



Full wwPDB EM Validation Report ⓘ

Jul 13, 2026 – 01:47 PM EDT

PDB ID : 9PEA / pdb_00009pea
EMDB ID : EMD-71555
Title : Cryo-EM structure of full-length human TRPV1 in complex with analgesic MSP20
Authors : Neuberger, A.; Talyzina, I.A.; Romeo, I.; Aiello, F.; Maramai, S.; Alcaro, S.; Artese, A.; Brizzi, A.; Sobolevsky, A.I.
Deposited on : 2025-07-01
Resolution : 2.60 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:

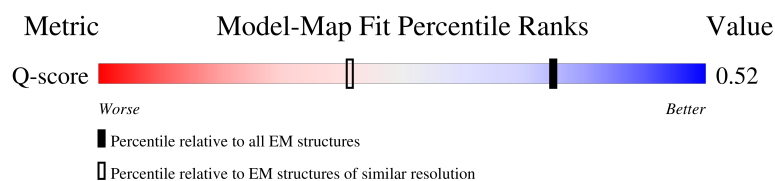
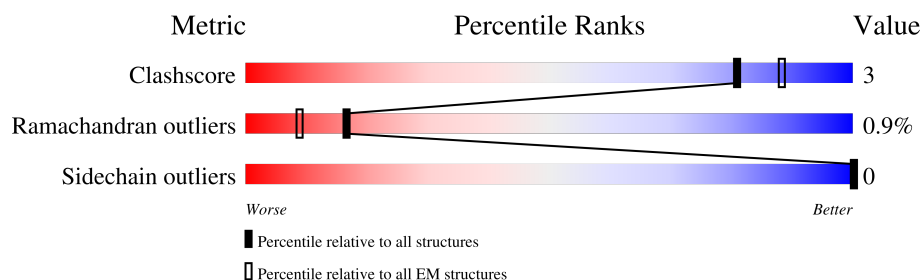
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 2.60 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	8728 (2.10 - 3.10)

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	1102	9% 44% 51%
1	B	1102	9% 44% 5% 51%
1	C	1102	9% 43% 5% 51%
1	D	1102	9% 44% 51%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18862 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 Transient receptor potential cation channel subfamily V member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	535	Total	C	N	O	S	0	0
			4338	2840	699	769	30		
1	B	535	Total	C	N	O	S	0	0
			4338	2840	699	769	30		
1	C	535	Total	C	N	O	S	0	0
			4338	2840	699	769	30		
1	D	535	Total	C	N	O	S	0	0
			4338	2840	699	769	30		

