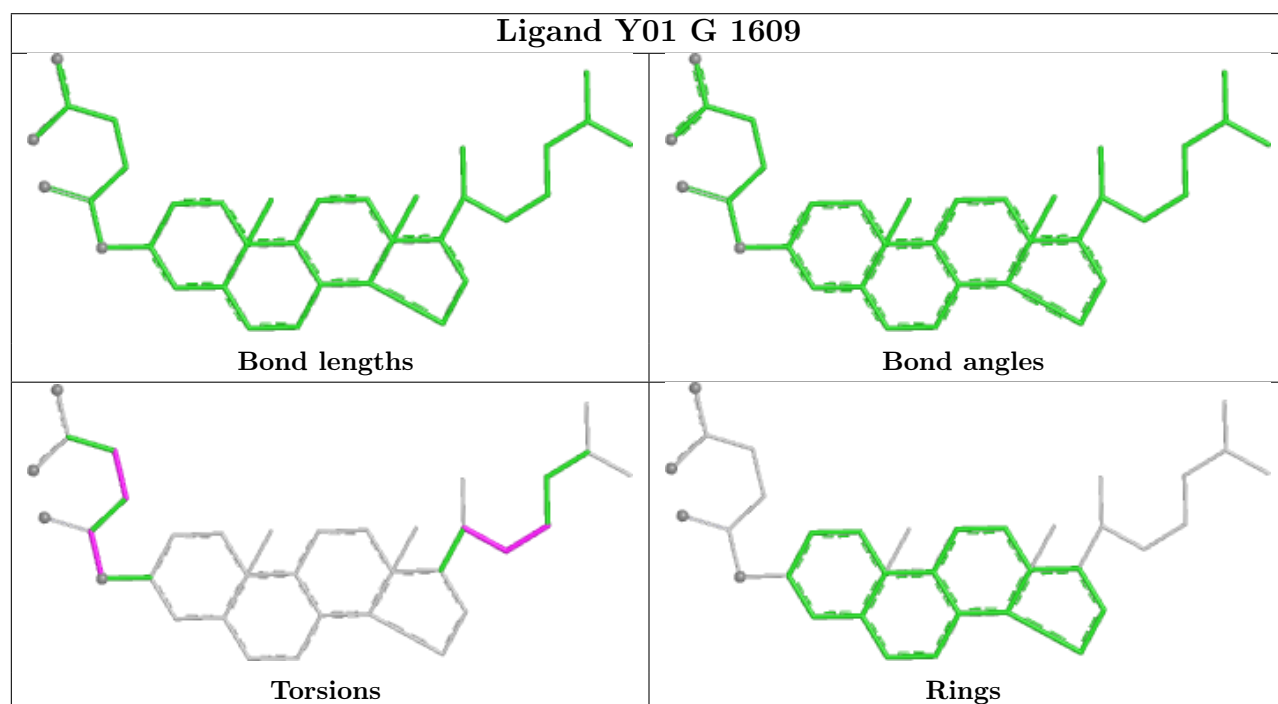
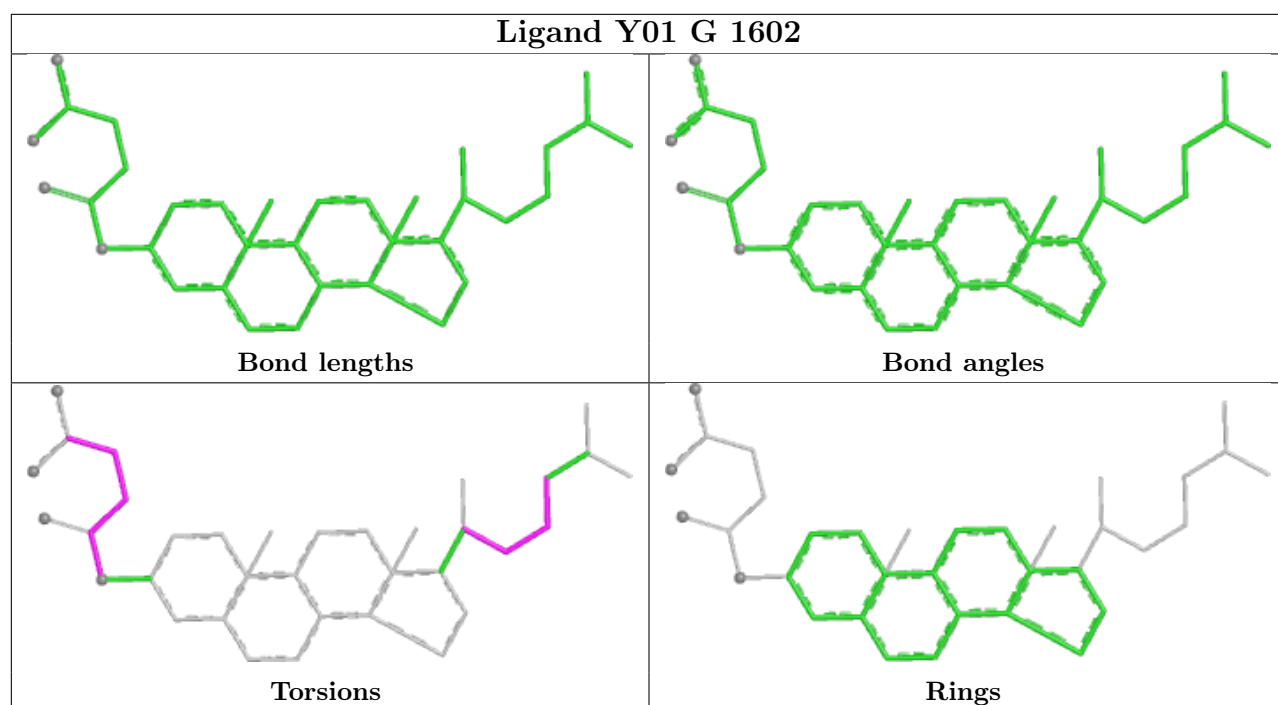


