Full wwPDB EM Validation Report ⓘ

May 13, 2025 – 03:24 PM EDT

PDB ID	:	9C1P / pdb_00009c1p
EMDB ID	:	EMD-45127
Title	:	Structure of Calcium-Sensing Receptor in complex with positive allosteric modulator '6218
Authors	:	Wu, C.; Skiniotis, G.
Deposited on	:	2024-05-29
Resolution	:	2.80 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:

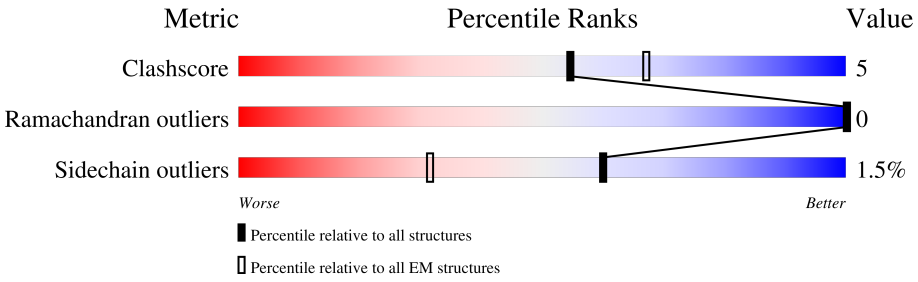
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 <=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	959	10% 69% 11% 19%
2	B	939	11% 71% 11% 18%

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
6	PO4	A	1007	-	-	X	-
6	PO4	B	1007	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12245 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
			Total	C	N	O	S		
1	A	772	6034	3920	983	1096	35	1	0

There are 83 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	TRP	-	expression tag	UNP P41180
A	-12	SER	-	expression tag	UNP P41180
A	-11	HIS	-	expression tag	UNP P41180
A	-10	PRO	-	expression tag	UNP P41180
A	-9	GLN	-	expression tag	UNP P41180
A	-8	PHE	-	expression tag	UNP P41180
A	-7	GLU	-	expression tag	UNP P41180
A	-6	LYS	-	expression tag	UNP P41180
A	-5	GLY	-	expression tag	UNP P41180
A	-4	GLY	-	expression tag	UNP P41180
A	-3	GLY	-	expression tag	UNP P41180
A	-2	SER	-	expression tag	UNP P41180
A	-1	GLY	-	expression tag	UNP P41180
A	0	GLY	-	expression tag	UNP P41180
A	1	GLY	-	expression tag	UNP P41180
A	2	SER	-	expression tag	UNP P41180
A	3	GLY	-	expression tag	UNP P41180
A	4	GLY	-	expression tag	UNP P41180
A	5	SER	-	expression tag	UNP P41180
A	6	ALA	-	expression tag	UNP P41180
A	7	TRP	-	expression tag	UNP P41180
A	8	SER	-	expression tag	UNP P41180
A	9	HIS	-	expression tag	UNP P41180
A	10	PRO	-	expression tag	UNP P41180
A	11	GLN	-	expression tag	UNP P41180
A	12	PHE	-	expression tag	UNP P41180
A	13	GLU	-	expression tag	UNP P41180
A	14	LYS	-	expression tag	UNP P41180

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	expression tag	UNP P41180
A	16	SER	-	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	GLY	-	expression tag	UNP P41180
A	897	SER	-	expression tag	UNP P41180
A	898	SER	-	expression tag	UNP P41180
A	899	THR	-	expression tag	UNP P41180
A	900	ASN	-	expression tag	UNP P41180
A	901	ASN	-	expression tag	UNP P41180
A	902	ASN	-	expression tag	UNP P41180
A	903	GLU	-	expression tag	UNP P41180
A	904	GLU	-	expression tag	UNP P41180
A	905	GLU	-	expression tag	UNP P41180
A	906	LYS	-	expression tag	UNP P41180
A	907	SER	-	expression tag	UNP P41180
A	908	ARG	-	expression tag	UNP P41180
A	909	LEU	-	expression tag	UNP P41180
A	910	LEU	-	expression tag	UNP P41180
A	911	GLU	-	expression tag	UNP P41180
A	912	LYS	-	expression tag	UNP P41180
A	913	GLU	-	expression tag	UNP P41180
A	914	ASN	-	expression tag	UNP P41180
A	915	ARG	-	expression tag	UNP P41180
A	916	GLU	-	expression tag	UNP P41180
A	917	LEU	-	expression tag	UNP P41180
A	918	GLU	-	expression tag	UNP P41180
A	919	LYS	-	expression tag	UNP P41180
A	920	ILE	-	expression tag	UNP P41180
A	921	ILE	-	expression tag	UNP P41180
A	922	ALA	-	expression tag	UNP P41180
A	923	GLU	-	expression tag	UNP P41180
A	924	LYS	-	expression tag	UNP P41180
A	925	GLU	-	expression tag	UNP P41180
A	926	GLU	-	expression tag	UNP P41180
A	927	ARG	-	expression tag	UNP P41180
A	928	VAL	-	expression tag	UNP P41180
A	929	SER	-	expression tag	UNP P41180
A	930	GLU	-	expression tag	UNP P41180
A	931	LEU	-	expression tag	UNP P41180
A	932	ARG	-	expression tag	UNP P41180

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Chain	Residue	Modelled	Actual	Comment	Reference
A	933	HIS	-	expression tag	UNP P41180
A	934	GLN	-	expression tag	UNP P41180
A	935	LEU	-	expression tag	UNP P41180
A	936	GLN	-	expression tag	UNP P41180
A	937	SER	-	expression tag	UNP P41180
A	938	ARG	-	expression tag	UNP P41180
A	939	GLN	-	expression tag	UNP P41180
A	940	GLN	-	expression tag	UNP P41180
A	941	LEU	-	expression tag	UNP P41180
A	942	LYS	-	expression tag	UNP P41180
A	943	LYS	-	expression tag	UNP P41180
A	944	THR	-	expression tag	UNP P41180
A	945	ASN	-	expression tag	UNP P41180

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	769	Total	C	N	O	S	0	0
			6031	3913	980	1104	34		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	ASP	-	expression tag	UNP P41180
B	10	TYR	-	expression tag	UNP P41180
B	11	LYS	-	expression tag	UNP P41180
B	12	ASP	-	expression tag	UNP P41180
B	13	ASP	-	expression tag	UNP P41180
B	14	ASP	-	expression tag	UNP P41180
B	15	ASP	-	expression tag	UNP P41180
B	16	LYS	-	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	SER	-	expression tag	UNP P41180
B	897	THR	-	expression tag	UNP P41180
B	898	SER	-	expression tag	UNP P41180
B	899	VAL	-	expression tag	UNP P41180
B	900	THR	-	expression tag	UNP P41180
B	901	SER	-	expression tag	UNP P41180
B	902	VAL	-	expression tag	UNP P41180
B	903	ASN	-	expression tag	UNP P41180

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Chain	Residue	Modelled	Actual	Comment	Reference
B	904	GLN	-	expression tag	UNP P41180
B	905	ALA	-	expression tag	UNP P41180
B	906	SER	-	expression tag	UNP P41180
B	907	THR	-	expression tag	UNP P41180
B	908	SER	-	expression tag	UNP P41180
B	909	ARG	-	expression tag	UNP P41180
B	910	LEU	-	expression tag	UNP P41180
B	911	GLU	-	expression tag	UNP P41180
B	912	GLY	-	expression tag	UNP P41180
B	913	LEU	-	expression tag	UNP P41180
B	914	GLN	-	expression tag	UNP P41180
B	915	SER	-	expression tag	UNP P41180
B	916	GLU	-	expression tag	UNP P41180
B	917	ASN	-	expression tag	UNP P41180
B	918	HIS	-	expression tag	UNP P41180
B	919	ARG	-	expression tag	UNP P41180
B	920	LEU	-	expression tag	UNP P41180
B	921	ARG	-	expression tag	UNP P41180
B	922	MET	-	expression tag	UNP P41180
B	923	LYS	-	expression tag	UNP P41180
B	924	ILE	-	expression tag	UNP P41180
B	925	THR	-	expression tag	UNP P41180
B	926	GLU	-	expression tag	UNP P41180
B	927	LEU	-	expression tag	UNP P41180
B	928	ASP	-	expression tag	UNP P41180
B	929	LYS	-	expression tag	UNP P41180
B	930	ASP	-	expression tag	UNP P41180
B	931	LEU	-	expression tag	UNP P41180
B	932	GLU	-	expression tag	UNP P41180
B	933	GLU	-	expression tag	UNP P41180
B	934	VAL	-	expression tag	UNP P41180
B	935	THR	-	expression tag	UNP P41180
B	936	MET	-	expression tag	UNP P41180
B	937	GLN	-	expression tag	UNP P41180
B	938	LEU	-	expression tag	UNP P41180
B	939	GLN	-	expression tag	UNP P41180
B	940	ASP	-	expression tag	UNP P41180
B	941	THR	-	expression tag	UNP P41180
B	942	PRO	-	expression tag	UNP P41180
B	943	GLU	-	expression tag	UNP P41180
B	944	LYS	-	expression tag	UNP P41180
B	945	LYS	-	expression tag	UNP P41180

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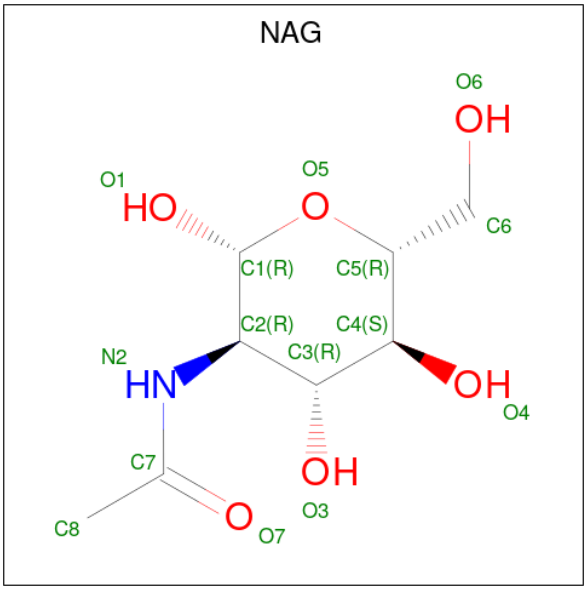
Chain	Residue	Modelled	Actual	Comment	Reference
B	946	THR	-	expression tag	UNP P41180
B	947	ASN	-	expression tag	UNP P41180

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

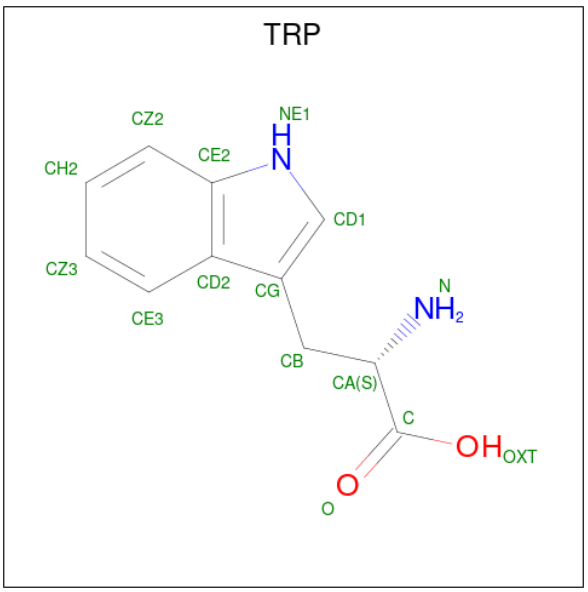


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

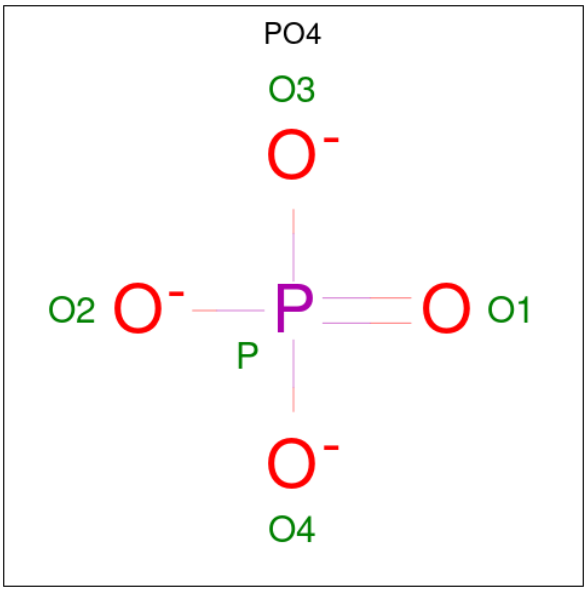
Mol	Chain	Residues	Atoms		AltConf
4	A	5	Total	Ca	0
			5	5	
4	B	3	Total	Ca	0
			3	3	