There are 1056 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q8NER1
A	0	THR	-	expression tag	UNP Q8NER1
A	1	SER	-	expression tag	UNP Q8NER1
A	840	LEU	-	expression tag	UNP Q8NER1
A	841	VAL	-	expression tag	UNP Q8NER1
A	842	PRO	-	expression tag	UNP Q8NER1
A	843	ARG	-	expression tag	UNP Q8NER1
A	844	GLY	-	expression tag	UNP Q8NER1
A	845	SER	-	expression tag	UNP Q8NER1
A	846	ALA	-	expression tag	UNP Q8NER1
A	847	ALA	-	expression tag	UNP Q8NER1
A	848	ALA	-	expression tag	UNP Q8NER1
A	849	ALA	-	expression tag	UNP Q8NER1
A	850	VAL	-	expression tag	UNP Q8NER1
A	851	SER	-	expression tag	UNP Q8NER1
A	852	LYS	-	expression tag	UNP Q8NER1
A	853	GLY	-	expression tag	UNP Q8NER1
A	854	GLU	-	expression tag	UNP Q8NER1
A	855	GLU	-	expression tag	UNP Q8NER1
A	856	LEU	-	expression tag	UNP Q8NER1
A	857	PHE	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	858	THR	-	expression tag	UNP Q8NER1
A	859	GLY	-	expression tag	UNP Q8NER1
A	860	VAL	-	expression tag	UNP Q8NER1
A	861	VAL	-	expression tag	UNP Q8NER1
A	862	PRO	-	expression tag	UNP Q8NER1
A	863	ILE	-	expression tag	UNP Q8NER1
A	864	LEU	-	expression tag	UNP Q8NER1
A	865	VAL	-	expression tag	UNP Q8NER1
A	866	GLU	-	expression tag	UNP Q8NER1
A	867	LEU	-	expression tag	UNP Q8NER1
A	868	ASP	-	expression tag	UNP Q8NER1
A	869	GLY	-	expression tag	UNP Q8NER1
A	870	ASP	-	expression tag	UNP Q8NER1
A	871	VAL	-	expression tag	UNP Q8NER1
A	872	ASN	-	expression tag	UNP Q8NER1
A	873	GLY	-	expression tag	UNP Q8NER1
A	874	HIS	-	expression tag	UNP Q8NER1
A	875	LYS	-	expression tag	UNP Q8NER1
A	876	PHE	-	expression tag	UNP Q8NER1
A	877	SER	-	expression tag	UNP Q8NER1
A	878	VAL	-	expression tag	UNP Q8NER1
A	879	SER	-	expression tag	UNP Q8NER1
A	880	GLY	-	expression tag	UNP Q8NER1
A	881	GLU	-	expression tag	UNP Q8NER1
A	882	GLY	-	expression tag	UNP Q8NER1
A	883	GLU	-	expression tag	UNP Q8NER1
A	884	GLY	-	expression tag	UNP Q8NER1
A	885	ASP	-	expression tag	UNP Q8NER1
A	886	ALA	-	expression tag	UNP Q8NER1
A	887	THR	-	expression tag	UNP Q8NER1
A	888	TYR	-	expression tag	UNP Q8NER1
A	889	GLY	-	expression tag	UNP Q8NER1
A	890	LYS	-	expression tag	UNP Q8NER1
A	891	LEU	-	expression tag	UNP Q8NER1
A	892	THR	-	expression tag	UNP Q8NER1
A	893	LEU	-	expression tag	UNP Q8NER1
A	894	LYS	-	expression tag	UNP Q8NER1
A	895	PHE	-	expression tag	UNP Q8NER1
A	896	ILE	-	expression tag	UNP Q8NER1
A	897	CYS	-	expression tag	UNP Q8NER1
A	898	THR	-	expression tag	UNP Q8NER1
A	899	THR	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	900	GLY	-	expression tag	UNP Q8NER1
A	901	LYS	-	expression tag	UNP Q8NER1
A	902	LEU	-	expression tag	UNP Q8NER1
A	903	PRO	-	expression tag	UNP Q8NER1
A	904	VAL	-	expression tag	UNP Q8NER1
A	905	PRO	-	expression tag	UNP Q8NER1
A	906	TRP	-	expression tag	UNP Q8NER1
A	907	PRO	-	expression tag	UNP Q8NER1
A	908	THR	-	expression tag	UNP Q8NER1
A	909	LEU	-	expression tag	UNP Q8NER1
A	910	VAL	-	expression tag	UNP Q8NER1
A	911	THR	-	expression tag	UNP Q8NER1
A	912	THR	-	expression tag	UNP Q8NER1
A	913	LEU	-	expression tag	UNP Q8NER1
A	914	THR	-	expression tag	UNP Q8NER1
A	915	TYR	-	expression tag	UNP Q8NER1
A	916	GLY	-	expression tag	UNP Q8NER1
A	917	VAL	-	expression tag	UNP Q8NER1
A	918	GLN	-	expression tag	UNP Q8NER1
A	919	CYS	-	expression tag	UNP Q8NER1
A	920	PHE	-	expression tag	UNP Q8NER1
A	921	SER	-	expression tag	UNP Q8NER1
A	922	ARG	-	expression tag	UNP Q8NER1
A	923	TYR	-	expression tag	UNP Q8NER1
A	924	PRO	-	expression tag	UNP Q8NER1
A	925	ASP	-	expression tag	UNP Q8NER1
A	926	HIS	-	expression tag	UNP Q8NER1
A	927	MET	-	expression tag	UNP Q8NER1
A	928	LYS	-	expression tag	UNP Q8NER1
A	929	GLN	-	expression tag	UNP Q8NER1
A	930	HIS	-	expression tag	UNP Q8NER1
A	931	ASP	-	expression tag	UNP Q8NER1
A	932	PHE	-	expression tag	UNP Q8NER1
A	933	PHE	-	expression tag	UNP Q8NER1
A	934	LYS	-	expression tag	UNP Q8NER1
A	935	SER	-	expression tag	UNP Q8NER1
A	936	ALA	-	expression tag	UNP Q8NER1
A	937	MET	-	expression tag	UNP Q8NER1
A	938	PRO	-	expression tag	UNP Q8NER1
A	939	GLU	-	expression tag	UNP Q8NER1
A	940	GLY	-	expression tag	UNP Q8NER1
A	941	TYR	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	942	VAL	-	expression tag	UNP Q8NER1
A	943	GLN	-	expression tag	UNP Q8NER1
A	944	GLU	-	expression tag	UNP Q8NER1
A	945	ARG	-	expression tag	UNP Q8NER1
A	946	THR	-	expression tag	UNP Q8NER1
A	947	ILE	-	expression tag	UNP Q8NER1
A	948	PHE	-	expression tag	UNP Q8NER1
A	949	PHE	-	expression tag	UNP Q8NER1
A	950	LYS	-	expression tag	UNP Q8NER1
A	951	ASP	-	expression tag	UNP Q8NER1
A	952	ASP	-	expression tag	UNP Q8NER1
A	953	GLY	-	expression tag	UNP Q8NER1
A	954	ASN	-	expression tag	UNP Q8NER1
A	955	TYR	-	expression tag	UNP Q8NER1
A	956	LYS	-	expression tag	UNP Q8NER1
A	957	THR	-	expression tag	UNP Q8NER1
A	958	ARG	-	expression tag	UNP Q8NER1
A	959	ALA	-	expression tag	UNP Q8NER1
A	960	GLU	-	expression tag	UNP Q8NER1
A	961	VAL	-	expression tag	UNP Q8NER1
A	962	LYS	-	expression tag	UNP Q8NER1
A	963	PHE	-	expression tag	UNP Q8NER1
A	964	GLU	-	expression tag	UNP Q8NER1
A	965	GLY	-	expression tag	UNP Q8NER1
A	966	ASP	-	expression tag	UNP Q8NER1
A	967	THR	-	expression tag	UNP Q8NER1
A	968	LEU	-	expression tag	UNP Q8NER1
A	969	VAL	-	expression tag	UNP Q8NER1
A	970	ASN	-	expression tag	UNP Q8NER1
A	971	ARG	-	expression tag	UNP Q8NER1
A	972	ILE	-	expression tag	UNP Q8NER1
A	973	GLU	-	expression tag	UNP Q8NER1
A	974	LEU	-	expression tag	UNP Q8NER1
A	975	LYS	-	expression tag	UNP Q8NER1
A	976	GLY	-	expression tag	UNP Q8NER1
A	977	ILE	-	expression tag	UNP Q8NER1
A	978	ASP	-	expression tag	UNP Q8NER1
A	979	PHE	-	expression tag	UNP Q8NER1
A	980	LYS	-	expression tag	UNP Q8NER1
A	981	GLU	-	expression tag	UNP Q8NER1
A	982	ASP	-	expression tag	UNP Q8NER1
A	983	GLY	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	984	ASN	-	expression tag	UNP Q8NER1
A	985	ILE	-	expression tag	UNP Q8NER1
A	986	LEU	-	expression tag	UNP Q8NER1
A	987	GLY	-	expression tag	UNP Q8NER1
A	988	HIS	-	expression tag	UNP Q8NER1
A	989	LYS	-	expression tag	UNP Q8NER1
A	990	LEU	-	expression tag	UNP Q8NER1
A	991	GLU	-	expression tag	UNP Q8NER1
A	992	TYR	-	expression tag	UNP Q8NER1
A	993	ASN	-	expression tag	UNP Q8NER1
A	994	TYR	-	expression tag	UNP Q8NER1
A	995	ASN	-	expression tag	UNP Q8NER1
A	996	SER	-	expression tag	UNP Q8NER1
A	997	HIS	-	expression tag	UNP Q8NER1
A	998	ASN	-	expression tag	UNP Q8NER1
A	999	VAL	-	expression tag	UNP Q8NER1
A	1000	TYR	-	expression tag	UNP Q8NER1
A	1001	ILE	-	expression tag	UNP Q8NER1
A	1002	MET	-	expression tag	UNP Q8NER1
A	1003	ALA	-	expression tag	UNP Q8NER1
A	1004	ASP	-	expression tag	UNP Q8NER1
A	1005	LYS	-	expression tag	UNP Q8NER1
A	1006	GLN	-	expression tag	UNP Q8NER1
A	1007	LYS	-	expression tag	UNP Q8NER1
A	1008	ASN	-	expression tag	UNP Q8NER1
A	1009	GLY	-	expression tag	UNP Q8NER1
A	1010	ILE	-	expression tag	UNP Q8NER1
A	1011	LYS	-	expression tag	UNP Q8NER1
A	1012	VAL	-	expression tag	UNP Q8NER1
A	1013	ASN	-	expression tag	UNP Q8NER1
A	1014	PHE	-	expression tag	UNP Q8NER1
A	1015	LYS	-	expression tag	UNP Q8NER1
A	1016	ILE	-	expression tag	UNP Q8NER1
A	1017	ARG	-	expression tag	UNP Q8NER1
A	1018	HIS	-	expression tag	UNP Q8NER1
A	1019	ASN	-	expression tag	UNP Q8NER1
A	1020	ILE	-	expression tag	UNP Q8NER1
A	1021	GLU	-	expression tag	UNP Q8NER1
A	1022	ASP	-	expression tag	UNP Q8NER1
A	1023	GLY	-	expression tag	UNP Q8NER1
A	1024	SER	-	expression tag	UNP Q8NER1
A	1025	VAL	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1026	GLN	-	expression tag	UNP Q8NER1
A	1027	LEU	-	expression tag	UNP Q8NER1
A	1028	ALA	-	expression tag	UNP Q8NER1
A	1029	ASP	-	expression tag	UNP Q8NER1
A	1030	HIS	-	expression tag	UNP Q8NER1
A	1031	TYR	-	expression tag	UNP Q8NER1
A	1032	GLN	-	expression tag	UNP Q8NER1
A	1033	GLN	-	expression tag	UNP Q8NER1
A	1034	ASN	-	expression tag	UNP Q8NER1
A	1035	THR	-	expression tag	UNP Q8NER1
A	1036	PRO	-	expression tag	UNP Q8NER1
A	1037	ILE	-	expression tag	UNP Q8NER1
A	1038	GLY	-	expression tag	UNP Q8NER1
A	1039	ASP	-	expression tag	UNP Q8NER1
A	1040	GLY	-	expression tag	UNP Q8NER1
A	1041	PRO	-	expression tag	UNP Q8NER1
A	1042	VAL	-	expression tag	UNP Q8NER1
A	1043	LEU	-	expression tag	UNP Q8NER1
A	1044	LEU	-	expression tag	UNP Q8NER1
A	1045	PRO	-	expression tag	UNP Q8NER1
A	1046	ASP	-	expression tag	UNP Q8NER1
A	1047	ASN	-	expression tag	UNP Q8NER1
A	1048	HIS	-	expression tag	UNP Q8NER1
A	1049	TYR	-	expression tag	UNP Q8NER1
A	1050	LEU	-	expression tag	UNP Q8NER1
A	1051	SER	-	expression tag	UNP Q8NER1
A	1052	THR	-	expression tag	UNP Q8NER1
A	1053	GLN	-	expression tag	UNP Q8NER1
A	1054	SER	-	expression tag	UNP Q8NER1
A	1055	LYS	-	expression tag	UNP Q8NER1
A	1056	LEU	-	expression tag	UNP Q8NER1
A	1057	SER	-	expression tag	UNP Q8NER1
A	1058	LYS	-	expression tag	UNP Q8NER1
A	1059	ASP	-	expression tag	UNP Q8NER1
A	1060	PRO	-	expression tag	UNP Q8NER1
A	1061	ASN	-	expression tag	UNP Q8NER1
A	1062	GLU	-	expression tag	UNP Q8NER1
A	1063	LYS	-	expression tag	UNP Q8NER1
A	1064	ARG	-	expression tag	UNP Q8NER1
A	1065	ASP	-	expression tag	UNP Q8NER1
A	1066	HIS	-	expression tag	UNP Q8NER1
A	1067	MET	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1068	VAL	-	expression tag	UNP Q8NER1
A	1069	LEU	-	expression tag	UNP Q8NER1
A	1070	LEU	-	expression tag	UNP Q8NER1
A	1071	GLU	-	expression tag	UNP Q8NER1
A	1072	PHE	-	expression tag	UNP Q8NER1
A	1073	VAL	-	expression tag	UNP Q8NER1
A	1074	THR	-	expression tag	UNP Q8NER1
A	1075	ALA	-	expression tag	UNP Q8NER1
A	1076	ALA	-	expression tag	UNP Q8NER1
A	1077	GLY	-	expression tag	UNP Q8NER1
A	1078	ILE	-	expression tag	UNP Q8NER1
A	1079	THR	-	expression tag	UNP Q8NER1
A	1080	LEU	-	expression tag	UNP Q8NER1
A	1081	GLY	-	expression tag	UNP Q8NER1
A	1082	MET	-	expression tag	UNP Q8NER1
A	1083	ASP	-	expression tag	UNP Q8NER1
A	1084	GLU	-	expression tag	UNP Q8NER1
A	1085	LEU	-	expression tag	UNP Q8NER1
A	1086	TYR	-	expression tag	UNP Q8NER1
A	1087	LYS	-	expression tag	UNP Q8NER1
A	1088	SER	-	expression tag	UNP Q8NER1
A	1089	GLY	-	expression tag	UNP Q8NER1
A	1090	LEU	-	expression tag	UNP Q8NER1
A	1091	ARG	-	expression tag	UNP Q8NER1
A	1092	SER	-	expression tag	UNP Q8NER1
A	1093	TRP	-	expression tag	UNP Q8NER1
A	1094	SER	-	expression tag	UNP Q8NER1
A	1095	HIS	-	expression tag	UNP Q8NER1
A	1096	PRO	-	expression tag	UNP Q8NER1
A	1097	GLN	-	expression tag	UNP Q8NER1
A	1098	PHE	-	expression tag	UNP Q8NER1
A	1099	GLU	-	expression tag	UNP Q8NER1
A	1100	LYS	-	expression tag	UNP Q8NER1
B	-1	MET	-	initiating methionine	UNP Q8NER1
B	0	THR	-	expression tag	UNP Q8NER1
B	1	SER	-	expression tag	UNP Q8NER1
B	840	LEU	-	expression tag	UNP Q8NER1
B	841	VAL	-	expression tag	UNP Q8NER1
B	842	PRO	-	expression tag	UNP Q8NER1
B	843	ARG	-	expression tag	UNP Q8NER1
B	844	GLY	-	expression tag	UNP Q8NER1
B	845	SER	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	846	ALA	-	expression tag	UNP Q8NER1
B	847	ALA	-	expression tag	UNP Q8NER1
B	848	ALA	-	expression tag	UNP Q8NER1
B	849	ALA	-	expression tag	UNP Q8NER1
B	850	VAL	-	expression tag	UNP Q8NER1
B	851	SER	-	expression tag	UNP Q8NER1
B	852	LYS	-	expression tag	UNP Q8NER1
B	853	GLY	-	expression tag	UNP Q8NER1
B	854	GLU	-	expression tag	UNP Q8NER1
B	855	GLU	-	expression tag	UNP Q8NER1
B	856	LEU	-	expression tag	UNP Q8NER1
B	857	PHE	-	expression tag	UNP Q8NER1
B	858	THR	-	expression tag	UNP Q8NER1
B	859	GLY	-	expression tag	UNP Q8NER1
B	860	VAL	-	expression tag	UNP Q8NER1
B	861	VAL	-	expression tag	UNP Q8NER1
B	862	PRO	-	expression tag	UNP Q8NER1
B	863	ILE	-	expression tag	UNP Q8NER1
B	864	LEU	-	expression tag	UNP Q8NER1
B	865	VAL	-	expression tag	UNP Q8NER1
B	866	GLU	-	expression tag	UNP Q8NER1
B	867	LEU	-	expression tag	UNP Q8NER1
B	868	ASP	-	expression tag	UNP Q8NER1
B	869	GLY	-	expression tag	UNP Q8NER1
B	870	ASP	-	expression tag	UNP Q8NER1
B	871	VAL	-	expression tag	UNP Q8NER1
B	872	ASN	-	expression tag	UNP Q8NER1
B	873	GLY	-	expression tag	UNP Q8NER1
B	874	HIS	-	expression tag	UNP Q8NER1
B	875	LYS	-	expression tag	UNP Q8NER1
B	876	PHE	-	expression tag	UNP Q8NER1
B	877	SER	-	expression tag	UNP Q8NER1
B	878	VAL	-	expression tag	UNP Q8NER1
B	879	SER	-	expression tag	UNP Q8NER1
B	880	GLY	-	expression tag	UNP Q8NER1
B	881	GLU	-	expression tag	UNP Q8NER1
B	882	GLY	-	expression tag	UNP Q8NER1
B	883	GLU	-	expression tag	UNP Q8NER1
B	884	GLY	-	expression tag	UNP Q8NER1
B	885	ASP	-	expression tag	UNP Q8NER1
B	886	ALA	-	expression tag	UNP Q8NER1
B	887	THR	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	888	TYR	-	expression tag	UNP Q8NER1
B	889	GLY	-	expression tag	UNP Q8NER1
B	890	LYS	-	expression tag	UNP Q8NER1
B	891	LEU	-	expression tag	UNP Q8NER1
B	892	THR	-	expression tag	UNP Q8NER1
B	893	LEU	-	expression tag	UNP Q8NER1
B	894	LYS	-	expression tag	UNP Q8NER1
B	895	PHE	-	expression tag	UNP Q8NER1
B	896	ILE	-	expression tag	UNP Q8NER1
B	897	CYS	-	expression tag	UNP Q8NER1
B	898	THR	-	expression tag	UNP Q8NER1
B	899	THR	-	expression tag	UNP Q8NER1
B	900	GLY	-	expression tag	UNP Q8NER1
B	901	LYS	-	expression tag	UNP Q8NER1
B	902	LEU	-	expression tag	UNP Q8NER1
B	903	PRO	-	expression tag	UNP Q8NER1
B	904	VAL	-	expression tag	UNP Q8NER1
B	905	PRO	-	expression tag	UNP Q8NER1
B	906	TRP	-	expression tag	UNP Q8NER1
B	907	PRO	-	expression tag	UNP Q8NER1
B	908	THR	-	expression tag	UNP Q8NER1
B	909	LEU	-	expression tag	UNP Q8NER1
B	910	VAL	-	expression tag	UNP Q8NER1
B	911	THR	-	expression tag	UNP Q8NER1
B	912	THR	-	expression tag	UNP Q8NER1
B	913	LEU	-	expression tag	UNP Q8NER1
B	914	THR	-	expression tag	UNP Q8NER1
B	915	TYR	-	expression tag	UNP Q8NER1
B	916	GLY	-	expression tag	UNP Q8NER1
B	917	VAL	-	expression tag	UNP Q8NER1
B	918	GLN	-	expression tag	UNP Q8NER1
B	919	CYS	-	expression tag	UNP Q8NER1
B	920	PHE	-	expression tag	UNP Q8NER1
B	921	SER	-	expression tag	UNP Q8NER1
B	922	ARG	-	expression tag	UNP Q8NER1
B	923	TYR	-	expression tag	UNP Q8NER1
B	924	PRO	-	expression tag	UNP Q8NER1
B	925	ASP	-	expression tag	UNP Q8NER1
B	926	HIS	-	expression tag	UNP Q8NER1
B	927	MET	-	expression tag	UNP Q8NER1
B	928	LYS	-	expression tag	UNP Q8NER1
B	929	GLN	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	930	HIS	-	expression tag	UNP Q8NER1
B	931	ASP	-	expression tag	UNP Q8NER1
B	932	PHE	-	expression tag	UNP Q8NER1
B	933	PHE	-	expression tag	UNP Q8NER1
B	934	LYS	-	expression tag	UNP Q8NER1
B	935	SER	-	expression tag	UNP Q8NER1
B	936	ALA	-	expression tag	UNP Q8NER1
B	937	MET	-	expression tag	UNP Q8NER1
B	938	PRO	-	expression tag	UNP Q8NER1
B	939	GLU	-	expression tag	UNP Q8NER1
B	940	GLY	-	expression tag	UNP Q8NER1
B	941	TYR	-	expression tag	UNP Q8NER1
B	942	VAL	-	expression tag	UNP Q8NER1
B	943	GLN	-	expression tag	UNP Q8NER1
B	944	GLU	-	expression tag	UNP Q8NER1
B	945	ARG	-	expression tag	UNP Q8NER1
B	946	THR	-	expression tag	UNP Q8NER1
B	947	ILE	-	expression tag	UNP Q8NER1
B	948	PHE	-	expression tag	UNP Q8NER1
B	949	PHE	-	expression tag	UNP Q8NER1
B	950	LYS	-	expression tag	UNP Q8NER1
B	951	ASP	-	expression tag	UNP Q8NER1
B	952	ASP	-	expression tag	UNP Q8NER1
B	953	GLY	-	expression tag	UNP Q8NER1
B	954	ASN	-	expression tag	UNP Q8NER1
B	955	TYR	-	expression tag	UNP Q8NER1
B	956	LYS	-	expression tag	UNP Q8NER1
B	957	THR	-	expression tag	UNP Q8NER1
B	958	ARG	-	expression tag	UNP Q8NER1
B	959	ALA	-	expression tag	UNP Q8NER1
B	960	GLU	-	expression tag	UNP Q8NER1
B	961	VAL	-	expression tag	UNP Q8NER1
B	962	LYS	-	expression tag	UNP Q8NER1
B	963	PHE	-	expression tag	UNP Q8NER1
B	964	GLU	-	expression tag	UNP Q8NER1
B	965	GLY	-	expression tag	UNP Q8NER1
B	966	ASP	-	expression tag	UNP Q8NER1
B	967	THR	-	expression tag	UNP Q8NER1
B	968	LEU	-	expression tag	UNP Q8NER1
B	969	VAL	-	expression tag	UNP Q8NER1
B	970	ASN	-	expression tag	UNP Q8NER1
B	971	ARG	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	972	ILE	-	expression tag	UNP Q8NER1
B	973	GLU	-	expression tag	UNP Q8NER1
B	974	LEU	-	expression tag	UNP Q8NER1
B	975	LYS	-	expression tag	UNP Q8NER1
B	976	GLY	-	expression tag	UNP Q8NER1
B	977	ILE	-	expression tag	UNP Q8NER1
B	978	ASP	-	expression tag	UNP Q8NER1
B	979	PHE	-	expression tag	UNP Q8NER1
B	980	LYS	-	expression tag	UNP Q8NER1
B	981	GLU	-	expression tag	UNP Q8NER1
B	982	ASP	-	expression tag	UNP Q8NER1
B	983	GLY	-	expression tag	UNP Q8NER1
B	984	ASN	-	expression tag	UNP Q8NER1
B	985	ILE	-	expression tag	UNP Q8NER1
B	986	LEU	-	expression tag	UNP Q8NER1
B	987	GLY	-	expression tag	UNP Q8NER1
B	988	HIS	-	expression tag	UNP Q8NER1
B	989	LYS	-	expression tag	UNP Q8NER1
B	990	LEU	-	expression tag	UNP Q8NER1
B	991	GLU	-	expression tag	UNP Q8NER1
B	992	TYR	-	expression tag	UNP Q8NER1
B	993	ASN	-	expression tag	UNP Q8NER1
B	994	TYR	-	expression tag	UNP Q8NER1
B	995	ASN	-	expression tag	UNP Q8NER1
B	996	SER	-	expression tag	UNP Q8NER1
B	997	HIS	-	expression tag	UNP Q8NER1
B	998	ASN	-	expression tag	UNP Q8NER1
B	999	VAL	-	expression tag	UNP Q8NER1
B	1000	TYR	-	expression tag	UNP Q8NER1
B	1001	ILE	-	expression tag	UNP Q8NER1
B	1002	MET	-	expression tag	UNP Q8NER1
B	1003	ALA	-	expression tag	UNP Q8NER1
B	1004	ASP	-	expression tag	UNP Q8NER1
B	1005	LYS	-	expression tag	UNP Q8NER1
B	1006	GLN	-	expression tag	UNP Q8NER1
B	1007	LYS	-	expression tag	UNP Q8NER1
B	1008	ASN	-	expression tag	UNP Q8NER1
B	1009	GLY	-	expression tag	UNP Q8NER1
B	1010	ILE	-	expression tag	UNP Q8NER1
B	1011	LYS	-	expression tag	UNP Q8NER1
B	1012	VAL	-	expression tag	UNP Q8NER1
B	1013	ASN	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1014	PHE	-	expression tag	UNP Q8NER1
B	1015	LYS	-	expression tag	UNP Q8NER1
B	1016	ILE	-	expression tag	UNP Q8NER1
B	1017	ARG	-	expression tag	UNP Q8NER1
B	1018	HIS	-	expression tag	UNP Q8NER1
B	1019	ASN	-	expression tag	UNP Q8NER1
B	1020	ILE	-	expression tag	UNP Q8NER1
B	1021	GLU	-	expression tag	UNP Q8NER1
B	1022	ASP	-	expression tag	UNP Q8NER1
B	1023	GLY	-	expression tag	UNP Q8NER1
B	1024	SER	-	expression tag	UNP Q8NER1
B	1025	VAL	-	expression tag	UNP Q8NER1
B	1026	GLN	-	expression tag	UNP Q8NER1
B	1027	LEU	-	expression tag	UNP Q8NER1
B	1028	ALA	-	expression tag	UNP Q8NER1
B	1029	ASP	-	expression tag	UNP Q8NER1
B	1030	HIS	-	expression tag	UNP Q8NER1
B	1031	TYR	-	expression tag	UNP Q8NER1
B	1032	GLN	-	expression tag	UNP Q8NER1
B	1033	GLN	-	expression tag	UNP Q8NER1
B	1034	ASN	-	expression tag	UNP Q8NER1
B	1035	THR	-	expression tag	UNP Q8NER1
B	1036	PRO	-	expression tag	UNP Q8NER1
B	1037	ILE	-	expression tag	UNP Q8NER1
B	1038	GLY	-	expression tag	UNP Q8NER1
B	1039	ASP	-	expression tag	UNP Q8NER1
B	1040	GLY	-	expression tag	UNP Q8NER1
B	1041	PRO	-	expression tag	UNP Q8NER1
B	1042	VAL	-	expression tag	UNP Q8NER1
B	1043	LEU	-	expression tag	UNP Q8NER1
B	1044	LEU	-	expression tag	UNP Q8NER1
B	1045	PRO	-	expression tag	UNP Q8NER1
B	1046	ASP	-	expression tag	UNP Q8NER1
B	1047	ASN	-	expression tag	UNP Q8NER1
B	1048	HIS	-	expression tag	UNP Q8NER1
B	1049	TYR	-	expression tag	UNP Q8NER1
B	1050	LEU	-	expression tag	UNP Q8NER1
B	1051	SER	-	expression tag	UNP Q8NER1
B	1052	THR	-	expression tag	UNP Q8NER1
B	1053	GLN	-	expression tag	UNP Q8NER1
B	1054	SER	-	expression tag	UNP Q8NER1
B	1055	LYS	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1056	LEU	-	expression tag	UNP Q8NER1
B	1057	SER	-	expression tag	UNP Q8NER1
B	1058	LYS	-	expression tag	UNP Q8NER1
B	1059	ASP	-	expression tag	UNP Q8NER1
B	1060	PRO	-	expression tag	UNP Q8NER1
B	1061	ASN	-	expression tag	UNP Q8NER1
B	1062	GLU	-	expression tag	UNP Q8NER1
B	1063	LYS	-	expression tag	UNP Q8NER1
B	1064	ARG	-	expression tag	UNP Q8NER1
B	1065	ASP	-	expression tag	UNP Q8NER1
B	1066	HIS	-	expression tag	UNP Q8NER1
B	1067	MET	-	expression tag	UNP Q8NER1
B	1068	VAL	-	expression tag	UNP Q8NER1
B	1069	LEU	-	expression tag	UNP Q8NER1
B	1070	LEU	-	expression tag	UNP Q8NER1
B	1071	GLU	-	expression tag	UNP Q8NER1
B	1072	PHE	-	expression tag	UNP Q8NER1
B	1073	VAL	-	expression tag	UNP Q8NER1
B	1074	THR	-	expression tag	UNP Q8NER1
B	1075	ALA	-	expression tag	UNP Q8NER1
B	1076	ALA	-	expression tag	UNP Q8NER1
B	1077	GLY	-	expression tag	UNP Q8NER1
B	1078	ILE	-	expression tag	UNP Q8NER1
B	1079	THR	-	expression tag	UNP Q8NER1
B	1080	LEU	-	expression tag	UNP Q8NER1
B	1081	GLY	-	expression tag	UNP Q8NER1
B	1082	MET	-	expression tag	UNP Q8NER1
B	1083	ASP	-	expression tag	UNP Q8NER1
B	1084	GLU	-	expression tag	UNP Q8NER1
B	1085	LEU	-	expression tag	UNP Q8NER1
B	1086	TYR	-	expression tag	UNP Q8NER1
B	1087	LYS	-	expression tag	UNP Q8NER1
B	1088	SER	-	expression tag	UNP Q8NER1
B	1089	GLY	-	expression tag	UNP Q8NER1
B	1090	LEU	-	expression tag	UNP Q8NER1
B	1091	ARG	-	expression tag	UNP Q8NER1
B	1092	SER	-	expression tag	UNP Q8NER1
B	1093	TRP	-	expression tag	UNP Q8NER1
B	1094	SER	-	expression tag	UNP Q8NER1
B	1095	HIS	-	expression tag	UNP Q8NER1
B	1096	PRO	-	expression tag	UNP Q8NER1
B	1097	GLN	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1098	PHE	-	expression tag	UNP Q8NER1
B	1099	GLU	-	expression tag	UNP Q8NER1
B	1100	LYS	-	expression tag	UNP Q8NER1
C	-1	MET	-	initiating methionine	UNP Q8NER1
C	0	THR	-	expression tag	UNP Q8NER1
C	1	SER	-	expression tag	UNP Q8NER1
C	840	LEU	-	expression tag	UNP Q8NER1
C	841	VAL	-	expression tag	UNP Q8NER1
C	842	PRO	-	expression tag	UNP Q8NER1
C	843	ARG	-	expression tag	UNP Q8NER1
C	844	GLY	-	expression tag	UNP Q8NER1
C	845	SER	-	expression tag	UNP Q8NER1
C	846	ALA	-	expression tag	UNP Q8NER1
C	847	ALA	-	expression tag	UNP Q8NER1
C	848	ALA	-	expression tag	UNP Q8NER1
C	849	ALA	-	expression tag	UNP Q8NER1
C	850	VAL	-	expression tag	UNP Q8NER1
C	851	SER	-	expression tag	UNP Q8NER1
C	852	LYS	-	expression tag	UNP Q8NER1
C	853	GLY	-	expression tag	UNP Q8NER1
C	854	GLU	-	expression tag	UNP Q8NER1
C	855	GLU	-	expression tag	UNP Q8NER1
C	856	LEU	-	expression tag	UNP Q8NER1
C	857	PHE	-	expression tag	UNP Q8NER1
C	858	THR	-	expression tag	UNP Q8NER1
C	859	GLY	-	expression tag	UNP Q8NER1
C	860	VAL	-	expression tag	UNP Q8NER1
C	861	VAL	-	expression tag	UNP Q8NER1
C	862	PRO	-	expression tag	UNP Q8NER1
C	863	ILE	-	expression tag	UNP Q8NER1
C	864	LEU	-	expression tag	UNP Q8NER1
C	865	VAL	-	expression tag	UNP Q8NER1
C	866	GLU	-	expression tag	UNP Q8NER1
C	867	LEU	-	expression tag	UNP Q8NER1
C	868	ASP	-	expression tag	UNP Q8NER1
C	869	GLY	-	expression tag	UNP Q8NER1
C	870	ASP	-	expression tag	UNP Q8NER1
C	871	VAL	-	expression tag	UNP Q8NER1
C	872	ASN	-	expression tag	UNP Q8NER1
C	873	GLY	-	expression tag	UNP Q8NER1
C	874	HIS	-	expression tag	UNP Q8NER1
C	875	LYS	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	876	PHE	-	expression tag	UNP Q8NER1
C	877	SER	-	expression tag	UNP Q8NER1
C	878	VAL	-	expression tag	UNP Q8NER1
C	879	SER	-	expression tag	UNP Q8NER1
C	880	GLY	-	expression tag	UNP Q8NER1
C	881	GLU	-	expression tag	UNP Q8NER1
C	882	GLY	-	expression tag	UNP Q8NER1
C	883	GLU	-	expression tag	UNP Q8NER1
C	884	GLY	-	expression tag	UNP Q8NER1
C	885	ASP	-	expression tag	UNP Q8NER1
C	886	ALA	-	expression tag	UNP Q8NER1
C	887	THR	-	expression tag	UNP Q8NER1
C	888	TYR	-	expression tag	UNP Q8NER1
C	889	GLY	-	expression tag	UNP Q8NER1
C	890	LYS	-	expression tag	UNP Q8NER1
C	891	LEU	-	expression tag	UNP Q8NER1
C	892	THR	-	expression tag	UNP Q8NER1
C	893	LEU	-	expression tag	UNP Q8NER1
C	894	LYS	-	expression tag	UNP Q8NER1
C	895	PHE	-	expression tag	UNP Q8NER1
C	896	ILE	-	expression tag	UNP Q8NER1
C	897	CYS	-	expression tag	UNP Q8NER1
C	898	THR	-	expression tag	UNP Q8NER1
C	899	THR	-	expression tag	UNP Q8NER1
C	900	GLY	-	expression tag	UNP Q8NER1
C	901	LYS	-	expression tag	UNP Q8NER1
C	902	LEU	-	expression tag	UNP Q8NER1
C	903	PRO	-	expression tag	UNP Q8NER1
C	904	VAL	-	expression tag	UNP Q8NER1
C	905	PRO	-	expression tag	UNP Q8NER1
C	906	TRP	-	expression tag	UNP Q8NER1
C	907	PRO	-	expression tag	UNP Q8NER1
C	908	THR	-	expression tag	UNP Q8NER1
C	909	LEU	-	expression tag	UNP Q8NER1
C	910	VAL	-	expression tag	UNP Q8NER1
C	911	THR	-	expression tag	UNP Q8NER1
C	912	THR	-	expression tag	UNP Q8NER1
C	913	LEU	-	expression tag	UNP Q8NER1
C	914	THR	-	expression tag	UNP Q8NER1
C	915	TYR	-	expression tag	UNP Q8NER1
C	916	GLY	-	expression tag	UNP Q8NER1
C	917	VAL	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	918	GLN	-	expression tag	UNP Q8NER1
C	919	CYS	-	expression tag	UNP Q8NER1
C	920	PHE	-	expression tag	UNP Q8NER1
C	921	SER	-	expression tag	UNP Q8NER1
C	922	ARG	-	expression tag	UNP Q8NER1
C	923	TYR	-	expression tag	UNP Q8NER1
C	924	PRO	-	expression tag	UNP Q8NER1
C	925	ASP	-	expression tag	UNP Q8NER1
C	926	HIS	-	expression tag	UNP Q8NER1
C	927	MET	-	expression tag	UNP Q8NER1
C	928	LYS	-	expression tag	UNP Q8NER1
C	929	GLN	-	expression tag	UNP Q8NER1
C	930	HIS	-	expression tag	UNP Q8NER1
C	931	ASP	-	expression tag	UNP Q8NER1
C	932	PHE	-	expression tag	UNP Q8NER1
C	933	PHE	-	expression tag	UNP Q8NER1
C	934	LYS	-	expression tag	UNP Q8NER1
C	935	SER	-	expression tag	UNP Q8NER1
C	936	ALA	-	expression tag	UNP Q8NER1
C	937	MET	-	expression tag	UNP Q8NER1
C	938	PRO	-	expression tag	UNP Q8NER1
C	939	GLU	-	expression tag	UNP Q8NER1
C	940	GLY	-	expression tag	UNP Q8NER1
C	941	TYR	-	expression tag	UNP Q8NER1
C	942	VAL	-	expression tag	UNP Q8NER1
C	943	GLN	-	expression tag	UNP Q8NER1
C	944	GLU	-	expression tag	UNP Q8NER1
C	945	ARG	-	expression tag	UNP Q8NER1
C	946	THR	-	expression tag	UNP Q8NER1
C	947	ILE	-	expression tag	UNP Q8NER1
C	948	PHE	-	expression tag	UNP Q8NER1
C	949	PHE	-	expression tag	UNP Q8NER1
C	950	LYS	-	expression tag	UNP Q8NER1
C	951	ASP	-	expression tag	UNP Q8NER1
C	952	ASP	-	expression tag	UNP Q8NER1
C	953	GLY	-	expression tag	UNP Q8NER1
C	954	ASN	-	expression tag	UNP Q8NER1
C	955	TYR	-	expression tag	UNP Q8NER1
C	956	LYS	-	expression tag	UNP Q8NER1
C	957	THR	-	expression tag	UNP Q8NER1
C	958	ARG	-	expression tag	UNP Q8NER1
C	959	ALA	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	960	GLU	-	expression tag	UNP Q8NER1
C	961	VAL	-	expression tag	UNP Q8NER1
C	962	LYS	-	expression tag	UNP Q8NER1
C	963	PHE	-	expression tag	UNP Q8NER1
C	964	GLU	-	expression tag	UNP Q8NER1
C	965	GLY	-	expression tag	UNP Q8NER1
C	966	ASP	-	expression tag	UNP Q8NER1
C	967	THR	-	expression tag	UNP Q8NER1
C	968	LEU	-	expression tag	UNP Q8NER1
C	969	VAL	-	expression tag	UNP Q8NER1
C	970	ASN	-	expression tag	UNP Q8NER1
C	971	ARG	-	expression tag	UNP Q8NER1
C	972	ILE	-	expression tag	UNP Q8NER1
C	973	GLU	-	expression tag	UNP Q8NER1
C	974	LEU	-	expression tag	UNP Q8NER1
C	975	LYS	-	expression tag	UNP Q8NER1
C	976	GLY	-	expression tag	UNP Q8NER1
C	977	ILE	-	expression tag	UNP Q8NER1
C	978	ASP	-	expression tag	UNP Q8NER1
C	979	PHE	-	expression tag	UNP Q8NER1
C	980	LYS	-	expression tag	UNP Q8NER1
C	981	GLU	-	expression tag	UNP Q8NER1
C	982	ASP	-	expression tag	UNP Q8NER1
C	983	GLY	-	expression tag	UNP Q8NER1
C	984	ASN	-	expression tag	UNP Q8NER1
C	985	ILE	-	expression tag	UNP Q8NER1
C	986	LEU	-	expression tag	UNP Q8NER1
C	987	GLY	-	expression tag	UNP Q8NER1
C	988	HIS	-	expression tag	UNP Q8NER1
C	989	LYS	-	expression tag	UNP Q8NER1
C	990	LEU	-	expression tag	UNP Q8NER1
C	991	GLU	-	expression tag	UNP Q8NER1
C	992	TYR	-	expression tag	UNP Q8NER1
C	993	ASN	-	expression tag	UNP Q8NER1
C	994	TYR	-	expression tag	UNP Q8NER1
C	995	ASN	-	expression tag	UNP Q8NER1
C	996	SER	-	expression tag	UNP Q8NER1
C	997	HIS	-	expression tag	UNP Q8NER1
C	998	ASN	-	expression tag	UNP Q8NER1
C	999	VAL	-	expression tag	UNP Q8NER1
C	1000	TYR	-	expression tag	UNP Q8NER1
C	1001	ILE	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1002	MET	-	expression tag	UNP Q8NER1
C	1003	ALA	-	expression tag	UNP Q8NER1
C	1004	ASP	-	expression tag	UNP Q8NER1
C	1005	LYS	-	expression tag	UNP Q8NER1
C	1006	GLN	-	expression tag	UNP Q8NER1
C	1007	LYS	-	expression tag	UNP Q8NER1
C	1008	ASN	-	expression tag	UNP Q8NER1
C	1009	GLY	-	expression tag	UNP Q8NER1
C	1010	ILE	-	expression tag	UNP Q8NER1
C	1011	LYS	-	expression tag	UNP Q8NER1
C	1012	VAL	-	expression tag	UNP Q8NER1
C	1013	ASN	-	expression tag	UNP Q8NER1
C	1014	PHE	-	expression tag	UNP Q8NER1
C	1015	LYS	-	expression tag	UNP Q8NER1
C	1016	ILE	-	expression tag	UNP Q8NER1
C	1017	ARG	-	expression tag	UNP Q8NER1
C	1018	HIS	-	expression tag	UNP Q8NER1
C	1019	ASN	-	expression tag	UNP Q8NER1
C	1020	ILE	-	expression tag	UNP Q8NER1
C	1021	GLU	-	expression tag	UNP Q8NER1
C	1022	ASP	-	expression tag	UNP Q8NER1
C	1023	GLY	-	expression tag	UNP Q8NER1
C	1024	SER	-	expression tag	UNP Q8NER1
C	1025	VAL	-	expression tag	UNP Q8NER1
C	1026	GLN	-	expression tag	UNP Q8NER1
C	1027	LEU	-	expression tag	UNP Q8NER1
C	1028	ALA	-	expression tag	UNP Q8NER1
C	1029	ASP	-	expression tag	UNP Q8NER1
C	1030	HIS	-	expression tag	UNP Q8NER1
C	1031	TYR	-	expression tag	UNP Q8NER1
C	1032	GLN	-	expression tag	UNP Q8NER1
C	1033	GLN	-	expression tag	UNP Q8NER1
C	1034	ASN	-	expression tag	UNP Q8NER1
C	1035	THR	-	expression tag	UNP Q8NER1
C	1036	PRO	-	expression tag	UNP Q8NER1
C	1037	ILE	-	expression tag	UNP Q8NER1
C	1038	GLY	-	expression tag	UNP Q8NER1
C	1039	ASP	-	expression tag	UNP Q8NER1
C	1040	GLY	-	expression tag	UNP Q8NER1
C	1041	PRO	-	expression tag	UNP Q8NER1
C	1042	VAL	-	expression tag	UNP Q8NER1
C	1043	LEU	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1044	LEU	-	expression tag	UNP Q8NER1
C	1045	PRO	-	expression tag	UNP Q8NER1
C	1046	ASP	-	expression tag	UNP Q8NER1
C	1047	ASN	-	expression tag	UNP Q8NER1
C	1048	HIS	-	expression tag	UNP Q8NER1
C	1049	TYR	-	expression tag	UNP Q8NER1
C	1050	LEU	-	expression tag	UNP Q8NER1
C	1051	SER	-	expression tag	UNP Q8NER1
C	1052	THR	-	expression tag	UNP Q8NER1
C	1053	GLN	-	expression tag	UNP Q8NER1
C	1054	SER	-	expression tag	UNP Q8NER1
C	1055	LYS	-	expression tag	UNP Q8NER1
C	1056	LEU	-	expression tag	UNP Q8NER1
C	1057	SER	-	expression tag	UNP Q8NER1
C	1058	LYS	-	expression tag	UNP Q8NER1
C	1059	ASP	-	expression tag	UNP Q8NER1
C	1060	PRO	-	expression tag	UNP Q8NER1
C	1061	ASN	-	expression tag	UNP Q8NER1
C	1062	GLU	-	expression tag	UNP Q8NER1
C	1063	LYS	-	expression tag	UNP Q8NER1
C	1064	ARG	-	expression tag	UNP Q8NER1
C	1065	ASP	-	expression tag	UNP Q8NER1
C	1066	HIS	-	expression tag	UNP Q8NER1
C	1067	MET	-	expression tag	UNP Q8NER1
C	1068	VAL	-	expression tag	UNP Q8NER1
C	1069	LEU	-	expression tag	UNP Q8NER1
C	1070	LEU	-	expression tag	UNP Q8NER1
C	1071	GLU	-	expression tag	UNP Q8NER1
C	1072	PHE	-	expression tag	UNP Q8NER1
C	1073	VAL	-	expression tag	UNP Q8NER1
C	1074	THR	-	expression tag	UNP Q8NER1
C	1075	ALA	-	expression tag	UNP Q8NER1
C	1076	ALA	-	expression tag	UNP Q8NER1
C	1077	GLY	-	expression tag	UNP Q8NER1
C	1078	ILE	-	expression tag	UNP Q8NER1
C	1079	THR	-	expression tag	UNP Q8NER1
C	1080	LEU	-	expression tag	UNP Q8NER1
C	1081	GLY	-	expression tag	UNP Q8NER1
C	1082	MET	-	expression tag	UNP Q8NER1
C	1083	ASP	-	expression tag	UNP Q8NER1
C	1084	GLU	-	expression tag	UNP Q8NER1
C	1085	LEU	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1086	TYR	-	expression tag	UNP Q8NER1
C	1087	LYS	-	expression tag	UNP Q8NER1
C	1088	SER	-	expression tag	UNP Q8NER1
C	1089	GLY	-	expression tag	UNP Q8NER1
C	1090	LEU	-	expression tag	UNP Q8NER1
C	1091	ARG	-	expression tag	UNP Q8NER1
C	1092	SER	-	expression tag	UNP Q8NER1
C	1093	TRP	-	expression tag	UNP Q8NER1
C	1094	SER	-	expression tag	UNP Q8NER1
C	1095	HIS	-	expression tag	UNP Q8NER1
C	1096	PRO	-	expression tag	UNP Q8NER1
C	1097	GLN	-	expression tag	UNP Q8NER1
C	1098	PHE	-	expression tag	UNP Q8NER1
C	1099	GLU	-	expression tag	UNP Q8NER1
C	1100	LYS	-	expression tag	UNP Q8NER1
D	-1	MET	-	initiating methionine	UNP Q8NER1
D	0	THR	-	expression tag	UNP Q8NER1
D	1	SER	-	expression tag	UNP Q8NER1
D	840	LEU	-	expression tag	UNP Q8NER1
D	841	VAL	-	expression tag	UNP Q8NER1
D	842	PRO	-	expression tag	UNP Q8NER1
D	843	ARG	-	expression tag	UNP Q8NER1
D	844	GLY	-	expression tag	UNP Q8NER1
D	845	SER	-	expression tag	UNP Q8NER1
D	846	ALA	-	expression tag	UNP Q8NER1
D	847	ALA	-	expression tag	UNP Q8NER1
D	848	ALA	-	expression tag	UNP Q8NER1
D	849	ALA	-	expression tag	UNP Q8NER1
D	850	VAL	-	expression tag	UNP Q8NER1
D	851	SER	-	expression tag	UNP Q8NER1
D	852	LYS	-	expression tag	UNP Q8NER1
D	853	GLY	-	expression tag	UNP Q8NER1
D	854	GLU	-	expression tag	UNP Q8NER1
D	855	GLU	-	expression tag	UNP Q8NER1
D	856	LEU	-	expression tag	UNP Q8NER1
D	857	PHE	-	expression tag	UNP Q8NER1
D	858	THR	-	expression tag	UNP Q8NER1
D	859	GLY	-	expression tag	UNP Q8NER1
D	860	VAL	-	expression tag	UNP Q8NER1
D	861	VAL	-	expression tag	UNP Q8NER1
D	862	PRO	-	expression tag	UNP Q8NER1
D	863	ILE	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	864	LEU	-	expression tag	UNP Q8NER1
D	865	VAL	-	expression tag	UNP Q8NER1
D	866	GLU	-	expression tag	UNP Q8NER1
D	867	LEU	-	expression tag	UNP Q8NER1
D	868	ASP	-	expression tag	UNP Q8NER1
D	869	GLY	-	expression tag	UNP Q8NER1
D	870	ASP	-	expression tag	UNP Q8NER1
D	871	VAL	-	expression tag	UNP Q8NER1
D	872	ASN	-	expression tag	UNP Q8NER1
D	873	GLY	-	expression tag	UNP Q8NER1
D	874	HIS	-	expression tag	UNP Q8NER1
D	875	LYS	-	expression tag	UNP Q8NER1
D	876	PHE	-	expression tag	UNP Q8NER1
D	877	SER	-	expression tag	UNP Q8NER1
D	878	VAL	-	expression tag	UNP Q8NER1
D	879	SER	-	expression tag	UNP Q8NER1
D	880	GLY	-	expression tag	UNP Q8NER1
D	881	GLU	-	expression tag	UNP Q8NER1
D	882	GLY	-	expression tag	UNP Q8NER1
D	883	GLU	-	expression tag	UNP Q8NER1
D	884	GLY	-	expression tag	UNP Q8NER1
D	885	ASP	-	expression tag	UNP Q8NER1
D	886	ALA	-	expression tag	UNP Q8NER1
D	887	THR	-	expression tag	UNP Q8NER1
D	888	TYR	-	expression tag	UNP Q8NER1
D	889	GLY	-	expression tag	UNP Q8NER1
D	890	LYS	-	expression tag	UNP Q8NER1
D	891	LEU	-	expression tag	UNP Q8NER1
D	892	THR	-	expression tag	UNP Q8NER1
D	893	LEU	-	expression tag	UNP Q8NER1
D	894	LYS	-	expression tag	UNP Q8NER1
D	895	PHE	-	expression tag	UNP Q8NER1
D	896	ILE	-	expression tag	UNP Q8NER1
D	897	CYS	-	expression tag	UNP Q8NER1
D	898	THR	-	expression tag	UNP Q8NER1
D	899	THR	-	expression tag	UNP Q8NER1
D	900	GLY	-	expression tag	UNP Q8NER1
D	901	LYS	-	expression tag	UNP Q8NER1
D	902	LEU	-	expression tag	UNP Q8NER1
D	903	PRO	-	expression tag	UNP Q8NER1
D	904	VAL	-	expression tag	UNP Q8NER1
D	905	PRO	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	906	TRP	-	expression tag	UNP Q8NER1
D	907	PRO	-	expression tag	UNP Q8NER1
D	908	THR	-	expression tag	UNP Q8NER1
D	909	LEU	-	expression tag	UNP Q8NER1
D	910	VAL	-	expression tag	UNP Q8NER1
D	911	THR	-	expression tag	UNP Q8NER1
D	912	THR	-	expression tag	UNP Q8NER1
D	913	LEU	-	expression tag	UNP Q8NER1
D	914	THR	-	expression tag	UNP Q8NER1
D	915	TYR	-	expression tag	UNP Q8NER1
D	916	GLY	-	expression tag	UNP Q8NER1
D	917	VAL	-	expression tag	UNP Q8NER1
D	918	GLN	-	expression tag	UNP Q8NER1
D	919	CYS	-	expression tag	UNP Q8NER1
D	920	PHE	-	expression tag	UNP Q8NER1
D	921	SER	-	expression tag	UNP Q8NER1
D	922	ARG	-	expression tag	UNP Q8NER1
D	923	TYR	-	expression tag	UNP Q8NER1
D	924	PRO	-	expression tag	UNP Q8NER1
D	925	ASP	-	expression tag	UNP Q8NER1
D	926	HIS	-	expression tag	UNP Q8NER1
D	927	MET	-	expression tag	UNP Q8NER1
D	928	LYS	-	expression tag	UNP Q8NER1
D	929	GLN	-	expression tag	UNP Q8NER1
D	930	HIS	-	expression tag	UNP Q8NER1
D	931	ASP	-	expression tag	UNP Q8NER1
D	932	PHE	-	expression tag	UNP Q8NER1
D	933	PHE	-	expression tag	UNP Q8NER1
D	934	LYS	-	expression tag	UNP Q8NER1
D	935	SER	-	expression tag	UNP Q8NER1
D	936	ALA	-	expression tag	UNP Q8NER1
D	937	MET	-	expression tag	UNP Q8NER1
D	938	PRO	-	expression tag	UNP Q8NER1
D	939	GLU	-	expression tag	UNP Q8NER1
D	940	GLY	-	expression tag	UNP Q8NER1
D	941	TYR	-	expression tag	UNP Q8NER1
D	942	VAL	-	expression tag	UNP Q8NER1
D	943	GLN	-	expression tag	UNP Q8NER1
D	944	GLU	-	expression tag	UNP Q8NER1
D	945	ARG	-	expression tag	UNP Q8NER1
D	946	THR	-	expression tag	UNP Q8NER1
D	947	ILE	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	948	PHE	-	expression tag	UNP Q8NER1
D	949	PHE	-	expression tag	UNP Q8NER1
D	950	LYS	-	expression tag	UNP Q8NER1
D	951	ASP	-	expression tag	UNP Q8NER1
D	952	ASP	-	expression tag	UNP Q8NER1
D	953	GLY	-	expression tag	UNP Q8NER1
D	954	ASN	-	expression tag	UNP Q8NER1
D	955	TYR	-	expression tag	UNP Q8NER1
D	956	LYS	-	expression tag	UNP Q8NER1
D	957	THR	-	expression tag	UNP Q8NER1
D	958	ARG	-	expression tag	UNP Q8NER1
D	959	ALA	-	expression tag	UNP Q8NER1
D	960	GLU	-	expression tag	UNP Q8NER1
D	961	VAL	-	expression tag	UNP Q8NER1
D	962	LYS	-	expression tag	UNP Q8NER1
D	963	PHE	-	expression tag	UNP Q8NER1
D	964	GLU	-	expression tag	UNP Q8NER1
D	965	GLY	-	expression tag	UNP Q8NER1
D	966	ASP	-	expression tag	UNP Q8NER1
D	967	THR	-	expression tag	UNP Q8NER1
D	968	LEU	-	expression tag	UNP Q8NER1
D	969	VAL	-	expression tag	UNP Q8NER1
D	970	ASN	-	expression tag	UNP Q8NER1
D	971	ARG	-	expression tag	UNP Q8NER1
D	972	ILE	-	expression tag	UNP Q8NER1
D	973	GLU	-	expression tag	UNP Q8NER1
D	974	LEU	-	expression tag	UNP Q8NER1
D	975	LYS	-	expression tag	UNP Q8NER1
D	976	GLY	-	expression tag	UNP Q8NER1
D	977	ILE	-	expression tag	UNP Q8NER1
D	978	ASP	-	expression tag	UNP Q8NER1
D	979	PHE	-	expression tag	UNP Q8NER1
D	980	LYS	-	expression tag	UNP Q8NER1
D	981	GLU	-	expression tag	UNP Q8NER1
D	982	ASP	-	expression tag	UNP Q8NER1
D	983	GLY	-	expression tag	UNP Q8NER1
D	984	ASN	-	expression tag	UNP Q8NER1
D	985	ILE	-	expression tag	UNP Q8NER1
D	986	LEU	-	expression tag	UNP Q8NER1
D	987	GLY	-	expression tag	UNP Q8NER1
D	988	HIS	-	expression tag	UNP Q8NER1
D	989	LYS	-	expression tag	UNP Q8NER1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	990	LEU	-	expression tag	UNP Q8NER1
D	991	GLU	-	expression tag	UNP Q8NER1
D	992	TYR	-	expression tag	UNP Q8NER1
D	993	ASN	-	expression tag	UNP Q8NER1
D	994	TYR	-	expression tag	UNP Q8NER1
D	995	ASN	-	expression tag	UNP Q8NER1
D	996	SER	-	expression tag	UNP Q8NER1
D	997	HIS	-	expression tag	UNP Q8NER1
D	998	ASN	-	expression tag	UNP Q8NER1
D	999	VAL	-	expression tag	UNP Q8NER1
D	1000	TYR	-	expression tag	UNP Q8NER1
D	1001	ILE	-	expression tag	UNP Q8NER1
D	1002	MET	-	expression tag	UNP Q8NER1
D	1003	ALA	-	expression tag	UNP Q8NER1
D	1004	ASP	-	expression tag	UNP Q8NER1
D	1005	LYS	-	expression tag	UNP Q8NER1
D	1006	GLN	-	expression tag	UNP Q8NER1
D	1007	LYS	-	expression tag	UNP Q8NER1
D	1008	ASN	-	expression tag	UNP Q8NER1
D	1009	GLY	-	expression tag	UNP Q8NER1
D	1010	ILE	-	expression tag	UNP Q8NER1
D	1011	LYS	-	expression tag	UNP Q8NER1
D	1012	VAL	-	expression tag	UNP Q8NER1
D	1013	ASN	-	expression tag	UNP Q8NER1
D	1014	PHE	-	expression tag	UNP Q8NER1
D	1015	LYS	-	expression tag	UNP Q8NER1
D	1016	ILE	-	expression tag	UNP Q8NER1
D	1017	ARG	-	expression tag	UNP Q8NER1
D	1018	HIS	-	expression tag	UNP Q8NER1
D	1019	ASN	-	expression tag	UNP Q8NER1
D	1020	ILE	-	expression tag	UNP Q8NER1
D	1021	GLU	-	expression tag	UNP Q8NER1
D	1022	ASP	-	expression tag	UNP Q8NER1
D	1023	GLY	-	expression tag	UNP Q8NER1
D	1024	SER	-	expression tag	UNP Q8NER1
D	1025	VAL	-	expression tag	UNP Q8NER1
D	1026	GLN	-	expression tag	UNP Q8NER1
D	1027	LEU	-	expression tag	UNP Q8NER1
D	1028	ALA	-	expression tag	UNP Q8NER1
D	1029	ASP	-	expression tag	UNP Q8NER1
D	1030	HIS	-	expression tag	UNP Q8NER1
D	1031	TYR	-	expression tag	UNP Q8NER1

