



Full wwPDB EM Validation Report ⓘ

Nov 24, 2022 – 10:58 AM EST

PDB ID : 7RZ5
EMDB ID : EMD-24751
Title : Structure of the complex of LBD-TMD part of AMPA receptor GluA2 with auxiliary subunit TARP gamma-5 bound to competitive antagonist ZK 200775
Authors : Gangwar, S.P.; Klykov, O.V.; Yelshanskaya, M.V.; Sobolevsky, A.I.
Deposited on : 2021-08-27
Resolution : 3.30 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

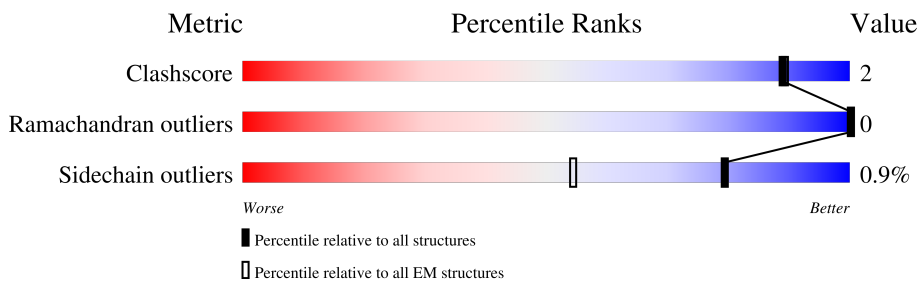
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1038	
1	B	1038	
1	C	1038	
1	D	1038	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 16770 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	611	4780	3112	770	866	32	0	0
1	B	412	3211	2079	521	590	21	0	0
1	C	611	4780	3112	770	866	32	0	0
1	D	412	3211	2079	521	590	21	0	0

There are 964 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	744	THR	ASN	conflict	UNP P19491
A	745	PRO	ALA	conflict	UNP P19491
A	754	SER	ASN	conflict	UNP P19491
A	758	VAL	LEU	conflict	UNP P19491
A	775	ALA	SER	conflict	UNP P19491
A	776	LYS	GLY	conflict	UNP P19491
A	777	ASP	GLY	conflict	UNP P19491
A	778	SER	GLY	conflict	UNP P19491
A	779	GLY	ASP	conflict	UNP P19491
A	827	GLY	-	expression tag	UNP P19491
A	828	THR	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	829	GLY	-	expression tag	UNP P19491
A	830	SER	-	expression tag	UNP P19491
A	831	ALA	-	expression tag	UNP P19491
A	832	CYS	-	expression tag	UNP P19491
A	833	GLY	-	expression tag	UNP P19491
A	834	ARG	-	expression tag	UNP P19491
A	835	LYS	-	expression tag	UNP P19491
A	836	ALA	-	expression tag	UNP P19491
A	837	LEU	-	expression tag	UNP P19491
A	838	THR	-	expression tag	UNP P19491
A	839	LEU	-	expression tag	UNP P19491
A	840	LEU	-	expression tag	UNP P19491
A	841	SER	-	expression tag	UNP P19491
A	842	SER	-	expression tag	UNP P19491
A	843	VAL	-	expression tag	UNP P19491
A	844	PHE	-	expression tag	UNP P19491
A	845	ALA	-	expression tag	UNP P19491
A	846	VAL	-	expression tag	UNP P19491
A	847	CYS	-	expression tag	UNP P19491
A	848	GLY	-	expression tag	UNP P19491
A	849	LEU	-	expression tag	UNP P19491
A	850	GLY	-	expression tag	UNP P19491
A	851	LEU	-	expression tag	UNP P19491
A	852	LEU	-	expression tag	UNP P19491
A	853	GLY	-	expression tag	UNP P19491
A	854	ILE	-	expression tag	UNP P19491
A	855	ALA	-	expression tag	UNP P19491
A	856	VAL	-	expression tag	UNP P19491
A	857	SER	-	expression tag	UNP P19491
A	858	THR	-	expression tag	UNP P19491
A	859	ASP	-	expression tag	UNP P19491
A	860	TYR	-	expression tag	UNP P19491
A	861	TRP	-	expression tag	UNP P19491
A	862	LEU	-	expression tag	UNP P19491
A	863	TYR	-	expression tag	UNP P19491
A	864	LEU	-	expression tag	UNP P19491
A	865	GLU	-	expression tag	UNP P19491
A	866	GLU	-	expression tag	UNP P19491
A	867	GLY	-	expression tag	UNP P19491
A	868	ILE	-	expression tag	UNP P19491
A	869	ILE	-	expression tag	UNP P19491
A	870	LEU	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	871	PRO	-	expression tag	UNP P19491
A	872	GLN	-	expression tag	UNP P19491
A	873	ASN	-	expression tag	UNP P19491
A	874	GLN	-	expression tag	UNP P19491
A	875	SER	-	expression tag	UNP P19491
A	876	THR	-	expression tag	UNP P19491
A	877	GLU	-	expression tag	UNP P19491
A	878	VAL	-	expression tag	UNP P19491
A	879	LYS	-	expression tag	UNP P19491
A	880	MET	-	expression tag	UNP P19491
A	881	SER	-	expression tag	UNP P19491
A	882	LEU	-	expression tag	UNP P19491
A	883	HIS	-	expression tag	UNP P19491
A	884	SER	-	expression tag	UNP P19491
A	885	GLY	-	expression tag	UNP P19491
A	886	LEU	-	expression tag	UNP P19491
A	887	TRP	-	expression tag	UNP P19491
A	888	ARG	-	expression tag	UNP P19491
A	889	VAL	-	expression tag	UNP P19491
A	890	CYS	-	expression tag	UNP P19491
A	891	PHE	-	expression tag	UNP P19491
A	892	LEU	-	expression tag	UNP P19491
A	893	ALA	-	expression tag	UNP P19491
A	894	GLY	-	expression tag	UNP P19491
A	895	GLU	-	expression tag	UNP P19491
A	896	GLU	-	expression tag	UNP P19491
A	897	ARG	-	expression tag	UNP P19491
A	898	GLY	-	expression tag	UNP P19491
A	899	ARG	-	expression tag	UNP P19491
A	900	CYS	-	expression tag	UNP P19491
A	901	PHE	-	expression tag	UNP P19491
A	902	THR	-	expression tag	UNP P19491
A	903	ILE	-	expression tag	UNP P19491
A	904	GLU	-	expression tag	UNP P19491
A	905	TYR	-	expression tag	UNP P19491
A	906	VAL	-	expression tag	UNP P19491
A	907	MET	-	expression tag	UNP P19491
A	908	PRO	-	expression tag	UNP P19491
A	909	MET	-	expression tag	UNP P19491
A	910	ASN	-	expression tag	UNP P19491
A	911	SER	-	expression tag	UNP P19491
A	912	GLN	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	913	MET	-	expression tag	UNP P19491
A	914	THR	-	expression tag	UNP P19491
A	915	SER	-	expression tag	UNP P19491
A	916	GLU	-	expression tag	UNP P19491
A	917	SER	-	expression tag	UNP P19491
A	918	THR	-	expression tag	UNP P19491
A	919	VAL	-	expression tag	UNP P19491
A	920	ASN	-	expression tag	UNP P19491
A	921	VAL	-	expression tag	UNP P19491
A	922	LEU	-	expression tag	UNP P19491
A	923	LYS	-	expression tag	UNP P19491
A	924	MET	-	expression tag	UNP P19491
A	925	ILE	-	expression tag	UNP P19491
A	926	ARG	-	expression tag	UNP P19491
A	927	SER	-	expression tag	UNP P19491
A	928	ALA	-	expression tag	UNP P19491
A	929	THR	-	expression tag	UNP P19491
A	930	PRO	-	expression tag	UNP P19491
A	931	PHE	-	expression tag	UNP P19491
A	932	PRO	-	expression tag	UNP P19491
A	933	LEU	-	expression tag	UNP P19491
A	934	VAL	-	expression tag	UNP P19491
A	935	SER	-	expression tag	UNP P19491
A	936	LEU	-	expression tag	UNP P19491
A	937	PHE	-	expression tag	UNP P19491
A	938	PHE	-	expression tag	UNP P19491
A	939	MET	-	expression tag	UNP P19491
A	940	PHE	-	expression tag	UNP P19491
A	941	ILE	-	expression tag	UNP P19491
A	942	GLY	-	expression tag	UNP P19491
A	943	PHE	-	expression tag	UNP P19491
A	944	ILE	-	expression tag	UNP P19491
A	945	LEU	-	expression tag	UNP P19491
A	946	SER	-	expression tag	UNP P19491
A	947	ASN	-	expression tag	UNP P19491
A	948	ILE	-	expression tag	UNP P19491
A	949	GLY	-	expression tag	UNP P19491
A	950	HIS	-	expression tag	UNP P19491
A	951	ILE	-	expression tag	UNP P19491
A	952	ARG	-	expression tag	UNP P19491
A	953	PRO	-	expression tag	UNP P19491
A	954	HIS	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	955	ARG	-	expression tag	UNP P19491
A	956	THR	-	expression tag	UNP P19491
A	957	ILE	-	expression tag	UNP P19491
A	958	LEU	-	expression tag	UNP P19491
A	959	ALA	-	expression tag	UNP P19491
A	960	PHE	-	expression tag	UNP P19491
A	961	VAL	-	expression tag	UNP P19491
A	962	SER	-	expression tag	UNP P19491
A	963	GLY	-	expression tag	UNP P19491
A	964	ILE	-	expression tag	UNP P19491
A	965	PHE	-	expression tag	UNP P19491
A	966	PHE	-	expression tag	UNP P19491
A	967	ILE	-	expression tag	UNP P19491
A	968	LEU	-	expression tag	UNP P19491
A	969	SER	-	expression tag	UNP P19491
A	970	GLY	-	expression tag	UNP P19491
A	971	LEU	-	expression tag	UNP P19491
A	972	SER	-	expression tag	UNP P19491
A	973	LEU	-	expression tag	UNP P19491
A	974	VAL	-	expression tag	UNP P19491
A	975	VAL	-	expression tag	UNP P19491
A	976	GLY	-	expression tag	UNP P19491
A	977	LEU	-	expression tag	UNP P19491
A	978	VAL	-	expression tag	UNP P19491
A	979	LEU	-	expression tag	UNP P19491
A	980	TYR	-	expression tag	UNP P19491
A	981	ILE	-	expression tag	UNP P19491
A	982	SER	-	expression tag	UNP P19491
A	983	SER	-	expression tag	UNP P19491
A	984	ILE	-	expression tag	UNP P19491
A	985	ASN	-	expression tag	UNP P19491
A	986	ASP	-	expression tag	UNP P19491
A	987	GLU	-	expression tag	UNP P19491
A	988	MET	-	expression tag	UNP P19491
A	989	LEU	-	expression tag	UNP P19491
A	990	ASN	-	expression tag	UNP P19491
A	991	ARG	-	expression tag	UNP P19491
A	992	THR	-	expression tag	UNP P19491
A	993	LYS	-	expression tag	UNP P19491
A	994	ASP	-	expression tag	UNP P19491
A	995	ALA	-	expression tag	UNP P19491
A	996	GLU	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	997	THR	-	expression tag	UNP P19491
A	998	TYR	-	expression tag	UNP P19491
A	999	PHE	-	expression tag	UNP P19491
A	1000	ASN	-	expression tag	UNP P19491
A	1001	TYR	-	expression tag	UNP P19491
A	1002	LYS	-	expression tag	UNP P19491
A	1003	TYR	-	expression tag	UNP P19491
A	1004	GLY	-	expression tag	UNP P19491
A	1005	TRP	-	expression tag	UNP P19491
A	1006	SER	-	expression tag	UNP P19491
A	1007	PHE	-	expression tag	UNP P19491
A	1008	ALA	-	expression tag	UNP P19491
A	1009	PHE	-	expression tag	UNP P19491
A	1010	ALA	-	expression tag	UNP P19491
A	1011	ALA	-	expression tag	UNP P19491
A	1012	ILE	-	expression tag	UNP P19491
A	1013	SER	-	expression tag	UNP P19491
A	1014	PHE	-	expression tag	UNP P19491
A	1015	LEU	-	expression tag	UNP P19491
A	1016	LEU	-	expression tag	UNP P19491
A	1017	THR	-	expression tag	UNP P19491
A	1018	GLU	-	expression tag	UNP P19491
A	1019	SER	-	expression tag	UNP P19491
A	1020	ALA	-	expression tag	UNP P19491
A	1021	GLY	-	expression tag	UNP P19491
A	1022	VAL	-	expression tag	UNP P19491
A	1023	MET	-	expression tag	UNP P19491
A	1024	SER	-	expression tag	UNP P19491
A	1025	VAL	-	expression tag	UNP P19491
A	1026	TYR	-	expression tag	UNP P19491
A	1027	LEU	-	expression tag	UNP P19491
A	1028	PHE	-	expression tag	UNP P19491
A	1029	MET	-	expression tag	UNP P19491
A	1030	LYS	-	expression tag	UNP P19491
A	1031	ARG	-	expression tag	UNP P19491
A	1032	TYR	-	expression tag	UNP P19491
A	1033	THR	-	expression tag	UNP P19491
A	1034	ALA	-	expression tag	UNP P19491
A	1035	GLU	-	expression tag	UNP P19491
A	1036	THR	-	expression tag	UNP P19491
A	1037	GLY	-	expression tag	UNP P19491
A	1038	GLY	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1039	LEU	-	expression tag	UNP P19491
A	1040	VAL	-	expression tag	UNP P19491
A	1041	PRO	-	expression tag	UNP P19491
A	1042	ARG	-	expression tag	UNP P19491
A	1043	GLY	-	expression tag	UNP P19491
A	1044	SER	-	expression tag	UNP P19491
A	1045	ALA	-	expression tag	UNP P19491
A	1046	ALA	-	expression tag	UNP P19491
A	1047	ALA	-	expression tag	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	744	THR	ASN	conflict	UNP P19491
B	745	PRO	ALA	conflict	UNP P19491
B	754	SER	ASN	conflict	UNP P19491
B	758	VAL	LEU	conflict	UNP P19491
B	775	ALA	SER	conflict	UNP P19491
B	776	LYS	GLY	conflict	UNP P19491
B	777	ASP	GLY	conflict	UNP P19491
B	778	SER	GLY	conflict	UNP P19491
B	779	GLY	ASP	conflict	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	THR	-	expression tag	UNP P19491
B	829	GLY	-	expression tag	UNP P19491
B	830	SER	-	expression tag	UNP P19491
B	831	ALA	-	expression tag	UNP P19491
B	832	CYS	-	expression tag	UNP P19491
B	833	GLY	-	expression tag	UNP P19491
B	834	ARG	-	expression tag	UNP P19491
B	835	LYS	-	expression tag	UNP P19491
B	836	ALA	-	expression tag	UNP P19491
B	837	LEU	-	expression tag	UNP P19491
B	838	THR	-	expression tag	UNP P19491
B	839	LEU	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	840	LEU	-	expression tag	UNP P19491
B	841	SER	-	expression tag	UNP P19491
B	842	SER	-	expression tag	UNP P19491
B	843	VAL	-	expression tag	UNP P19491
B	844	PHE	-	expression tag	UNP P19491
B	845	ALA	-	expression tag	UNP P19491
B	846	VAL	-	expression tag	UNP P19491
B	847	CYS	-	expression tag	UNP P19491
B	848	GLY	-	expression tag	UNP P19491
B	849	LEU	-	expression tag	UNP P19491
B	850	GLY	-	expression tag	UNP P19491
B	851	LEU	-	expression tag	UNP P19491
B	852	LEU	-	expression tag	UNP P19491
B	853	GLY	-	expression tag	UNP P19491
B	854	ILE	-	expression tag	UNP P19491
B	855	ALA	-	expression tag	UNP P19491
B	856	VAL	-	expression tag	UNP P19491
B	857	SER	-	expression tag	UNP P19491
B	858	THR	-	expression tag	UNP P19491
B	859	ASP	-	expression tag	UNP P19491
B	860	TYR	-	expression tag	UNP P19491
B	861	TRP	-	expression tag	UNP P19491
B	862	LEU	-	expression tag	UNP P19491
B	863	TYR	-	expression tag	UNP P19491
B	864	LEU	-	expression tag	UNP P19491
B	865	GLU	-	expression tag	UNP P19491
B	866	GLU	-	expression tag	UNP P19491
B	867	GLY	-	expression tag	UNP P19491
B	868	ILE	-	expression tag	UNP P19491
B	869	ILE	-	expression tag	UNP P19491
B	870	LEU	-	expression tag	UNP P19491
B	871	PRO	-	expression tag	UNP P19491
B	872	GLN	-	expression tag	UNP P19491
B	873	ASN	-	expression tag	UNP P19491
B	874	GLN	-	expression tag	UNP P19491
B	875	SER	-	expression tag	UNP P19491
B	876	THR	-	expression tag	UNP P19491
B	877	GLU	-	expression tag	UNP P19491
B	878	VAL	-	expression tag	UNP P19491
B	879	LYS	-	expression tag	UNP P19491
B	880	MET	-	expression tag	UNP P19491
B	881	SER	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	882	LEU	-	expression tag	UNP P19491
B	883	HIS	-	expression tag	UNP P19491
B	884	SER	-	expression tag	UNP P19491
B	885	GLY	-	expression tag	UNP P19491
B	886	LEU	-	expression tag	UNP P19491
B	887	TRP	-	expression tag	UNP P19491
B	888	ARG	-	expression tag	UNP P19491
B	889	VAL	-	expression tag	UNP P19491
B	890	CYS	-	expression tag	UNP P19491
B	891	PHE	-	expression tag	UNP P19491
B	892	LEU	-	expression tag	UNP P19491
B	893	ALA	-	expression tag	UNP P19491
B	894	GLY	-	expression tag	UNP P19491
B	895	GLU	-	expression tag	UNP P19491
B	896	GLU	-	expression tag	UNP P19491
B	897	ARG	-	expression tag	UNP P19491
B	898	GLY	-	expression tag	UNP P19491
B	899	ARG	-	expression tag	UNP P19491
B	900	CYS	-	expression tag	UNP P19491
B	901	PHE	-	expression tag	UNP P19491
B	902	THR	-	expression tag	UNP P19491
B	903	ILE	-	expression tag	UNP P19491
B	904	GLU	-	expression tag	UNP P19491
B	905	TYR	-	expression tag	UNP P19491
B	906	VAL	-	expression tag	UNP P19491
B	907	MET	-	expression tag	UNP P19491
B	908	PRO	-	expression tag	UNP P19491
B	909	MET	-	expression tag	UNP P19491
B	910	ASN	-	expression tag	UNP P19491
B	911	SER	-	expression tag	UNP P19491
B	912	GLN	-	expression tag	UNP P19491
B	913	MET	-	expression tag	UNP P19491
B	914	THR	-	expression tag	UNP P19491
B	915	SER	-	expression tag	UNP P19491
B	916	GLU	-	expression tag	UNP P19491
B	917	SER	-	expression tag	UNP P19491
B	918	THR	-	expression tag	UNP P19491
B	919	VAL	-	expression tag	UNP P19491
B	920	ASN	-	expression tag	UNP P19491
B	921	VAL	-	expression tag	UNP P19491
B	922	LEU	-	expression tag	UNP P19491
B	923	LYS	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	924	MET	-	expression tag	UNP P19491
B	925	ILE	-	expression tag	UNP P19491
B	926	ARG	-	expression tag	UNP P19491
B	927	SER	-	expression tag	UNP P19491
B	928	ALA	-	expression tag	UNP P19491
B	929	THR	-	expression tag	UNP P19491
B	930	PRO	-	expression tag	UNP P19491
B	931	PHE	-	expression tag	UNP P19491
B	932	PRO	-	expression tag	UNP P19491
B	933	LEU	-	expression tag	UNP P19491
B	934	VAL	-	expression tag	UNP P19491
B	935	SER	-	expression tag	UNP P19491
B	936	LEU	-	expression tag	UNP P19491
B	937	PHE	-	expression tag	UNP P19491
B	938	PHE	-	expression tag	UNP P19491
B	939	MET	-	expression tag	UNP P19491
B	940	PHE	-	expression tag	UNP P19491
B	941	ILE	-	expression tag	UNP P19491
B	942	GLY	-	expression tag	UNP P19491
B	943	PHE	-	expression tag	UNP P19491
B	944	ILE	-	expression tag	UNP P19491
B	945	LEU	-	expression tag	UNP P19491
B	946	SER	-	expression tag	UNP P19491
B	947	ASN	-	expression tag	UNP P19491
B	948	ILE	-	expression tag	UNP P19491
B	949	GLY	-	expression tag	UNP P19491
B	950	HIS	-	expression tag	UNP P19491
B	951	ILE	-	expression tag	UNP P19491
B	952	ARG	-	expression tag	UNP P19491
B	953	PRO	-	expression tag	UNP P19491
B	954	HIS	-	expression tag	UNP P19491
B	955	ARG	-	expression tag	UNP P19491
B	956	THR	-	expression tag	UNP P19491
B	957	ILE	-	expression tag	UNP P19491
B	958	LEU	-	expression tag	UNP P19491
B	959	ALA	-	expression tag	UNP P19491
B	960	PHE	-	expression tag	UNP P19491
B	961	VAL	-	expression tag	UNP P19491
B	962	SER	-	expression tag	UNP P19491
B	963	GLY	-	expression tag	UNP P19491
B	964	ILE	-	expression tag	UNP P19491
B	965	PHE	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	966	PHE	-	expression tag	UNP P19491
B	967	ILE	-	expression tag	UNP P19491
B	968	LEU	-	expression tag	UNP P19491
B	969	SER	-	expression tag	UNP P19491
B	970	GLY	-	expression tag	UNP P19491
B	971	LEU	-	expression tag	UNP P19491
B	972	SER	-	expression tag	UNP P19491
B	973	LEU	-	expression tag	UNP P19491
B	974	VAL	-	expression tag	UNP P19491
B	975	VAL	-	expression tag	UNP P19491
B	976	GLY	-	expression tag	UNP P19491
B	977	LEU	-	expression tag	UNP P19491
B	978	VAL	-	expression tag	UNP P19491
B	979	LEU	-	expression tag	UNP P19491
B	980	TYR	-	expression tag	UNP P19491
B	981	ILE	-	expression tag	UNP P19491
B	982	SER	-	expression tag	UNP P19491
B	983	SER	-	expression tag	UNP P19491
B	984	ILE	-	expression tag	UNP P19491
B	985	ASN	-	expression tag	UNP P19491
B	986	ASP	-	expression tag	UNP P19491
B	987	GLU	-	expression tag	UNP P19491
B	988	MET	-	expression tag	UNP P19491
B	989	LEU	-	expression tag	UNP P19491
B	990	ASN	-	expression tag	UNP P19491
B	991	ARG	-	expression tag	UNP P19491
B	992	THR	-	expression tag	UNP P19491
B	993	LYS	-	expression tag	UNP P19491
B	994	ASP	-	expression tag	UNP P19491
B	995	ALA	-	expression tag	UNP P19491
B	996	GLU	-	expression tag	UNP P19491
B	997	THR	-	expression tag	UNP P19491
B	998	TYR	-	expression tag	UNP P19491
B	999	PHE	-	expression tag	UNP P19491
B	1000	ASN	-	expression tag	UNP P19491
B	1001	TYR	-	expression tag	UNP P19491
B	1002	LYS	-	expression tag	UNP P19491
B	1003	TYR	-	expression tag	UNP P19491
B	1004	GLY	-	expression tag	UNP P19491
B	1005	TRP	-	expression tag	UNP P19491
B	1006	SER	-	expression tag	UNP P19491
B	1007	PHE	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1008	ALA	-	expression tag	UNP P19491
B	1009	PHE	-	expression tag	UNP P19491
B	1010	ALA	-	expression tag	UNP P19491
B	1011	ALA	-	expression tag	UNP P19491
B	1012	ILE	-	expression tag	UNP P19491
B	1013	SER	-	expression tag	UNP P19491
B	1014	PHE	-	expression tag	UNP P19491
B	1015	LEU	-	expression tag	UNP P19491
B	1016	LEU	-	expression tag	UNP P19491
B	1017	THR	-	expression tag	UNP P19491
B	1018	GLU	-	expression tag	UNP P19491
B	1019	SER	-	expression tag	UNP P19491
B	1020	ALA	-	expression tag	UNP P19491
B	1021	GLY	-	expression tag	UNP P19491
B	1022	VAL	-	expression tag	UNP P19491
B	1023	MET	-	expression tag	UNP P19491
B	1024	SER	-	expression tag	UNP P19491
B	1025	VAL	-	expression tag	UNP P19491
B	1026	TYR	-	expression tag	UNP P19491
B	1027	LEU	-	expression tag	UNP P19491
B	1028	PHE	-	expression tag	UNP P19491
B	1029	MET	-	expression tag	UNP P19491
B	1030	LYS	-	expression tag	UNP P19491
B	1031	ARG	-	expression tag	UNP P19491
B	1032	TYR	-	expression tag	UNP P19491
B	1033	THR	-	expression tag	UNP P19491
B	1034	ALA	-	expression tag	UNP P19491
B	1035	GLU	-	expression tag	UNP P19491
B	1036	THR	-	expression tag	UNP P19491
B	1037	GLY	-	expression tag	UNP P19491
B	1038	GLY	-	expression tag	UNP P19491
B	1039	LEU	-	expression tag	UNP P19491
B	1040	VAL	-	expression tag	UNP P19491
B	1041	PRO	-	expression tag	UNP P19491
B	1042	ARG	-	expression tag	UNP P19491
B	1043	GLY	-	expression tag	UNP P19491
B	1044	SER	-	expression tag	UNP P19491
B	1045	ALA	-	expression tag	UNP P19491
B	1046	ALA	-	expression tag	UNP P19491
B	1047	ALA	-	expression tag	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	744	THR	ASN	conflict	UNP P19491
C	745	PRO	ALA	conflict	UNP P19491
C	754	SER	ASN	conflict	UNP P19491
C	758	VAL	LEU	conflict	UNP P19491
C	775	ALA	SER	conflict	UNP P19491
C	776	LYS	GLY	conflict	UNP P19491
C	777	ASP	GLY	conflict	UNP P19491
C	778	SER	GLY	conflict	UNP P19491
C	779	GLY	ASP	conflict	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	THR	-	expression tag	UNP P19491
C	829	GLY	-	expression tag	UNP P19491
C	830	SER	-	expression tag	UNP P19491
C	831	ALA	-	expression tag	UNP P19491
C	832	CYS	-	expression tag	UNP P19491
C	833	GLY	-	expression tag	UNP P19491
C	834	ARG	-	expression tag	UNP P19491
C	835	LYS	-	expression tag	UNP P19491
C	836	ALA	-	expression tag	UNP P19491
C	837	LEU	-	expression tag	UNP P19491
C	838	THR	-	expression tag	UNP P19491
C	839	LEU	-	expression tag	UNP P19491
C	840	LEU	-	expression tag	UNP P19491
C	841	SER	-	expression tag	UNP P19491
C	842	SER	-	expression tag	UNP P19491
C	843	VAL	-	expression tag	UNP P19491
C	844	PHE	-	expression tag	UNP P19491
C	845	ALA	-	expression tag	UNP P19491
C	846	VAL	-	expression tag	UNP P19491
C	847	CYS	-	expression tag	UNP P19491
C	848	GLY	-	expression tag	UNP P19491
C	849	LEU	-	expression tag	UNP P19491
C	850	GLY	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	851	LEU	-	expression tag	UNP P19491
C	852	LEU	-	expression tag	UNP P19491
C	853	GLY	-	expression tag	UNP P19491
C	854	ILE	-	expression tag	UNP P19491
C	855	ALA	-	expression tag	UNP P19491
C	856	VAL	-	expression tag	UNP P19491
C	857	SER	-	expression tag	UNP P19491
C	858	THR	-	expression tag	UNP P19491
C	859	ASP	-	expression tag	UNP P19491
C	860	TYR	-	expression tag	UNP P19491
C	861	TRP	-	expression tag	UNP P19491
C	862	LEU	-	expression tag	UNP P19491
C	863	TYR	-	expression tag	UNP P19491
C	864	LEU	-	expression tag	UNP P19491
C	865	GLU	-	expression tag	UNP P19491
C	866	GLU	-	expression tag	UNP P19491
C	867	GLY	-	expression tag	UNP P19491
C	868	ILE	-	expression tag	UNP P19491
C	869	ILE	-	expression tag	UNP P19491
C	870	LEU	-	expression tag	UNP P19491
C	871	PRO	-	expression tag	UNP P19491
C	872	GLN	-	expression tag	UNP P19491
C	873	ASN	-	expression tag	UNP P19491
C	874	GLN	-	expression tag	UNP P19491
C	875	SER	-	expression tag	UNP P19491
C	876	THR	-	expression tag	UNP P19491
C	877	GLU	-	expression tag	UNP P19491
C	878	VAL	-	expression tag	UNP P19491
C	879	LYS	-	expression tag	UNP P19491
C	880	MET	-	expression tag	UNP P19491
C	881	SER	-	expression tag	UNP P19491
C	882	LEU	-	expression tag	UNP P19491
C	883	HIS	-	expression tag	UNP P19491
C	884	SER	-	expression tag	UNP P19491
C	885	GLY	-	expression tag	UNP P19491
C	886	LEU	-	expression tag	UNP P19491
C	887	TRP	-	expression tag	UNP P19491
C	888	ARG	-	expression tag	UNP P19491
C	889	VAL	-	expression tag	UNP P19491
C	890	CYS	-	expression tag	UNP P19491
C	891	PHE	-	expression tag	UNP P19491
C	892	LEU	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	893	ALA	-	expression tag	UNP P19491
C	894	GLY	-	expression tag	UNP P19491
C	895	GLU	-	expression tag	UNP P19491
C	896	GLU	-	expression tag	UNP P19491
C	897	ARG	-	expression tag	UNP P19491
C	898	GLY	-	expression tag	UNP P19491
C	899	ARG	-	expression tag	UNP P19491
C	900	CYS	-	expression tag	UNP P19491
C	901	PHE	-	expression tag	UNP P19491
C	902	THR	-	expression tag	UNP P19491
C	903	ILE	-	expression tag	UNP P19491
C	904	GLU	-	expression tag	UNP P19491
C	905	TYR	-	expression tag	UNP P19491
C	906	VAL	-	expression tag	UNP P19491
C	907	MET	-	expression tag	UNP P19491
C	908	PRO	-	expression tag	UNP P19491
C	909	MET	-	expression tag	UNP P19491
C	910	ASN	-	expression tag	UNP P19491
C	911	SER	-	expression tag	UNP P19491
C	912	GLN	-	expression tag	UNP P19491
C	913	MET	-	expression tag	UNP P19491
C	914	THR	-	expression tag	UNP P19491
C	915	SER	-	expression tag	UNP P19491
C	916	GLU	-	expression tag	UNP P19491
C	917	SER	-	expression tag	UNP P19491
C	918	THR	-	expression tag	UNP P19491
C	919	VAL	-	expression tag	UNP P19491
C	920	ASN	-	expression tag	UNP P19491
C	921	VAL	-	expression tag	UNP P19491
C	922	LEU	-	expression tag	UNP P19491
C	923	LYS	-	expression tag	UNP P19491
C	924	MET	-	expression tag	UNP P19491
C	925	ILE	-	expression tag	UNP P19491
C	926	ARG	-	expression tag	UNP P19491
C	927	SER	-	expression tag	UNP P19491
C	928	ALA	-	expression tag	UNP P19491
C	929	THR	-	expression tag	UNP P19491
C	930	PRO	-	expression tag	UNP P19491
C	931	PHE	-	expression tag	UNP P19491
C	932	PRO	-	expression tag	UNP P19491
C	933	LEU	-	expression tag	UNP P19491
C	934	VAL	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	935	SER	-	expression tag	UNP P19491
C	936	LEU	-	expression tag	UNP P19491
C	937	PHE	-	expression tag	UNP P19491
C	938	PHE	-	expression tag	UNP P19491
C	939	MET	-	expression tag	UNP P19491
C	940	PHE	-	expression tag	UNP P19491
C	941	ILE	-	expression tag	UNP P19491
C	942	GLY	-	expression tag	UNP P19491
C	943	PHE	-	expression tag	UNP P19491
C	944	ILE	-	expression tag	UNP P19491
C	945	LEU	-	expression tag	UNP P19491
C	946	SER	-	expression tag	UNP P19491
C	947	ASN	-	expression tag	UNP P19491
C	948	ILE	-	expression tag	UNP P19491
C	949	GLY	-	expression tag	UNP P19491
C	950	HIS	-	expression tag	UNP P19491
C	951	ILE	-	expression tag	UNP P19491
C	952	ARG	-	expression tag	UNP P19491
C	953	PRO	-	expression tag	UNP P19491
C	954	HIS	-	expression tag	UNP P19491
C	955	ARG	-	expression tag	UNP P19491
C	956	THR	-	expression tag	UNP P19491
C	957	ILE	-	expression tag	UNP P19491
C	958	LEU	-	expression tag	UNP P19491
C	959	ALA	-	expression tag	UNP P19491
C	960	PHE	-	expression tag	UNP P19491
C	961	VAL	-	expression tag	UNP P19491
C	962	SER	-	expression tag	UNP P19491
C	963	GLY	-	expression tag	UNP P19491
C	964	ILE	-	expression tag	UNP P19491
C	965	PHE	-	expression tag	UNP P19491
C	966	PHE	-	expression tag	UNP P19491
C	967	ILE	-	expression tag	UNP P19491
C	968	LEU	-	expression tag	UNP P19491
C	969	SER	-	expression tag	UNP P19491
C	970	GLY	-	expression tag	UNP P19491
C	971	LEU	-	expression tag	UNP P19491
C	972	SER	-	expression tag	UNP P19491
C	973	LEU	-	expression tag	UNP P19491
C	974	VAL	-	expression tag	UNP P19491
C	975	VAL	-	expression tag	UNP P19491
C	976	GLY	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	977	LEU	-	expression tag	UNP P19491
C	978	VAL	-	expression tag	UNP P19491
C	979	LEU	-	expression tag	UNP P19491
C	980	TYR	-	expression tag	UNP P19491
C	981	ILE	-	expression tag	UNP P19491
C	982	SER	-	expression tag	UNP P19491
C	983	SER	-	expression tag	UNP P19491
C	984	ILE	-	expression tag	UNP P19491
C	985	ASN	-	expression tag	UNP P19491
C	986	ASP	-	expression tag	UNP P19491
C	987	GLU	-	expression tag	UNP P19491
C	988	MET	-	expression tag	UNP P19491
C	989	LEU	-	expression tag	UNP P19491
C	990	ASN	-	expression tag	UNP P19491
C	991	ARG	-	expression tag	UNP P19491
C	992	THR	-	expression tag	UNP P19491
C	993	LYS	-	expression tag	UNP P19491
C	994	ASP	-	expression tag	UNP P19491
C	995	ALA	-	expression tag	UNP P19491
C	996	GLU	-	expression tag	UNP P19491
C	997	THR	-	expression tag	UNP P19491
C	998	TYR	-	expression tag	UNP P19491
C	999	PHE	-	expression tag	UNP P19491
C	1000	ASN	-	expression tag	UNP P19491
C	1001	TYR	-	expression tag	UNP P19491
C	1002	LYS	-	expression tag	UNP P19491
C	1003	TYR	-	expression tag	UNP P19491
C	1004	GLY	-	expression tag	UNP P19491
C	1005	TRP	-	expression tag	UNP P19491
C	1006	SER	-	expression tag	UNP P19491
C	1007	PHE	-	expression tag	UNP P19491
C	1008	ALA	-	expression tag	UNP P19491
C	1009	PHE	-	expression tag	UNP P19491
C	1010	ALA	-	expression tag	UNP P19491
C	1011	ALA	-	expression tag	UNP P19491
C	1012	ILE	-	expression tag	UNP P19491
C	1013	SER	-	expression tag	UNP P19491
C	1014	PHE	-	expression tag	UNP P19491
C	1015	LEU	-	expression tag	UNP P19491
C	1016	LEU	-	expression tag	UNP P19491
C	1017	THR	-	expression tag	UNP P19491
C	1018	GLU	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1019	SER	-	expression tag	UNP P19491
C	1020	ALA	-	expression tag	UNP P19491
C	1021	GLY	-	expression tag	UNP P19491
C	1022	VAL	-	expression tag	UNP P19491
C	1023	MET	-	expression tag	UNP P19491
C	1024	SER	-	expression tag	UNP P19491
C	1025	VAL	-	expression tag	UNP P19491
C	1026	TYR	-	expression tag	UNP P19491
C	1027	LEU	-	expression tag	UNP P19491
C	1028	PHE	-	expression tag	UNP P19491
C	1029	MET	-	expression tag	UNP P19491
C	1030	LYS	-	expression tag	UNP P19491
C	1031	ARG	-	expression tag	UNP P19491
C	1032	TYR	-	expression tag	UNP P19491
C	1033	THR	-	expression tag	UNP P19491
C	1034	ALA	-	expression tag	UNP P19491
C	1035	GLU	-	expression tag	UNP P19491
C	1036	THR	-	expression tag	UNP P19491
C	1037	GLY	-	expression tag	UNP P19491
C	1038	GLY	-	expression tag	UNP P19491
C	1039	LEU	-	expression tag	UNP P19491
C	1040	VAL	-	expression tag	UNP P19491
C	1041	PRO	-	expression tag	UNP P19491
C	1042	ARG	-	expression tag	UNP P19491
C	1043	GLY	-	expression tag	UNP P19491
C	1044	SER	-	expression tag	UNP P19491
C	1045	ALA	-	expression tag	UNP P19491
C	1046	ALA	-	expression tag	UNP P19491
C	1047	ALA	-	expression tag	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	744	THR	ASN	conflict	UNP P19491
D	745	PRO	ALA	conflict	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	754	SER	ASN	conflict	UNP P19491
D	758	VAL	LEU	conflict	UNP P19491
D	775	ALA	SER	conflict	UNP P19491
D	776	LYS	GLY	conflict	UNP P19491
D	777	ASP	GLY	conflict	UNP P19491
D	778	SER	GLY	conflict	UNP P19491
D	779	GLY	ASP	conflict	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	THR	-	expression tag	UNP P19491
D	829	GLY	-	expression tag	UNP P19491
D	830	SER	-	expression tag	UNP P19491
D	831	ALA	-	expression tag	UNP P19491
D	832	CYS	-	expression tag	UNP P19491
D	833	GLY	-	expression tag	UNP P19491
D	834	ARG	-	expression tag	UNP P19491
D	835	LYS	-	expression tag	UNP P19491
D	836	ALA	-	expression tag	UNP P19491
D	837	LEU	-	expression tag	UNP P19491
D	838	THR	-	expression tag	UNP P19491
D	839	LEU	-	expression tag	UNP P19491
D	840	LEU	-	expression tag	UNP P19491
D	841	SER	-	expression tag	UNP P19491
D	842	SER	-	expression tag	UNP P19491
D	843	VAL	-	expression tag	UNP P19491
D	844	PHE	-	expression tag	UNP P19491
D	845	ALA	-	expression tag	UNP P19491
D	846	VAL	-	expression tag	UNP P19491
D	847	CYS	-	expression tag	UNP P19491
D	848	GLY	-	expression tag	UNP P19491
D	849	LEU	-	expression tag	UNP P19491
D	850	GLY	-	expression tag	UNP P19491
D	851	LEU	-	expression tag	UNP P19491
D	852	LEU	-	expression tag	UNP P19491
D	853	GLY	-	expression tag	UNP P19491
D	854	ILE	-	expression tag	UNP P19491
D	855	ALA	-	expression tag	UNP P19491
D	856	VAL	-	expression tag	UNP P19491
D	857	SER	-	expression tag	UNP P19491
D	858	THR	-	expression tag	UNP P19491
D	859	ASP	-	expression tag	UNP P19491
D	860	TYR	-	expression tag	UNP P19491
D	861	TRP	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	862	LEU	-	expression tag	UNP P19491
D	863	TYR	-	expression tag	UNP P19491
D	864	LEU	-	expression tag	UNP P19491
D	865	GLU	-	expression tag	UNP P19491
D	866	GLU	-	expression tag	UNP P19491
D	867	GLY	-	expression tag	UNP P19491
D	868	ILE	-	expression tag	UNP P19491
D	869	ILE	-	expression tag	UNP P19491
D	870	LEU	-	expression tag	UNP P19491
D	871	PRO	-	expression tag	UNP P19491
D	872	GLN	-	expression tag	UNP P19491
D	873	ASN	-	expression tag	UNP P19491
D	874	GLN	-	expression tag	UNP P19491
D	875	SER	-	expression tag	UNP P19491
D	876	THR	-	expression tag	UNP P19491
D	877	GLU	-	expression tag	UNP P19491
D	878	VAL	-	expression tag	UNP P19491
D	879	LYS	-	expression tag	UNP P19491
D	880	MET	-	expression tag	UNP P19491
D	881	SER	-	expression tag	UNP P19491
D	882	LEU	-	expression tag	UNP P19491
D	883	HIS	-	expression tag	UNP P19491
D	884	SER	-	expression tag	UNP P19491
D	885	GLY	-	expression tag	UNP P19491
D	886	LEU	-	expression tag	UNP P19491
D	887	TRP	-	expression tag	UNP P19491
D	888	ARG	-	expression tag	UNP P19491
D	889	VAL	-	expression tag	UNP P19491
D	890	CYS	-	expression tag	UNP P19491
D	891	PHE	-	expression tag	UNP P19491
D	892	LEU	-	expression tag	UNP P19491
D	893	ALA	-	expression tag	UNP P19491
D	894	GLY	-	expression tag	UNP P19491
D	895	GLU	-	expression tag	UNP P19491
D	896	GLU	-	expression tag	UNP P19491
D	897	ARG	-	expression tag	UNP P19491
D	898	GLY	-	expression tag	UNP P19491
D	899	ARG	-	expression tag	UNP P19491
D	900	CYS	-	expression tag	UNP P19491
D	901	PHE	-	expression tag	UNP P19491
D	902	THR	-	expression tag	UNP P19491
D	903	ILE	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	904	GLU	-	expression tag	UNP P19491
D	905	TYR	-	expression tag	UNP P19491
D	906	VAL	-	expression tag	UNP P19491
D	907	MET	-	expression tag	UNP P19491
D	908	PRO	-	expression tag	UNP P19491
D	909	MET	-	expression tag	UNP P19491
D	910	ASN	-	expression tag	UNP P19491
D	911	SER	-	expression tag	UNP P19491
D	912	GLN	-	expression tag	UNP P19491
D	913	MET	-	expression tag	UNP P19491
D	914	THR	-	expression tag	UNP P19491
D	915	SER	-	expression tag	UNP P19491
D	916	GLU	-	expression tag	UNP P19491
D	917	SER	-	expression tag	UNP P19491
D	918	THR	-	expression tag	UNP P19491
D	919	VAL	-	expression tag	UNP P19491
D	920	ASN	-	expression tag	UNP P19491
D	921	VAL	-	expression tag	UNP P19491
D	922	LEU	-	expression tag	UNP P19491
D	923	LYS	-	expression tag	UNP P19491
D	924	MET	-	expression tag	UNP P19491
D	925	ILE	-	expression tag	UNP P19491
D	926	ARG	-	expression tag	UNP P19491
D	927	SER	-	expression tag	UNP P19491
D	928	ALA	-	expression tag	UNP P19491
D	929	THR	-	expression tag	UNP P19491
D	930	PRO	-	expression tag	UNP P19491
D	931	PHE	-	expression tag	UNP P19491
D	932	PRO	-	expression tag	UNP P19491
D	933	LEU	-	expression tag	UNP P19491
D	934	VAL	-	expression tag	UNP P19491
D	935	SER	-	expression tag	UNP P19491
D	936	LEU	-	expression tag	UNP P19491
D	937	PHE	-	expression tag	UNP P19491
D	938	PHE	-	expression tag	UNP P19491
D	939	MET	-	expression tag	UNP P19491
D	940	PHE	-	expression tag	UNP P19491
D	941	ILE	-	expression tag	UNP P19491
D	942	GLY	-	expression tag	UNP P19491
D	943	PHE	-	expression tag	UNP P19491
D	944	ILE	-	expression tag	UNP P19491
D	945	LEU	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	946	SER	-	expression tag	UNP P19491
D	947	ASN	-	expression tag	UNP P19491
D	948	ILE	-	expression tag	UNP P19491
D	949	GLY	-	expression tag	UNP P19491
D	950	HIS	-	expression tag	UNP P19491
D	951	ILE	-	expression tag	UNP P19491
D	952	ARG	-	expression tag	UNP P19491
D	953	PRO	-	expression tag	UNP P19491
D	954	HIS	-	expression tag	UNP P19491
D	955	ARG	-	expression tag	UNP P19491
D	956	THR	-	expression tag	UNP P19491
D	957	ILE	-	expression tag	UNP P19491
D	958	LEU	-	expression tag	UNP P19491
D	959	ALA	-	expression tag	UNP P19491
D	960	PHE	-	expression tag	UNP P19491
D	961	VAL	-	expression tag	UNP P19491
D	962	SER	-	expression tag	UNP P19491
D	963	GLY	-	expression tag	UNP P19491
D	964	ILE	-	expression tag	UNP P19491
D	965	PHE	-	expression tag	UNP P19491
D	966	PHE	-	expression tag	UNP P19491
D	967	ILE	-	expression tag	UNP P19491
D	968	LEU	-	expression tag	UNP P19491
D	969	SER	-	expression tag	UNP P19491
D	970	GLY	-	expression tag	UNP P19491
D	971	LEU	-	expression tag	UNP P19491
D	972	SER	-	expression tag	UNP P19491
D	973	LEU	-	expression tag	UNP P19491
D	974	VAL	-	expression tag	UNP P19491
D	975	VAL	-	expression tag	UNP P19491
D	976	GLY	-	expression tag	UNP P19491
D	977	LEU	-	expression tag	UNP P19491
D	978	VAL	-	expression tag	UNP P19491
D	979	LEU	-	expression tag	UNP P19491
D	980	TYR	-	expression tag	UNP P19491
D	981	ILE	-	expression tag	UNP P19491
D	982	SER	-	expression tag	UNP P19491
D	983	SER	-	expression tag	UNP P19491
D	984	ILE	-	expression tag	UNP P19491
D	985	ASN	-	expression tag	UNP P19491
D	986	ASP	-	expression tag	UNP P19491
D	987	GLU	-	expression tag	UNP P19491