- Molecule 5 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



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

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

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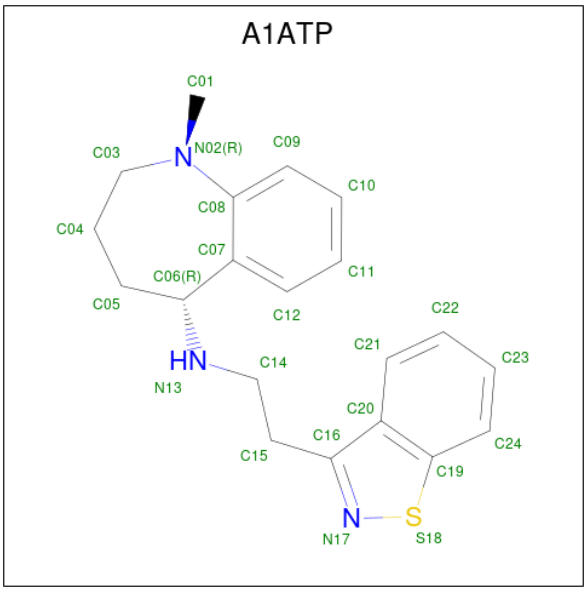
Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total O P 5 4 1	0

- Molecule 7 is (5R)-N-[2-(1,2-benzothiazol-3-yl)ethyl]-1-methyl-2,3,4,5-tetrahydro-1H-1-benzazepin-5-amine (CCD ID: A1ATP) (formula: $C_{20}H_{23}N_3S$) (labeled as "Ligand of Interest" by depositor).



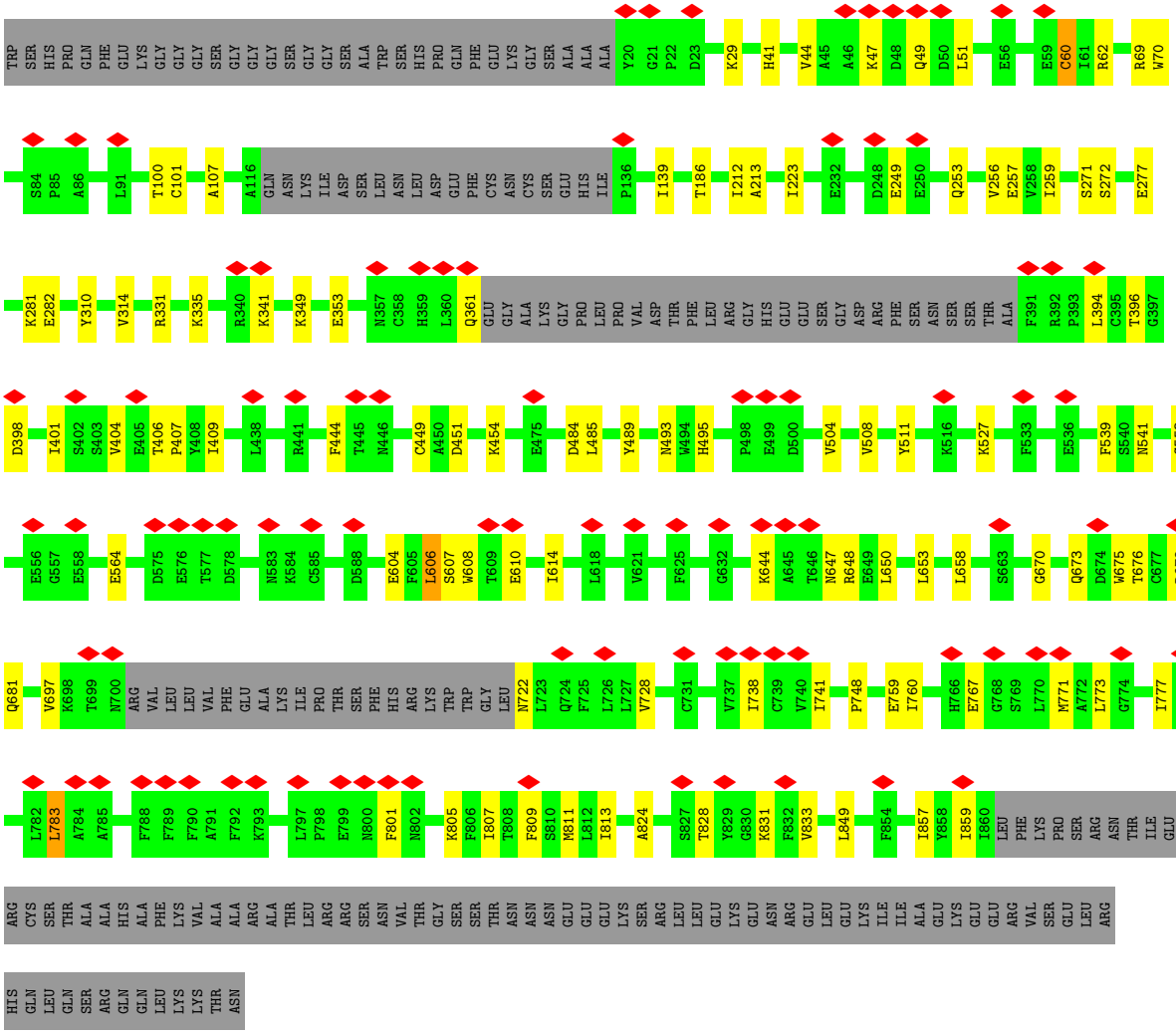
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C N S 24 20 3 1	0
7	B	1	Total C N S 24 20 3 1	0

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.

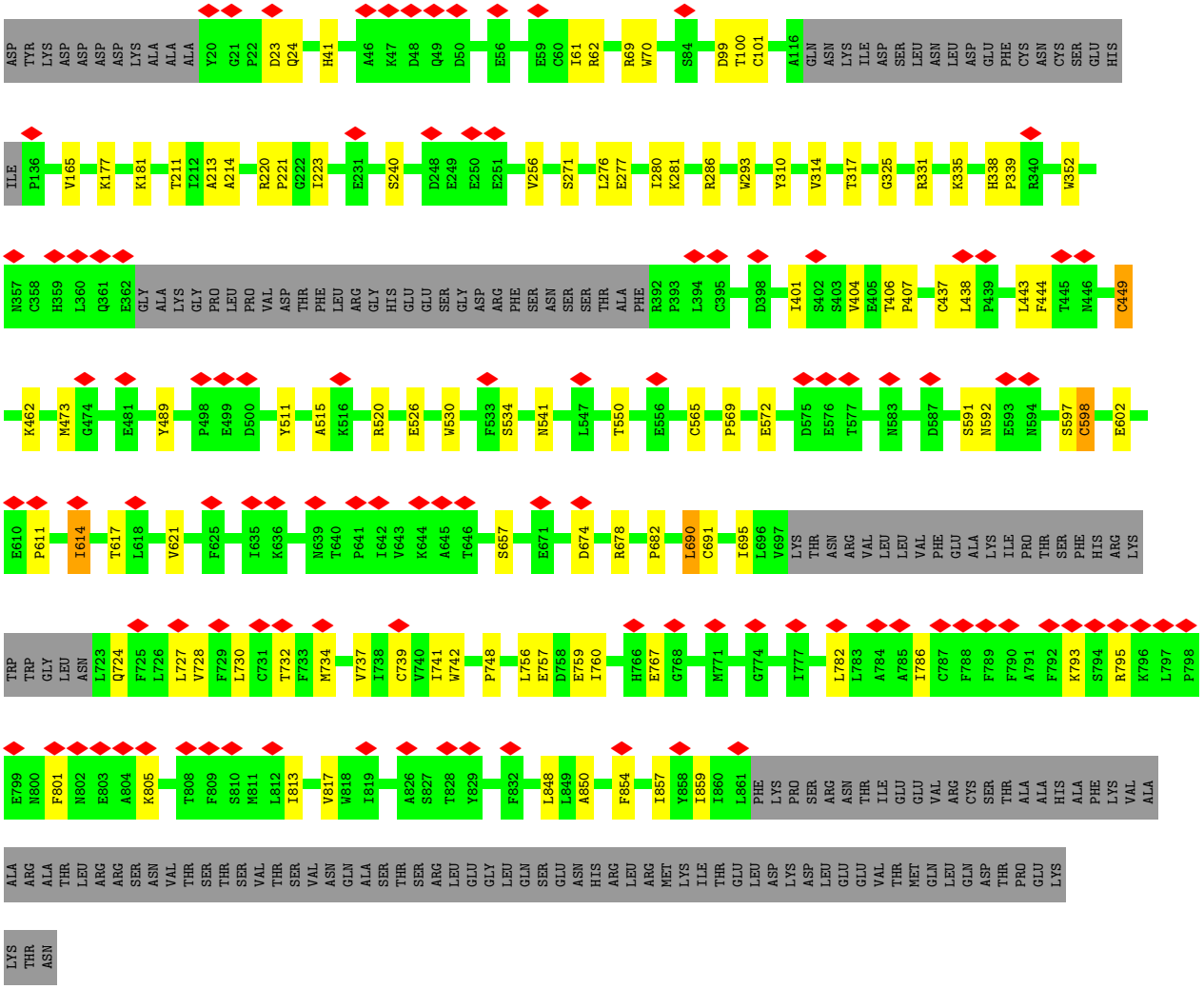
• Molecule 1: Extracellular calcium-sensing receptor

Chain A:



• Molecule 2: Extracellular calcium-sensing receptor

Chain B:


ASP TYR LYS ASP ASP ASP LYS ALA ALA ALA Y20 G21 P22 D23 Q24 H41 A46 K47 D48 Q49 D50 E56 E59 C60 I61 R62 R69 W70 S84 D99 T100 C101 A116 GLN ASN LYS ILE ASP SER LEU ASN LEU ASP GLU PHE CYS ASN CYS SER GLU HIS
ILE P136 V165 K177 K181 T211 I212 A213 A214 R220 P221 G222 I223 E231 S240 D248 E249 E250 E251 V256 S271 L276 E277 I280 K281 R286 W293 Y310 V314 T317 G325 R331 K335 H338 P339 R340 W352
N357 C358 H359 L360 Q361 E362 GLY ALA LYS GLY PRO LEU PRO VAL ASP THR PHE LEU ARG GLY HIS GLU GLU SER GLY ASP ARG PHE SER ASN SER SER THR ALA PHE R392 P393 L394 C396 D398 I401 S402 S403 V404 E405 T406 P407 C437 L438 P439 L443 F444 T445 N446 C449
K462 M473 G474 E481 Y489 P498 E499 D500 Y511 A515 K516 R520 E526 W530 F533 S534 N541 L547 T550 E556 C565 P569 E572 D575 E576 T577 N583 D587 S591 N592 E593 N594 S597 C598 E602
E610 P611 I614 T617 L618 V621 F625 I635 K636 N639 T640 P641 I642 V643 K644 A645 T646 S657 E671 D674 R678 P682 L690 C691 I695 L696 V697 LYS THR ASN ARG VAL LEU LEU VAL PHE GLU ALA LYS ILE PRO THR SER PHE HIS ARG LYS
TRP TRP GLY LEU ASN L723 Q724 F725 L726 L727 V728 F729 L730 C731 T732 F733 M734 V737 I738 C739 Y740 I741 W742 P748 L756 E757 D758 E759 I760 H766 E767 G768 M771 G774 I777 L782 L783 A784 A785 I786 C787 F788 F789 F790 A791 F792 K793 S794 R795 K796 L797 P798
E799 N800 F801 N802 E803 A804 K805 T808 F809 S810 M811 L812 I813 V817 W818 I819 A826 S827 T828 Y829 F832 L848 L849 A850 F854 I857 Y858 I859 I860 L861 PHE LYS PRO SER ARG ASN THR ILE GLU GLU VAL ARG CYS SER THR ALA ALA HIS ALA PHE LYS VAL ALA
ALA ARG ALA THR LEU ARG ARG SER ASN VAL THR SER THR SER VAL THR SER VAL ASN GLN ALA SER THR SER ARG LEU GLU GLY LEU GLN SER GLU ASN HIS ARG LEU ARG MET LYS ILE THR GLU LEU ASP LYS ASP LEU GLU GLU VAL THR MET GLN LEU GLN ASP THR PRO GLU LYS
LYS THR ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	346741	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.543	Depositor
Minimum map value	-0.526	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.384	Depositor
Map size (Å)	444.2624, 444.2624, 444.2624	wwPDB
Map dimensions	512, 512, 512	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, CA, A1ATP, 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	A	0.16	0/6184	0.31	0/8399
2	B	0.12	0/6182	0.28	0/8395
All	All	0.14	0/12366	0.30	0/16794

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

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	6034	0	5888	60	0
2	B	6031	0	5872	59	0
3	A	42	0	39	1	0
3	B	42	0	39	1	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
5	A	15	0	9	0	0
5	B	15	0	9	0	0
6	A	5	0	0	2	0
6	B	5	0	0	2	0
7	A	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	24	0	0	0	0
All	All	12245	0	11856	118	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 5.

All (118) 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:213:ALA:HB2	2:B:223:ILE:HG13	1.65	0.79
1:A:644:LYS:HG3	1:A:648:ARG:HH21	1.57	0.69
1:A:213:ALA:HB2	1:A:223:ILE:HG13	1.73	0.69
1:A:44:VAL:HA	1:A:60:CYS:HA	1.74	0.68
1:A:647:ASN:HB2	1:A:650:LEU:HB2	1.78	0.66
1:A:608:TRP:O	1:A:614:ILE:CD1	2.45	0.65
2:B:277:GLU:HG2	2:B:281:LYS:HE2	1.81	0.63
2:B:657:SER:OG	2:B:691:CYS:SG	2.57	0.63
2:B:813:ILE:O	2:B:817:VAL:HG23	1.98	0.62
1:A:673:GLN:OE1	1:A:675:TRP:NE1	2.30	0.62
1:A:70:TRP:NE1	6:A:1007:PO4:O4	2.30	0.62
2:B:795:ARG:HG3	2:B:805:LYS:HG2	1.83	0.61
1:A:47:LYS:HE3	1:A:49:GLN:HG3	1.81	0.61
1:A:444:PHE:HD2	1:A:449:CYS:HA	1.65	0.60
2:B:592:ASN:ND2	2:B:597:SER:O	2.34	0.60
1:A:828:THR:HG23	1:A:833:VAL:HG22	1.84	0.60
2:B:682:PRO:HB3	2:B:739:CYS:SG	2.42	0.60
1:A:69:ARG:NH2	6:A:1007:PO4:O2	2.34	0.59
2:B:41:HIS:ND1	2:B:62:ARG:O	2.33	0.59
2:B:530:TRP:O	2:B:534:SER:OG	2.21	0.59
2:B:69:ARG:NH2	6:B:1007:PO4:O2	2.35	0.58
1:A:69:ARG:NH1	1:A:407:PRO:O	2.37	0.58
1:A:361:GLN:HG2	1:A:394:LEU:HD11	1.85	0.58
1:A:396:THR:HG23	1:A:398:ASP:H	1.69	0.57
1:A:349:LYS:O	1:A:353:GLU:HG2	2.04	0.57
2:B:69:ARG:NH1	2:B:407:PRO:O	2.37	0.57
2:B:256:VAL:HG11	2:B:286:ARG:HD3	1.88	0.56
2:B:759:GLU:O	2:B:759:GLU:HG2	2.06	0.56
2:B:617:THR:O	2:B:621:VAL:HG22	2.07	0.55
1:A:100:THR:HG23	1:A:107:ALA:HB2	1.87	0.55
2:B:23:ASP:OD1	2:B:24:GLN:N	2.40	0.55
2:B:214:ALA:HB2	2:B:271:SER:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:TRP:NE1	6:B:1007:PO4:O3	2.36	0.54
2:B:293:TRP:HB2	2:B:317:THR:HG23	1.89	0.54
1:A:51:LEU:HB2	2:B:462:LYS:HB2	1.90	0.54
1:A:271:SER:OG	1:A:272:SER:N	2.40	0.54
2:B:444:PHE:HD2	2:B:449:CYS:HA	1.72	0.53
2:B:489:TYR:HB2	2:B:511:TYR:HB3	1.90	0.53
2:B:550:THR:HG21	2:B:565:CYS:HB3	1.91	0.53
2:B:437:CYS:SG	2:B:438:LEU:N	2.82	0.53
1:A:539:PHE:CZ	1:A:541:ASN:HB2	2.44	0.52
2:B:331:ARG:HG2	2:B:335:LYS:HD2	1.90	0.52
1:A:608:TRP:O	1:A:614:ILE:HD11	2.08	0.52
1:A:606:LEU:HD12	1:A:610:GLU:HG2	1.92	0.51
1:A:678:ARG:HA	1:A:748:PRO:HG2	1.92	0.51
2:B:515:ALA:O	2:B:520:ARG:NH1	2.44	0.51
1:A:801:PHE:HE2	1:A:859:ILE:HG21	1.76	0.51
1:A:809:PHE:O	1:A:813:ILE:HG22	2.10	0.51
2:B:727:LEU:HD12	2:B:730:LEU:HD11	1.94	0.50
2:B:443:LEU:O	2:B:462:LYS:NZ	2.44	0.50
1:A:489:TYR:HB2	1:A:511:TYR:HB3	1.95	0.48
2:B:591:SER:HA	2:B:598:CYS:HB3	1.96	0.48
1:A:454:LYS:HE2	1:A:454:LYS:HB2	1.71	0.48
2:B:211:THR:OG1	2:B:240:SER:OG	2.27	0.48
1:A:773:LEU:O	1:A:777:ILE:HG13	2.14	0.48
2:B:737:VAL:O	2:B:741:ILE:HG12	2.13	0.47
2:B:310:TYR:O	2:B:314:VAL:HG22	2.15	0.47
1:A:335:LYS:HA	1:A:401:ILE:HD11	1.96	0.47
2:B:742:TRP:HE1	2:B:748:PRO:HD3	1.80	0.47
2:B:782:LEU:O	2:B:786:ILE:HG22	2.15	0.47
1:A:310:TYR:O	1:A:314:VAL:HG22	2.15	0.47
2:B:338:HIS:ND1	2:B:339:PRO:HD2	2.30	0.47
2:B:602:GLU:HB2	2:B:760:ILE:HD13	1.96	0.47
2:B:674:ASP:O	2:B:678:ARG:HG3	2.14	0.46
2:B:748:PRO:HB3	2:B:767:GLU:HA	1.97	0.46
1:A:212:ILE:HD11	1:A:259:ILE:HD11	1.96	0.46
1:A:404:VAL:HG12	1:A:406:THR:HG23	1.96	0.46
1:A:541:ASN:OD1	3:A:1011:NAG:N2	2.48	0.46
1:A:604:GLU:HG3	1:A:831:LYS:HD3	1.96	0.46
2:B:690:LEU:HD12	2:B:732:THR:OG1	2.16	0.45
1:A:771:MET:HE2	1:A:771:MET:HA	1.99	0.45
1:A:41:HIS:ND1	1:A:62:ARG:O	2.50	0.45
1:A:607:SER:HA	1:A:670:GLY:HA2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:GLY:HA2	2:B:473:MET:HE1	1.99	0.45
1:A:331:ARG:NH2	1:A:409:ILE:O	2.51	0.44
2:B:61:ILE:HG22	2:B:62:ARG:HG3	1.98	0.44
1:A:29:LYS:HE3	1:A:29:LYS:HA	1.98	0.44
2:B:177:LYS:HA	2:B:177:LYS:HD3	1.62	0.44
2:B:541:ASN:HD21	3:B:1009:NAG:H2	1.81	0.44
1:A:658:LEU:HD13	1:A:849:LEU:HB2	1.99	0.44
1:A:807:ILE:O	1:A:811:MET:HG2	2.18	0.44
1:A:680:ARG:HG3	1:A:681:GLN:HG2	2.00	0.44
2:B:850:ALA:HA	2:B:854:PHE:CD2	2.53	0.44
1:A:277:GLU:HG2	1:A:281:LYS:HD2	2.00	0.43
1:A:249:GLU:O	1:A:253:GLN:HG3	2.18	0.43
1:A:253:GLN:O	1:A:257:GLU:HG3	2.19	0.43
2:B:404:VAL:HG12	2:B:406:THR:HG23	2.00	0.43
2:B:742:TRP:CD1	2:B:742:TRP:C	2.96	0.43
1:A:493:ASN:HD22	1:A:495:HIS:CD2	2.37	0.43
1:A:553:GLY:N	1:A:564:GLU:O	2.51	0.43
1:A:857:ILE:HD13	1:A:857:ILE:HA	1.86	0.43
2:B:99:ASP:OD1	2:B:100:THR:N	2.51	0.43
1:A:186:THR:HA	1:A:485:LEU:HD12	2.00	0.43
2:B:220:ARG:HB2	2:B:221:PRO:HD3	2.01	0.43
2:B:41:HIS:HB2	2:B:101:CYS:SG	2.59	0.42
1:A:697:VAL:HG21	1:A:728:VAL:HG23	1.99	0.42
1:A:759:GLU:OE1	1:A:759:GLU:N	2.51	0.42
2:B:438:LEU:HD23	2:B:438:LEU:HA	1.85	0.42
2:B:742:TRP:NE1	2:B:748:PRO:HD3	2.34	0.42
1:A:508:VAL:HG12	1:A:527:LYS:HB2	2.01	0.42
1:A:256:VAL:HG21	1:A:282:GLU:HG2	2.01	0.42
1:A:738:ILE:HA	1:A:741:ILE:HG22	2.01	0.41
2:B:801:PHE:CE2	2:B:859:ILE:HG13	2.54	0.41
1:A:748:PRO:HB3	1:A:767:GLU:HA	2.02	0.41
1:A:783:LEU:HD23	1:A:783:LEU:HA	1.82	0.41
2:B:569:PRO:HG2	2:B:572:GLU:HG3	2.01	0.41
2:B:793:LYS:HE2	2:B:793:LYS:HB3	1.86	0.41
1:A:451:ASP:N	1:A:451:ASP:OD1	2.51	0.41
2:B:352:TRP:CZ3	2:B:401:ILE:HD11	2.55	0.41
2:B:181:LYS:HZ2	2:B:181:LYS:HG2	1.77	0.41
2:B:756:LEU:HB3	2:B:757:GLU:OE2	2.20	0.41
1:A:341:LYS:HZ3	1:A:341:LYS:HG3	1.80	0.41
1:A:805:LYS:HB3	1:A:805:LYS:HE3	1.85	0.41
2:B:276:LEU:HG	2:B:280:ILE:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:611:PRO:O	2:B:614:ILE:HG22	2.21	0.41
1:A:60:CYS:HB3	1:A:101:CYS:HB3	1.90	0.41
1:A:824:ALA:O	1:A:828:THR:HG22	2.21	0.41
2:B:724:GLN:O	2:B:728:VAL:HG12	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	A	765/959 (80%)	746 (98%)	19 (2%)	0	100	100
2	B	761/939 (81%)	742 (98%)	19 (2%)	0	100	100
All	All	1526/1898 (80%)	1488 (98%)	38 (2%)	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	646/827 (78%)	636 (98%)	10 (2%)	60	86
2	B	648/817 (79%)	638 (98%)	10 (2%)	60	86
All	All	1294/1644 (79%)	1274 (98%)	20 (2%)	60	86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	CYS
1	A	139	ILE
1	A	484	ASP
1	A	504	VAL
1	A	606	LEU
1	A	653	LEU
1	A	676	THR
1	A	722	ASN
1	A	760	ILE
1	A	783	LEU
2	B	165	VAL
2	B	449	CYS
2	B	526	GLU
2	B	598	CYS
2	B	614	ILE
2	B	690	LEU
2	B	695	ILE
2	B	734	MET
2	B	848	LEU
2	B	857	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	72	GLN
1	A	344	HIS
1	A	345	ASN
1	A	463	HIS
1	A	493	ASN
2	B	24	GLN
2	B	344	HIS
2	B	400	ASN
2	B	459	GLN
2	B	472	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
7	A1ATP	A	1008	-	22,27,27	0.44	0	23,37,37	1.03	1 (4%)
5	TRP	A	1006	-	14,16,16	0.88	1 (7%)	13,22,22	1.16	1 (7%)
3	NAG	A	1011	1	14,14,15	0.82	0	17,19,21	1.09	1 (5%)
5	TRP	B	1003	-	14,16,16	0.88	1 (7%)	13,22,22	1.17	1 (7%)
3	NAG	B	1002	2	14,14,15	0.69	0	17,19,21	0.95	0
7	A1ATP	B	1008	-	22,27,27	0.45	0	23,37,37	1.00	1 (4%)
3	NAG	A	1010	1	14,14,15	0.72	0	17,19,21	1.01	1 (5%)
6	PO4	B	1007	-	4,4,4	1.53	1 (25%)	6,6,6	0.51	0
3	NAG	B	1001	2	14,14,15	0.70	0	17,19,21	1.22	1 (5%)
3	NAG	B	1009	-	14,14,15	0.71	0	17,19,21	0.98	0
6	PO4	A	1007	-	4,4,4	1.53	1 (25%)	6,6,6	0.47	0
3	NAG	A	1001	1	14,14,15	0.72	0	17,19,21	0.79	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
7	A1ATP	A	1008	-	-	3/4/20/20	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TRP	A	1006	-	-	0/7/8/8	0/2/2/2
3	NAG	A	1011	1	-	0/6/23/26	0/1/1/1
5	TRP	B	1003	-	-	1/7/8/8	0/2/2/2
3	NAG	B	1002	2	-	0/6/23/26	0/1/1/1
7	A1ATP	B	1008	-	-	1/4/20/20	0/4/4/4
3	NAG	A	1010	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1009	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1001	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1007	PO4	P-O1	2.69	1.56	1.50
6	A	1007	PO4	P-O1	2.68	1.56	1.50
5	B	1003	TRP	OXT-C	-2.28	1.23	1.30
5	A	1006	TRP	OXT-C	-2.27	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1008	A1ATP	C20-C19-S18	-4.36	108.67	112.25
7	B	1008	A1ATP	C20-C19-S18	-4.25	108.76	112.25
3	B	1001	NAG	C2-N2-C7	3.18	127.16	122.90
3	A	1011	NAG	C1-O5-C5	2.87	116.03	112.19
5	B	1003	TRP	OXT-C-O	-2.73	117.90	124.08
5	A	1006	TRP	OXT-C-O	-2.69	117.98	124.08
3	A	1010	NAG	C1-O5-C5	2.55	115.61	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