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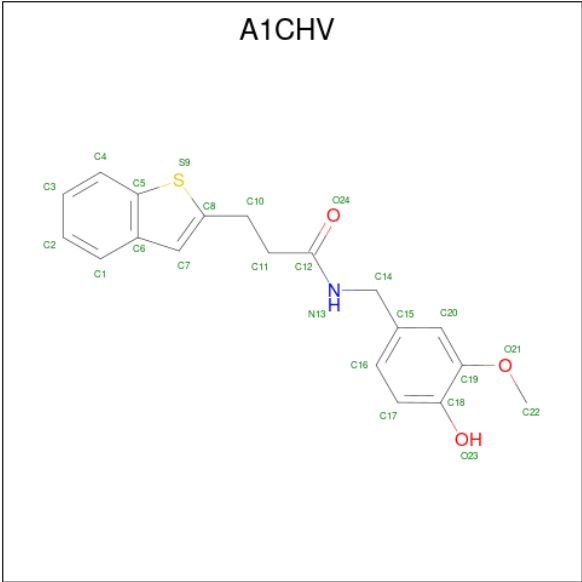
Chain	Residue	Modelled	Actual	Comment	Reference
D	1032	GLN	-	expression tag	UNP Q8NER1
D	1033	GLN	-	expression tag	UNP Q8NER1
D	1034	ASN	-	expression tag	UNP Q8NER1
D	1035	THR	-	expression tag	UNP Q8NER1
D	1036	PRO	-	expression tag	UNP Q8NER1
D	1037	ILE	-	expression tag	UNP Q8NER1
D	1038	GLY	-	expression tag	UNP Q8NER1
D	1039	ASP	-	expression tag	UNP Q8NER1
D	1040	GLY	-	expression tag	UNP Q8NER1
D	1041	PRO	-	expression tag	UNP Q8NER1
D	1042	VAL	-	expression tag	UNP Q8NER1
D	1043	LEU	-	expression tag	UNP Q8NER1
D	1044	LEU	-	expression tag	UNP Q8NER1
D	1045	PRO	-	expression tag	UNP Q8NER1
D	1046	ASP	-	expression tag	UNP Q8NER1
D	1047	ASN	-	expression tag	UNP Q8NER1
D	1048	HIS	-	expression tag	UNP Q8NER1
D	1049	TYR	-	expression tag	UNP Q8NER1
D	1050	LEU	-	expression tag	UNP Q8NER1
D	1051	SER	-	expression tag	UNP Q8NER1
D	1052	THR	-	expression tag	UNP Q8NER1
D	1053	GLN	-	expression tag	UNP Q8NER1
D	1054	SER	-	expression tag	UNP Q8NER1
D	1055	LYS	-	expression tag	UNP Q8NER1
D	1056	LEU	-	expression tag	UNP Q8NER1
D	1057	SER	-	expression tag	UNP Q8NER1
D	1058	LYS	-	expression tag	UNP Q8NER1
D	1059	ASP	-	expression tag	UNP Q8NER1
D	1060	PRO	-	expression tag	UNP Q8NER1
D	1061	ASN	-	expression tag	UNP Q8NER1
D	1062	GLU	-	expression tag	UNP Q8NER1
D	1063	LYS	-	expression tag	UNP Q8NER1
D	1064	ARG	-	expression tag	UNP Q8NER1
D	1065	ASP	-	expression tag	UNP Q8NER1
D	1066	HIS	-	expression tag	UNP Q8NER1
D	1067	MET	-	expression tag	UNP Q8NER1
D	1068	VAL	-	expression tag	UNP Q8NER1
D	1069	LEU	-	expression tag	UNP Q8NER1
D	1070	LEU	-	expression tag	UNP Q8NER1
D	1071	GLU	-	expression tag	UNP Q8NER1
D	1072	PHE	-	expression tag	UNP Q8NER1
D	1073	VAL	-	expression tag	UNP Q8NER1

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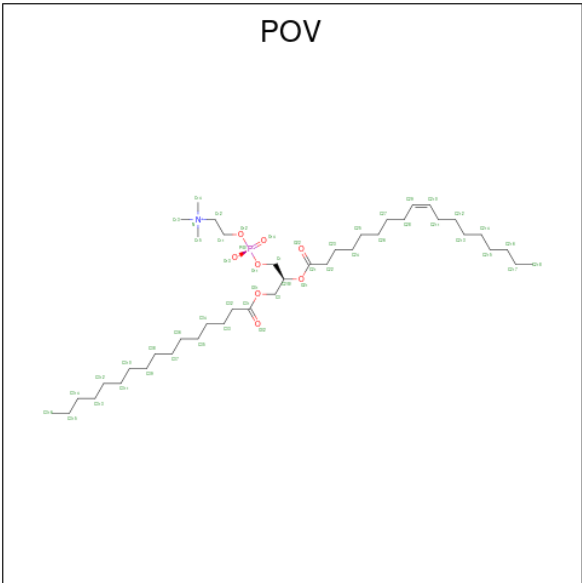
Chain	Residue	Modelled	Actual	Comment	Reference
D	1074	THR	-	expression tag	UNP Q8NER1
D	1075	ALA	-	expression tag	UNP Q8NER1
D	1076	ALA	-	expression tag	UNP Q8NER1
D	1077	GLY	-	expression tag	UNP Q8NER1
D	1078	ILE	-	expression tag	UNP Q8NER1
D	1079	THR	-	expression tag	UNP Q8NER1
D	1080	LEU	-	expression tag	UNP Q8NER1
D	1081	GLY	-	expression tag	UNP Q8NER1
D	1082	MET	-	expression tag	UNP Q8NER1
D	1083	ASP	-	expression tag	UNP Q8NER1
D	1084	GLU	-	expression tag	UNP Q8NER1
D	1085	LEU	-	expression tag	UNP Q8NER1
D	1086	TYR	-	expression tag	UNP Q8NER1
D	1087	LYS	-	expression tag	UNP Q8NER1
D	1088	SER	-	expression tag	UNP Q8NER1
D	1089	GLY	-	expression tag	UNP Q8NER1
D	1090	LEU	-	expression tag	UNP Q8NER1
D	1091	ARG	-	expression tag	UNP Q8NER1
D	1092	SER	-	expression tag	UNP Q8NER1
D	1093	TRP	-	expression tag	UNP Q8NER1
D	1094	SER	-	expression tag	UNP Q8NER1
D	1095	HIS	-	expression tag	UNP Q8NER1
D	1096	PRO	-	expression tag	UNP Q8NER1
D	1097	GLN	-	expression tag	UNP Q8NER1
D	1098	PHE	-	expression tag	UNP Q8NER1
D	1099	GLU	-	expression tag	UNP Q8NER1
D	1100	LYS	-	expression tag	UNP Q8NER1

- Molecule 2 is 3-(1-benzothiophen-2-yl)-N-[(4-hydroxy-3-methoxyphenyl)methyl]propanamide (CCD ID: A1CHV) (formula: C₁₉H₁₉NO₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			24	19	1	3	1	
2	B	1	Total	C	N	O	S	0
			24	19	1	3	1	
2	C	1	Total	C	N	O	S	0
			24	19	1	3	1	
2	D	1	Total	C	N	O	S	0
			24	19	1	3	1	

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



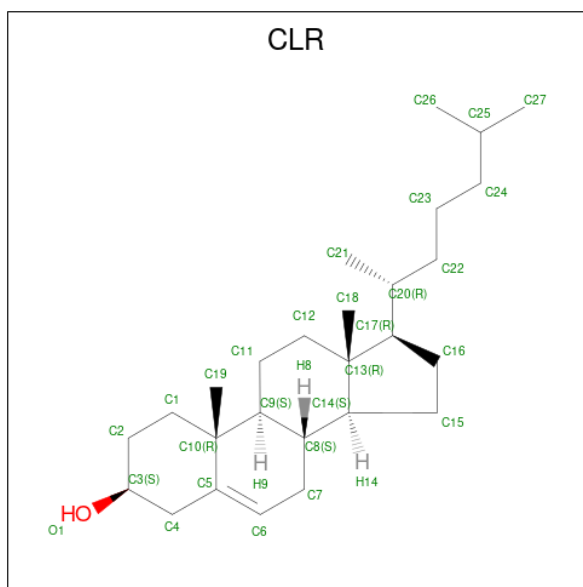
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

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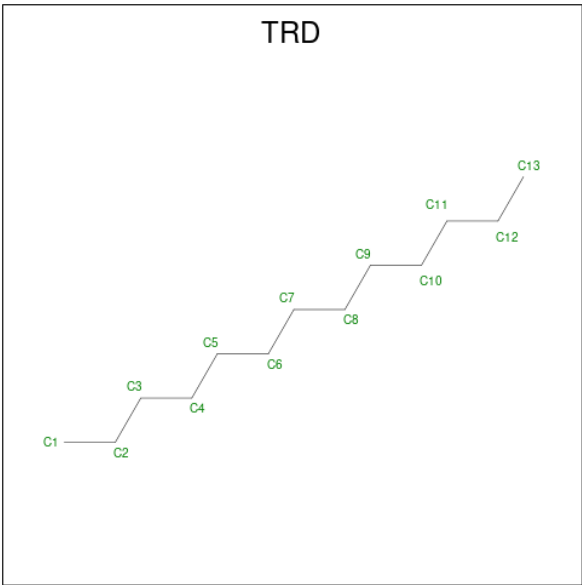
Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	C	1	Total	C	O	0
			28	27	1	
4	D	1	Total	C	O	0
			28	27	1	

- Molecule 5 is TRIDECANE (CCD ID: TRD) (formula: $C_{13}H_{28}$).



Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	C	0
			13	13	
5	B	1	Total	C	0
			13	13	
5	C	1	Total	C	0
			13	13	
5	D	1	Total	C	0
			13	13	

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Na	0
			1	1	
6	C	1	Total	Na	0
			1	1	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	249242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.503	Depositor
Minimum map value	-0.295	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	212.48, 212.48, 212.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, CLR, A1CHV, TRD, NA

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	0.31	0/4441	0.51	2/6009 (0.0%)
1	B	0.31	0/4441	0.51	2/6009 (0.0%)
1	C	0.31	0/4441	0.51	2/6009 (0.0%)
1	D	0.31	0/4441	0.51	2/6009 (0.0%)
All	All	0.31	0/17764	0.51	8/24036 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	VAL	CG1-CB-CG2	5.56	123.04	110.80
1	B	396	VAL	CG1-CB-CG2	5.54	123.00	110.80
1	C	396	VAL	CG1-CB-CG2	5.53	122.97	110.80
1	D	396	VAL	CG1-CB-CG2	5.52	122.95	110.80
1	A	295	VAL	CG1-CB-CG2	5.25	122.36	110.80
1	B	295	VAL	CG1-CB-CG2	5.22	122.30	110.80
1	D	295	VAL	CG1-CB-CG2	5.22	122.30	110.80
1	C	295	VAL	CG1-CB-CG2	5.22	122.28	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	462	PRO	Peptide
1	B	462	PRO	Peptide
1	C	462	PRO	Peptide
1	D	462	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4338	0	4368	26	0
1	B	4338	0	4368	27	0
1	C	4338	0	4368	28	0
1	D	4338	0	4368	24	0
2	A	24	0	0	0	0
2	B	24	0	0	0	0
2	C	24	0	0	0	0
2	D	24	0	0	0	0
3	A	312	0	492	2	0
3	B	312	0	492	2	0
3	C	312	0	492	2	0
3	D	312	0	492	2	0
4	A	28	0	46	0	0
4	B	28	0	46	0	0
4	C	28	0	46	0	0
4	D	28	0	46	0	0
5	A	13	0	28	0	0
5	B	13	0	28	0	0
5	C	13	0	28	0	0
5	D	13	0	28	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
All	All	18862	0	19736	101	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 3.

All (101) 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:D:399:VAL:O	1:D:403:SER:OG	2.02	0.78
1:C:399:VAL:O	1:C:403:SER:OG	2.02	0.77
1:B:399:VAL:O	1:B:403:SER:OG	2.02	0.76
1:A:399:VAL:O	1:A:403:SER:OG	2.02	0.73
1:D:491:ARG:NH1	3:D:1204:POV:O13	2.21	0.73
1:C:491:ARG:NH1	3:C:1204:POV:O13	2.21	0.73
1:A:491:ARG:NH1	3:A:1202:POV:O13	2.22	0.72
1:B:491:ARG:NH1	3:B:1204:POV:O13	2.22	0.72
1:B:446:MET:O	1:B:450:THR:OG1	2.06	0.71
1:B:517:PHE:O	1:B:520:SER:OG	2.08	0.70
1:C:517:PHE:O	1:C:520:SER:OG	2.08	0.69
1:D:517:PHE:O	1:D:520:SER:OG	2.08	0.69
1:A:446:MET:O	1:A:450:THR:OG1	2.06	0.69
1:D:327:GLU:OE2	1:D:356:ARG:NH1	2.26	0.69
1:C:446:MET:O	1:C:450:THR:OG1	2.06	0.69
1:B:327:GLU:OE2	1:B:356:ARG:NH1	2.26	0.68
1:C:213:ARG:NH2	1:C:261:GLN:OE1	2.27	0.68
1:D:213:ARG:NH2	1:D:261:GLN:OE1	2.26	0.68
1:C:211:GLU:OE1	1:C:212:ARG:NH1	2.27	0.68
1:D:211:GLU:OE1	1:D:212:ARG:NH1	2.27	0.68
1:C:327:GLU:OE2	1:C:356:ARG:NH1	2.26	0.68
1:A:211:GLU:OE1	1:A:212:ARG:NH1	2.27	0.68
1:A:213:ARG:NH2	1:A:261:GLN:OE1	2.26	0.68
1:B:211:GLU:OE1	1:B:212:ARG:NH1	2.27	0.67
1:B:213:ARG:NH2	1:B:261:GLN:OE1	2.27	0.67
1:A:327:GLU:OE2	1:A:356:ARG:NH1	2.26	0.67
1:A:517:PHE:O	1:A:520:SER:OG	2.08	0.66
1:C:255:LEU:O	1:C:259:THR:OG1	2.12	0.65
1:A:576:ASP:OD1	1:A:579:ARG:NH1	2.31	0.63
1:C:576:ASP:OD1	1:C:579:ARG:NH1	2.32	0.63
1:B:576:ASP:OD1	1:B:579:ARG:NH1	2.32	0.63
1:D:576:ASP:OD1	1:D:579:ARG:NH1	2.31	0.63
1:D:255:LEU:O	1:D:259:THR:OG1	2.12	0.62
1:A:429:ARG:NH1	1:A:723:SER:OG	2.34	0.61
1:B:429:ARG:NH1	1:B:723:SER:OG	2.34	0.61
1:C:429:ARG:NH1	1:C:723:SER:OG	2.34	0.61
1:D:429:ARG:NH1	1:D:723:SER:OG	2.34	0.61
1:A:255:LEU:O	1:A:259:THR:OG1	2.12	0.60
1:A:695:LYS:O	1:A:698:TRP:NE1	2.36	0.59
1:C:695:LYS:O	1:C:698:TRP:NE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:LYS:O	1:B:698:TRP:NE1	2.36	0.59
1:B:402:TYR:OH	1:B:708:ASP:OD1	2.21	0.58
1:D:695:LYS:O	1:D:698:TRP:NE1	2.36	0.58
1:D:402:TYR:OH	1:D:708:ASP:OD1	2.21	0.58
1:C:402:TYR:OH	1:C:708:ASP:OD1	2.21	0.58
1:B:728:GLN:NE2	1:B:730:GLY:O	2.37	0.58
1:D:446:MET:O	1:D:450:THR:OG1	2.06	0.58
1:A:402:TYR:OH	1:A:708:ASP:OD1	2.21	0.57
1:D:728:GLN:NE2	1:D:730:GLY:O	2.37	0.57
1:A:728:GLN:NE2	1:A:730:GLY:O	2.37	0.56
1:C:728:GLN:NE2	1:C:730:GLY:O	2.37	0.56
1:A:282:ASP:OD1	1:A:286:ASN:N	2.39	0.56
1:B:282:ASP:OD1	1:B:286:ASN:N	2.39	0.56
1:B:255:LEU:O	1:B:259:THR:OG1	2.12	0.55
1:C:282:ASP:OD1	1:C:286:ASN:N	2.39	0.55
1:D:282:ASP:OD1	1:D:286:ASN:N	2.39	0.55
1:D:425:ASP:O	1:D:429:ARG:NE	2.45	0.50
1:A:425:ASP:O	1:A:429:ARG:NE	2.45	0.50
1:C:425:ASP:O	1:C:429:ARG:NE	2.45	0.50
1:B:425:ASP:O	1:B:429:ARG:NE	2.45	0.50
1:B:757:VAL:O	1:C:260:ASN:ND2	2.45	0.50
1:A:557:ARG:NH1	1:A:570:GLU:OE1	2.44	0.50
1:A:260:ASN:ND2	1:D:757:VAL:O	2.45	0.49
1:C:757:VAL:O	1:D:260:ASN:ND2	2.44	0.49
1:B:557:ARG:NH1	1:B:570:GLU:OE1	2.44	0.49
1:D:293:VAL:O	1:D:346:LYS:NZ	2.41	0.49
1:D:495:TYR:OH	1:D:499:ARG:NH1	2.46	0.48
1:B:588:LEU:O	1:B:592:SER:OG	2.28	0.48
1:B:495:TYR:OH	1:B:499:ARG:NH1	2.47	0.48
1:A:495:TYR:OH	1:A:499:ARG:NH1	2.46	0.48
1:C:495:TYR:OH	1:C:499:ARG:NH1	2.46	0.48
1:A:757:VAL:O	1:B:260:ASN:ND2	2.46	0.47
1:C:293:VAL:O	1:C:346:LYS:NZ	2.41	0.47
1:A:293:VAL:O	1:A:346:LYS:NZ	2.42	0.47
1:B:293:VAL:O	1:B:346:LYS:NZ	2.42	0.47
1:B:667:TYR:O	1:B:671:THR:OG1	2.28	0.47
1:C:557:ARG:NH1	1:C:570:GLU:OE1	2.44	0.46
1:C:732:THR:OG1	1:C:734:ASP:O	2.19	0.45
1:D:251:LEU:O	1:D:253:LEU:N	2.50	0.45
1:C:251:LEU:O	1:C:253:LEU:N	2.50	0.45
1:B:251:LEU:O	1:B:253:LEU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:THR:OG1	1:B:734:ASP:O	2.19	0.45
1:A:251:LEU:O	1:A:253:LEU:N	2.50	0.44
1:D:557:ARG:NH1	1:D:570:GLU:OE1	2.44	0.44
1:A:471:ASP:OD1	1:A:474:ARG:NH1	2.48	0.43
1:C:667:TYR:O	1:C:671:THR:OG1	2.28	0.43
1:B:444:LEU:HD21	3:B:1209:POV:H218	2.01	0.42
1:D:444:LEU:HD21	3:D:1209:POV:H218	2.01	0.42
1:C:444:LEU:HD21	3:C:1209:POV:H218	2.01	0.42
1:D:261:GLN:HG2	1:D:264:ILE:HD12	2.02	0.42
1:A:444:LEU:HD21	3:A:1207:POV:H218	2.02	0.41
1:A:588:LEU:O	1:A:592:SER:OG	2.28	0.41
1:C:261:GLN:HG2	1:C:264:ILE:HD12	2.02	0.41
1:C:682:LEU:O	1:C:686:THR:N	2.52	0.41
1:A:261:GLN:HG2	1:A:264:ILE:HD12	2.02	0.41
1:B:356:ARG:NH2	1:B:366:LEU:O	2.47	0.41
1:B:261:GLN:HG2	1:B:264:ILE:HD12	2.02	0.41
1:C:471:ASP:OD1	1:C:474:ARG:NH1	2.48	0.41
1:A:356:ARG:NH2	1:A:366:LEU:O	2.47	0.41
1:C:401:ALA:HA	1:C:700:LEU:HD11	2.03	0.40
1:D:401:ALA:HA	1:D:700:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	531/1102 (48%)	496 (93%)	30 (6%)	5 (1%)	14	30
1	B	531/1102 (48%)	496 (93%)	30 (6%)	5 (1%)	14	30
1	C	531/1102 (48%)	496 (93%)	30 (6%)	5 (1%)	14	30
1	D	531/1102 (48%)	496 (93%)	30 (6%)	5 (1%)	14	30
All	All	2124/4408 (48%)	1984 (93%)	120 (6%)	20 (1%)	16	30

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	GLU
1	B	250	GLU
1	C	250	GLU
1	D	250	GLU
1	A	463	PRO
1	B	463	PRO
1	C	463	PRO
1	D	463	PRO
1	A	252	PRO
1	B	252	PRO
1	C	252	PRO
1	D	252	PRO
1	A	462	PRO
1	B	462	PRO
1	C	462	PRO
1	D	462	PRO
1	A	251	LEU
1	B	251	LEU
1	C	251	LEU
1	D	251	LEU

