Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 03:50 PM EDT

PDB ID	:	8SZG
EMDB ID	:	EMD-40915
Title	:	Cryo-EM structure of cinacalcet-bound human calcium-sensing receptor CaSR-Gq complex in lipid nanodiscs
Authors	:	He, F.; Wu, C.; Gao, Y.; Skiniotis, G.
Deposited on	:	2023-05-29
Resolution	:	3.60 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:

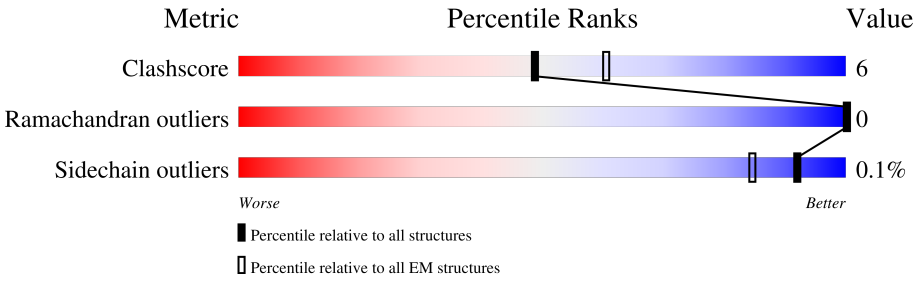
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)
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 <=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	D	369	17% 76% 15% 9%
2	E	71	25% 66% 11% 23%
3	A	1101	68% 8% 25%
4	B	959	74% 9% 17%
5	C	353	11% 52% 10% 38%
6	F	2	50% 100%
6	G	2	100%
6	H	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	PO4	B	1406	-	-	X	-
9	PCW	A	1204	X	-	-	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 17571 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 Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	335	Total	C	N	O	S	0	0
			2404	1502	431	453	18		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP P62873
D	-1	SER	-	expression tag	UNP P62873
D	0	SER	-	expression tag	UNP P62873
D	1	GLY	-	expression tag	UNP P62873
D	341	GLY	-	expression tag	UNP P62873
D	342	SER	-	expression tag	UNP P62873
D	343	SER	-	expression tag	UNP P62873
D	344	GLY	-	expression tag	UNP P62873
D	345	GLY	-	expression tag	UNP P62873
D	346	GLY	-	expression tag	UNP P62873
D	347	GLY	-	expression tag	UNP P62873
D	348	SER	-	expression tag	UNP P62873
D	349	GLY	-	expression tag	UNP P62873
D	350	GLY	-	expression tag	UNP P62873
D	351	GLY	-	expression tag	UNP P62873
D	352	GLY	-	expression tag	UNP P62873
D	353	SER	-	expression tag	UNP P62873
D	354	SER	-	expression tag	UNP P62873
D	355	GLY	-	expression tag	UNP P62873
D	356	VAL	-	expression tag	UNP P62873
D	357	SER	-	expression tag	UNP P62873
D	358	GLY	-	expression tag	UNP P62873
D	359	TRP	-	expression tag	UNP P62873
D	360	ARG	-	expression tag	UNP P62873
D	361	LEU	-	expression tag	UNP P62873
D	362	PHE	-	expression tag	UNP P62873
D	363	LYS	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
D	364	LYS	-	expression tag	UNP P62873
D	365	ILE	-	expression tag	UNP P62873
D	366	SER	-	expression tag	UNP P62873

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	55	Total	C	N	O	S	0	0
			368	231	64	70	3		

- Molecule 3 is a protein called Extracellular calcium-sensing receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	830	Total	C	N	O	S	0	0
			6520	4242	1073	1169	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 4 is a protein called Extracellular calcium-sensing receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	796	Total	C	N	O	S	0	0
			6279	4080	1026	1138	35		

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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	906	LYS	-	expression tag	UNP P41180
B	907	SER	-	expression tag	UNP P41180
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 5 is a protein called Guanine nucleotide-binding protein G(q) subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	219	Total	C	N	O	S	0	0
			1640	1057	281	294	8		

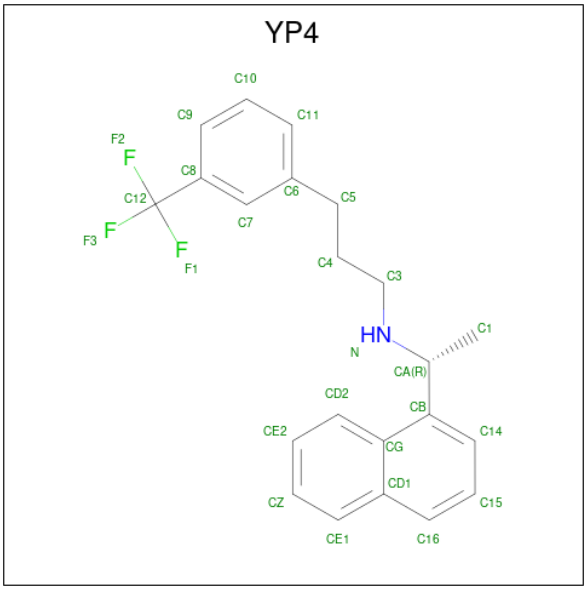
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	7	MET	-	initiating methionine	UNP P50148
C	8	GLY	-	expression tag	UNP P50148
C	9	CYS	-	expression tag	UNP P50148
C	10	THR	-	expression tag	UNP P50148
C	11	LEU	-	expression tag	UNP P50148
C	12	SER	-	expression tag	UNP P50148
C	13	ALA	-	expression tag	UNP P50148
C	14	GLU	-	expression tag	UNP P50148
C	15	ASP	-	expression tag	UNP P50148
C	16	LYS	-	expression tag	UNP P50148
C	17	ALA	-	expression tag	UNP P50148
C	18	ALA	-	expression tag	UNP P50148
C	19	VAL	-	expression tag	UNP P50148
C	20	GLU	-	expression tag	UNP P50148
C	21	ARG	-	expression tag	UNP P50148
C	22	SER	-	expression tag	UNP P50148
C	23	LYS	-	expression tag	UNP P50148
C	24	MET	-	expression tag	UNP P50148
C	25	ILE	-	expression tag	UNP P50148
C	26	ASP	-	expression tag	UNP P50148
C	27	ARG	-	expression tag	UNP P50148
C	28	ASN	-	expression tag	UNP P50148

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

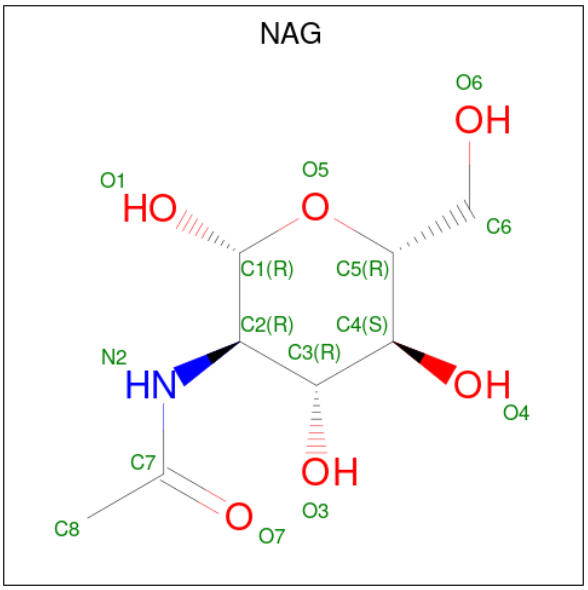
Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	2	Total	C	N	O	0	0
			28	16	2	10		
6	G	2	Total	C	N	O	0	0
			28	16	2	10		
6	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is N-[(1R)-1-(naphthalen-1-yl)ethyl]-3-[3-(trifluoromethyl)phenyl]propan-1-amine (three-letter code: YP4) (formula: $C_{22}H_{22}F_3N$) (labeled as "Ligand of Interest" by depositor).



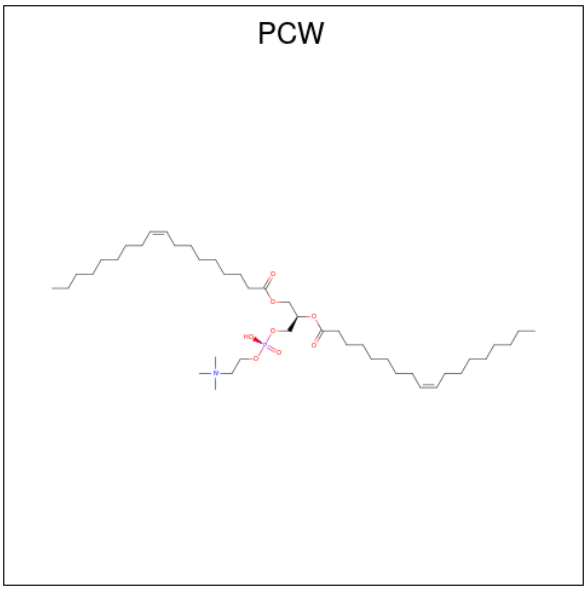
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	F	N	0
			26	22	3	1	
7	B	1	Total	C	F	N	0
			26	22	3	1	

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



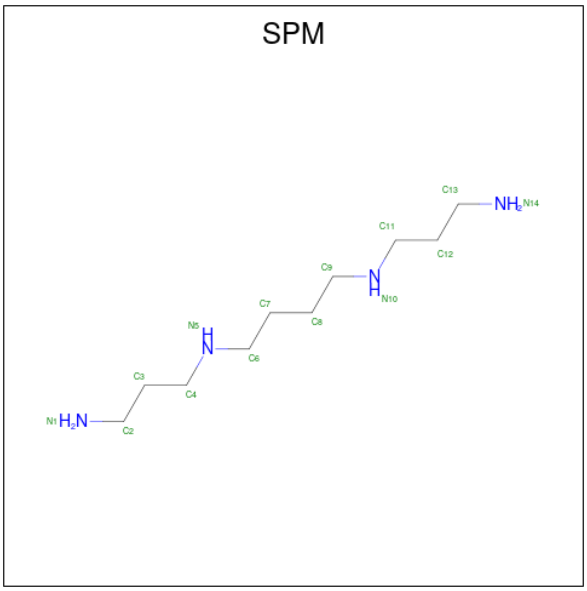
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	

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

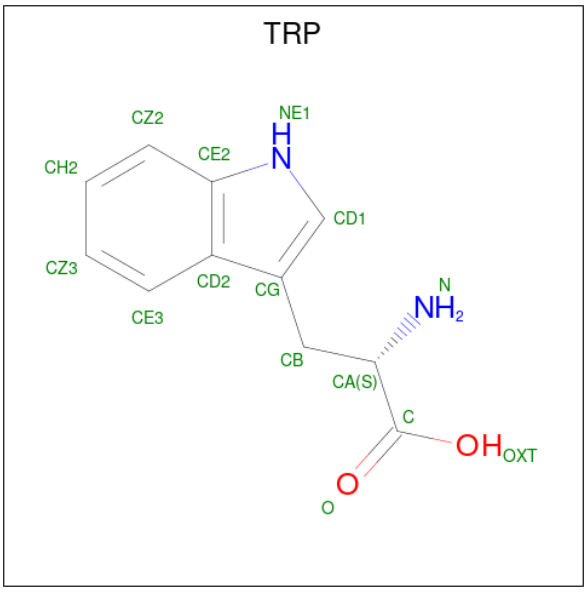


Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C N 14 10 4	0
10	A	1	Total C N 14 10 4	0
10	B	1	Total C N 14 10 4	0

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

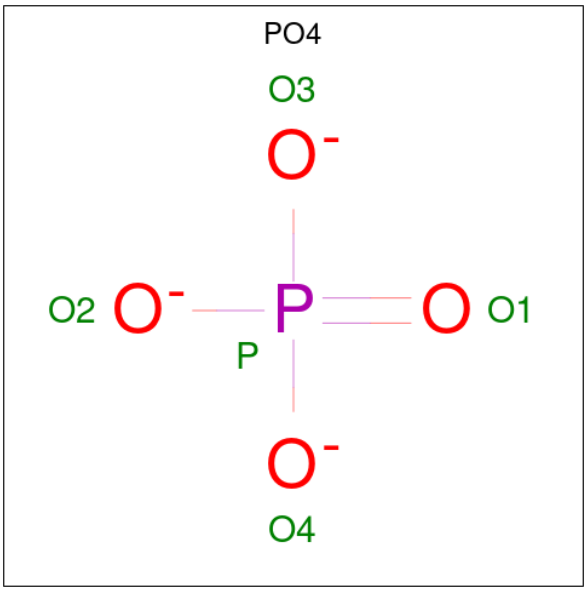
Mol	Chain	Residues	Atoms	AltConf
11	A	3	Total Ca 3 3	0

- Molecule 12 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
12	A	1	Total	C	N	O	0
			15	11	2	2	
12	B	1	Total	C	N	O	0
			15	11	2	2	

- Molecule 13 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



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

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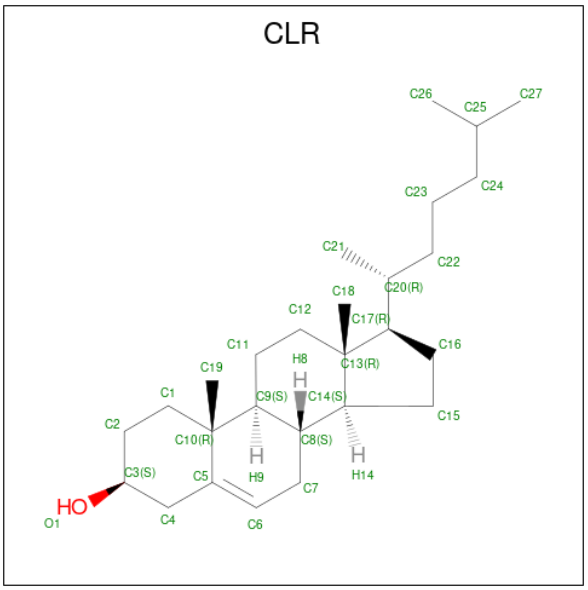
Mol	Chain	Residues	Atoms	AltConf
13	B	1	Total O P 5 4 1	0

- Molecule 14 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 15 is water.

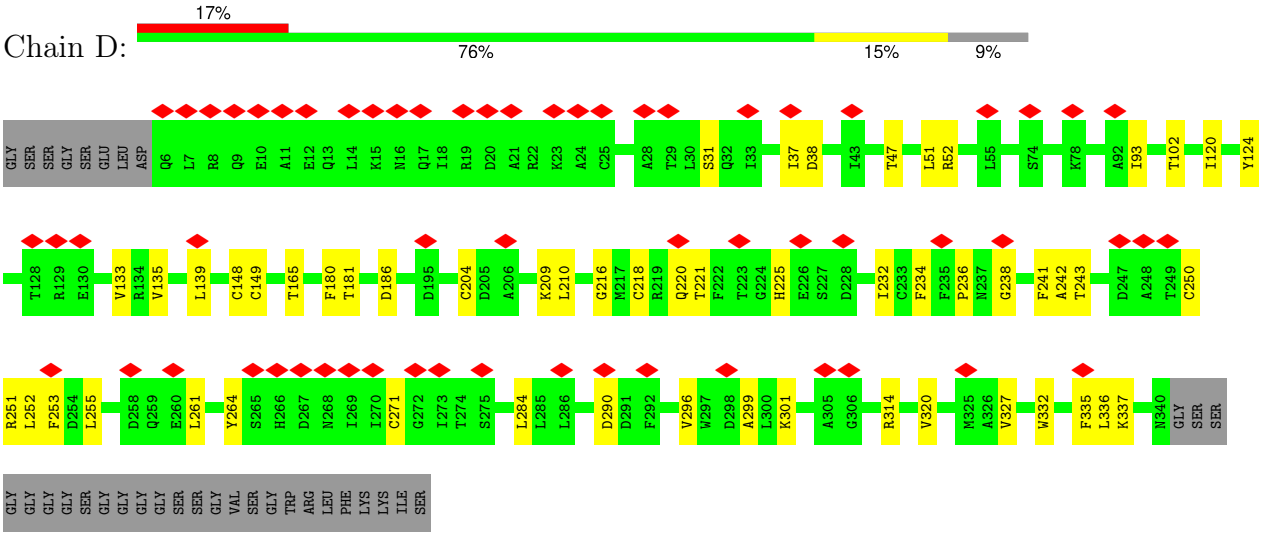
Mol	Chain	Residues	Atoms	AltConf
15	B	1	Total O 1 1	0

3 Residue-property plots (i)

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.