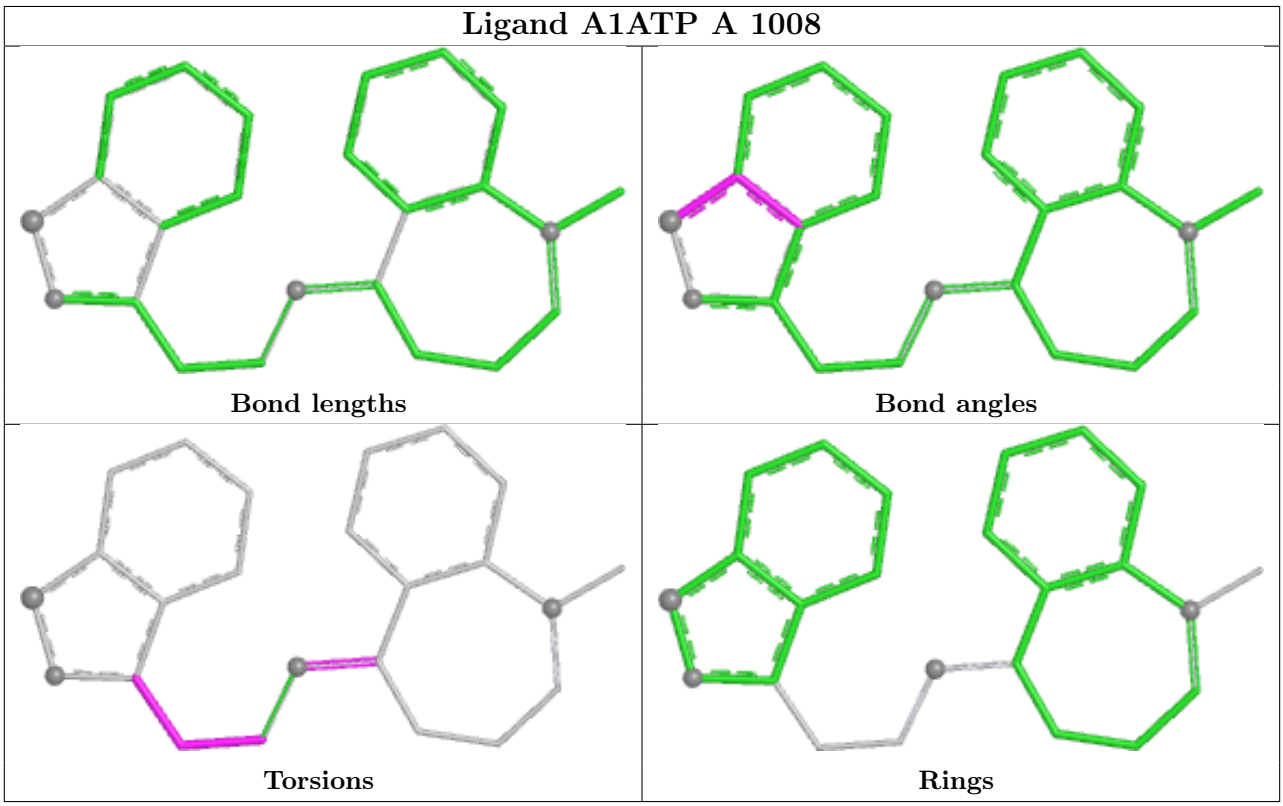
Mol	Chain	Res	Type	Atoms
7	A	1008	A1ATP	C14-C15-C16-C20
7	A	1008	A1ATP	C07-C06-N13-C14
7	A	1008	A1ATP	N13-C14-C15-C16
5	B	1003	TRP	CA-CB-CG-CD1
7	B	1008	A1ATP	C15-C14-N13-C06
3	B	1001	NAG	C3-C2-N2-C7
3	B	1001	NAG	C1-C2-N2-C7

There are no ring outliers.

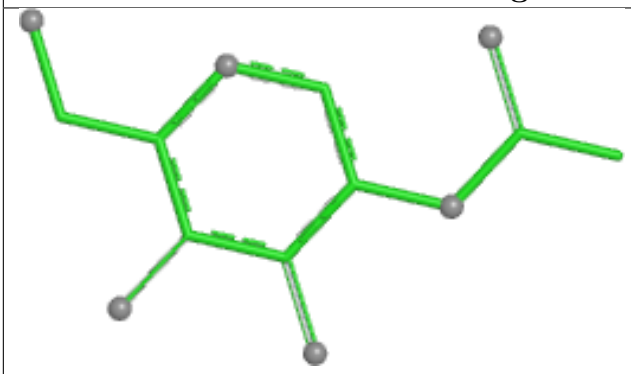
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1011	NAG	1	0
6	B	1007	PO4	2	0
3	B	1009	NAG	1	0
6	A	1007	PO4	2	0

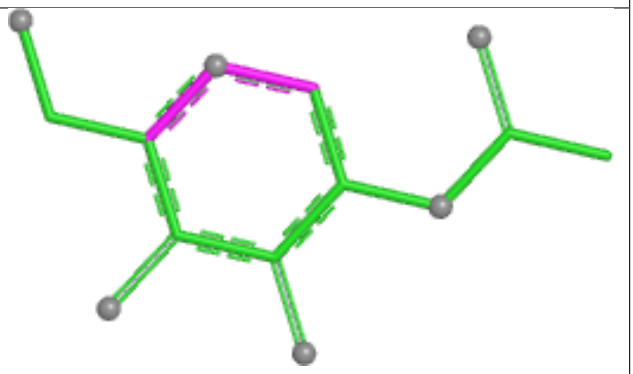
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