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	470/963 (49%)	470 (100%)	0	100	100
1	B	470/963 (49%)	470 (100%)	0	100	100
1	C	470/963 (49%)	470 (100%)	0	100	100
1	D	470/963 (49%)	470 (100%)	0	100	100
All	All	1880/3852 (49%)	1880 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	ASN
1	A	629	ASN
1	A	701	GLN
1	B	233	HIS
1	B	302	ASN
1	B	379	HIS
1	B	533	HIS
1	B	629	ASN
1	B	701	GLN
1	C	302	ASN
1	C	420	ASN
1	C	533	HIS
1	C	629	ASN
1	C	701	GLN
1	D	302	ASN
1	D	420	ASN
1	D	533	HIS
1	D	629	ASN
1	D	701	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 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	$\# Z > 2$
3	POV	C	1207	-	51,51,51	0.29	0	57,59,59	0.30	0
3	POV	A	1208	-	51,51,51	0.30	0	57,59,59	0.41	0
3	POV	B	1204	-	51,51,51	0.35	0	57,59,59	0.66	1 (1%)
3	POV	A	1206	-	51,51,51	0.31	0	57,59,59	0.45	0
3	POV	B	1201	-	51,51,51	0.30	0	57,59,59	0.41	0
3	POV	B	1202	-	51,51,51	0.29	0	57,59,59	0.41	0
3	POV	B	1209	-	51,51,51	0.37	0	57,59,59	0.66	1 (1%)
3	POV	D	1201	-	51,51,51	0.30	0	57,59,59	0.41	0
4	CLR	D	1205	-	31,31,31	0.16	0	48,48,48	0.28	0
5	TRD	B	1206	-	12,12,12	0.17	0	11,11,11	0.18	0
3	POV	B	1208	-	51,51,51	0.30	0	57,59,59	0.45	0
3	POV	D	1207	-	51,51,51	0.30	0	57,59,59	0.30	0
3	POV	C	1201	-	51,51,51	0.30	0	57,59,59	0.41	0
3	POV	C	1208	-	51,51,51	0.30	0	57,59,59	0.45	0
5	TRD	C	1206	-	12,12,12	0.17	0	11,11,11	0.17	0
2	A1CHV	D	1203	-	26,26,26	0.19	0	35,35,35	0.50	1 (2%)
3	POV	C	1202	-	51,51,51	0.29	0	57,59,59	0.41	0
5	TRD	D	1206	-	12,12,12	0.17	0	11,11,11	0.17	0
2	A1CHV	B	1203	-	26,26,26	0.19	0	35,35,35	0.50	1 (2%)
3	POV	D	1202	-	51,51,51	0.29	0	57,59,59	0.41	0
4	CLR	B	1205	-	31,31,31	0.16	0	48,48,48	0.28	0
3	POV	B	1207	-	51,51,51	0.29	0	57,59,59	0.30	0
3	POV	A	1205	-	51,51,51	0.29	0	57,59,59	0.30	0
3	POV	D	1208	-	51,51,51	0.30	0	57,59,59	0.45	0
2	A1CHV	A	1201	-	26,26,26	0.20	0	35,35,35	0.50	1 (2%)
3	POV	C	1209	-	51,51,51	0.37	0	57,59,59	0.66	1 (1%)
3	POV	A	1209	-	51,51,51	0.29	0	57,59,59	0.41	0
3	POV	C	1204	-	51,51,51	0.36	0	57,59,59	0.66	1 (1%)
5	TRD	A	1204	-	12,12,12	0.17	0	11,11,11	0.17	0
4	CLR	C	1205	-	31,31,31	0.15	0	48,48,48	0.28	0
3	POV	A	1202	-	51,51,51	0.35	0	57,59,59	0.66	1 (1%)
3	POV	A	1207	-	51,51,51	0.37	0	57,59,59	0.66	1 (1%)
3	POV	D	1209	-	51,51,51	0.37	0	57,59,59	0.66	1 (1%)
2	A1CHV	C	1203	-	26,26,26	0.18	0	35,35,35	0.49	1 (2%)
4	CLR	A	1203	-	31,31,31	0.16	0	48,48,48	0.28	0
3	POV	D	1204	-	51,51,51	0.35	0	57,59,59	0.66	1 (1%)

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	POV	C	1207	-	-	11/55/55/55	-
3	POV	A	1208	-	-	15/55/55/55	-
3	POV	B	1204	-	-	19/55/55/55	-
3	POV	A	1206	-	-	16/55/55/55	-
3	POV	B	1201	-	-	15/55/55/55	-
3	POV	B	1202	-	-	16/55/55/55	-
3	POV	B	1209	-	-	24/55/55/55	-
3	POV	D	1201	-	-	15/55/55/55	-
4	CLR	D	1205	-	-	4/10/68/68	0/4/4/4
5	TRD	B	1206	-	-	2/10/10/10	-
3	POV	B	1208	-	-	16/55/55/55	-
3	POV	D	1207	-	-	11/55/55/55	-
3	POV	C	1201	-	-	14/55/55/55	-
3	POV	C	1208	-	-	16/55/55/55	-
5	TRD	C	1206	-	-	2/10/10/10	-
2	A1CHV	D	1203	-	-	3/12/12/12	0/3/3/3
3	POV	C	1202	-	-	16/55/55/55	-
5	TRD	D	1206	-	-	2/10/10/10	-
2	A1CHV	B	1203	-	-	3/12/12/12	0/3/3/3
3	POV	D	1202	-	-	16/55/55/55	-
4	CLR	B	1205	-	-	4/10/68/68	0/4/4/4
3	POV	B	1207	-	-	11/55/55/55	-
3	POV	A	1205	-	-	11/55/55/55	-
3	POV	D	1208	-	-	16/55/55/55	-
2	A1CHV	A	1201	-	-	3/12/12/12	0/3/3/3
3	POV	C	1209	-	-	23/55/55/55	-
3	POV	A	1209	-	-	16/55/55/55	-
3	POV	C	1204	-	-	19/55/55/55	-
5	TRD	A	1204	-	-	2/10/10/10	-
4	CLR	C	1205	-	-	4/10/68/68	0/4/4/4
3	POV	A	1202	-	-	19/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	A	1207	-	-	23/55/55/55	-
3	POV	D	1209	-	-	23/55/55/55	-
2	A1CHV	C	1203	-	-	3/12/12/12	0/3/3/3
4	CLR	A	1203	-	-	4/10/68/68	0/4/4/4
3	POV	D	1204	-	-	19/55/55/55	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	A1CHV	C11-C10-C8	2.44	116.86	112.11
3	D	1204	POV	C2-O21-C21	2.44	123.64	117.80
3	A	1202	POV	C2-O21-C21	2.44	123.63	117.80
3	C	1204	POV	C2-O21-C21	2.42	123.60	117.80
2	B	1203	A1CHV	C11-C10-C8	2.42	116.83	112.11
2	D	1203	A1CHV	C11-C10-C8	2.41	116.81	112.11
3	C	1209	POV	C2-O21-C21	2.39	123.52	117.80
3	B	1204	POV	C2-O21-C21	2.39	123.52	117.80
3	D	1209	POV	C2-O21-C21	2.38	123.50	117.80
3	A	1207	POV	C2-O21-C21	2.38	123.49	117.80
3	B	1209	POV	C2-O21-C21	2.37	123.48	117.80
2	C	1203	A1CHV	C11-C10-C8	2.36	116.71	112.11

There are no chirality outliers.

All (436) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	POV	C1-O11-P-O12
3	A	1202	POV	C1-O11-P-O13
3	A	1202	POV	C11-O12-P-O13
3	A	1202	POV	O12-C11-C12-N
3	A	1202	POV	C22-C21-O21-C2
3	A	1202	POV	O22-C21-O21-C2
3	A	1202	POV	C32-C31-O31-C3
3	A	1202	POV	O32-C31-O31-C3
3	A	1205	POV	C1-O11-P-O12
3	A	1205	POV	C1-O11-P-O13
3	A	1206	POV	C11-O12-P-O11
3	A	1206	POV	C11-O12-P-O14
3	A	1206	POV	O12-C11-C12-N

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Mol	Chain	Res	Type	Atoms
3	A	1206	POV	O22-C21-O21-C2
3	A	1207	POV	C1-O11-P-O12
3	A	1207	POV	C11-O12-P-O14
3	A	1207	POV	O22-C21-O21-C2
3	A	1207	POV	C32-C31-O31-C3
3	A	1207	POV	O32-C31-O31-C3
3	A	1208	POV	C11-O12-P-O11
3	A	1208	POV	C11-O12-P-O13
3	A	1208	POV	C11-O12-P-O14
3	A	1208	POV	C32-C31-O31-C3
3	A	1208	POV	O32-C31-O31-C3
3	A	1209	POV	C11-O12-P-O11
3	A	1209	POV	C11-O12-P-O14
3	A	1209	POV	O21-C2-C3-O31
3	B	1201	POV	C11-O12-P-O11
3	B	1201	POV	C11-O12-P-O13
3	B	1201	POV	C11-O12-P-O14
3	B	1201	POV	C32-C31-O31-C3
3	B	1201	POV	O32-C31-O31-C3
3	B	1202	POV	C11-O12-P-O11
3	B	1202	POV	C11-O12-P-O14
3	B	1202	POV	O21-C2-C3-O31
3	B	1204	POV	C1-O11-P-O12
3	B	1204	POV	C1-O11-P-O13
3	B	1204	POV	C11-O12-P-O13
3	B	1204	POV	O12-C11-C12-N
3	B	1204	POV	C22-C21-O21-C2
3	B	1204	POV	O22-C21-O21-C2
3	B	1204	POV	C32-C31-O31-C3
3	B	1204	POV	O32-C31-O31-C3
3	B	1207	POV	C1-O11-P-O12
3	B	1207	POV	C1-O11-P-O13
3	B	1208	POV	C11-O12-P-O11
3	B	1208	POV	C11-O12-P-O14
3	B	1208	POV	O12-C11-C12-N
3	B	1208	POV	O22-C21-O21-C2
3	B	1209	POV	C1-O11-P-O12
3	B	1209	POV	C11-O12-P-O14
3	B	1209	POV	O22-C21-O21-C2
3	B	1209	POV	C32-C31-O31-C3
3	B	1209	POV	O32-C31-O31-C3
3	C	1201	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
3	C	1201	POV	C11-O12-P-O13
3	C	1201	POV	C11-O12-P-O14
3	C	1201	POV	C32-C31-O31-C3
3	C	1201	POV	O32-C31-O31-C3
3	C	1202	POV	C11-O12-P-O11
3	C	1202	POV	C11-O12-P-O14
3	C	1202	POV	O21-C2-C3-O31
3	C	1204	POV	C1-O11-P-O12
3	C	1204	POV	C1-O11-P-O13
3	C	1204	POV	C11-O12-P-O13
3	C	1204	POV	O12-C11-C12-N
3	C	1204	POV	C22-C21-O21-C2
3	C	1204	POV	O22-C21-O21-C2
3	C	1204	POV	C32-C31-O31-C3
3	C	1204	POV	O32-C31-O31-C3
3	C	1207	POV	C1-O11-P-O12
3	C	1207	POV	C1-O11-P-O13
3	C	1208	POV	C11-O12-P-O11
3	C	1208	POV	C11-O12-P-O14
3	C	1208	POV	O12-C11-C12-N
3	C	1208	POV	O22-C21-O21-C2
3	C	1209	POV	C1-O11-P-O12
3	C	1209	POV	C11-O12-P-O14
3	C	1209	POV	O22-C21-O21-C2
3	C	1209	POV	C32-C31-O31-C3
3	C	1209	POV	O32-C31-O31-C3
3	D	1201	POV	C11-O12-P-O11
3	D	1201	POV	C11-O12-P-O13
3	D	1201	POV	C11-O12-P-O14
3	D	1201	POV	C32-C31-O31-C3
3	D	1201	POV	O32-C31-O31-C3
3	D	1202	POV	C11-O12-P-O11
3	D	1202	POV	C11-O12-P-O14
3	D	1202	POV	O21-C2-C3-O31
3	D	1204	POV	C1-O11-P-O12
3	D	1204	POV	C1-O11-P-O13
3	D	1204	POV	C11-O12-P-O13
3	D	1204	POV	O12-C11-C12-N
3	D	1204	POV	C22-C21-O21-C2
3	D	1204	POV	O22-C21-O21-C2
3	D	1204	POV	C32-C31-O31-C3
3	D	1204	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
3	D	1207	POV	C1-O11-P-O12
3	D	1207	POV	C1-O11-P-O13
3	D	1208	POV	C11-O12-P-O11
3	D	1208	POV	C11-O12-P-O14
3	D	1208	POV	O12-C11-C12-N
3	D	1208	POV	O22-C21-O21-C2
3	D	1209	POV	C1-O11-P-O12
3	D	1209	POV	C11-O12-P-O14
3	D	1209	POV	O22-C21-O21-C2
3	D	1209	POV	C32-C31-O31-C3
3	D	1209	POV	O32-C31-O31-C3
3	A	1206	POV	C22-C21-O21-C2
3	A	1207	POV	C22-C21-O21-C2
3	B	1208	POV	C22-C21-O21-C2
3	B	1209	POV	C22-C21-O21-C2
3	C	1208	POV	C22-C21-O21-C2
3	C	1209	POV	C22-C21-O21-C2
3	D	1208	POV	C22-C21-O21-C2
3	D	1209	POV	C22-C21-O21-C2
3	A	1206	POV	O21-C2-C3-O31
3	B	1208	POV	O21-C2-C3-O31
3	C	1208	POV	O21-C2-C3-O31
3	D	1208	POV	O21-C2-C3-O31
3	A	1202	POV	C31-C32-C33-C34
3	B	1204	POV	C31-C32-C33-C34
3	C	1204	POV	C31-C32-C33-C34
3	D	1204	POV	C31-C32-C33-C34
4	A	1203	CLR	C17-C20-C22-C23
4	B	1205	CLR	C17-C20-C22-C23
4	C	1205	CLR	C17-C20-C22-C23
4	D	1205	CLR	C17-C20-C22-C23
4	B	1205	CLR	C21-C20-C22-C23
4	D	1205	CLR	C21-C20-C22-C23
4	A	1203	CLR	C21-C20-C22-C23
4	C	1205	CLR	C21-C20-C22-C23
3	A	1208	POV	C31-C32-C33-C34
3	B	1201	POV	C31-C32-C33-C34
3	C	1201	POV	C31-C32-C33-C34
3	D	1201	POV	C31-C32-C33-C34
4	A	1203	CLR	C20-C22-C23-C24
4	B	1205	CLR	C20-C22-C23-C24
4	C	1205	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
4	D	1205	CLR	C20-C22-C23-C24
3	A	1208	POV	C21-C22-C23-C24
3	B	1201	POV	C21-C22-C23-C24
3	C	1201	POV	C21-C22-C23-C24
3	D	1201	POV	C21-C22-C23-C24
3	C	1209	POV	C32-C33-C34-C35
3	D	1209	POV	C32-C33-C34-C35
3	A	1207	POV	C32-C33-C34-C35
3	B	1209	POV	C32-C33-C34-C35
3	A	1202	POV	C33-C34-C35-C36
3	B	1204	POV	C33-C34-C35-C36
3	C	1204	POV	C33-C34-C35-C36
3	D	1204	POV	C33-C34-C35-C36
3	B	1204	POV	C24-C25-C26-C27
3	C	1204	POV	C24-C25-C26-C27
3	D	1204	POV	C24-C25-C26-C27
3	A	1202	POV	C24-C25-C26-C27
3	B	1208	POV	C39-C310-C311-C312
3	C	1208	POV	C39-C310-C311-C312
3	D	1208	POV	C39-C310-C311-C312
3	A	1206	POV	C39-C310-C311-C312
3	A	1207	POV	C311-C310-C39-C38
3	A	1209	POV	C25-C26-C27-C28
3	B	1202	POV	C25-C26-C27-C28
3	C	1202	POV	C25-C26-C27-C28
3	D	1202	POV	C25-C26-C27-C28
3	B	1209	POV	C311-C310-C39-C38
3	C	1209	POV	C311-C310-C39-C38
3	D	1209	POV	C311-C310-C39-C38
3	A	1208	POV	C24-C25-C26-C27
3	B	1202	POV	C35-C36-C37-C38
3	C	1202	POV	C35-C36-C37-C38
3	D	1201	POV	C24-C25-C26-C27
3	D	1202	POV	C35-C36-C37-C38
3	A	1209	POV	C35-C36-C37-C38
3	B	1201	POV	C24-C25-C26-C27
3	C	1201	POV	C24-C25-C26-C27
3	D	1208	POV	C36-C37-C38-C39
3	B	1208	POV	C36-C37-C38-C39
3	C	1208	POV	C36-C37-C38-C39
3	B	1209	POV	C213-C214-C215-C216
3	A	1206	POV	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
3	D	1209	POV	C213-C214-C215-C216
3	C	1209	POV	C213-C214-C215-C216
3	B	1209	POV	C33-C34-C35-C36
3	C	1209	POV	C33-C34-C35-C36
3	A	1207	POV	C33-C34-C35-C36
3	D	1209	POV	C33-C34-C35-C36
3	A	1206	POV	C214-C215-C216-C217
3	B	1208	POV	C214-C215-C216-C217
3	C	1201	POV	C214-C215-C216-C217
3	C	1208	POV	C214-C215-C216-C217
3	D	1208	POV	C214-C215-C216-C217
3	A	1205	POV	O21-C2-C3-O31
3	B	1207	POV	O21-C2-C3-O31
3	B	1209	POV	C210-C211-C212-C213
3	C	1207	POV	O21-C2-C3-O31
3	D	1207	POV	O21-C2-C3-O31
3	A	1207	POV	C213-C214-C215-C216
3	D	1201	POV	C39-C310-C311-C312
3	A	1208	POV	C214-C215-C216-C217
3	B	1201	POV	C39-C310-C311-C312
3	A	1208	POV	C39-C310-C311-C312
3	C	1201	POV	C39-C310-C311-C312
3	B	1201	POV	C214-C215-C216-C217
3	D	1201	POV	C214-C215-C216-C217
3	C	1204	POV	C211-C212-C213-C214
3	C	1209	POV	C210-C211-C212-C213
3	D	1209	POV	C210-C211-C212-C213
3	B	1204	POV	C211-C212-C213-C214
3	D	1204	POV	C211-C212-C213-C214
3	A	1202	POV	C211-C212-C213-C214
3	A	1209	POV	C1-C2-C3-O31
3	B	1202	POV	C1-C2-C3-O31
3	C	1202	POV	C1-C2-C3-O31
3	D	1202	POV	C1-C2-C3-O31
3	A	1207	POV	C210-C211-C212-C213
3	A	1207	POV	C1-C2-O21-C21
3	B	1209	POV	C1-C2-O21-C21
3	C	1209	POV	C1-C2-O21-C21
3	D	1209	POV	C1-C2-O21-C21
3	A	1206	POV	C23-C24-C25-C26
3	D	1208	POV	C23-C24-C25-C26
3	B	1208	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	C	1208	POV	C23-C24-C25-C26
5	B	1206	TRD	C4-C5-C6-C7
5	A	1204	TRD	C4-C5-C6-C7
5	C	1206	TRD	C4-C5-C6-C7
5	D	1206	TRD	C4-C5-C6-C7
3	A	1208	POV	C35-C36-C37-C38
3	B	1209	POV	C36-C37-C38-C39
3	C	1209	POV	C36-C37-C38-C39
3	D	1201	POV	C35-C36-C37-C38
3	D	1209	POV	C36-C37-C38-C39
3	B	1201	POV	C35-C36-C37-C38
3	C	1201	POV	C35-C36-C37-C38
3	A	1207	POV	C36-C37-C38-C39
3	B	1204	POV	C215-C216-C217-C218
3	C	1204	POV	C215-C216-C217-C218
3	D	1204	POV	C215-C216-C217-C218
3	A	1202	POV	C215-C216-C217-C218
3	A	1205	POV	C210-C211-C212-C213
3	C	1207	POV	C210-C211-C212-C213
3	D	1207	POV	C210-C211-C212-C213
3	B	1202	POV	C310-C311-C312-C313
3	D	1202	POV	C310-C311-C312-C313
3	C	1202	POV	C310-C311-C312-C313
3	A	1209	POV	C310-C311-C312-C313
3	B	1207	POV	C210-C211-C212-C213
3	A	1207	POV	C215-C216-C217-C218
3	D	1209	POV	C215-C216-C217-C218
3	C	1209	POV	C215-C216-C217-C218
3	B	1209	POV	C215-C216-C217-C218
3	A	1206	POV	C1-C2-C3-O31
3	B	1207	POV	C1-C2-C3-O31
3	B	1208	POV	C1-C2-C3-O31
3	C	1207	POV	C1-C2-C3-O31
3	C	1208	POV	C1-C2-C3-O31
3	D	1207	POV	C1-C2-C3-O31
3	D	1208	POV	C1-C2-C3-O31
3	A	1209	POV	O11-C1-C2-O21
3	B	1202	POV	O11-C1-C2-O21
3	C	1202	POV	O11-C1-C2-O21
3	D	1202	POV	O11-C1-C2-O21
3	C	1209	POV	C311-C312-C313-C314
3	B	1209	POV	C311-C312-C313-C314

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Mol	Chain	Res	Type	Atoms
3	A	1207	POV	C311-C312-C313-C314
3	D	1209	POV	C311-C312-C313-C314
2	A	1201	A1CHV	C11-C10-C8-S9
2	C	1203	A1CHV	C11-C10-C8-S9
2	D	1203	A1CHV	C11-C10-C8-S9
3	A	1209	POV	O11-C1-C2-C3
3	B	1202	POV	O11-C1-C2-C3
3	C	1202	POV	O11-C1-C2-C3
3	D	1202	POV	O11-C1-C2-C3
3	A	1205	POV	C1-C2-C3-O31
2	B	1203	A1CHV	C11-C10-C8-S9
3	D	1204	POV	C311-C312-C313-C314
3	B	1204	POV	C311-C312-C313-C314
3	C	1204	POV	C311-C312-C313-C314
3	A	1208	POV	O12-C11-C12-N
3	B	1201	POV	O12-C11-C12-N
3	C	1201	POV	O12-C11-C12-N
3	D	1201	POV	O12-C11-C12-N
3	A	1202	POV	C311-C312-C313-C314
3	A	1209	POV	C313-C314-C315-C316
3	C	1202	POV	C313-C314-C315-C316
3	D	1202	POV	C313-C314-C315-C316
2	A	1201	A1CHV	C11-C10-C8-C7
2	B	1203	A1CHV	C11-C10-C8-C7
2	C	1203	A1CHV	C11-C10-C8-C7
2	D	1203	A1CHV	C11-C10-C8-C7
3	B	1202	POV	C313-C314-C315-C316
3	A	1202	POV	C1-O11-P-O14
3	A	1202	POV	C11-O12-P-O11
3	A	1207	POV	C1-O11-P-O14
3	A	1207	POV	C11-O12-P-O11
3	A	1208	POV	C1-O11-P-O14
3	A	1209	POV	C11-O12-P-O13
3	B	1201	POV	C1-O11-P-O14
3	B	1202	POV	C11-O12-P-O13
3	B	1204	POV	C1-O11-P-O14
3	B	1204	POV	C11-O12-P-O11
3	B	1209	POV	C1-O11-P-O14
3	B	1209	POV	C11-O12-P-O11
3	C	1201	POV	C1-O11-P-O14
3	C	1202	POV	C11-O12-P-O13
3	C	1204	POV	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
3	C	1204	POV	C11-O12-P-O11
3	C	1209	POV	C1-O11-P-O14
3	C	1209	POV	C11-O12-P-O11
3	D	1201	POV	C1-O11-P-O14
3	D	1202	POV	C11-O12-P-O13
3	D	1204	POV	C1-O11-P-O14
3	D	1204	POV	C11-O12-P-O11
3	D	1209	POV	C1-O11-P-O14
3	D	1209	POV	C11-O12-P-O11
3	B	1209	POV	C27-C28-C29-C210
3	C	1209	POV	C27-C28-C29-C210
3	D	1209	POV	C27-C28-C29-C210
3	A	1207	POV	C27-C28-C29-C210
3	C	1208	POV	C213-C214-C215-C216
3	B	1208	POV	C213-C214-C215-C216
3	D	1208	POV	C213-C214-C215-C216
3	A	1202	POV	C32-C33-C34-C35
4	A	1203	CLR	C22-C23-C24-C25
4	D	1205	CLR	C22-C23-C24-C25
4	B	1205	CLR	C22-C23-C24-C25
4	C	1205	CLR	C22-C23-C24-C25
3	A	1206	POV	C29-C210-C211-C212
3	B	1208	POV	C29-C210-C211-C212
3	A	1206	POV	C213-C214-C215-C216
3	C	1204	POV	C32-C33-C34-C35
3	A	1206	POV	C27-C28-C29-C210
3	B	1208	POV	C27-C28-C29-C210
3	C	1208	POV	C29-C210-C211-C212
3	C	1208	POV	C27-C28-C29-C210
3	D	1208	POV	C27-C28-C29-C210
3	B	1204	POV	C32-C33-C34-C35
3	D	1204	POV	C32-C33-C34-C35
3	A	1207	POV	C25-C26-C27-C28
3	A	1202	POV	C29-C210-C211-C212
3	B	1204	POV	C29-C210-C211-C212
3	C	1204	POV	C29-C210-C211-C212
3	D	1204	POV	C29-C210-C211-C212
3	D	1208	POV	C29-C210-C211-C212
2	A	1201	A1CHV	C8-C10-C11-C12
2	B	1203	A1CHV	C8-C10-C11-C12
2	C	1203	A1CHV	C8-C10-C11-C12
2	D	1203	A1CHV	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	B	1209	POV	C25-C26-C27-C28
3	C	1209	POV	C25-C26-C27-C28
3	D	1209	POV	C25-C26-C27-C28
3	C	1208	POV	C215-C216-C217-C218
3	D	1208	POV	C215-C216-C217-C218
3	B	1208	POV	C215-C216-C217-C218
3	A	1206	POV	C215-C216-C217-C218
3	B	1207	POV	C34-C35-C36-C37
3	D	1207	POV	C34-C35-C36-C37
3	A	1205	POV	C34-C35-C36-C37
3	C	1207	POV	C34-C35-C36-C37
3	B	1209	POV	C2-C1-O11-P
3	D	1207	POV	C211-C212-C213-C214
3	B	1207	POV	C211-C212-C213-C214
3	A	1205	POV	C211-C212-C213-C214
3	C	1207	POV	C211-C212-C213-C214
3	C	1207	POV	C32-C33-C34-C35
3	D	1207	POV	C32-C33-C34-C35
3	B	1207	POV	C32-C33-C34-C35
3	A	1207	POV	C2-C1-O11-P
3	C	1209	POV	C2-C1-O11-P
3	D	1209	POV	C2-C1-O11-P
3	A	1205	POV	C32-C33-C34-C35
3	C	1202	POV	C311-C312-C313-C314
3	A	1208	POV	C311-C310-C39-C38
3	A	1209	POV	C311-C312-C313-C314
3	C	1201	POV	C311-C310-C39-C38
3	A	1202	POV	C210-C211-C212-C213
3	C	1204	POV	C210-C211-C212-C213
3	D	1204	POV	C210-C211-C212-C213
3	A	1207	POV	C11-C12-N-C13
3	B	1209	POV	C11-C12-N-C13
3	C	1209	POV	C11-C12-N-C13
3	D	1209	POV	C11-C12-N-C13
5	B	1206	TRD	C11-C10-C9-C8
3	B	1204	POV	C210-C211-C212-C213
5	D	1206	TRD	C11-C10-C9-C8
3	D	1201	POV	C311-C310-C39-C38
5	C	1206	TRD	C11-C10-C9-C8
3	B	1201	POV	C311-C310-C39-C38
5	A	1204	TRD	C11-C10-C9-C8
3	A	1205	POV	C310-C311-C312-C313