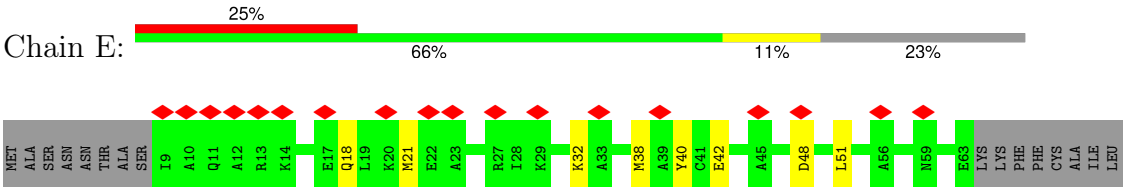
• Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain D:



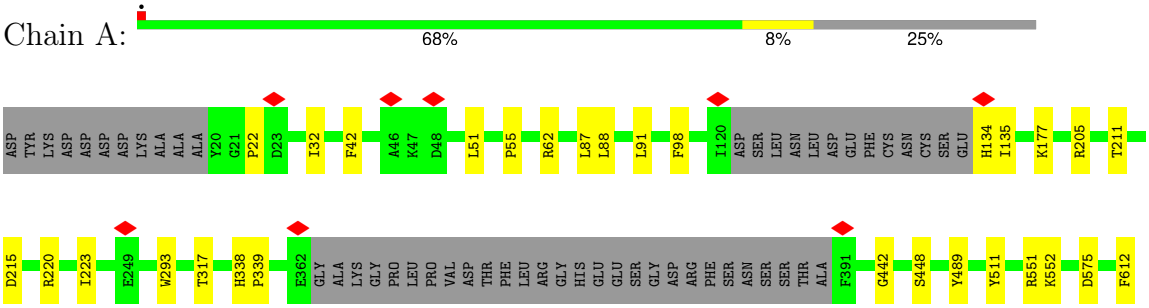
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

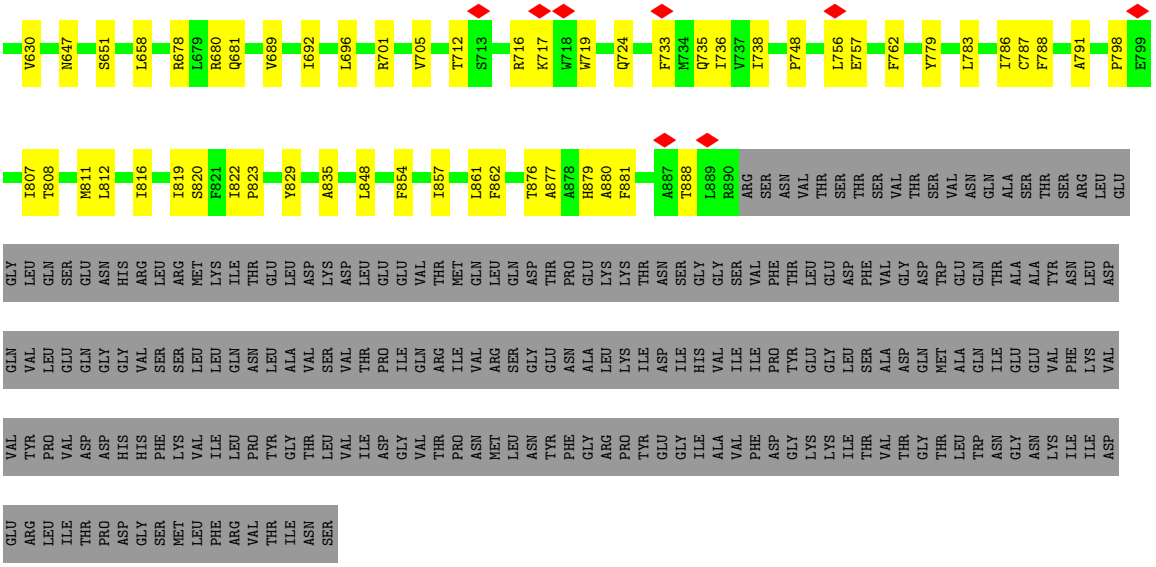
Chain E:



• Molecule 3: Extracellular calcium-sensing receptor

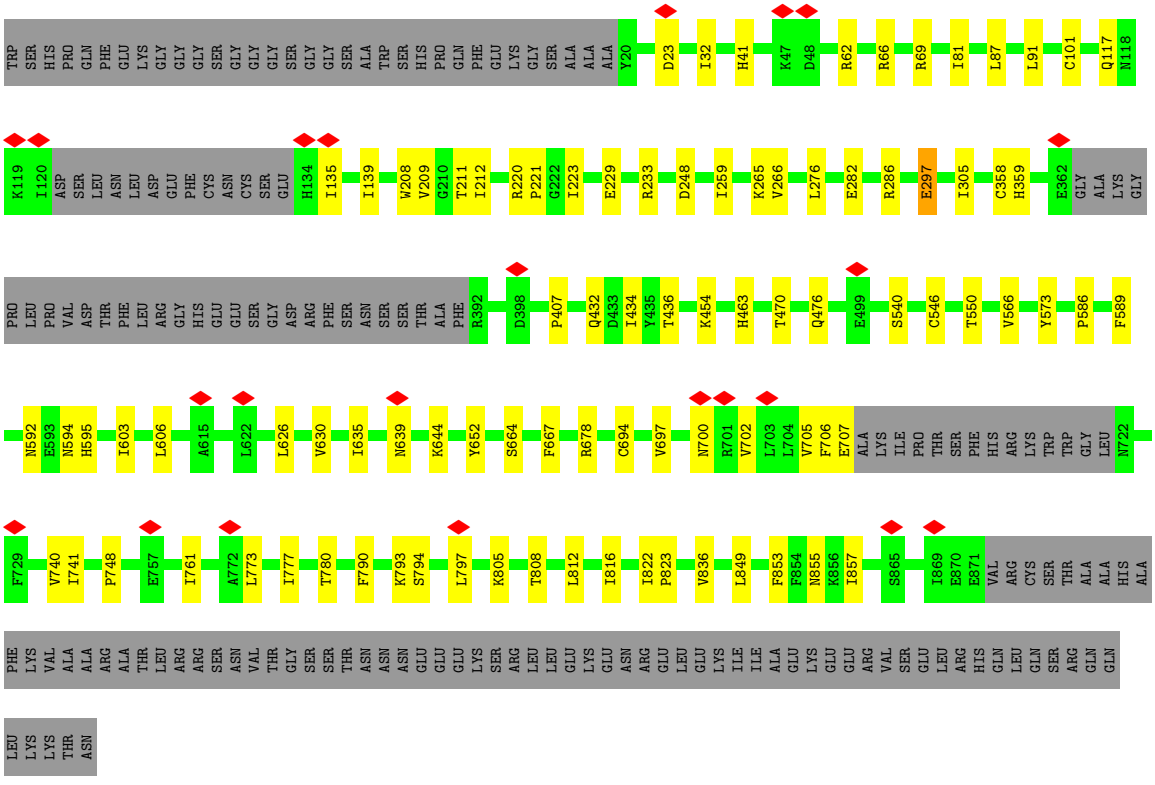
Chain A:





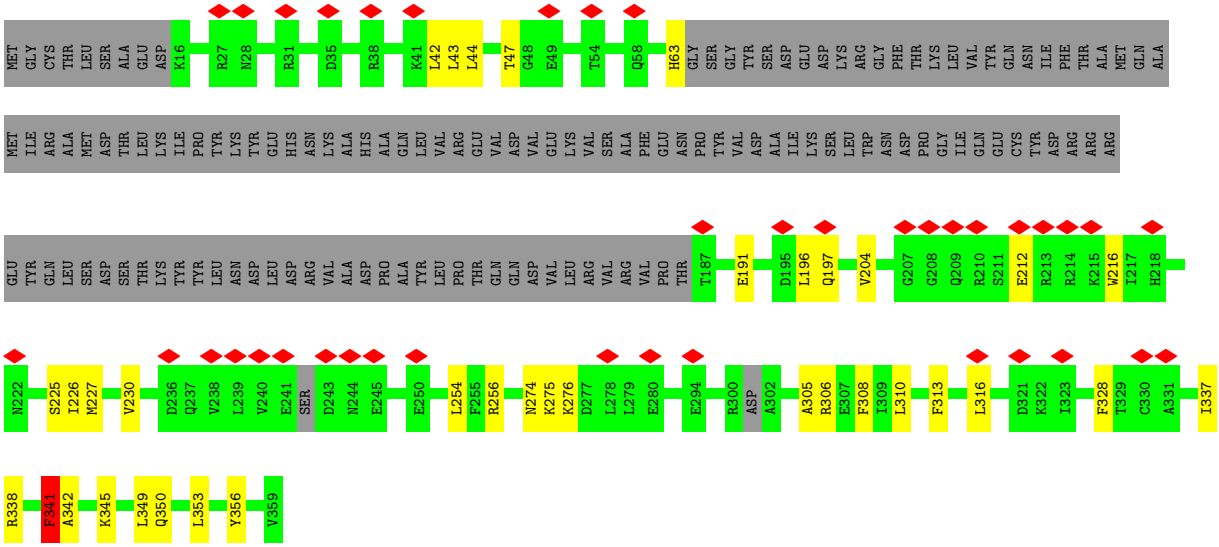
• Molecule 4: Extracellular calcium-sensing receptor

Chain B:



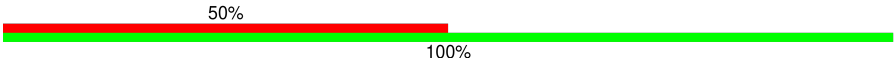
• Molecule 5: Guanine nucleotide-binding protein G(q) subunit alpha

Chain C:



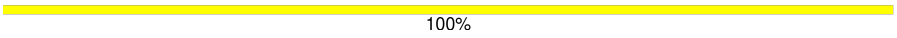
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



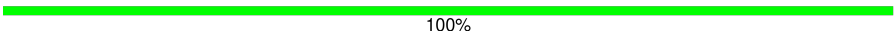
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89192	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 ($e^-/Å^2$)	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	7.747	Depositor
Minimum map value	-0.495	Depositor
Average map value	0.048	Depositor
Map value standard deviation	0.126	Depositor
Recommended contour level	1	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

5.1 Standard geometry

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

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	D	0.28	0/2448	0.54	0/3338
2	E	0.24	0/373	0.42	0/510
3	A	0.33	0/6689	0.54	0/9084
4	B	0.34	0/6439	0.54	0/8741
5	C	0.34	0/1668	0.64	1/2257 (0.0%)
All	All	0.33	0/17617	0.55	1/23930 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	341	PHE	CB-CA-C	-10.76	88.88	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2404	0	2238	37	0
2	E	368	0	326	6	0
3	A	6520	0	6369	75	0
4	B	6279	0	6122	56	0
5	C	1640	0	1536	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	28	0	25	0	0
6	G	28	0	25	2	0
6	H	28	0	25	0	0
7	A	26	0	0	0	0
7	B	26	0	0	1	0
8	A	28	0	26	1	0
8	B	28	0	26	0	0
9	A	54	0	84	8	0
10	A	28	0	52	0	0
10	B	14	0	26	0	0
11	A	3	0	0	0	0
12	A	15	0	9	0	0
12	B	15	0	9	0	0
13	A	5	0	0	0	0
13	B	5	0	0	2	0
14	B	28	0	46	3	0
15	B	1	0	0	0	0
All	All	17571	0	16944	193	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 6.