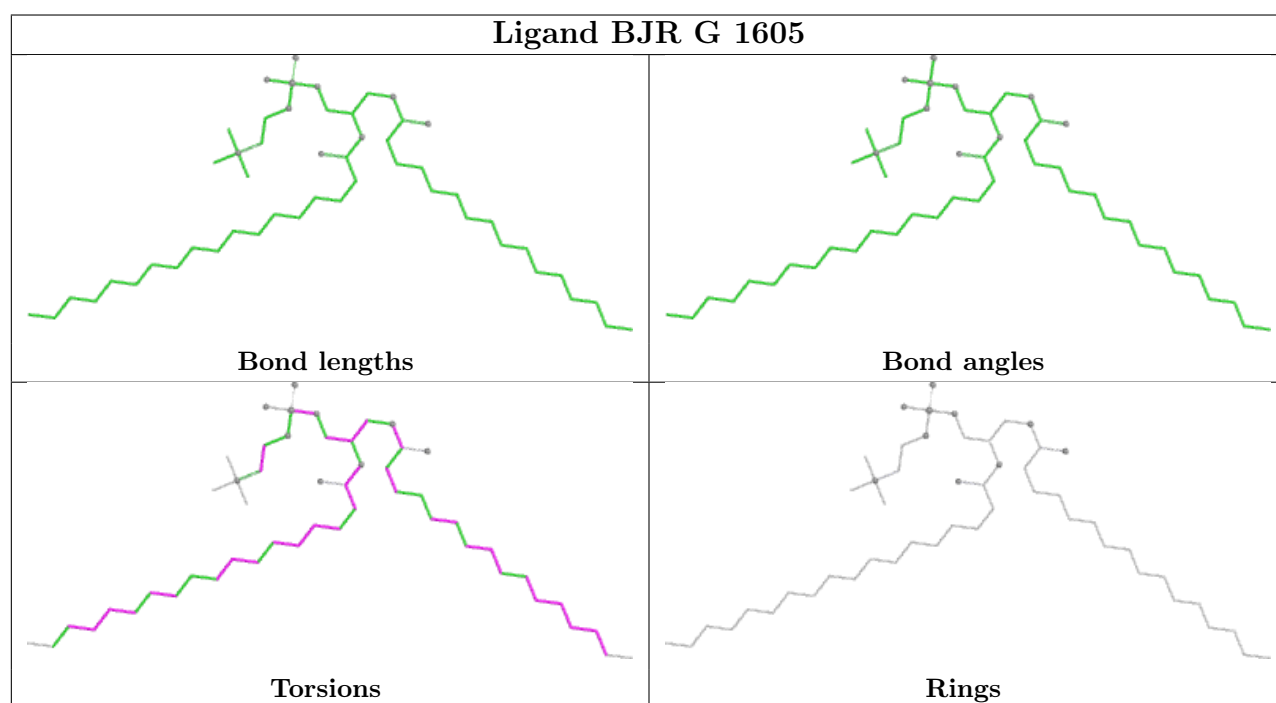
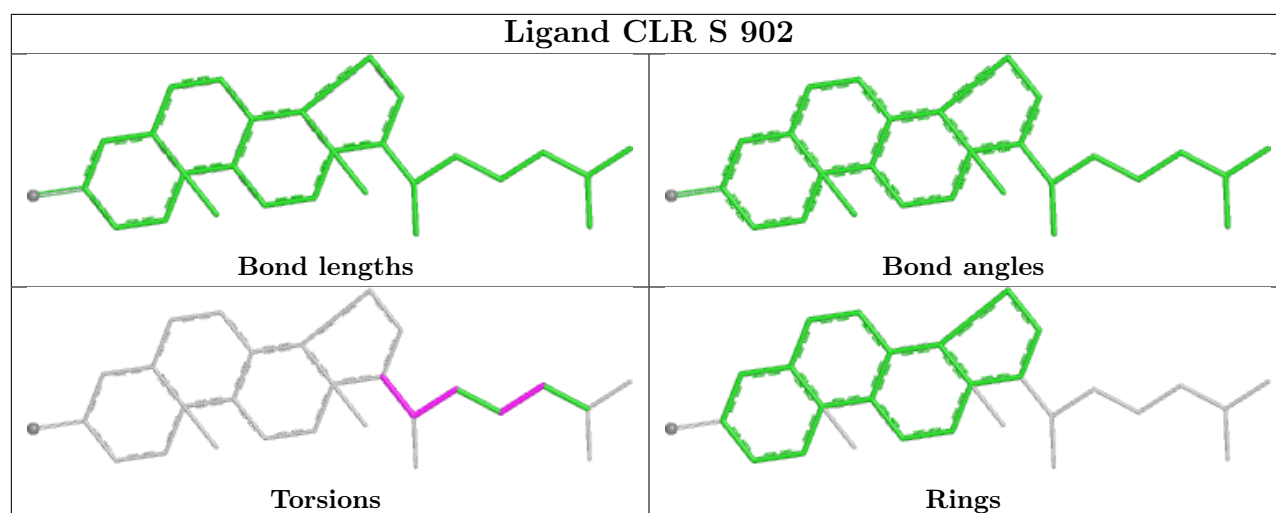


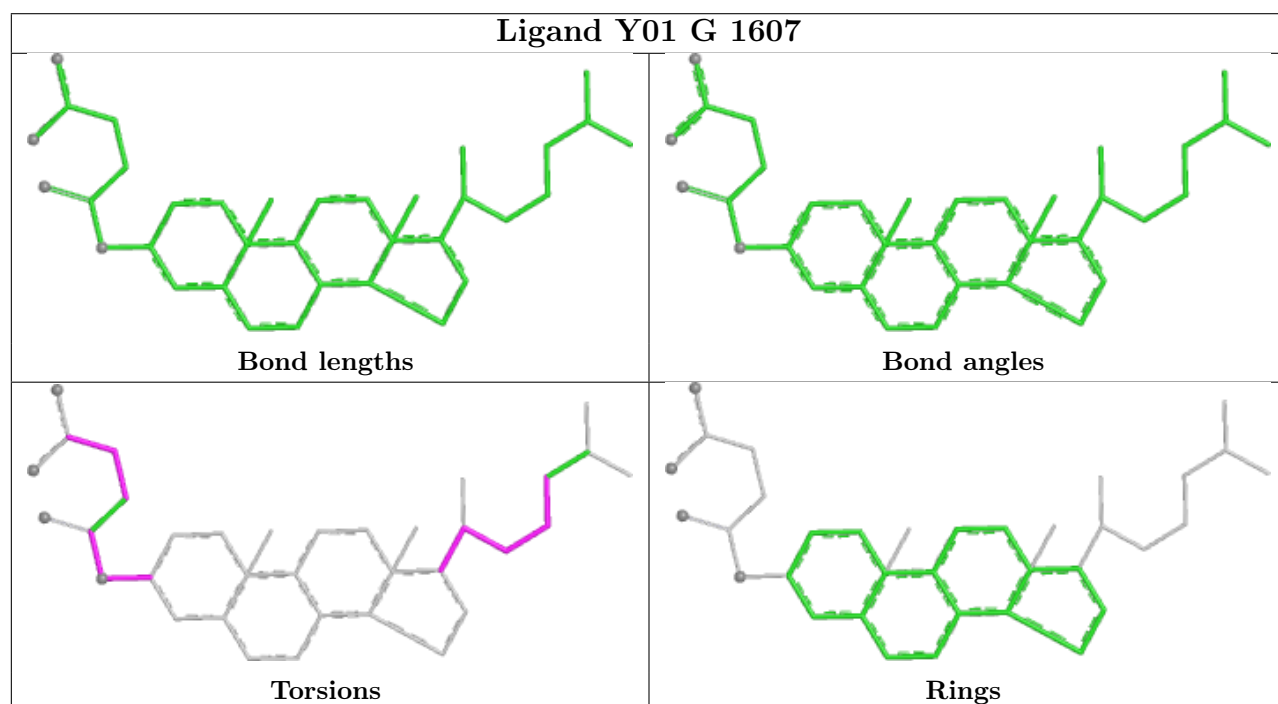
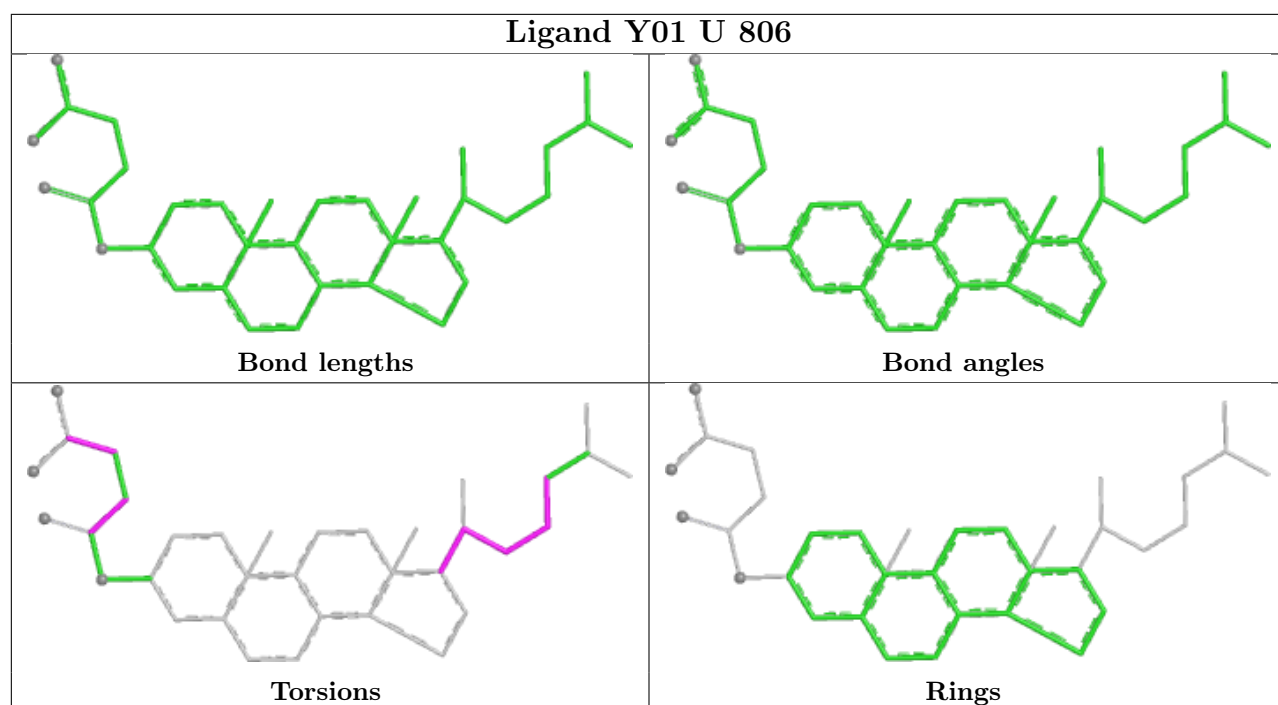