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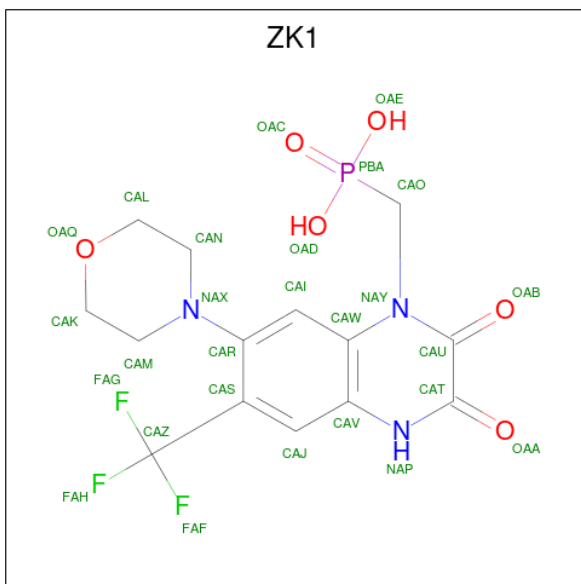
Chain	Residue	Modelled	Actual	Comment	Reference
D	988	MET	-	expression tag	UNP P19491
D	989	LEU	-	expression tag	UNP P19491
D	990	ASN	-	expression tag	UNP P19491
D	991	ARG	-	expression tag	UNP P19491
D	992	THR	-	expression tag	UNP P19491
D	993	LYS	-	expression tag	UNP P19491
D	994	ASP	-	expression tag	UNP P19491
D	995	ALA	-	expression tag	UNP P19491
D	996	GLU	-	expression tag	UNP P19491
D	997	THR	-	expression tag	UNP P19491
D	998	TYR	-	expression tag	UNP P19491
D	999	PHE	-	expression tag	UNP P19491
D	1000	ASN	-	expression tag	UNP P19491
D	1001	TYR	-	expression tag	UNP P19491
D	1002	LYS	-	expression tag	UNP P19491
D	1003	TYR	-	expression tag	UNP P19491
D	1004	GLY	-	expression tag	UNP P19491
D	1005	TRP	-	expression tag	UNP P19491
D	1006	SER	-	expression tag	UNP P19491
D	1007	PHE	-	expression tag	UNP P19491
D	1008	ALA	-	expression tag	UNP P19491
D	1009	PHE	-	expression tag	UNP P19491
D	1010	ALA	-	expression tag	UNP P19491
D	1011	ALA	-	expression tag	UNP P19491
D	1012	ILE	-	expression tag	UNP P19491
D	1013	SER	-	expression tag	UNP P19491
D	1014	PHE	-	expression tag	UNP P19491
D	1015	LEU	-	expression tag	UNP P19491
D	1016	LEU	-	expression tag	UNP P19491
D	1017	THR	-	expression tag	UNP P19491
D	1018	GLU	-	expression tag	UNP P19491
D	1019	SER	-	expression tag	UNP P19491
D	1020	ALA	-	expression tag	UNP P19491
D	1021	GLY	-	expression tag	UNP P19491
D	1022	VAL	-	expression tag	UNP P19491
D	1023	MET	-	expression tag	UNP P19491
D	1024	SER	-	expression tag	UNP P19491
D	1025	VAL	-	expression tag	UNP P19491
D	1026	TYR	-	expression tag	UNP P19491
D	1027	LEU	-	expression tag	UNP P19491
D	1028	PHE	-	expression tag	UNP P19491
D	1029	MET	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1030	LYS	-	expression tag	UNP P19491
D	1031	ARG	-	expression tag	UNP P19491
D	1032	TYR	-	expression tag	UNP P19491
D	1033	THR	-	expression tag	UNP P19491
D	1034	ALA	-	expression tag	UNP P19491
D	1035	GLU	-	expression tag	UNP P19491
D	1036	THR	-	expression tag	UNP P19491
D	1037	GLY	-	expression tag	UNP P19491
D	1038	GLY	-	expression tag	UNP P19491
D	1039	LEU	-	expression tag	UNP P19491
D	1040	VAL	-	expression tag	UNP P19491
D	1041	PRO	-	expression tag	UNP P19491
D	1042	ARG	-	expression tag	UNP P19491
D	1043	GLY	-	expression tag	UNP P19491
D	1044	SER	-	expression tag	UNP P19491
D	1045	ALA	-	expression tag	UNP P19491
D	1046	ALA	-	expression tag	UNP P19491
D	1047	ALA	-	expression tag	UNP P19491

- Molecule 2 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C₁₄H₁₅F₃N₃O₆P) (labeled as "Ligand of Interest" by depositor).