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Mol	Chain	Res	Type	Atoms
3	B	1202	POV	C29-C210-C211-C212
3	D	1202	POV	C29-C210-C211-C212
3	C	1207	POV	C310-C311-C312-C313
3	D	1202	POV	C311-C312-C313-C314
3	A	1209	POV	C29-C210-C211-C212
3	B	1202	POV	C311-C312-C313-C314
3	D	1207	POV	C310-C311-C312-C313
3	B	1202	POV	O21-C21-C22-C23
3	D	1202	POV	O21-C21-C22-C23
3	B	1207	POV	C310-C311-C312-C313
3	A	1209	POV	O21-C21-C22-C23
3	C	1202	POV	O21-C21-C22-C23
3	C	1202	POV	C29-C210-C211-C212
3	B	1209	POV	C11-C12-N-C15
3	A	1209	POV	C24-C25-C26-C27
3	A	1207	POV	C11-C12-N-C14
3	A	1207	POV	C11-C12-N-C15
3	B	1209	POV	C11-C12-N-C14
3	C	1209	POV	C11-C12-N-C15
3	D	1209	POV	C11-C12-N-C15
3	C	1202	POV	C24-C25-C26-C27
3	B	1208	POV	O31-C31-C32-C33
3	C	1208	POV	O31-C31-C32-C33
3	D	1202	POV	C24-C25-C26-C27
3	B	1202	POV	C24-C25-C26-C27
3	C	1209	POV	C11-C12-N-C14
3	D	1209	POV	C11-C12-N-C14
3	A	1205	POV	O21-C21-C22-C23
3	D	1208	POV	O31-C31-C32-C33
3	D	1207	POV	O21-C21-C22-C23
3	D	1207	POV	C24-C25-C26-C27
3	B	1207	POV	O21-C21-C22-C23
3	C	1207	POV	O21-C21-C22-C23
3	B	1202	POV	C312-C313-C314-C315
3	D	1201	POV	C312-C313-C314-C315
3	D	1202	POV	C312-C313-C314-C315
3	B	1207	POV	C24-C25-C26-C27
3	C	1207	POV	C24-C25-C26-C27
3	B	1201	POV	C312-C313-C314-C315
3	A	1206	POV	O31-C31-C32-C33
3	A	1209	POV	C312-C313-C314-C315
3	A	1208	POV	C312-C313-C314-C315

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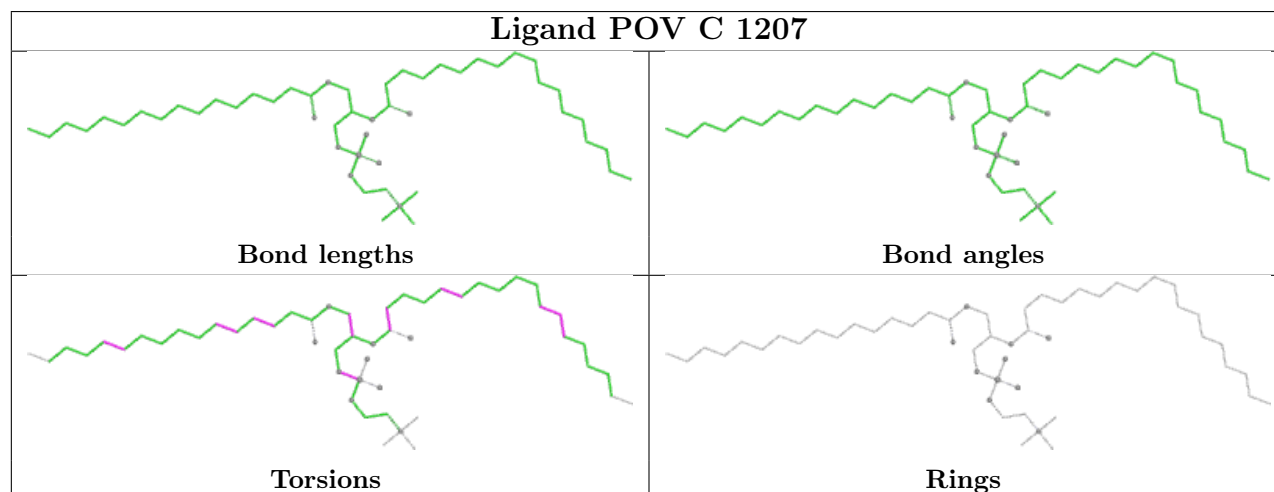
Mol	Chain	Res	Type	Atoms
3	C	1202	POV	C312-C313-C314-C315
3	B	1209	POV	C34-C35-C36-C37
3	A	1205	POV	C24-C25-C26-C27

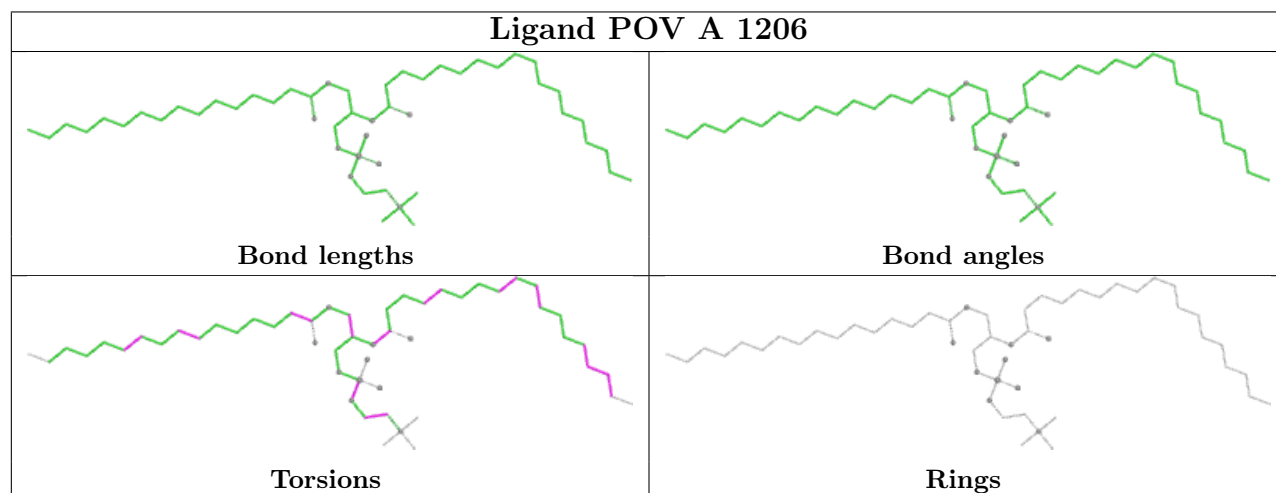
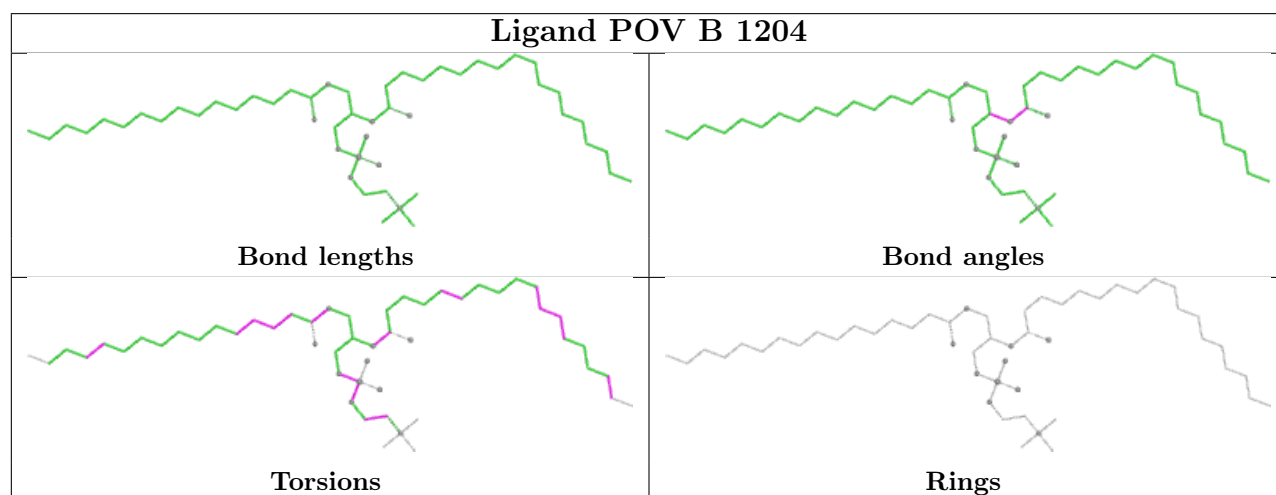
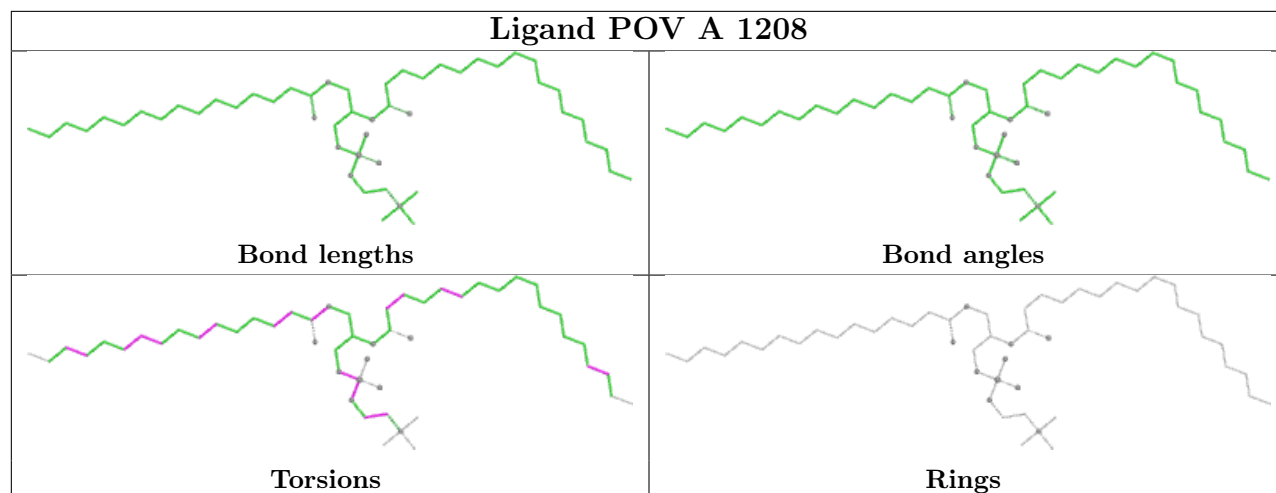
There are no ring outliers.

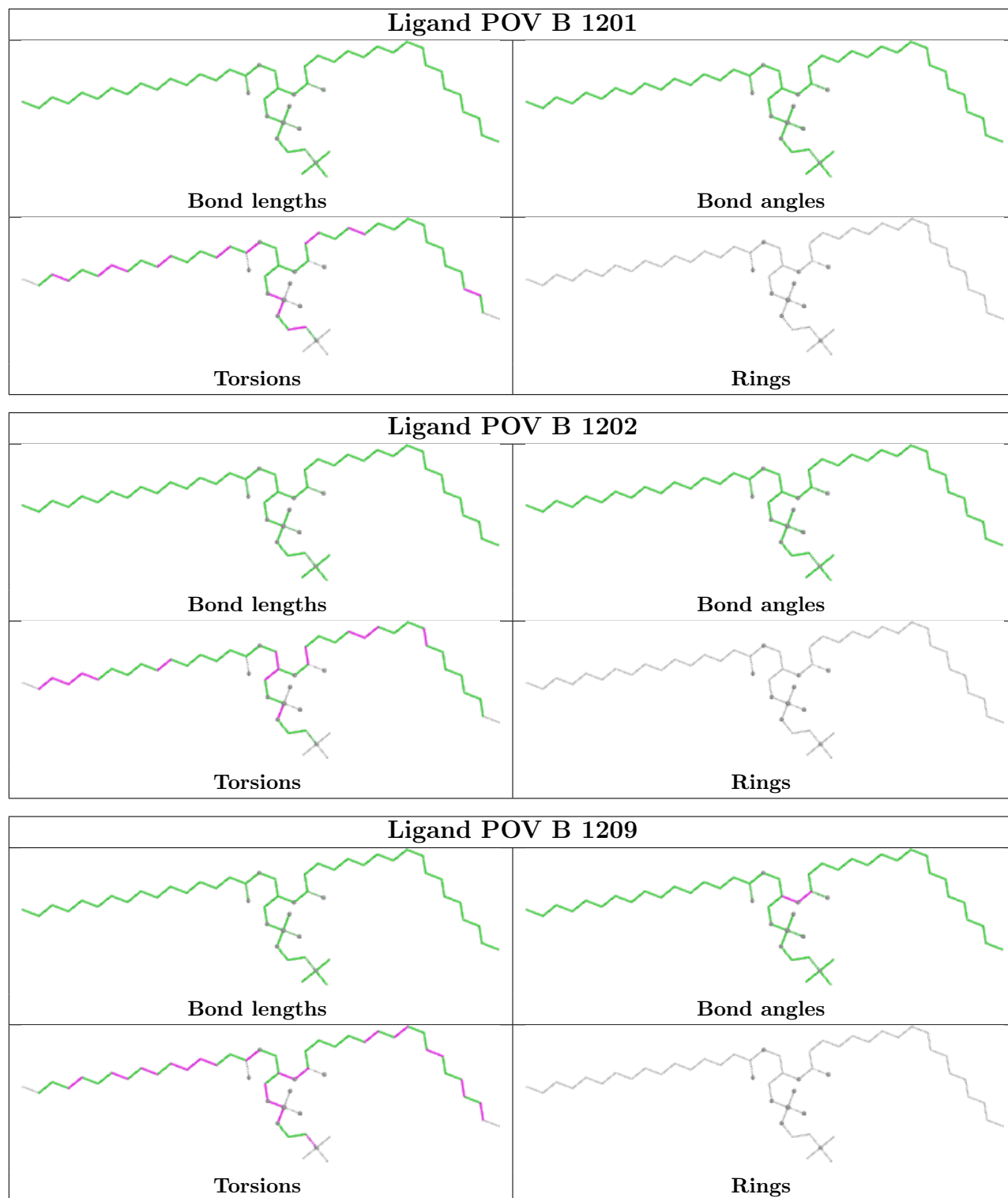
8 monomers are involved in 8 short contacts:

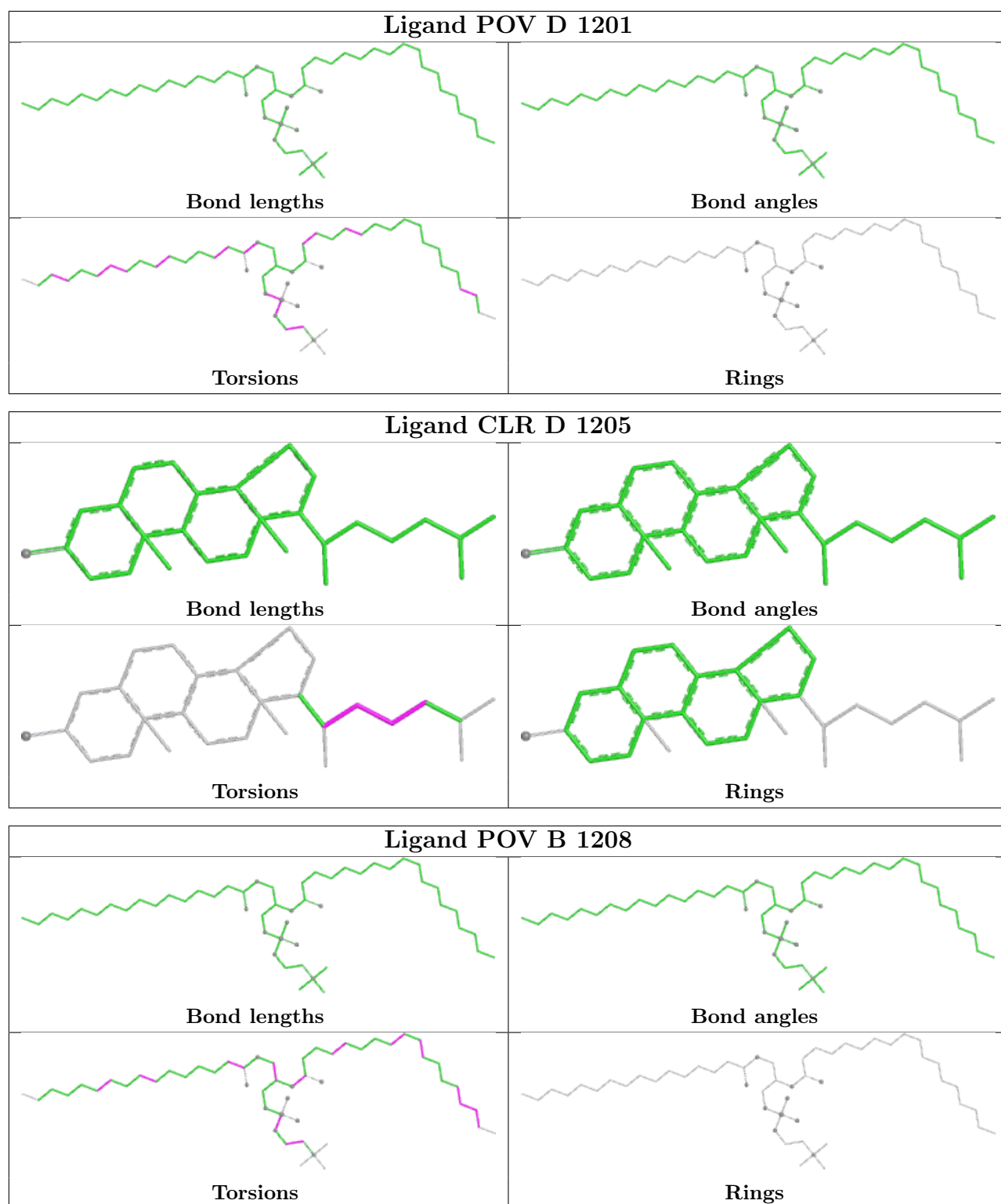
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1204	POV	1	0
3	B	1209	POV	1	0
3	C	1209	POV	1	0
3	C	1204	POV	1	0
3	A	1202	POV	1	0
3	A	1207	POV	1	0
3	D	1209	POV	1	0
3	D	1204	POV	1	0

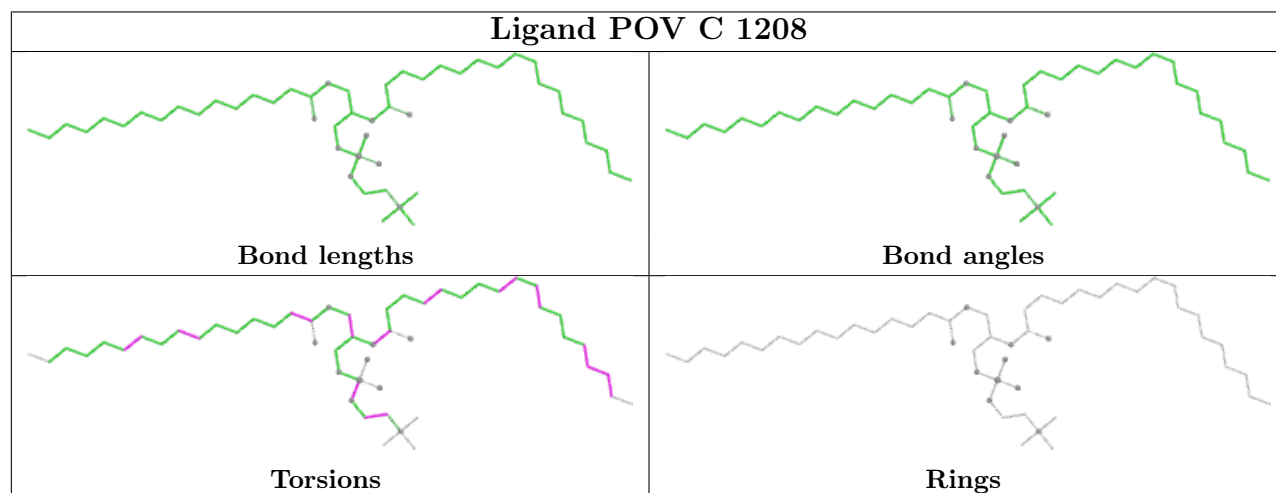
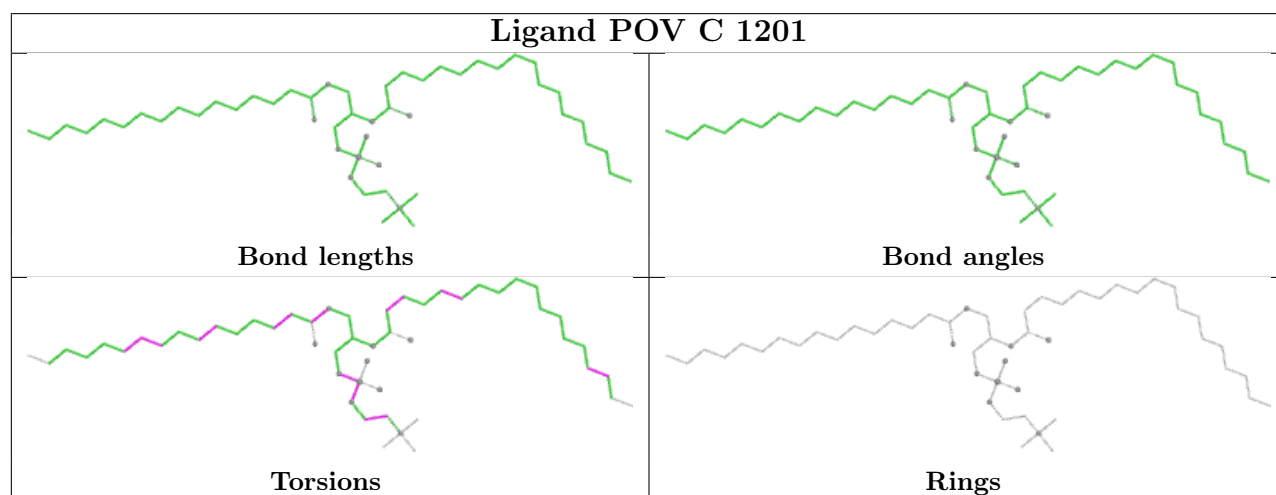
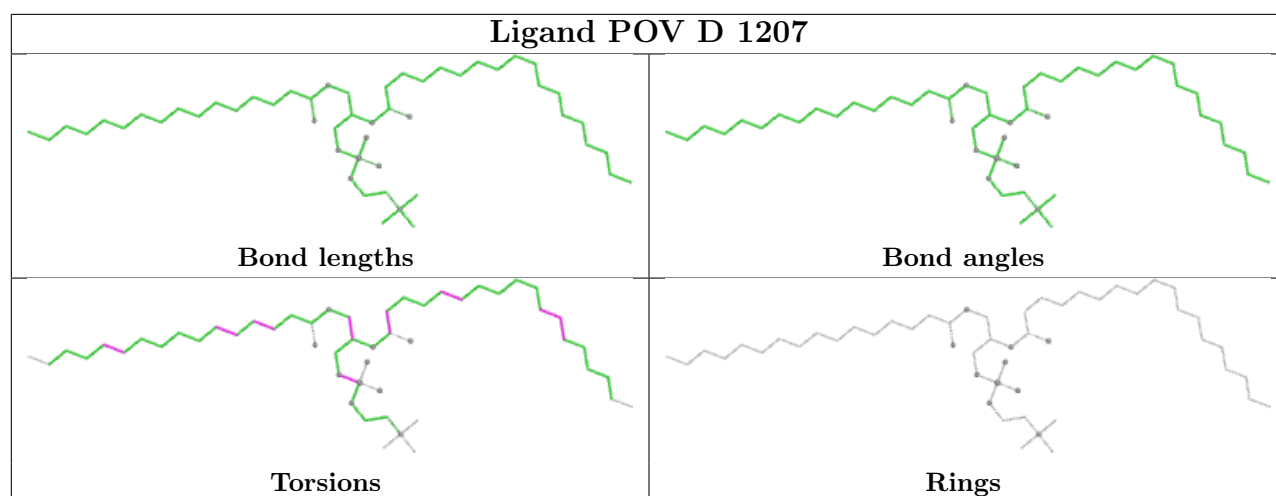
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

