Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 04:17 pm GMT

PDB ID	:	7OCF
EMDB ID	:	EMD-12806
Title	:	Active state GluA1/A2 AMPA receptor in complex with TARP gamma 8 and CNIH2 (LBD-TMD)
Authors	:	Zhang, D.; Watson, J.F.; Matthews, P.M.; Cais, O.; Greger, I.H.
Deposited on	:	2021-04-26
Resolution	:	3.60 Å(reported)
Based on initial models	:	6QKC, 6PEQ

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

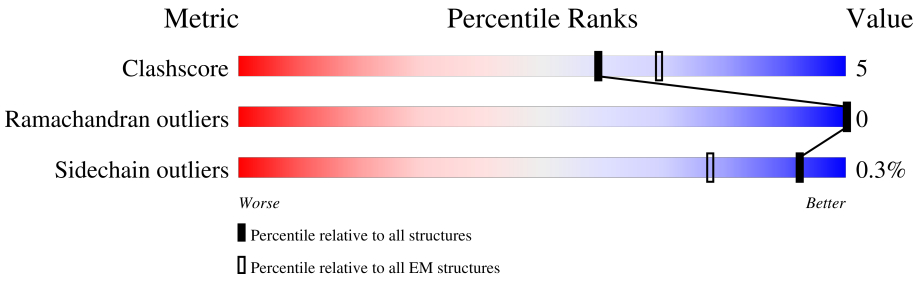
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	915	8% 39% 6% 56%
1	C	915	8% 39% 5% 56%
2	B	860	5% 42% · 54%
2	D	860	5% 42% 5% 54%
3	E	188	25% 77% 7% 16%
3	G	188	26% 77% 7% 16%
4	I	423	· 40% · 57%
4	J	423	· 39% · 57%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17088 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 Isoform Flip of Glutamate receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	406	Total 2803	C 1831	N 456	O 504	S 12	0	0
1	C	406	Total 2803	C 1831	N 456	O 504	S 12	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	insertion	UNP P19490
A	-5	TYR	-	insertion	UNP P19490
A	-4	LYS	-	insertion	UNP P19490
A	-3	ASP	-	insertion	UNP P19490
A	-2	ASP	-	insertion	UNP P19490
A	-1	ASP	-	insertion	UNP P19490
A	0	ASP	-	insertion	UNP P19490
A	1	LYS	-	insertion	UNP P19490
C	-6	ASP	-	insertion	UNP P19490
C	-5	TYR	-	insertion	UNP P19490
C	-4	LYS	-	insertion	UNP P19490
C	-3	ASP	-	insertion	UNP P19490
C	-2	ASP	-	insertion	UNP P19490
C	-1	ASP	-	insertion	UNP P19490
C	0	ASP	-	insertion	UNP P19490
C	1	LYS	-	insertion	UNP P19490

- Molecule 2 is a protein called Isoform Flip of Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	399	Total 2878	C 1870	N 477	O 513	S 18	0	0
2	D	399	Total 2878	C 1870	N 477	O 513	S 18	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	586	ARG	GLN	variant	UNP P19491
D	586	ARG	GLN	variant	UNP P19491