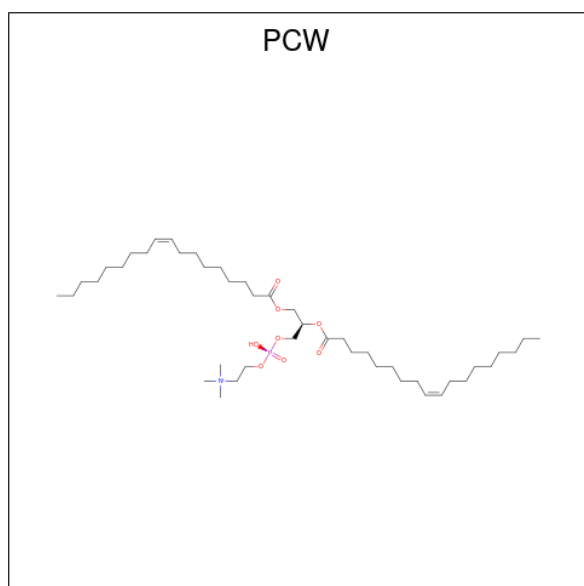
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	F	N	O		P
2	A	1	27	14	3	3	6	1	0

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Mol	Chain	Residues	Atoms					AltConf	
			Total	C	F	N	O		P
2	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C₄₄H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total	C	N	O	P	0
			183	153	3	24	3	
3	A	1	Total	C	N	O	P	0
			183	153	3	24	3	
3	A	1	Total	C	N	O	P	0
			183	153	3	24	3	
3	A	1	Total	C	N	O	P	0
			183	153	3	24	3	
3	A	1	Total	C	N	O	P	0
			183	153	3	24	3	
3	A	1	Total	C	N	O	P	0
			183	153	3	24	3	
3	B	1	Total	C	N	O	P	0
			157	127	3	24	3	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	B	1	Total 157	C 127	N 3	O 24	P 3	0
3	B	1	Total 157	C 127	N 3	O 24	P 3	0
3	B	1	Total 157	C 127	N 3	O 24	P 3	0
3	B	1	Total 157	C 127	N 3	O 24	P 3	0
3	C	1	Total 170	C 140	N 3	O 24	P 3	0
3	C	1	Total 170	C 140	N 3	O 24	P 3	0
3	C	1	Total 170	C 140	N 3	O 24	P 3	0
3	C	1	Total 170	C 140	N 3	O 24	P 3	0
3	C	1	Total 170	C 140	N 3	O 24	P 3	0
3	C	1	Total 170	C 140	N 3	O 24	P 3	0
3	C	1	Total 170	C 140	N 3	O 24	P 3	0
3	D	1	Total 170	C 140	N 3	O 24	P 3	0
3	D	1	Total 170	C 140	N 3	O 24	P 3	0
3	D	1	Total 170	C 140	N 3	O 24	P 3	0
3	D	1	Total 170	C 140	N 3	O 24	P 3	0
3	D	1	Total 170	C 140	N 3	O 24	P 3	0
3	D	1	Total 170	C 140	N 3	O 24	P 3	0

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	111527	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.137	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (\AA)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PCW, ZK1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/4885	0.52	1/6596 (0.0%)
1	B	0.32	0/3280	0.49	0/4425
1	C	0.32	0/4885	0.51	1/6596 (0.0%)
1	D	0.32	0/3280	0.49	0/4425
All	All	0.32	0/16330	0.50	2/22042 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	882	LEU	CA-CB-CG	6.71	130.75	115.30
1	C	882	LEU	CA-CB-CG	6.71	130.72	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4780	0	4844	11	0
1	B	3211	0	3257	6	0
1	C	4780	0	4844	14	0
1	D	3211	0	3257	6	0
2	A	27	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	13	0	0
2	C	27	0	13	0	0
2	D	27	0	13	0	0
3	A	183	0	258	5	0
3	B	157	0	218	6	0
3	C	170	0	238	6	0
3	D	170	0	238	8	0
All	All	16770	0	17206	61	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 2.

All (61) 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)
1:C:544:SER:OG	1:C:569:ASN:ND2	2.37	0.58
1:A:869:ILE:HG22	1:A:876:THR:HG22	1.87	0.57
1:A:544:SER:OG	1:A:569:ASN:ND2	2.37	0.56
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.88	0.55
1:D:651:ASP:OD2	1:D:684:ARG:NH2	2.40	0.55
1:C:869:ILE:HG22	1:C:876:THR:HG22	1.87	0.55
1:B:466:GLU:HG2	1:B:471:LYS:HE3	1.89	0.55
1:B:651:ASP:OD2	1:B:684:ARG:NH2	2.40	0.55
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.88	0.54
1:D:466:GLU:HG2	1:D:471:LYS:HE3	1.89	0.54
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.94	0.49
1:C:650:LEU:HD23	1:C:652:SER:H	1.78	0.49
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.94	0.49
1:A:650:LEU:HD23	1:A:652:SER:H	1.78	0.49
1:A:671:TRP:HE1	1:A:675:ARG:HH21	1.63	0.47
3:A:1102:PCW:H152	3:A:1102:PCW:H121	1.69	0.47
1:B:489:ILE:HD12	1:B:735:ALA:HB1	1.97	0.47
1:C:489:ILE:HD12	1:C:735:ALA:HB1	1.97	0.47
1:D:526:TRP:HB3	3:D:1103:PCW:H361	1.97	0.46
1:A:489:ILE:HD12	1:A:735:ALA:HB1	1.97	0.46
3:B:1106:PCW:H211	3:B:1106:PCW:H182	1.71	0.46
3:D:1103:PCW:H322	3:D:1103:PCW:H351	1.65	0.46
1:C:544:SER:HG	1:C:569:ASN:HD21	1.63	0.45
1:A:948:ILE:HG13	1:A:958:LEU:HD13	1.98	0.45
1:D:489:ILE:HD12	1:D:735:ALA:HB1	1.97	0.45
1:C:671:TRP:HE1	1:C:675:ARG:HH21	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1101:PCW:H211	3:D:1101:PCW:H182	1.70	0.45
2:A:1101:ZK1:HAI	2:A:1101:ZK1:HAOA	1.76	0.45
1:A:922:LEU:HD23	1:A:925:ILE:HD12	1.99	0.44
1:C:922:LEU:HD23	1:C:925:ILE:HD12	1.99	0.44
1:C:466:GLU:HG2	1:C:471:LYS:HE3	1.99	0.44
1:A:831:ALA:HB1	1:A:834:ARG:HB2	2.00	0.44
3:B:1102:PCW:H11	3:B:1103:PCW:H32	2.00	0.44
1:A:466:GLU:HG2	1:A:471:LYS:HE3	1.99	0.44
1:C:948:ILE:HG13	1:C:958:LEU:HD13	1.98	0.44
3:D:1103:PCW:H121	3:D:1103:PCW:H152	1.76	0.44
3:A:1102:PCW:H40	3:A:1102:PCW:H372	1.80	0.44
1:C:831:ALA:HB1	1:C:834:ARG:HB2	2.00	0.43
3:C:1102:PCW:H141	3:C:1102:PCW:H171	1.84	0.43
3:A:1104:PCW:H142	3:A:1104:PCW:H171	1.79	0.43
3:A:1102:PCW:H321	3:A:1102:PCW:H352	1.83	0.43
3:C:1102:PCW:H121	3:C:1102:PCW:H152	1.71	0.43
3:C:1103:PCW:H382	3:C:1103:PCW:H412	1.82	0.43
1:A:399:THR:HG21	1:A:406:VAL:HG21	2.01	0.43
3:C:1102:PCW:H372	3:C:1102:PCW:H40	1.63	0.42
3:A:1104:PCW:H372	3:A:1104:PCW:H342	1.79	0.42
3:D:1101:PCW:H142	3:D:1101:PCW:H171	1.67	0.42
1:C:399:THR:HG21	1:C:406:VAL:HG21	2.01	0.42
1:D:405:TYR:CD2	1:D:478:PRO:HG3	2.55	0.42
3:D:1103:PCW:H282	3:D:1103:PCW:H252	1.92	0.42
3:C:1104:PCW:H171	3:C:1104:PCW:H142	1.82	0.41
3:B:1106:PCW:H171	3:B:1106:PCW:H142	1.67	0.41
3:B:1102:PCW:H121	3:B:1102:PCW:H152	1.76	0.41
3:B:1102:PCW:H351	3:B:1102:PCW:H322	1.66	0.41
3:C:1107:PCW:H171	3:C:1107:PCW:H142	1.79	0.41
1:B:606:TRP:CG	1:C:587:GLN:HG3	2.56	0.41
3:D:1103:PCW:H11	3:D:1104:PCW:H32	2.03	0.41
1:C:546:PHE:HD2	1:C:548:PRO:HD2	1.86	0.40
3:D:1103:PCW:H41	3:D:1103:PCW:H82	1.89	0.40
3:B:1103:PCW:H73	3:B:1103:PCW:H42	1.84	0.40
1:B:405:TYR:CD2	1:B:478:PRO:HG3	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	603/1038 (58%)	580 (96%)	23 (4%)	0	100	100
1	B	408/1038 (39%)	395 (97%)	13 (3%)	0	100	100
1	C	603/1038 (58%)	580 (96%)	23 (4%)	0	100	100
1	D	408/1038 (39%)	396 (97%)	12 (3%)	0	100	100
All	All	2022/4152 (49%)	1951 (96%)	71 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/883 (59%)	511 (99%)	6 (1%)	71	83
1	B	347/883 (39%)	345 (99%)	2 (1%)	86	91
1	C	517/883 (59%)	511 (99%)	6 (1%)	71	83
1	D	347/883 (39%)	345 (99%)	2 (1%)	86	91
All	All	1728/3532 (49%)	1712 (99%)	16 (1%)	79	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	393	LYS
1	A	873	ASN

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Mol	Chain	Res	Type
1	A	882	LEU
1	A	907	MET
1	A	920	ASN
1	A	993	LYS
1	B	410	LYS
1	B	764	ASN
1	C	393	LYS
1	C	873	ASN
1	C	882	LEU
1	C	907	MET
1	C	920	ASN
1	C	993	LYS
1	D	410	LYS
1	D	764	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	873	ASN
1	A	920	ASN
1	B	764	ASN
1	C	873	ASN
1	C	920	ASN
1	D	764	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

28 ligands 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
3	PCW	D	1106	-	10,10,53	0.78	0	9,9,61	0.32	0
3	PCW	A	1105	-	10,10,53	0.78	0	9,9,61	0.27	0
3	PCW	D	1104	-	42,42,53	1.24	3 (7%)	48,50,61	1.10	3 (6%)
3	PCW	B	1106	-	10,10,53	0.78	0	9,9,61	0.33	0
3	PCW	C	1105	-	10,10,53	0.80	0	9,9,61	0.23	0
2	ZK1	B	1101	-	28,29,29	2.75	8 (28%)	42,45,45	1.81	11 (26%)
3	PCW	C	1104	-	40,40,53	1.23	4 (10%)	46,48,61	1.05	3 (6%)
3	PCW	D	1103	-	50,50,53	1.16	4 (8%)	56,58,61	0.99	3 (5%)
3	PCW	B	1102	-	50,50,53	1.16	4 (8%)	56,58,61	0.99	3 (5%)
3	PCW	A	1106	-	12,12,53	0.79	0	11,11,61	0.39	0
3	PCW	C	1106	-	12,12,53	0.79	0	11,11,61	0.38	0
3	PCW	C	1103	-	42,42,53	1.22	4 (9%)	48,50,61	1.03	3 (6%)
3	PCW	D	1105	-	40,40,53	1.25	5 (12%)	46,48,61	1.07	3 (6%)
3	PCW	C	1107	-	10,10,53	0.78	0	9,9,61	0.36	0
2	ZK1	D	1102	-	28,29,29	2.76	8 (28%)	42,45,45	1.81	11 (26%)
2	ZK1	A	1101	-	28,29,29	2.76	8 (28%)	42,45,45	1.77	11 (26%)
2	ZK1	C	1101	-	28,29,29	2.76	8 (28%)	42,45,45	1.76	11 (26%)
3	PCW	D	1101	-	10,10,53	0.78	0	9,9,61	0.33	0
3	PCW	A	1102	-	50,50,53	1.18	4 (8%)	56,58,61	1.03	3 (5%)
3	PCW	B	1104	-	40,40,53	1.24	5 (12%)	46,48,61	1.07	3 (6%)
3	PCW	C	1102	-	50,50,53	1.17	4 (8%)	56,58,61	1.02	3 (5%)
3	PCW	B	1103	-	42,42,53	1.24	3 (7%)	48,50,61	1.10	3 (6%)
3	PCW	A	1104	-	40,40,53	1.23	4 (10%)	46,48,61	1.06	3 (6%)
3	PCW	A	1108	-	10,10,53	0.78	0	9,9,61	0.36	0
3	PCW	A	1103	-	42,42,53	1.22	4 (9%)	48,50,61	1.03	3 (6%)
3	PCW	D	1107	-	12,12,53	0.80	0	11,11,61	0.35	0
3	PCW	B	1105	-	10,10,53	0.78	0	9,9,61	0.32	0
3	PCW	A	1107	-	12,12,53	0.80	0	11,11,61	0.36	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
3	PCW	D	1106	-	-	3/8/8/57	-
3	PCW	A	1105	-	-	3/8/8/57	-
3	PCW	D	1104	-	-	24/46/46/57	-
3	PCW	B	1106	-	-	4/8/8/57	-
3	PCW	C	1105	-	-	5/8/8/57	-
2	ZK1	B	1101	-	-	4/13/23/23	0/3/3/3
3	PCW	C	1104	-	-	25/44/44/57	-
3	PCW	D	1103	-	-	26/54/54/57	-
3	PCW	B	1102	-	-	25/54/54/57	-
3	PCW	A	1106	-	-	5/10/10/57	-
3	PCW	C	1106	-	-	5/10/10/57	-
3	PCW	C	1103	-	-	21/46/46/57	-
3	PCW	D	1105	-	-	18/44/44/57	-
3	PCW	C	1107	-	-	3/8/8/57	-
2	ZK1	D	1102	-	-	4/13/23/23	0/3/3/3
2	ZK1	A	1101	-	-	4/13/23/23	0/3/3/3
2	ZK1	C	1101	-	-	5/13/23/23	0/3/3/3
3	PCW	D	1101	-	-	4/8/8/57	-
3	PCW	A	1102	-	-	29/54/54/57	-
3	PCW	B	1104	-	-	22/44/44/57	-
3	PCW	C	1102	-	-	30/54/54/57	-
3	PCW	B	1103	-	-	24/46/46/57	-
3	PCW	A	1104	-	-	28/44/44/57	-
3	PCW	A	1108	-	-	3/8/8/57	-
3	PCW	A	1103	-	-	20/46/46/57	-
3	PCW	D	1107	-	-	3/10/10/57	-
3	PCW	B	1105	-	-	3/8/8/57	-
3	PCW	A	1107	-	-	3/10/10/57	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1102	ZK1	OAA-CAT	8.68	1.40	1.23
2	B	1101	ZK1	OAA-CAT	8.65	1.40	1.23
2	A	1101	ZK1	OAA-CAT	8.55	1.39	1.23
2	C	1101	ZK1	OAA-CAT	8.53	1.39	1.23
2	D	1102	ZK1	OAB-CAU	7.97	1.39	1.23
2	C	1101	ZK1	OAB-CAU	7.96	1.39	1.23
2	B	1101	ZK1	OAB-CAU	7.95	1.39	1.23
2	A	1101	ZK1	OAB-CAU	7.92	1.39	1.23
2	B	1101	ZK1	CAW-NAY	-3.84	1.34	1.41
2	D	1102	ZK1	CAW-NAY	-3.80	1.34	1.41
2	A	1101	ZK1	CAW-NAY	-3.76	1.34	1.41
2	C	1101	ZK1	CAW-NAY	-3.76	1.34	1.41
2	C	1101	ZK1	CAV-NAP	-3.43	1.34	1.39
2	D	1102	ZK1	CAU-NAY	-3.39	1.31	1.38
2	A	1101	ZK1	CAV-NAP	-3.38	1.34	1.39
2	B	1101	ZK1	CAU-NAY	-3.35	1.31	1.38
3	A	1102	PCW	O3-C11	3.34	1.43	1.33
3	C	1102	PCW	O3-C11	3.31	1.43	1.33
3	B	1103	PCW	O3-C11	3.24	1.42	1.33
3	D	1104	PCW	O3-C11	3.24	1.42	1.33
3	A	1103	PCW	O3-C11	3.23	1.42	1.33
3	C	1103	PCW	O3-C11	3.22	1.42	1.33
2	C	1101	ZK1	CAV-CAW	-3.22	1.36	1.40
3	B	1102	PCW	O3-C11	3.20	1.42	1.33
3	D	1103	PCW	O3-C11	3.20	1.42	1.33
3	D	1105	PCW	O3-C11	3.19	1.42	1.33
2	A	1101	ZK1	CAV-CAW	-3.17	1.37	1.40
2	C	1101	ZK1	CAU-NAY	-3.17	1.32	1.38
3	B	1104	PCW	O3-C11	3.16	1.42	1.33
2	A	1101	ZK1	CAU-NAY	-3.16	1.32	1.38
2	D	1102	ZK1	CAV-NAP	-3.14	1.34	1.39
2	B	1101	ZK1	CAV-NAP	-3.13	1.34	1.39
3	C	1104	PCW	O3-C11	3.13	1.42	1.33
3	A	1104	PCW	O3-C11	3.11	1.42	1.33
2	B	1101	ZK1	CAV-CAW	-3.08	1.37	1.40
2	D	1102	ZK1	CAV-CAW	-3.07	1.37	1.40
3	A	1104	PCW	O2-C31	3.06	1.42	1.34
3	C	1104	PCW	O2-C31	3.05	1.42	1.34
3	D	1105	PCW	O2-C31	3.02	1.42	1.34
2	C	1101	ZK1	CAT-NAP	-3.01	1.31	1.35
2	A	1101	ZK1	CAT-NAP	-2.99	1.31	1.35
3	B	1104	PCW	O2-C31	2.99	1.42	1.34
3	D	1104	PCW	O2-C31	2.99	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1103	PCW	O2-C31	2.98	1.42	1.34
3	A	1102	PCW	O2-C31	2.94	1.42	1.34
3	B	1102	PCW	O2-C31	2.93	1.42	1.34
3	D	1103	PCW	O2-C31	2.91	1.42	1.34
3	C	1102	PCW	O2-C31	2.90	1.42	1.34
3	C	1103	PCW	O2-C31	2.87	1.42	1.34
3	A	1103	PCW	O2-C31	2.84	1.42	1.34
3	A	1103	PCW	O2-C2	-2.67	1.39	1.46
3	C	1103	PCW	O2-C2	-2.64	1.40	1.46
3	A	1102	PCW	O2-C2	-2.63	1.40	1.46
3	C	1102	PCW	O2-C2	-2.62	1.40	1.46
2	D	1102	ZK1	CAT-NAP	-2.55	1.32	1.35
2	B	1101	ZK1	CAT-NAP	-2.54	1.32	1.35
3	B	1104	PCW	O2-C2	-2.41	1.40	1.46
3	D	1105	PCW	O2-C2	-2.40	1.40	1.46
3	D	1104	PCW	O2-C2	-2.40	1.40	1.46
3	B	1103	PCW	O2-C2	-2.37	1.40	1.46
3	B	1102	PCW	O2-C2	-2.32	1.40	1.46
3	D	1103	PCW	O2-C2	-2.30	1.40	1.46
3	C	1104	PCW	O2-C2	-2.28	1.40	1.46
3	A	1104	PCW	O2-C2	-2.21	1.41	1.46
2	D	1102	ZK1	CAR-NAX	2.10	1.45	1.41
3	B	1104	PCW	P-O4P	2.09	1.67	1.59
3	B	1102	PCW	P-O4P	2.09	1.67	1.59
2	B	1101	ZK1	CAR-NAX	2.09	1.45	1.41
2	A	1101	ZK1	CAR-NAX	2.08	1.45	1.41
3	D	1105	PCW	P-O4P	2.07	1.67	1.59
3	D	1103	PCW	P-O4P	2.07	1.67	1.59
3	A	1102	PCW	P-O4P	2.07	1.67	1.59
3	C	1103	PCW	P-O4P	2.07	1.67	1.59
3	A	1103	PCW	P-O4P	2.07	1.67	1.59
2	C	1101	ZK1	CAR-NAX	2.07	1.45	1.41
3	C	1102	PCW	P-O4P	2.07	1.67	1.59
3	A	1104	PCW	P-O4P	2.04	1.67	1.59
3	D	1105	PCW	P-O3P	2.04	1.67	1.59
3	B	1104	PCW	P-O3P	2.02	1.67	1.59
3	C	1104	PCW	P-O4P	2.01	1.67	1.59

