



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 11:42 PM EST

PDB ID : 8SZF
EMDB ID : EMD-40914
Title : Cryo-EM structure of cinacalcet-bound active-state human calcium-sensing receptor CaSR in lipid nanodiscs
Authors : He, F.; Wu, C.; Gao, Y.; Skiniotis, G.
Deposited on : 2023-05-29
Resolution : 2.80 Å(reported)

This is a wwPDB EM Validation Summary 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

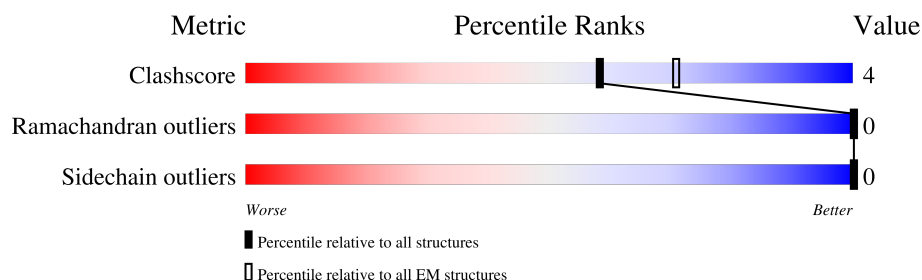
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1101	
2	B	959	
3	C	2	
3	D	2	
3	E	2	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12813 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 Extracellular calcium-sensing receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	799	Total	C	N	O	S	0	0
			6243	4054	1023	1130	36		

There are 225 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ASP	-	expression tag	UNP P41180
A	10	TYR	-	expression tag	UNP P41180
A	11	LYS	-	expression tag	UNP P41180
A	12	ASP	-	expression tag	UNP P41180
A	13	ASP	-	expression tag	UNP P41180
A	14	ASP	-	expression tag	UNP P41180
A	15	ASP	-	expression tag	UNP P41180
A	16	LYS	-	expression tag	UNP P41180
A	17	ALA	-	expression tag	UNP P41180
A	18	ALA	-	expression tag	UNP P41180
A	895	THR	-	expression tag	UNP P41180
A	896	SER	-	expression tag	UNP P41180
A	897	THR	-	expression tag	UNP P41180
A	898	SER	-	expression tag	UNP P41180
A	899	VAL	-	expression tag	UNP P41180
A	900	THR	-	expression tag	UNP P41180
A	901	SER	-	expression tag	UNP P41180
A	902	VAL	-	expression tag	UNP P41180
A	903	ASN	-	expression tag	UNP P41180
A	904	GLN	-	expression tag	UNP P41180
A	905	ALA	-	expression tag	UNP P41180
A	906	SER	-	expression tag	UNP P41180
A	907	THR	-	expression tag	UNP P41180
A	908	SER	-	expression tag	UNP P41180
A	909	ARG	-	expression tag	UNP P41180
A	910	LEU	-	expression tag	UNP P41180
A	911	GLU	-	expression tag	UNP P41180
A	912	GLY	-	expression tag	UNP P41180

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Chain	Residue	Modelled	Actual	Comment	Reference
A	913	LEU	-	expression tag	UNP P41180
A	914	GLN	-	expression tag	UNP P41180
A	915	SER	-	expression tag	UNP P41180
A	916	GLU	-	expression tag	UNP P41180
A	917	ASN	-	expression tag	UNP P41180
A	918	HIS	-	expression tag	UNP P41180
A	919	ARG	-	expression tag	UNP P41180
A	920	LEU	-	expression tag	UNP P41180
A	921	ARG	-	expression tag	UNP P41180
A	922	MET	-	expression tag	UNP P41180
A	923	LYS	-	expression tag	UNP P41180
A	924	ILE	-	expression tag	UNP P41180
A	925	THR	-	expression tag	UNP P41180
A	926	GLU	-	expression tag	UNP P41180
A	927	LEU	-	expression tag	UNP P41180
A	928	ASP	-	expression tag	UNP P41180
A	929	LYS	-	expression tag	UNP P41180
A	930	ASP	-	expression tag	UNP P41180
A	931	LEU	-	expression tag	UNP P41180
A	932	GLU	-	expression tag	UNP P41180
A	933	GLU	-	expression tag	UNP P41180
A	934	VAL	-	expression tag	UNP P41180
A	935	THR	-	expression tag	UNP P41180
A	936	MET	-	expression tag	UNP P41180
A	937	GLN	-	expression tag	UNP P41180
A	938	LEU	-	expression tag	UNP P41180
A	939	GLN	-	expression tag	UNP P41180
A	940	ASP	-	expression tag	UNP P41180
A	941	THR	-	expression tag	UNP P41180
A	942	PRO	-	expression tag	UNP P41180
A	943	GLU	-	expression tag	UNP P41180
A	944	LYS	-	expression tag	UNP P41180
A	945	LYS	-	expression tag	UNP P41180
A	946	THR	-	expression tag	UNP P41180
A	947	ASN	-	expression tag	UNP P41180
A	948	SER	-	expression tag	UNP P41180
A	949	GLY	-	expression tag	UNP P41180
A	950	GLY	-	expression tag	UNP P41180
A	951	SER	-	expression tag	UNP P41180
A	952	VAL	-	expression tag	UNP P41180
A	953	PHE	-	expression tag	UNP P41180
A	954	THR	-	expression tag	UNP P41180

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Chain	Residue	Modelled	Actual	Comment	Reference
A	955	LEU	-	expression tag	UNP P41180
A	956	GLU	-	expression tag	UNP P41180
A	957	ASP	-	expression tag	UNP P41180
A	958	PHE	-	expression tag	UNP P41180
A	959	VAL	-	expression tag	UNP P41180
A	960	GLY	-	expression tag	UNP P41180
A	961	ASP	-	expression tag	UNP P41180
A	962	TRP	-	expression tag	UNP P41180
A	963	GLU	-	expression tag	UNP P41180
A	964	GLN	-	expression tag	UNP P41180
A	965	THR	-	expression tag	UNP P41180
A	966	ALA	-	expression tag	UNP P41180
A	967	ALA	-	expression tag	UNP P41180
A	968	TYR	-	expression tag	UNP P41180
A	969	ASN	-	expression tag	UNP P41180
A	970	LEU	-	expression tag	UNP P41180
A	971	ASP	-	expression tag	UNP P41180
A	972	GLN	-	expression tag	UNP P41180
A	973	VAL	-	expression tag	UNP P41180
A	974	LEU	-	expression tag	UNP P41180
A	975	GLU	-	expression tag	UNP P41180
A	976	GLN	-	expression tag	UNP P41180
A	977	GLY	-	expression tag	UNP P41180
A	978	GLY	-	expression tag	UNP P41180
A	979	VAL	-	expression tag	UNP P41180
A	980	SER	-	expression tag	UNP P41180
A	981	SER	-	expression tag	UNP P41180
A	982	LEU	-	expression tag	UNP P41180
A	983	LEU	-	expression tag	UNP P41180
A	984	GLN	-	expression tag	UNP P41180
A	985	ASN	-	expression tag	UNP P41180
A	986	LEU	-	expression tag	UNP P41180
A	987	ALA	-	expression tag	UNP P41180
A	988	VAL	-	expression tag	UNP P41180
A	989	SER	-	expression tag	UNP P41180
A	990	VAL	-	expression tag	UNP P41180
A	991	THR	-	expression tag	UNP P41180
A	992	PRO	-	expression tag	UNP P41180
A	993	ILE	-	expression tag	UNP P41180
A	994	GLN	-	expression tag	UNP P41180
A	995	ARG	-	expression tag	UNP P41180
A	996	ILE	-	expression tag	UNP P41180

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Chain	Residue	Modelled	Actual	Comment	Reference
A	997	VAL	-	expression tag	UNP P41180
A	998	ARG	-	expression tag	UNP P41180
A	999	SER	-	expression tag	UNP P41180
A	1000	GLY	-	expression tag	UNP P41180
A	1001	GLU	-	expression tag	UNP P41180
A	1002	ASN	-	expression tag	UNP P41180
A	1003	ALA	-	expression tag	UNP P41180
A	1004	LEU	-	expression tag	UNP P41180
A	1005	LYS	-	expression tag	UNP P41180
A	1006	ILE	-	expression tag	UNP P41180
A	1007	ASP	-	expression tag	UNP P41180
A	1008	ILE	-	expression tag	UNP P41180
A	1009	HIS	-	expression tag	UNP P41180
A	1010	VAL	-	expression tag	UNP P41180
A	1011	ILE	-	expression tag	UNP P41180
A	1012	ILE	-	expression tag	UNP P41180
A	1013	PRO	-	expression tag	UNP P41180
A	1014	TYR	-	expression tag	UNP P41180
A	1015	GLU	-	expression tag	UNP P41180
A	1016	GLY	-	expression tag	UNP P41180
A	1017	LEU	-	expression tag	UNP P41180
A	1018	SER	-	expression tag	UNP P41180
A	1019	ALA	-	expression tag	UNP P41180
A	1020	ASP	-	expression tag	UNP P41180
A	1021	GLN	-	expression tag	UNP P41180
A	1022	MET	-	expression tag	UNP P41180
A	1023	ALA	-	expression tag	UNP P41180
A	1024	GLN	-	expression tag	UNP P41180
A	1025	ILE	-	expression tag	UNP P41180
A	1026	GLU	-	expression tag	UNP P41180
A	1027	GLU	-	expression tag	UNP P41180
A	1028	VAL	-	expression tag	UNP P41180
A	1029	PHE	-	expression tag	UNP P41180
A	1030	LYS	-	expression tag	UNP P41180
A	1031	VAL	-	expression tag	UNP P41180
A	1032	VAL	-	expression tag	UNP P41180
A	1033	TYR	-	expression tag	UNP P41180
A	1034	PRO	-	expression tag	UNP P41180
A	1035	VAL	-	expression tag	UNP P41180
A	1036	ASP	-	expression tag	UNP P41180
A	1037	ASP	-	expression tag	UNP P41180
A	1038	HIS	-	expression tag	UNP P41180

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1039	HIS	-	expression tag	UNP P41180
A	1040	PHE	-	expression tag	UNP P41180
A	1041	LYS	-	expression tag	UNP P41180
A	1042	VAL	-	expression tag	UNP P41180
A	1043	ILE	-	expression tag	UNP P41180
A	1044	LEU	-	expression tag	UNP P41180
A	1045	PRO	-	expression tag	UNP P41180
A	1046	TYR	-	expression tag	UNP P41180
A	1047	GLY	-	expression tag	UNP P41180
A	1048	THR	-	expression tag	UNP P41180
A	1049	LEU	-	expression tag	UNP P41180
A	1050	VAL	-	expression tag	UNP P41180
A	1051	ILE	-	expression tag	UNP P41180
A	1052	ASP	-	expression tag	UNP P41180
A	1053	GLY	-	expression tag	UNP P41180
A	1054	VAL	-	expression tag	UNP P41180
A	1055	THR	-	expression tag	UNP P41180
A	1056	PRO	-	expression tag	UNP P41180
A	1057	ASN	-	expression tag	UNP P41180
A	1058	MET	-	expression tag	UNP P41180
A	1059	LEU	-	expression tag	UNP P41180
A	1060	ASN	-	expression tag	UNP P41180
A	1061	TYR	-	expression tag	UNP P41180
A	1062	PHE	-	expression tag	UNP P41180
A	1063	GLY	-	expression tag	UNP P41180
A	1064	ARG	-	expression tag	UNP P41180
A	1065	PRO	-	expression tag	UNP P41180
A	1066	TYR	-	expression tag	UNP P41180
A	1067	GLU	-	expression tag	UNP P41180
A	1068	GLY	-	expression tag	UNP P41180
A	1069	ILE	-	expression tag	UNP P41180
A	1070	ALA	-	expression tag	UNP P41180
A	1071	VAL	-	expression tag	UNP P41180
A	1072	PHE	-	expression tag	UNP P41180
A	1073	ASP	-	expression tag	UNP P41180
A	1074	GLY	-	expression tag	UNP P41180
A	1075	LYS	-	expression tag	UNP P41180
A	1076	LYS	-	expression tag	UNP P41180
A	1077	ILE	-	expression tag	UNP P41180
A	1078	THR	-	expression tag	UNP P41180
A	1079	VAL	-	expression tag	UNP P41180
A	1080	THR	-	expression tag	UNP P41180