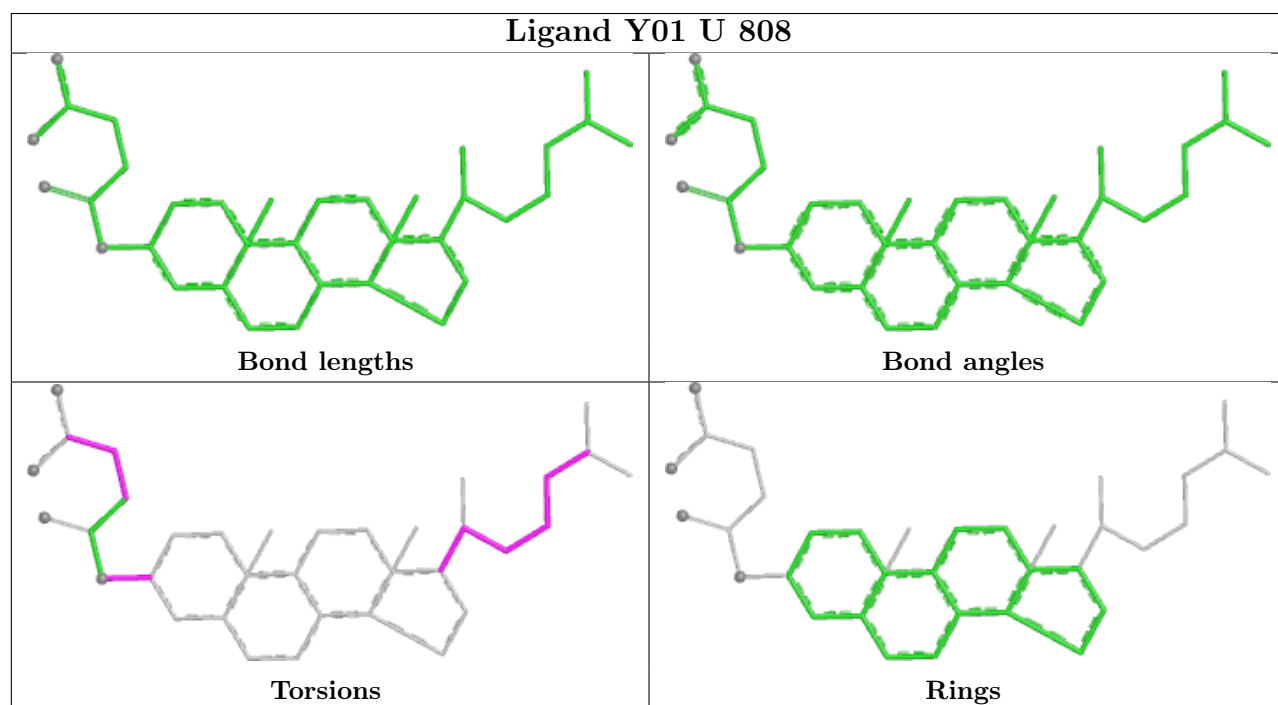
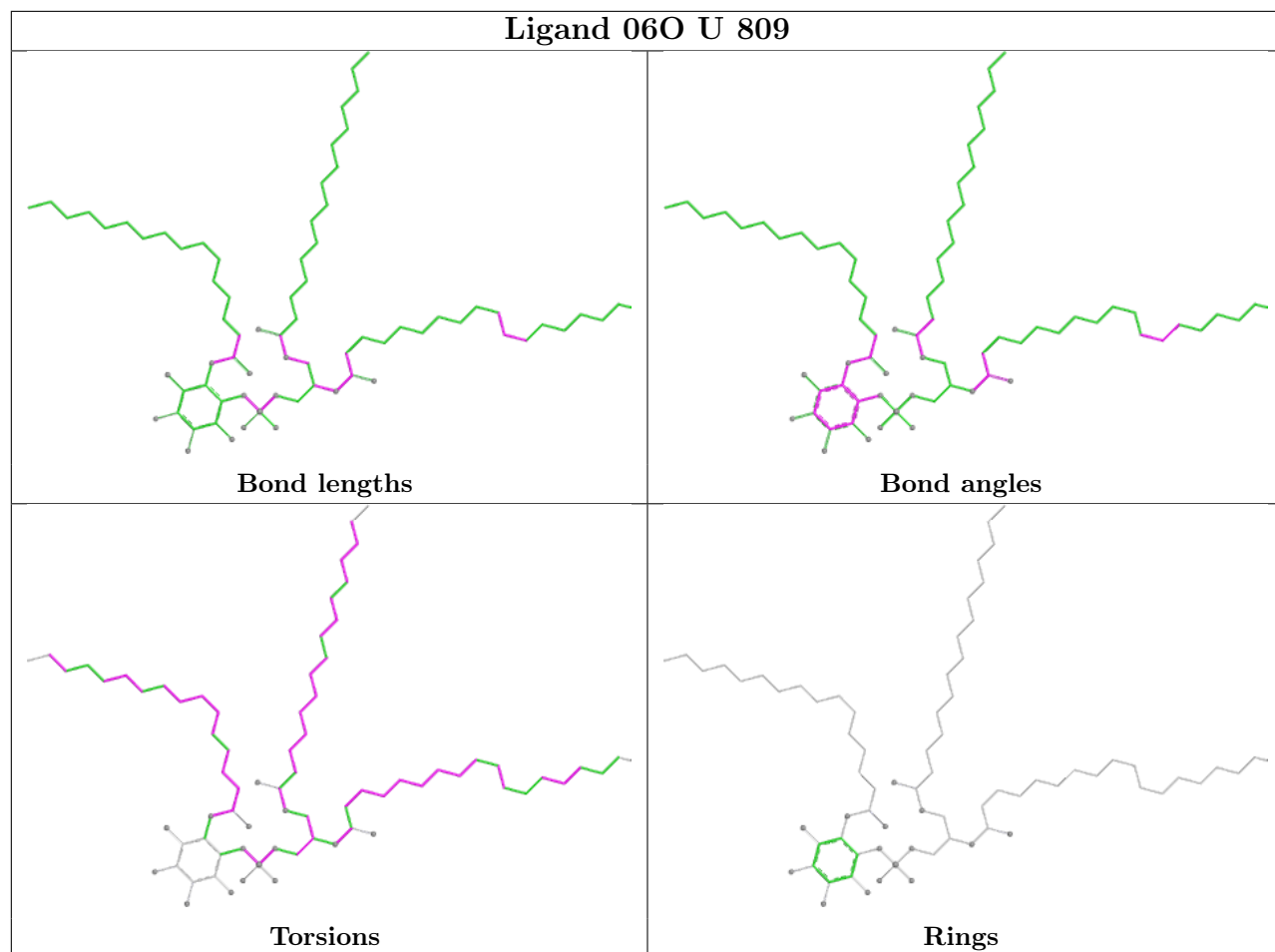