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1102	ZK1	CAN-NAX-CAM	5.24	123.08	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	ZK1	CAN-NAX-CAM	5.19	122.98	111.52
2	C	1101	ZK1	CAN-NAX-CAM	5.08	122.73	111.52
2	A	1101	ZK1	CAN-NAX-CAM	5.05	122.67	111.52
2	B	1101	ZK1	CAI-CAR-NAX	-4.32	116.13	122.52
2	D	1102	ZK1	CAI-CAR-NAX	-4.28	116.19	122.52
3	C	1102	PCW	O2-C31-C32	4.00	120.11	111.50
3	D	1104	PCW	O2-C31-C32	3.97	120.05	111.50
3	B	1103	PCW	O2-C31-C32	3.95	120.01	111.50
2	A	1101	ZK1	CAV-NAP-CAT	-3.94	119.78	124.80
3	A	1102	PCW	O2-C31-C32	3.93	119.97	111.50
3	D	1105	PCW	O2-C31-C32	3.91	119.94	111.50
3	B	1102	PCW	C8-N-C6	3.91	119.03	108.97
3	D	1103	PCW	C8-N-C6	3.90	119.00	108.97
2	C	1101	ZK1	CAV-NAP-CAT	-3.87	119.87	124.80
3	B	1104	PCW	C8-N-C6	3.87	118.91	108.97
3	D	1105	PCW	C8-N-C6	3.86	118.89	108.97
3	B	1104	PCW	O2-C31-C32	3.85	119.81	111.50
3	D	1104	PCW	C8-N-C6	3.85	118.87	108.97
3	B	1103	PCW	C8-N-C6	3.83	118.82	108.97
2	B	1101	ZK1	CAS-CAR-NAX	3.82	124.29	119.92
3	D	1103	PCW	O2-C31-C32	3.80	119.69	111.50
3	B	1102	PCW	O2-C31-C32	3.79	119.66	111.50
2	D	1102	ZK1	CAS-CAR-NAX	3.77	124.24	119.92
2	B	1101	ZK1	CAV-NAP-CAT	-3.76	120.01	124.80
2	D	1102	ZK1	CAV-NAP-CAT	-3.76	120.01	124.80
3	A	1104	PCW	C8-N-C6	3.71	118.52	108.97
3	C	1104	PCW	C8-N-C6	3.69	118.47	108.97
3	A	1103	PCW	O2-C31-C32	3.65	119.36	111.50
3	C	1103	PCW	O2-C31-C32	3.63	119.32	111.50
2	C	1101	ZK1	CAI-CAR-NAX	-3.60	117.20	122.52
2	A	1101	ZK1	CAI-CAR-NAX	-3.59	117.21	122.52
3	A	1103	PCW	C8-N-C6	3.45	117.84	108.97
3	C	1103	PCW	C8-N-C6	3.44	117.83	108.97
3	C	1102	PCW	C8-N-C6	3.44	117.83	108.97
3	A	1104	PCW	O2-C31-C32	3.43	118.89	111.50
3	A	1102	PCW	C8-N-C6	3.43	117.79	108.97
2	C	1101	ZK1	CAO-NAY-CAU	3.33	119.76	116.51
2	A	1101	ZK1	CAO-NAY-CAU	3.30	119.73	116.51
3	C	1104	PCW	O2-C31-C32	3.27	118.54	111.50
3	A	1102	PCW	O3-C11-C12	3.26	122.13	111.91
3	C	1102	PCW	O3-C11-C12	3.15	121.79	111.91
2	C	1101	ZK1	CAS-CAR-NAX	2.95	123.31	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	ZK1	CAS-CAR-NAX	2.95	123.30	119.92
3	C	1104	PCW	O3-C11-C12	2.77	120.59	111.91
2	C	1101	ZK1	CAT-CAU-NAY	2.77	120.49	117.32
2	A	1101	ZK1	CAT-CAU-NAY	2.75	120.47	117.32
3	A	1103	PCW	O3-C11-C12	2.73	120.47	111.91
3	D	1104	PCW	O3-C11-C12	2.69	120.34	111.91
3	B	1103	PCW	O3-C11-C12	2.68	120.32	111.91
3	C	1103	PCW	O3-C11-C12	2.68	120.31	111.91
2	D	1102	ZK1	CAT-CAU-NAY	2.67	120.38	117.32
2	C	1101	ZK1	FAG-CAZ-CAS	-2.66	108.06	112.70
2	A	1101	ZK1	FAG-CAZ-CAS	-2.66	108.07	112.70
3	B	1104	PCW	O3-C11-C12	2.65	120.23	111.91
2	B	1101	ZK1	CAT-CAU-NAY	2.63	120.34	117.32
3	D	1105	PCW	O3-C11-C12	2.62	120.13	111.91
2	D	1102	ZK1	CAO-NAY-CAU	2.60	119.04	116.51
3	A	1104	PCW	O3-C11-C12	2.58	120.00	111.91
2	B	1101	ZK1	CAO-NAY-CAU	2.53	118.97	116.51
2	A	1101	ZK1	CAW-NAY-CAU	-2.51	119.68	122.79
2	C	1101	ZK1	CAW-NAY-CAU	-2.50	119.70	122.79
2	D	1102	ZK1	FAG-CAZ-CAS	-2.49	108.36	112.70
3	B	1102	PCW	O3-C11-C12	2.47	119.67	111.91
3	D	1103	PCW	O3-C11-C12	2.47	119.66	111.91
2	B	1101	ZK1	FAG-CAZ-CAS	-2.47	108.40	112.70
2	A	1101	ZK1	CAU-CAT-NAP	2.41	119.97	117.49
2	D	1102	ZK1	CAL-CAN-NAX	2.38	114.41	110.02
2	D	1102	ZK1	CAK-CAM-NAX	2.34	114.34	110.02
2	C	1101	ZK1	CAU-CAT-NAP	2.33	119.89	117.49
2	B	1101	ZK1	CAL-CAN-NAX	2.32	114.30	110.02
2	B	1101	ZK1	CAK-CAM-NAX	2.28	114.23	110.02
2	B	1101	ZK1	CAU-CAT-NAP	2.26	119.82	117.49
2	D	1102	ZK1	CAU-CAT-NAP	2.24	119.80	117.49
2	D	1102	ZK1	CAW-NAY-CAU	-2.24	120.02	122.79
2	B	1101	ZK1	CAW-NAY-CAU	-2.23	120.02	122.79
2	A	1101	ZK1	CAK-CAM-NAX	2.12	113.93	110.02
2	C	1101	ZK1	CAL-CAN-NAX	2.07	113.84	110.02
2	C	1101	ZK1	CAK-CAM-NAX	2.07	113.84	110.02
2	A	1101	ZK1	CAL-CAN-NAX	2.07	113.83	110.02

There are no chirality outliers.

All (353) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	ZK1	NAY-CAO-PBA-OAD
2	A	1101	ZK1	NAY-CAO-PBA-OAE
2	C	1101	ZK1	NAY-CAO-PBA-OAD
2	C	1101	ZK1	NAY-CAO-PBA-OAE
3	A	1102	PCW	O3P-C1-C2-O2
3	A	1102	PCW	O4P-C4-C5-N
3	A	1102	PCW	C12-C11-O3-C3
3	A	1102	PCW	O11-C11-O3-C3
3	A	1102	PCW	C32-C31-O2-C2
3	A	1102	PCW	C4-O4P-P-O1P
3	A	1102	PCW	C4-O4P-P-O2P
3	A	1103	PCW	O3P-C1-C2-O2
3	A	1103	PCW	O4P-C4-C5-N
3	A	1103	PCW	C12-C11-O3-C3
3	A	1103	PCW	C4-O4P-P-O1P
3	A	1103	PCW	C4-O4P-P-O2P
3	A	1104	PCW	C1-O3P-P-O1P
3	A	1104	PCW	C1-O3P-P-O2P
3	A	1104	PCW	C1-O3P-P-O4P
3	A	1104	PCW	C4-O4P-P-O3P
3	B	1102	PCW	O4P-C4-C5-N
3	B	1102	PCW	O31-C31-O2-C2
3	B	1103	PCW	O4P-C4-C5-N
3	B	1103	PCW	C4-O4P-P-O2P
3	B	1103	PCW	C4-O4P-P-O3P
3	B	1104	PCW	O4P-C4-C5-N
3	B	1104	PCW	C1-O3P-P-O1P
3	B	1104	PCW	C1-O3P-P-O2P
3	B	1104	PCW	C1-O3P-P-O4P
3	B	1106	PCW	C20-C21-C22-C23
3	C	1102	PCW	O3P-C1-C2-O2
3	C	1102	PCW	O4P-C4-C5-N
3	C	1102	PCW	C12-C11-O3-C3
3	C	1102	PCW	O11-C11-O3-C3
3	C	1102	PCW	C32-C31-O2-C2
3	C	1102	PCW	C4-O4P-P-O1P
3	C	1102	PCW	C4-O4P-P-O2P
3	C	1103	PCW	O3P-C1-C2-O2
3	C	1103	PCW	O4P-C4-C5-N
3	C	1103	PCW	C12-C11-O3-C3
3	C	1103	PCW	C4-O4P-P-O2P
3	C	1104	PCW	C1-O3P-P-O1P
3	C	1104	PCW	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
3	D	1101	PCW	C20-C21-C22-C23
3	D	1103	PCW	O4P-C4-C5-N
3	D	1103	PCW	O31-C31-O2-C2
3	D	1104	PCW	O4P-C4-C5-N
3	D	1104	PCW	C4-O4P-P-O2P
3	D	1104	PCW	C4-O4P-P-O3P
3	D	1105	PCW	O4P-C4-C5-N
3	D	1105	PCW	C1-O3P-P-O1P
3	D	1105	PCW	C1-O3P-P-O2P
3	D	1105	PCW	C1-O3P-P-O4P
3	A	1103	PCW	O11-C11-O3-C3
3	C	1103	PCW	O11-C11-O3-C3
3	B	1103	PCW	O11-C11-O3-C3
3	D	1104	PCW	O11-C11-O3-C3
3	B	1103	PCW	C12-C11-O3-C3
3	D	1104	PCW	C12-C11-O3-C3
3	B	1102	PCW	C32-C31-O2-C2
3	D	1103	PCW	C32-C31-O2-C2
3	D	1105	PCW	C12-C11-O3-C3
3	A	1102	PCW	O31-C31-O2-C2
3	C	1102	PCW	O31-C31-O2-C2
3	D	1105	PCW	O11-C11-O3-C3
3	B	1104	PCW	C12-C11-O3-C3
3	A	1104	PCW	C32-C31-O2-C2
3	B	1104	PCW	O11-C11-O3-C3
3	C	1103	PCW	C32-C31-O2-C2
3	A	1104	PCW	O31-C31-O2-C2
3	B	1104	PCW	C11-C12-C13-C14
3	B	1102	PCW	O3P-C1-C2-O2
3	B	1103	PCW	O3P-C1-C2-O2
3	D	1103	PCW	O3P-C1-C2-O2
3	B	1104	PCW	C13-C14-C15-C16
3	A	1103	PCW	C32-C31-O2-C2
3	C	1104	PCW	C32-C31-O2-C2
3	D	1105	PCW	C13-C14-C15-C16
3	D	1105	PCW	C11-C12-C13-C14
3	C	1104	PCW	C11-C12-C13-C14
3	C	1103	PCW	O31-C31-O2-C2
3	C	1104	PCW	O31-C31-O2-C2
3	A	1104	PCW	C11-C12-C13-C14
3	C	1102	PCW	C11-C12-C13-C14
3	B	1104	PCW	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
3	A	1102	PCW	C4-O4P-P-O3P
3	A	1103	PCW	C4-O4P-P-O3P
3	B	1102	PCW	C4-O4P-P-O3P
3	C	1102	PCW	C4-O4P-P-O3P
3	C	1103	PCW	C4-O4P-P-O3P
3	C	1104	PCW	C1-O3P-P-O4P
3	C	1104	PCW	C4-O4P-P-O3P
3	D	1103	PCW	C4-O4P-P-O3P
3	A	1104	PCW	C12-C11-O3-C3
3	A	1102	PCW	C11-C12-C13-C14
3	A	1103	PCW	O31-C31-O2-C2
3	A	1103	PCW	C11-C12-C13-C14
3	A	1104	PCW	C31-C32-C33-C34
3	D	1103	PCW	C13-C14-C15-C16
3	A	1103	PCW	C34-C35-C36-C37
3	B	1102	PCW	C13-C14-C15-C16
3	D	1104	PCW	C33-C34-C35-C36
3	C	1104	PCW	C12-C11-O3-C3
3	A	1107	PCW	C14-C15-C16-C17
3	C	1102	PCW	C12-C13-C14-C15
3	D	1105	PCW	C34-C35-C36-C37
3	D	1107	PCW	C14-C15-C16-C17
3	C	1104	PCW	C32-C33-C34-C35
3	D	1104	PCW	O3P-C1-C2-O2
3	B	1104	PCW	C32-C33-C34-C35
3	D	1104	PCW	C35-C36-C37-C38
3	D	1105	PCW	C33-C34-C35-C36
3	B	1104	PCW	C34-C35-C36-C37
3	C	1102	PCW	C13-C14-C15-C16
3	A	1103	PCW	C12-C13-C14-C15
3	B	1103	PCW	C33-C34-C35-C36
3	A	1102	PCW	C13-C14-C15-C16
3	B	1106	PCW	C14-C15-C16-C17
3	D	1101	PCW	C14-C15-C16-C17
3	A	1102	PCW	C12-C13-C14-C15
3	B	1103	PCW	C35-C36-C37-C38
3	C	1103	PCW	C34-C35-C36-C37
3	D	1105	PCW	C36-C37-C38-C39
3	A	1103	PCW	C31-C32-C33-C34
3	C	1103	PCW	C11-C12-C13-C14
3	C	1103	PCW	C31-C32-C33-C34
3	A	1104	PCW	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
3	B	1105	PCW	C20-C21-C22-C23
3	D	1106	PCW	C20-C21-C22-C23
3	C	1103	PCW	C12-C13-C14-C15
3	D	1103	PCW	C23-C24-C25-C26
3	A	1104	PCW	C33-C34-C35-C36
3	D	1105	PCW	C35-C36-C37-C38
3	A	1104	PCW	O11-C11-O3-C3
3	B	1103	PCW	C13-C14-C15-C16
3	D	1104	PCW	C13-C14-C15-C16
3	A	1102	PCW	C40-C41-C42-C43
3	C	1102	PCW	C33-C34-C35-C36
3	C	1104	PCW	C13-C14-C15-C16
3	C	1104	PCW	O11-C11-O3-C3
3	A	1102	PCW	C33-C34-C35-C36
3	A	1102	PCW	C41-C42-C43-C44
3	A	1102	PCW	C36-C37-C38-C39
3	A	1105	PCW	C16-C17-C18-C19
3	B	1102	PCW	C20-C21-C22-C23
3	C	1102	PCW	C36-C37-C38-C39
3	C	1105	PCW	C16-C17-C18-C19
3	B	1102	PCW	C32-C33-C34-C35
3	A	1102	PCW	C34-C35-C36-C37
3	D	1103	PCW	C22-C23-C24-C25
3	D	1105	PCW	C32-C33-C34-C35
3	D	1103	PCW	C32-C33-C34-C35
3	D	1104	PCW	C15-C16-C17-C18
3	A	1102	PCW	C14-C15-C16-C17
3	B	1103	PCW	C15-C16-C17-C18
3	C	1104	PCW	C40-C41-C42-C43
3	B	1102	PCW	C21-C22-C23-C24
3	C	1105	PCW	C13-C14-C15-C16
3	B	1102	PCW	C23-C24-C25-C26
3	A	1103	PCW	O3P-C1-C2-C3
3	B	1102	PCW	O3P-C1-C2-C3
3	B	1103	PCW	O3P-C1-C2-C3
3	B	1104	PCW	O3P-C1-C2-C3
3	C	1102	PCW	O3P-C1-C2-C3
3	D	1103	PCW	O3P-C1-C2-C3
3	C	1102	PCW	C41-C42-C43-C44
3	B	1103	PCW	C14-C15-C16-C17
3	D	1104	PCW	C14-C15-C16-C17
3	A	1104	PCW	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
3	A	1106	PCW	C20-C21-C22-C23
3	C	1106	PCW	C20-C21-C22-C23
3	C	1102	PCW	C14-C15-C16-C17
3	A	1102	PCW	C39-C40-C41-C42
3	C	1102	PCW	C35-C36-C37-C38
3	A	1102	PCW	C42-C43-C44-C45
3	C	1102	PCW	C34-C35-C36-C37
3	C	1102	PCW	C42-C43-C44-C45
3	A	1104	PCW	C32-C33-C34-C35
3	C	1102	PCW	C39-C40-C41-C42
3	B	1102	PCW	C22-C23-C24-C25
3	B	1102	PCW	C12-C13-C14-C15
3	C	1104	PCW	C16-C17-C18-C19
3	C	1104	PCW	C1-C2-O2-C31
3	D	1103	PCW	C12-C13-C14-C15
3	A	1106	PCW	C12-C13-C14-C15
3	A	1103	PCW	C13-C14-C15-C16
3	A	1104	PCW	C14-C15-C16-C17
3	A	1102	PCW	C37-C38-C39-C40
3	C	1103	PCW	C13-C14-C15-C16
3	D	1104	PCW	C39-C40-C41-C42
3	A	1102	PCW	O3P-C1-C2-C3
3	D	1104	PCW	O3P-C1-C2-C3
3	D	1105	PCW	O3P-C1-C2-C3
3	A	1106	PCW	C21-C22-C23-C24
3	C	1106	PCW	C21-C22-C23-C24
3	B	1102	PCW	C2-C1-O3P-P
3	B	1104	PCW	C2-C1-O3P-P
3	D	1103	PCW	C2-C1-O3P-P
3	D	1105	PCW	C2-C1-O3P-P
3	B	1103	PCW	C39-C40-C41-C42
3	A	1104	PCW	C34-C35-C36-C37
3	B	1104	PCW	C33-C34-C35-C36
3	C	1104	PCW	C1-C2-C3-O3
3	A	1104	PCW	C16-C17-C18-C19
3	D	1103	PCW	C21-C22-C23-C24
3	C	1106	PCW	C12-C13-C14-C15
3	B	1102	PCW	C11-C12-C13-C14
3	C	1102	PCW	C40-C41-C42-C43
3	B	1103	PCW	C42-C43-C44-C45
3	B	1104	PCW	O2-C2-C3-O3
3	C	1102	PCW	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	C	1105	PCW	C14-C15-C16-C17
3	D	1103	PCW	C11-C12-C13-C14
3	A	1103	PCW	C32-C33-C34-C35
3	C	1103	PCW	O3P-C1-C2-C3
3	A	1108	PCW	C19-C20-C21-C22
3	C	1107	PCW	C19-C20-C21-C22
3	D	1103	PCW	C20-C21-C22-C23
3	C	1104	PCW	O2-C31-C32-C33
3	D	1104	PCW	C42-C43-C44-C45
3	C	1103	PCW	C33-C34-C35-C36
3	C	1104	PCW	C14-C15-C16-C17
3	A	1104	PCW	C1-C2-O2-C31
3	A	1107	PCW	C16-C17-C18-C19
3	D	1107	PCW	C16-C17-C18-C19
3	B	1103	PCW	C2-C1-O3P-P
3	D	1104	PCW	C2-C1-O3P-P
3	A	1103	PCW	C33-C34-C35-C36
3	B	1102	PCW	O2-C2-C3-O3
3	C	1103	PCW	C14-C15-C16-C17
2	B	1101	ZK1	NAY-CAO-PBA-OAD
2	B	1101	ZK1	NAY-CAO-PBA-OAE
2	D	1102	ZK1	NAY-CAO-PBA-OAD
2	D	1102	ZK1	NAY-CAO-PBA-OAE
2	A	1101	ZK1	NAY-CAO-PBA-OAC
2	B	1101	ZK1	NAY-CAO-PBA-OAC
2	C	1101	ZK1	NAY-CAO-PBA-OAC
2	D	1102	ZK1	NAY-CAO-PBA-OAC
3	C	1103	PCW	C32-C33-C34-C35
3	A	1103	PCW	C14-C15-C16-C17
2	B	1101	ZK1	CAI-CAR-NAX-CAN
2	D	1102	ZK1	CAI-CAR-NAX-CAN
3	D	1103	PCW	C35-C36-C37-C38
3	A	1102	PCW	C1-O3P-P-O2P
3	A	1104	PCW	C4-O4P-P-O1P
3	B	1102	PCW	C1-O3P-P-O2P
3	B	1102	PCW	C4-O4P-P-O1P
3	C	1102	PCW	C1-O3P-P-O2P
3	C	1103	PCW	C4-O4P-P-O1P
3	C	1104	PCW	C4-O4P-P-O1P
3	D	1103	PCW	C1-O3P-P-O2P
3	D	1103	PCW	C4-O4P-P-O1P
3	B	1102	PCW	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
3	D	1106	PCW	C13-C14-C15-C16
3	B	1104	PCW	O3P-C1-C2-O2
3	D	1105	PCW	O3P-C1-C2-O2
3	B	1105	PCW	C13-C14-C15-C16
3	A	1104	PCW	C39-C40-C41-C42
3	C	1104	PCW	C39-C40-C41-C42
3	C	1104	PCW	C31-C32-C33-C34
3	D	1104	PCW	C11-C12-C13-C14
3	A	1104	PCW	C1-C2-C3-O3
3	A	1104	PCW	O4P-C4-C5-N
3	C	1104	PCW	O4P-C4-C5-N
3	A	1104	PCW	O2-C2-C3-O3
3	B	1103	PCW	O2-C2-C3-O3
3	C	1104	PCW	O2-C2-C3-O3
3	D	1103	PCW	O2-C2-C3-O3
3	B	1103	PCW	C11-C12-C13-C14
3	D	1103	PCW	C33-C34-C35-C36
3	D	1104	PCW	C12-C13-C14-C15
3	B	1102	PCW	C33-C34-C35-C36
3	A	1102	PCW	C35-C36-C37-C38
3	A	1108	PCW	C14-C15-C16-C17
3	C	1102	PCW	C21-C22-C23-C24
3	B	1104	PCW	C35-C36-C37-C38
3	C	1102	PCW	C25-C26-C27-C28
3	C	1104	PCW	C36-C37-C38-C39
2	A	1101	ZK1	CAI-CAR-NAX-CAN
2	C	1101	ZK1	CAI-CAR-NAX-CAN
3	B	1103	PCW	C12-C13-C14-C15
3	C	1107	PCW	C14-C15-C16-C17
3	B	1103	PCW	C37-C38-C39-C40
3	A	1106	PCW	C13-C14-C15-C16
3	C	1106	PCW	C13-C14-C15-C16
3	C	1104	PCW	O3-C11-C12-C13
3	A	1102	PCW	C25-C26-C27-C28
3	C	1102	PCW	C19-C20-C21-C22
3	A	1102	PCW	C32-C33-C34-C35
3	B	1104	PCW	C4-O4P-P-O3P
3	D	1105	PCW	C4-O4P-P-O3P
3	A	1105	PCW	C14-C15-C16-C17
3	A	1102	PCW	C19-C20-C21-C22
3	D	1104	PCW	C37-C38-C39-C40
3	B	1103	PCW	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
3	C	1105	PCW	C20-C21-C22-C23
3	B	1104	PCW	C31-C32-C33-C34
3	A	1104	PCW	C2-C1-O3P-P
3	A	1103	PCW	C41-C42-C43-C44
3	B	1102	PCW	C37-C38-C39-C40
3	D	1103	PCW	C19-C20-C21-C22
3	B	1102	PCW	C19-C20-C21-C22
3	D	1103	PCW	C37-C38-C39-C40
3	D	1103	PCW	C24-C25-C26-C27
3	D	1105	PCW	O2-C2-C3-O3
3	D	1101	PCW	C15-C16-C17-C18
3	B	1106	PCW	C15-C16-C17-C18
3	D	1104	PCW	C36-C37-C38-C39
3	A	1102	PCW	C21-C22-C23-C24
3	A	1107	PCW	C17-C18-C19-C20
3	B	1105	PCW	C17-C18-C19-C20
3	D	1106	PCW	C17-C18-C19-C20
3	D	1107	PCW	C17-C18-C19-C20
3	A	1104	PCW	O2-C31-C32-C33
3	A	1105	PCW	C13-C14-C15-C16
3	A	1104	PCW	O3-C11-C12-C13
3	C	1103	PCW	C41-C42-C43-C44
3	C	1102	PCW	C16-C17-C18-C19
3	A	1103	PCW	O2-C2-C3-O3
3	D	1104	PCW	O2-C2-C3-O3
3	C	1104	PCW	C37-C38-C39-C40
3	A	1106	PCW	C17-C18-C19-C20
3	C	1106	PCW	C17-C18-C19-C20
3	B	1103	PCW	C1-C2-C3-O3
3	D	1103	PCW	C1-C2-C3-O3
3	C	1103	PCW	O2-C2-C3-O3
3	A	1104	PCW	C37-C38-C39-C40
3	C	1102	PCW	C37-C38-C39-C40
3	A	1108	PCW	C13-C14-C15-C16
3	C	1107	PCW	C13-C14-C15-C16
3	B	1104	PCW	O2-C31-C32-C33
3	B	1103	PCW	C36-C37-C38-C39
3	B	1106	PCW	C16-C17-C18-C19
3	D	1101	PCW	C16-C17-C18-C19
3	B	1102	PCW	C1-C2-C3-O3
3	B	1104	PCW	C1-C2-C3-O3
3	D	1104	PCW	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	1102	PCW	C1-O3P-P-O4P
3	C	1102	PCW	C1-O3P-P-O4P
3	D	1103	PCW	C1-O3P-P-O4P
3	D	1104	PCW	C41-C42-C43-C44
3	B	1103	PCW	C1-O3P-P-O2P
3	D	1104	PCW	C1-O3P-P-O2P
3	B	1104	PCW	O31-C31-C32-C33
3	C	1105	PCW	C15-C16-C17-C18
3	A	1102	PCW	C16-C17-C18-C19
3	B	1103	PCW	C5-C4-O4P-P
3	D	1104	PCW	C5-C4-O4P-P
3	D	1103	PCW	C31-C32-C33-C34
3	C	1103	PCW	C2-C1-O3P-P
3	B	1102	PCW	C14-C15-C16-C17
2	C	1101	ZK1	CAI-CAR-NAX-CAM
3	A	1104	PCW	C12-C13-C14-C15

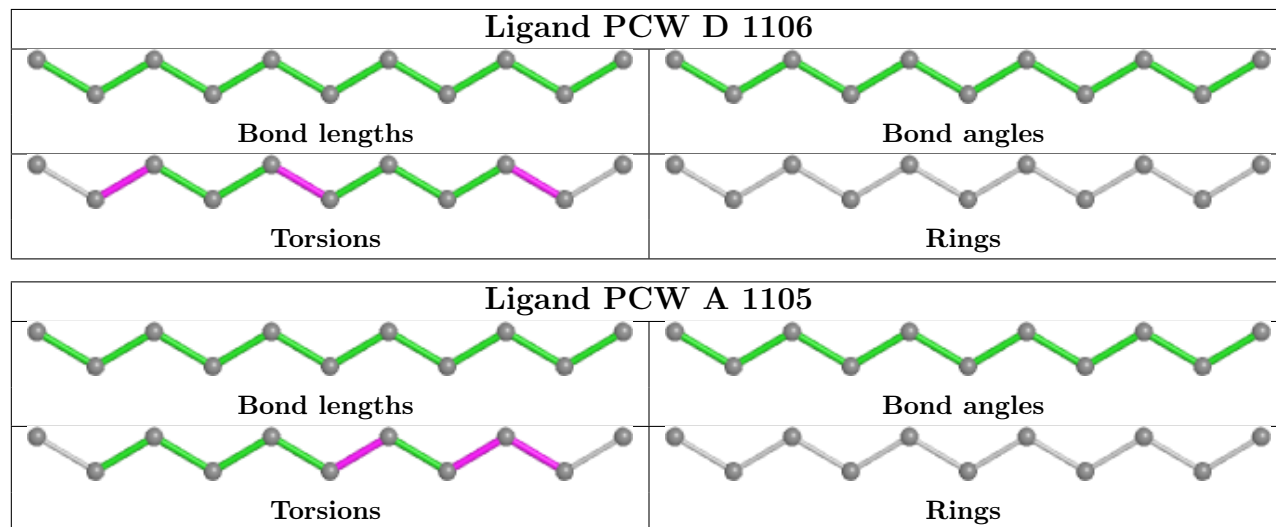
There are no ring outliers.