- Molecule 3 is a protein called Protein cornichon homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	158	Total	C	N	O	S	0	0
			1222	829	191	190	12		
3	E	158	Total	C	N	O	S	0	0
			1222	829	191	190	12		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	161	GLU	-	expression tag	UNP Q5BJU5
G	162	ASN	-	expression tag	UNP Q5BJU5
G	163	LEU	-	expression tag	UNP Q5BJU5
G	164	TYR	-	expression tag	UNP Q5BJU5
G	165	PHE	-	expression tag	UNP Q5BJU5
G	166	GLN	-	expression tag	UNP Q5BJU5
G	167	SER	-	expression tag	UNP Q5BJU5
G	168	GLY	-	expression tag	UNP Q5BJU5
G	169	GLY	-	expression tag	UNP Q5BJU5
G	170	SER	-	expression tag	UNP Q5BJU5
G	171	THR	-	expression tag	UNP Q5BJU5
G	172	GLU	-	expression tag	UNP Q5BJU5
G	173	THR	-	expression tag	UNP Q5BJU5
G	174	SER	-	expression tag	UNP Q5BJU5
G	175	GLN	-	expression tag	UNP Q5BJU5
G	176	VAL	-	expression tag	UNP Q5BJU5
G	177	ALA	-	expression tag	UNP Q5BJU5
G	178	PRO	-	expression tag	UNP Q5BJU5
G	179	ALA	-	expression tag	UNP Q5BJU5
G	180	TYR	-	expression tag	UNP Q5BJU5
G	181	PRO	-	expression tag	UNP Q5BJU5
G	182	TYR	-	expression tag	UNP Q5BJU5
G	183	ASP	-	expression tag	UNP Q5BJU5
G	184	VAL	-	expression tag	UNP Q5BJU5
G	185	PRO	-	expression tag	UNP Q5BJU5
G	186	ASP	-	expression tag	UNP Q5BJU5
G	187	TYR	-	expression tag	UNP Q5BJU5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	188	ALA	-	expression tag	UNP Q5BJU5
E	161	GLU	-	expression tag	UNP Q5BJU5
E	162	ASN	-	expression tag	UNP Q5BJU5
E	163	LEU	-	expression tag	UNP Q5BJU5
E	164	TYR	-	expression tag	UNP Q5BJU5
E	165	PHE	-	expression tag	UNP Q5BJU5
E	166	GLN	-	expression tag	UNP Q5BJU5
E	167	SER	-	expression tag	UNP Q5BJU5
E	168	GLY	-	expression tag	UNP Q5BJU5
E	169	GLY	-	expression tag	UNP Q5BJU5
E	170	SER	-	expression tag	UNP Q5BJU5
E	171	THR	-	expression tag	UNP Q5BJU5
E	172	GLU	-	expression tag	UNP Q5BJU5
E	173	THR	-	expression tag	UNP Q5BJU5
E	174	SER	-	expression tag	UNP Q5BJU5
E	175	GLN	-	expression tag	UNP Q5BJU5
E	176	VAL	-	expression tag	UNP Q5BJU5
E	177	ALA	-	expression tag	UNP Q5BJU5
E	178	PRO	-	expression tag	UNP Q5BJU5
E	179	ALA	-	expression tag	UNP Q5BJU5
E	180	TYR	-	expression tag	UNP Q5BJU5
E	181	PRO	-	expression tag	UNP Q5BJU5
E	182	TYR	-	expression tag	UNP Q5BJU5
E	183	ASP	-	expression tag	UNP Q5BJU5
E	184	VAL	-	expression tag	UNP Q5BJU5
E	185	PRO	-	expression tag	UNP Q5BJU5
E	186	ASP	-	expression tag	UNP Q5BJU5
E	187	TYR	-	expression tag	UNP Q5BJU5
E	188	ALA	-	expression tag	UNP Q5BJU5

- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	184	Total	C	N	O	S	0	0
			1322	867	223	226	6		
4	J	184	Total	C	N	O	S	0	0
			1322	867	223	226	6		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	GLY	-	expression tag	UNP Q8VHW5

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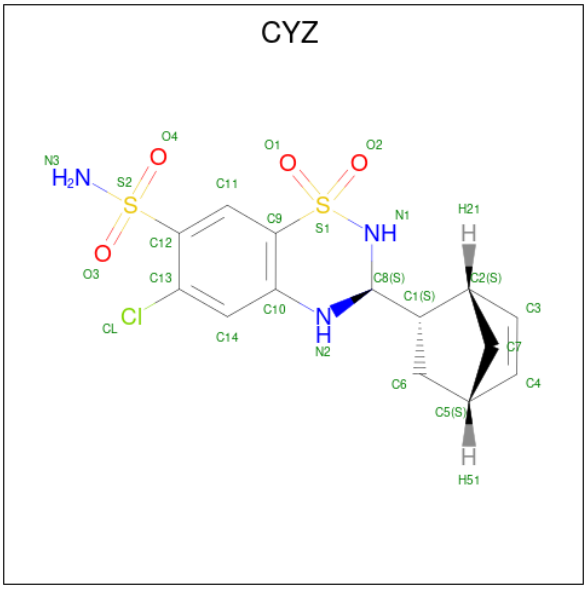
Chain	Residue	Modelled	Actual	Comment	Reference
I	418	LEU	-	expression tag	UNP Q8VHW5
I	419	GLU	-	expression tag	UNP Q8VHW5
I	420	VAL	-	expression tag	UNP Q8VHW5
I	421	LEU	-	expression tag	UNP Q8VHW5
I	422	PHE	-	expression tag	UNP Q8VHW5
I	423	GLN	-	expression tag	UNP Q8VHW5
J	1	GLY	-	expression tag	UNP Q8VHW5
J	418	LEU	-	expression tag	UNP Q8VHW5
J	419	GLU	-	expression tag	UNP Q8VHW5
J	420	VAL	-	expression tag	UNP Q8VHW5
J	421	LEU	-	expression tag	UNP Q8VHW5
J	422	PHE	-	expression tag	UNP Q8VHW5
J	423	GLN	-	expression tag	UNP Q8VHW5