All (193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:888:THR:HB	5:C:341:PHE:CE1	1.66	1.29
3:A:888:THR:CB	5:C:341:PHE:CE1	2.60	0.80
3:A:888:THR:HB	5:C:341:PHE:HE1	1.44	0.79
3:A:658:LEU:HD11	3:A:848:LEU:HD22	1.63	0.78
1:D:234:PHE:HE2	1:D:238:GLY:HA2	1.48	0.78
3:A:791:ALA:HB2	3:A:807:ILE:HG21	1.66	0.78
4:B:780:THR:HG21	7:B:1407:YP4:CE1	2.15	0.75
1:D:209:LYS:NZ	1:D:218:CYS:SG	2.63	0.71
3:A:716:ARG:HH21	3:A:719:TRP:HB2	1.56	0.70
1:D:210:LEU:HD12	1:D:220:GLN:HB2	1.72	0.70
5:C:276:LYS:HD3	5:C:306:ARG:HH21	1.56	0.70
3:A:88:LEU:HD22	3:A:91:LEU:HD23	1.73	0.69
5:C:196:LEU:HD13	5:C:341:PHE:CE1	2.30	0.66
3:A:756:LEU:HD12	3:A:757:GLU:N	2.11	0.66
3:A:808:THR:HG21	9:A:1204:PCW:H342	1.77	0.65
4:B:706:PHE:O	4:B:707:GLU:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:229:GLU:OE1	4:B:233:ARG:NH1	2.31	0.64
1:D:250:CYS:HB2	1:D:264:TYR:HB2	1.79	0.64
1:D:47:THR:HG21	1:D:337:LYS:HD3	1.80	0.62
3:A:756:LEU:HD11	3:A:762:PHE:CE2	2.34	0.62
4:B:358:CYS:SG	4:B:359:HIS:N	2.72	0.62
4:B:702:VAL:O	4:B:705:VAL:HG12	1.99	0.62
5:C:212:GLU:O	5:C:216:TRP:NE1	2.33	0.62
1:D:225:HIS:CD2	1:D:251:ARG:HH11	2.17	0.62
4:B:69:ARG:NH2	13:B:1406:PO4:O2	2.33	0.62
5:C:196:LEU:HD21	5:C:337:ILE:HD11	1.81	0.61
1:D:225:HIS:HD2	1:D:251:ARG:HH11	1.48	0.61
3:A:696:LEU:HD11	3:A:786:ILE:HG22	1.83	0.61
3:A:134:HIS:O	3:A:135:ILE:HG13	2.01	0.61
3:A:816:ILE:HA	9:A:1204:PCW:H252	1.83	0.61
3:A:854:PHE:HA	3:A:857:ILE:HG22	1.82	0.61
4:B:630:VAL:HG13	4:B:857:ILE:HD11	1.83	0.61
1:D:93:ILE:HG12	1:D:133:VAL:HG11	1.84	0.59
3:A:293:TRP:HB2	3:A:317:THR:HG23	1.85	0.59
3:A:787:CYS:SG	3:A:807:ILE:HG23	2.42	0.59
1:D:102:THR:HG21	1:D:148:CYS:HA	1.85	0.58
3:A:647:ASN:HD22	3:A:724:GLN:NE2	2.01	0.58
4:B:626:LEU:HD22	4:B:849:LEU:HD21	1.85	0.58
3:A:32:ILE:HD12	3:A:91:LEU:HD21	1.83	0.58
5:C:191:GLU:HB3	5:C:204:VAL:HG12	1.84	0.58
3:A:647:ASN:HD22	3:A:724:GLN:HE22	1.52	0.57
1:D:37:ILE:HB	1:D:301:LYS:HD3	1.85	0.57
3:A:692:ILE:HG21	3:A:783:LEU:HB3	1.86	0.57
1:D:165:THR:HG22	1:D:181:THR:HG22	1.87	0.57
3:A:678:ARG:HG2	3:A:748:PRO:HD2	1.85	0.56
3:A:51:LEU:HD22	3:A:55:PRO:HG3	1.87	0.56
1:D:51:LEU:HB2	1:D:336:LEU:HB2	1.87	0.55
1:D:38:ASP:O	1:D:301:LYS:NZ	2.33	0.55
4:B:603:ILE:HG22	4:B:761:ILE:HB	1.88	0.55
4:B:276:LEU:HD23	4:B:305:ILE:HD13	1.88	0.55
8:A:1202:NAG:H83	8:A:1202:NAG:H3	1.88	0.55
4:B:66:ARG:NH2	13:B:1406:PO4:O1	2.33	0.55
3:A:876:THR:CG2	5:C:349:LEU:HD22	2.37	0.55
3:A:551:ARG:NH1	3:A:552:LYS:O	2.39	0.54
1:D:236:PRO:HB2	2:E:40:TYR:HE2	1.73	0.53
3:A:861:LEU:HD12	3:A:862:PHE:N	2.24	0.53
9:A:1204:PCW:H131	14:B:1401:CLR:H151	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:205:ARG:NH1	6:G:2:NAG:O6	2.41	0.53
3:A:489:TYR:HB2	3:A:511:TYR:HB3	1.89	0.53
5:C:43:LEU:HD21	5:C:226:ILE:HG13	1.91	0.53
1:D:225:HIS:HD2	1:D:251:ARG:HD2	1.73	0.53
4:B:700:ASN:ND2	4:B:794:SER:HB3	2.24	0.52
4:B:209:VAL:HG12	4:B:266:VAL:HB	1.91	0.52
1:D:209:LYS:HG2	1:D:221:THR:HG22	1.92	0.52
3:A:791:ALA:HB2	3:A:807:ILE:CG2	2.38	0.52
3:A:712:THR:HG22	5:C:356:TYR:HE1	1.75	0.51
3:A:735:GLN:HA	3:A:738:ILE:HG22	1.92	0.51
3:A:876:THR:HG21	5:C:349:LEU:HD22	1.93	0.51
1:D:234:PHE:CE2	1:D:238:GLY:HA2	2.36	0.51
3:A:211:THR:HB	3:A:223:ILE:HD11	1.92	0.51
4:B:282:GLU:HG3	4:B:286:ARG:HH12	1.75	0.51
3:A:880:ALA:HA	5:C:345:LYS:NZ	2.26	0.50
4:B:69:ARG:NH1	4:B:407:PRO:O	2.44	0.50
4:B:212:ILE:HD11	4:B:259:ILE:HD11	1.94	0.50
4:B:635:ILE:HG22	4:B:652:TYR:CE1	2.46	0.50
5:C:310:LEU:HD12	5:C:328:PHE:HZ	1.77	0.50
5:C:230:VAL:HG21	5:C:313:PHE:HE2	1.76	0.49
4:B:32:ILE:HD12	4:B:91:LEU:HD21	1.94	0.49
5:C:256:ARG:HB2	5:C:316:LEU:HD21	1.95	0.49
2:E:48:ASP:HB3	2:E:51:LEU:HB2	1.93	0.49
1:D:271:CYS:HB2	1:D:290:ASP:HB2	1.95	0.49
3:A:735:GLN:HE21	3:A:779:TYR:HB3	1.78	0.49
5:C:47:THR:HG22	5:C:254:LEU:HD23	1.94	0.49
1:D:186:ASP:O	1:D:204:CYS:N	2.46	0.48
3:A:756:LEU:HD11	3:A:762:PHE:CD2	2.48	0.48
4:B:694:CYS:O	4:B:697:VAL:HG12	2.13	0.48
5:C:197:GLN:HG2	5:C:341:PHE:HZ	1.78	0.48
5:C:44:LEU:HD13	5:C:227:MET:HE2	1.95	0.48
3:A:630:VAL:HG22	3:A:857:ILE:HD12	1.95	0.48
3:A:756:LEU:HD21	3:A:762:PHE:HD2	1.79	0.48
4:B:822:ILE:HB	4:B:823:PRO:HD3	1.95	0.48
6:G:1:NAG:H61	6:G:2:NAG:HN2	1.77	0.48
4:B:41:HIS:ND1	4:B:62:ARG:O	2.37	0.48
1:D:320:VAL:HG22	1:D:327:VAL:HG22	1.95	0.48
3:A:705:VAL:HG11	5:C:353:LEU:HD12	1.96	0.48
4:B:573:TYR:HA	4:B:595:HIS:O	2.14	0.47
1:D:284:LEU:HD13	1:D:296:VAL:HG11	1.97	0.47
3:A:712:THR:HG22	5:C:356:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:215:ASP:OD1	3:A:220:ARG:NH1	2.48	0.47
3:A:716:ARG:NH2	3:A:719:TRP:HB2	2.26	0.47
4:B:777:ILE:O	4:B:780:THR:HG22	2.15	0.47
4:B:434:ILE:HG12	4:B:463:HIS:CE1	2.50	0.47
4:B:81:ILE:HG23	4:B:87:LEU:HD23	1.97	0.47
4:B:220:ARG:HB2	4:B:221:PRO:HD3	1.95	0.47
3:A:689:VAL:HG21	3:A:735:GLN:NE2	2.31	0.46
3:A:788:PHE:CE1	3:A:811:MET:HB2	2.50	0.46
3:A:680:ARG:HG3	3:A:681:GLN:HG3	1.98	0.46
5:C:274:ASN:OD1	5:C:275:LYS:N	2.48	0.46
4:B:855:ASN:HB3	14:B:1401:CLR:H191	1.98	0.46
3:A:658:LEU:HD11	3:A:848:LEU:CD2	2.39	0.46
3:A:808:THR:HG21	9:A:1204:PCW:C34	2.45	0.46
1:D:252:LEU:HD22	1:D:261:LEU:HD12	1.97	0.46
1:D:232:ILE:HD12	1:D:243:THR:HG22	1.98	0.46
3:A:42:PHE:HB2	3:A:62:ARG:HB2	1.97	0.46
9:A:1204:PCW:H72	9:A:1204:PCW:H41	1.75	0.46
3:A:823:PRO:HG2	4:B:836:VAL:HG22	1.98	0.46
4:B:678:ARG:HG2	4:B:748:PRO:HD2	1.97	0.46
3:A:876:THR:O	3:A:877:ALA:C	2.55	0.45
1:D:314:ARG:HG2	1:D:332:TRP:CD2	2.50	0.45
3:A:733:PHE:O	3:A:736:ILE:HG22	2.17	0.45
3:A:861:LEU:HD11	3:A:862:PHE:CE2	2.51	0.45
4:B:700:ASN:HD22	4:B:797:LEU:HD22	1.80	0.45
1:D:124:TYR:HE1	1:D:135:VAL:HG22	1.81	0.45
4:B:117:GLN:NE2	4:B:135:ILE:O	2.40	0.45
1:D:124:TYR:CE1	1:D:135:VAL:HG22	2.52	0.44
3:A:647:ASN:O	3:A:651:SER:HB3	2.18	0.44
4:B:639:ASN:HA	4:B:644:LYS:HE2	1.98	0.44
3:A:812:LEU:HD23	3:A:812:LEU:HA	1.87	0.44
4:B:211:THR:HB	4:B:223:ILE:HD11	1.98	0.44
5:C:42:LEU:HD23	5:C:225:SER:HB2	2.00	0.44
3:A:808:THR:CG2	9:A:1204:PCW:H342	2.46	0.44
4:B:773:LEU:O	4:B:777:ILE:HG12	2.18	0.44
1:D:148:CYS:SG	1:D:149:CYS:N	2.90	0.44
1:D:210:LEU:HD11	1:D:255:LEU:HG	1.99	0.44
3:A:575:ASP:N	3:A:575:ASP:OD1	2.50	0.44
3:A:888:THR:HG23	5:C:338:ARG:HD3	1.99	0.44
5:C:63:HIS:O	5:C:337:ILE:HD13	2.18	0.44
4:B:41:HIS:HB2	4:B:101:CYS:SG	2.58	0.44
1:D:301:LYS:HB2	1:D:301:LYS:HE2	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:881:PHE:CD1	5:C:342:ALA:HB1	2.53	0.43
3:A:701:ARG:O	3:A:705:VAL:HG23	2.18	0.43
4:B:297:GLU:O	4:B:297:GLU:HG2	2.18	0.43
1:D:180:PHE:HE1	1:D:216:GLY:HA2	1.84	0.43
4:B:432:GLN:O	4:B:436:THR:HG22	2.18	0.43
4:B:790:PHE:O	4:B:793:LYS:HB3	2.19	0.43
3:A:816:ILE:HG23	9:A:1204:PCW:H272	2.00	0.43
1:D:120:ILE:HG13	1:D:139:LEU:O	2.19	0.43
2:E:18:GLN:O	2:E:21:MET:HG3	2.18	0.43
4:B:664:SER:O	4:B:667:PHE:HB2	2.19	0.43
4:B:849:LEU:O	4:B:853:PHE:HB2	2.19	0.43
4:B:546:CYS:HB3	4:B:550:THR:HG23	2.00	0.43
5:C:305:ALA:HB3	5:C:308:PHE:CE2	2.54	0.43
3:A:87:LEU:HD12	3:A:87:LEU:HA	1.88	0.42
1:D:31:SER:O	1:D:31:SER:OG	2.28	0.42
4:B:454:LYS:HB3	4:B:454:LYS:HE2	1.76	0.42
4:B:592:ASN:HB3	4:B:594:ASN:O	2.18	0.42
3:A:22:PRO:HG2	3:A:98:PHE:CD1	2.54	0.42
1:D:241:PHE:CE1	1:D:253:PHE:HB2	2.55	0.42
1:D:52:ARG:HG2	1:D:335:PHE:CE1	2.55	0.42
3:A:880:ALA:HA	5:C:345:LYS:HZ3	1.84	0.42
3:A:338:HIS:CD2	3:A:339:PRO:HD2	2.55	0.42
3:A:881:PHE:CE1	5:C:342:ALA:HB1	2.54	0.42
4:B:23:ASP:OD1	4:B:23:ASP:N	2.51	0.42
4:B:805:LYS:O	4:B:808:THR:HG22	2.19	0.42
3:A:787:CYS:SG	3:A:807:ILE:CG2	3.08	0.42
14:B:1401:CLR:H183	14:B:1401:CLR:H20	1.84	0.42
4:B:208:TRP:O	4:B:540:SER:OG	2.38	0.42
4:B:248:ASP:OD1	4:B:248:ASP:N	2.48	0.41
3:A:888:THR:HB	5:C:341:PHE:CD1	2.42	0.41
3:A:820:SER:HB2	9:A:1204:PCW:H281	2.02	0.41
4:B:32:ILE:HG23	4:B:139:ILE:HG13	2.02	0.41
4:B:265:LYS:HB3	4:B:265:LYS:HE3	1.93	0.41
3:A:756:LEU:HD13	3:A:829:TYR:CE1	2.55	0.41
5:C:349:LEU:O	5:C:350:GLN:C	2.59	0.41
1:D:232:ILE:HA	1:D:242:ALA:O	2.20	0.41
3:A:442:GLY:HA3	3:A:448:SER:O	2.20	0.41
3:A:612:PHE:HE2	3:A:835:ALA:HB1	1.86	0.41
2:E:38:MET:O	2:E:42:GLU:HG2	2.21	0.41
4:B:81:ILE:HG12	4:B:87:LEU:HD23	2.01	0.41
4:B:470:THR:OG1	4:B:476:GLN:OE1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:812:LEU:O	4:B:816:ILE:HG13	2.21	0.41
4:B:606:LEU:HD12	4:B:606:LEU:HA	1.89	0.41
1:D:236:PRO:HB2	2:E:40:TYR:CE2	2.54	0.40
3:A:177:LYS:HA	3:A:177:LYS:HD3	1.84	0.40
3:A:717:LYS:HB3	3:A:717:LYS:HE2	1.80	0.40
3:A:798:PRO:HG3	3:A:879:HIS:HB2	2.03	0.40
4:B:586:PRO:HB2	4:B:589:PHE:HD2	1.86	0.40
4:B:740:VAL:O	4:B:741:ILE:C	2.58	0.40
1:D:264:TYR:OH	1:D:299:ALA:HA	2.21	0.40
2:E:32:LYS:HE3	2:E:32:LYS:HB3	1.92	0.40
3:A:854:PHE:O	3:A:857:ILE:HG22	2.22	0.40
4:B:550:THR:OG1	4:B:566:VAL:O	2.28	0.40
3:A:819:ILE:O	3:A:822:ILE:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	333/369 (90%)	316 (95%)	17 (5%)	0	100	100
2	E	53/71 (75%)	52 (98%)	1 (2%)	0	100	100
3	A	824/1101 (75%)	785 (95%)	39 (5%)	0	100	100
4	B	788/959 (82%)	751 (95%)	37 (5%)	0	100	100
5	C	211/353 (60%)	200 (95%)	11 (5%)	0	100	100
All	All	2209/2853 (77%)	2104 (95%)	105 (5%)	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	D	232/299 (78%)	232 (100%)	0	100 100
2	E	29/58 (50%)	29 (100%)	0	100 100
3	A	694/957 (72%)	694 (100%)	0	100 100
4	B	675/827 (82%)	674 (100%)	1 (0%)	92 97
5	C	157/320 (49%)	156 (99%)	1 (1%)	84 92
All	All	1787/2461 (73%)	1785 (100%)	2 (0%)	92 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	297	GLU
5	C	341	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	225	HIS
3	A	724	GLN
3	A	735	GLN
4	B	471	ASN
4	B	700	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	$\#\|Z\|>2$
6	NAG	F	1	6,3	14,14,15	0.28	0	17,19,21	0.62	0
6	NAG	F	2	6	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	G	1	6,3	14,14,15	0.23	0	17,19,21	0.47	0
6	NAG	G	2	6	14,14,15	0.33	0	17,19,21	0.50	0
6	NAG	H	1	6,4	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	H	2	6	14,14,15	0.28	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
6	NAG	F	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	NAG	G	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	2/6/23/26	0/1/1/1
6	NAG	H	1	6,4	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	1	NAG	O5-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	H	1	NAG	C4-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
6	G	2	NAG	C4-C5-C6-O6

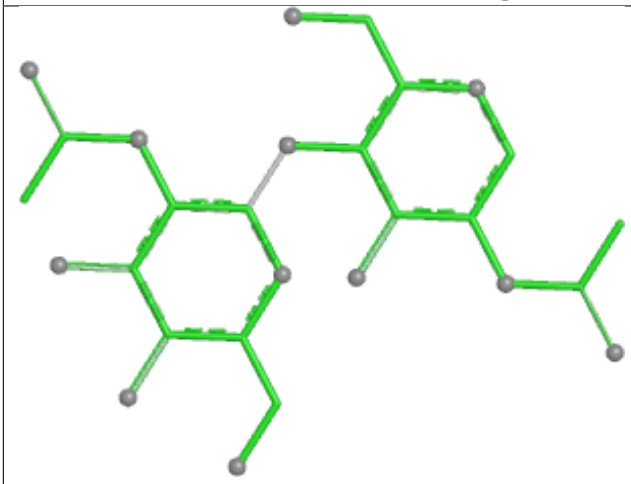
There are no ring outliers.