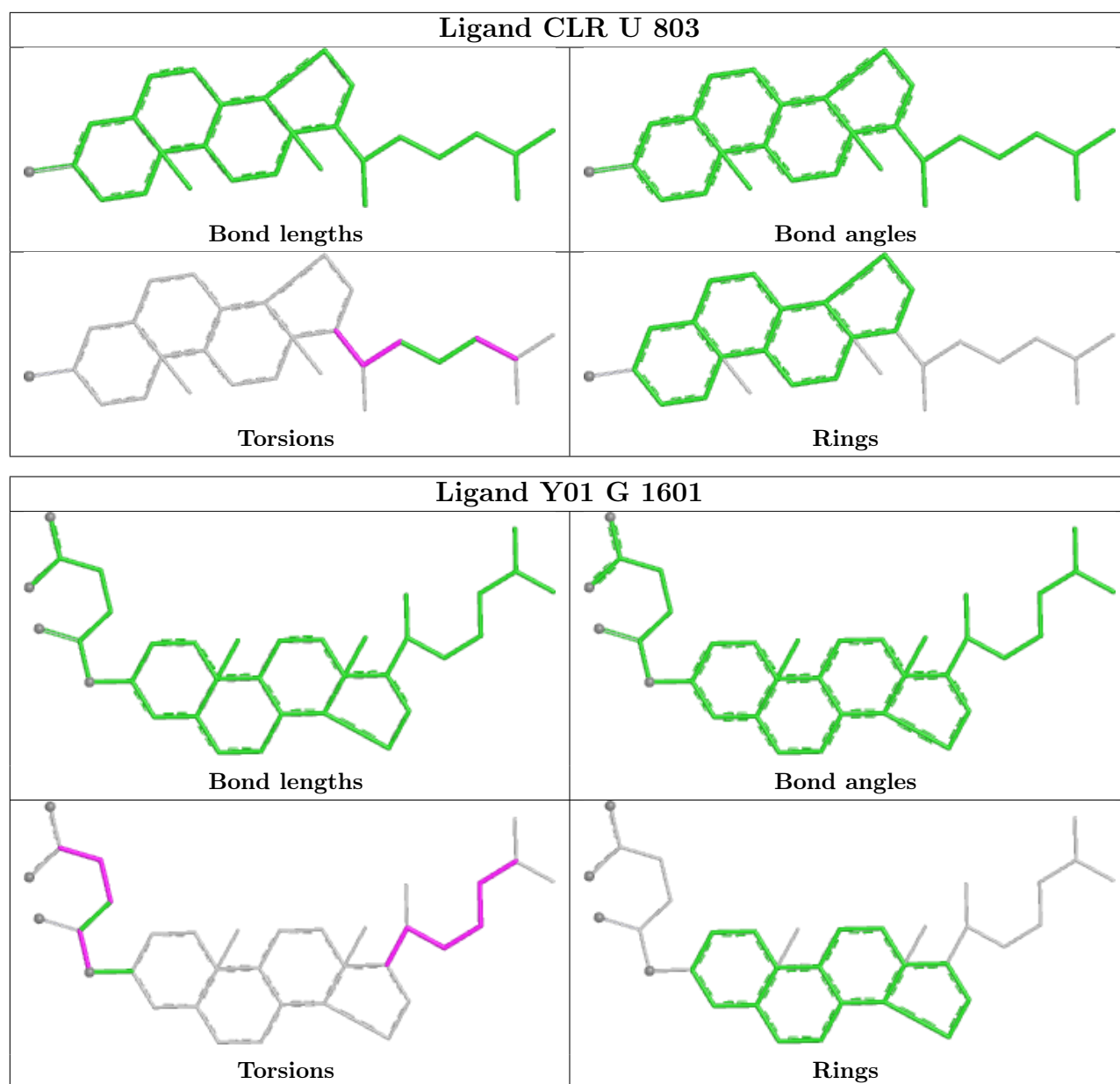












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

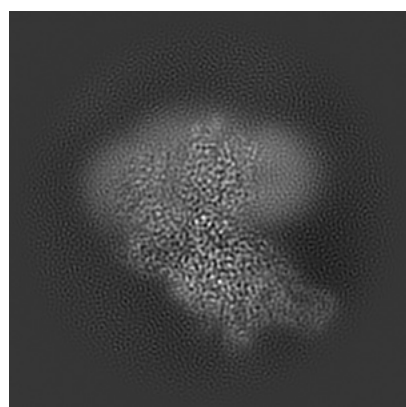
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32582. These allow visual inspection of the internal detail of the map and identification of artifacts.