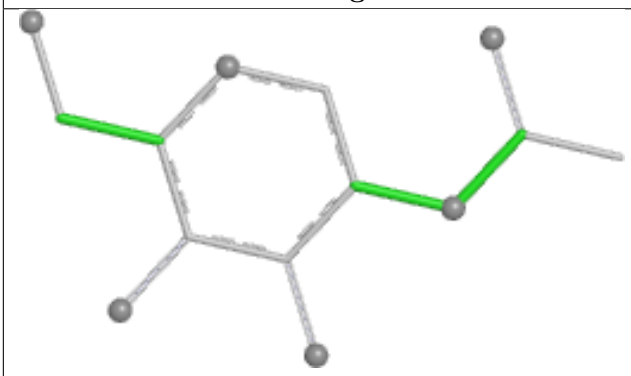
Ligand NAG A 1011



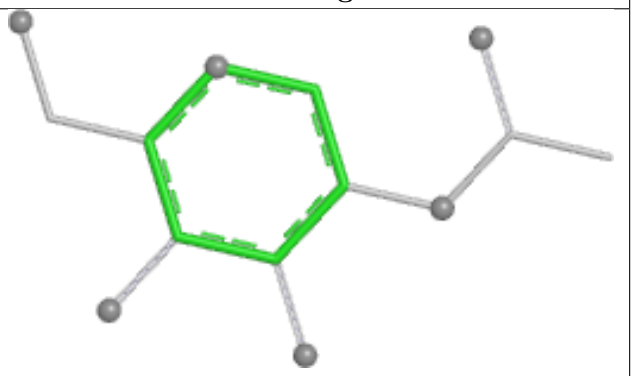
Bond lengths



Bond angles

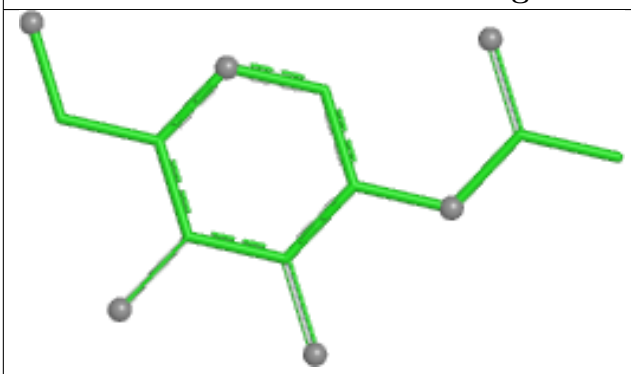


Torsions

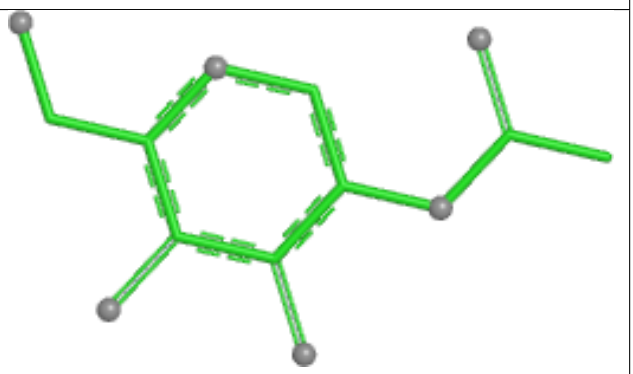


Rings

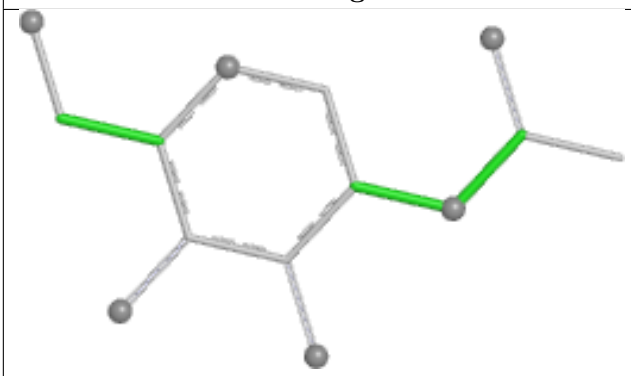
Ligand NAG B 1002



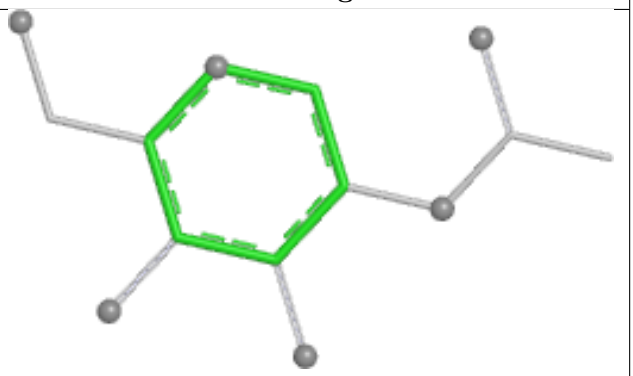
Bond lengths



Bond angles

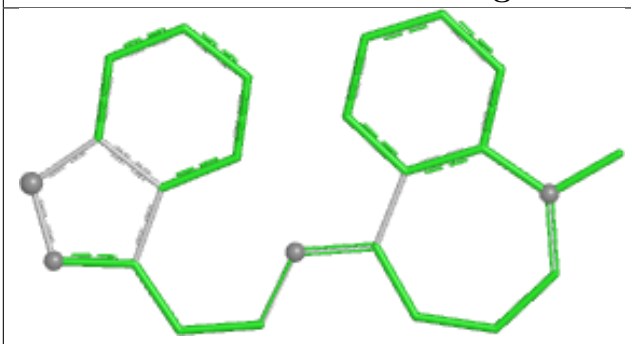


Torsions

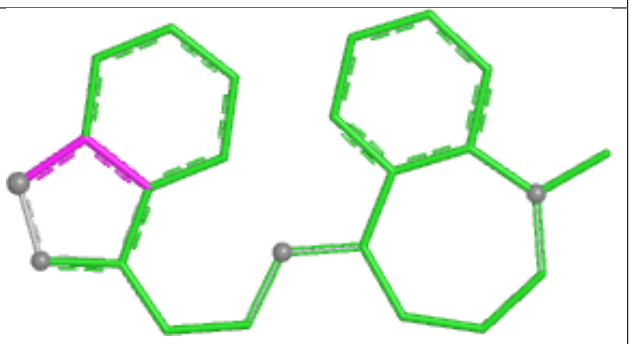


Rings

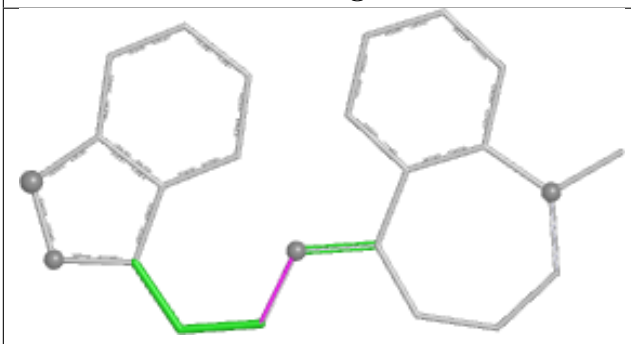
Ligand A1ATP B 1008



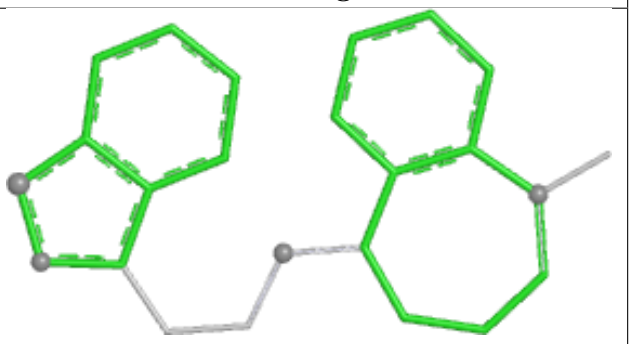
Bond lengths



Bond angles

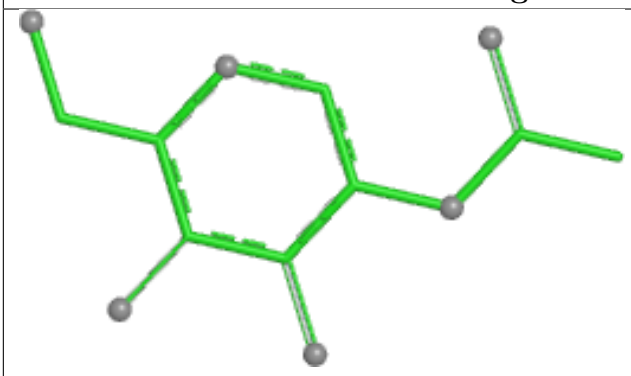


Torsions

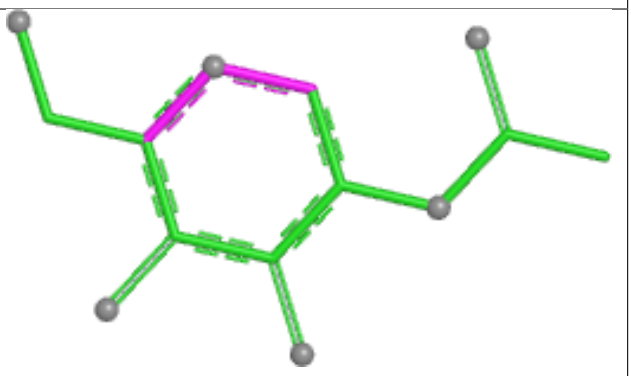


Rings

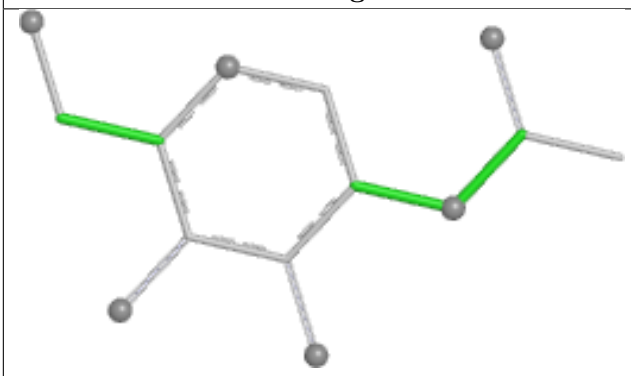
Ligand NAG A 1010



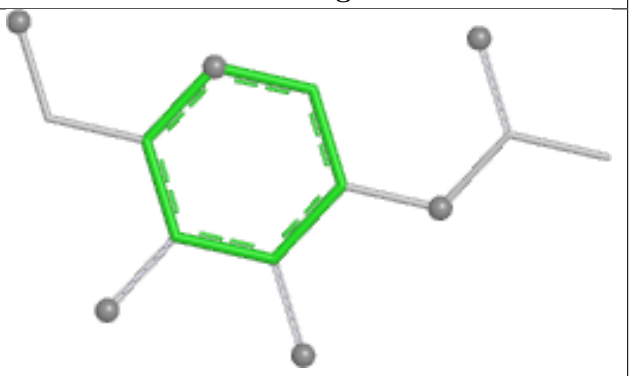
Bond lengths



Bond angles

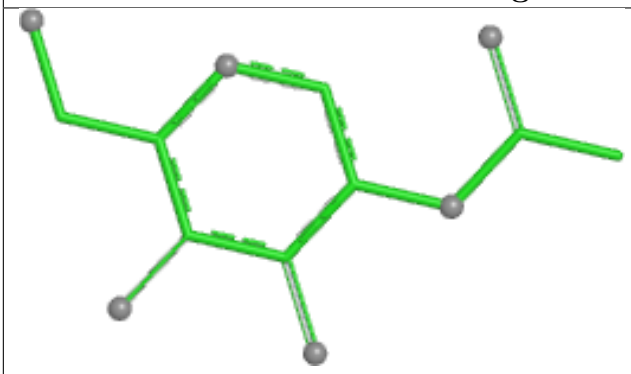


Torsions

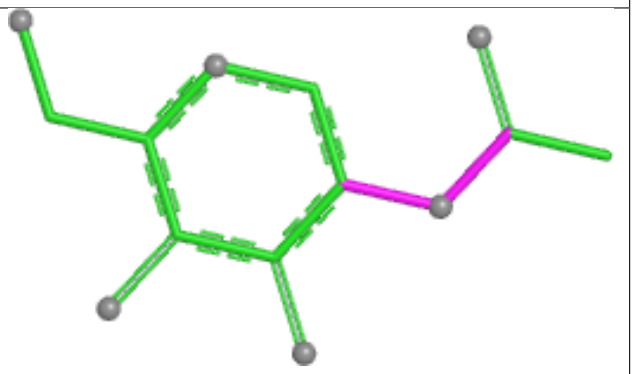


Rings

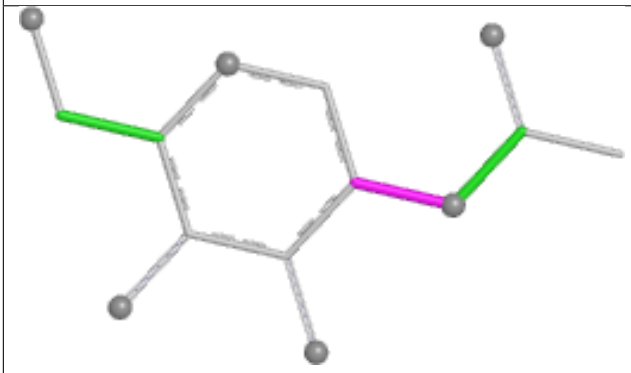
Ligand NAG B 1001



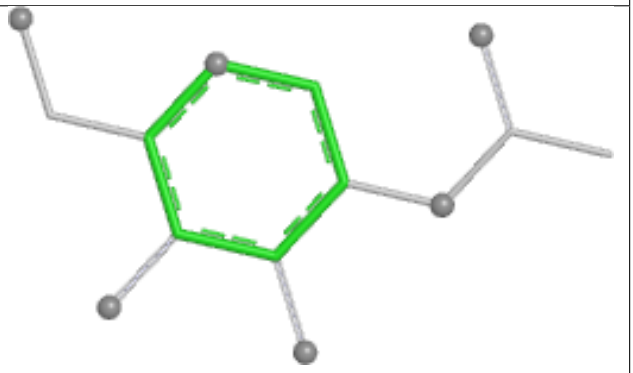
Bond lengths



Bond angles

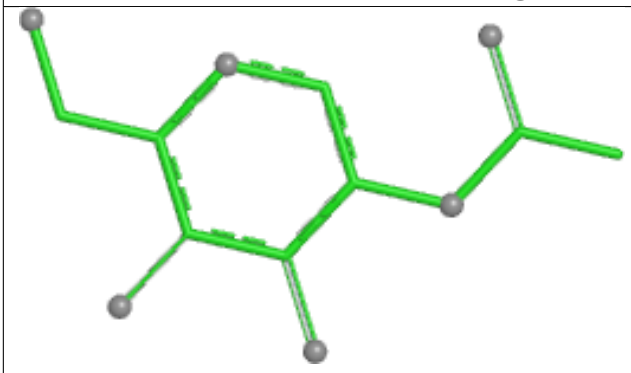


Torsions

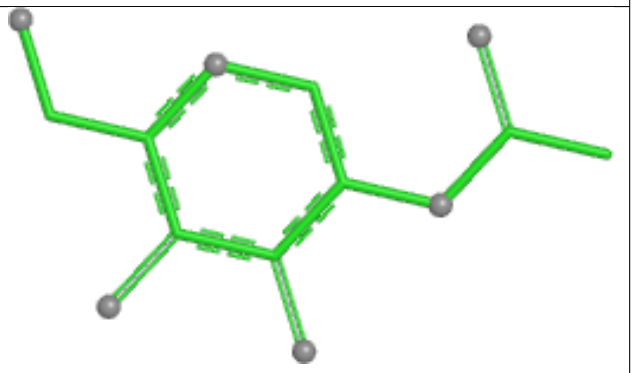


Rings

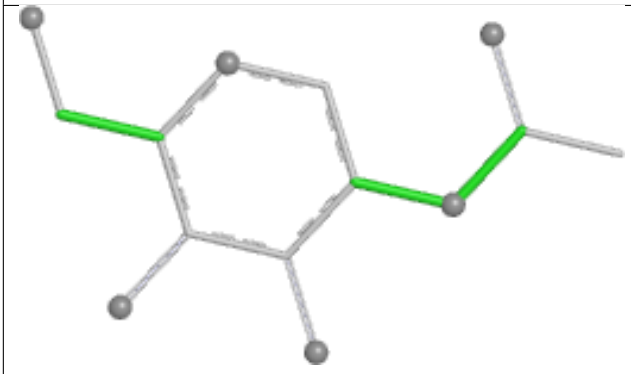
Ligand NAG B 1009



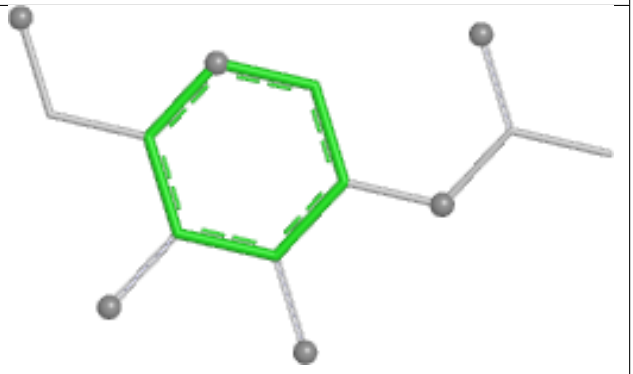
Bond lengths



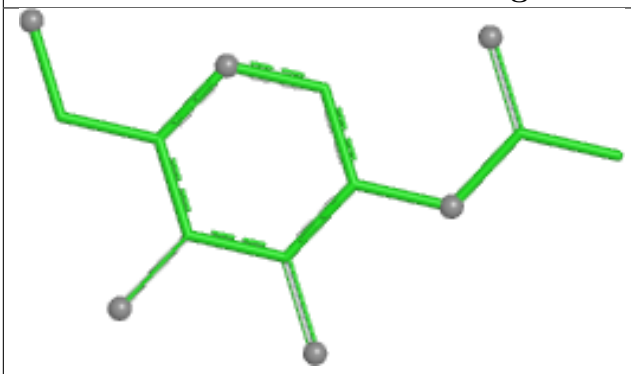