2 monomers are involved in 2 short contacts:

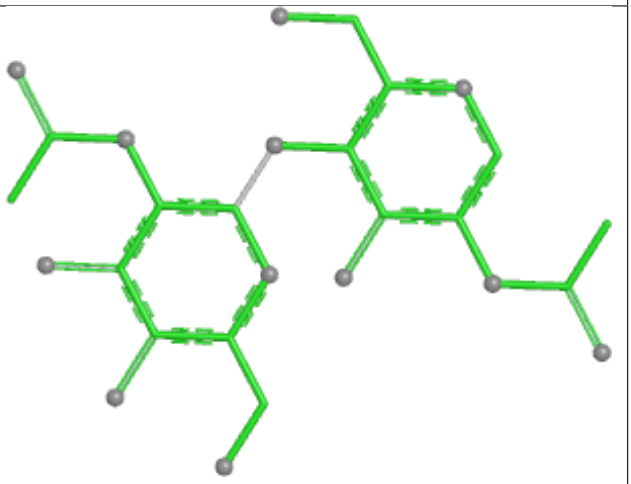
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	2	NAG	2	0
6	G	1	NAG	1	0

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

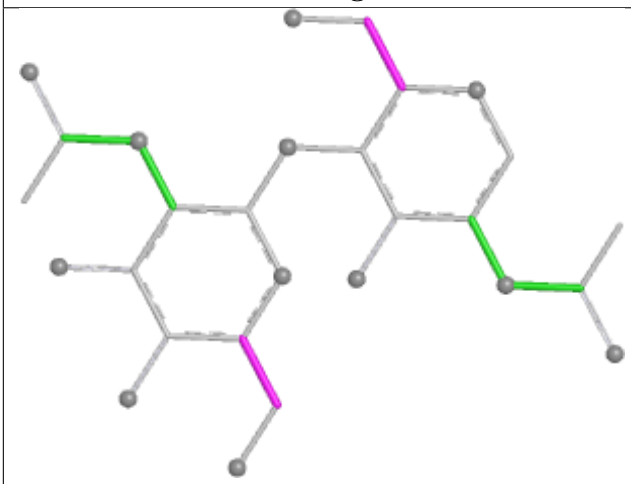
Oligosaccharide Chain F



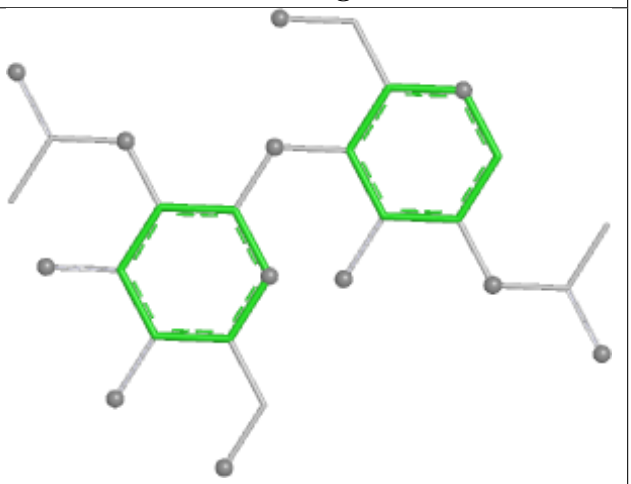
Bond lengths



Bond angles

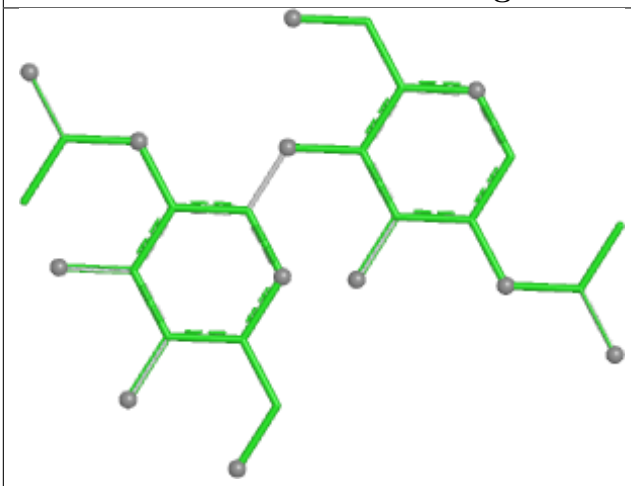


Torsions

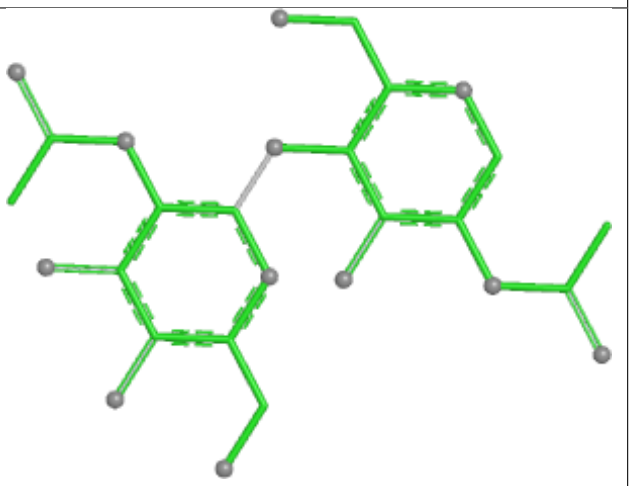


Rings

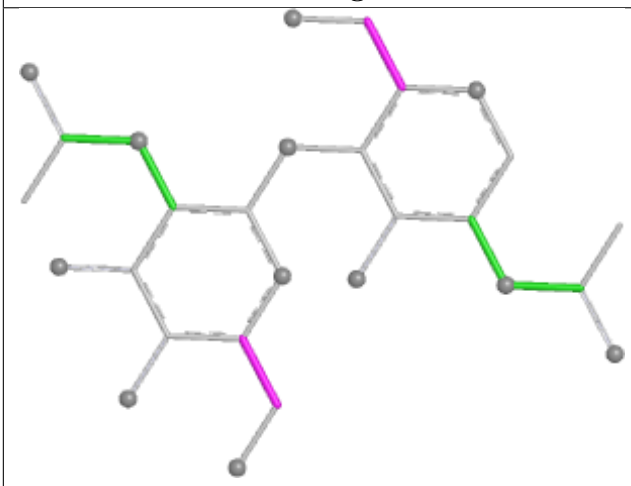
Oligosaccharide Chain G



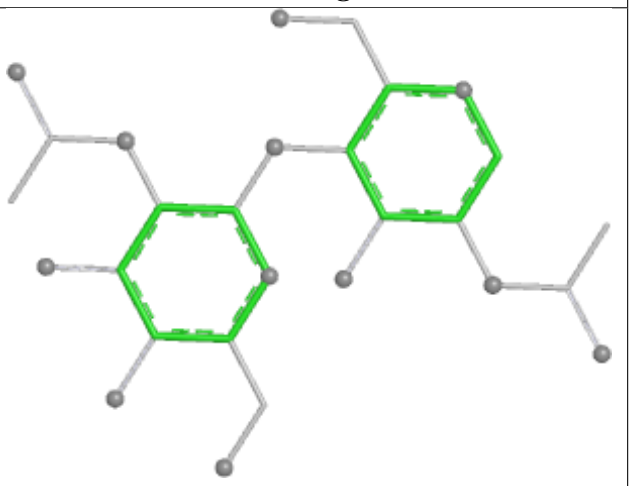
Bond lengths



Bond angles

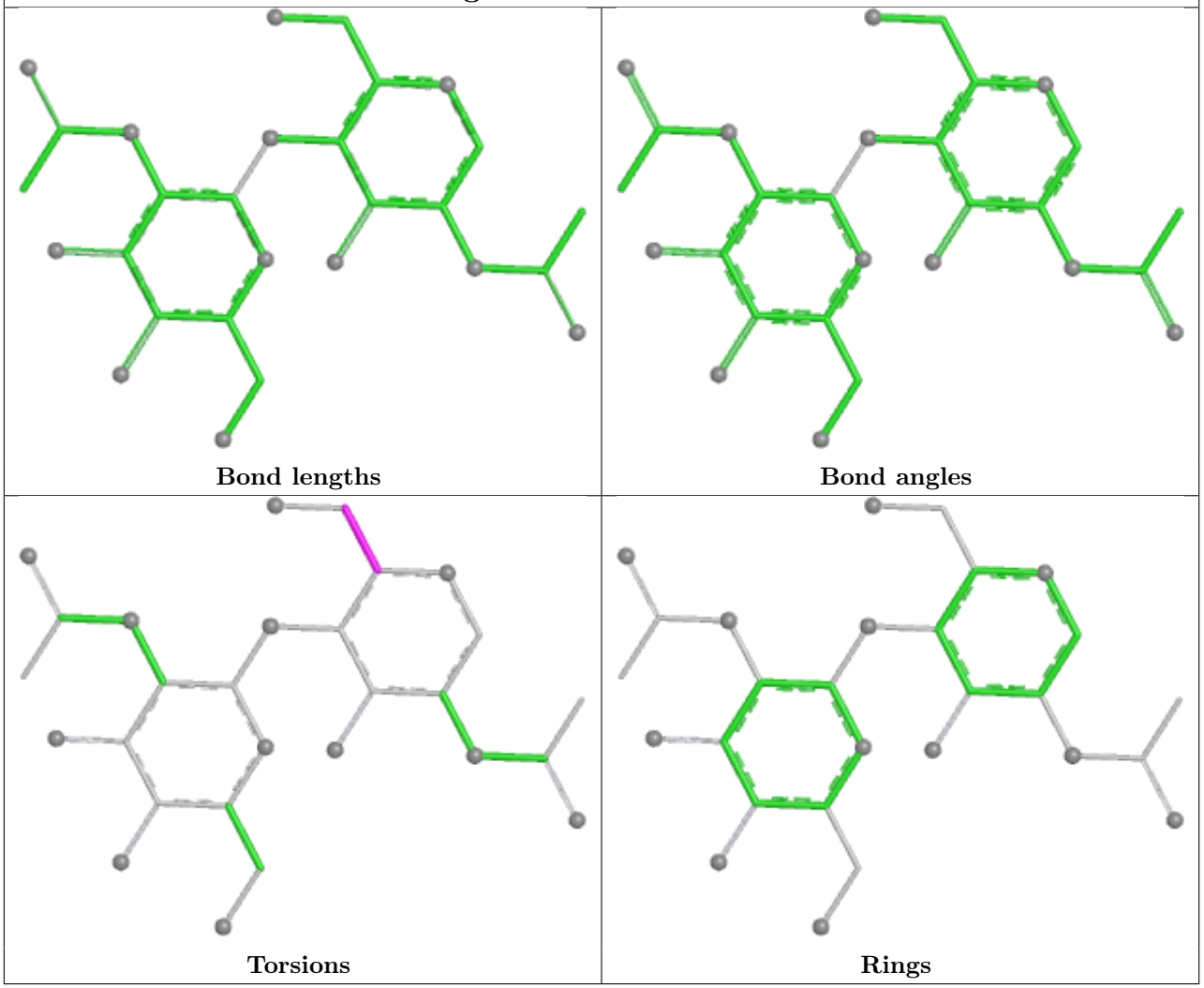


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
7	YP4	B	1407	-	28,28,28	1.11	1 (3%)	39,39,39	1.14	2 (5%)
8	NAG	A	1203	3	14,14,15	0.19	0	17,19,21	0.46	0
8	NAG	A	1202	3	14,14,15	0.45	0	17,19,21	1.33	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	B	1403	4	14,14,15	0.23	0	17,19,21	0.50	0
7	YP4	A	1201	-	28,28,28	1.04	1 (3%)	39,39,39	0.99	1 (2%)
10	SPM	A	1210	-	13,13,13	0.47	0	12,12,12	0.55	0
12	TRP	B	1405	-	14,16,16	0.92	1 (7%)	13,22,22	1.14	1 (7%)
14	CLR	B	1401	-	31,31,31	0.58	0	48,48,48	1.12	4 (8%)
10	SPM	A	1205	-	13,13,13	0.35	0	12,12,12	0.96	0
8	NAG	B	1402	4	14,14,15	0.23	0	17,19,21	0.64	0
12	TRP	A	1208	-	14,16,16	0.92	1 (7%)	13,22,22	1.15	1 (7%)
10	SPM	B	1404	-	13,13,13	0.35	0	12,12,12	0.94	0
13	PO4	B	1406	-	4,4,4	1.04	0	6,6,6	0.42	0
13	PO4	A	1209	-	4,4,4	1.04	0	6,6,6	0.47	0
9	PCW	A	1204	-	53,53,53	1.53	8 (15%)	59,61,61	1.00	3 (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
7	YP4	B	1407	-	-	8/17/17/17	0/3/3/3
8	NAG	A	1203	3	-	2/6/23/26	0/1/1/1
8	NAG	A	1202	3	-	4/6/23/26	0/1/1/1
8	NAG	B	1403	4	-	2/6/23/26	0/1/1/1
7	YP4	A	1201	-	-	7/17/17/17	0/3/3/3
10	SPM	A	1210	-	-	2/11/11/11	-
12	TRP	B	1405	-	-	2/7/8/8	0/2/2/2
14	CLR	B	1401	-	-	6/10/68/68	0/4/4/4
10	SPM	A	1205	-	-	0/11/11/11	-
8	NAG	B	1402	4	-	4/6/23/26	0/1/1/1
12	TRP	A	1208	-	-	0/7/8/8	0/2/2/2
10	SPM	B	1404	-	-	1/11/11/11	-
9	PCW	A	1204	-	1/1/5/9	30/57/57/57	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1204	PCW	O2-C31	5.28	1.49	1.34
7	B	1407	YP4	CG-CD1	-4.04	1.35	1.43
9	A	1204	PCW	C32-C31	3.39	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1201	YP4	CG-CD1	-3.29	1.36	1.43
9	A	1204	PCW	O3-C11	3.02	1.42	1.33
9	A	1204	PCW	C1-C2	2.63	1.59	1.50
9	A	1204	PCW	P-O3P	2.34	1.68	1.59
9	A	1204	PCW	C3-C2	2.30	1.58	1.50
12	A	1208	TRP	OXT-C	-2.28	1.23	1.30
12	B	1405	TRP	OXT-C	-2.28	1.23	1.30
9	A	1204	PCW	C17-C18	2.25	1.61	1.52
9	A	1204	PCW	C17-C16	2.20	1.62	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1202	NAG	C2-N2-C7	4.56	129.01	122.90
9	A	1204	PCW	O2-C31-C32	4.09	120.33	111.48
9	A	1204	PCW	C18-C19-C20	3.70	152.56	124.83
14	B	1401	CLR	C13-C17-C20	-3.66	113.85	119.50
12	A	1208	TRP	OXT-C-O	-2.67	118.02	124.08
7	B	1407	YP4	C3-N-CA	-2.66	109.29	113.42
9	A	1204	PCW	O3-C11-C12	2.62	119.83	111.83
7	A	1201	YP4	CD2-CG-CB	-2.57	120.24	123.37
12	B	1405	TRP	OXT-C-O	-2.57	118.24	124.08
7	B	1407	YP4	CD2-CG-CB	-2.48	120.36	123.37
14	B	1401	CLR	C19-C10-C9	-2.41	108.96	111.66
14	B	1401	CLR	C11-C12-C13	-2.33	108.81	112.74
14	B	1401	CLR	C10-C9-C8	-2.20	109.50	112.71
8	A	1202	NAG	C1-C2-N2	2.11	113.76	110.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1204	PCW	C2

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1201	YP4	C1-CA-N-C3
7	A	1201	YP4	CB-CA-N-C3
9	A	1204	PCW	O4P-C4-C5-N
9	A	1204	PCW	C32-C31-O2-C2
9	A	1204	PCW	O31-C31-O2-C2
9	A	1204	PCW	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
9	A	1204	PCW	C4-O4P-P-O2P
9	A	1204	PCW	C4-O4P-P-O3P
14	B	1401	CLR	C13-C17-C20-C22
14	B	1401	CLR	C13-C17-C20-C21
8	B	1403	NAG	O5-C5-C6-O6
8	A	1203	NAG	O5-C5-C6-O6
14	B	1401	CLR	C17-C20-C22-C23
9	A	1204	PCW	C12-C11-O3-C3
9	A	1204	PCW	O11-C11-O3-C3
8	B	1403	NAG	C4-C5-C6-O6
8	A	1202	NAG	C8-C7-N2-C2
8	A	1202	NAG	O7-C7-N2-C2
9	A	1204	PCW	C11-C12-C13-C14
9	A	1204	PCW	C31-C32-C33-C34
9	A	1204	PCW	C16-C17-C18-C19
14	B	1401	CLR	C21-C20-C22-C23
14	B	1401	CLR	C16-C17-C20-C21
8	A	1203	NAG	C4-C5-C6-O6
9	A	1204	PCW	C23-C24-C25-C26
9	A	1204	PCW	C35-C36-C37-C38
9	A	1204	PCW	C43-C44-C45-C46
9	A	1204	PCW	C32-C33-C34-C35
7	A	1201	YP4	C3-C4-C5-C6
9	A	1204	PCW	C44-C45-C46-C47
9	A	1204	PCW	C34-C35-C36-C37
14	B	1401	CLR	C16-C17-C20-C22
9	A	1204	PCW	C20-C21-C22-C23
12	B	1405	TRP	N-CA-CB-CG
9	A	1204	PCW	C36-C37-C38-C39
9	A	1204	PCW	C12-C13-C14-C15
10	A	1210	SPM	C6-C7-C8-C9
9	A	1204	PCW	C39-C40-C41-C42
9	A	1204	PCW	O3P-C1-C2-O2
9	A	1204	PCW	C33-C34-C35-C36
9	A	1204	PCW	C42-C43-C44-C45
7	A	1201	YP4	C4-C3-N-CA
10	B	1404	SPM	N5-C6-C7-C8
8	B	1402	NAG	C4-C5-C6-O6
9	A	1204	PCW	C37-C38-C39-C40
8	B	1402	NAG	C3-C2-N2-C7
12	B	1405	TRP	C-CA-CB-CG
7	B	1407	YP4	N-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
7	A	1201	YP4	C4-C5-C6-C7
9	A	1204	PCW	C1-C2-C3-O3
7	A	1201	YP4	C4-C5-C6-C11
8	B	1402	NAG	O5-C5-C6-O6
8	A	1202	NAG	C1-C2-N2-C7
8	B	1402	NAG	C1-C2-N2-C7
9	A	1204	PCW	C22-C23-C24-C25
9	A	1204	PCW	C40-C41-C42-C43
8	A	1202	NAG	C3-C2-N2-C7
7	B	1407	YP4	C4-C5-C6-C11
9	A	1204	PCW	O3P-C1-C2-C3
7	B	1407	YP4	C4-C5-C6-C7
7	B	1407	YP4	N-CA-CB-C14
7	B	1407	YP4	N-CA-CB-CG
10	A	1210	SPM	C8-C9-N10-C11
7	A	1201	YP4	N-C3-C4-C5
7	B	1407	YP4	C1-CA-CB-C14
7	B	1407	YP4	C1-CA-CB-CG
7	B	1407	YP4	CB-CA-N-C3
9	A	1204	PCW	O2-C2-C3-O3

There are no ring outliers.