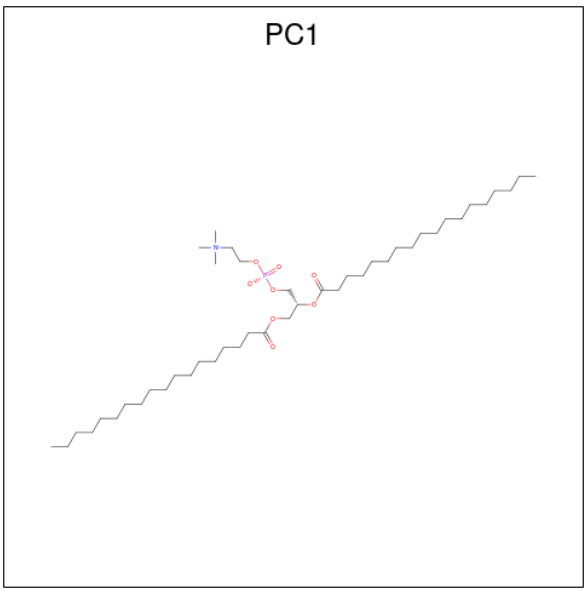
- Molecule 5 is CYCLOTHIAZIDE (three-letter code: CYZ) (formula: $C_{14}H_{16}ClN_3O_4S_2$).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
5	B	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
5	C	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
5	D	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1)

(formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C O 114 102 12	0
6	A	1	Total C O 114 102 12	0
6	A	1	Total C O 114 102 12	0
6	A	1	Total C O 114 102 12	0
6	A	1	Total C O 114 102 12	0
6	A	1	Total C O 114 102 12	0
6	B	1	Total C O 99 87 12	0
6	B	1	Total C O 99 87 12	0
6	B	1	Total C O 99 87 12	0
6	B	1	Total C O 99 87 12	0
6	B	1	Total C O 99 87 12	0
6	I	1	Total C O 40 36 4	0
6	I	1	Total C O 40 36 4	0

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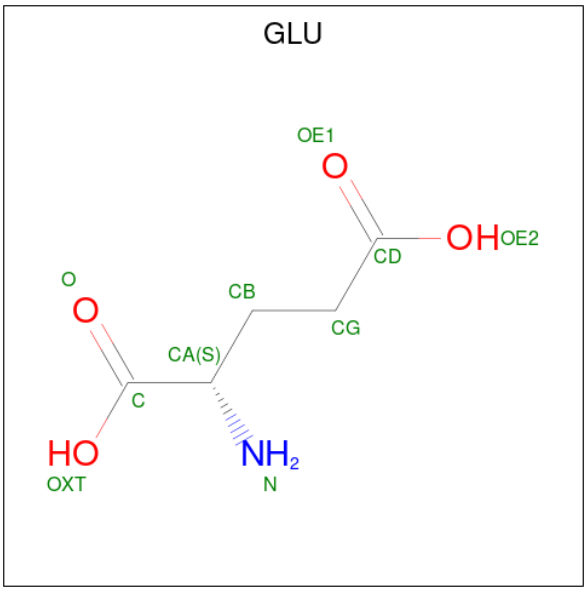
Mol	Chain	Residues	Atoms			AltConf
6	C	1	Total 114	C 102	O 12	0
6	C	1	Total 114	C 102	O 12	0
6	C	1	Total 114	C 102	O 12	0
6	C	1	Total 114	C 102	O 12	0
6	C	1	Total 114	C 102	O 12	0
6	C	1	Total 114	C 102	O 12	0
6	E	1	Total 18	C 16	O 2	0
6	J	1	Total 40	C 36	O 4	0
6	J	1	Total 40	C 36	O 4	0
6	D	1	Total 81	C 71	O 10	0
6	D	1	Total 81	C 71	O 10	0
6	D	1	Total 81	C 71	O 10	0
6	D	1	Total 81	C 71	O 10	0