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1081	GLY	-	expression tag	UNP P41180
A	1082	THR	-	expression tag	UNP P41180
A	1083	LEU	-	expression tag	UNP P41180
A	1084	TRP	-	expression tag	UNP P41180
A	1085	ASN	-	expression tag	UNP P41180
A	1086	GLY	-	expression tag	UNP P41180
A	1087	ASN	-	expression tag	UNP P41180
A	1088	LYS	-	expression tag	UNP P41180
A	1089	ILE	-	expression tag	UNP P41180
A	1090	ILE	-	expression tag	UNP P41180
A	1091	ASP	-	expression tag	UNP P41180
A	1092	GLU	-	expression tag	UNP P41180
A	1093	ARG	-	expression tag	UNP P41180
A	1094	LEU	-	expression tag	UNP P41180
A	1095	ILE	-	expression tag	UNP P41180
A	1096	THR	-	expression tag	UNP P41180
A	1097	PRO	-	expression tag	UNP P41180
A	1098	ASP	-	expression tag	UNP P41180
A	1099	GLY	-	expression tag	UNP P41180
A	1100	SER	-	expression tag	UNP P41180
A	1101	MET	-	expression tag	UNP P41180
A	1102	LEU	-	expression tag	UNP P41180
A	1103	PHE	-	expression tag	UNP P41180
A	1104	ARG	-	expression tag	UNP P41180
A	1105	VAL	-	expression tag	UNP P41180
A	1106	THR	-	expression tag	UNP P41180
A	1107	ILE	-	expression tag	UNP P41180
A	1108	ASN	-	expression tag	UNP P41180
A	1109	SER	-	expression tag	UNP P41180

- Molecule 2 is a protein called Extracellular calcium-sensing receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	801	Total	C	N	O	S	0	0
			6306	4087	1029	1154	36		

There are 83 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	TRP	-	expression tag	UNP P41180
B	-12	SER	-	expression tag	UNP P41180
B	-11	HIS	-	expression tag	UNP P41180

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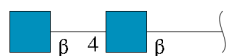
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	PRO	-	expression tag	UNP P41180
B	-9	GLN	-	expression tag	UNP P41180
B	-8	PHE	-	expression tag	UNP P41180
B	-7	GLU	-	expression tag	UNP P41180
B	-6	LYS	-	expression tag	UNP P41180
B	-5	GLY	-	expression tag	UNP P41180
B	-4	GLY	-	expression tag	UNP P41180
B	-3	GLY	-	expression tag	UNP P41180
B	-2	SER	-	expression tag	UNP P41180
B	-1	GLY	-	expression tag	UNP P41180
B	0	GLY	-	expression tag	UNP P41180
B	1	GLY	-	expression tag	UNP P41180
B	2	SER	-	expression tag	UNP P41180
B	3	GLY	-	expression tag	UNP P41180
B	4	GLY	-	expression tag	UNP P41180
B	5	SER	-	expression tag	UNP P41180
B	6	ALA	-	expression tag	UNP P41180
B	7	TRP	-	expression tag	UNP P41180
B	8	SER	-	expression tag	UNP P41180
B	9	HIS	-	expression tag	UNP P41180
B	10	PRO	-	expression tag	UNP P41180
B	11	GLN	-	expression tag	UNP P41180
B	12	PHE	-	expression tag	UNP P41180
B	13	GLU	-	expression tag	UNP P41180
B	14	LYS	-	expression tag	UNP P41180
B	15	GLY	-	expression tag	UNP P41180
B	16	SER	-	expression tag	UNP P41180
B	17	ALA	-	expression tag	UNP P41180
B	18	ALA	-	expression tag	UNP P41180
B	895	THR	-	expression tag	UNP P41180
B	896	GLY	-	expression tag	UNP P41180
B	897	SER	-	expression tag	UNP P41180
B	898	SER	-	expression tag	UNP P41180
B	899	THR	-	expression tag	UNP P41180
B	900	ASN	-	expression tag	UNP P41180
B	901	ASN	-	expression tag	UNP P41180
B	902	ASN	-	expression tag	UNP P41180
B	903	GLU	-	expression tag	UNP P41180
B	904	GLU	-	expression tag	UNP P41180
B	905	GLU	-	expression tag	UNP P41180
B	906	LYS	-	expression tag	UNP P41180
B	907	SER	-	expression tag	UNP P41180

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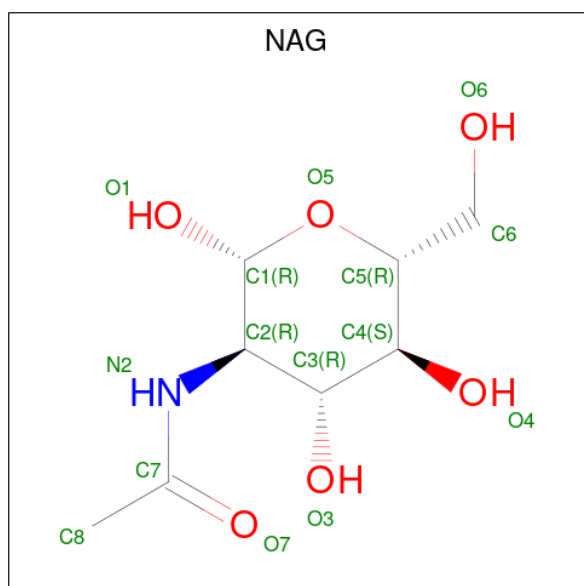
Chain	Residue	Modelled	Actual	Comment	Reference
B	908	ARG	-	expression tag	UNP P41180
B	909	LEU	-	expression tag	UNP P41180
B	910	LEU	-	expression tag	UNP P41180
B	911	GLU	-	expression tag	UNP P41180
B	912	LYS	-	expression tag	UNP P41180
B	913	GLU	-	expression tag	UNP P41180
B	914	ASN	-	expression tag	UNP P41180
B	915	ARG	-	expression tag	UNP P41180
B	916	GLU	-	expression tag	UNP P41180
B	917	LEU	-	expression tag	UNP P41180
B	918	GLU	-	expression tag	UNP P41180
B	919	LYS	-	expression tag	UNP P41180
B	920	ILE	-	expression tag	UNP P41180
B	921	ILE	-	expression tag	UNP P41180
B	922	ALA	-	expression tag	UNP P41180
B	923	GLU	-	expression tag	UNP P41180
B	924	LYS	-	expression tag	UNP P41180
B	925	GLU	-	expression tag	UNP P41180
B	926	GLU	-	expression tag	UNP P41180
B	927	ARG	-	expression tag	UNP P41180
B	928	VAL	-	expression tag	UNP P41180
B	929	SER	-	expression tag	UNP P41180
B	930	GLU	-	expression tag	UNP P41180
B	931	LEU	-	expression tag	UNP P41180
B	932	ARG	-	expression tag	UNP P41180
B	933	HIS	-	expression tag	UNP P41180
B	934	GLN	-	expression tag	UNP P41180
B	935	LEU	-	expression tag	UNP P41180
B	936	GLN	-	expression tag	UNP P41180
B	937	SER	-	expression tag	UNP P41180
B	938	ARG	-	expression tag	UNP P41180
B	939	GLN	-	expression tag	UNP P41180
B	940	GLN	-	expression tag	UNP P41180
B	941	LEU	-	expression tag	UNP P41180
B	942	LYS	-	expression tag	UNP P41180
B	943	LYS	-	expression tag	UNP P41180
B	944	THR	-	expression tag	UNP P41180
B	945	ASN	-	expression tag	UNP P41180

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		

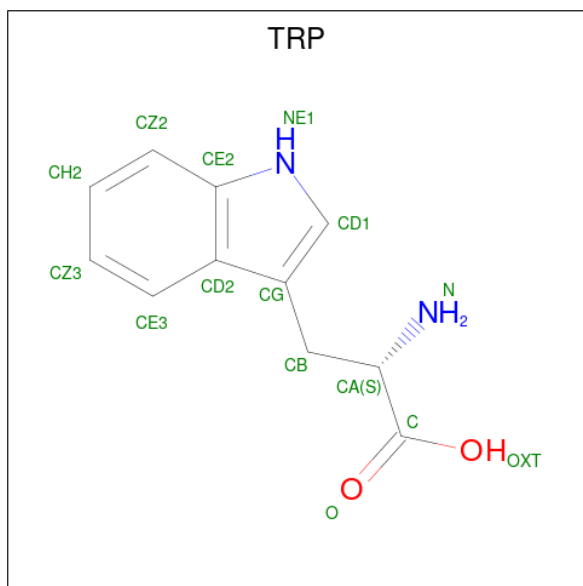
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			15	11	2	2	
5	B	1	Total	C	N	O	0
			15	11	2	2	

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

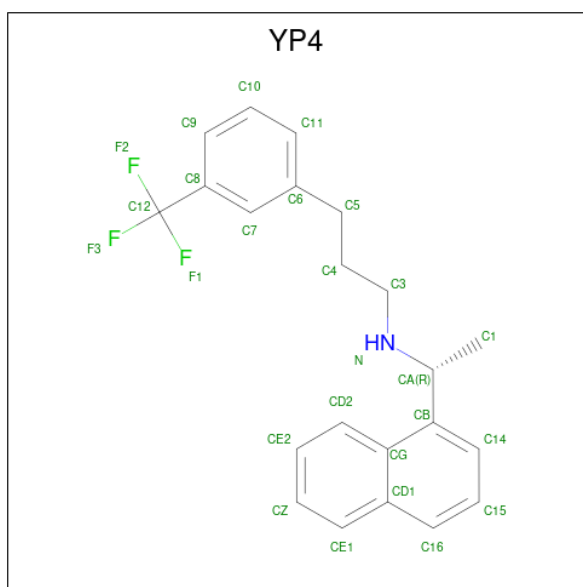
Mol	Chain	Residues	Atoms		AltConf
6	A	3	Total	Ca	0
			3	3	
6	B	1	Total	Ca	0
			1	1	

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	O	P	0
			5	4	1	
7	B	1	Total	O	P	0
			5	4	1	

- Molecule 8 is N-[(1R)-1-(naphthalen-1-yl)ethyl]-3-[3-(trifluoromethyl)phenyl]propan-1-amine (three-letter code: YP4) (formula: C₂₂H₂₂F₃N) (labeled as "Ligand of Interest" by depositor).



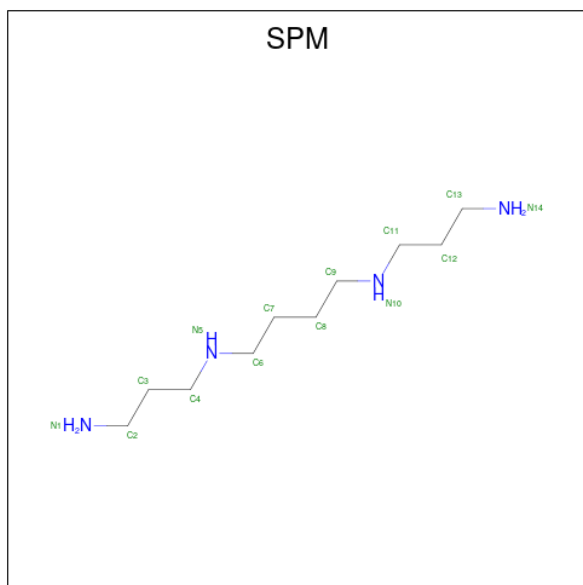
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	F	N	0
			26	22	3	1	

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Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	F	N	0
			26	22	3	1	

- Molecule 9 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).