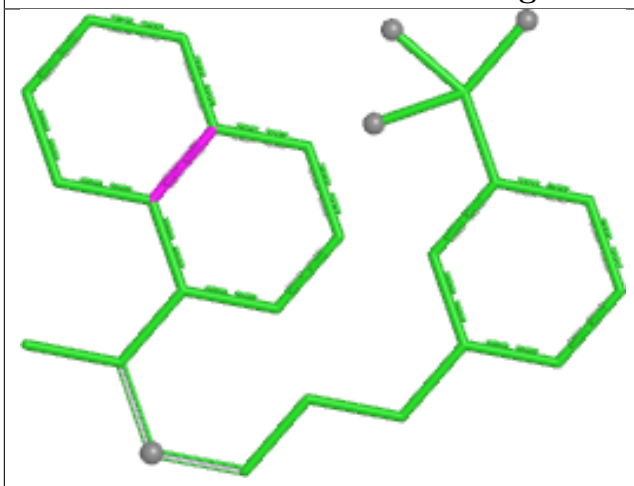
5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1407	YP4	1	0
8	A	1202	NAG	1	0
14	B	1401	CLR	3	0
13	B	1406	PO4	2	0
9	A	1204	PCW	8	0

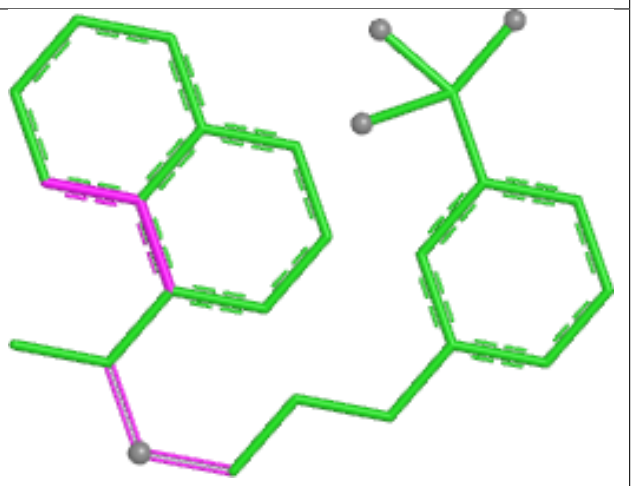
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

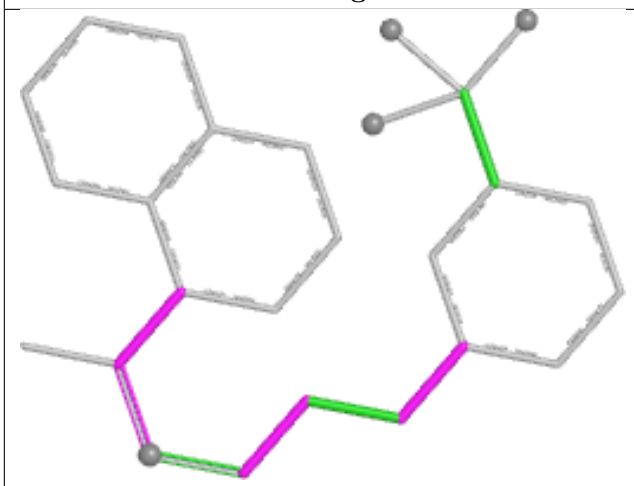
Ligand YP4 B 1407



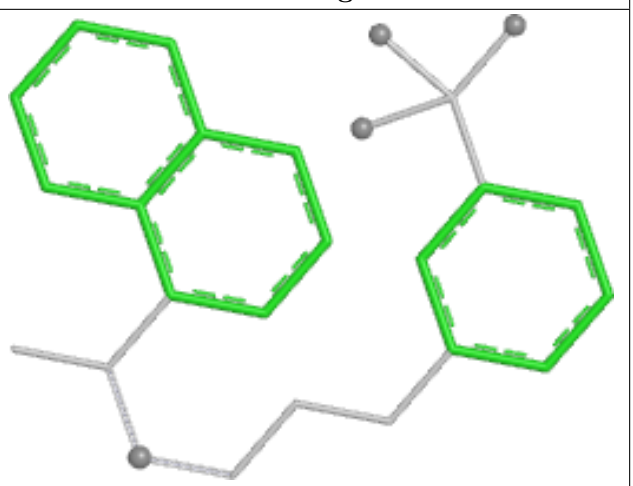
Bond lengths



Bond angles

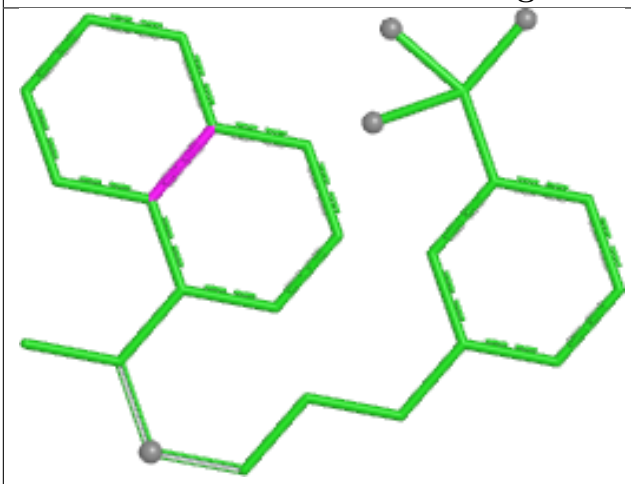


Torsions

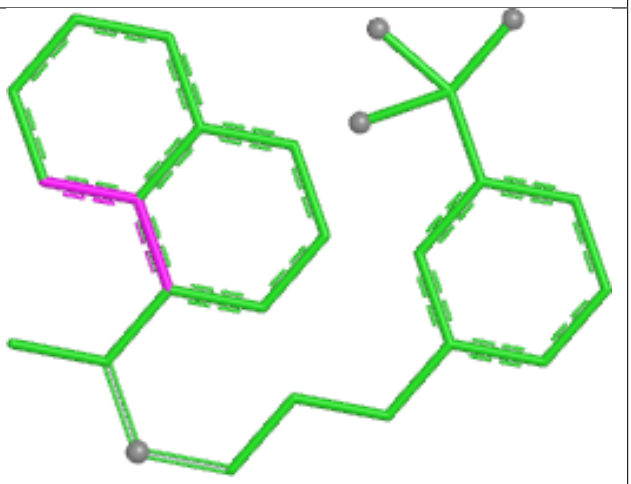


Rings

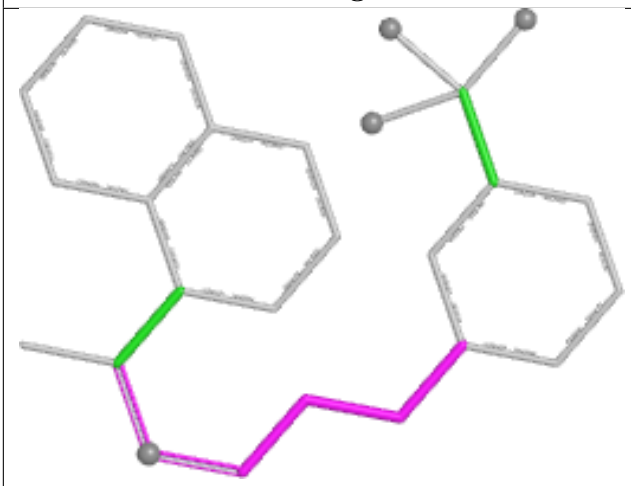
Ligand YP4 A 1201



Bond lengths



Bond angles



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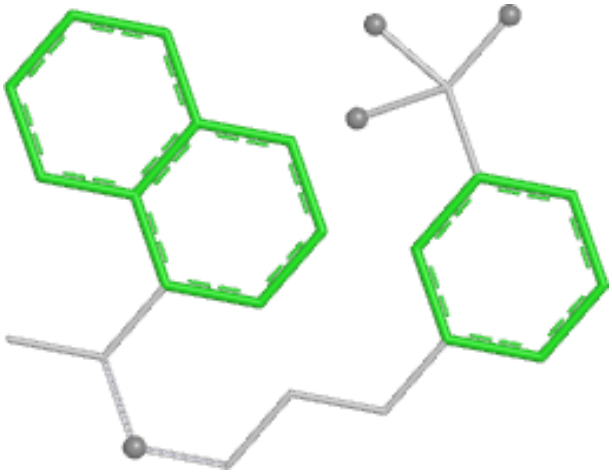
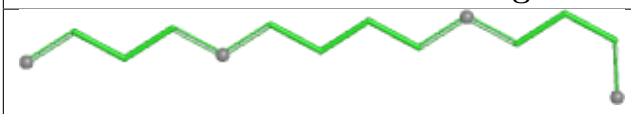
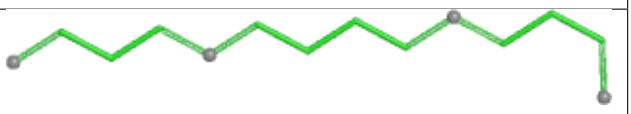


Rings

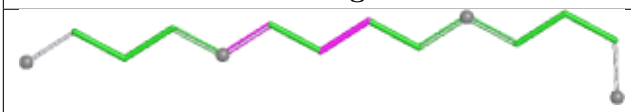
Ligand SPM A 1210



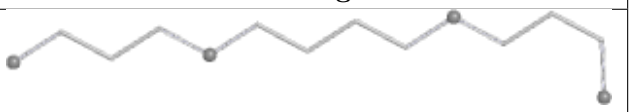
Bond lengths



Bond angles

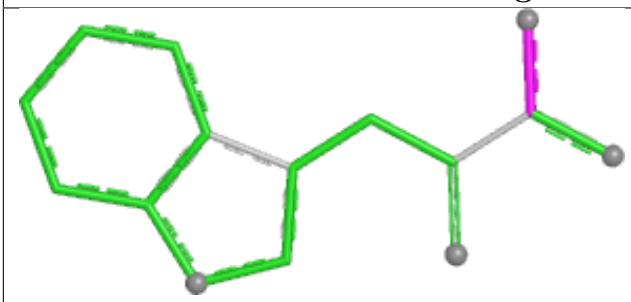


Torsions

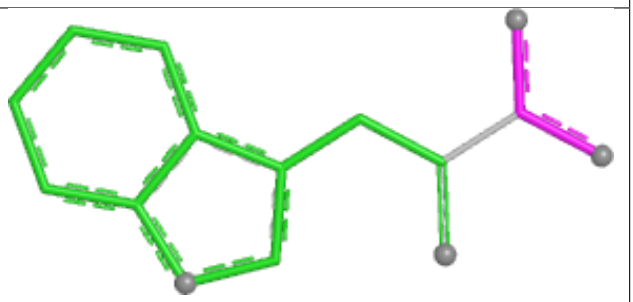


Rings

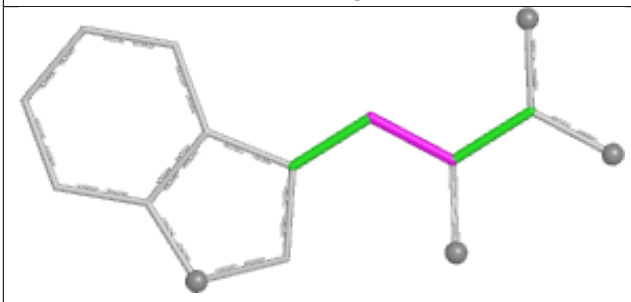
Ligand TRP B 1405



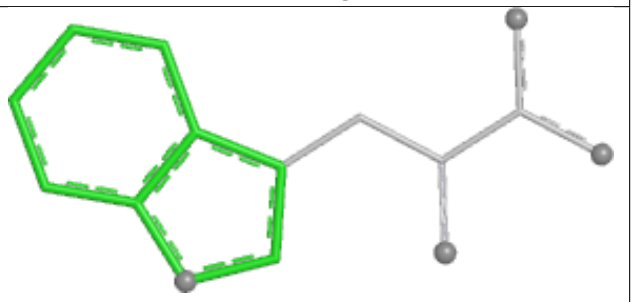
Bond lengths



Bond angles

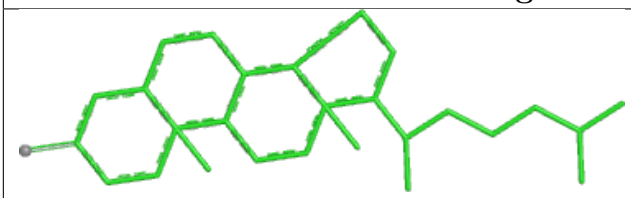


Torsions

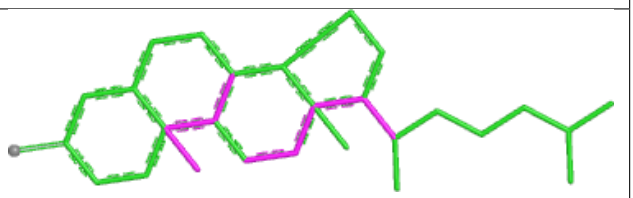


Rings

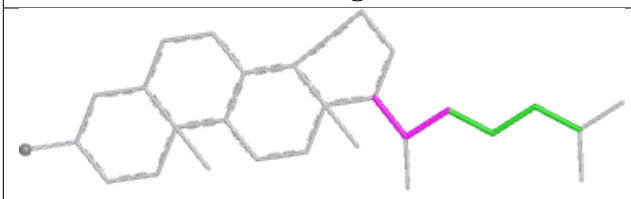
Ligand CLR B 1401



Bond lengths



Bond angles



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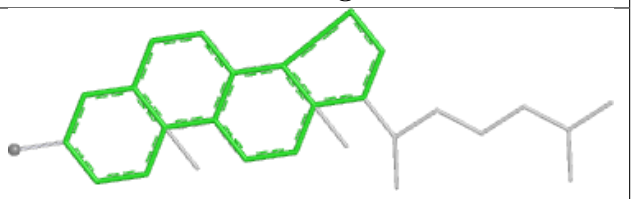
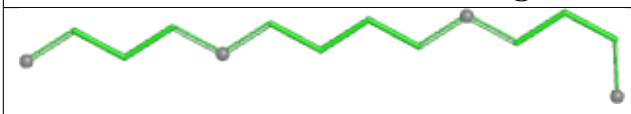