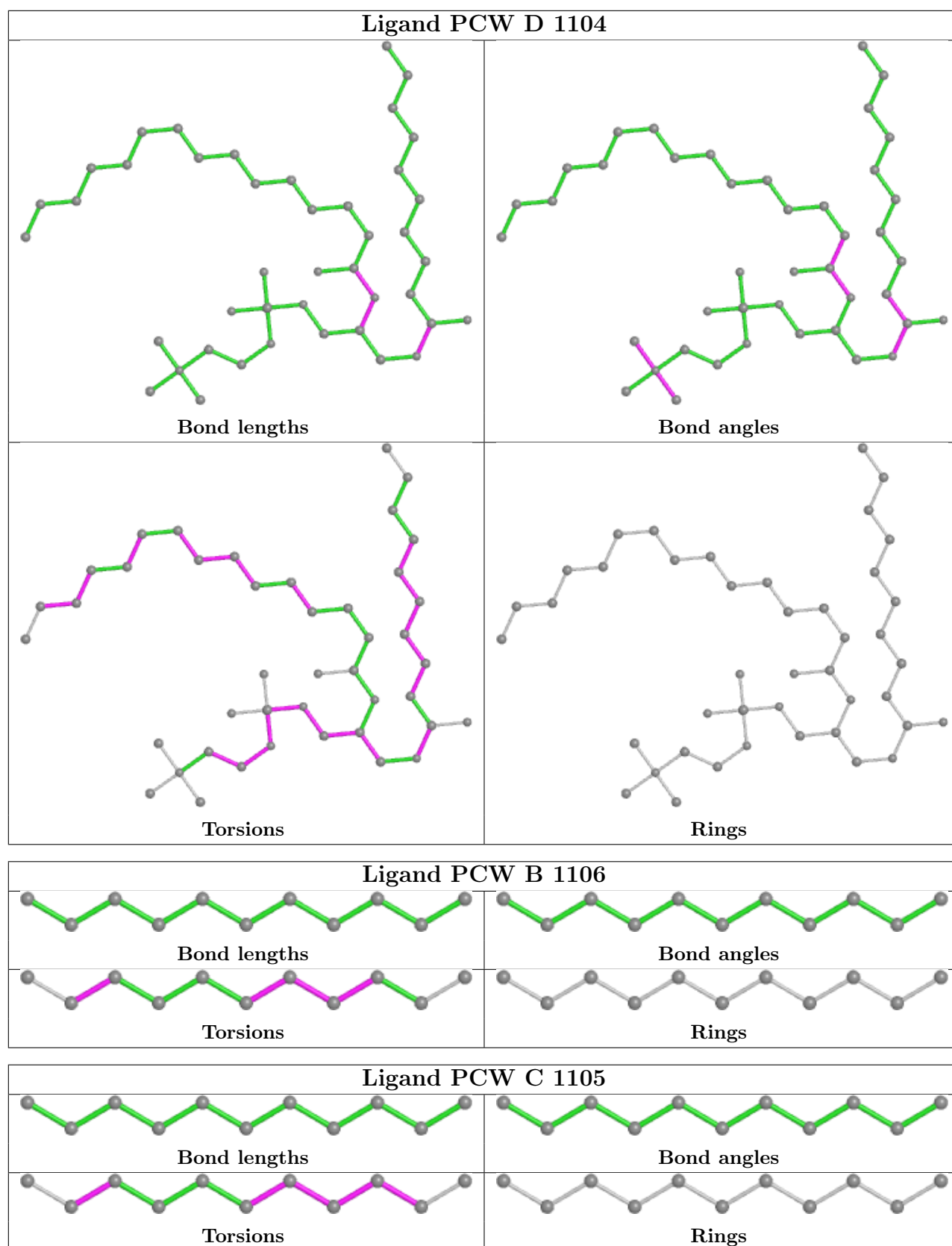
13 monomers are involved in 26 short contacts:

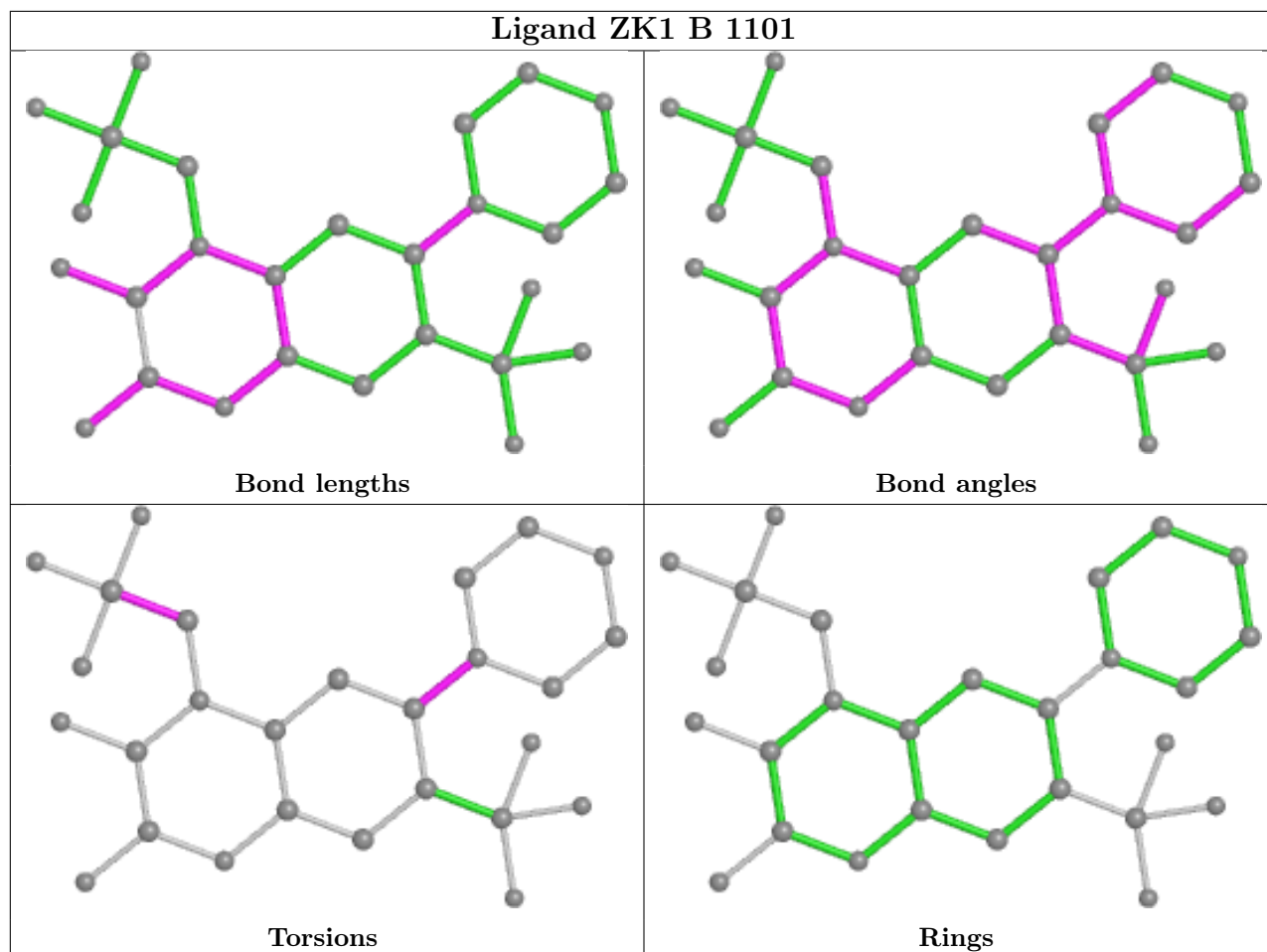
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1104	PCW	1	0
3	B	1106	PCW	2	0
3	C	1104	PCW	1	0
3	D	1103	PCW	6	0
3	B	1102	PCW	3	0
3	C	1103	PCW	1	0
3	C	1107	PCW	1	0
2	A	1101	ZK1	1	0
3	D	1101	PCW	2	0
3	A	1102	PCW	3	0
3	C	1102	PCW	3	0
3	B	1103	PCW	2	0
3	A	1104	PCW	2	0

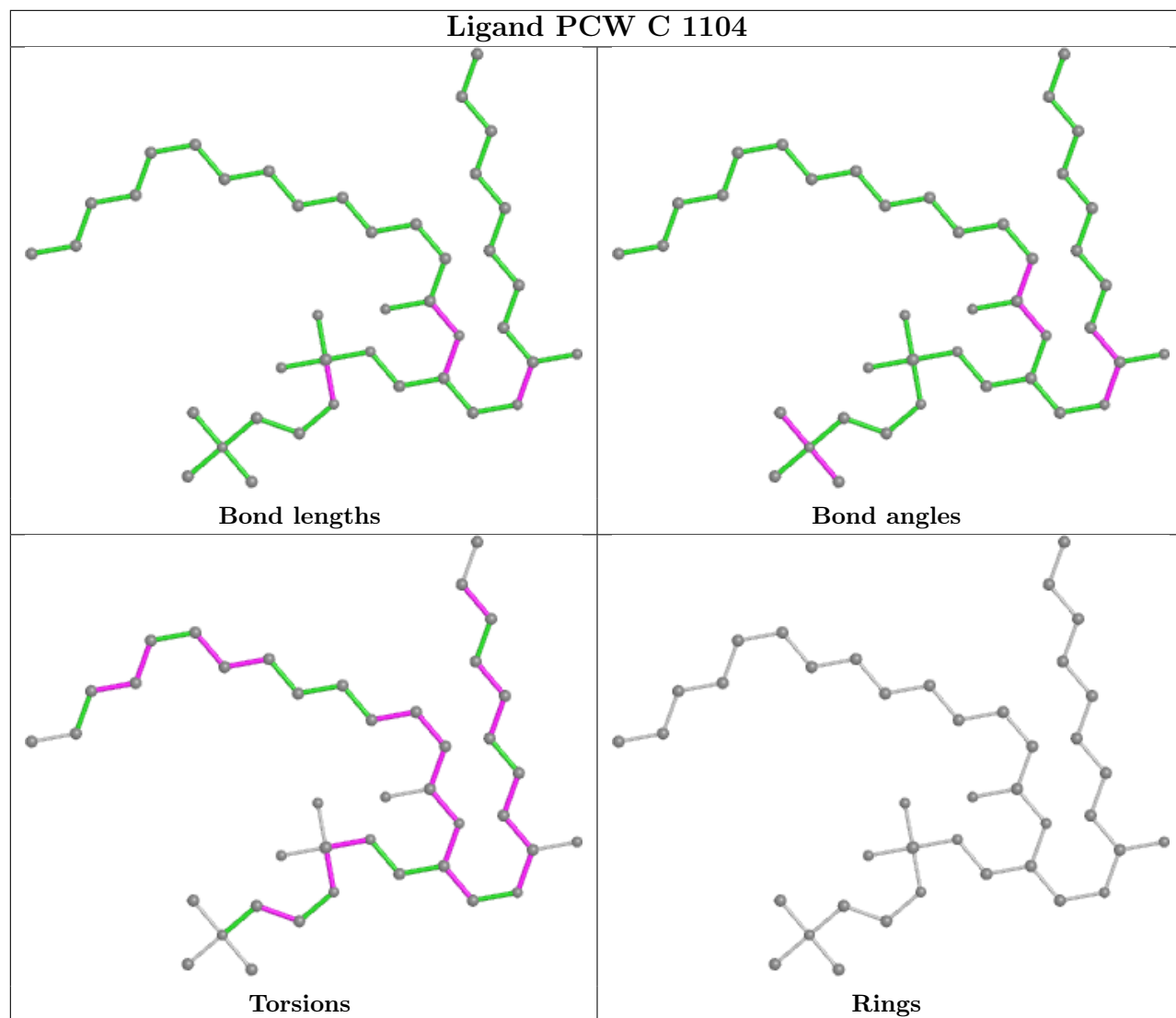
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

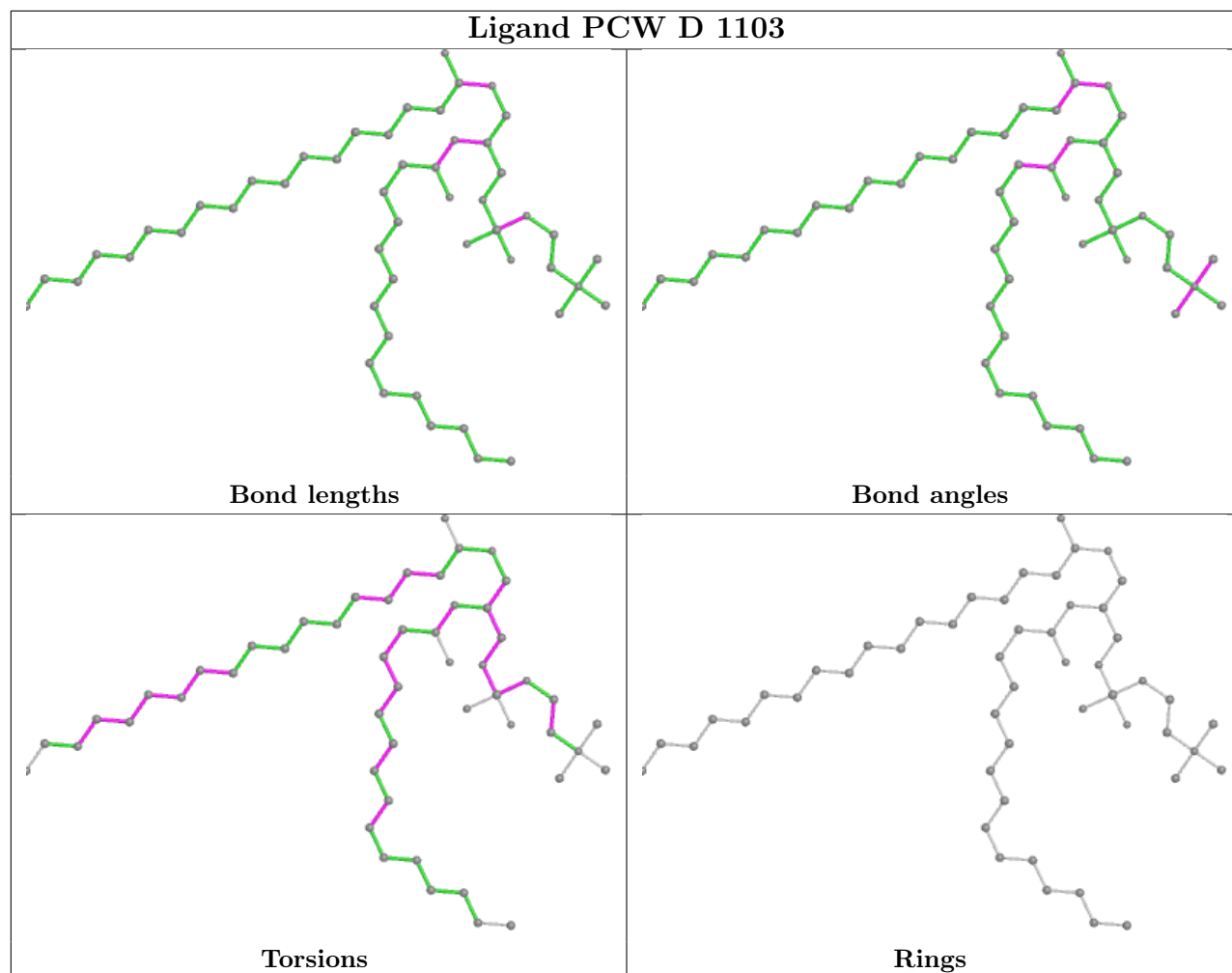
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

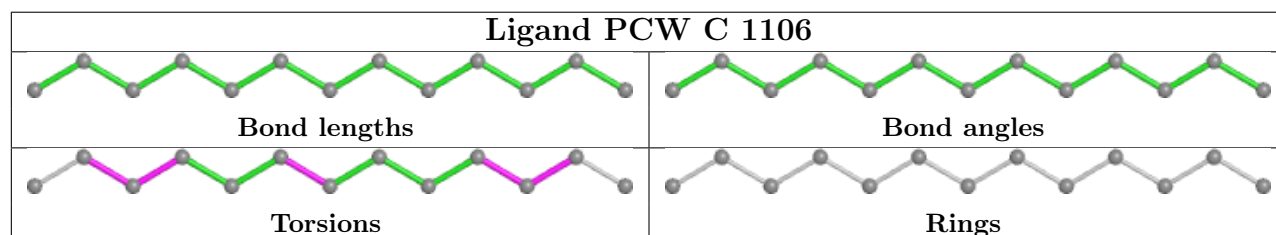
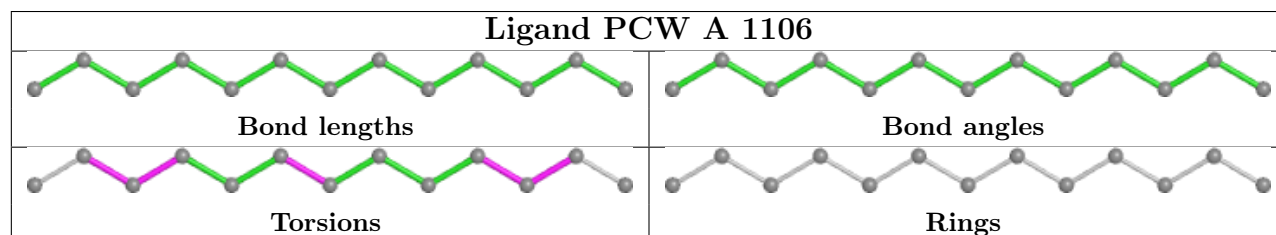
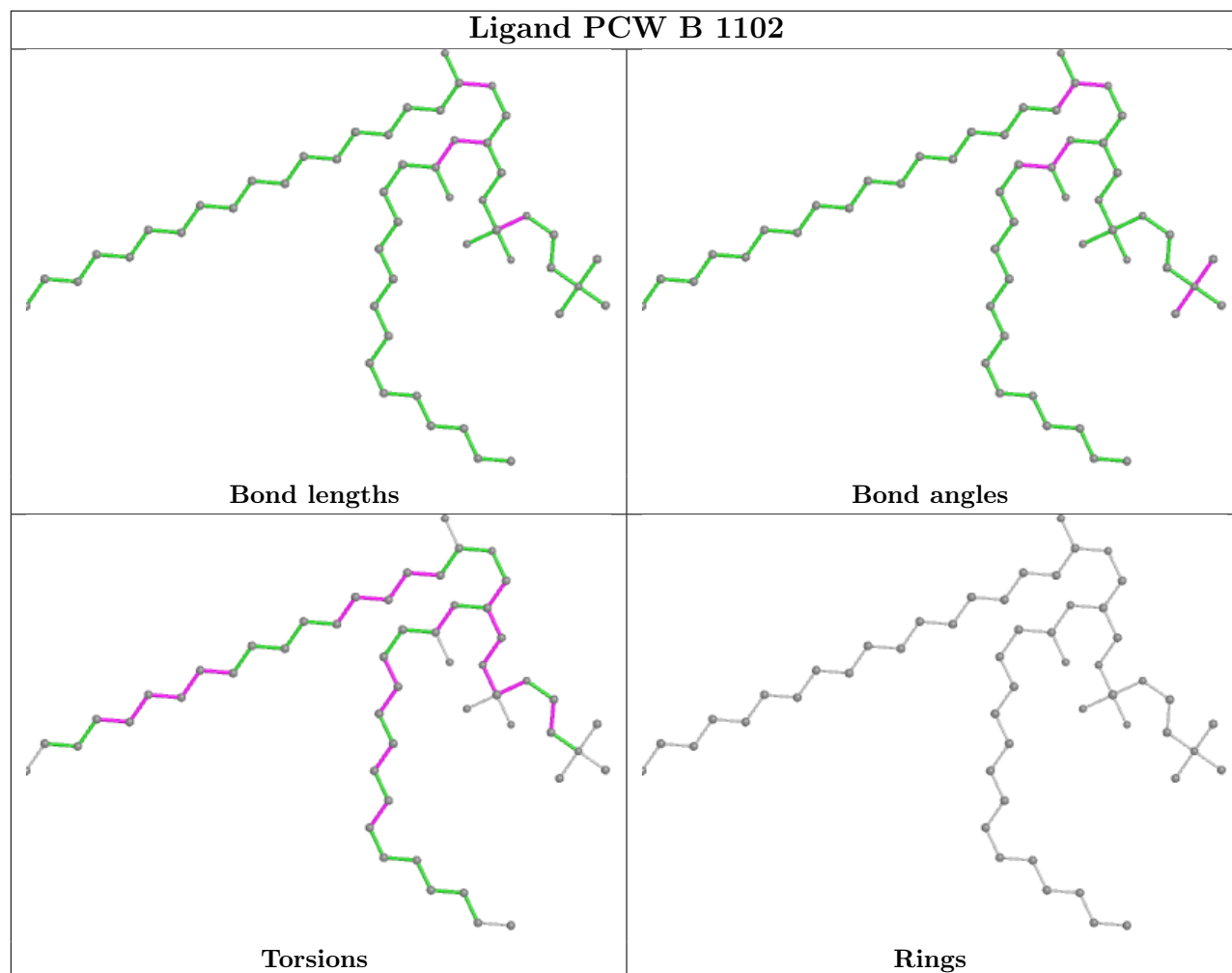