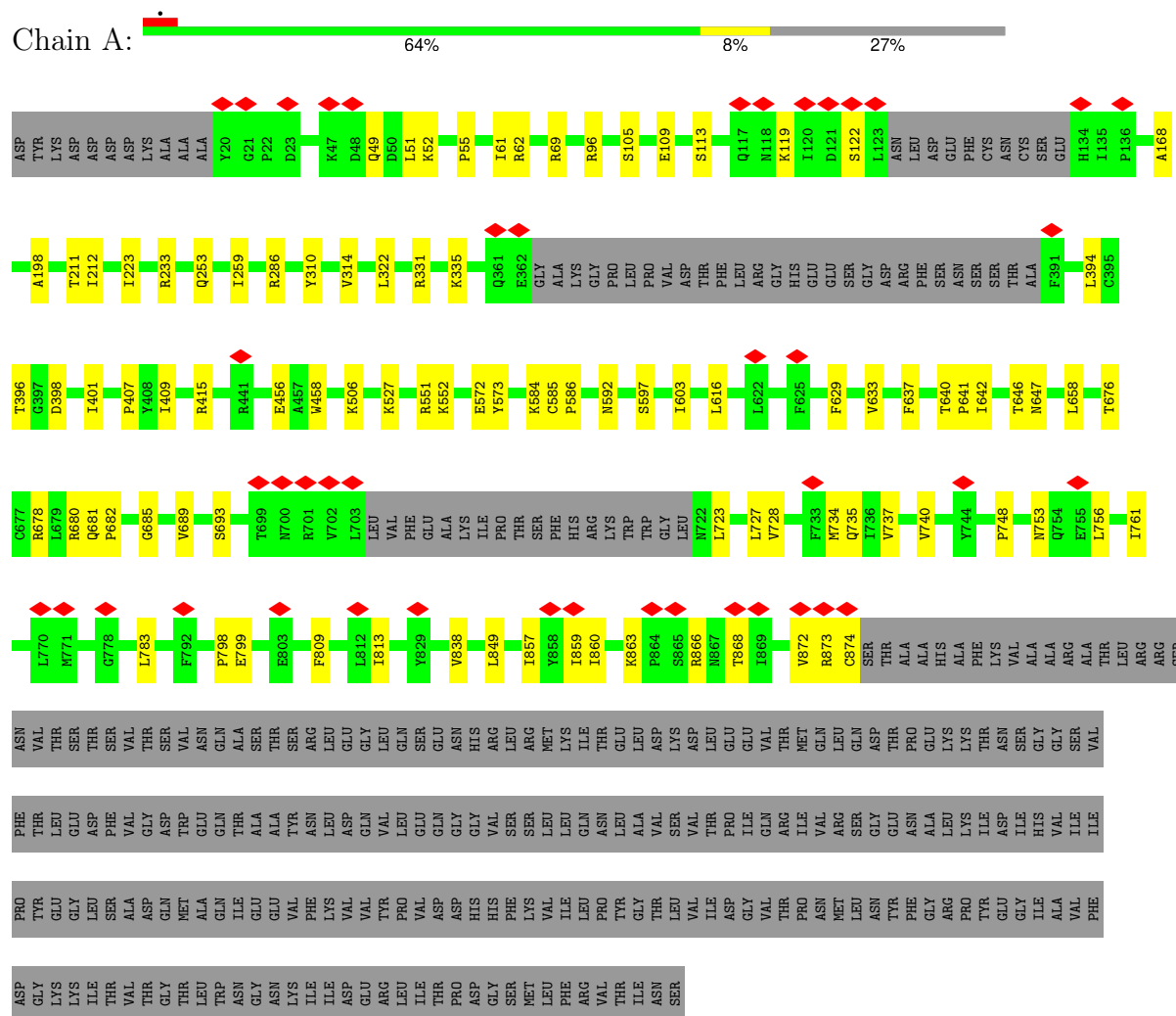


Mol	Chain	Residues	Atoms				AltConf
9	B	1	Total	C	N		0
			14	10	4		

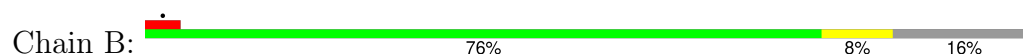
3 Residue-property plots

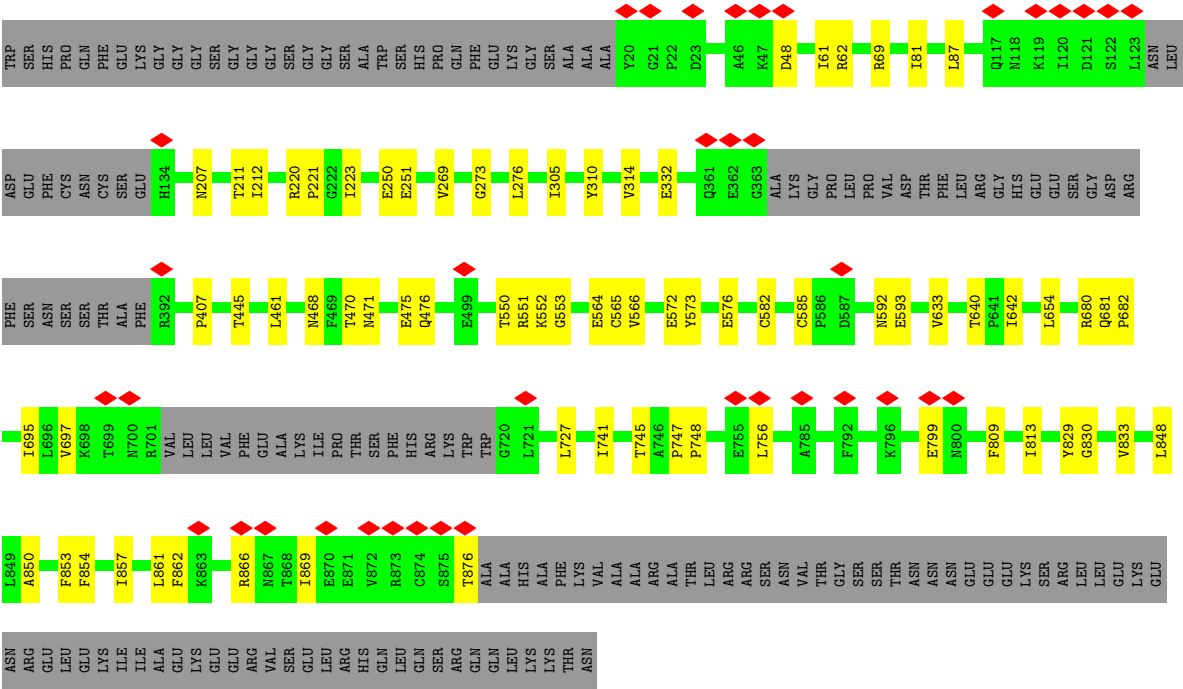
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Extracellular calcium-sensing receptor

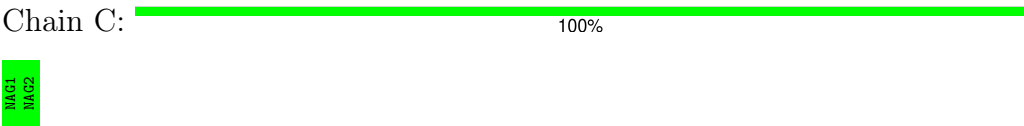


• Molecule 2: Extracellular calcium-sensing receptor

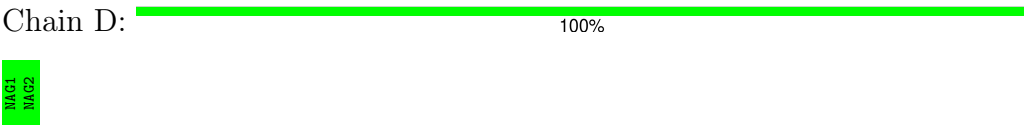




• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	234170	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.896	Depositor
Minimum map value	-0.800	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	416.496, 416.496, 416.496	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8677, 0.8677, 0.8677	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, SPM, NAG, CA, YP4

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	0.30	0/6399	0.50	0/8691
2	B	0.30	0/6464	0.51	0/8774
All	All	0.30	0/12863	0.50	0/17465

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6243	0	6079	64	0
2	B	6306	0	6137	51	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
3	E	28	0	25	1	0
4	A	28	0	26	0	0
4	B	42	0	39	0	0
5	A	15	0	9	1	0
5	B	15	0	9	0	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	5	0	0	1	0
7	B	5	0	0	1	0
8	A	26	0	0	0	0
8	B	26	0	0	0	0
9	B	14	0	26	0	0
All	All	12813	0	12400	113	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 4.

The worst 5 of 113 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:642:ILE:HD11	2:B:869:ILE:HA	1.67	0.77
2:B:866:ARG:HA	2:B:869:ILE:HG22	1.68	0.75
1:A:642:ILE:HG12	1:A:868:THR:HG22	1.70	0.73
2:B:866:ARG:HA	2:B:869:ILE:CG2	2.19	0.72
1:A:799:GLU:HA	1:A:872:VAL:HG21	1.70	0.72

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	791/1101 (72%)	766 (97%)	25 (3%)	0	100	100
2	B	793/959 (83%)	769 (97%)	24 (3%)	0	100	100
All	All	1584/2060 (77%)	1535 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	667/957 (70%)	667 (100%)	0	100	100
2	B	680/827 (82%)	680 (100%)	0	100	100
All	All	1347/1784 (76%)	1347 (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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	722	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1	1,3	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	C	2	3	14,14,15	0.21	0	17,19,21	0.47	0
3	NAG	D	1	1,3	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	D	2	3	14,14,15	0.43	0	17,19,21	0.54	0
3	NAG	E	1	2,3	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	E	2	3	14,14,15	0.24	0	17,19,21	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

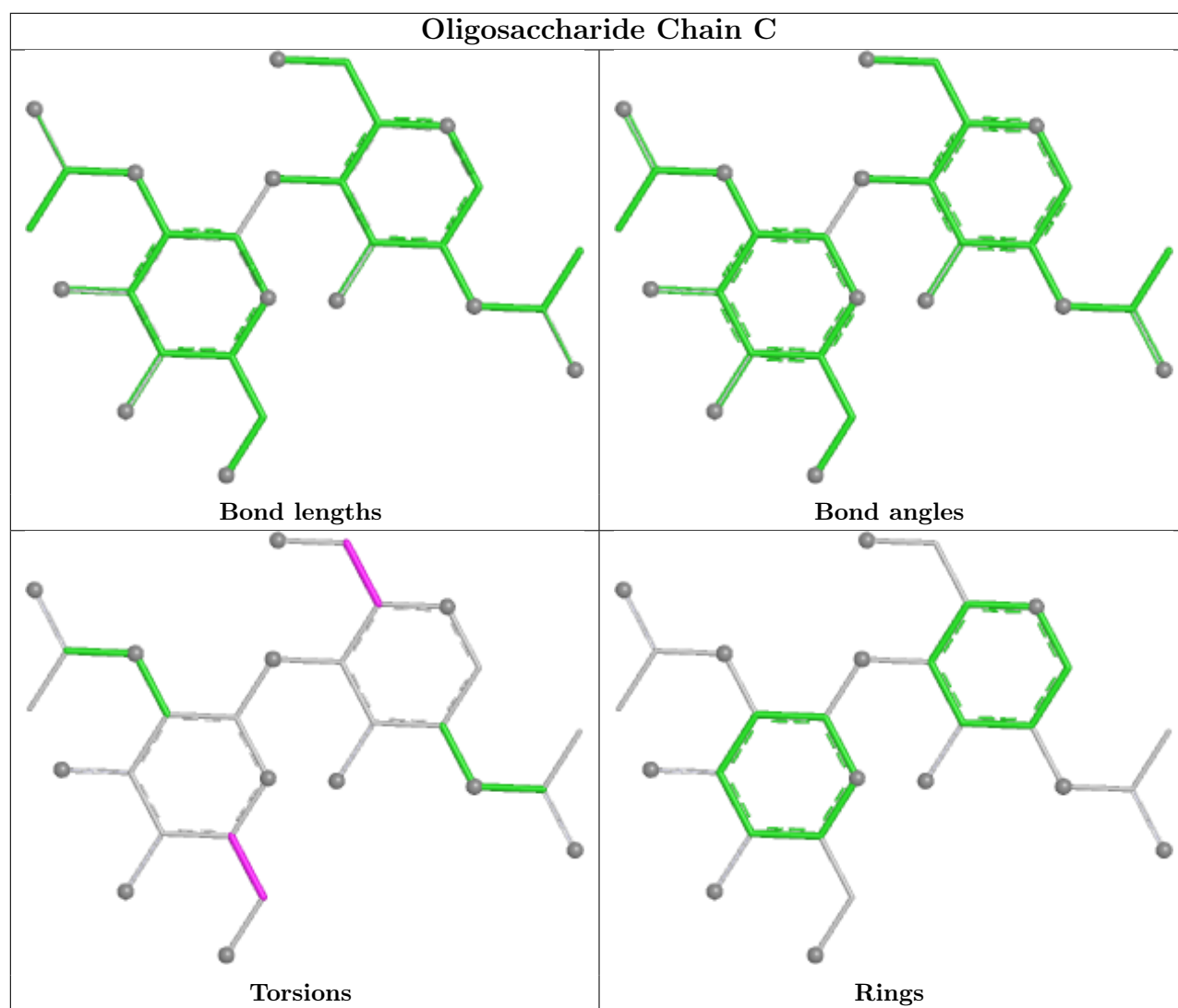
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6