Rings

Ligand SPM A 1205



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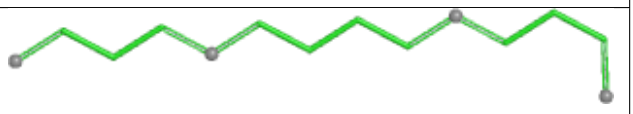
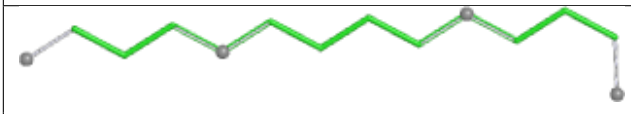


Bond angles



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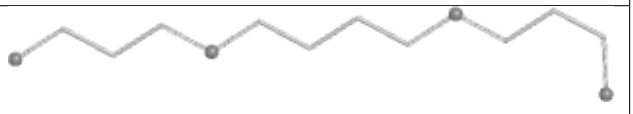
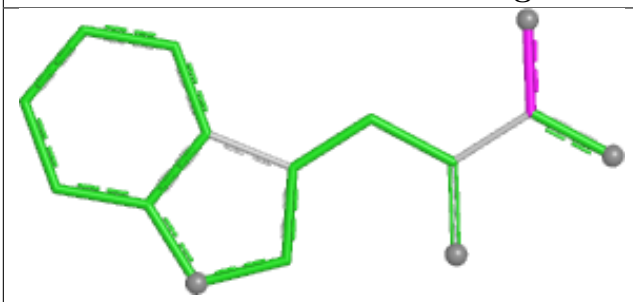
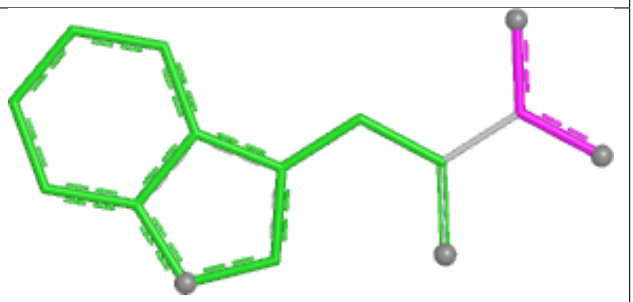


Rings

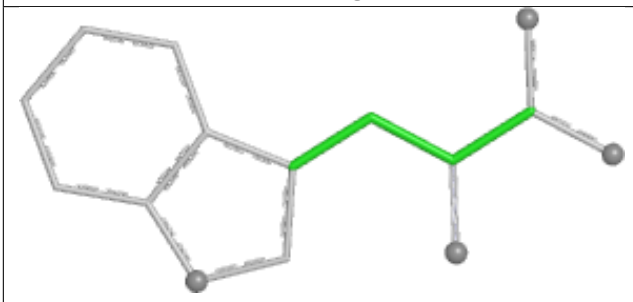
Ligand TRP A 1208



Bond lengths



Bond angles



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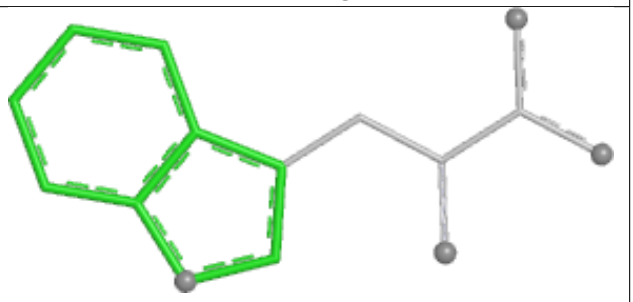
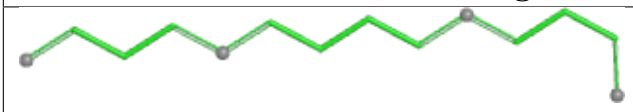
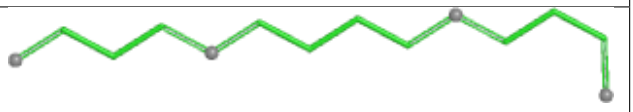