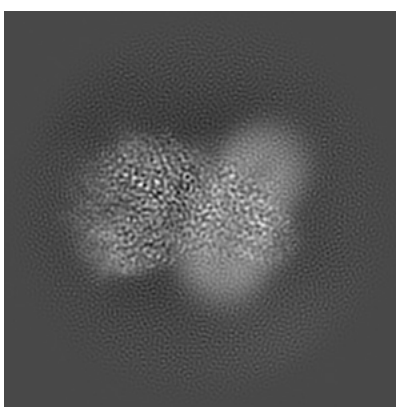
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

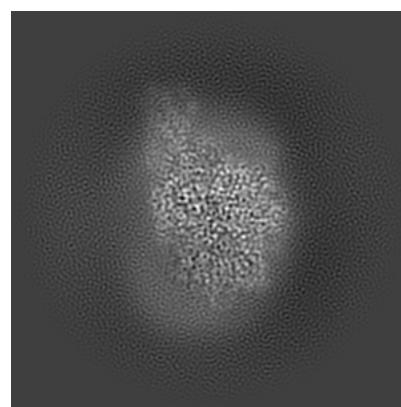
6.1.1 Primary map



X



Y

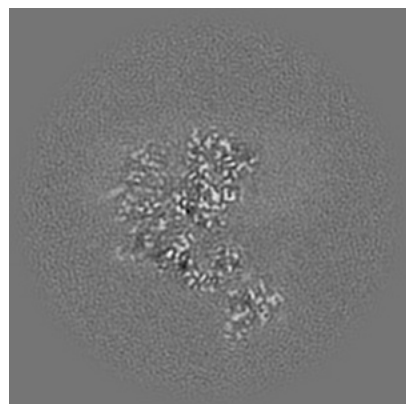


Z

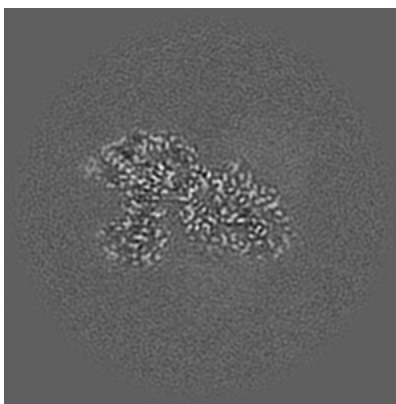
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

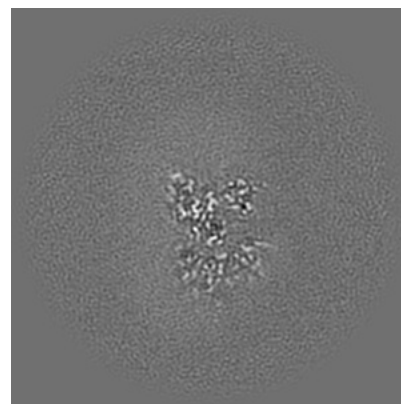
6.2.1 Primary map



X Index: 140



Y Index: 140

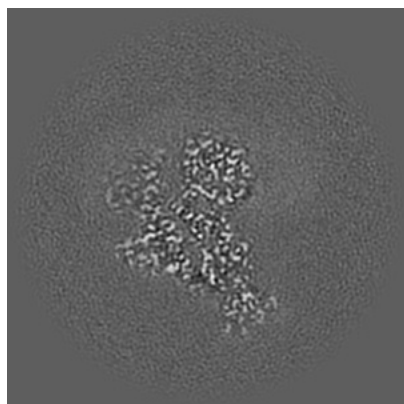


Z Index: 140

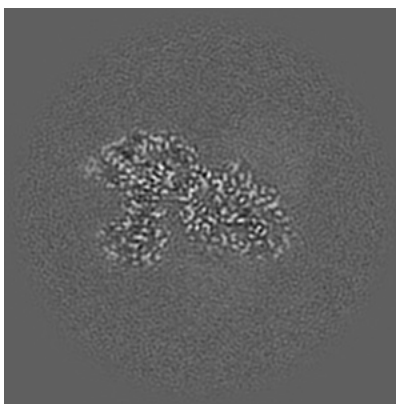
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

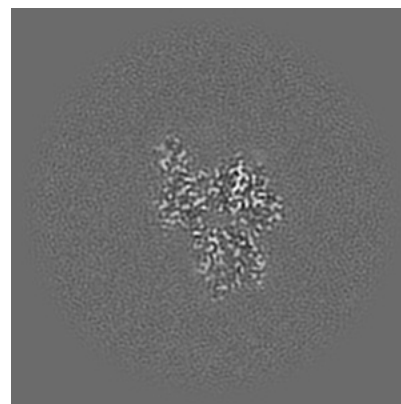
6.3.1 Primary map



X Index: 147



Y Index: 140

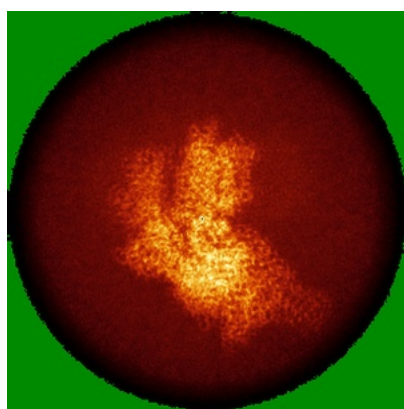


Z Index: 107

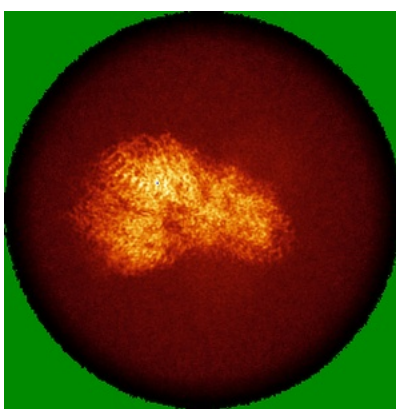
The images above show the largest variance slices of the map in three orthogonal directions.