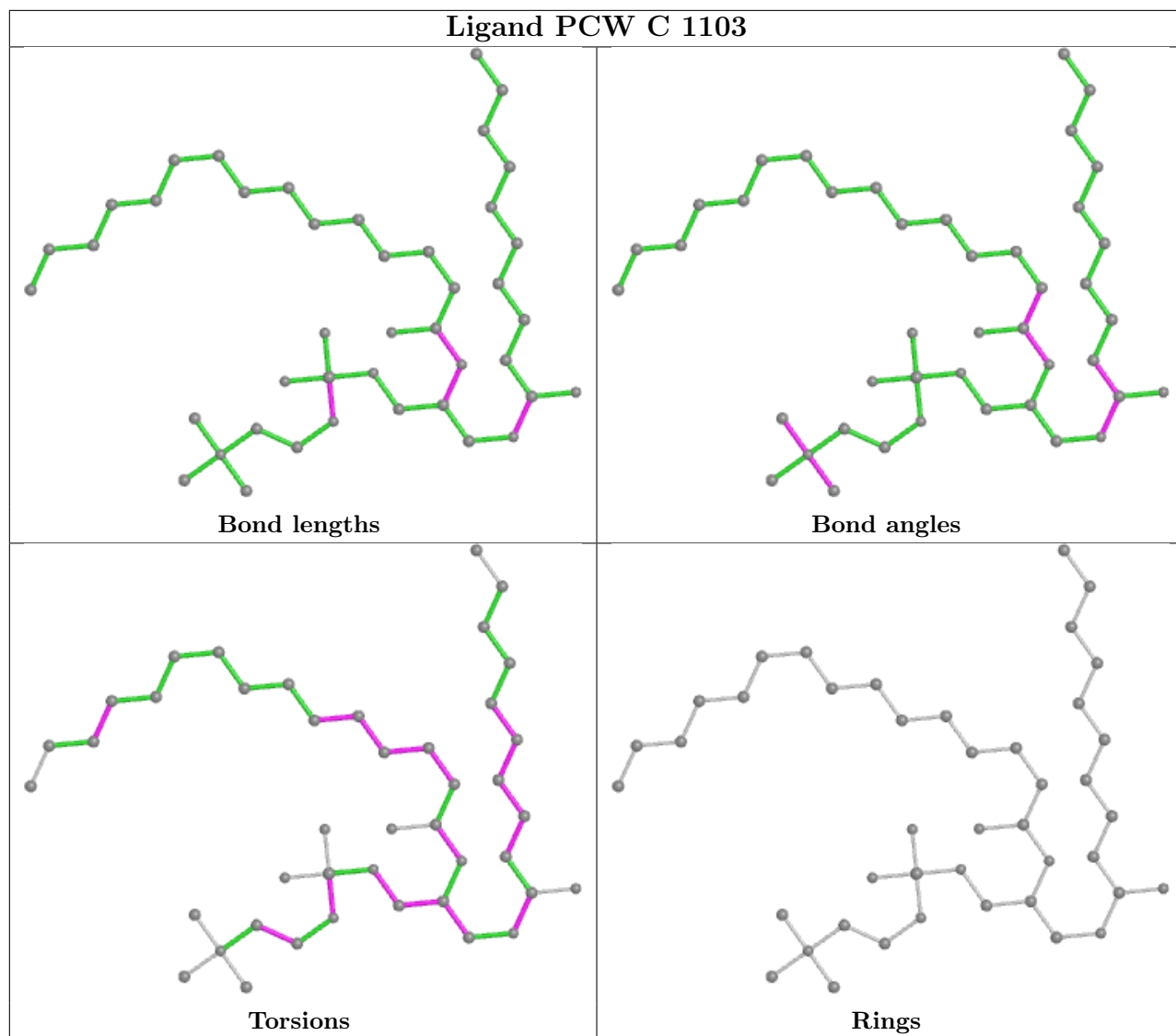


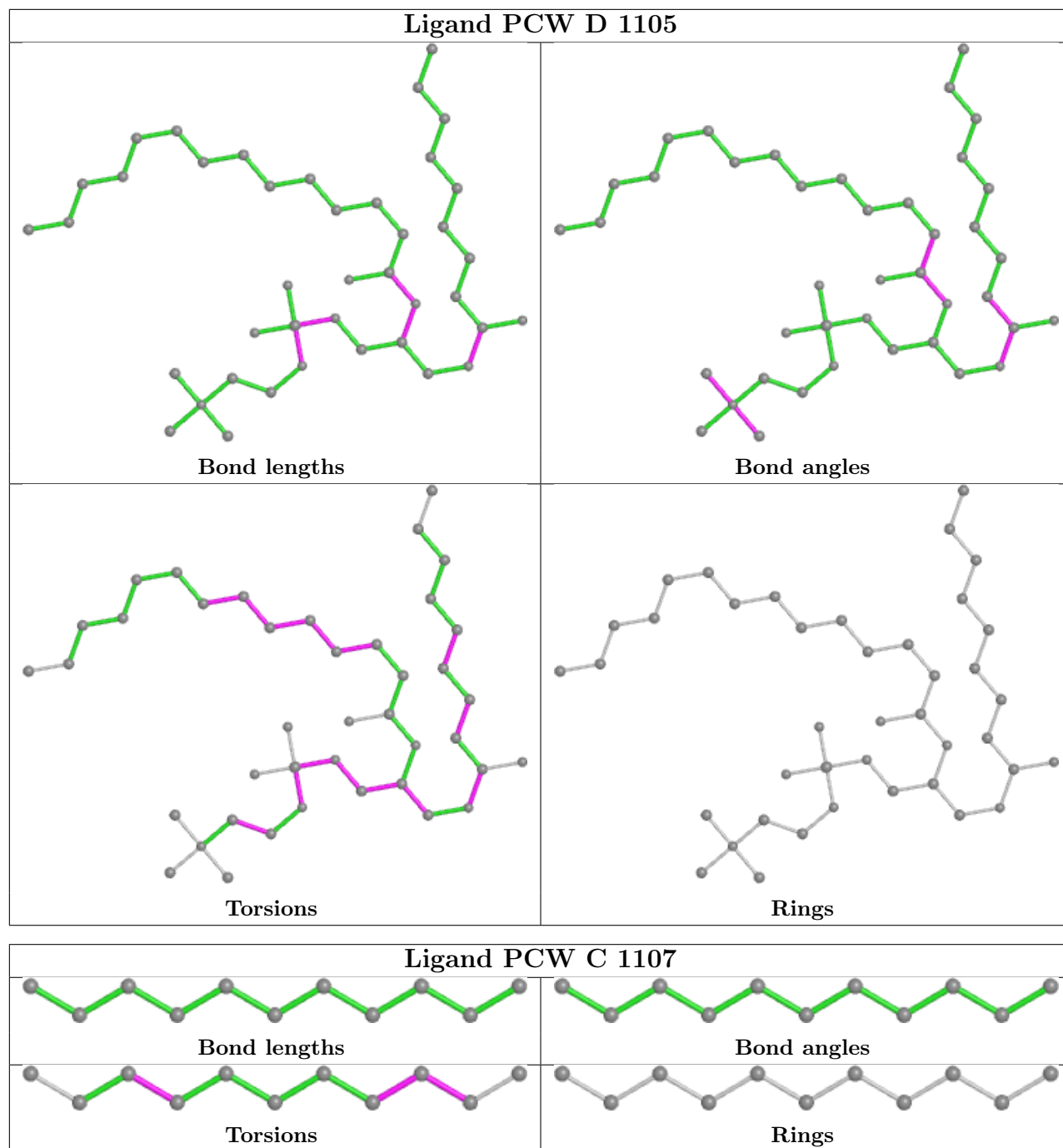


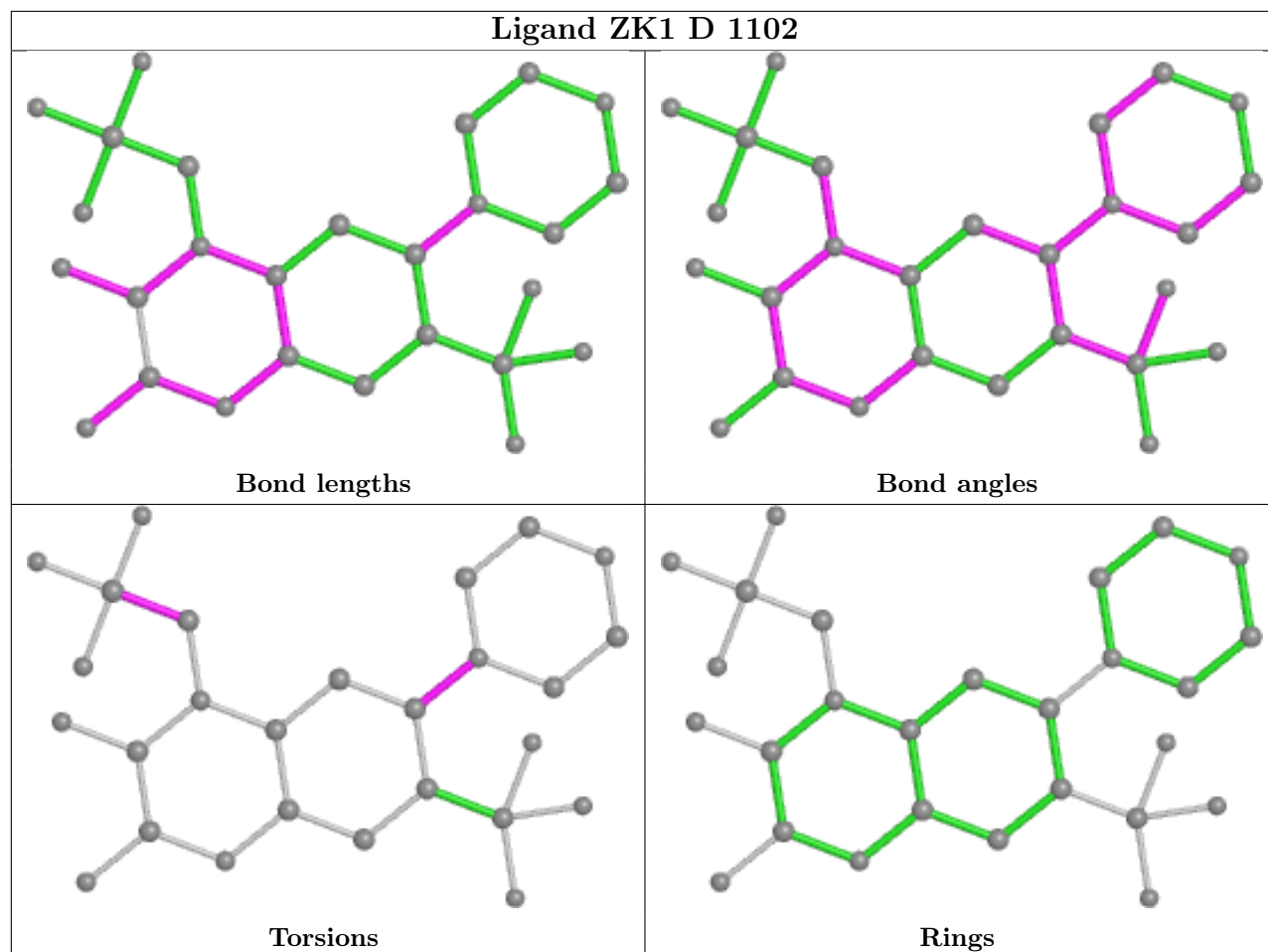


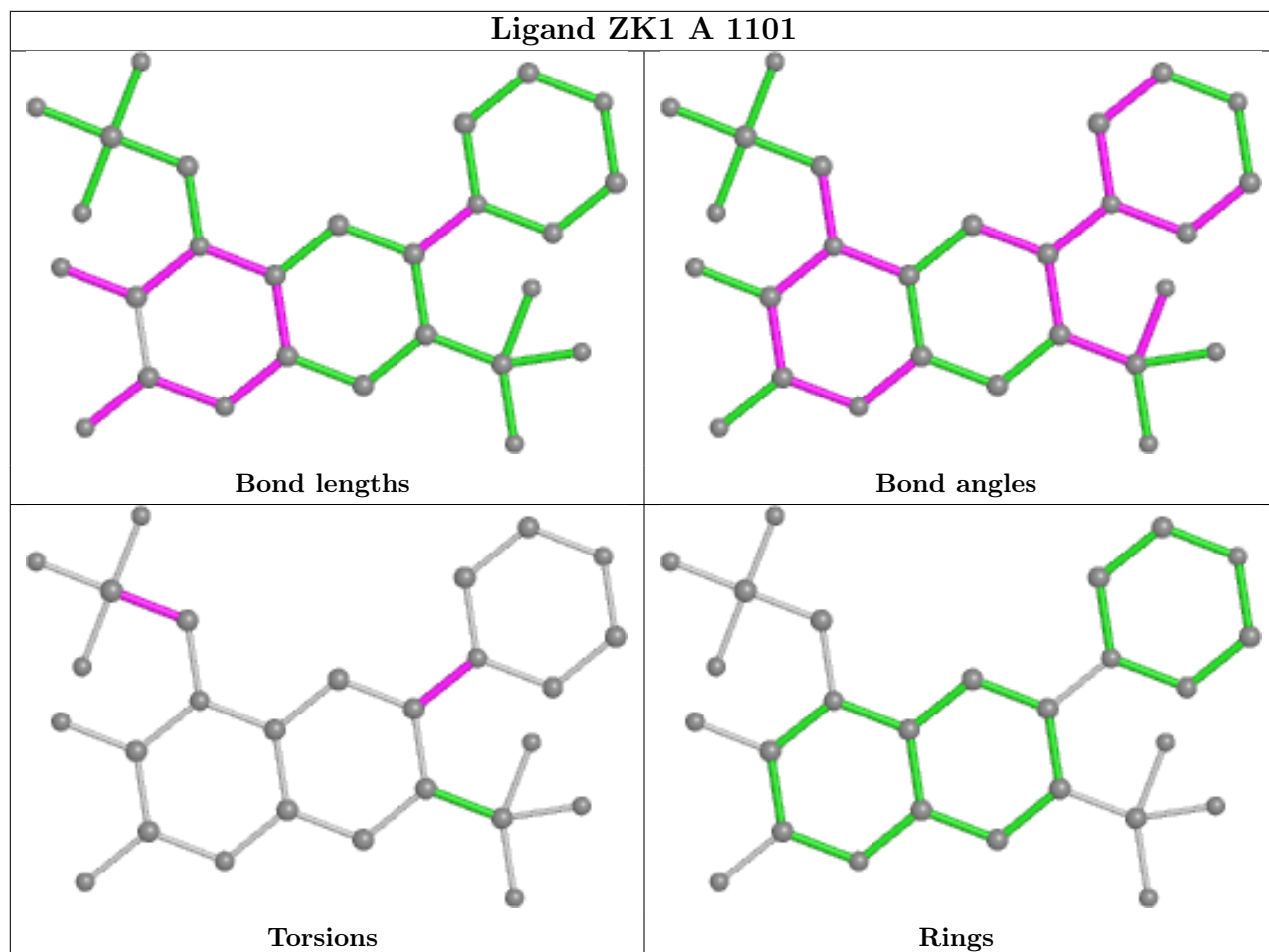


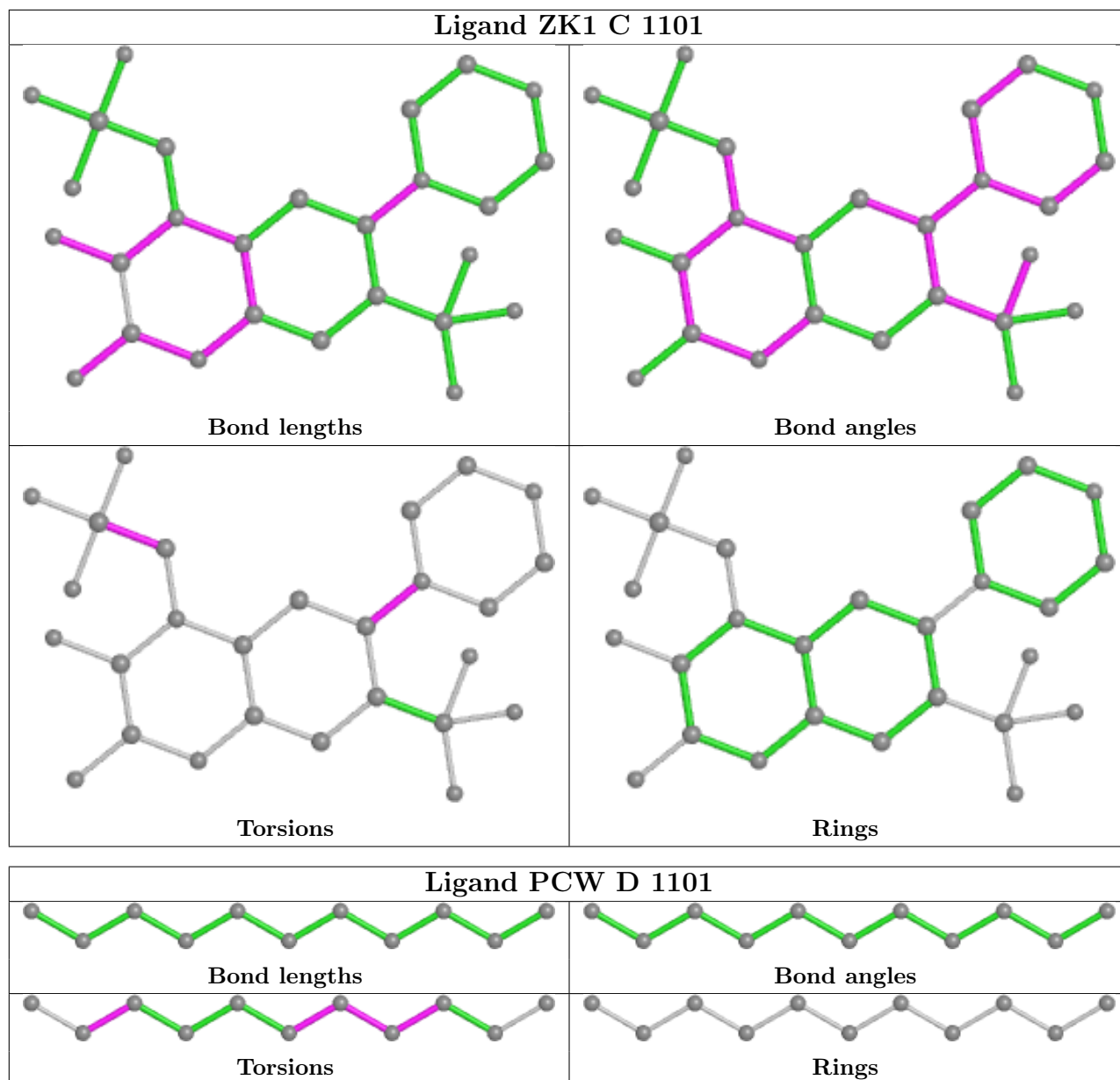


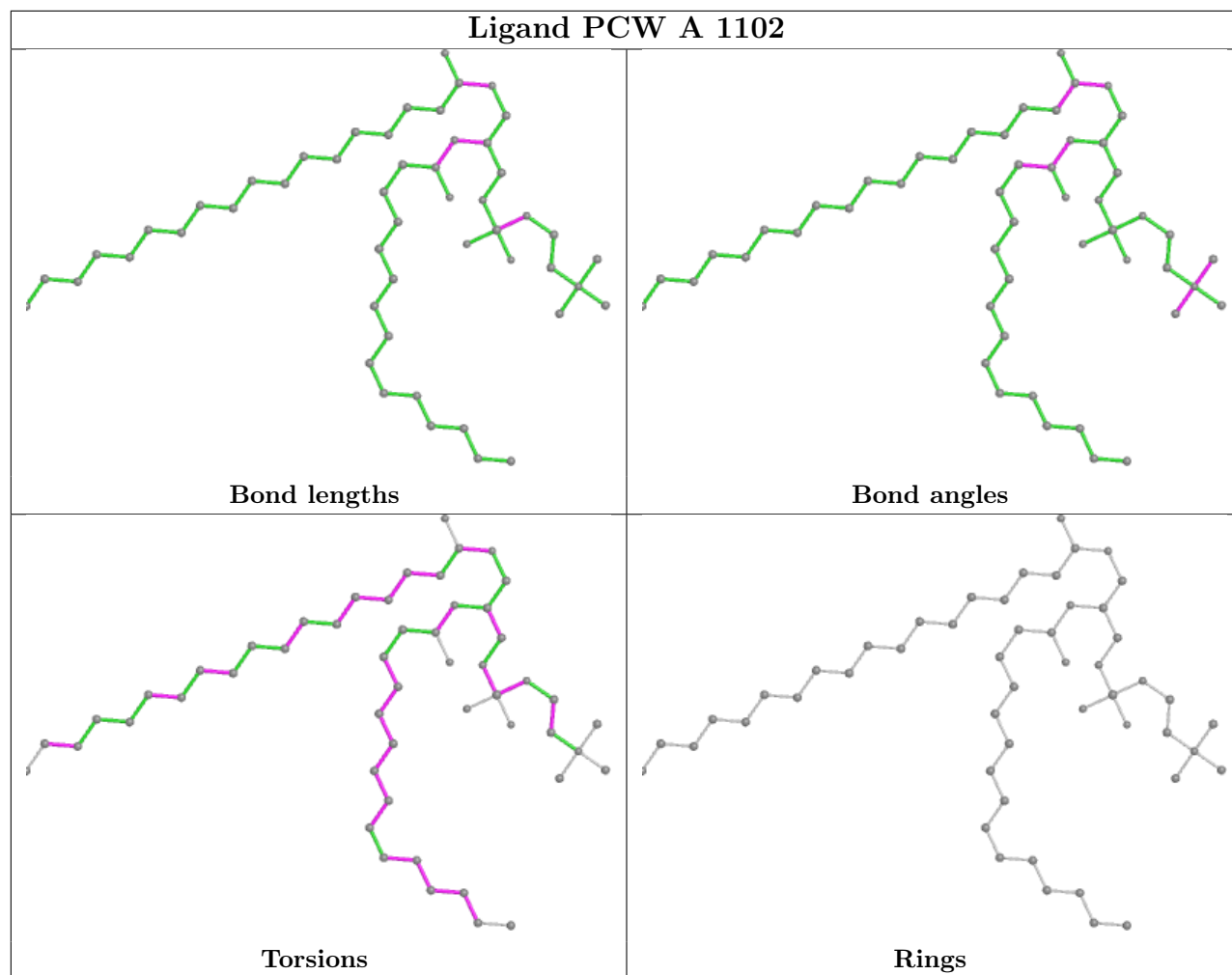


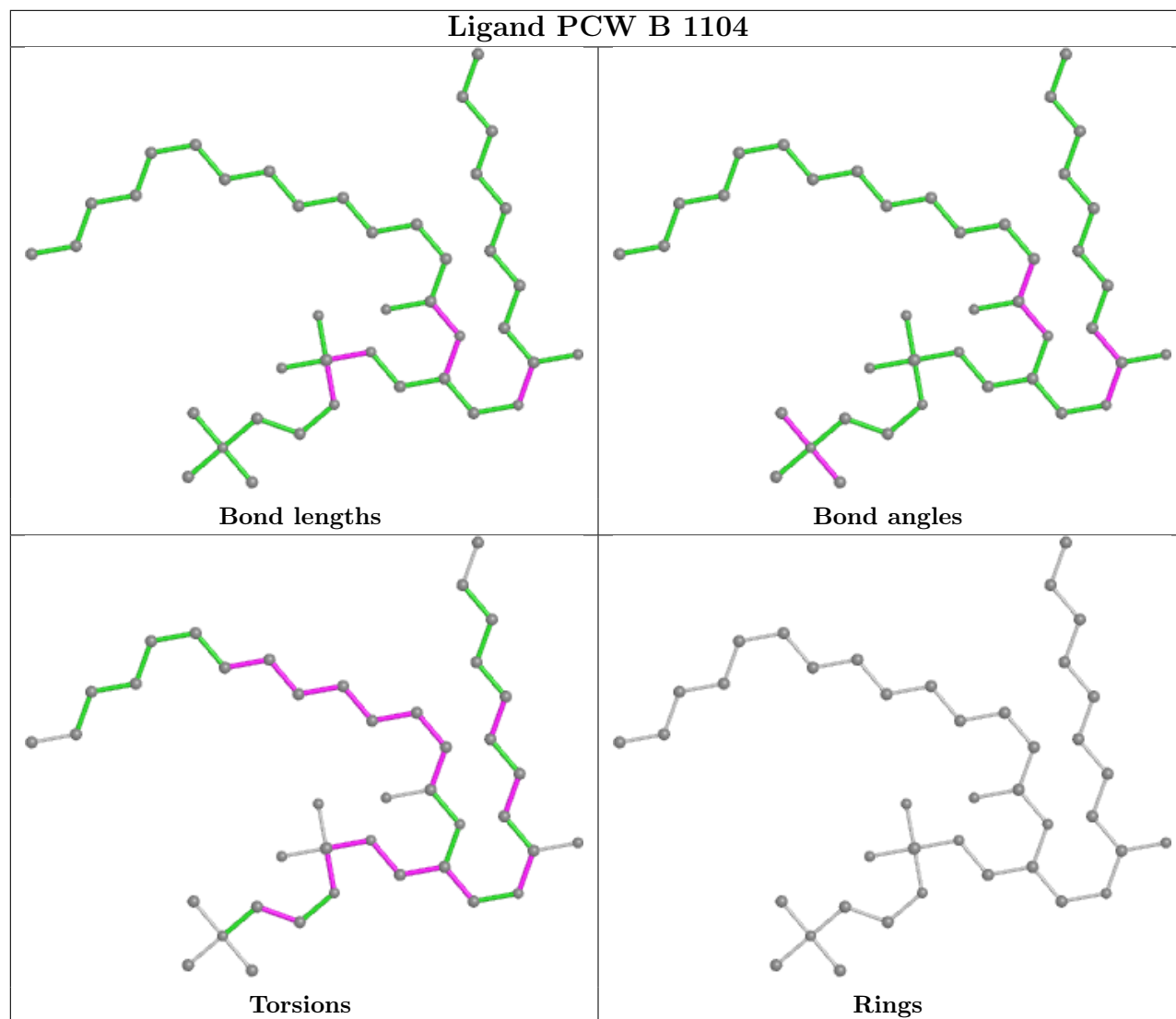


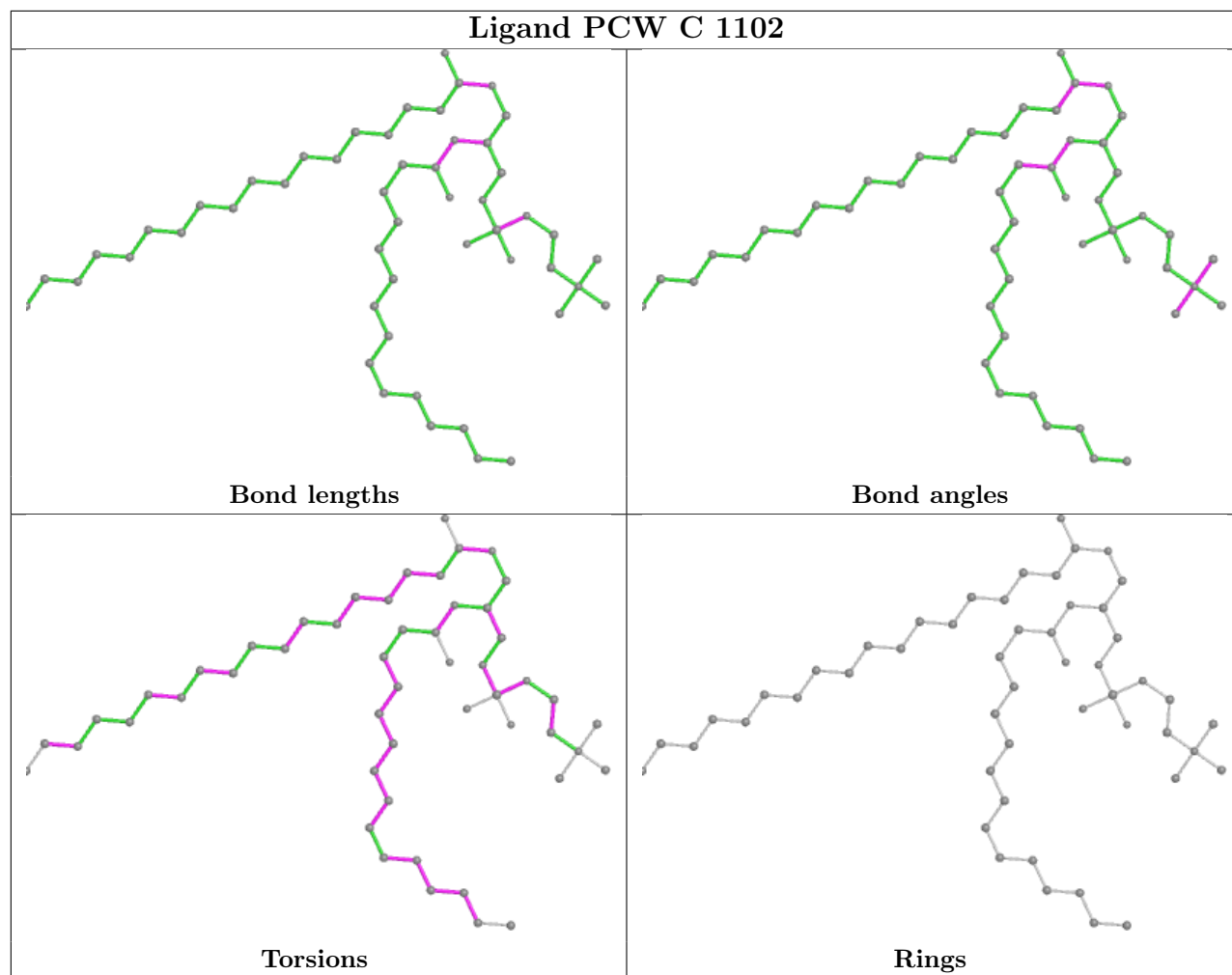


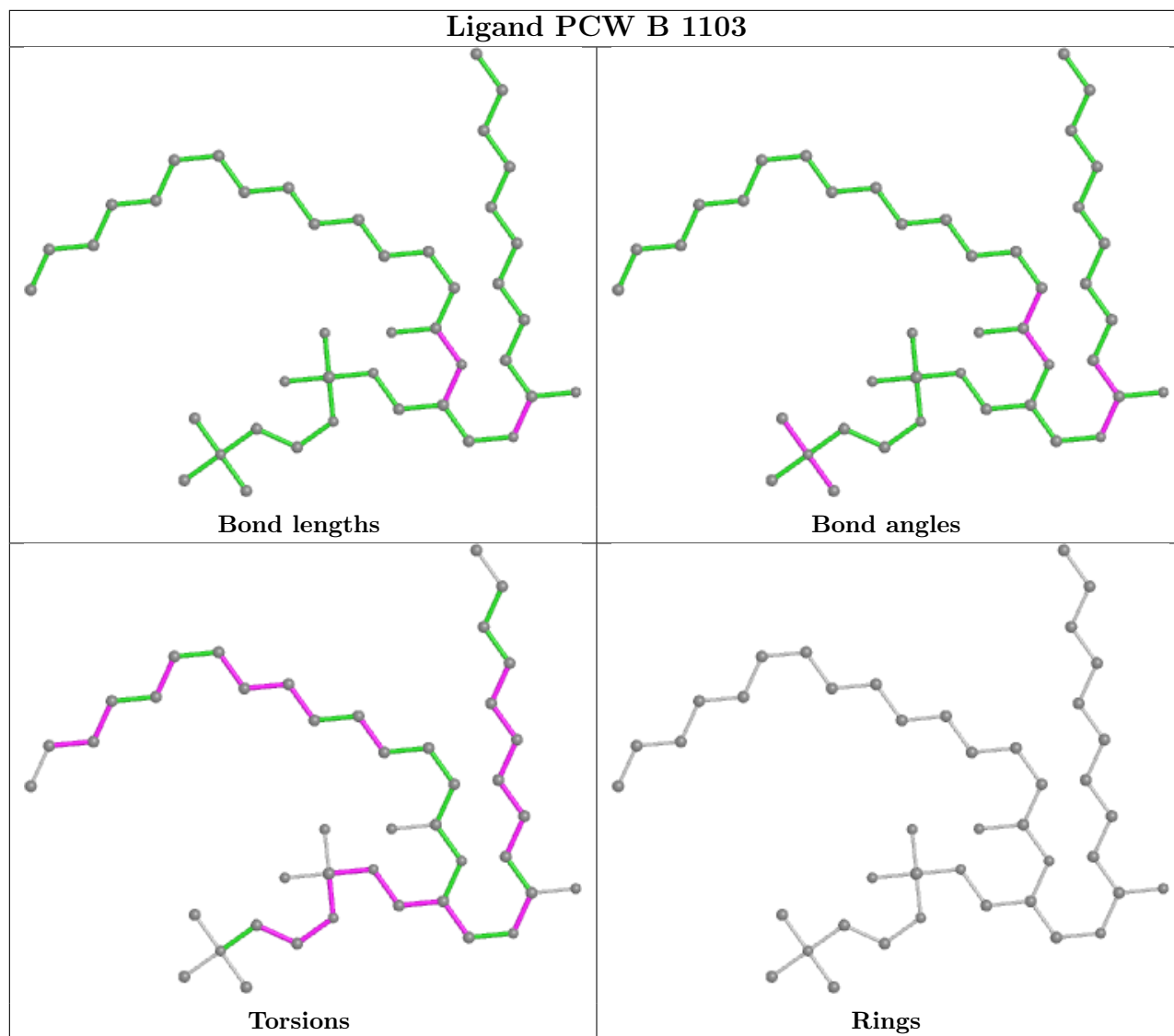


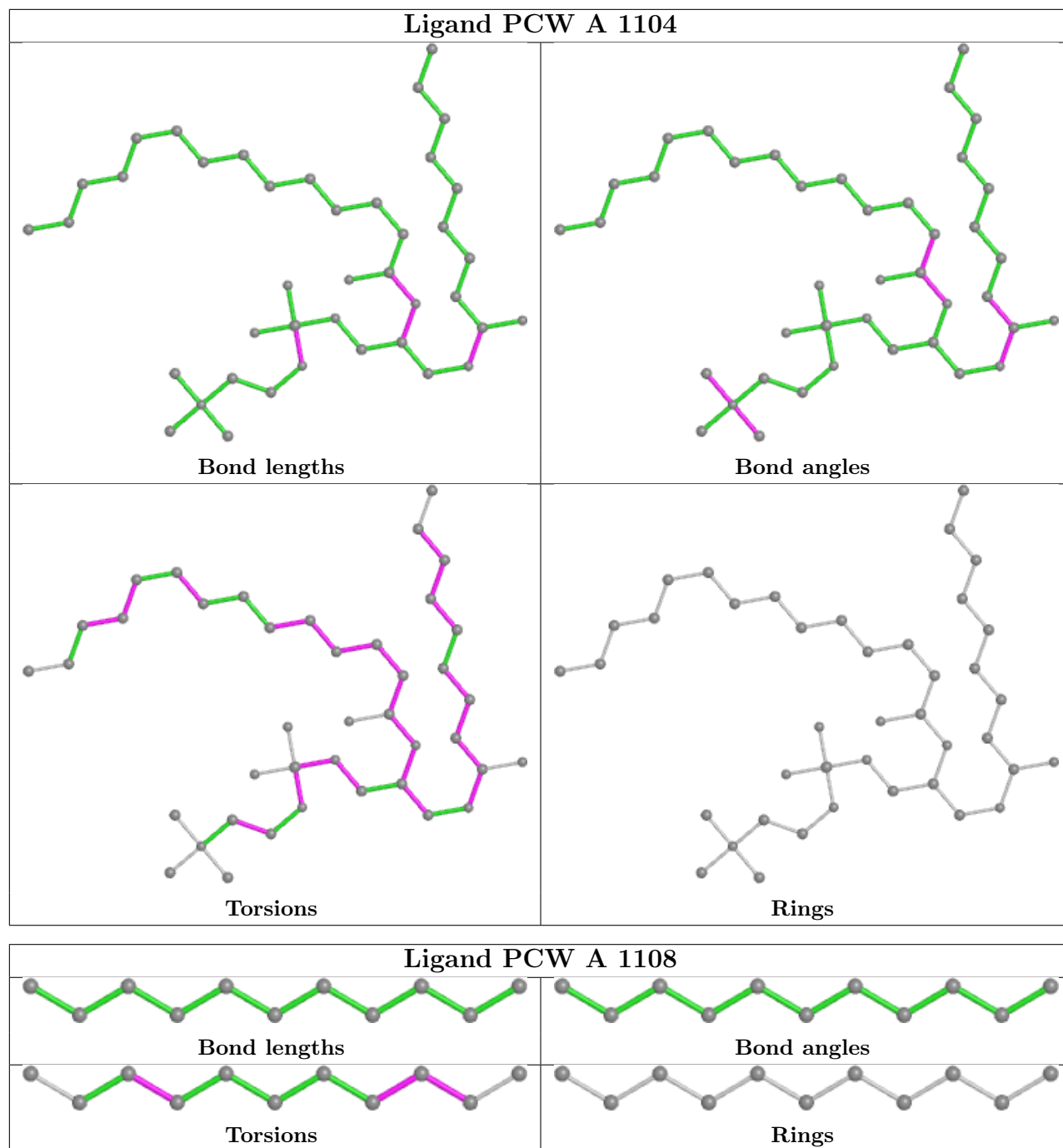


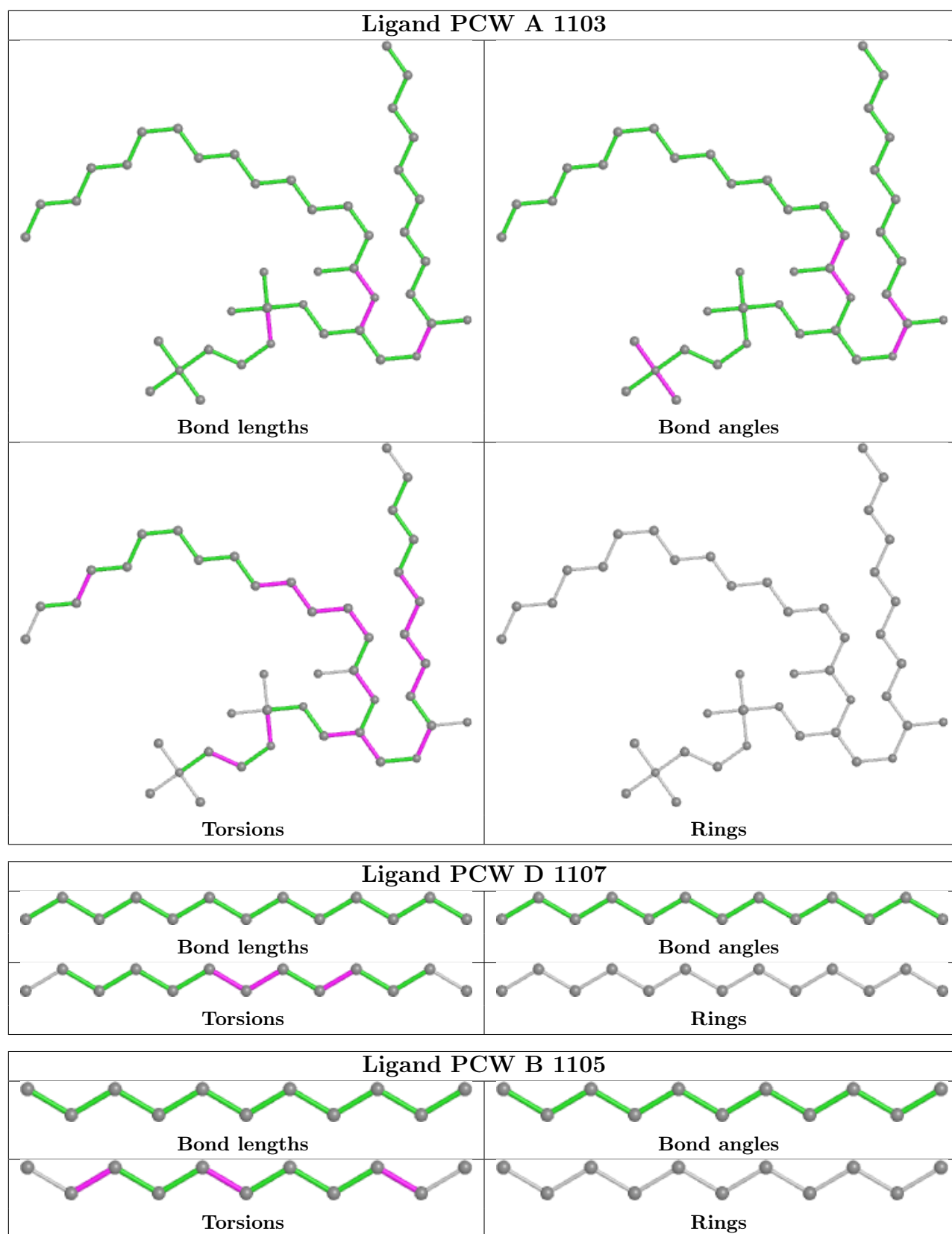


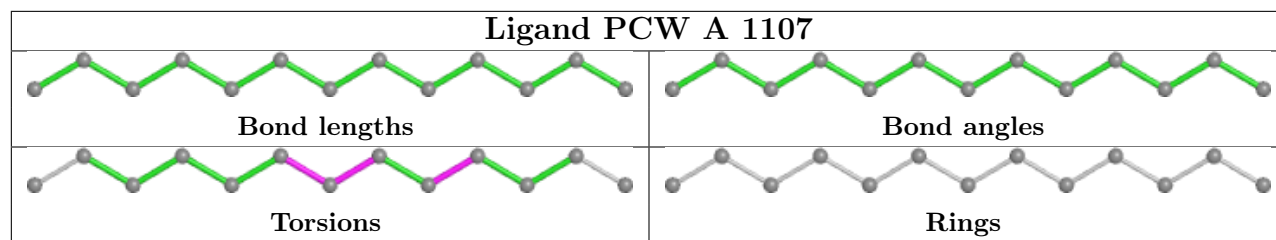












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

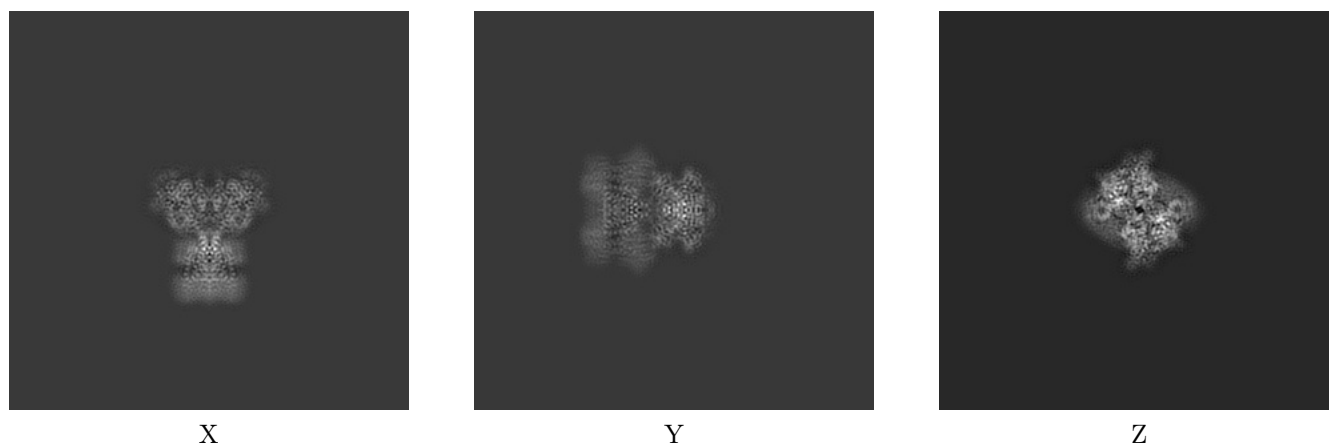