Rings

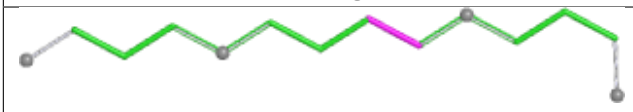
Ligand SPM B 1404



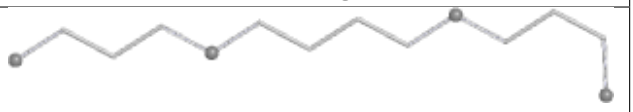
Bond lengths



Bond angles

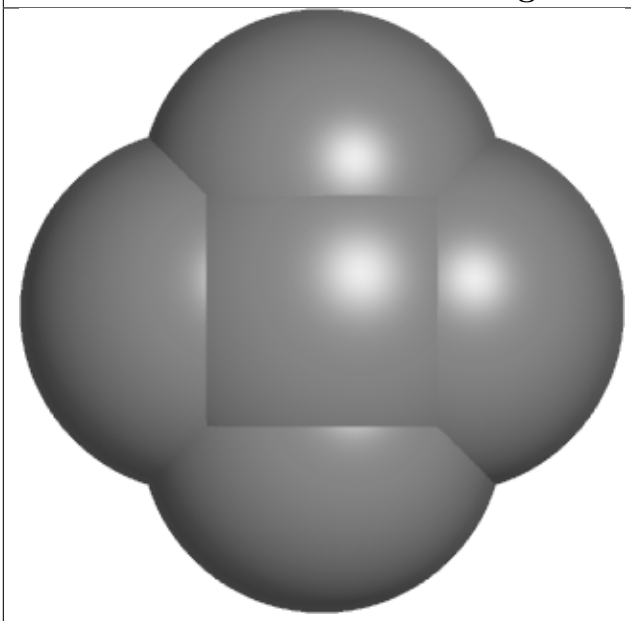


Torsions

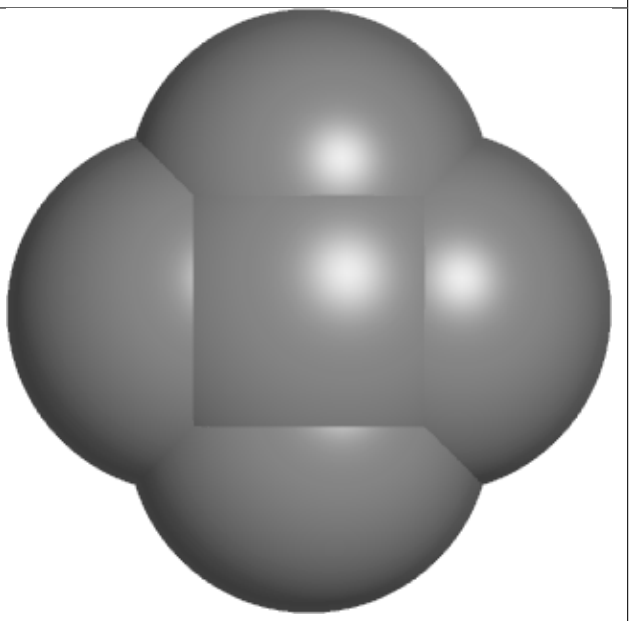


Rings

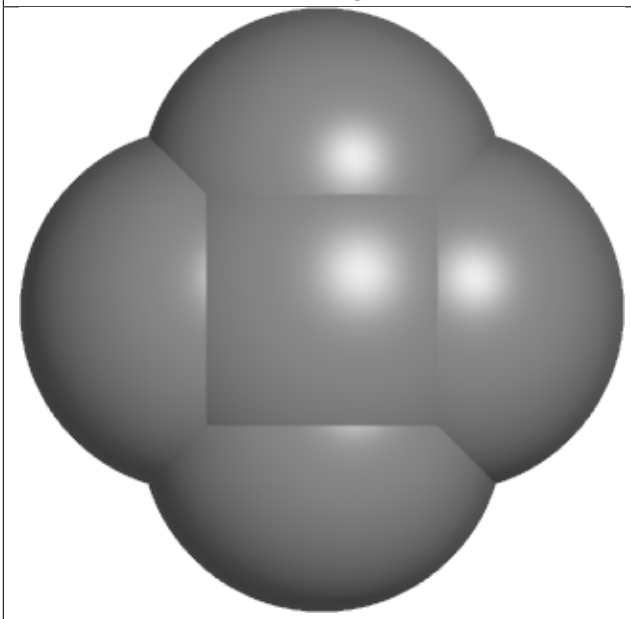
Ligand PO4 B 1406



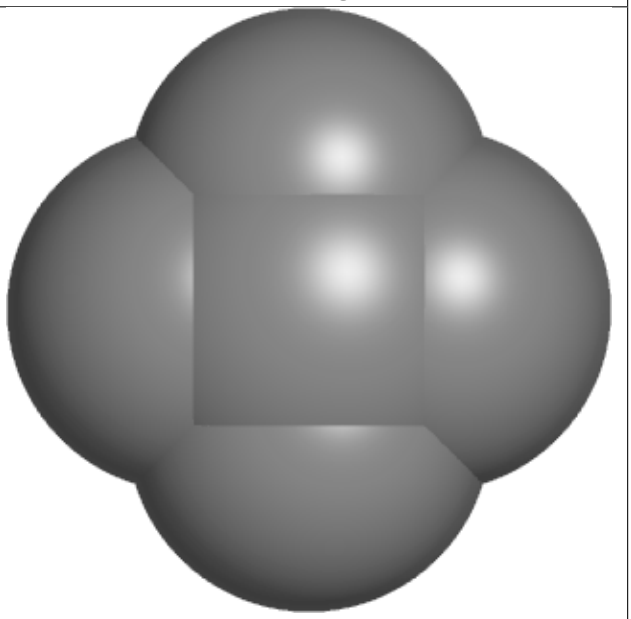
Bond lengths



Bond angles

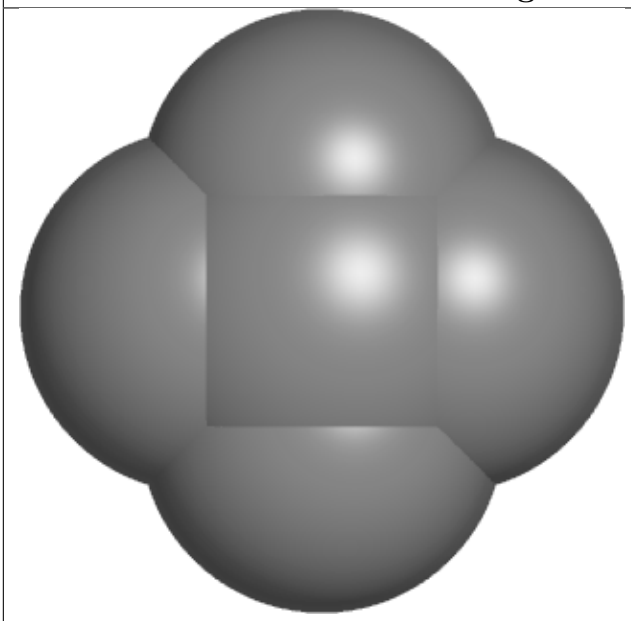


Torsions

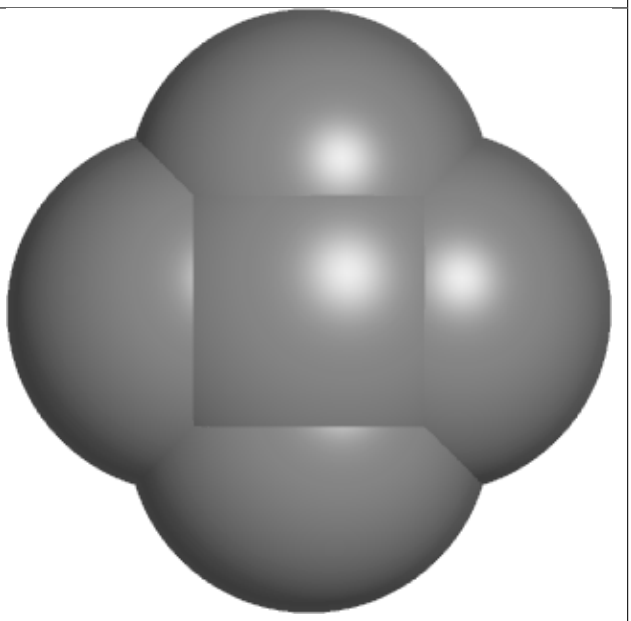


Rings

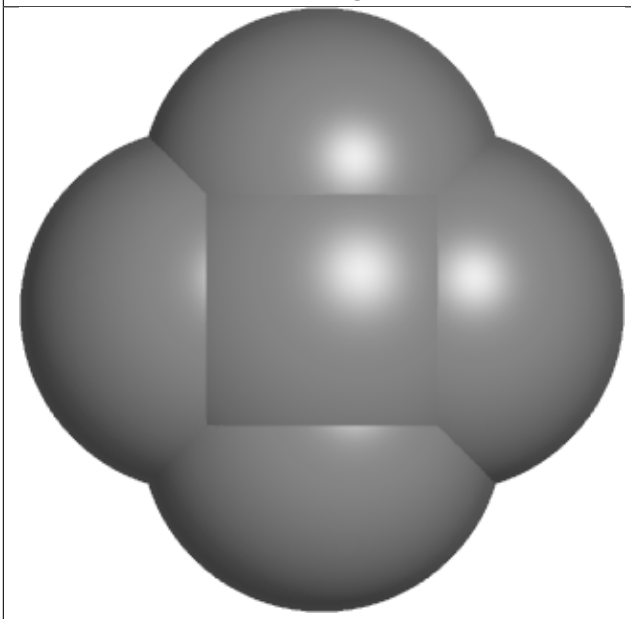
Ligand PO4 A 1209



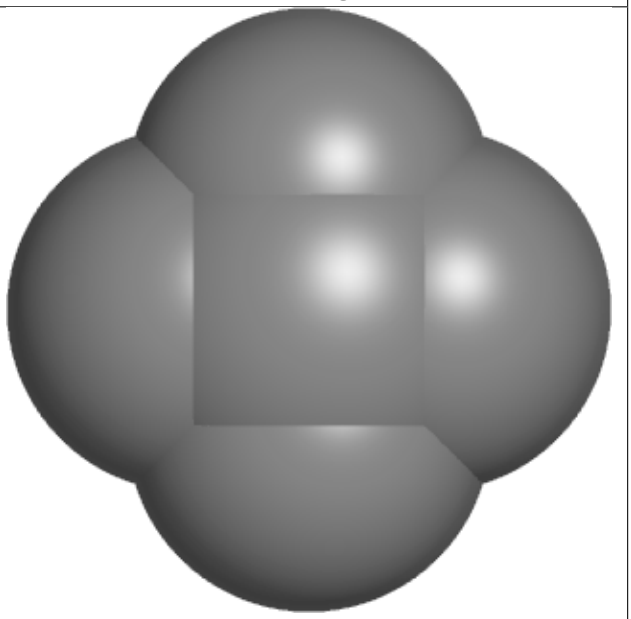
Bond lengths



Bond angles

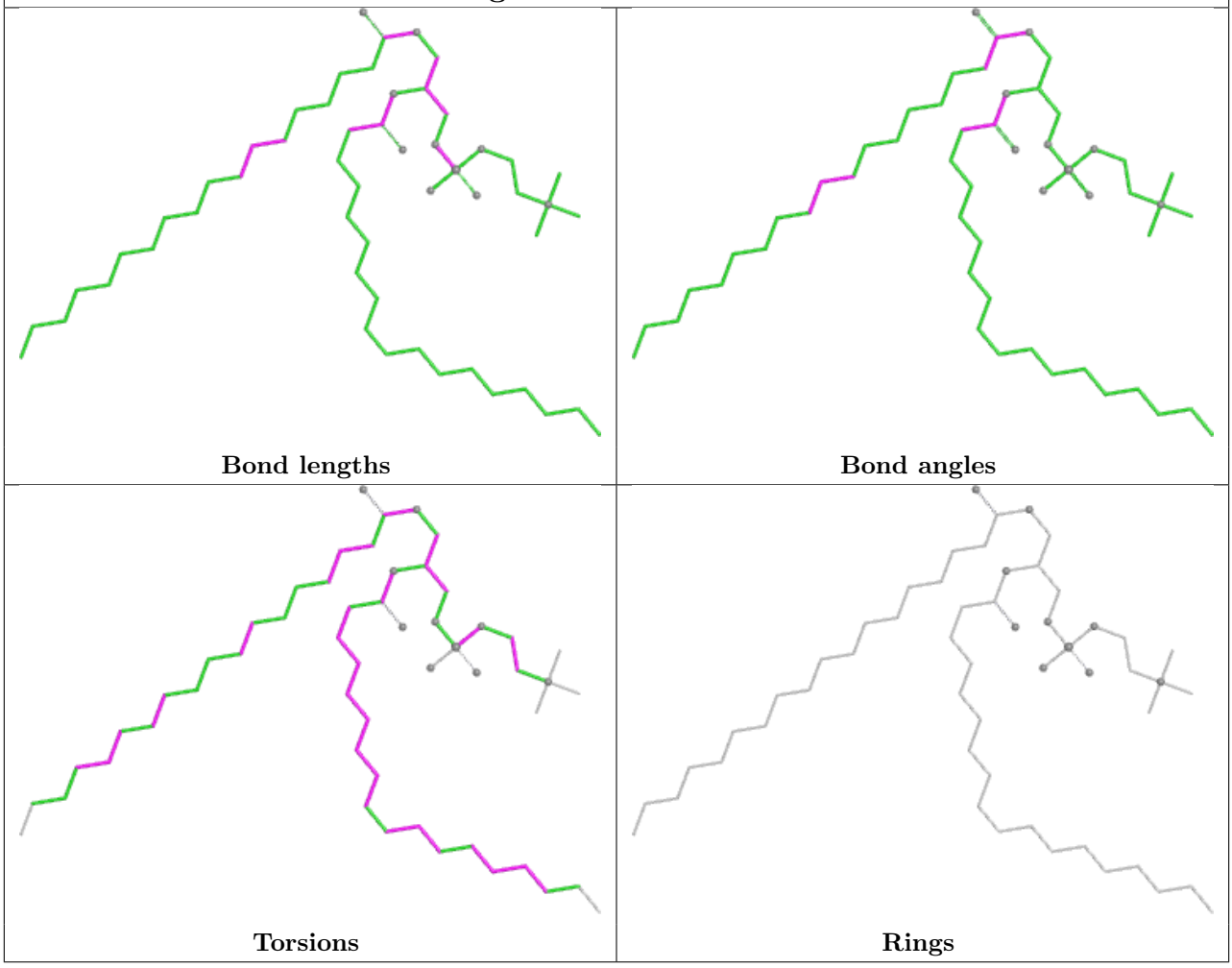


Torsions



Rings

Ligand PCW A 1204



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.

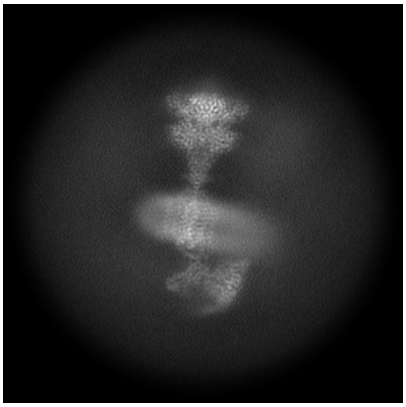
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40915. These allow visual inspection of the internal detail of the map and identification of artifacts.

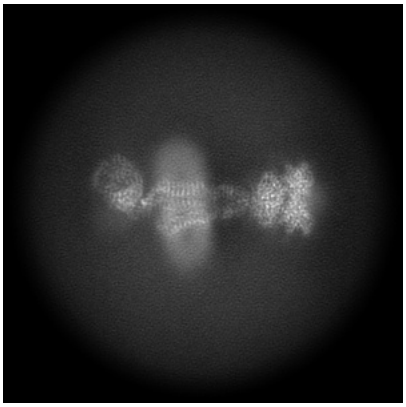
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

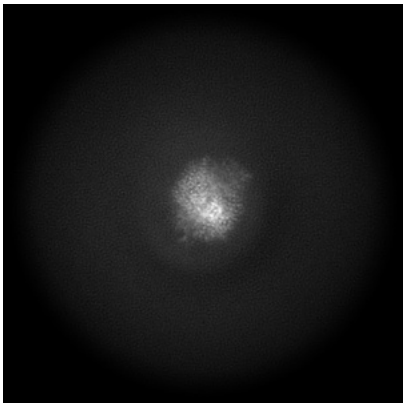
6.1.1 Primary map



X



Y

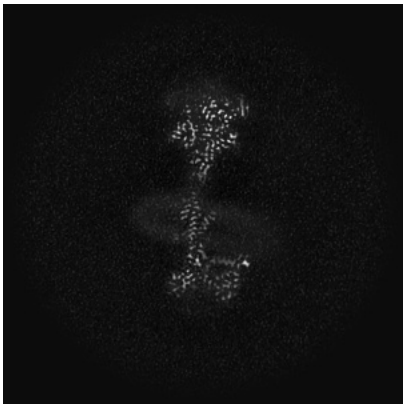


Z

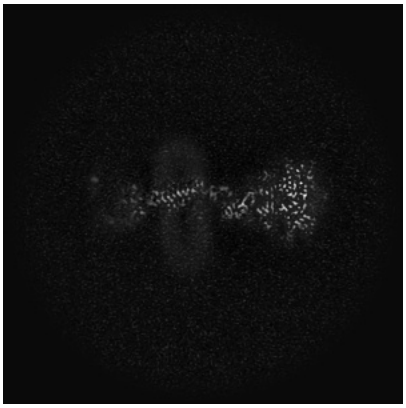
The images above show the map projected in three orthogonal directions.

6.2 Central slices

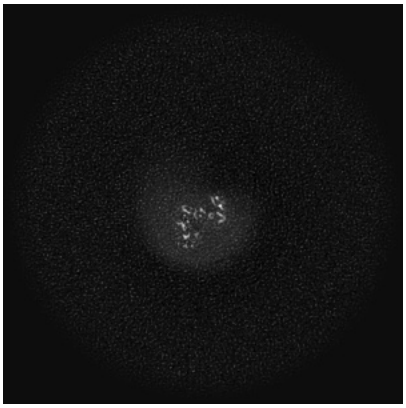
6.2.1 Primary map



X Index: 240



Y Index: 240

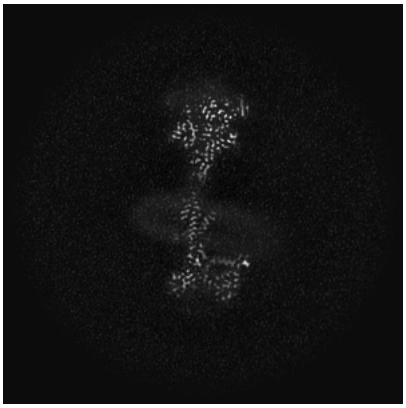


Z Index: 240

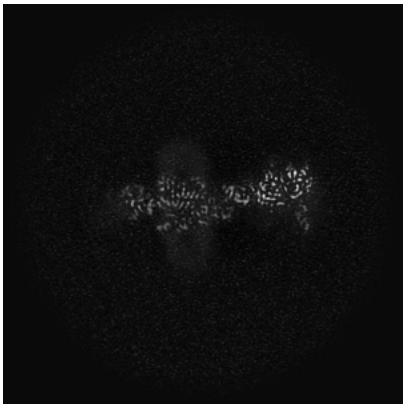
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

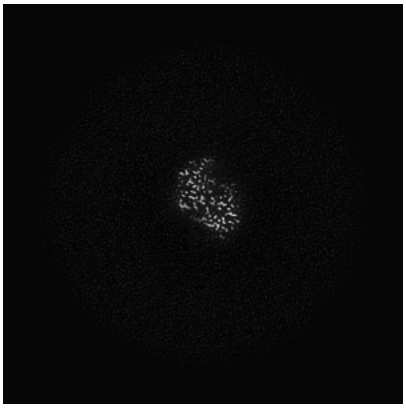
6.3.1 Primary map



X Index: 240



Y Index: 226

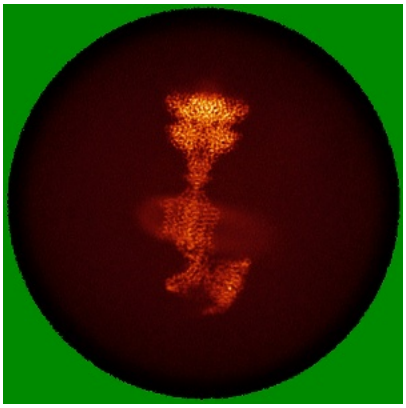


Z Index: 350

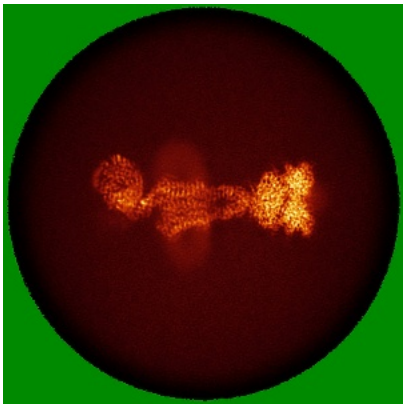
The images above show the largest variance slices of the map in three orthogonal directions.

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

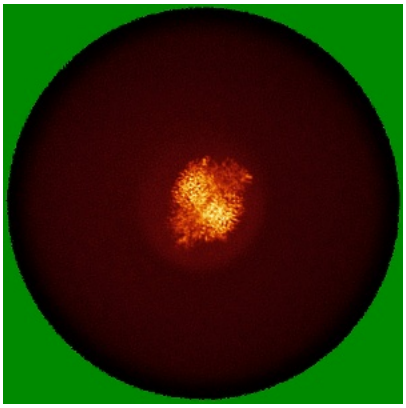
6.4.1 Primary map



X



Y

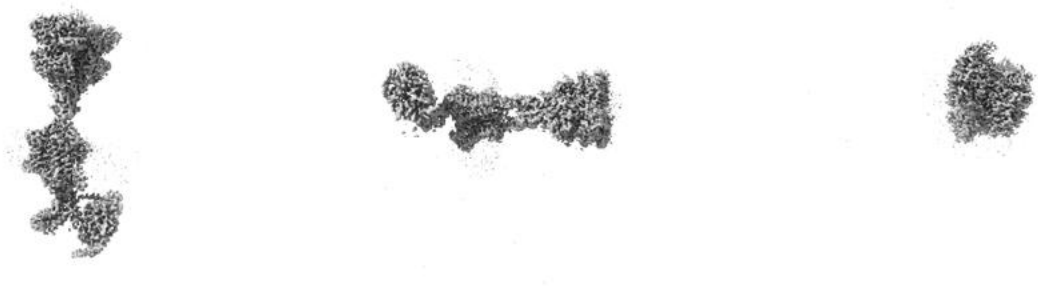


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

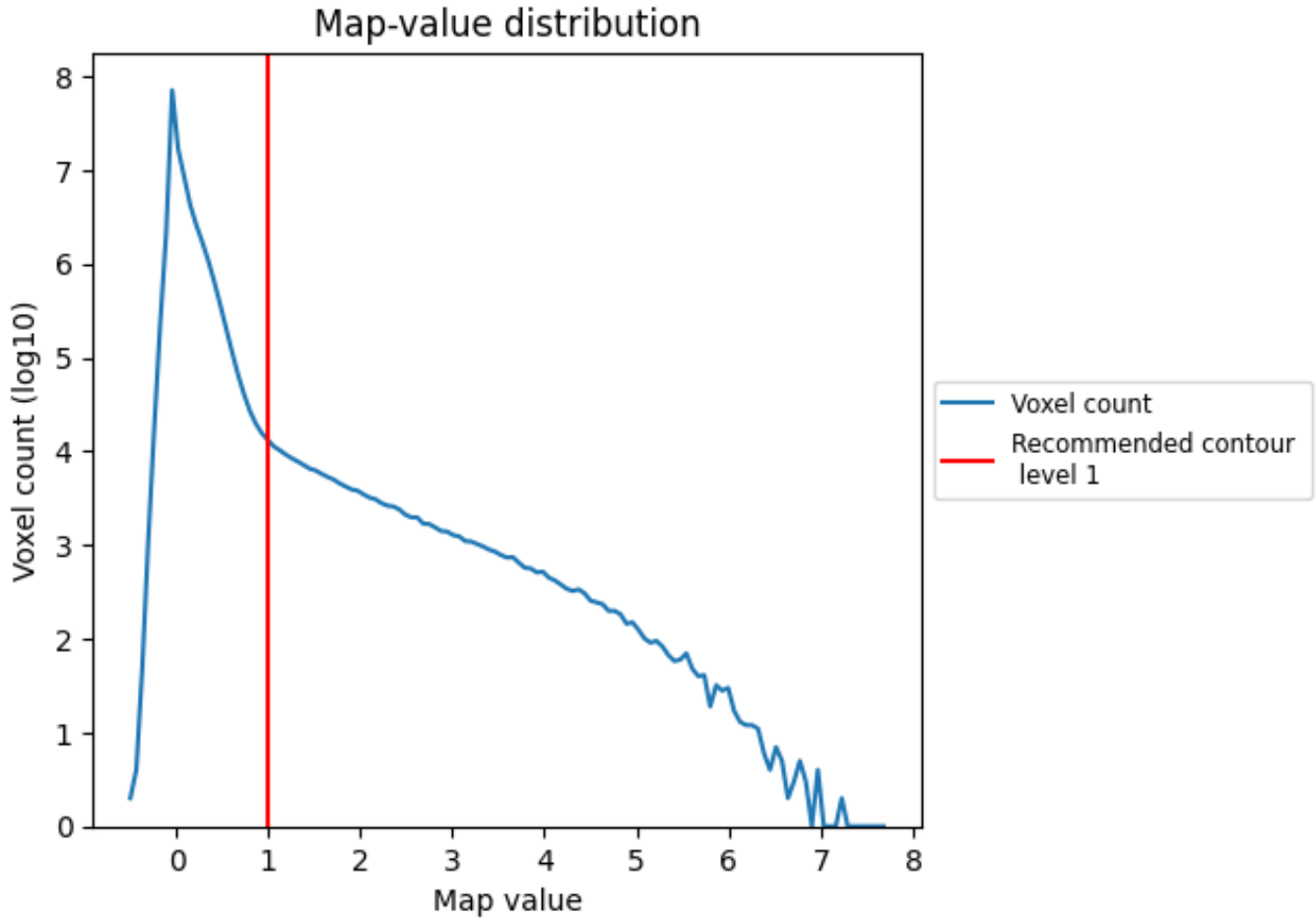
6.6 Mask visualisation (i)