- Molecule 7 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



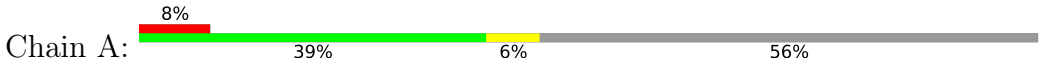
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			9	5	1	3	
7	B	1	Total	C	N	O	0
			9	5	1	3	
7	C	1	Total	C	N	O	0
			9	5	1	3	
7	D	1	Total	C	N	O	0
			9	5	1	3	

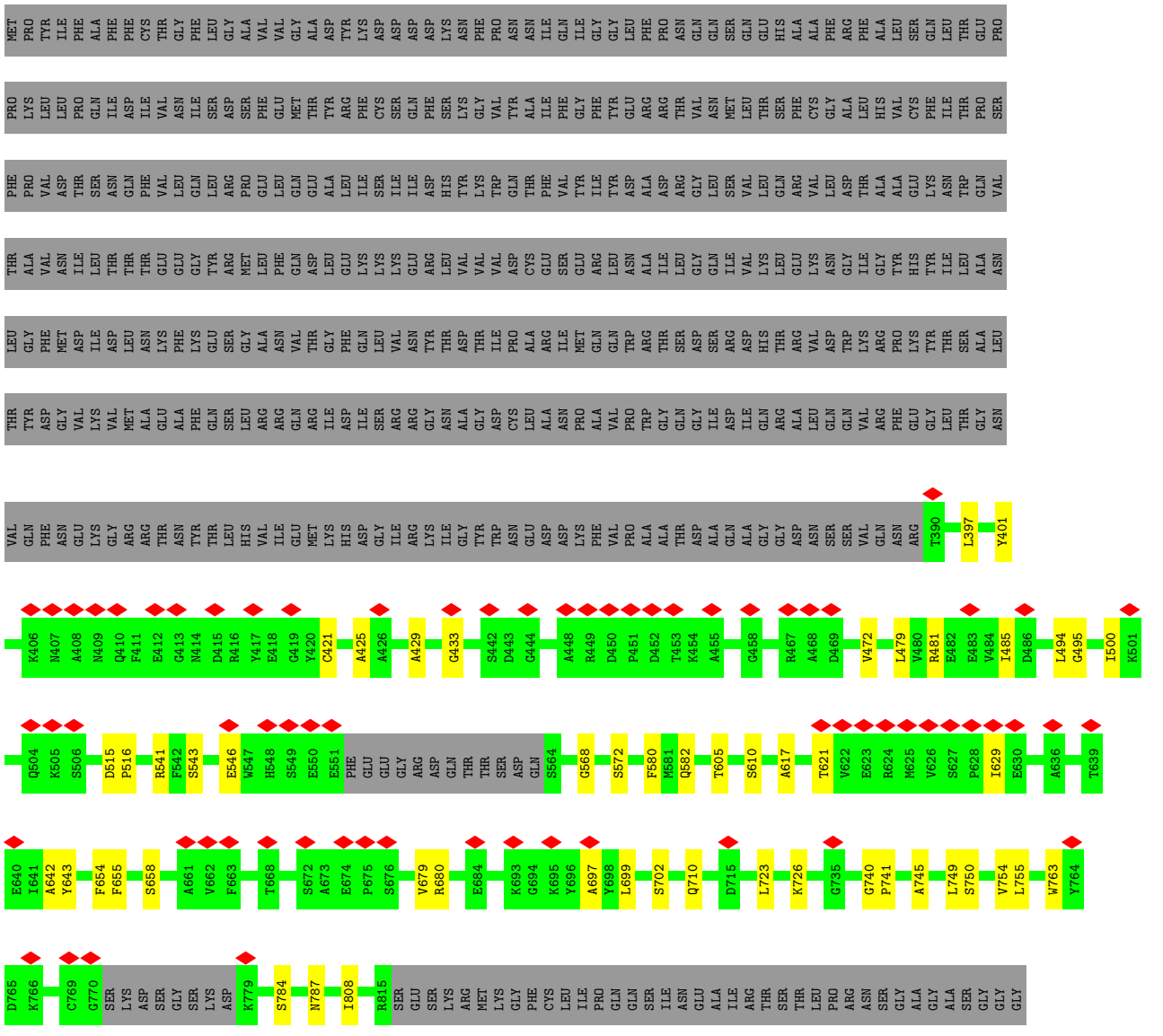
3 Residue-property plots (i)

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: Isoform Flip of Glutamate receptor 1