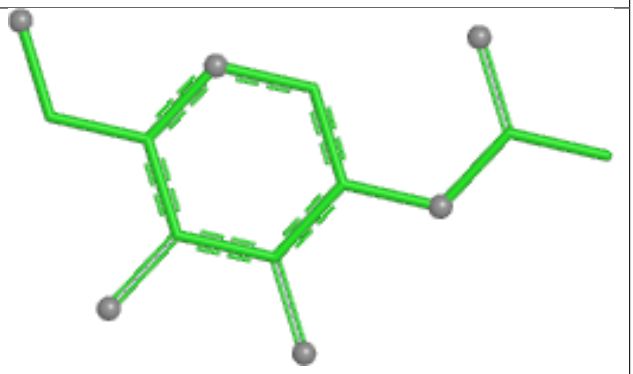
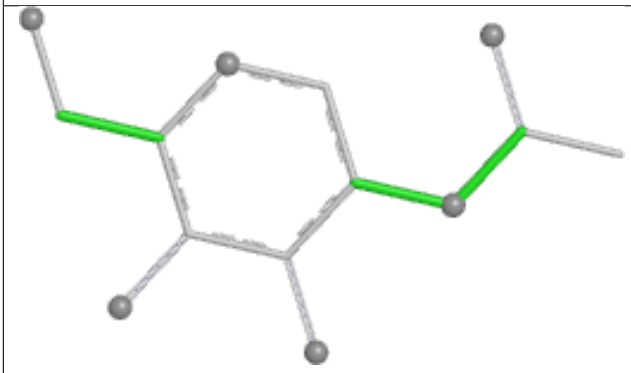
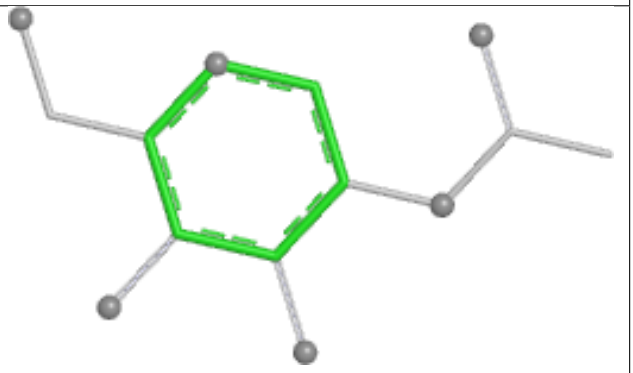
Bond angles



Torsions



Rings

Ligand NAG A 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

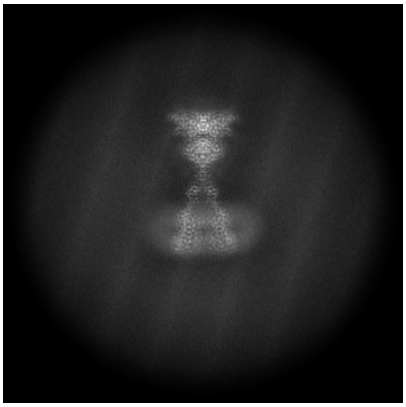
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45127. These allow visual inspection of the internal detail of the map and identification of artifacts.

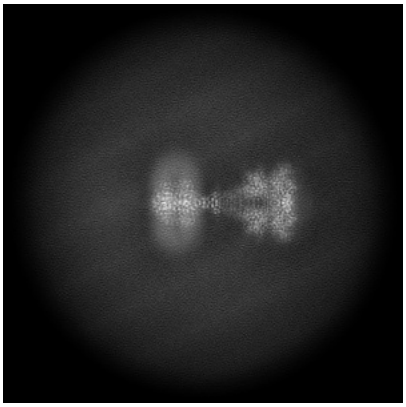
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

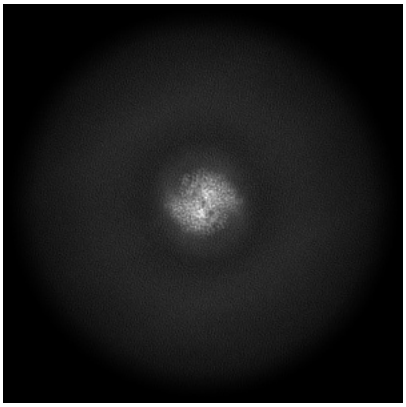
6.1.1 Primary map



X



Y

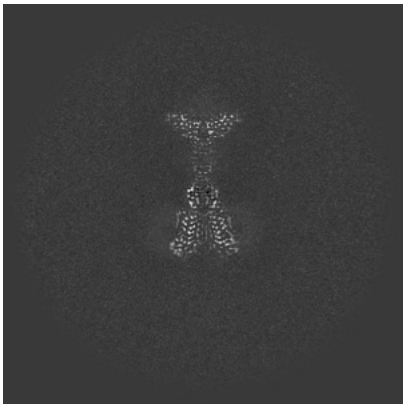


Z

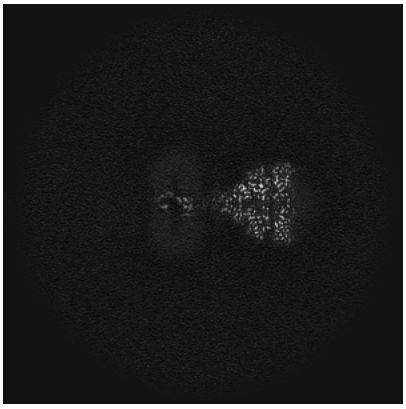
The images above show the map projected in three orthogonal directions.

6.2 Central slices

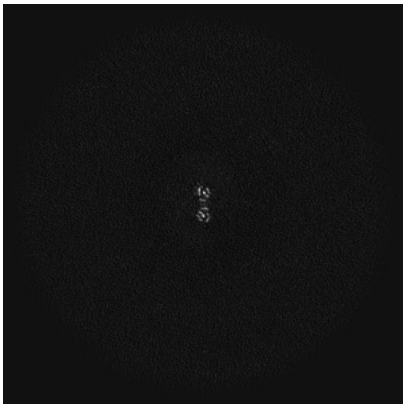
6.2.1 Primary map



X Index: 256



Y Index: 256

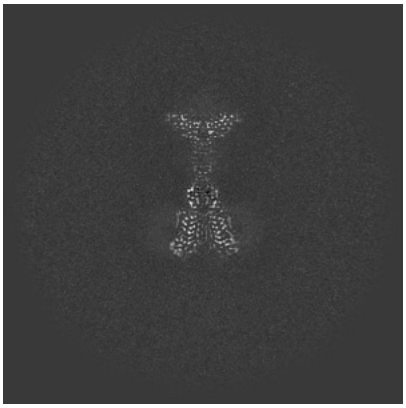


Z Index: 256

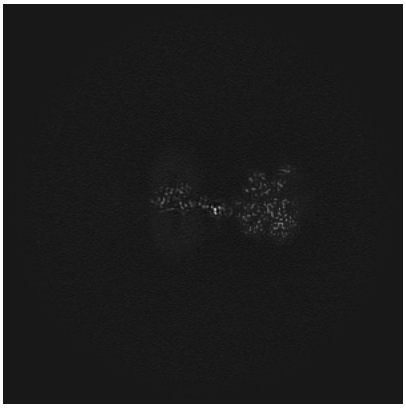
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

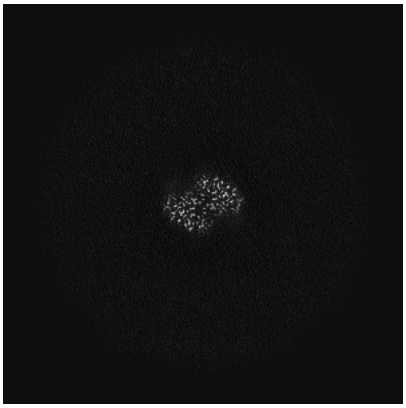
6.3.1 Primary map



X Index: 256



Y Index: 245

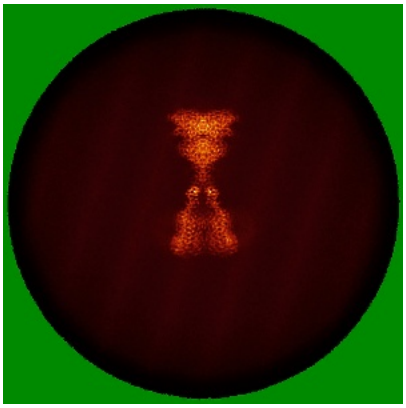


Z Index: 357

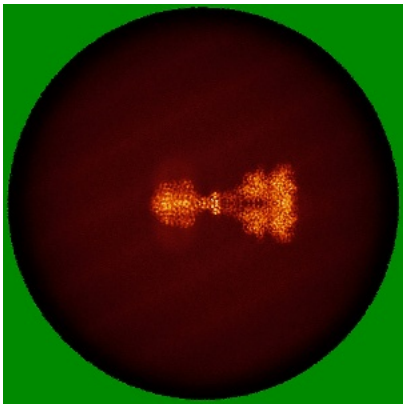
The images above show the largest variance slices of the map in three orthogonal directions.