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

7 Map analysis

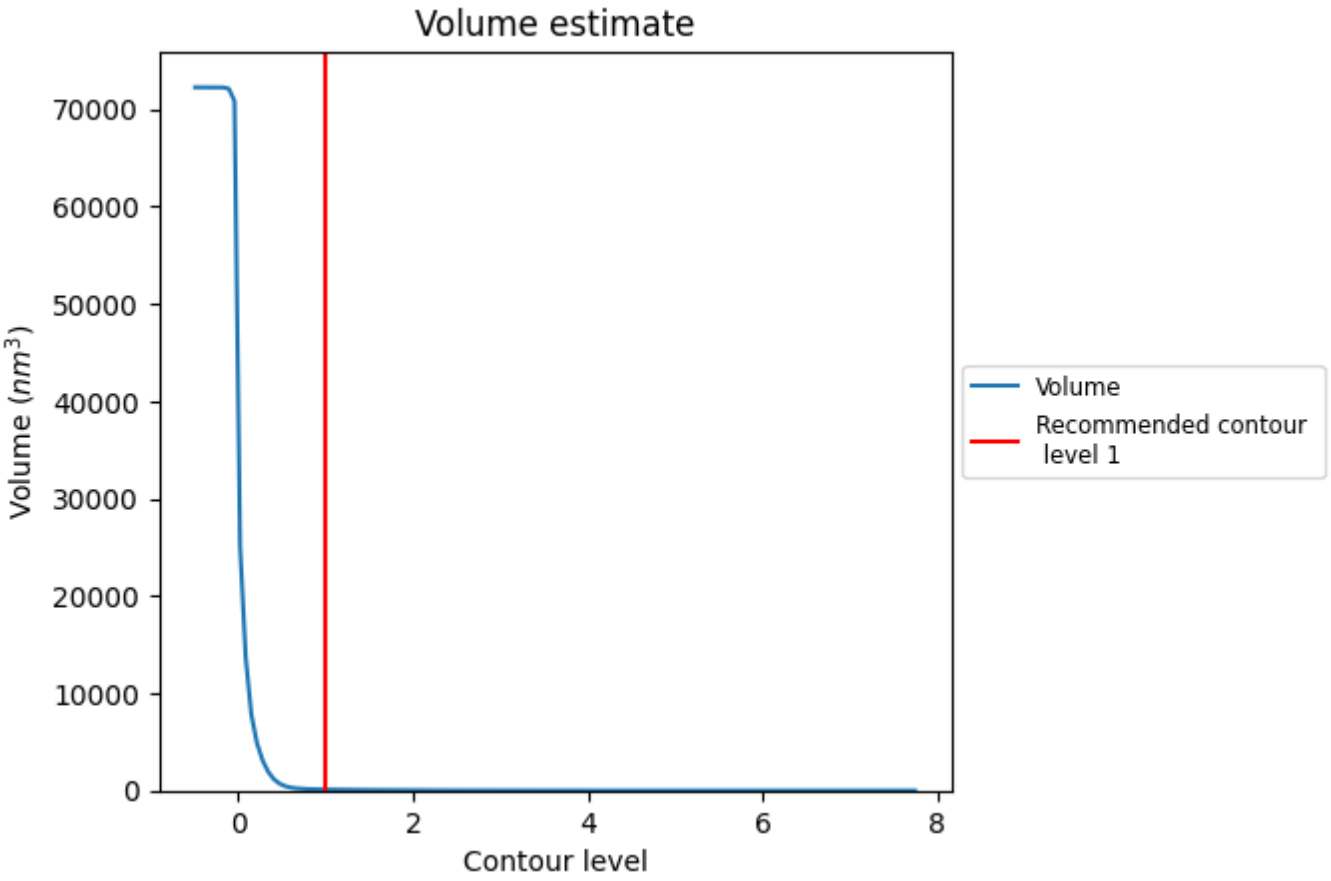
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

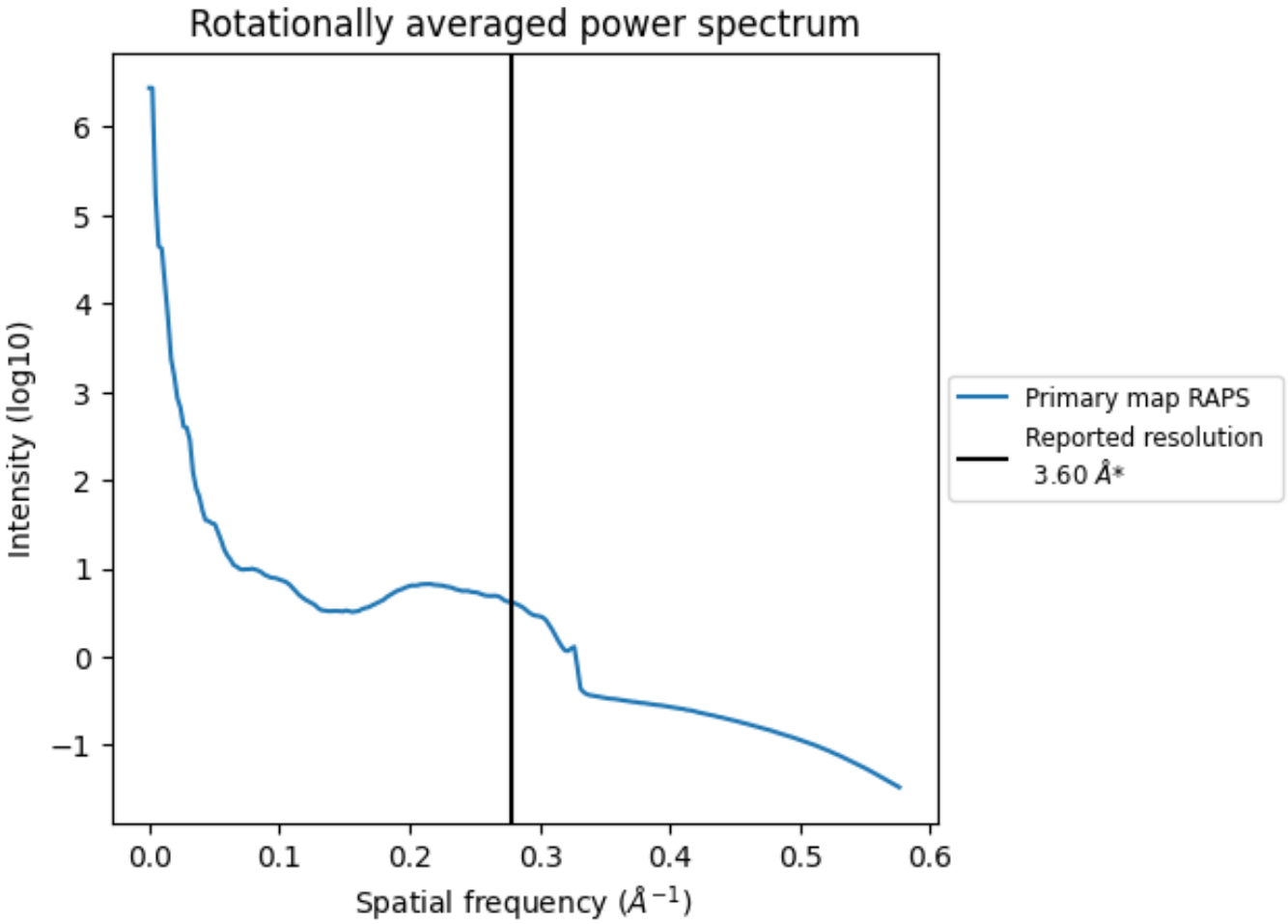
7.2 Volume estimate (i)



The volume at the recommended contour level is 108 nm^3; this corresponds to an approximate mass of 98 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

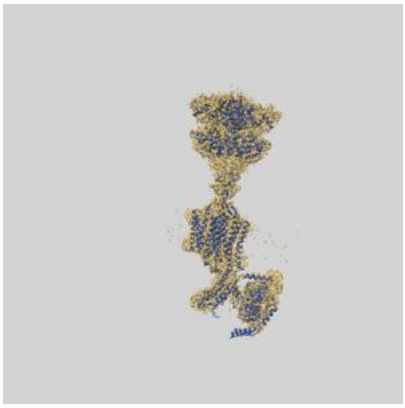
8 Fourier-Shell correlation

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

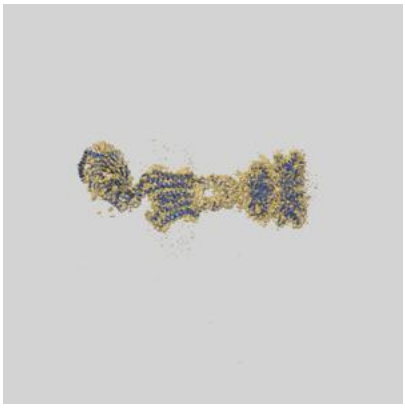
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40915 and PDB model 8SZG. Per-residue inclusion information can be found in section 3 on page 19.

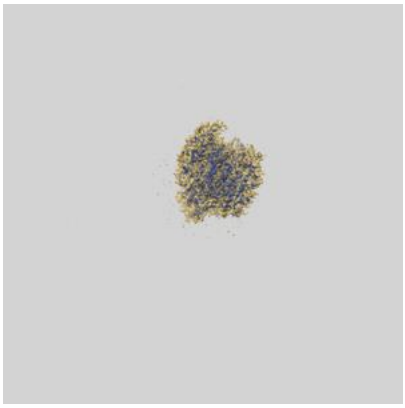
9.1 Map-model overlay



X



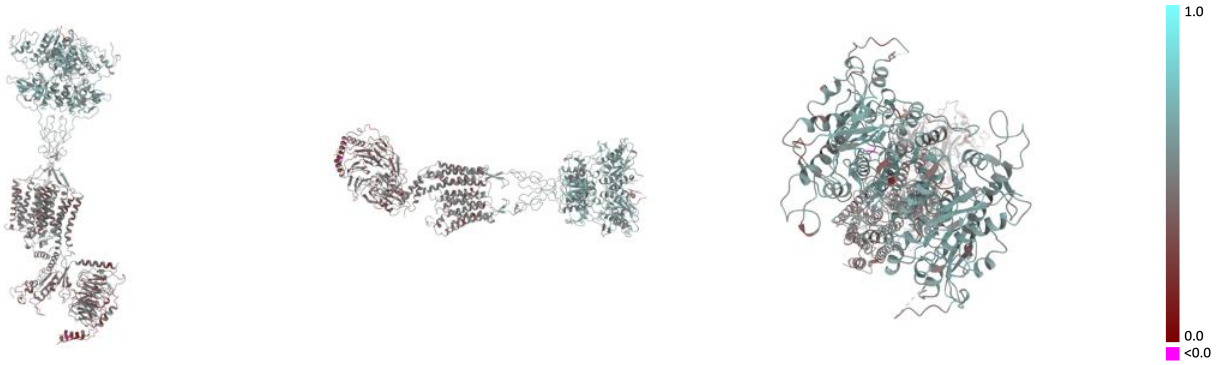
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

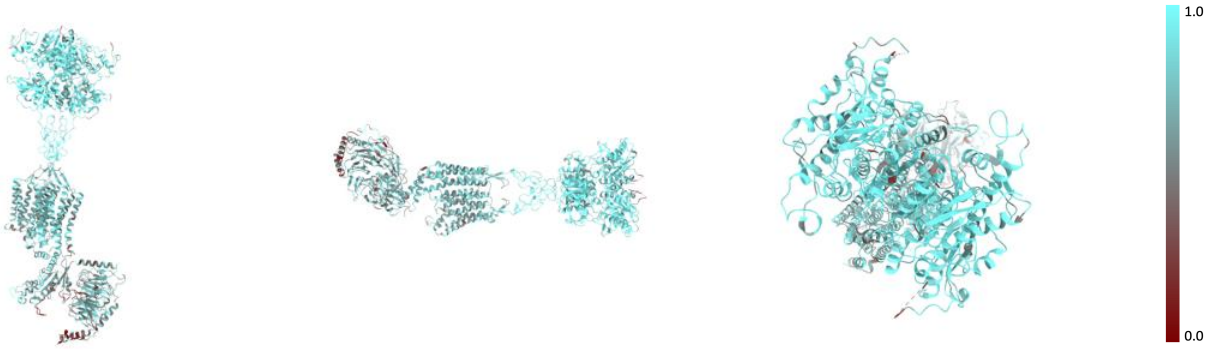
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

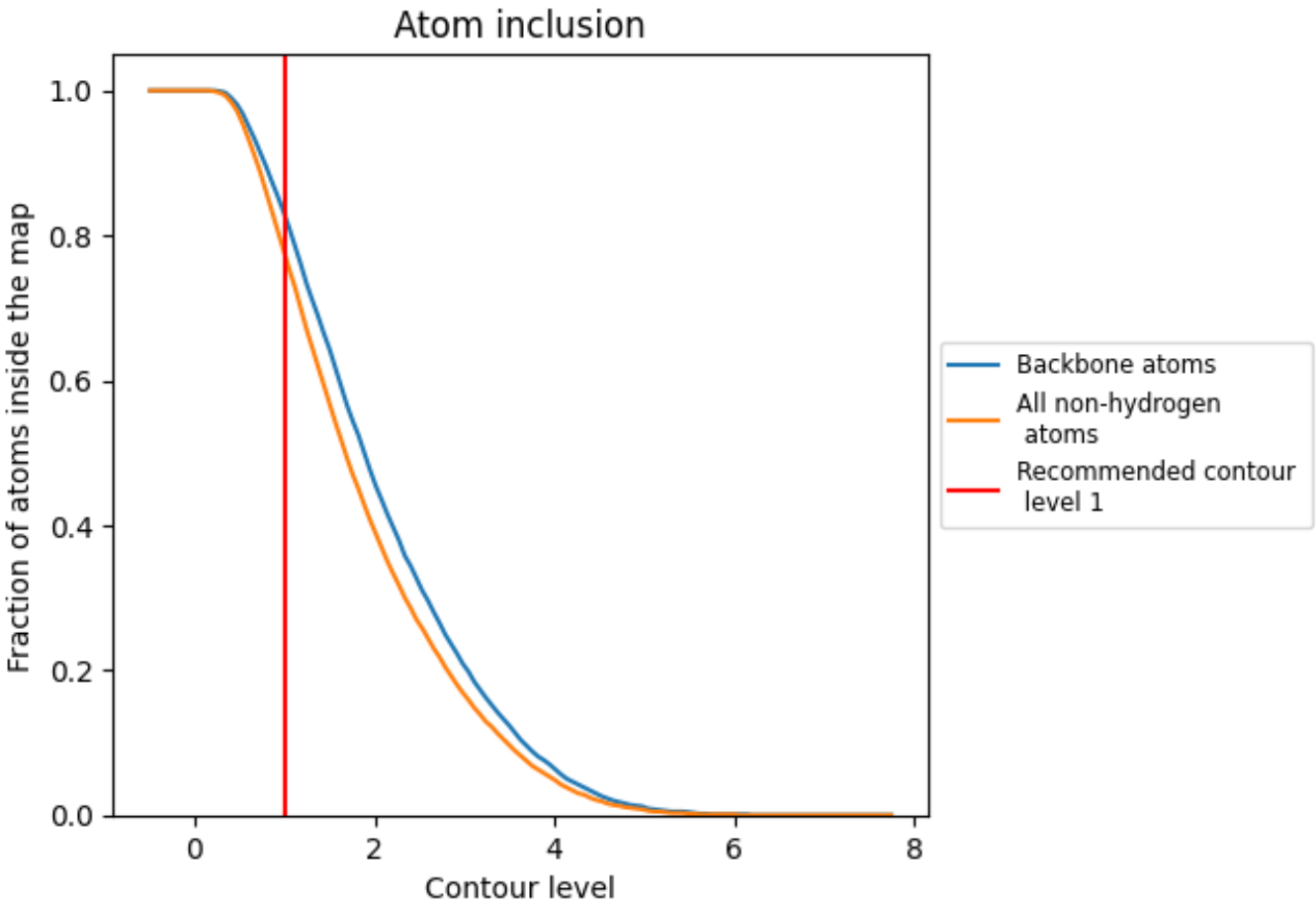
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (1).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7750	0.4910
A	0.8350	0.5250
B	0.8200	0.5160
C	0.6240	0.4060
D	0.6360	0.4070
E	0.5480	0.3710
F	0.5000	0.4580
G	0.8570	0.5050
H	0.8930	0.5500