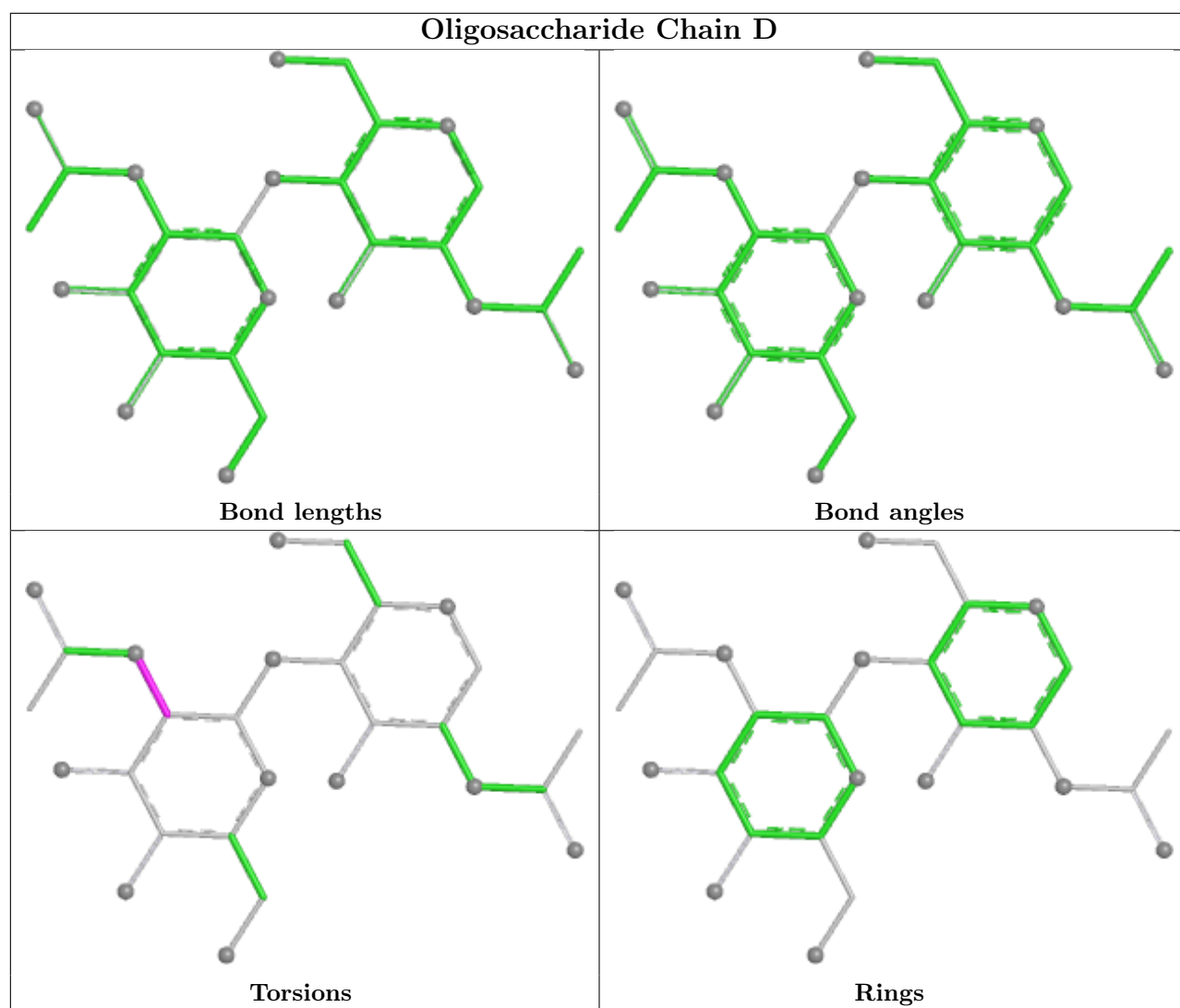
There are no ring outliers.

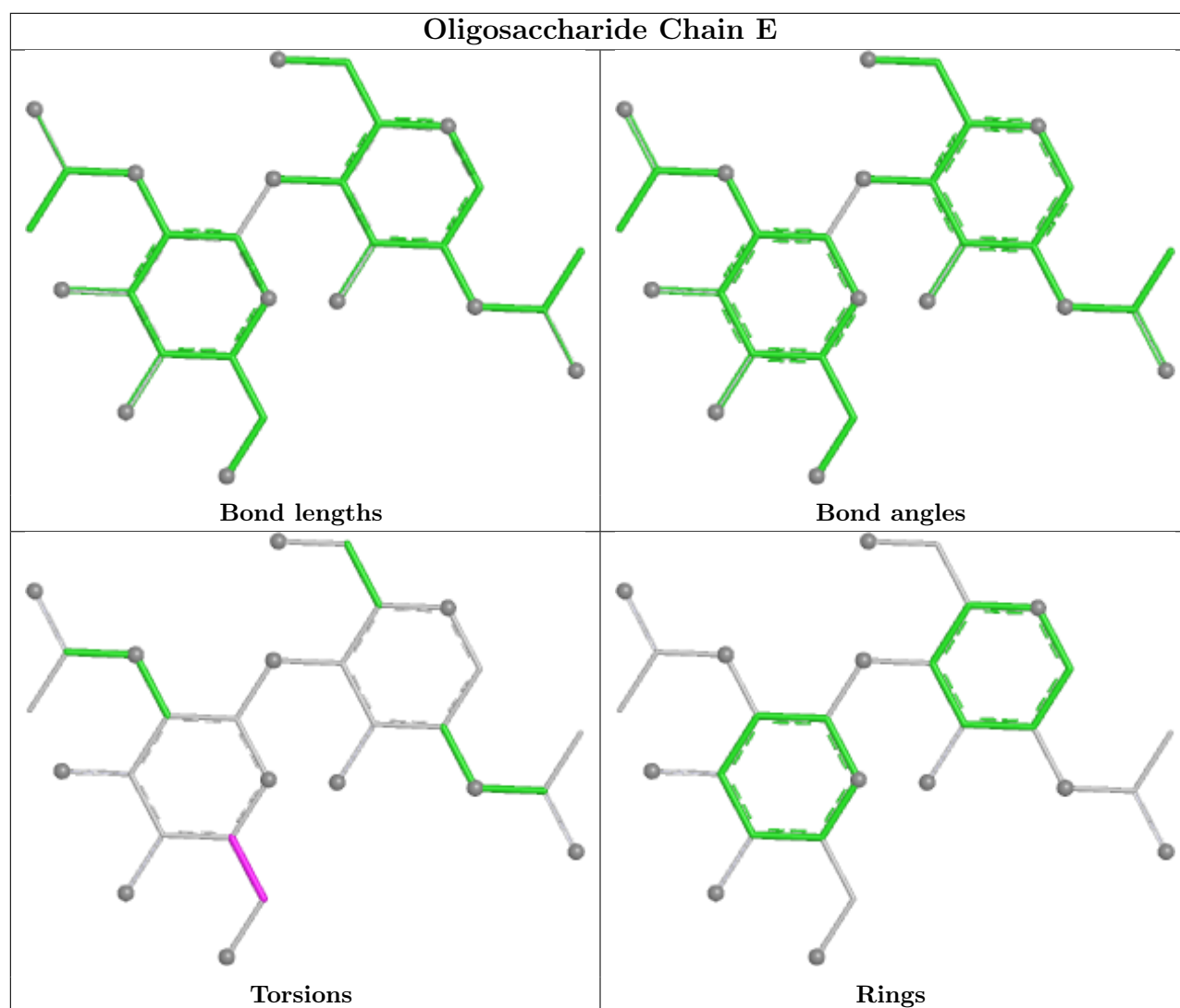
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	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 oligosaccharide.







5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
5	TRP	A	1203	-	14,16,16	0.89	1 (7%)	13,22,22	1.13	1 (7%)
4	NAG	A	1202	1	14,14,15	0.27	0	17,19,21	0.49	0
8	YP4	A	1208	-	28,28,28	1.02	1 (3%)	39,39,39	1.11	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	TRP	B	1003	-	14,16,16	0.89	1 (7%)	13,22,22	1.17	1 (7%)
7	PO4	B	1005	-	4,4,4	1.06	0	6,6,6	0.42	0
4	NAG	B	1007	2	14,14,15	1.14	1 (7%)	17,19,21	1.13	2 (11%)
4	NAG	B	1002	2	14,14,15	0.27	0	17,19,21	0.51	0
7	PO4	A	1207	-	4,4,4	1.06	0	6,6,6	0.46	0
9	SPM	B	1008	-	13,13,13	0.47	0	12,12,12	0.57	0
4	NAG	B	1001	2	14,14,15	0.29	0	17,19,21	0.54	0
4	NAG	A	1201	1	14,14,15	0.29	0	17,19,21	0.63	1 (5%)
8	YP4	B	1006	-	28,28,28	1.01	1 (3%)	39,39,39	1.08	2 (5%)

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
5	TRP	A	1203	-	-	3/7/8/8	0/2/2/2
4	NAG	A	1202	1	-	0/6/23/26	0/1/1/1
8	YP4	A	1208	-	-	6/17/17/17	0/3/3/3
5	TRP	B	1003	-	-	1/7/8/8	0/2/2/2
4	NAG	B	1007	2	-	1/6/23/26	0/1/1/1
4	NAG	B	1002	2	-	2/6/23/26	0/1/1/1
9	SPM	B	1008	-	-	2/11/11/11	-
4	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1201	1	-	0/6/23/26	0/1/1/1
8	YP4	B	1006	-	-	6/17/17/17	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1007	NAG	C1-C2	4.05	1.57	1.52
8	A	1208	YP4	CG-CD1	-3.81	1.35	1.43
8	B	1006	YP4	CG-CD1	-3.68	1.36	1.43
5	B	1003	TRP	OXT-C	-2.31	1.23	1.30
5	A	1203	TRP	OXT-C	-2.28	1.23	1.30

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1006	YP4	CB-CA-N	-3.42	105.71	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1208	YP4	C3-N-CA	-3.04	108.69	113.42
8	A	1208	YP4	CD2-CG-CB	-2.99	119.74	123.37
5	B	1003	TRP	OXT-C-O	-2.70	117.95	124.08
5	A	1203	TRP	OXT-C-O	-2.64	118.08	124.08