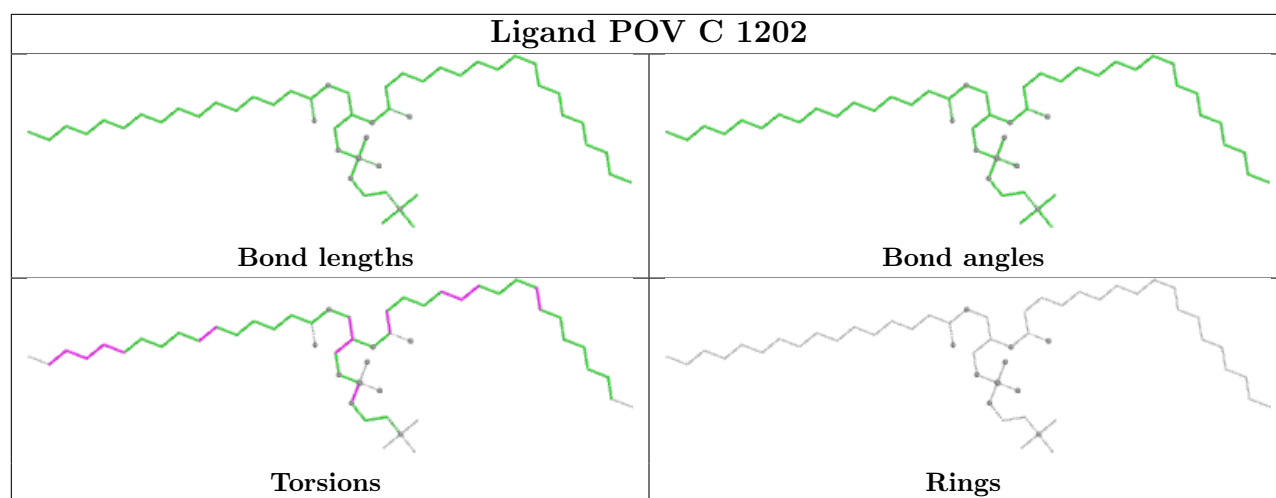
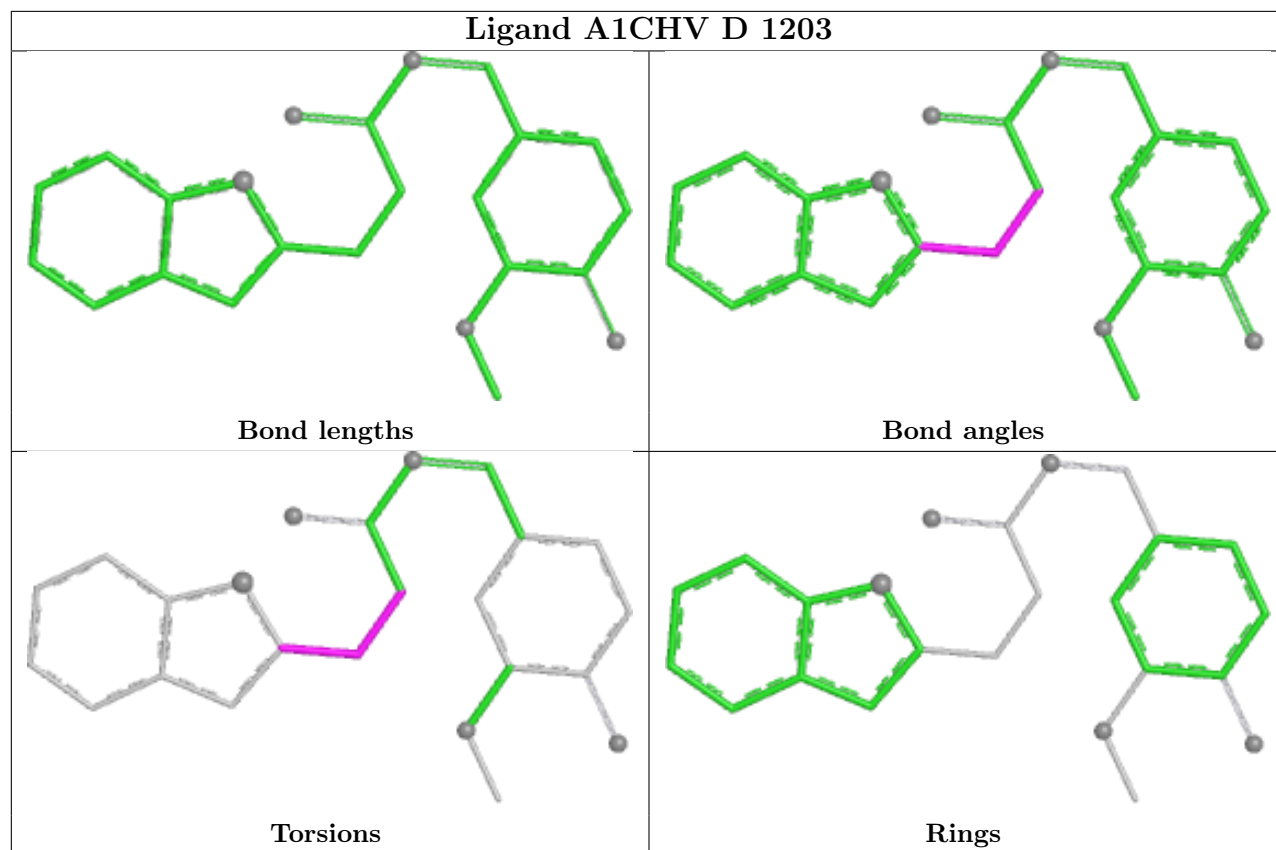


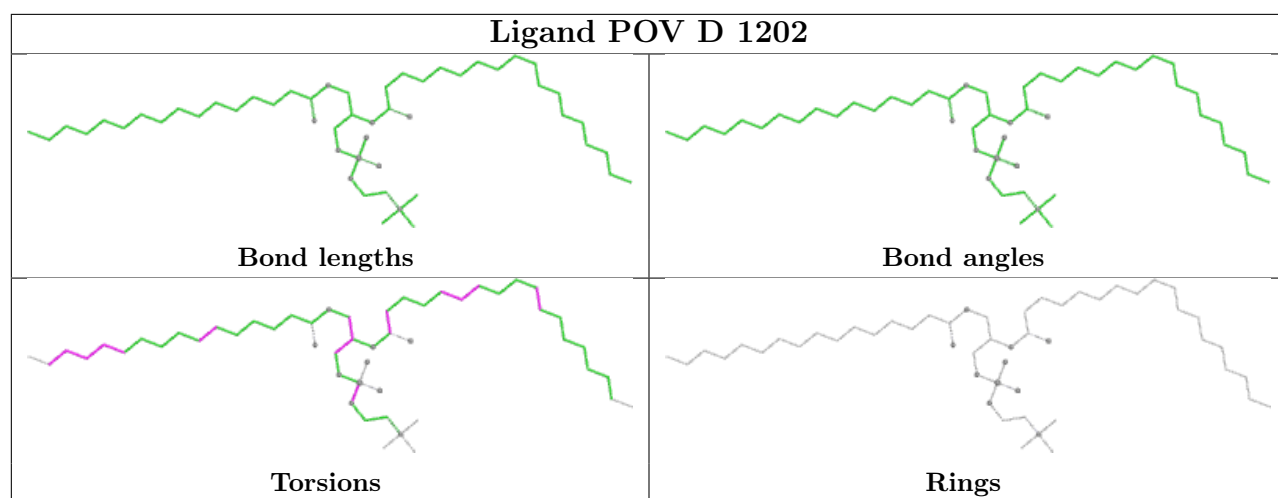
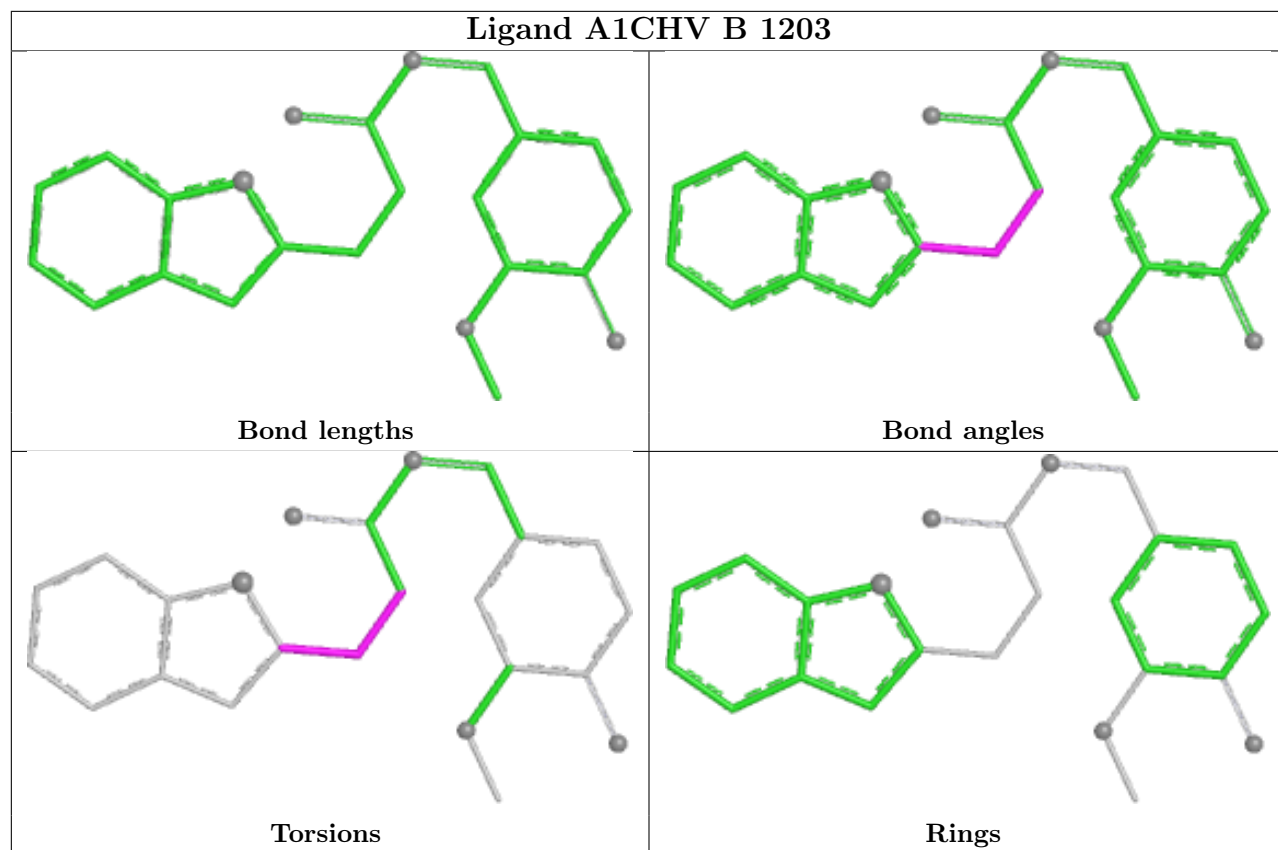


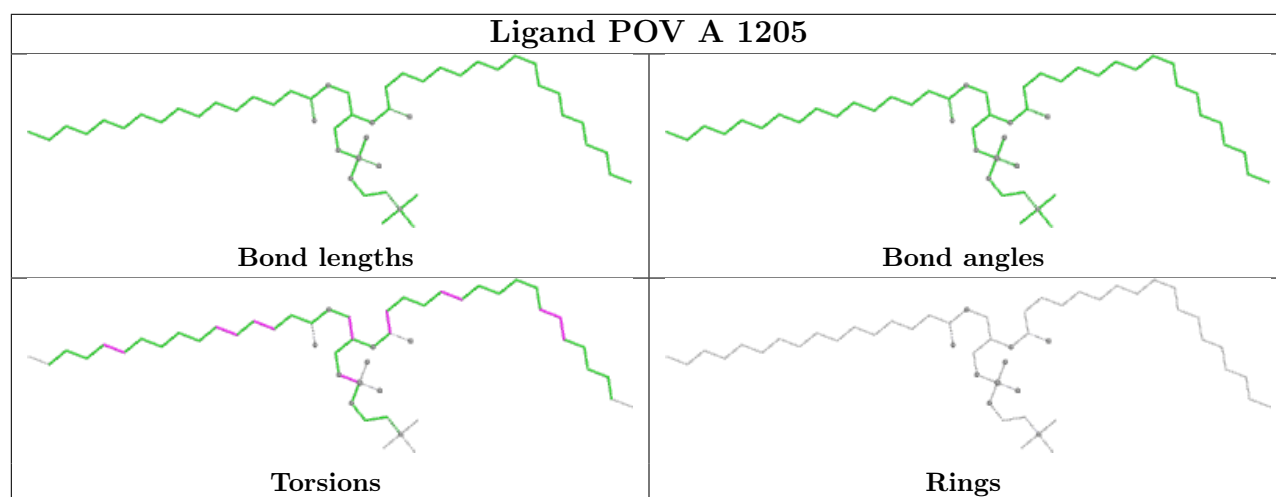
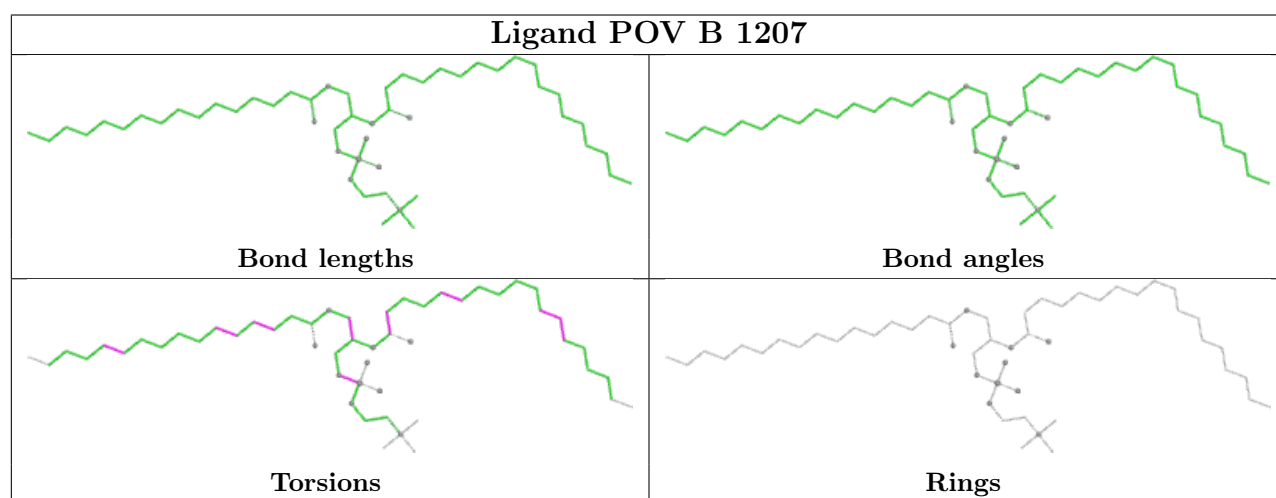
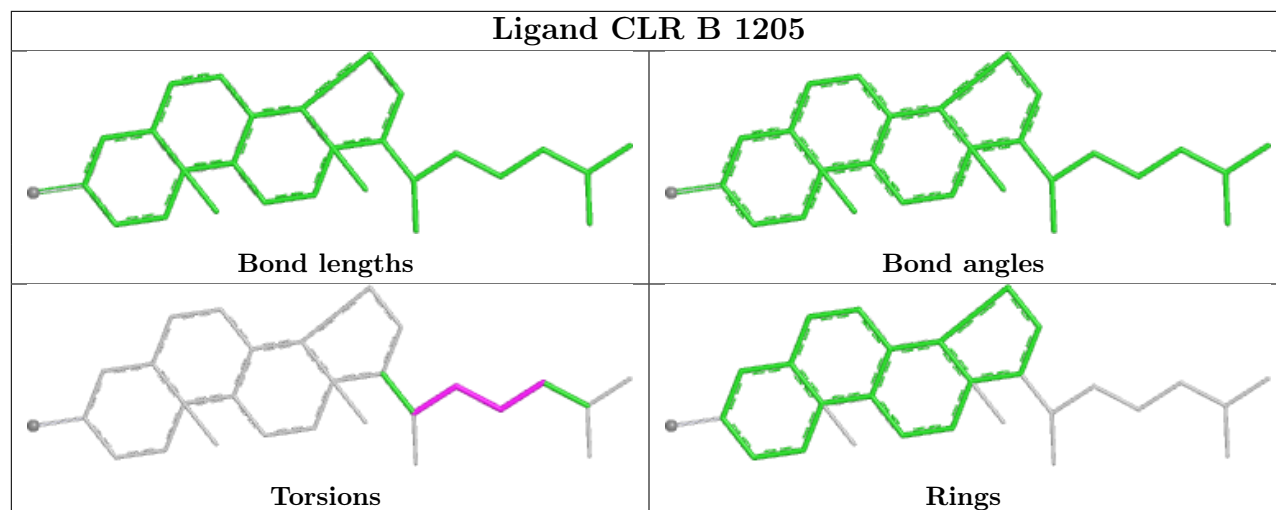


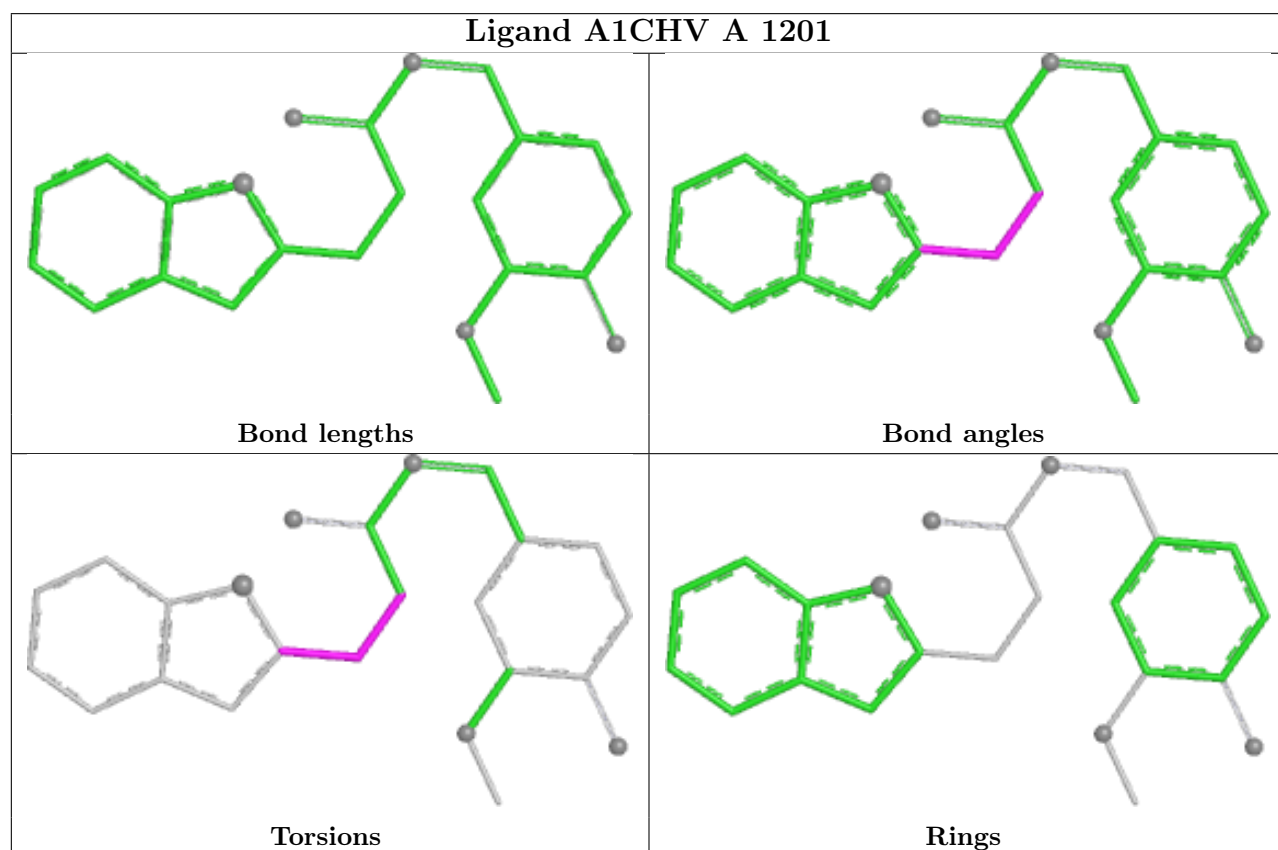
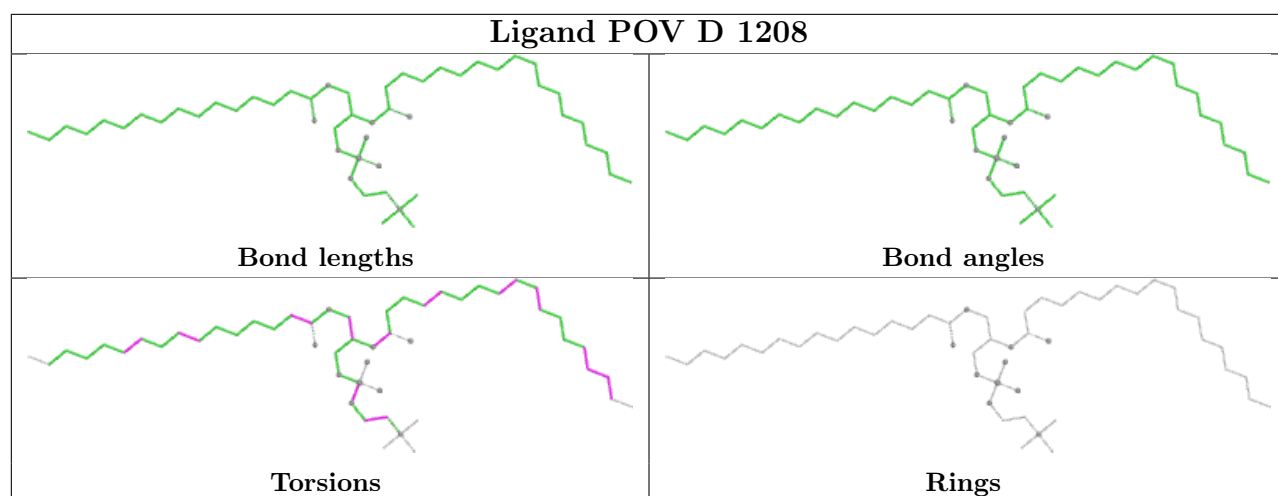


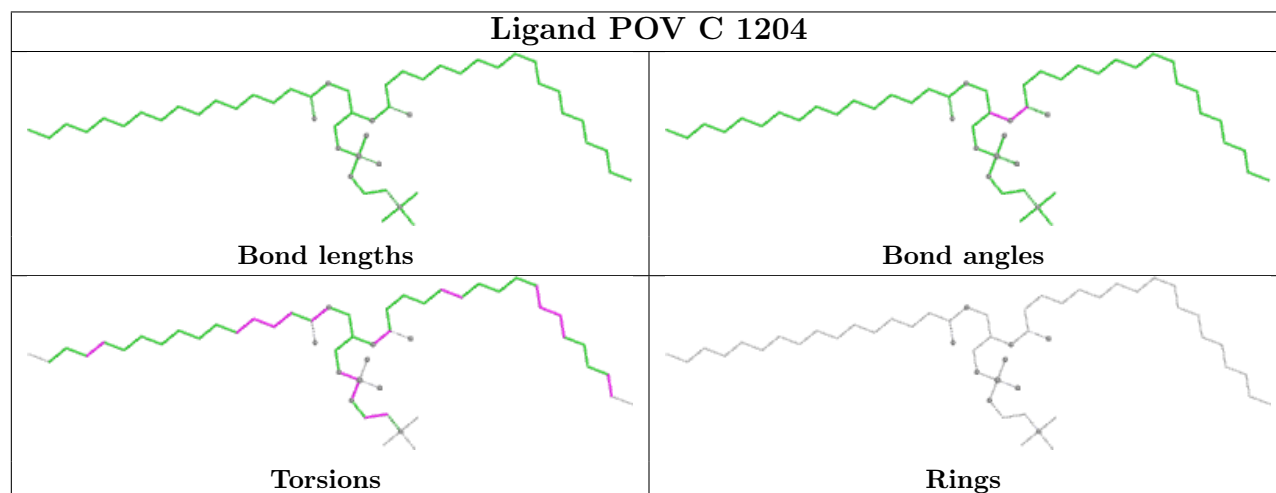
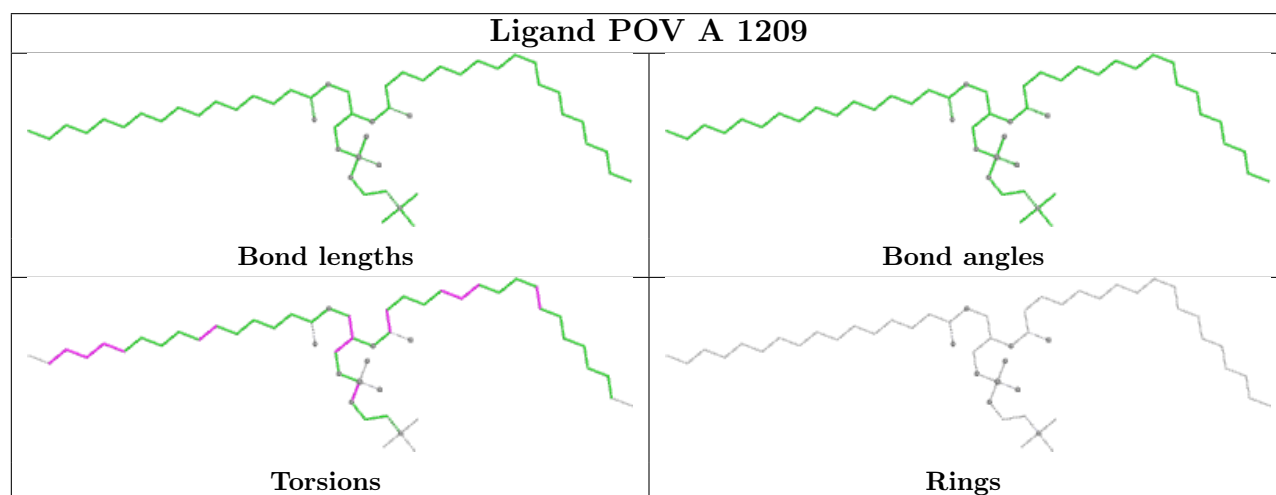
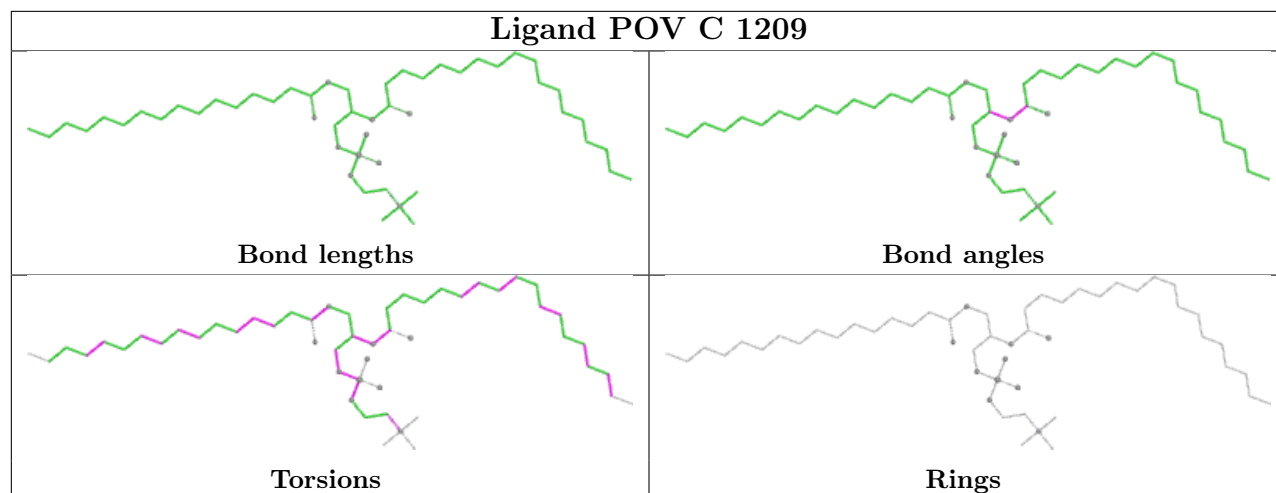