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

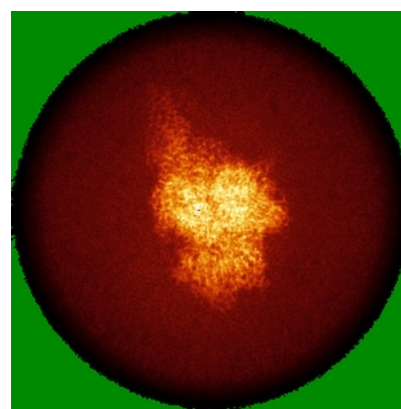
6.4.1 Primary map



X



Y

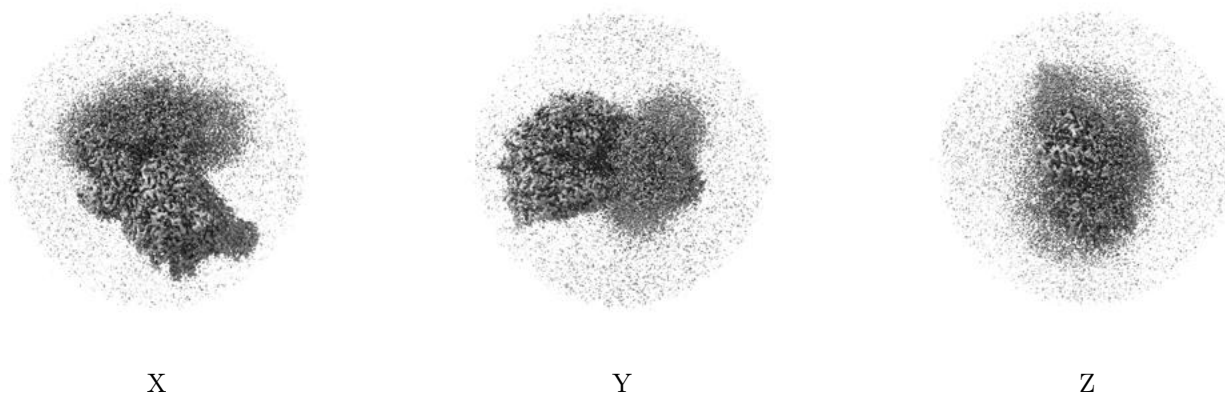


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

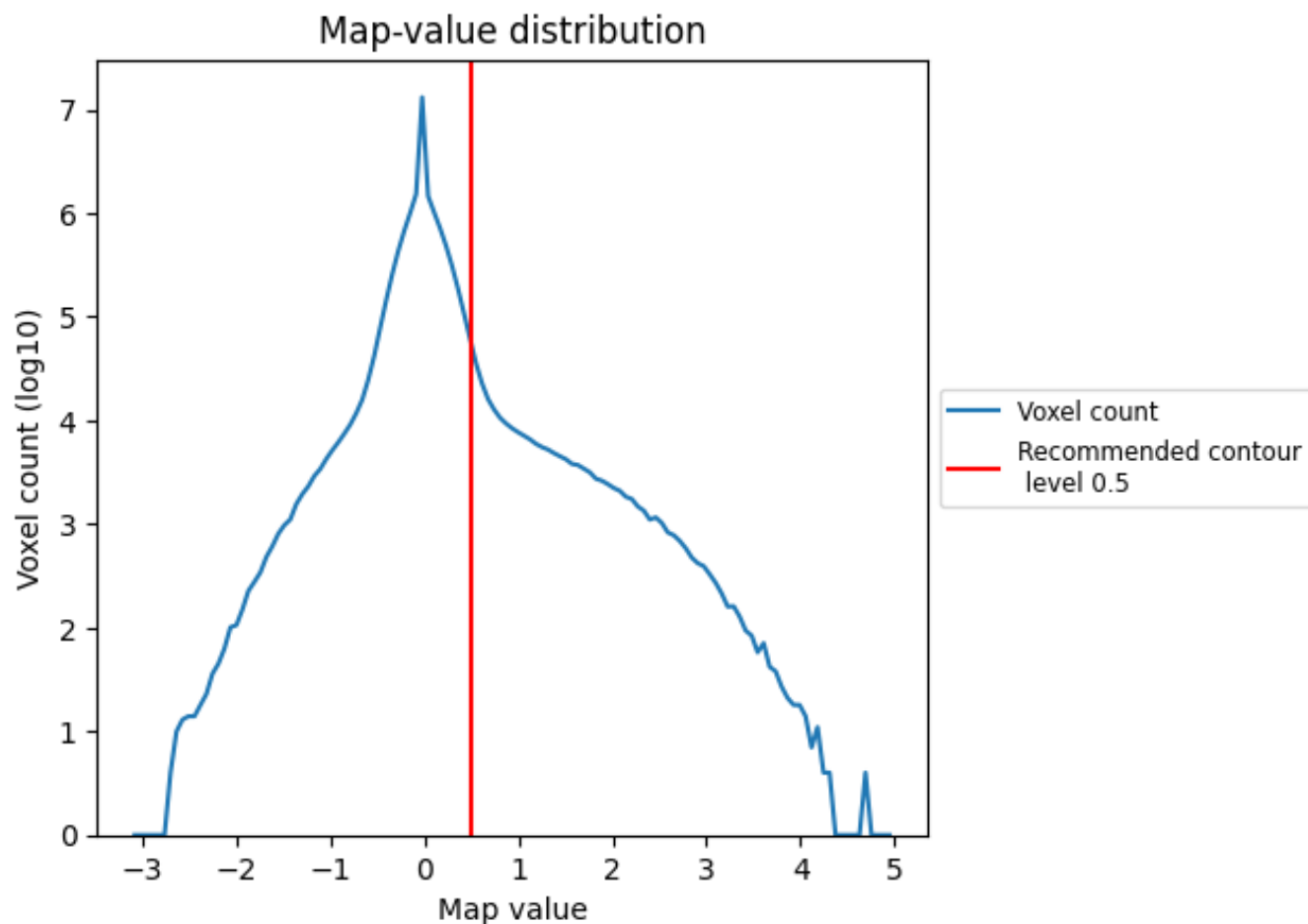
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

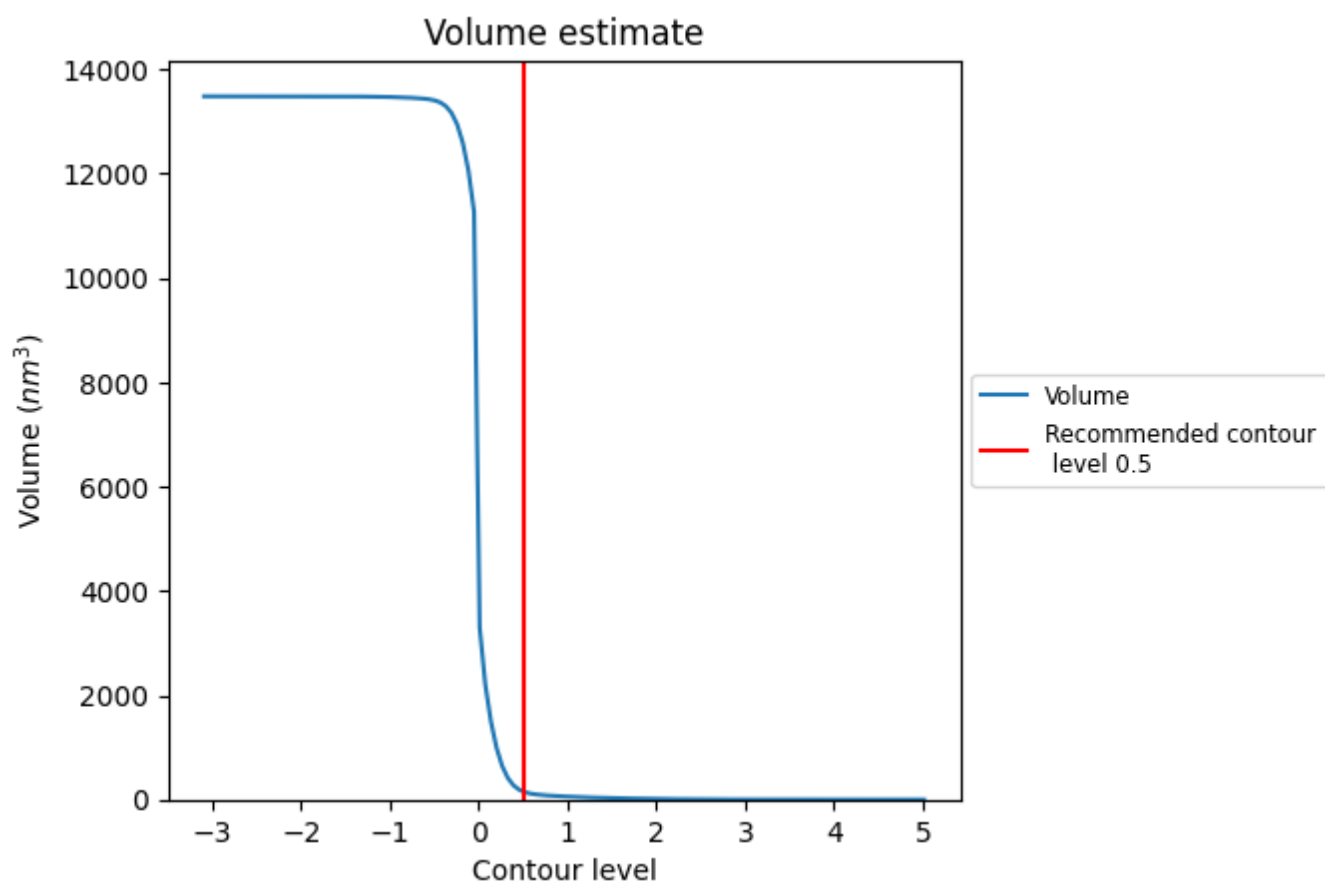
This section contains the results of statistical analysis of the map.