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

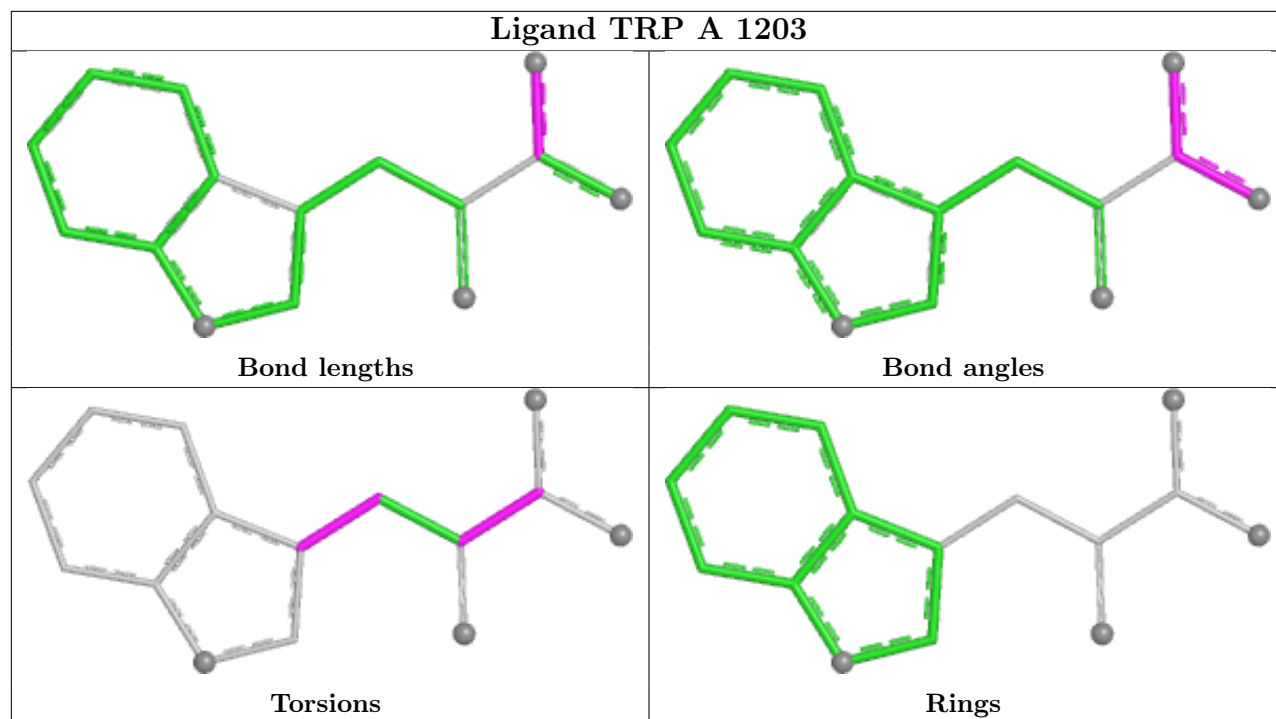
Mol	Chain	Res	Type	Atoms
5	A	1203	TRP	CA-CB-CG-CD1
8	B	1006	YP4	C1-CA-N-C3
8	B	1006	YP4	CB-CA-N-C3
4	B	1002	NAG	C4-C5-C6-O6
4	B	1001	NAG	O5-C5-C6-O6

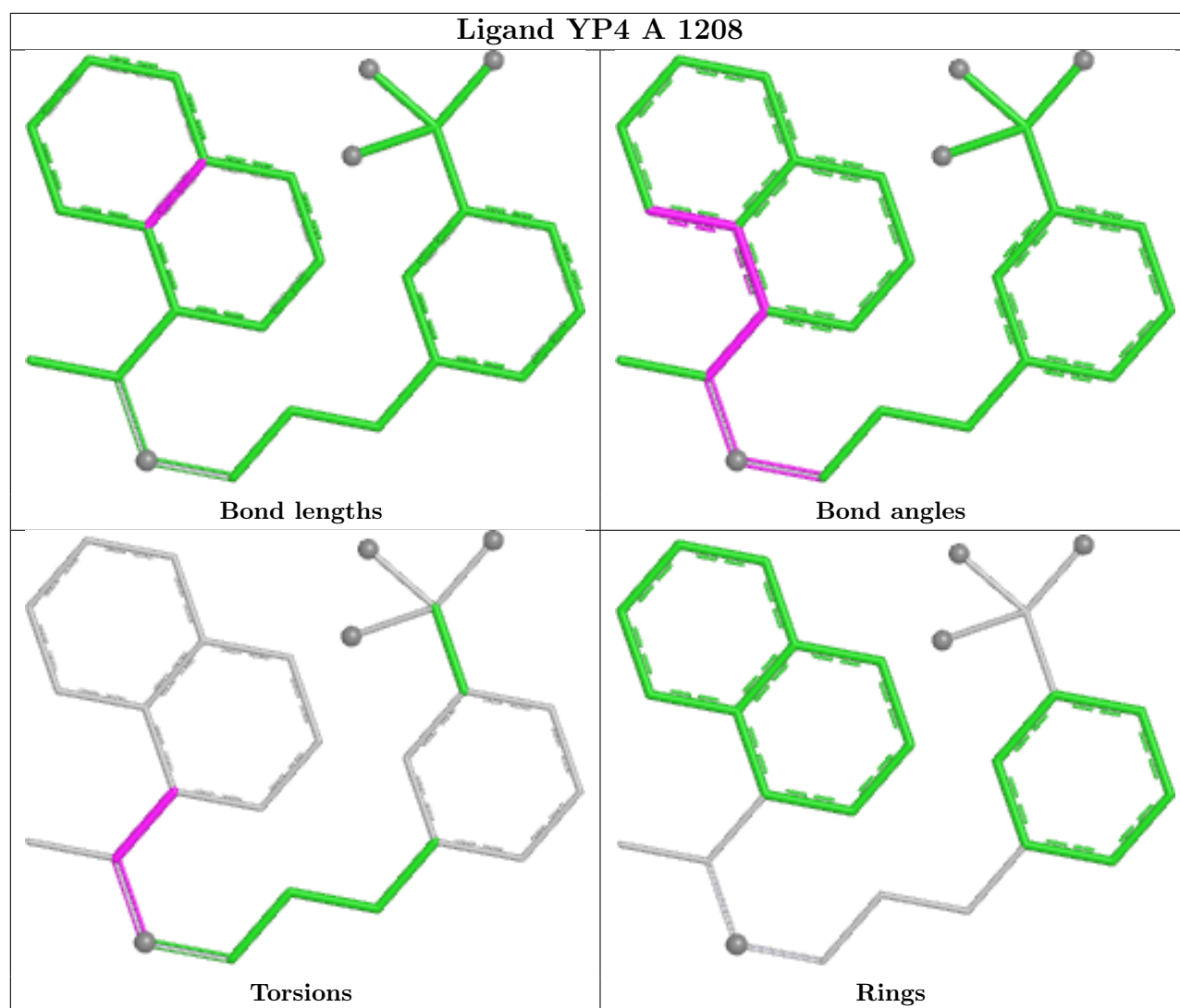
There are no ring outliers.

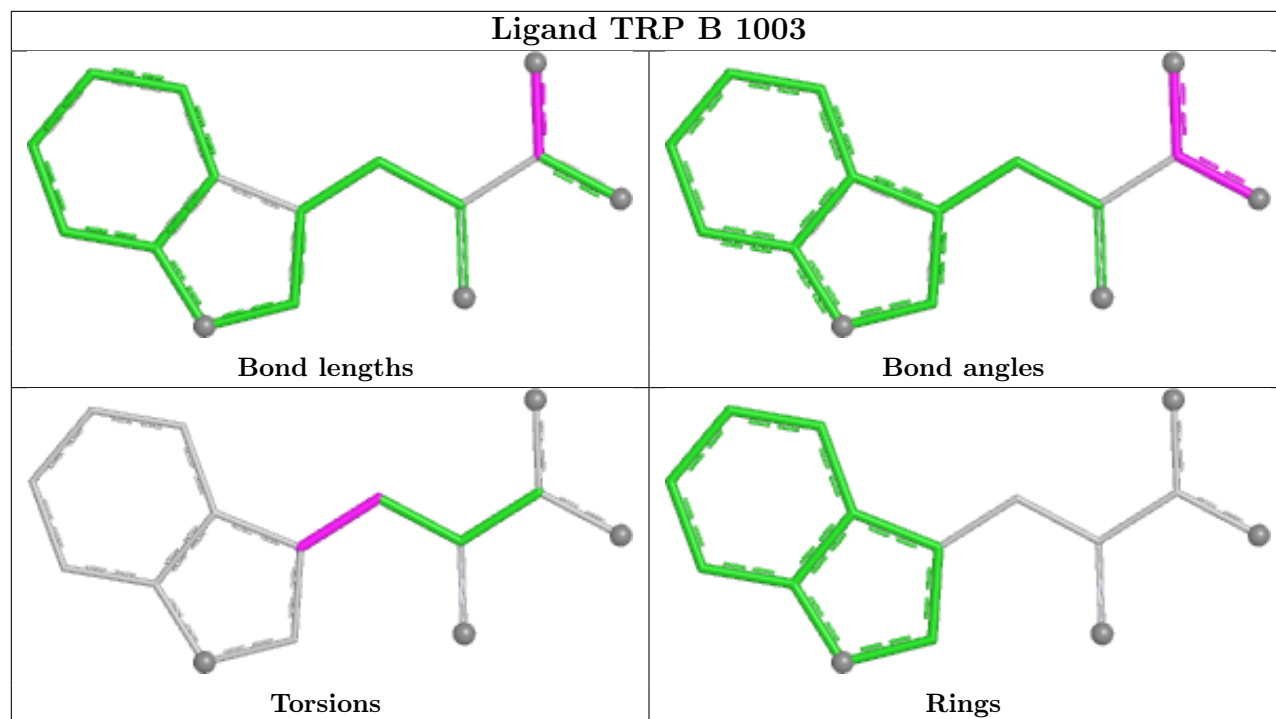
3 monomers are involved in 3 short contacts:

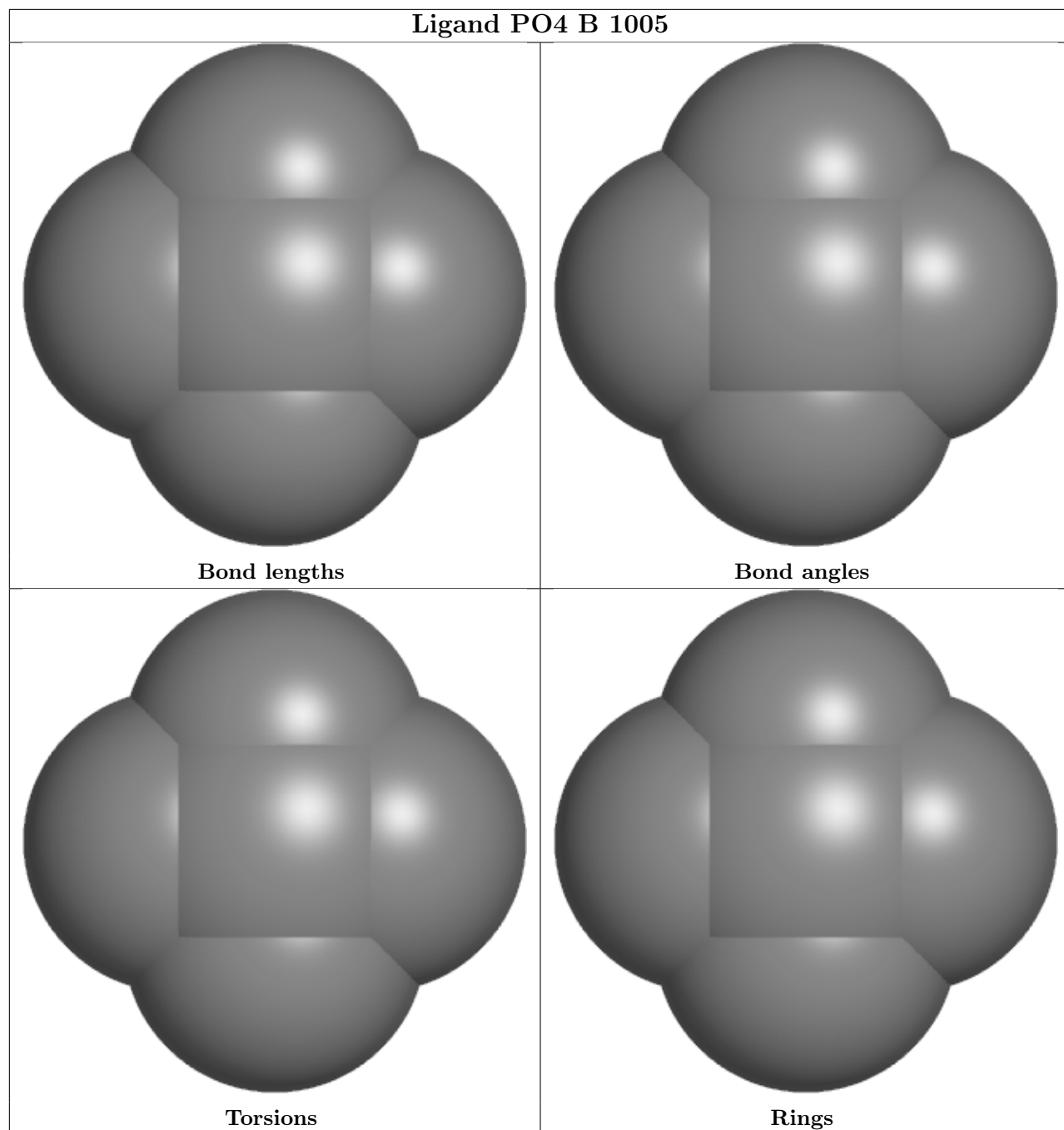
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1203	TRP	1	0
7	B	1005	PO4	1	0
7	A	1207	PO4	1	0