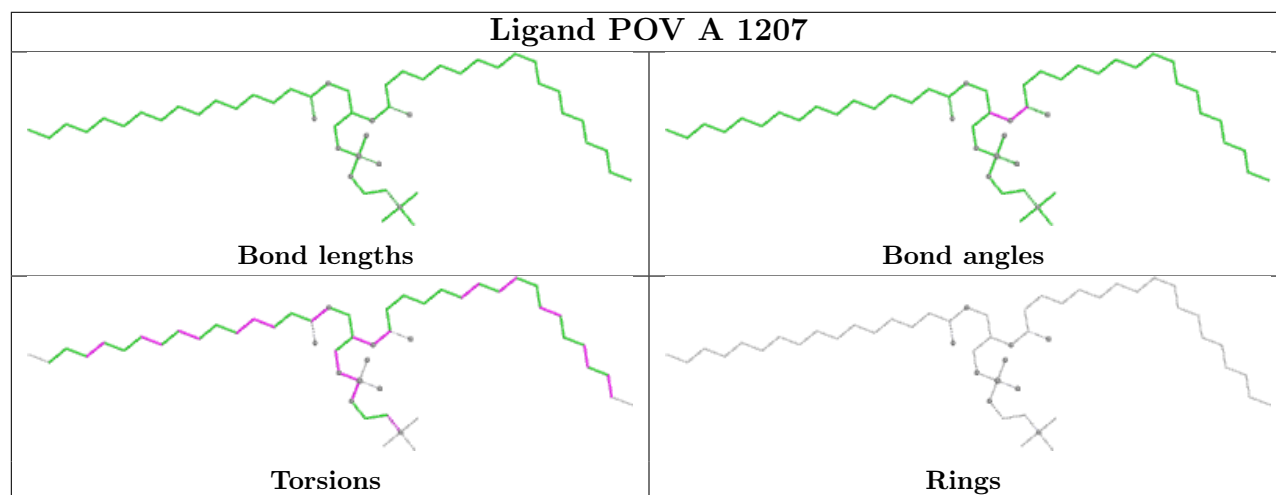
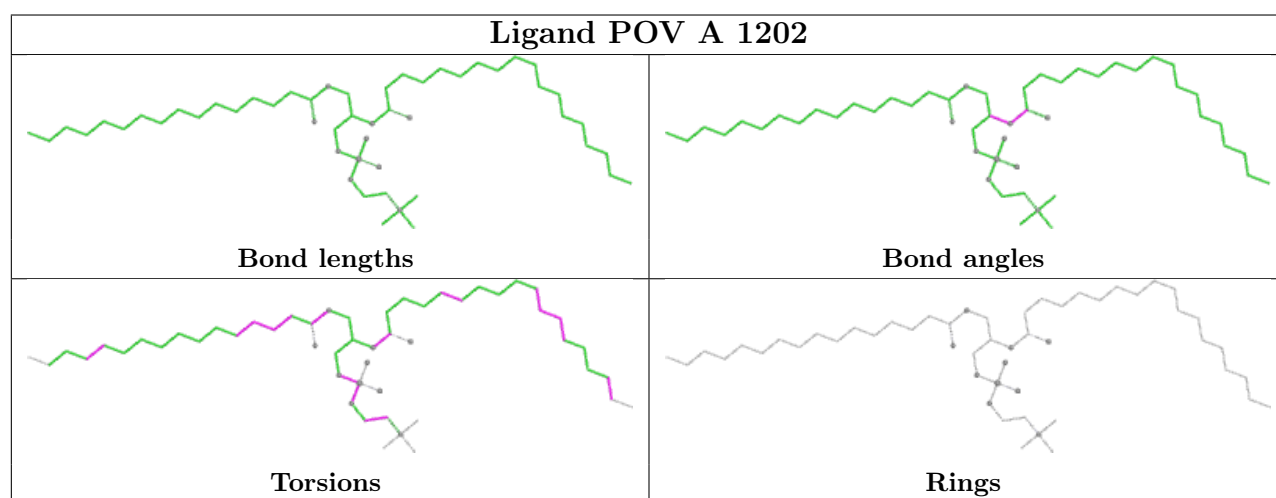
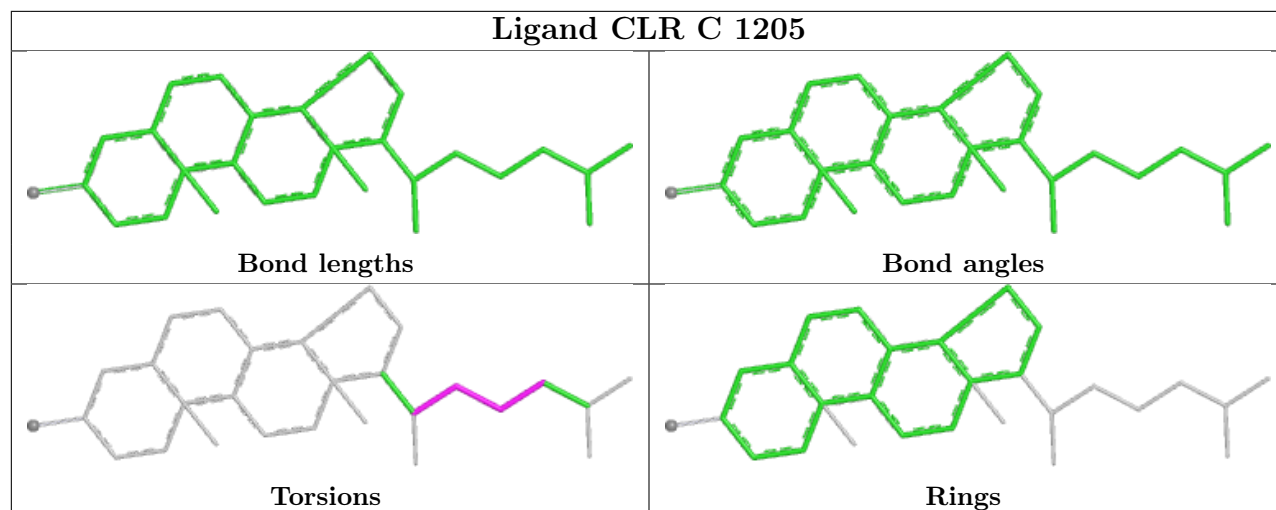


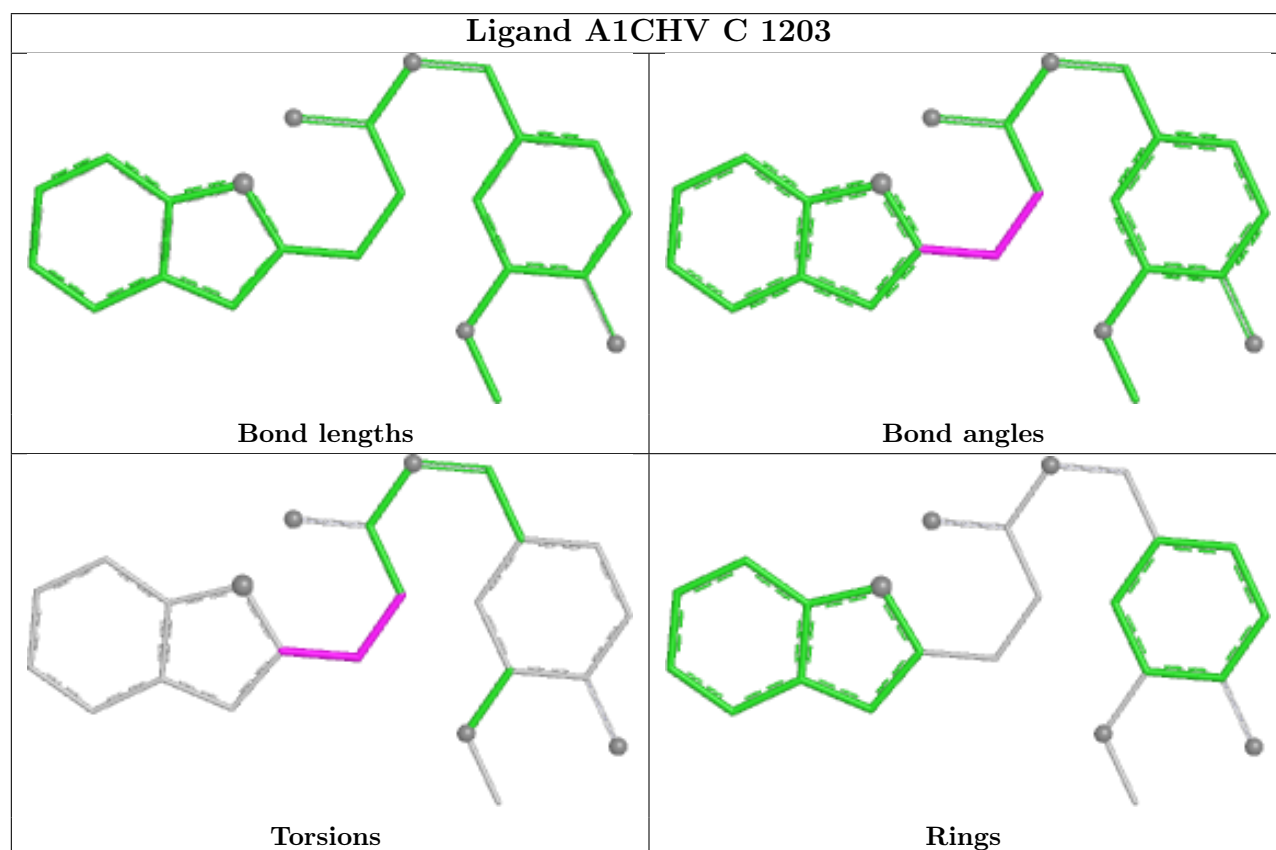
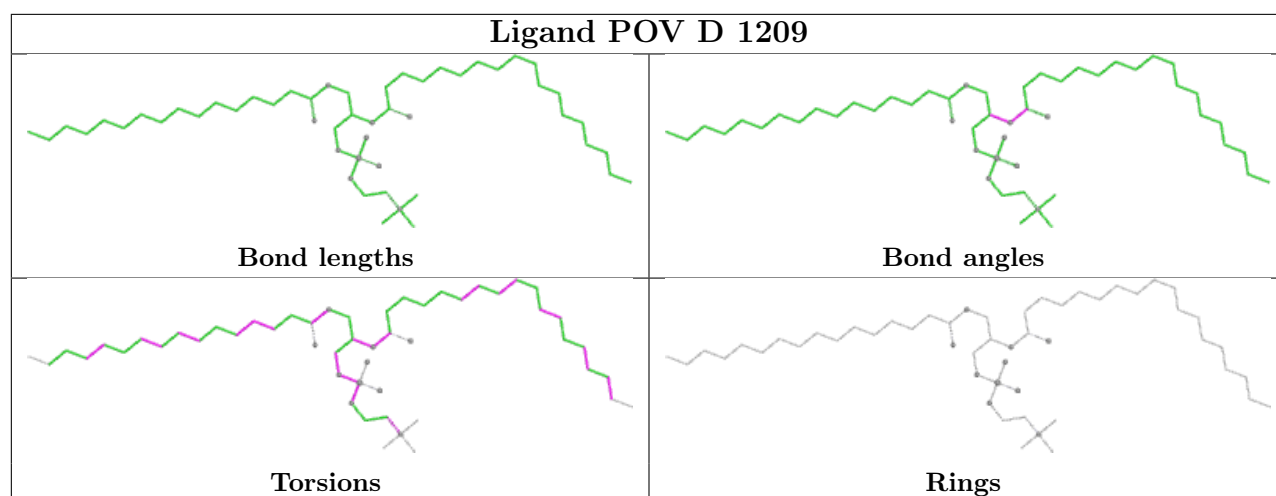


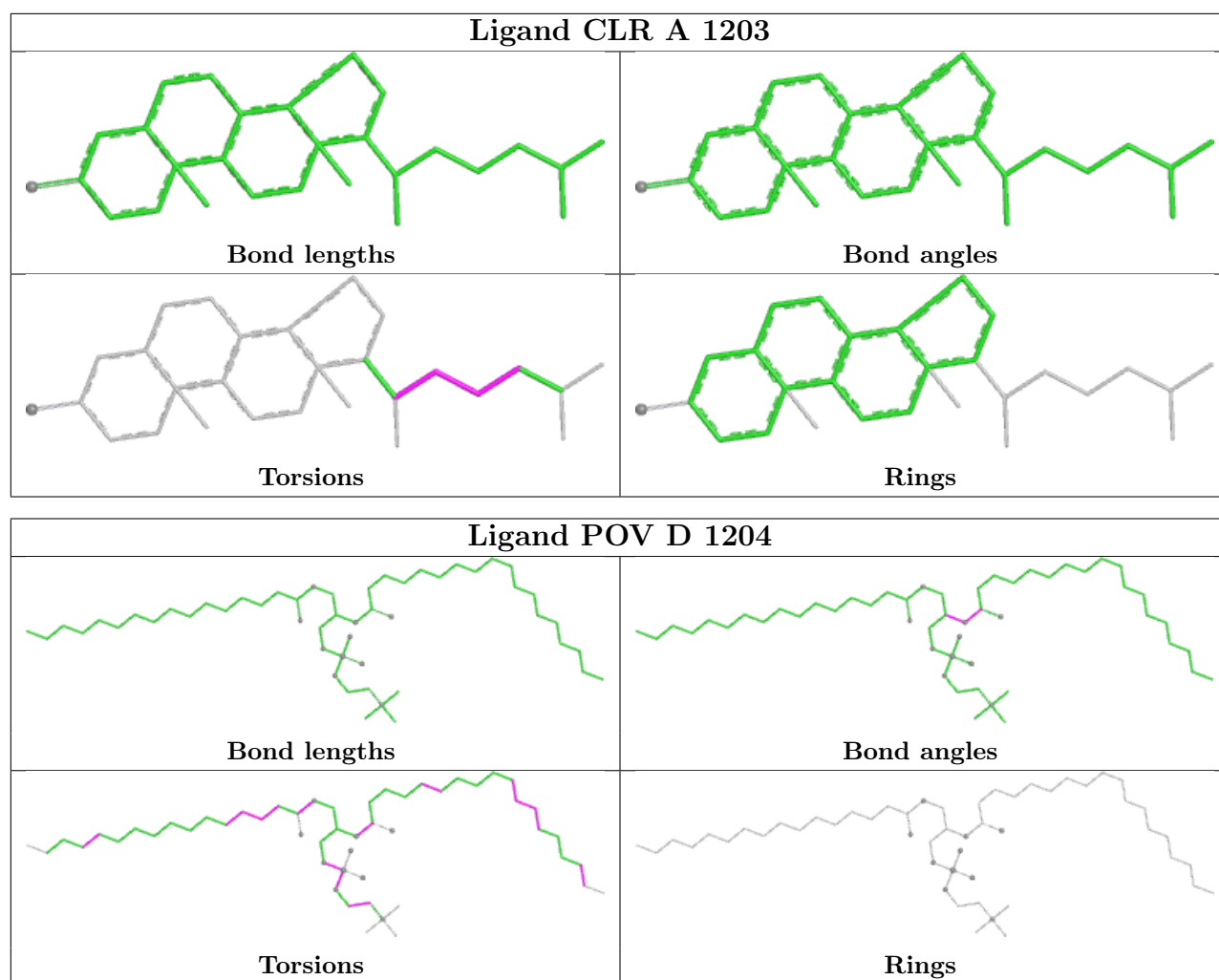












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

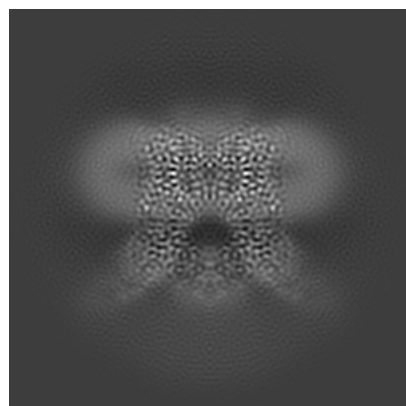
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71555. These allow visual inspection of the internal detail of the map and identification of artifacts.

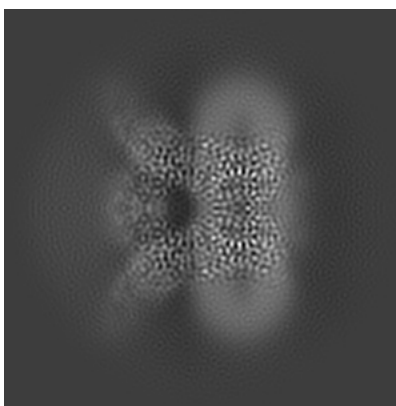
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

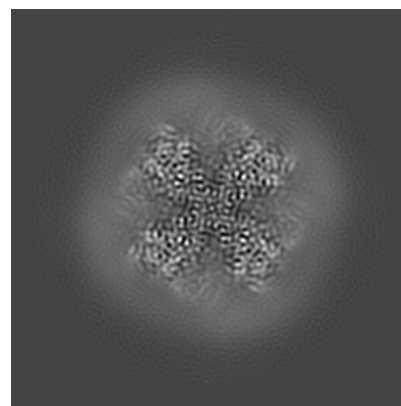
6.1.1 Primary map



X

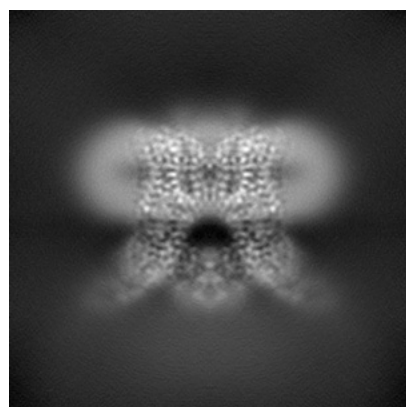


Y

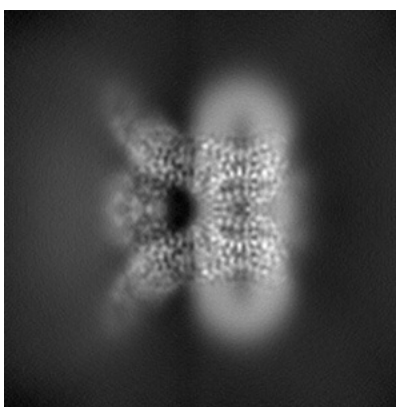


Z

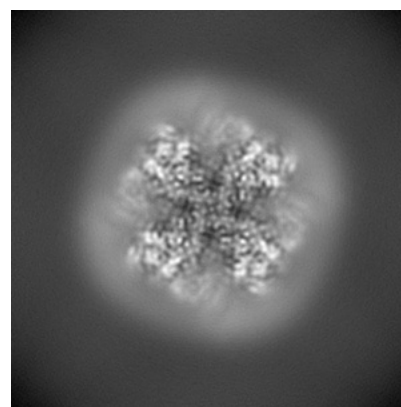
6.1.2 Raw map



X



Y

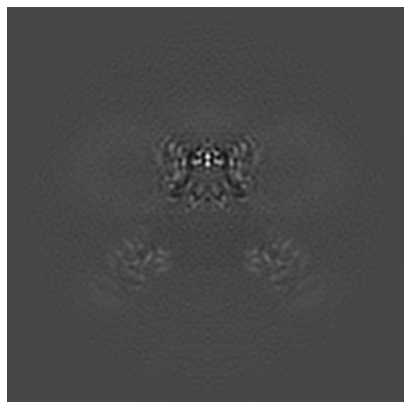


Z

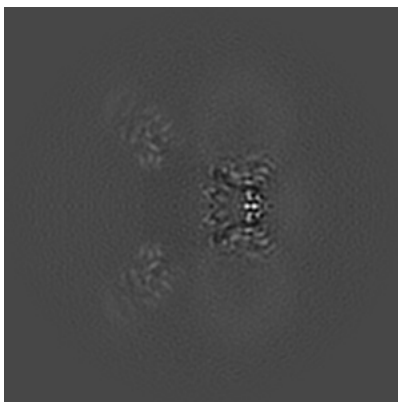
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

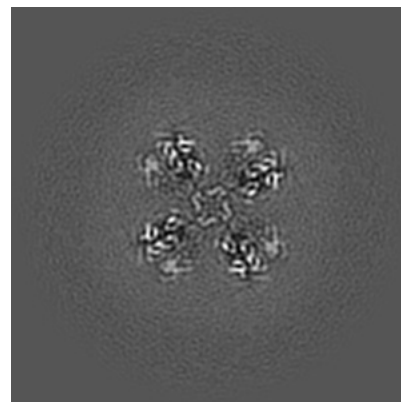
6.2.1 Primary map



X Index: 128

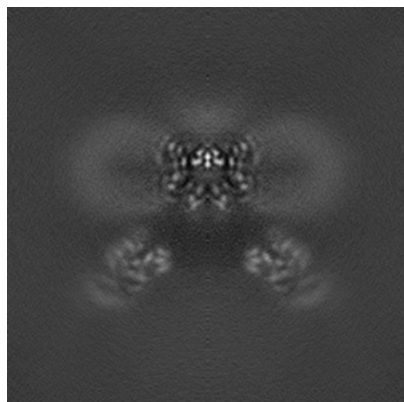


Y Index: 128

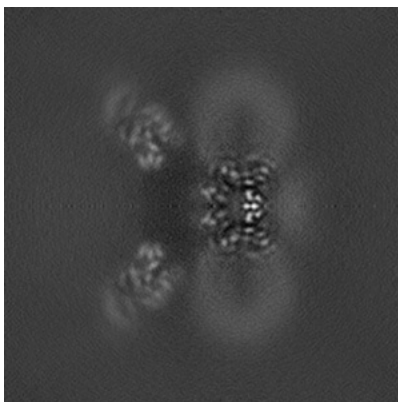


Z Index: 128

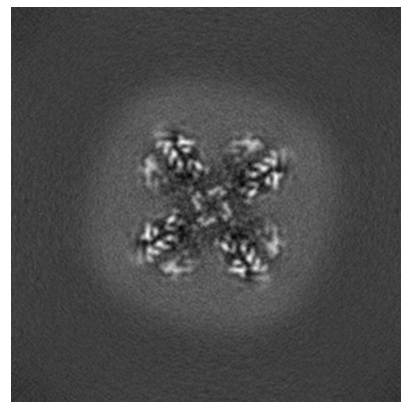
6.2.2 Raw map



X Index: 128



Y Index: 128

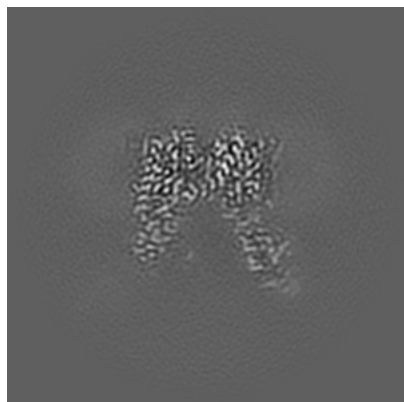


Z Index: 128

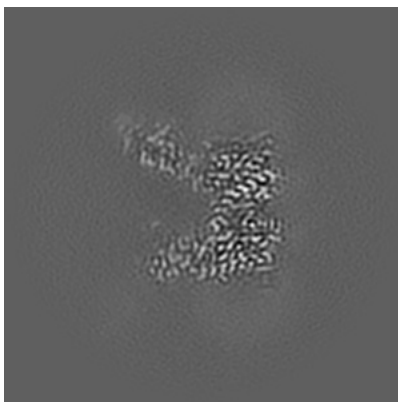
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

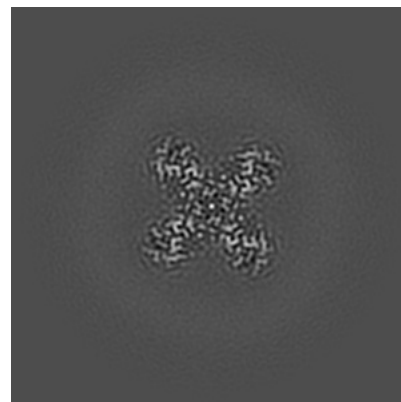
6.3.1 Primary map



X Index: 148

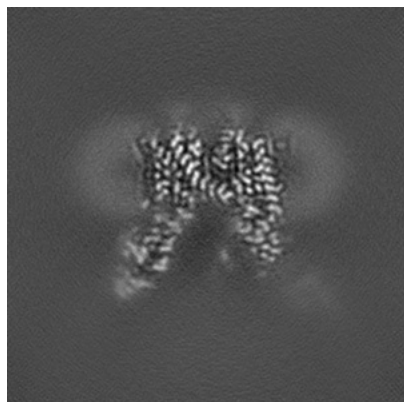


Y Index: 108

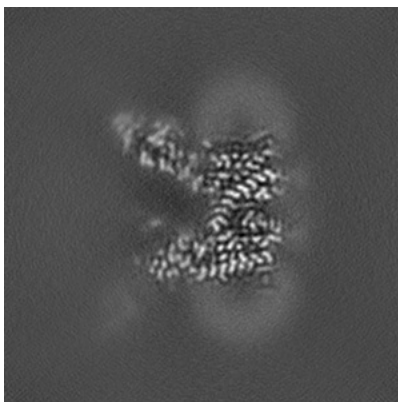


Z Index: 155

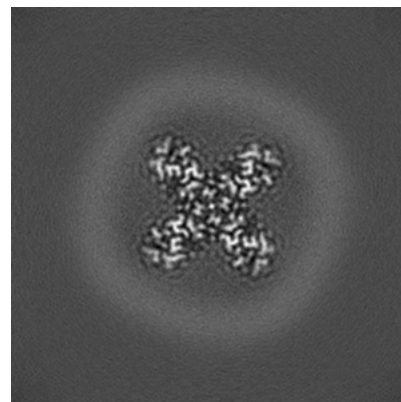
6.3.2 Raw map



X Index: 108



Y Index: 108

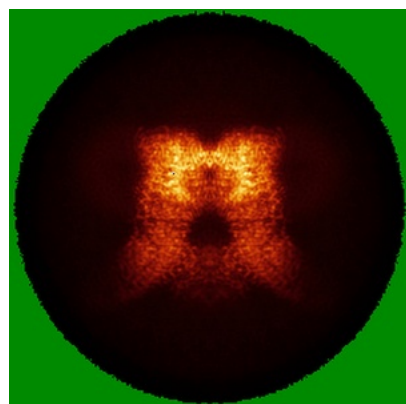


Z Index: 155

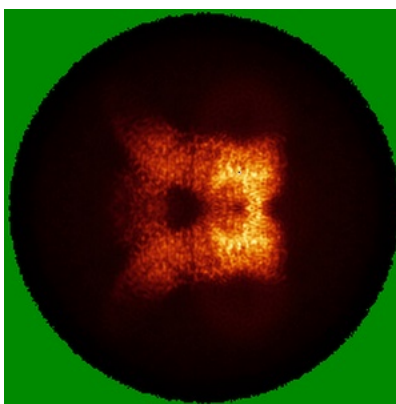
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