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.

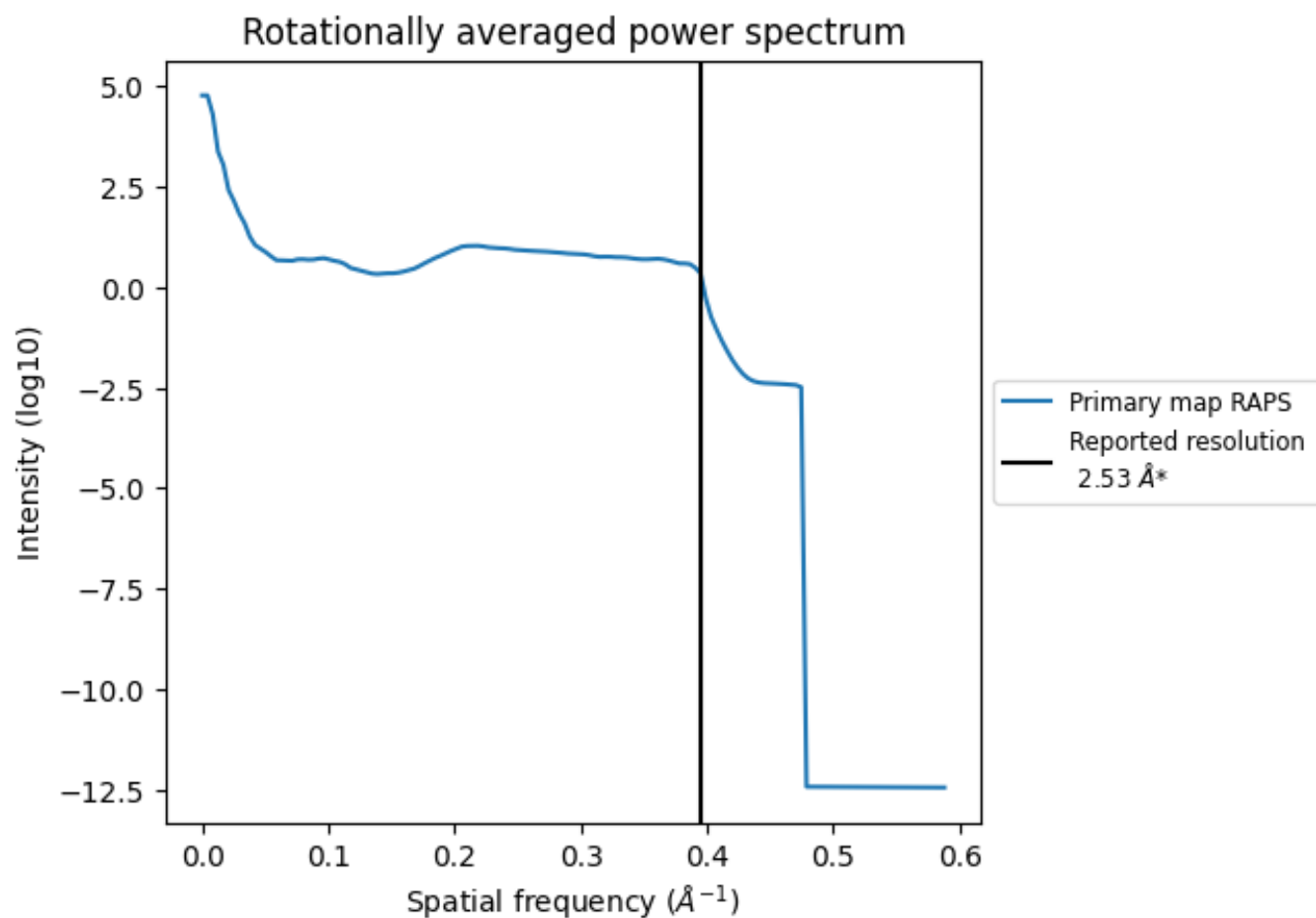
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 157 nm³; this corresponds to an approximate mass of 142 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 0.395 Å⁻¹

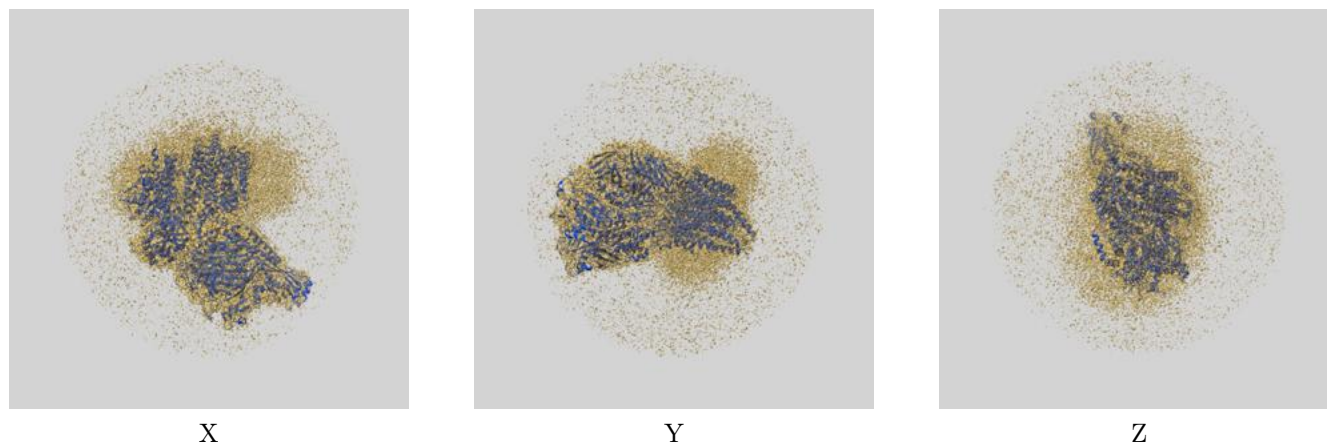
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