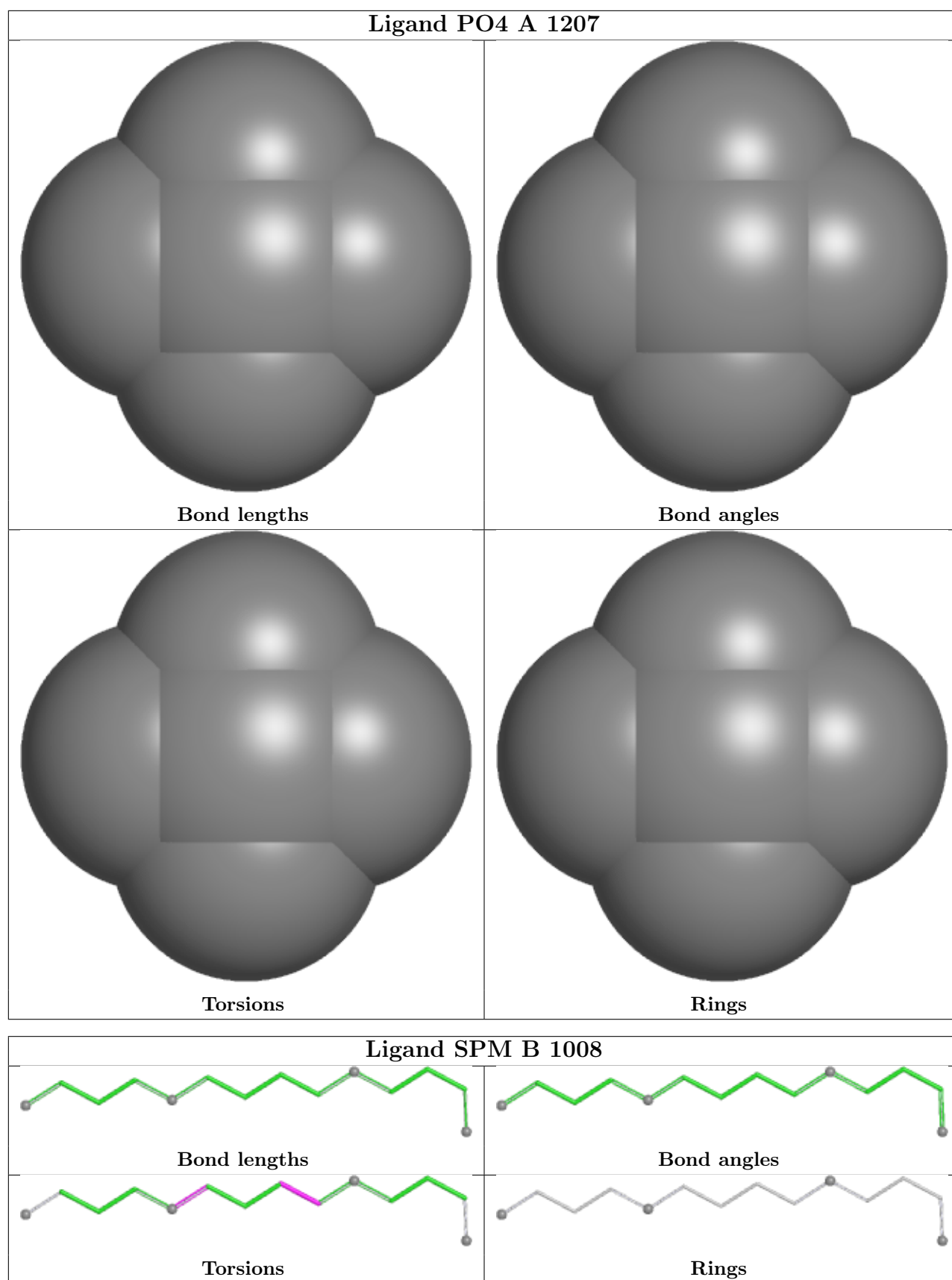
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

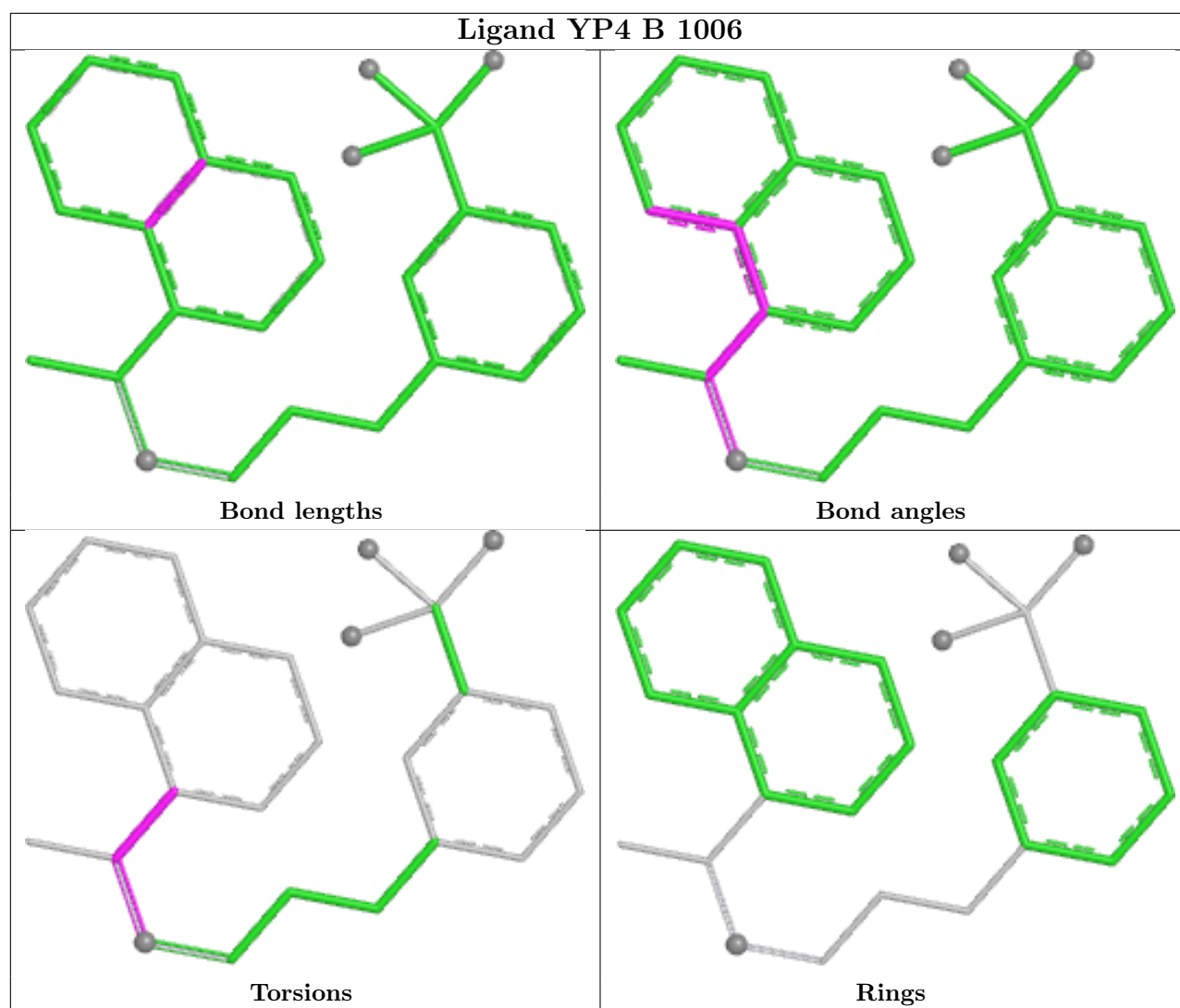












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

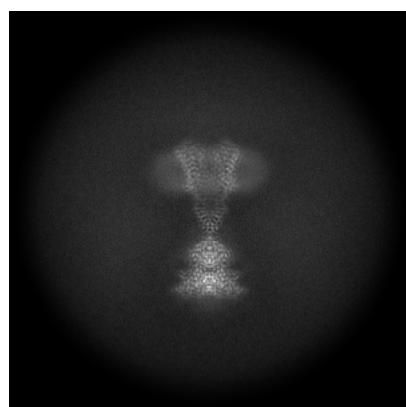
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40914. These allow visual inspection of the internal detail of the map and identification of artifacts.

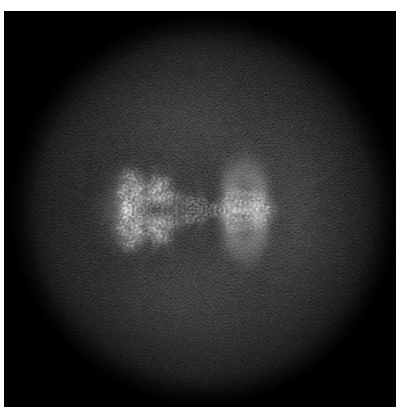
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

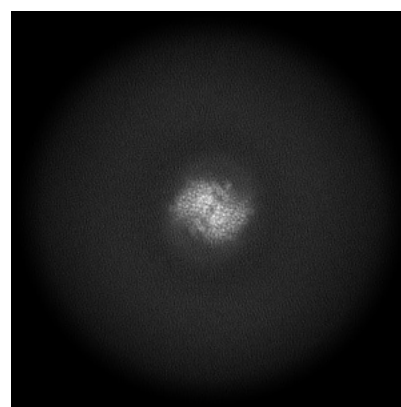
6.1.1 Primary map



X



Y

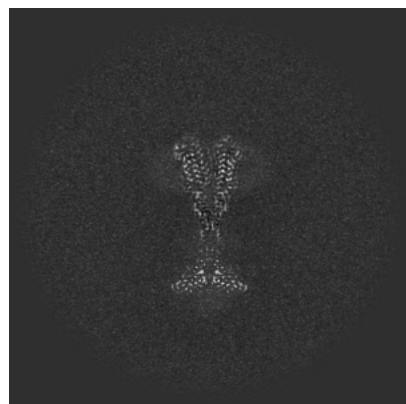


Z

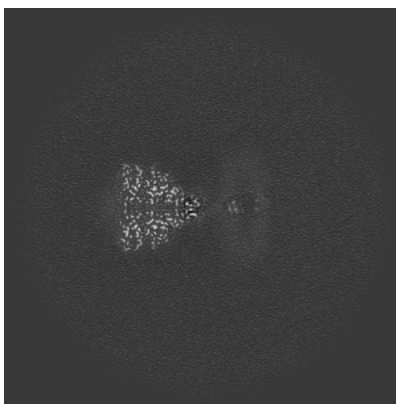
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

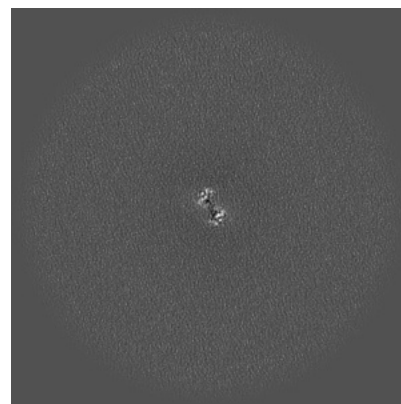
6.2.1 Primary map



X Index: 240



Y Index: 240

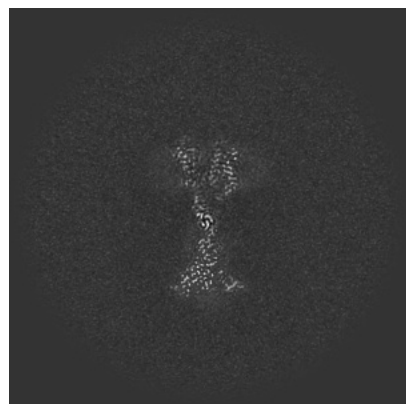


Z Index: 240

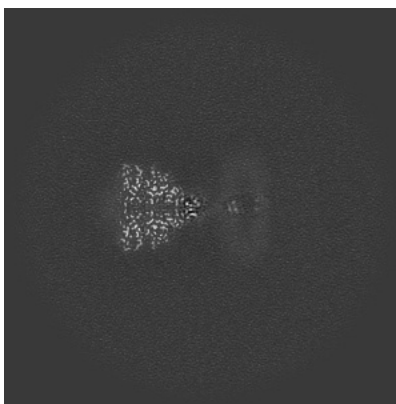
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