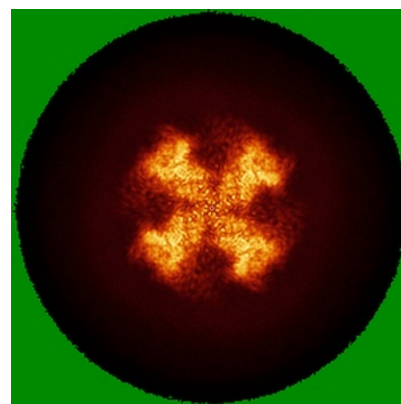
6.4.1 Primary map



X

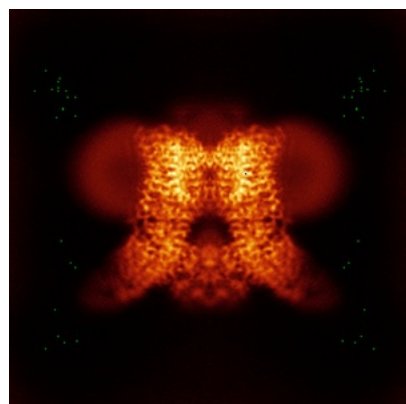


Y

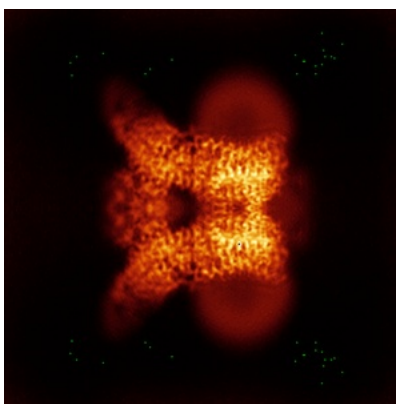


Z

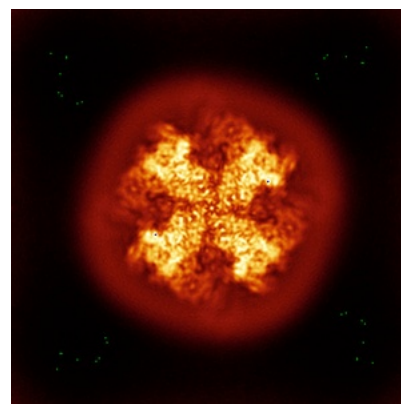
6.4.2 Raw map



X



Y

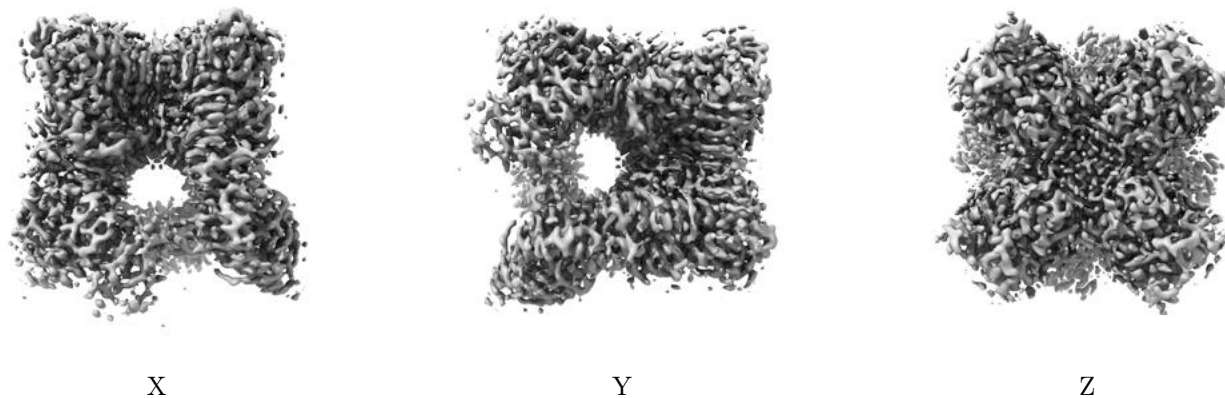


Z

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

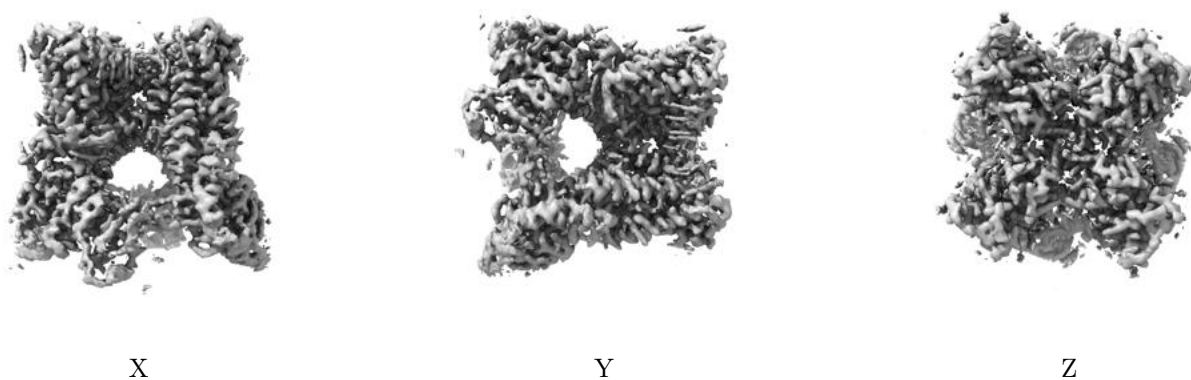
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

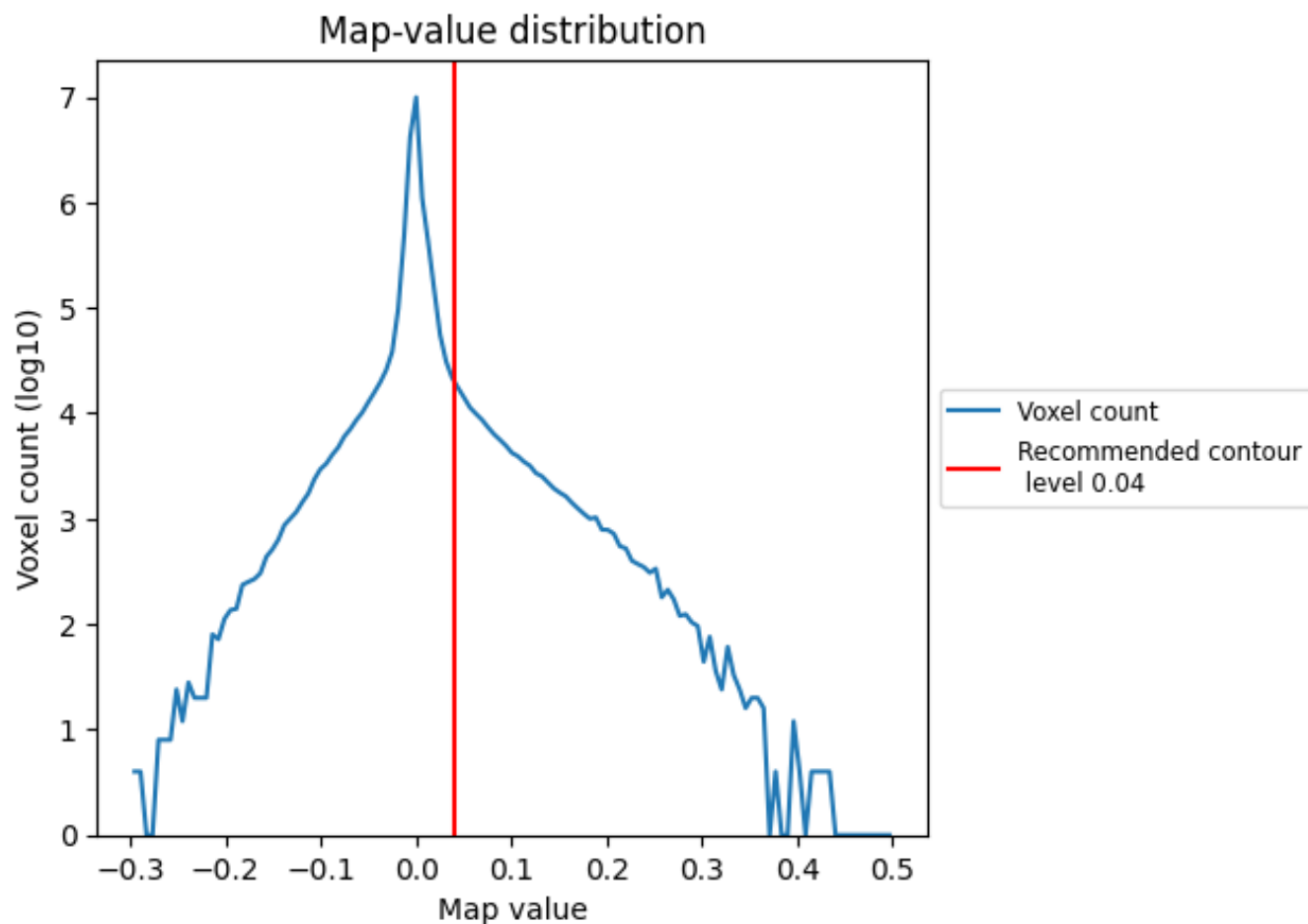
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

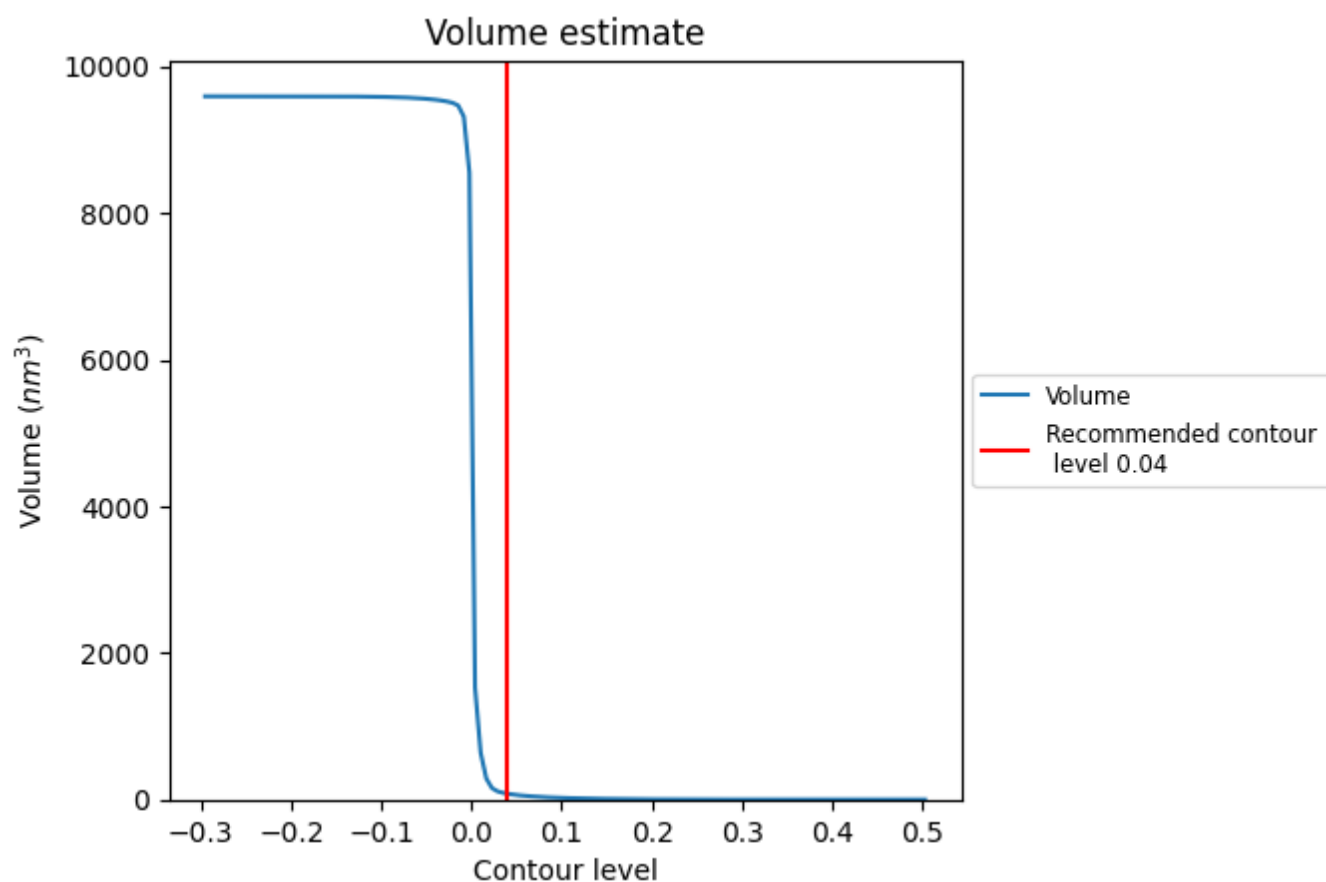
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

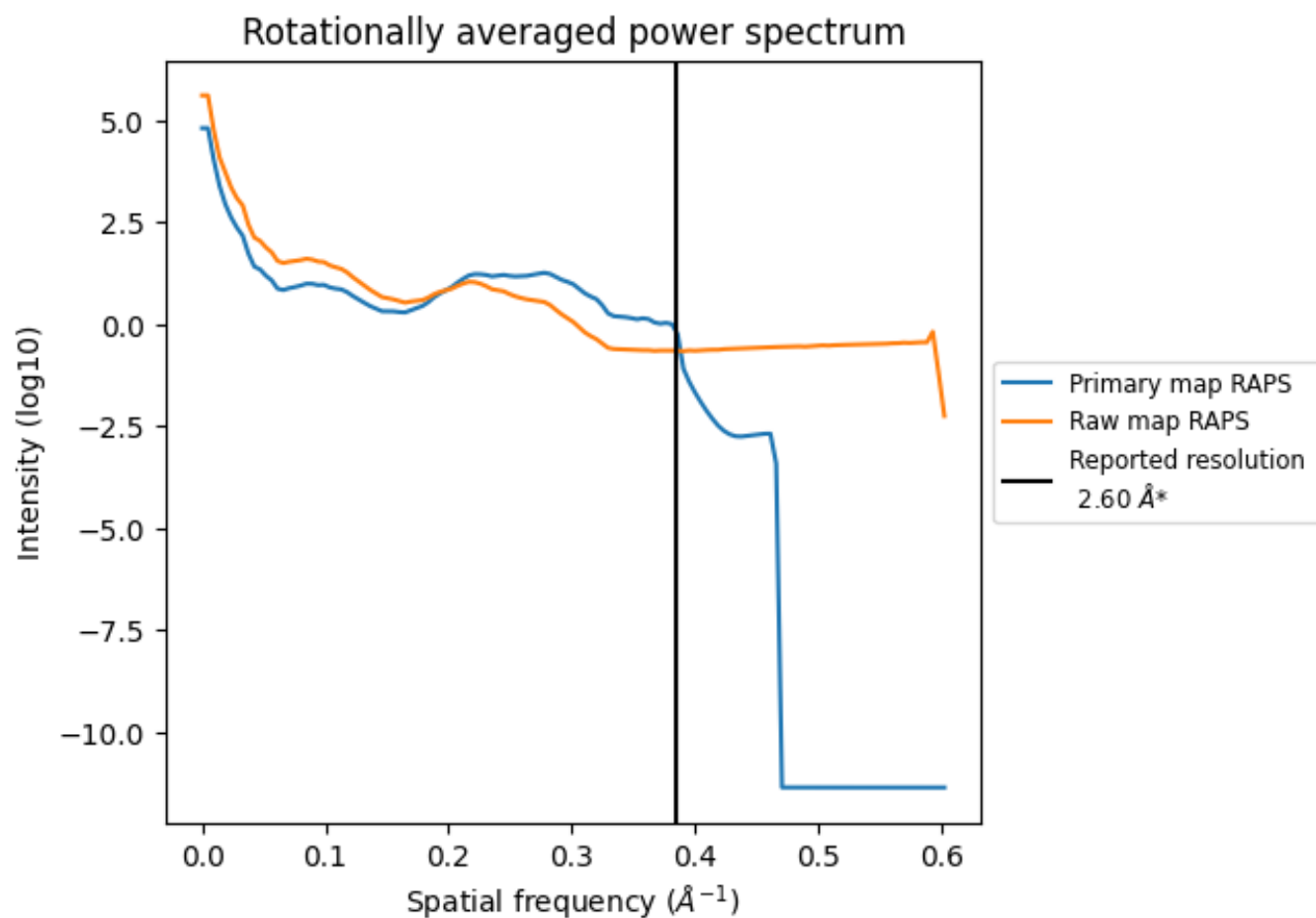
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm³; this corresponds to an approximate mass of 72 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 ⓘ

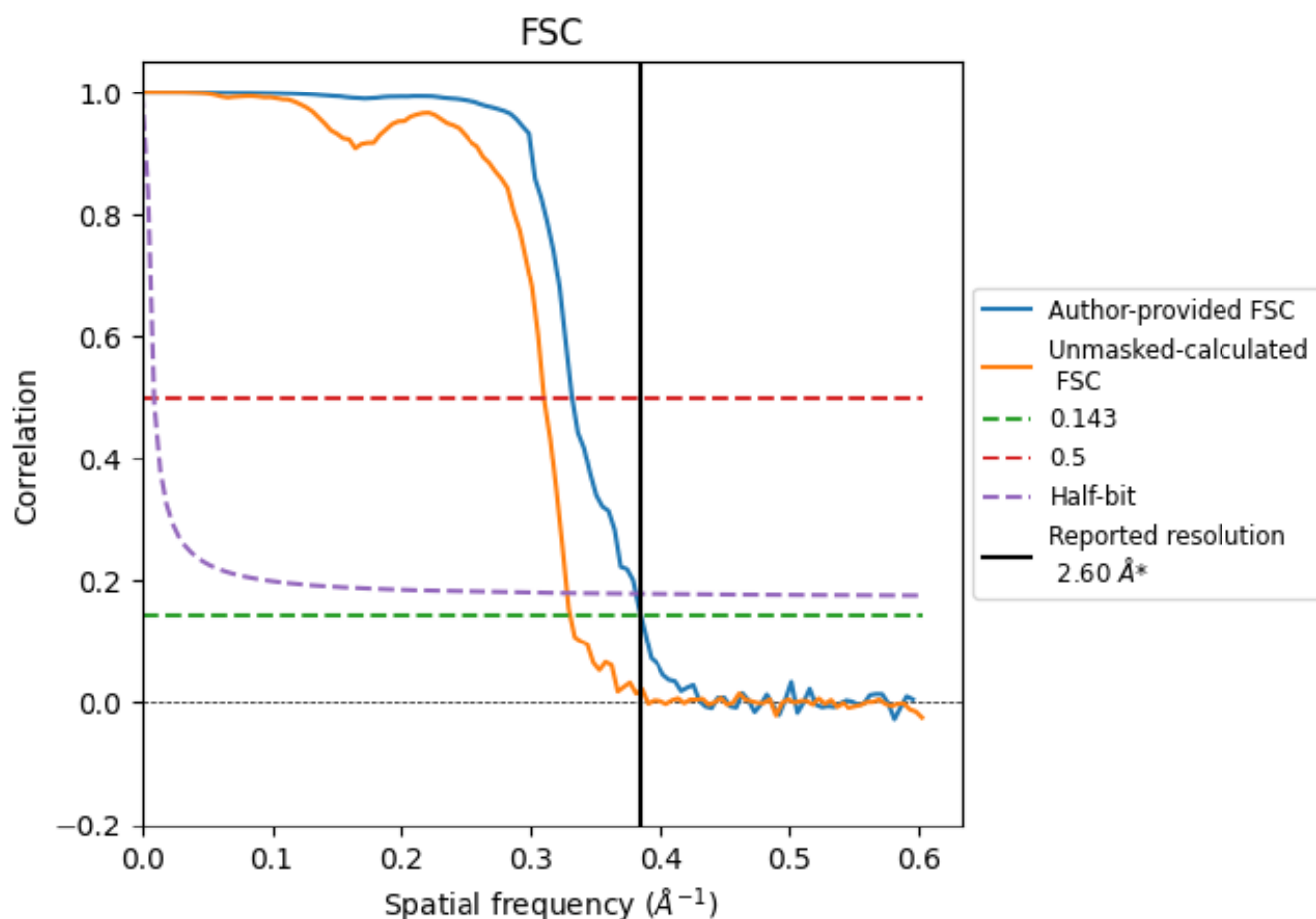


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 $0.385 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

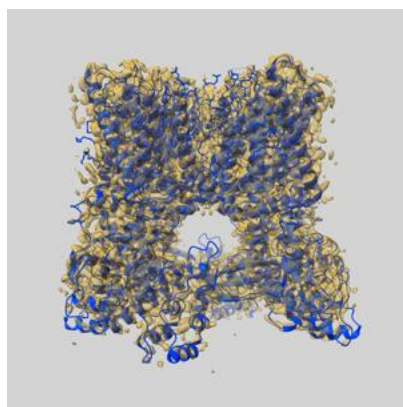
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	3.01	2.62
Unmasked-calculated*	3.02	3.22	3.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.02 differs from the reported value 2.6 by more than 10 %

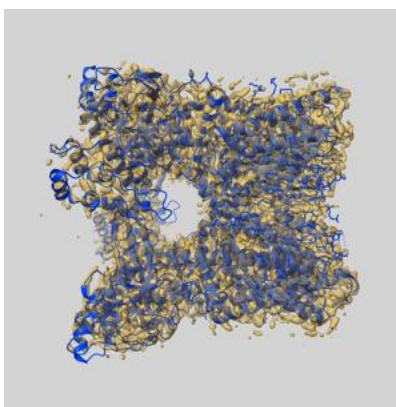
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71555 and PDB model 9PEA. Per-residue inclusion information can be found in section 3 on page 33.

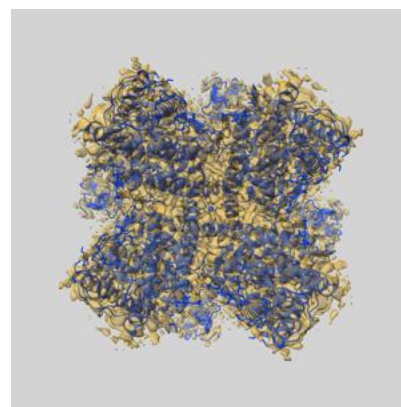
9.1 Map-model overlay [i](#)



X



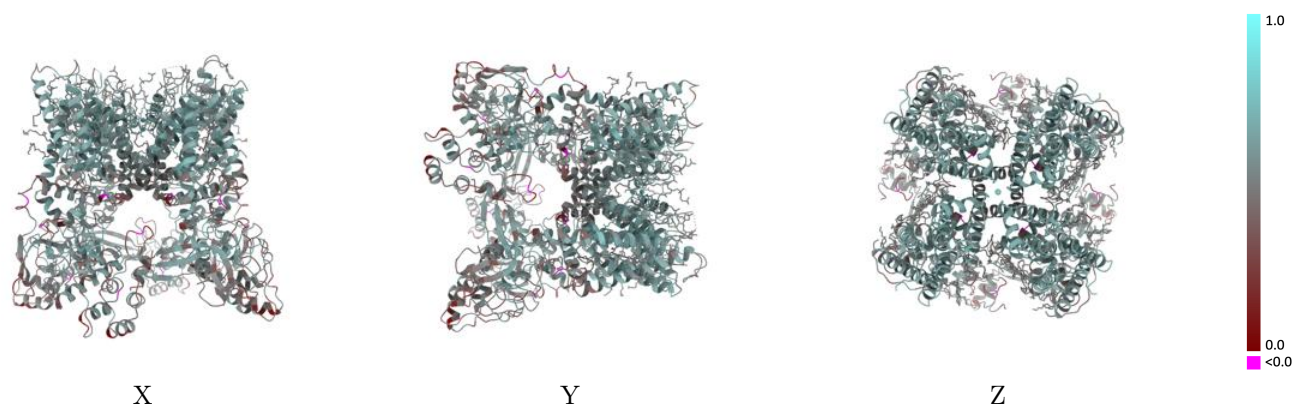
Y



Z

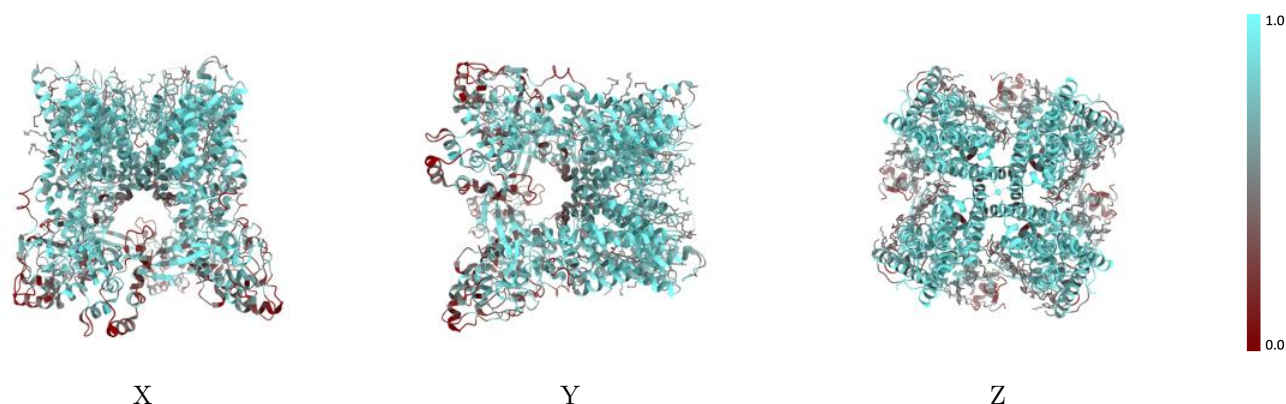
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



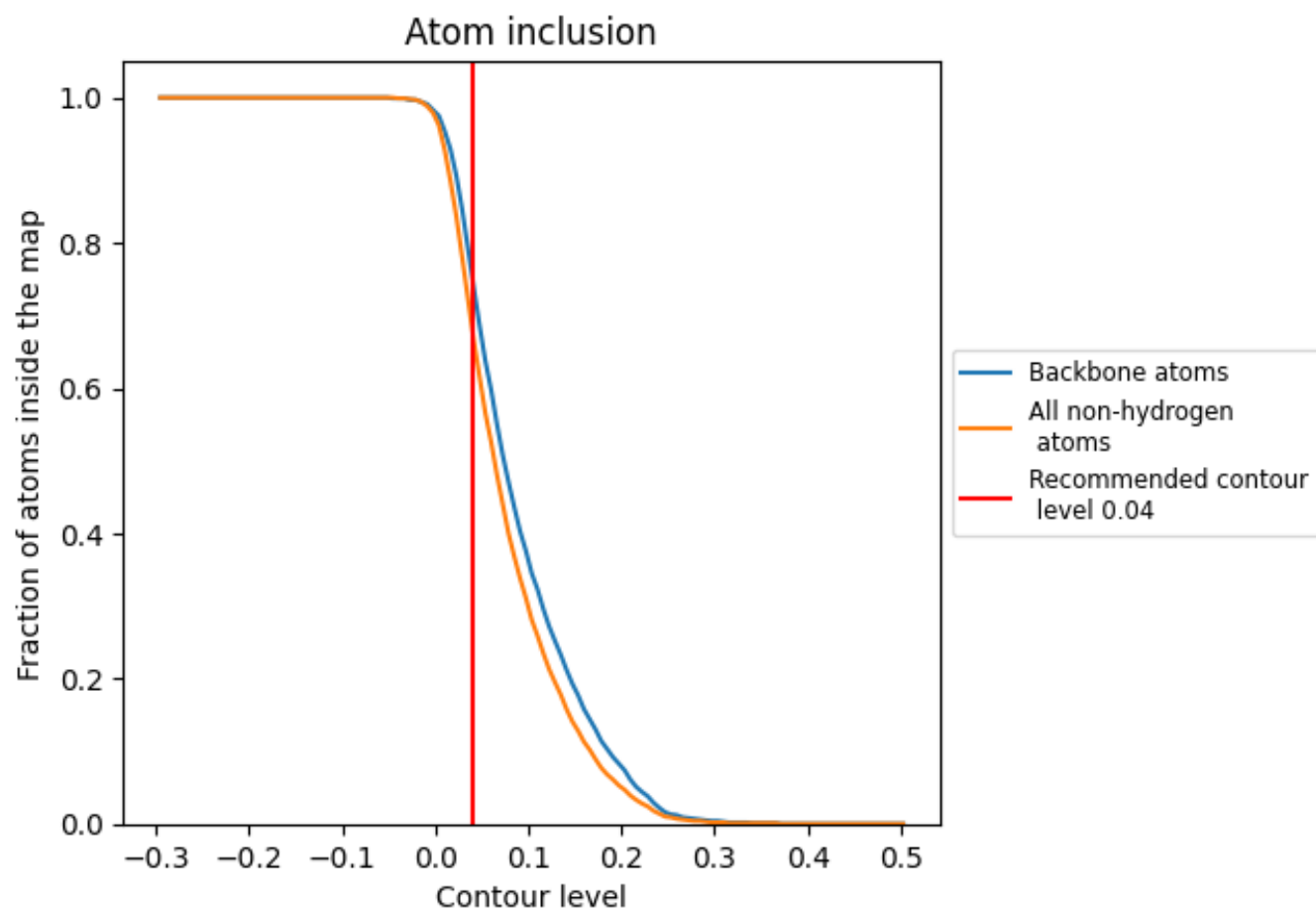
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6780	0.5200
A	0.6770	0.5200
B	0.6780	0.5200
C	0.6790	0.5190
D	0.6780	0.5200