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

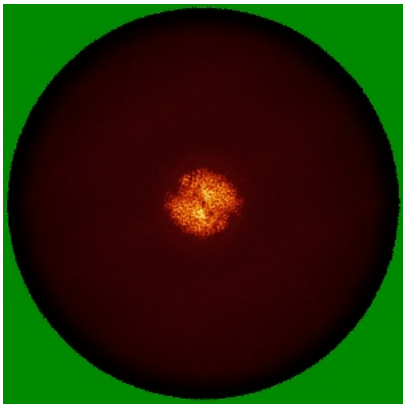
6.4.1 Primary map



X



Y

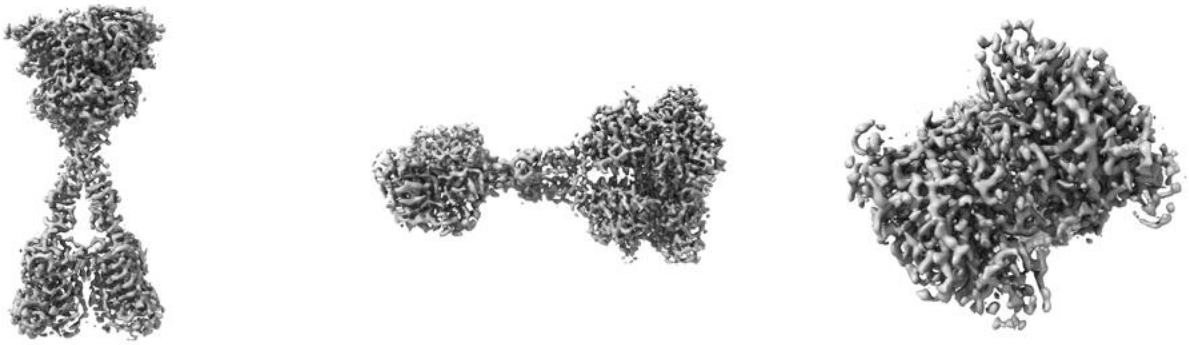


Z

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 0.384. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

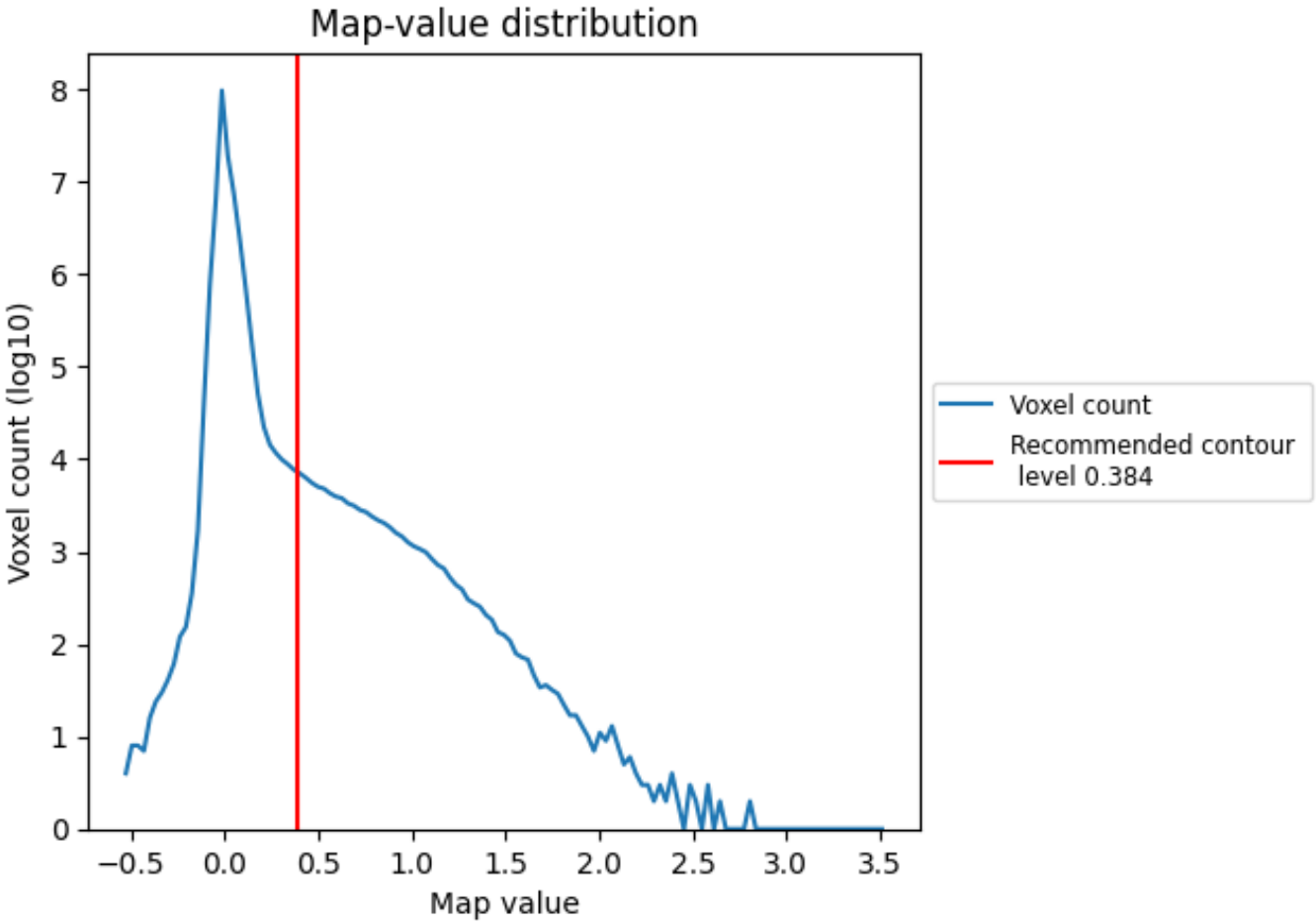
6.6 Mask visualisation (i)

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

7 Map analysis

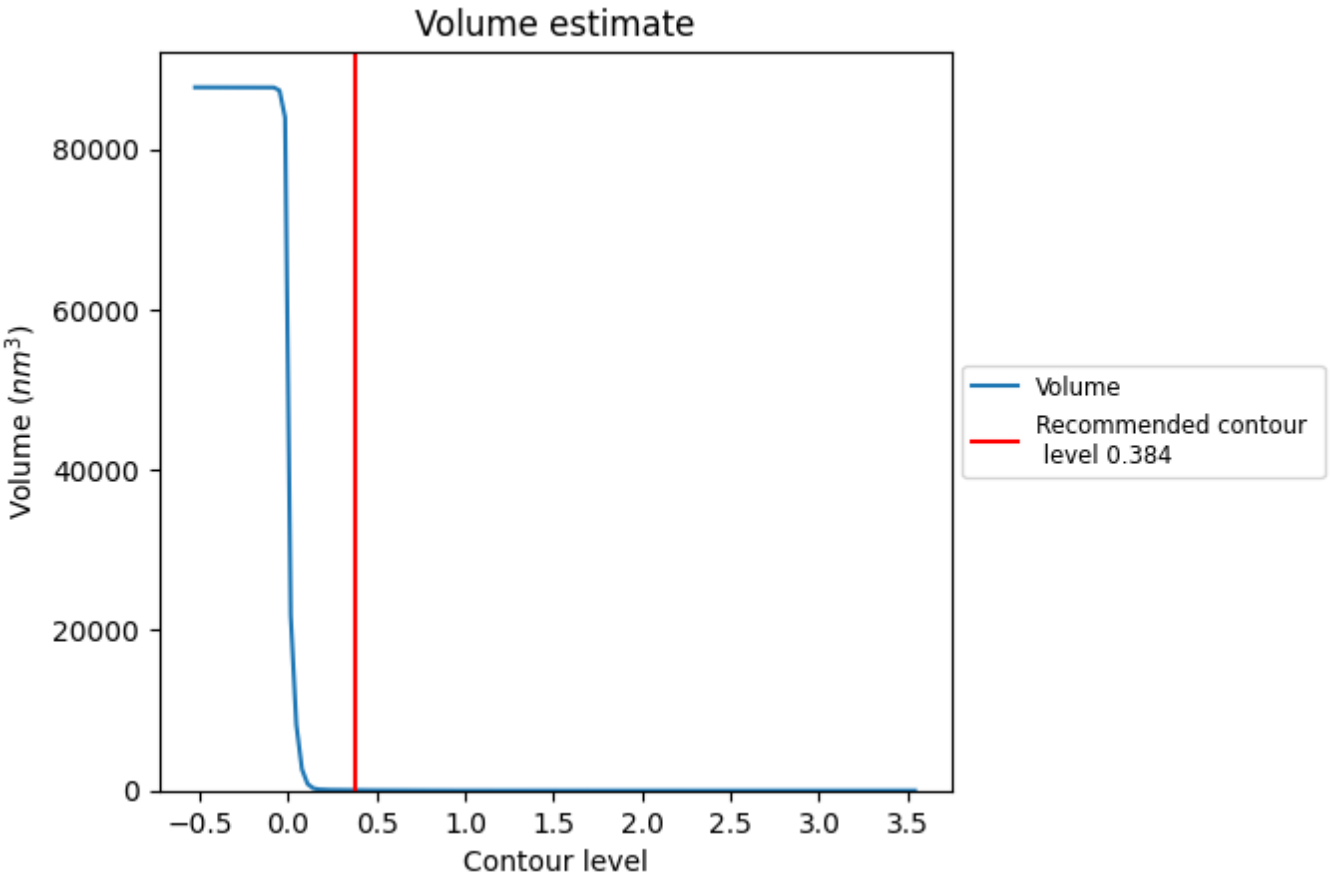
This section contains the results of statistical analysis of the map.

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.