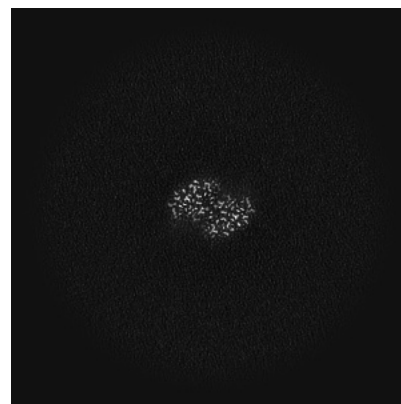
6.3.1 Primary map



X Index: 247



Y Index: 240

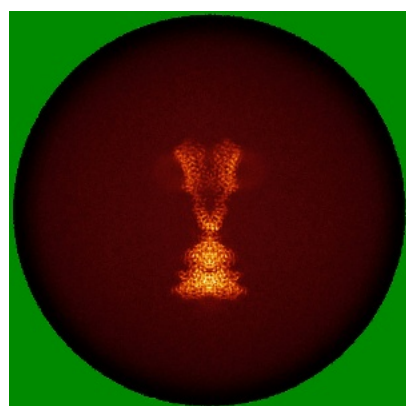


Z Index: 153

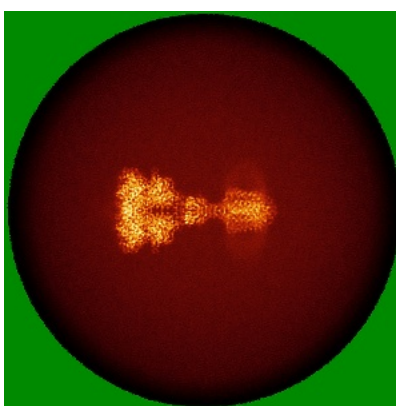
The images above show the largest variance slices of the map in three orthogonal directions.

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

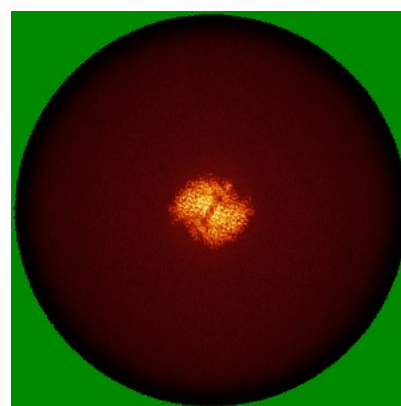
6.4.1 Primary map



X



Y

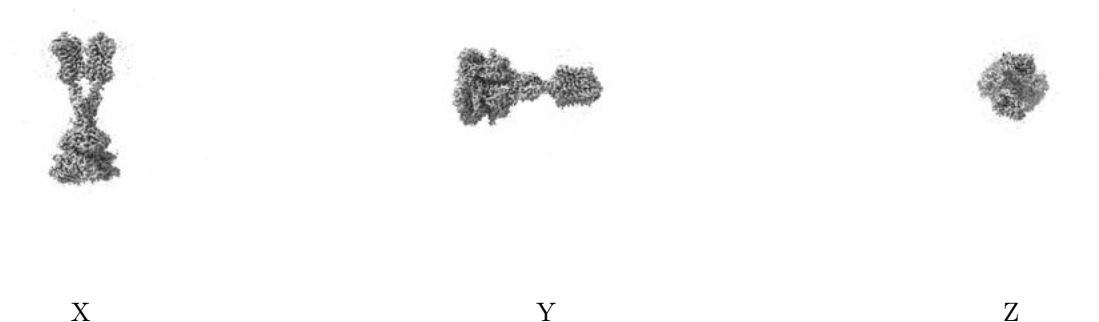


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

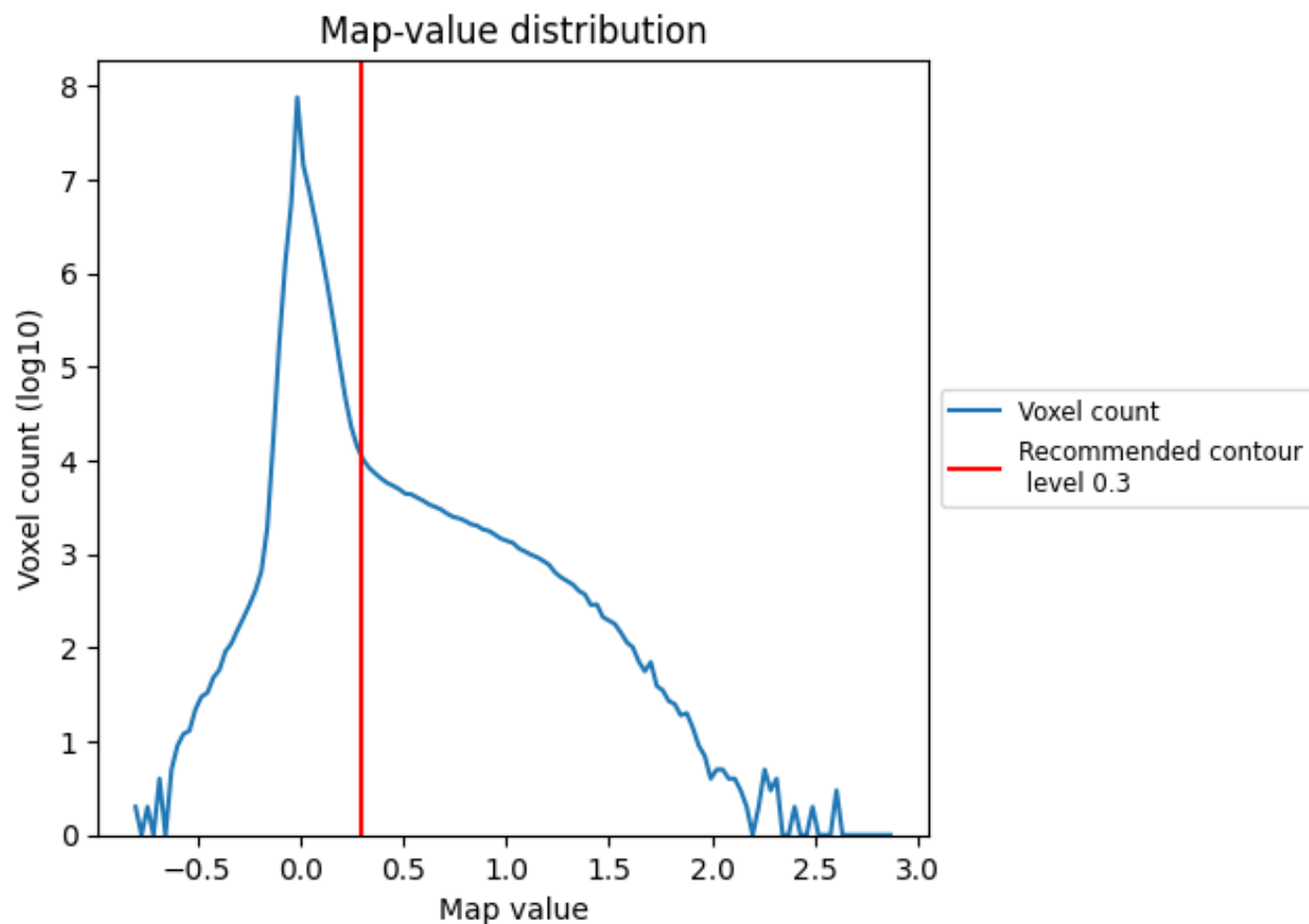
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

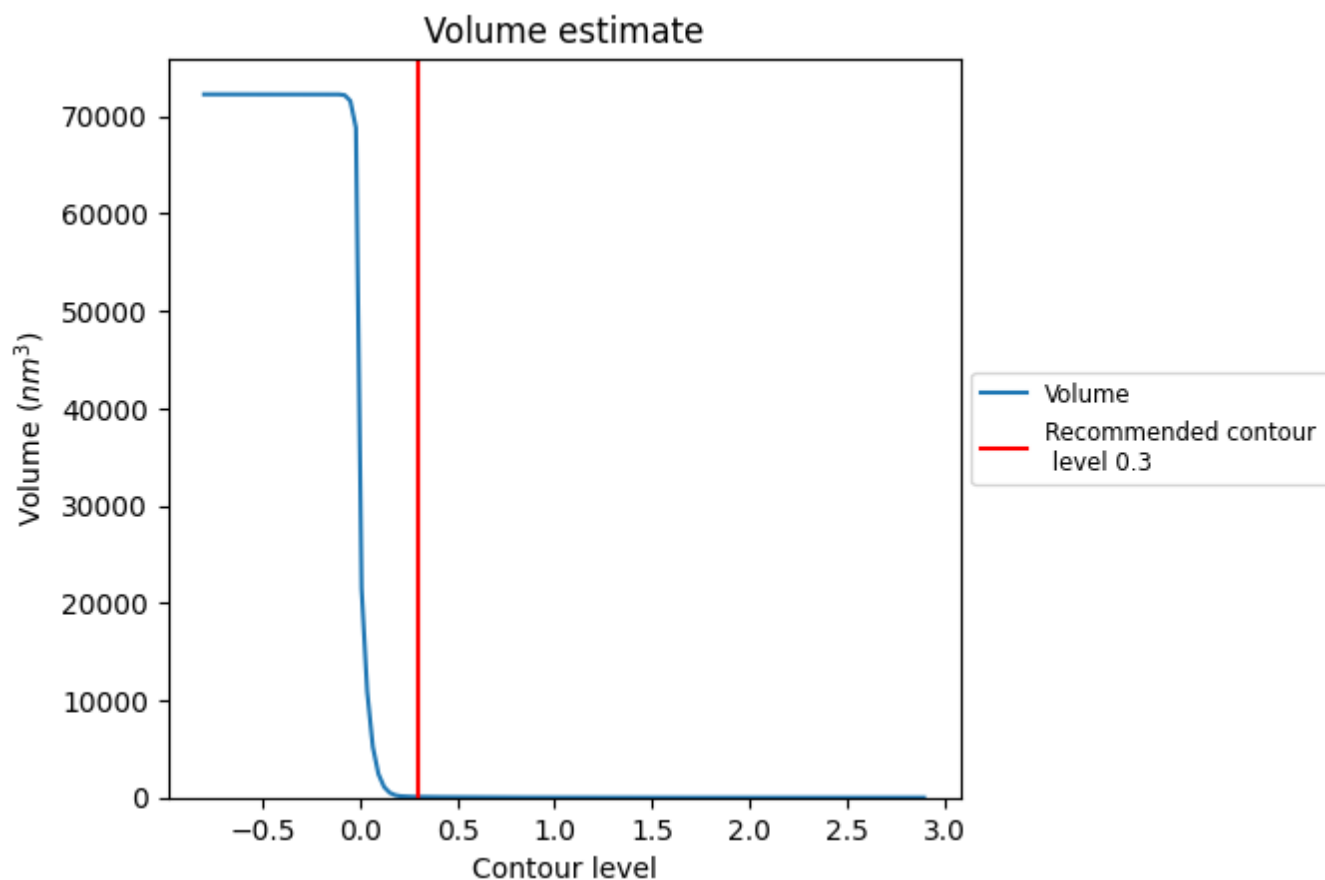
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