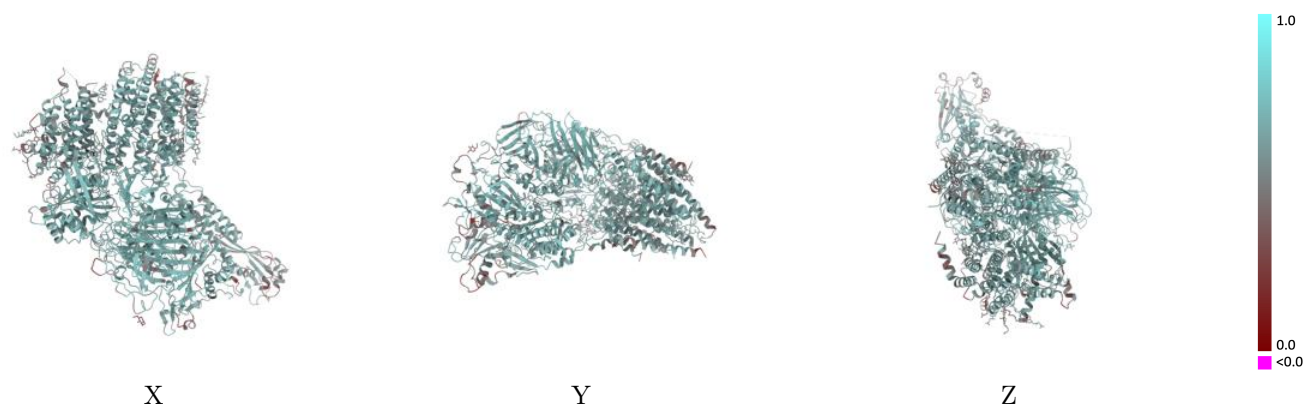
This section contains information regarding the fit between EMDB map EMD-32582 and PDB model 7WLD. Per-residue inclusion information can be found in section [3](#) on page [45](#).

9.1 Map-model overlay [i](#)



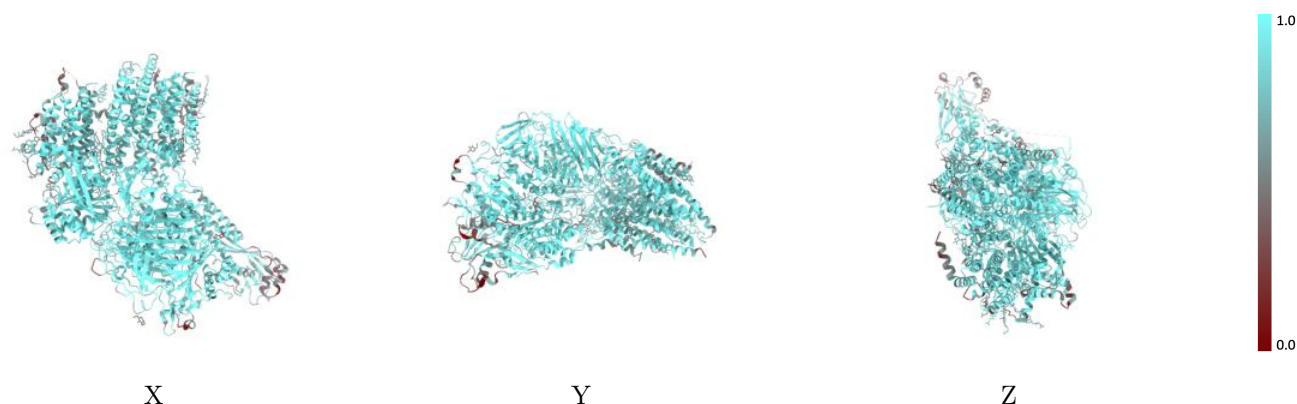
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



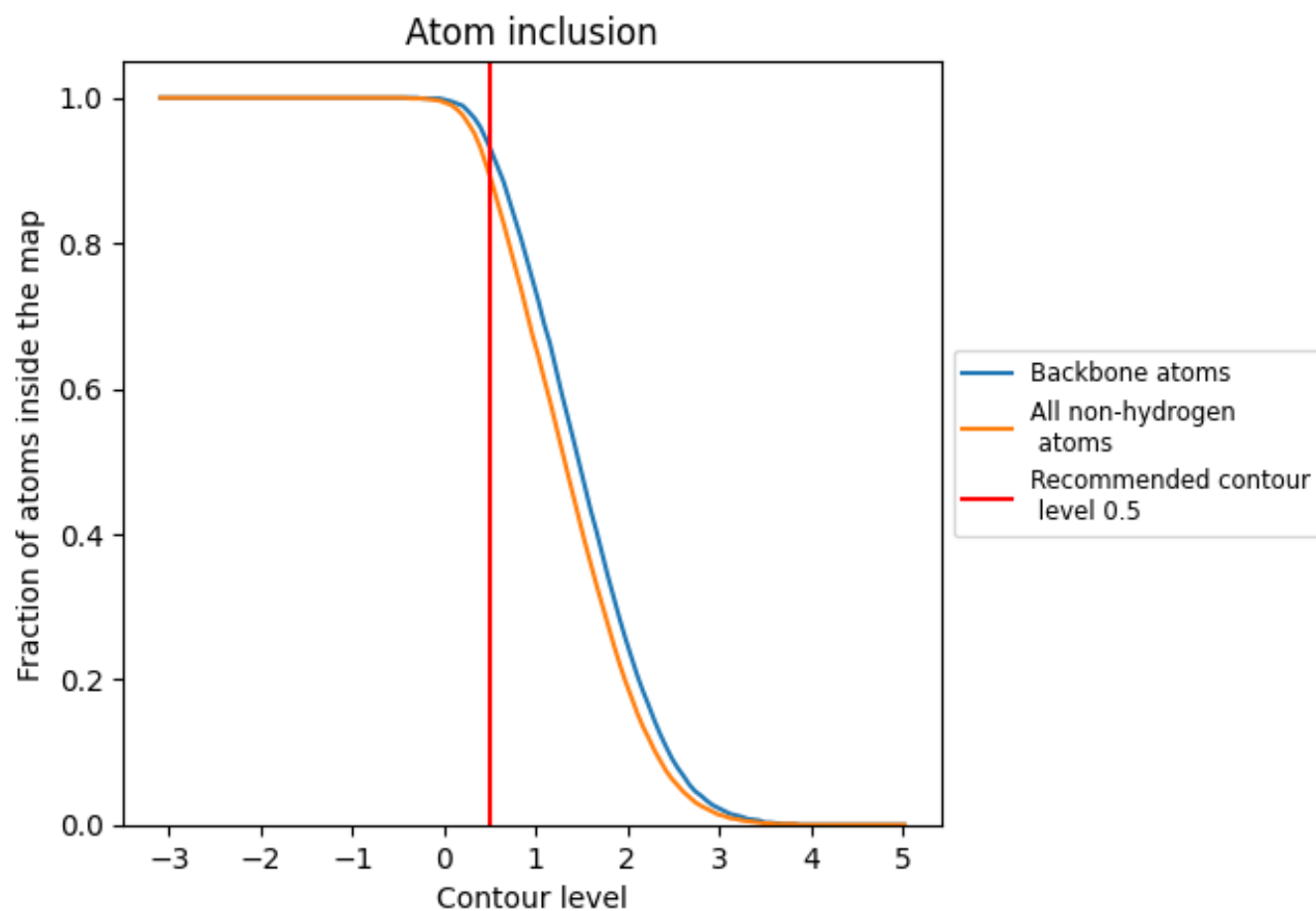
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8920	0.6150
A	0.9640	0.6270
G	0.8760	0.6050
K	0.9260	0.6310
S	0.8060	0.5740
T	0.9430	0.6420
U	0.9210	0.6290

1.0

0.0

<0.0