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24751. 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](#)

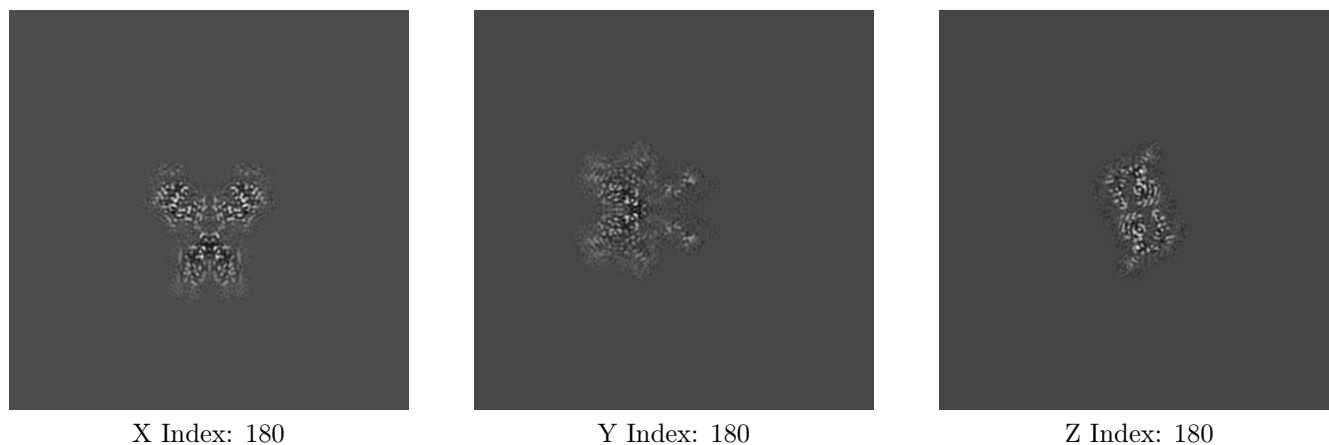
6.1.1 Primary map



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

6.2 Central slices [i](#)

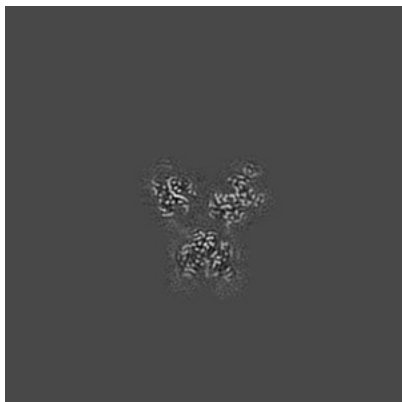
6.2.1 Primary map



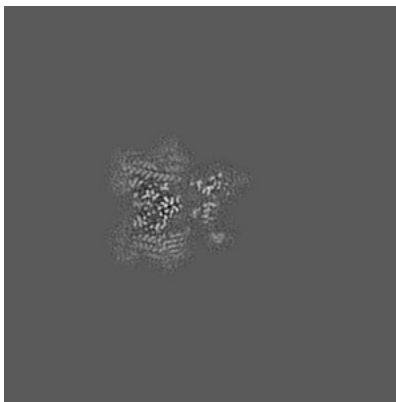
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

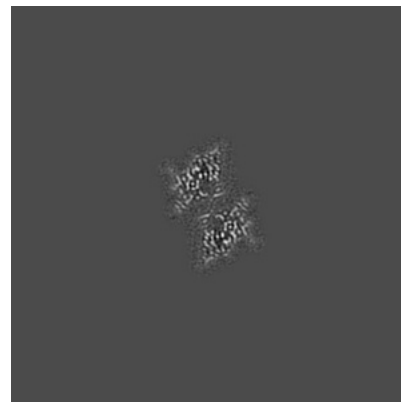
6.3.1 Primary map



X Index: 185



Y Index: 175

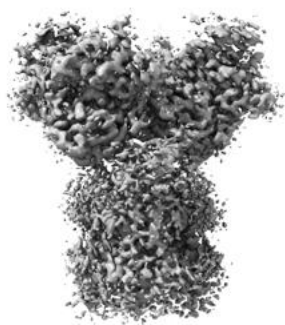


Z Index: 190

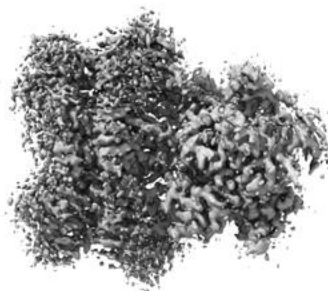
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