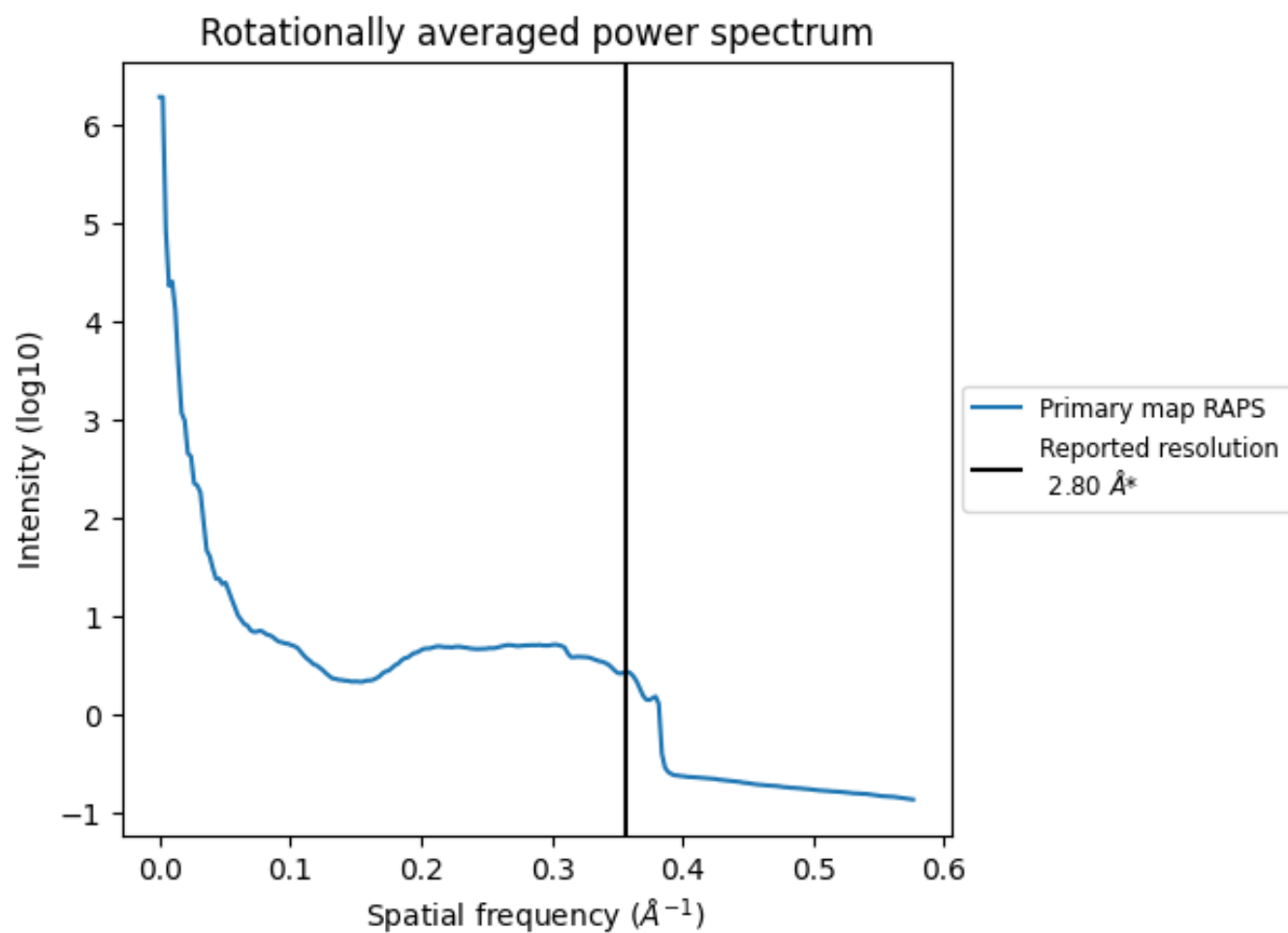
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 72 nm^3 ; this corresponds to an approximate mass of 65 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 0.357 Å⁻¹

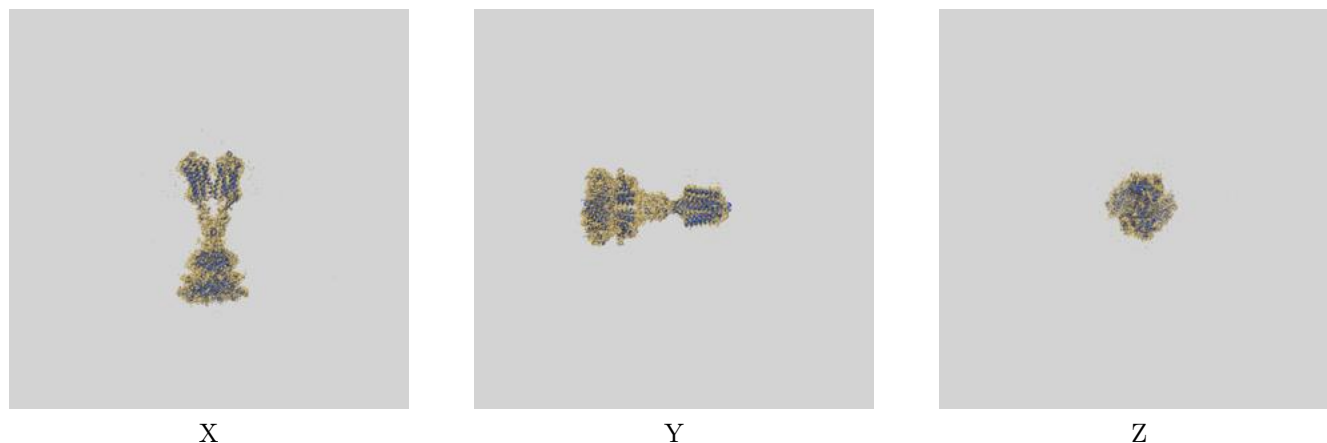
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

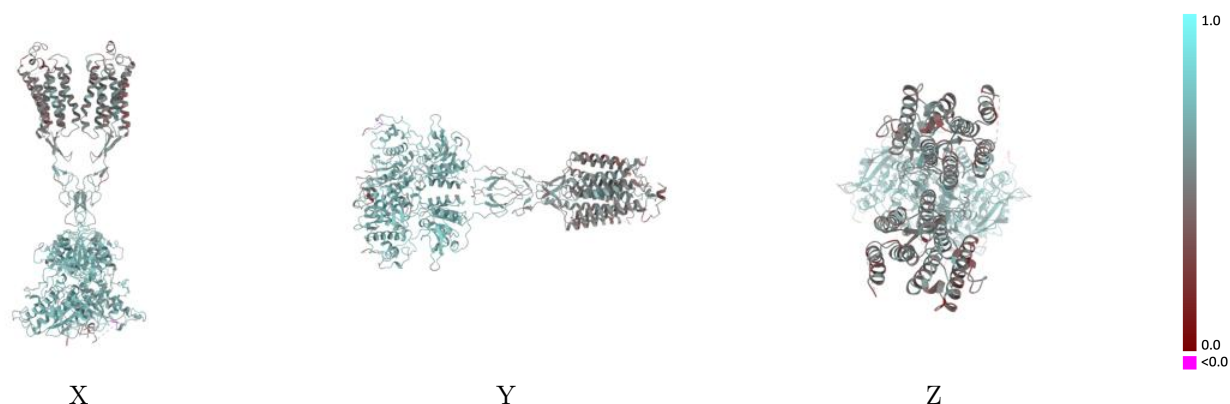
This section contains information regarding the fit between EMDB map EMD-40914 and PDB model 8SZF. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



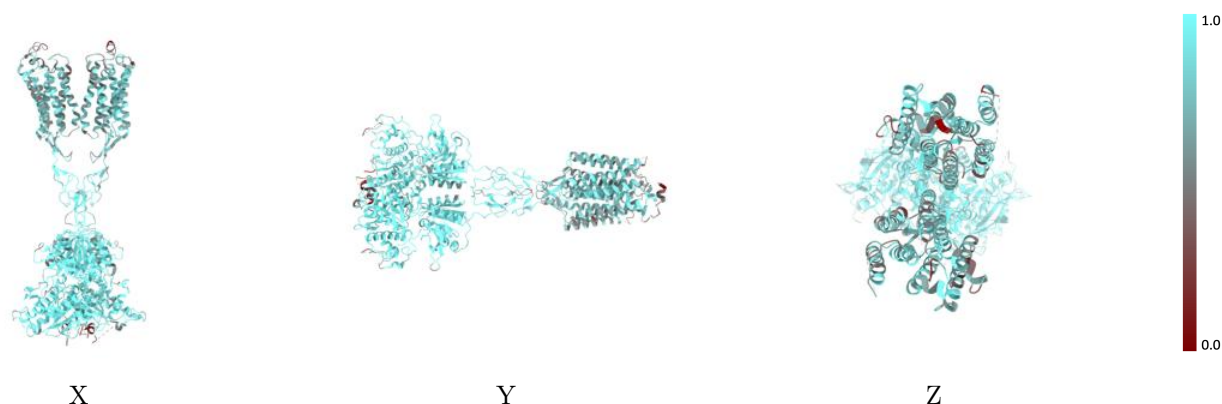
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



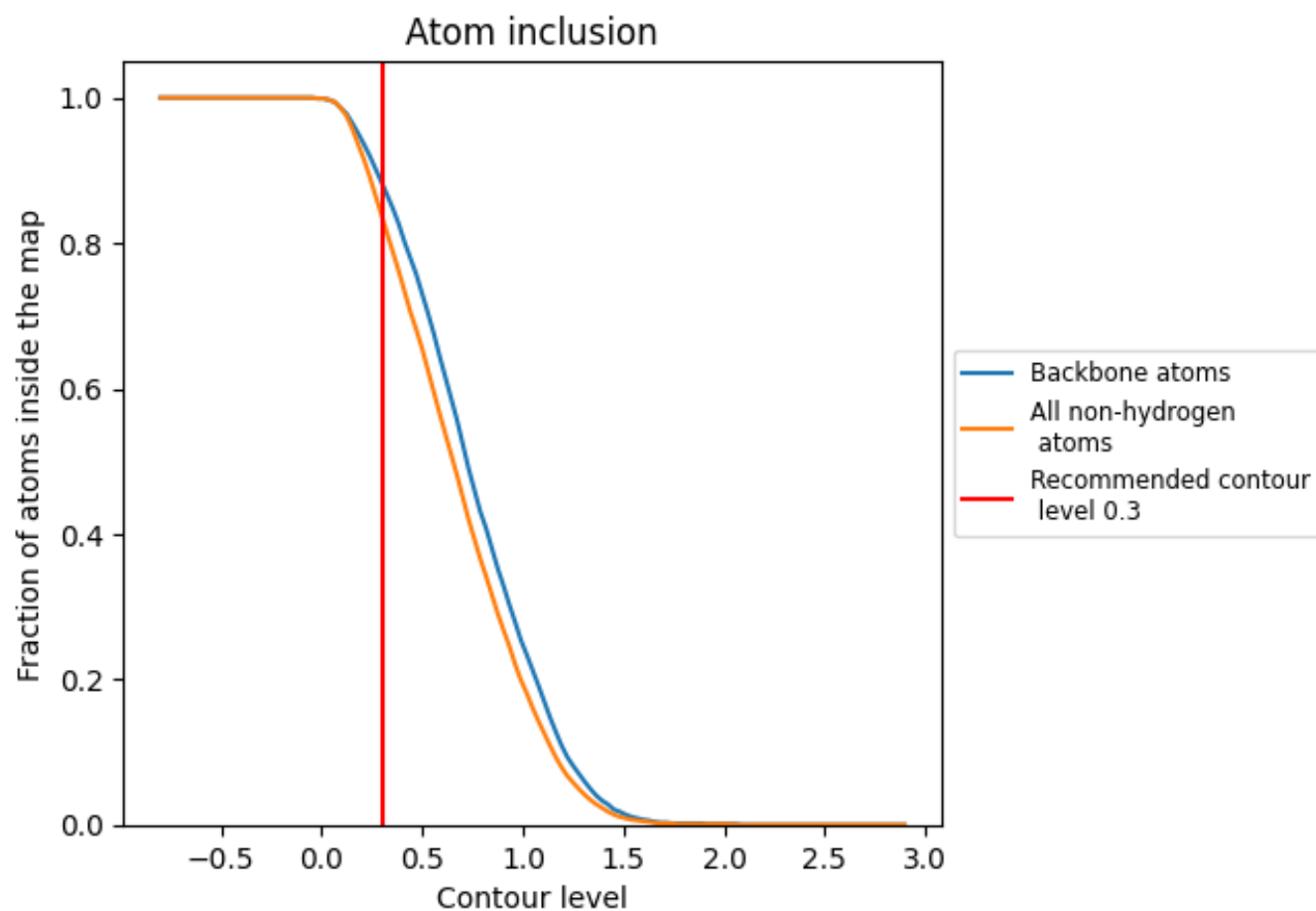
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8360	<div></div> 0.5870
A	<div></div> 0.8370	<div></div> 0.5870
B	<div></div> 0.8360	<div></div> 0.5880
C	<div></div> 0.8930	<div></div> 0.6040
D	<div></div> 0.6070	<div></div> 0.5010
E	<div></div> 0.8210	<div></div> 0.5760