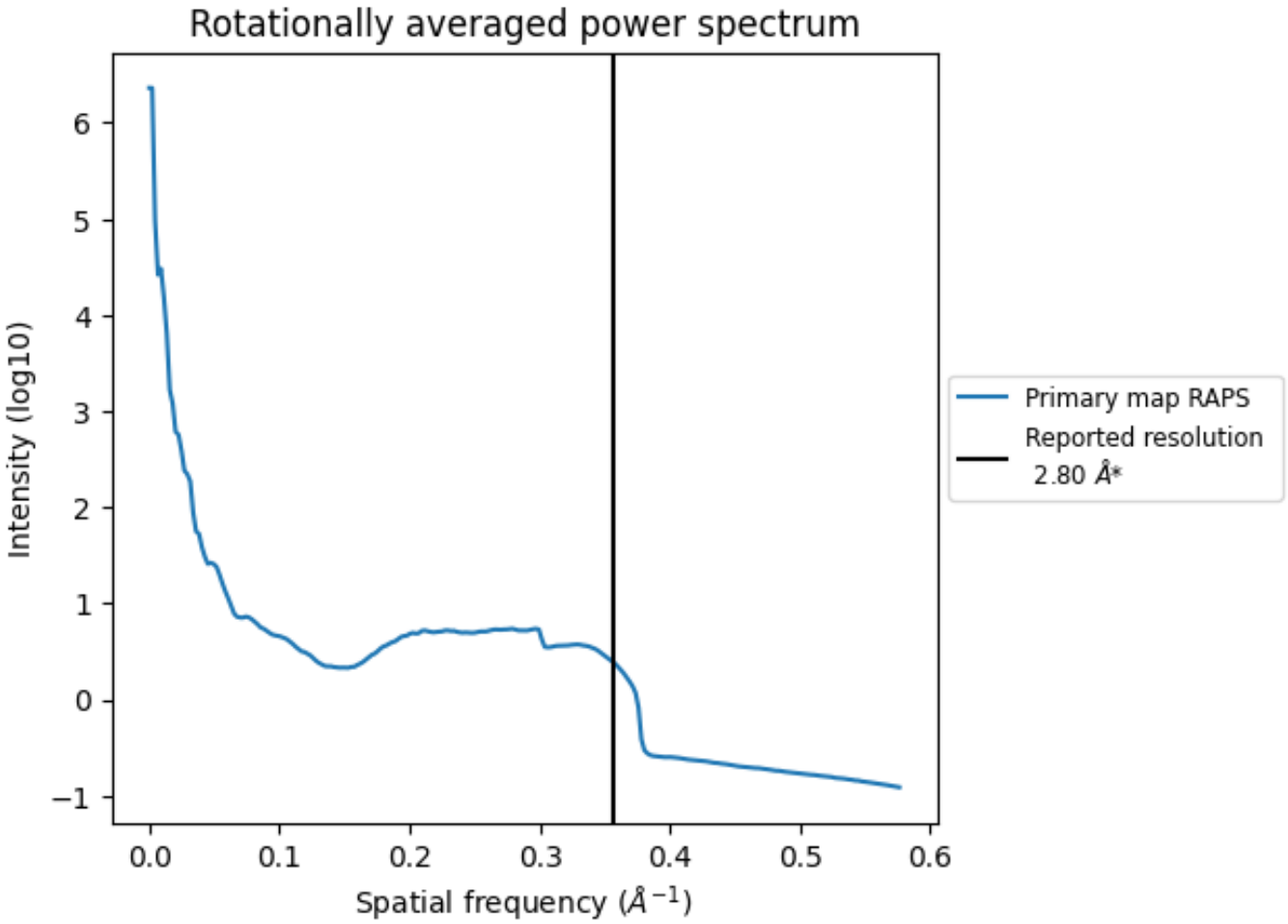
7.2 Volume estimate



The volume at the recommended contour level is 52 nm^3; this corresponds to an approximate mass of 47 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 0.357 Å^{-1}

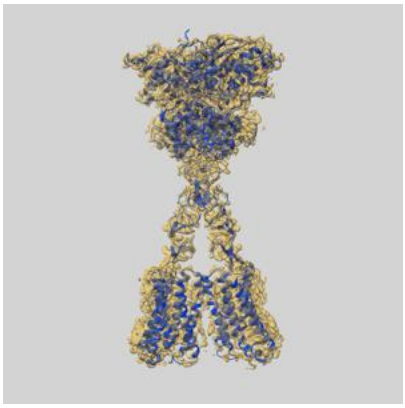
8 Fourier-Shell correlation

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

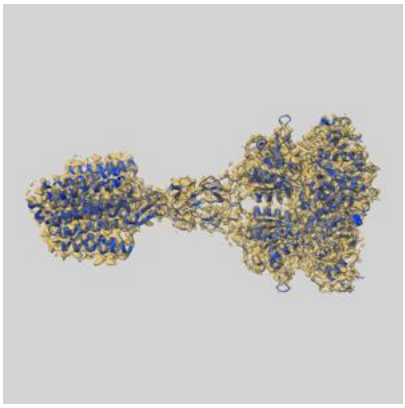
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45127 and PDB model 9C1P. Per-residue inclusion information can be found in section 3 on page 10.

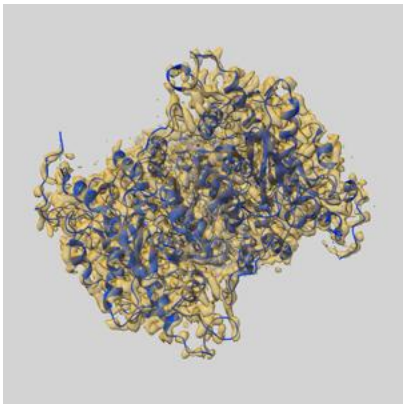
9.1 Map-model overlay



X



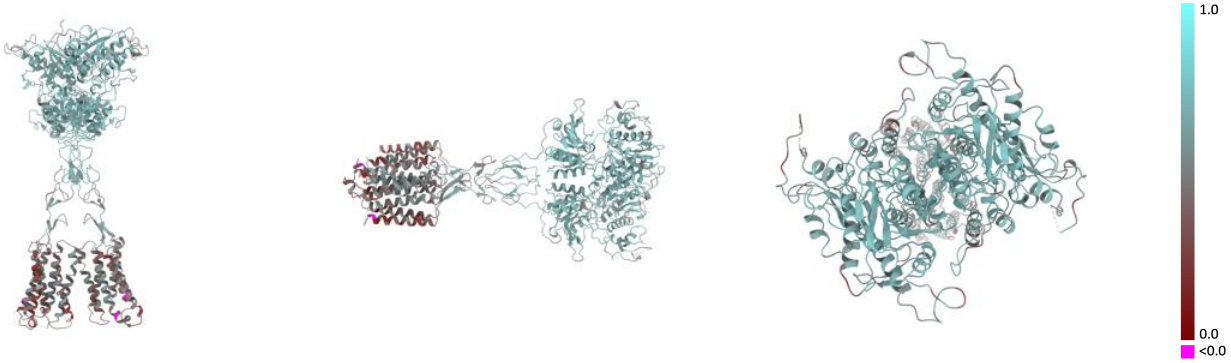
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.384 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.

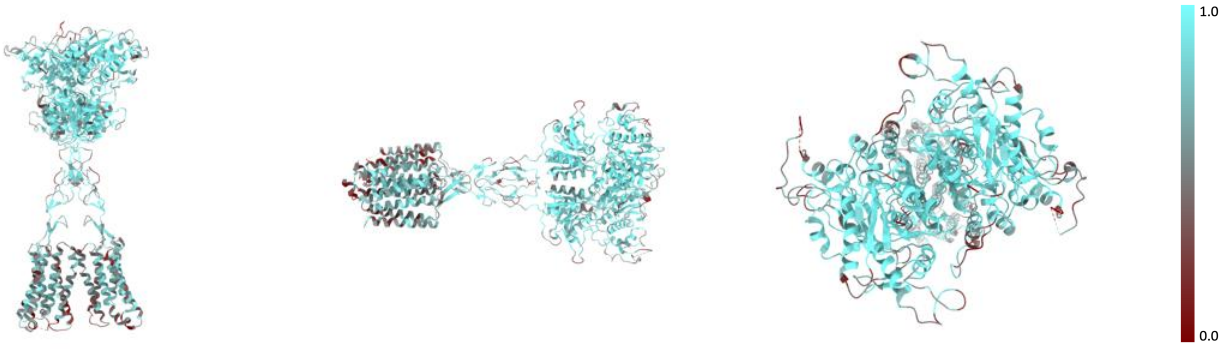
9.2 Q-score mapped to coordinate model (i)



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.

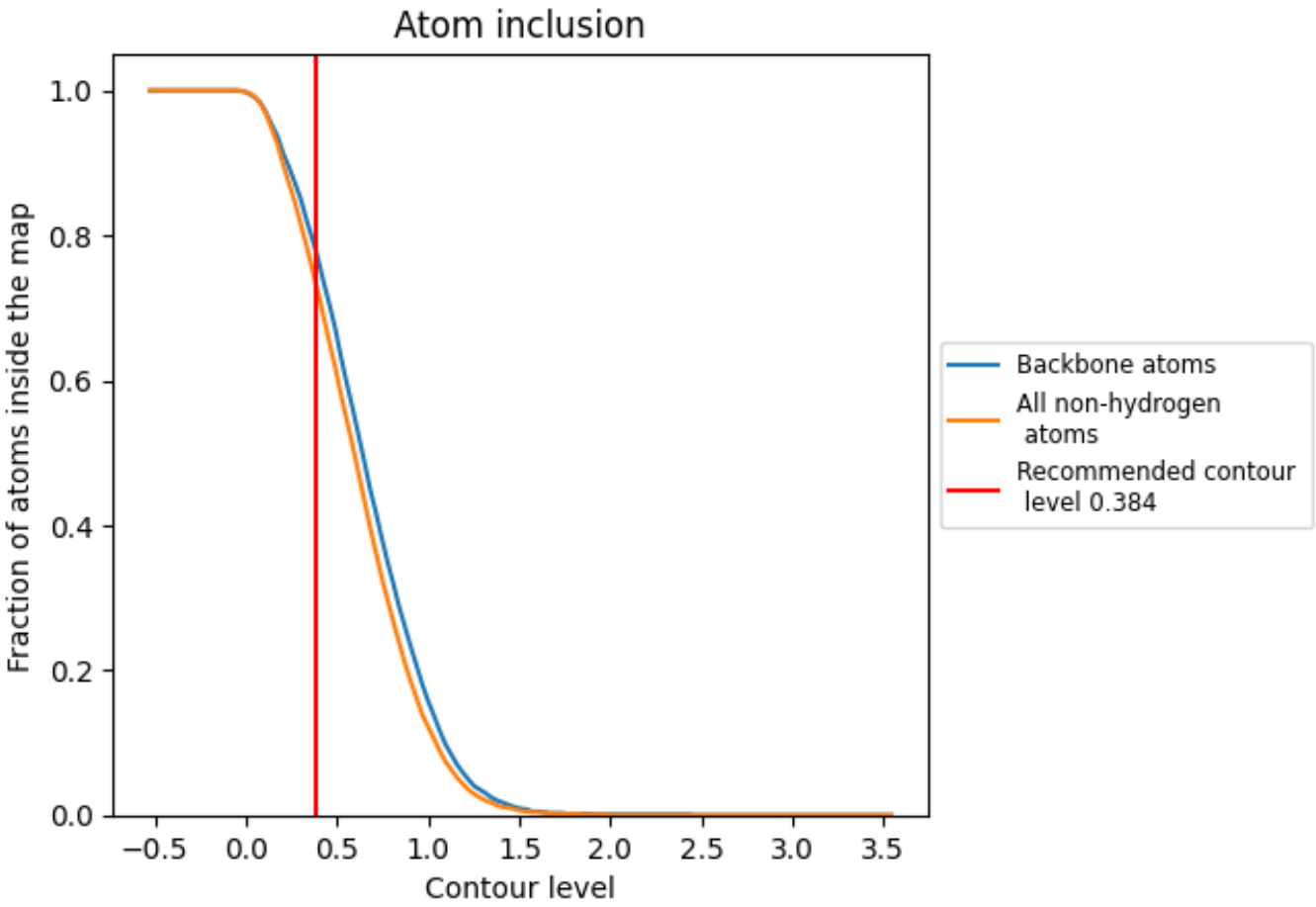
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.384).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.384) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7330	0.5680
A	0.7360	0.5660
B	0.7300	0.5690