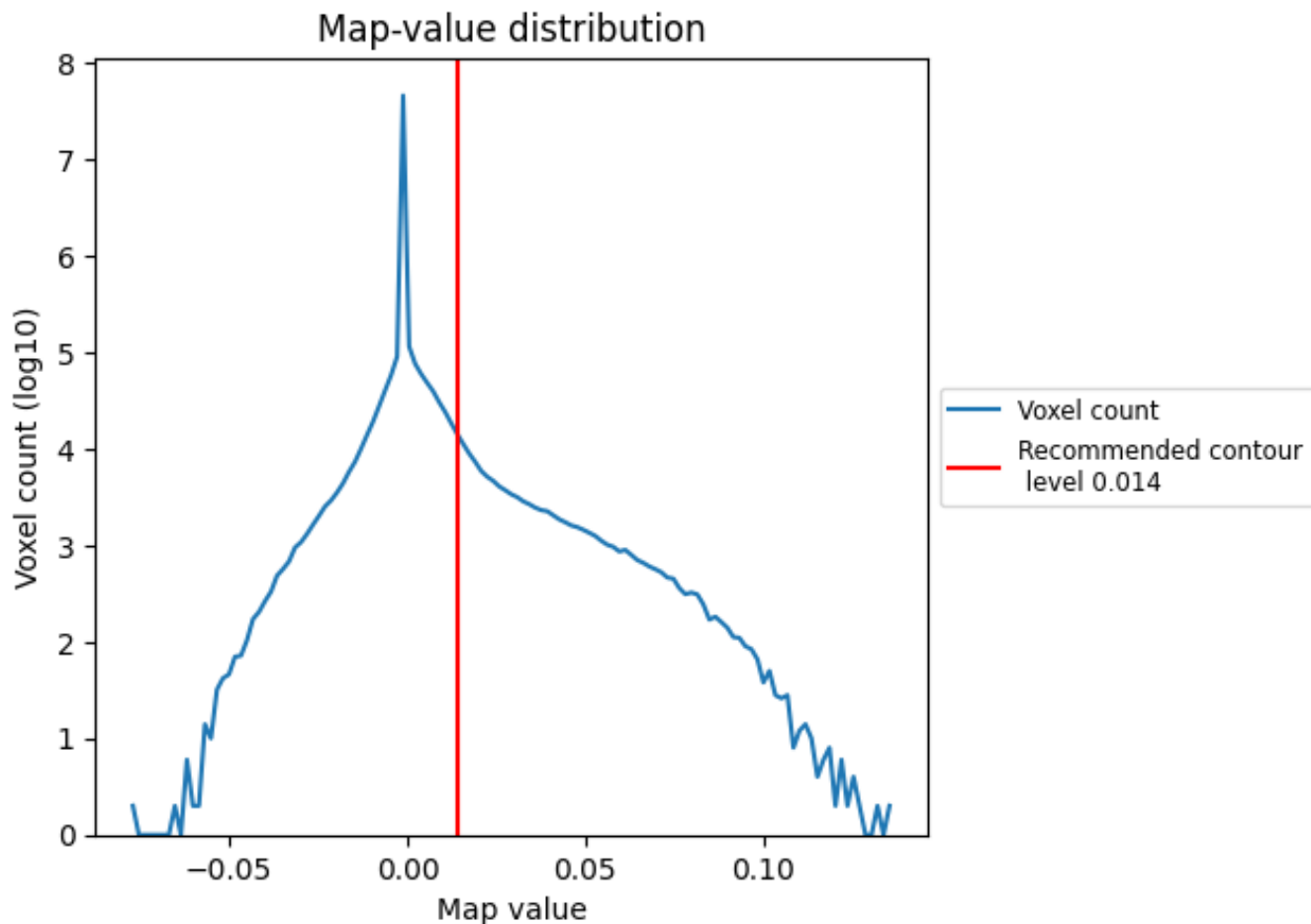
6.5 Mask visualisation

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

7 Map analysis [i](#)

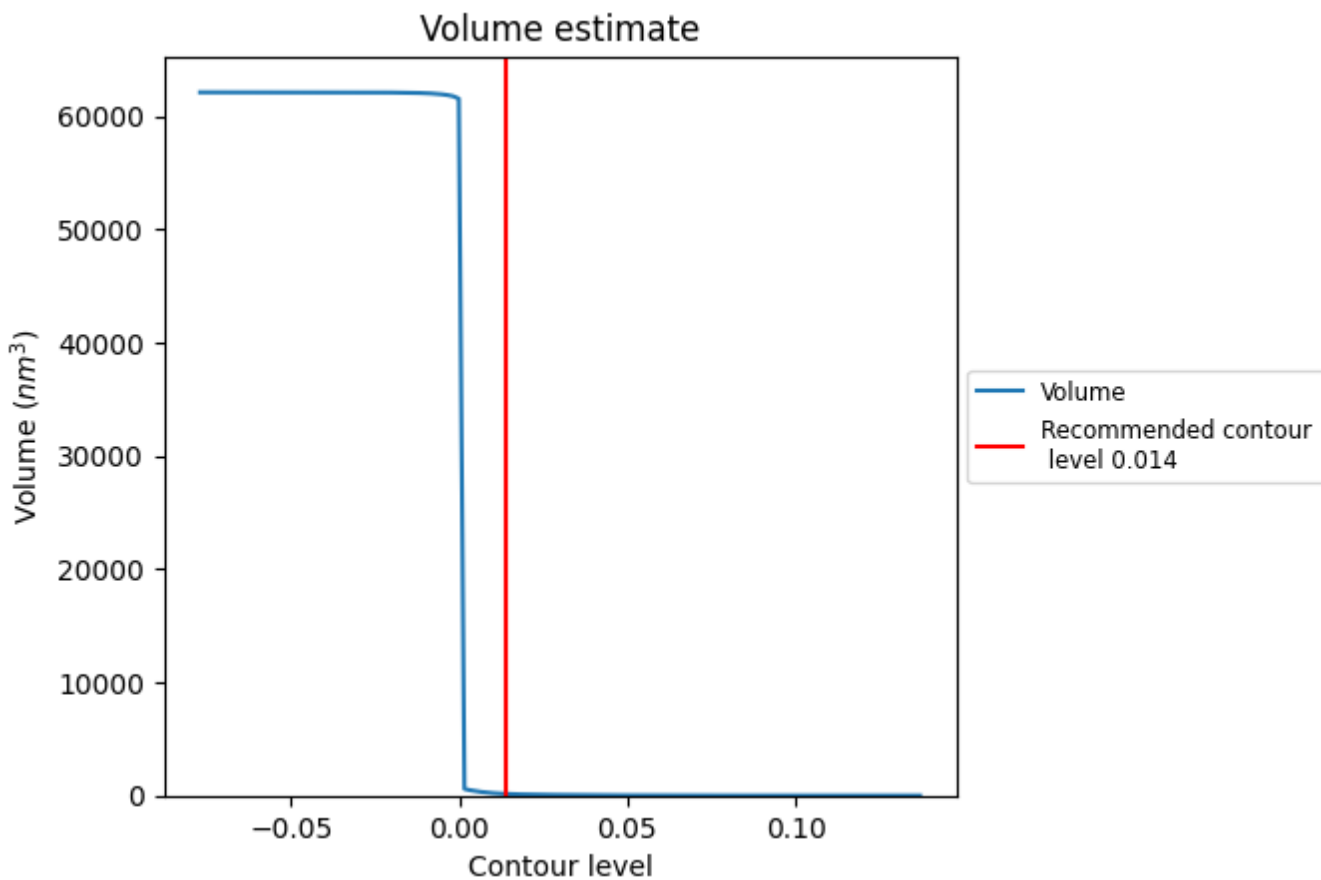
This section contains the results of statistical analysis of the map.

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.

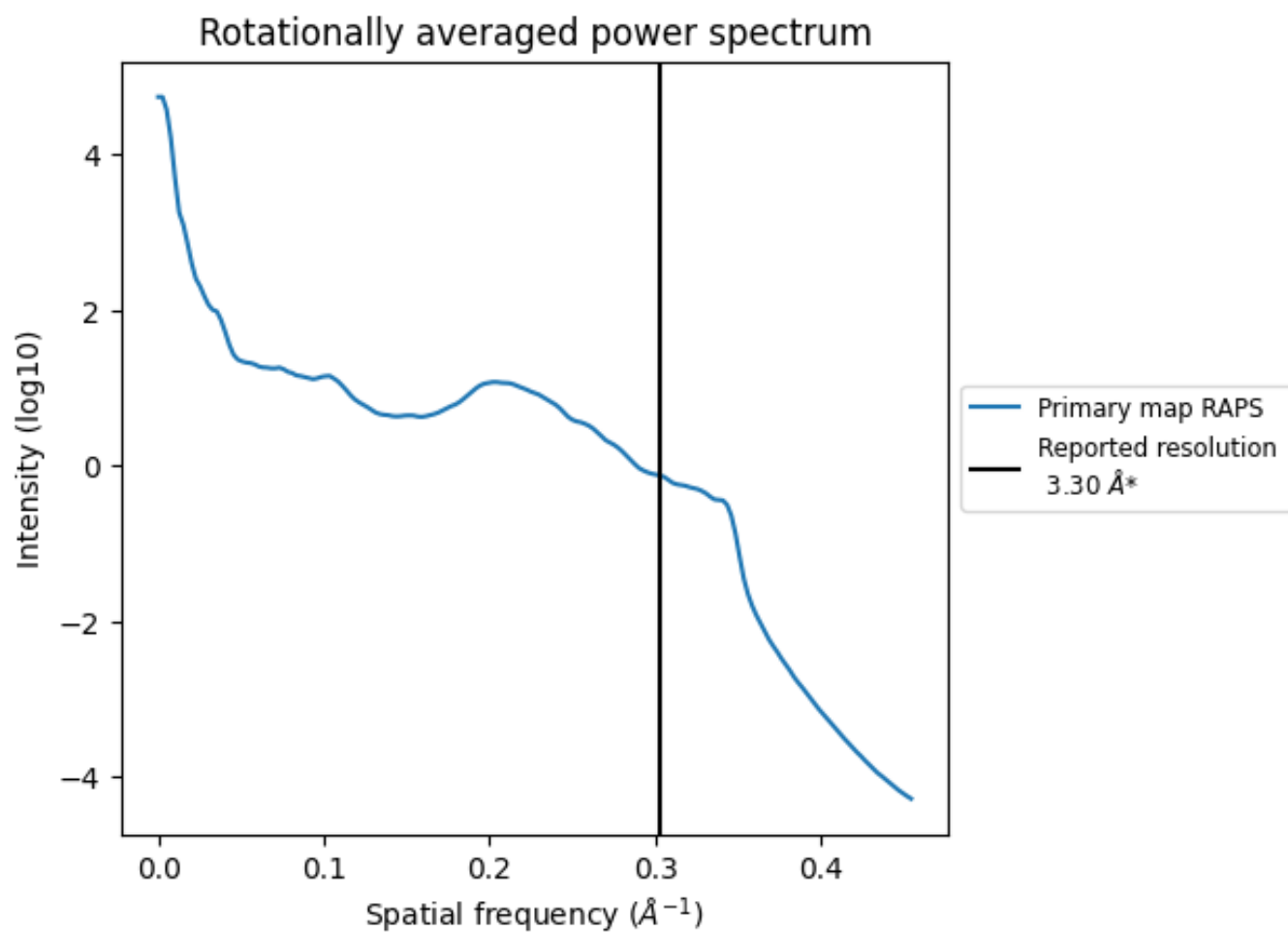
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147 nm³; this corresponds to an approximate mass of 133 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 [i](#)

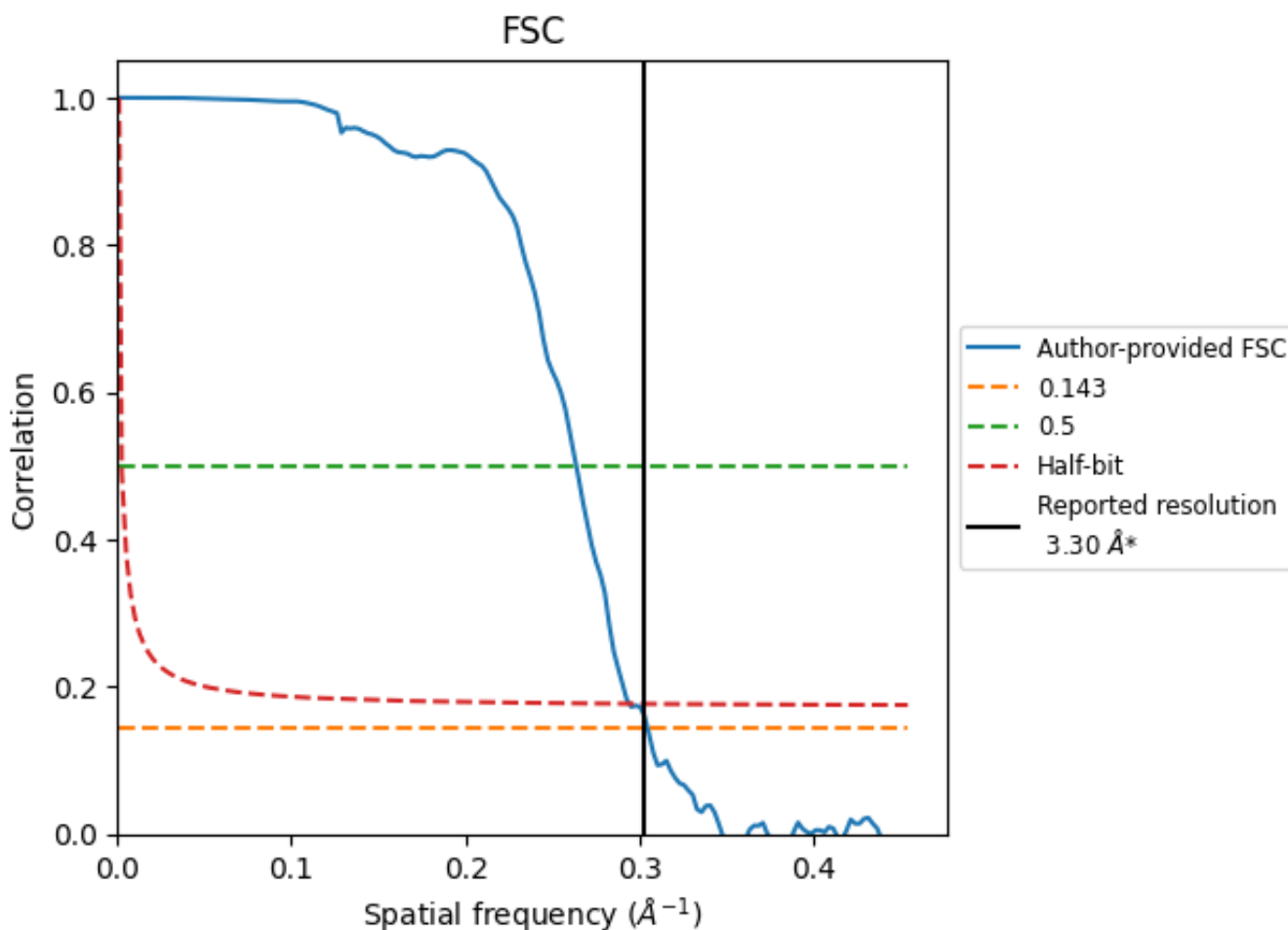


*Reported resolution corresponds to spatial frequency of 0.303\AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

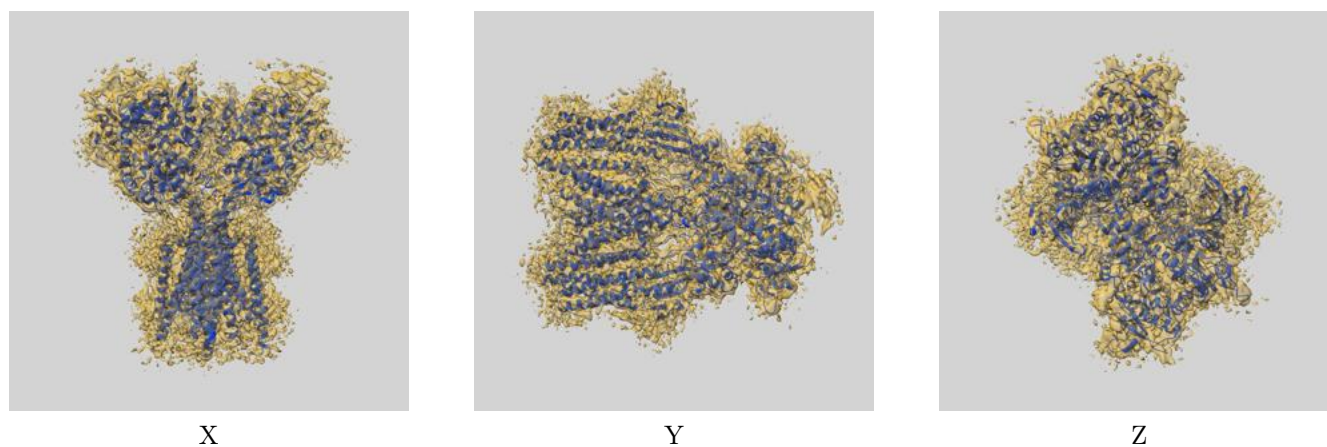
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	3.79	3.40
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

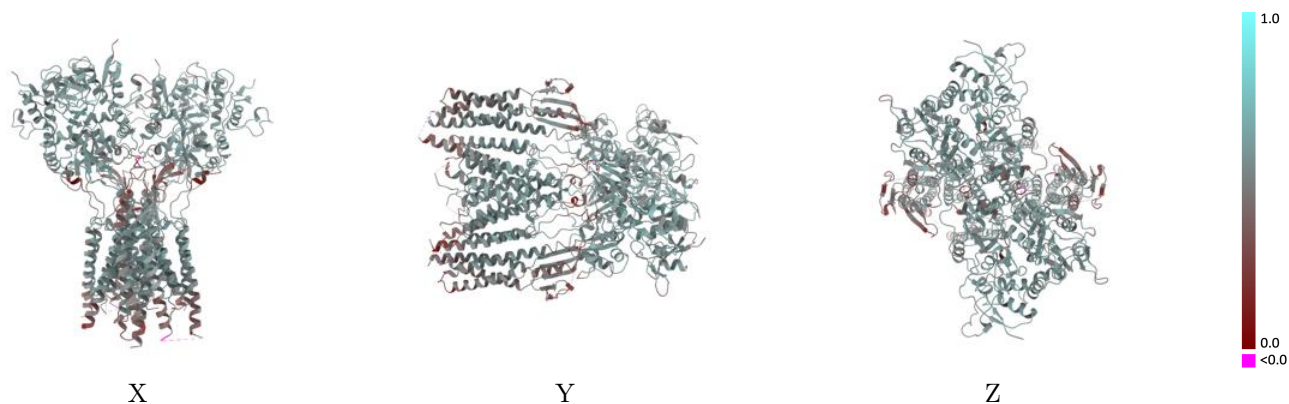
This section contains information regarding the fit between EMDB map EMD-24751 and PDB model 7RZ5. Per-residue inclusion information can be found in section 3 on page 29.

9.1 Map-model overlay [i](#)



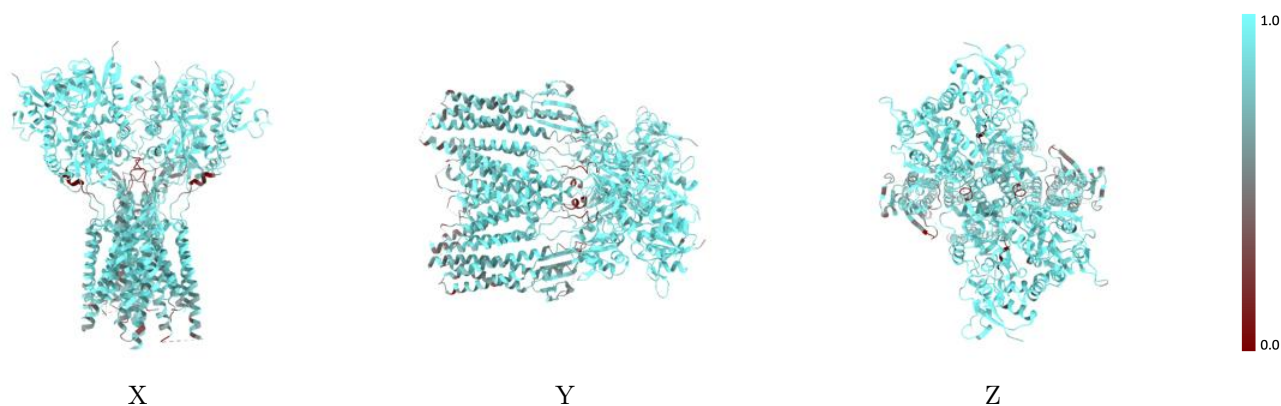
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



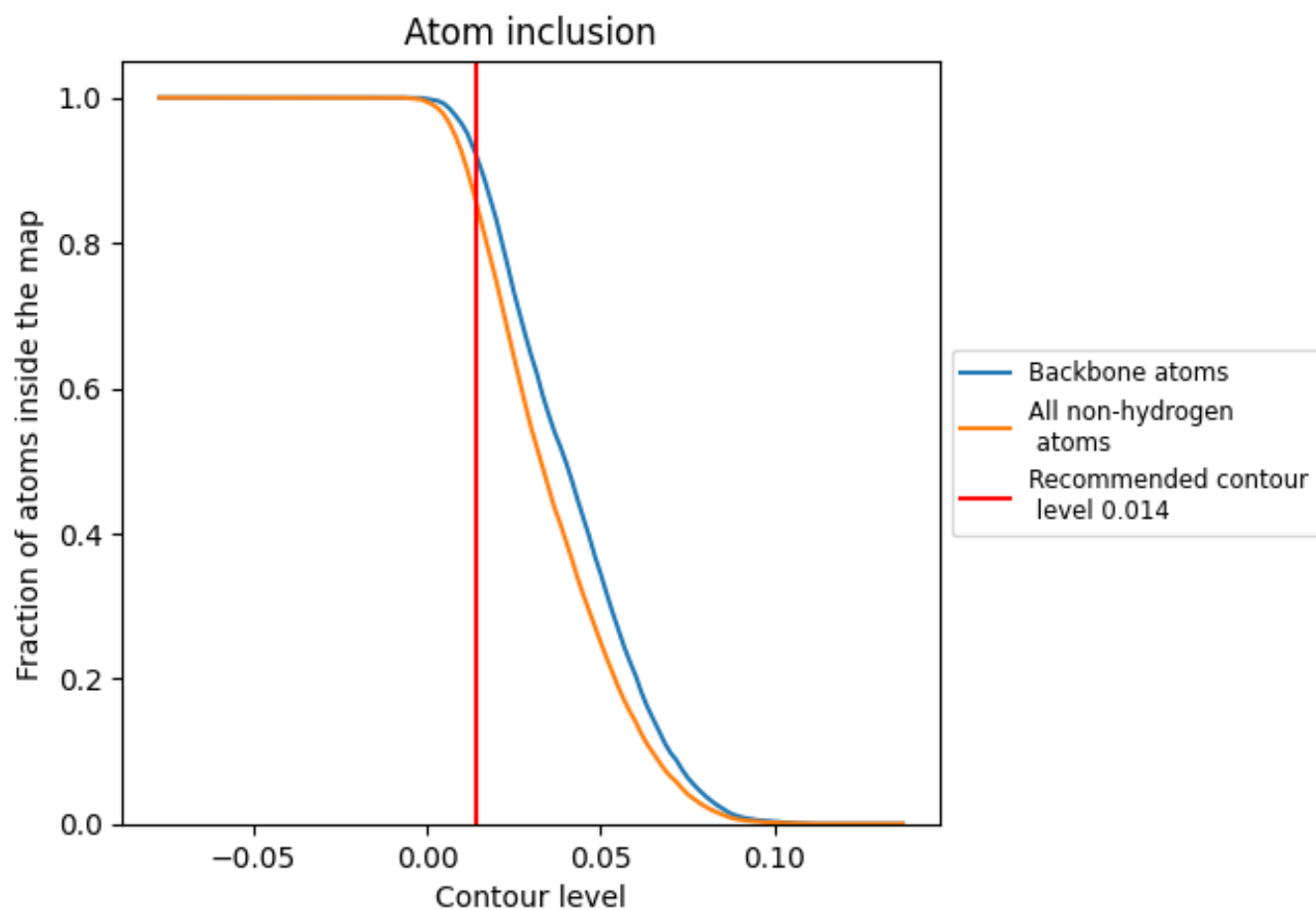
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).








9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8605	 0.5180
A	 0.8486	 0.5110
B	 0.8840	 0.5350
C	 0.8386	 0.5040
D	 0.8866	 0.5330