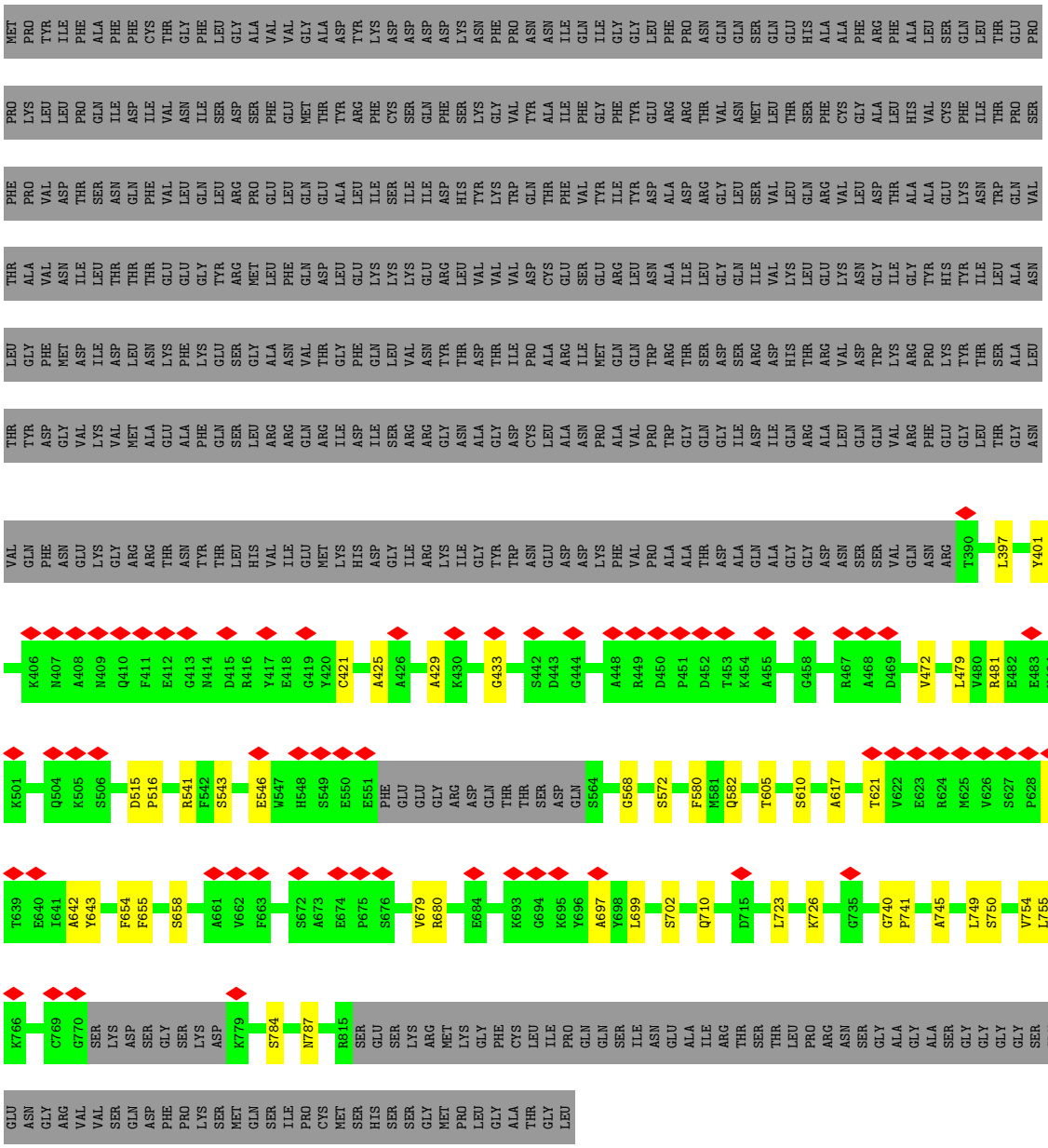
Chain A:





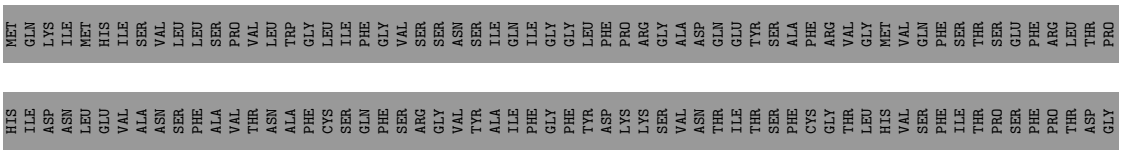
• Molecule 1: Isoform Flip of Glutamate receptor 1

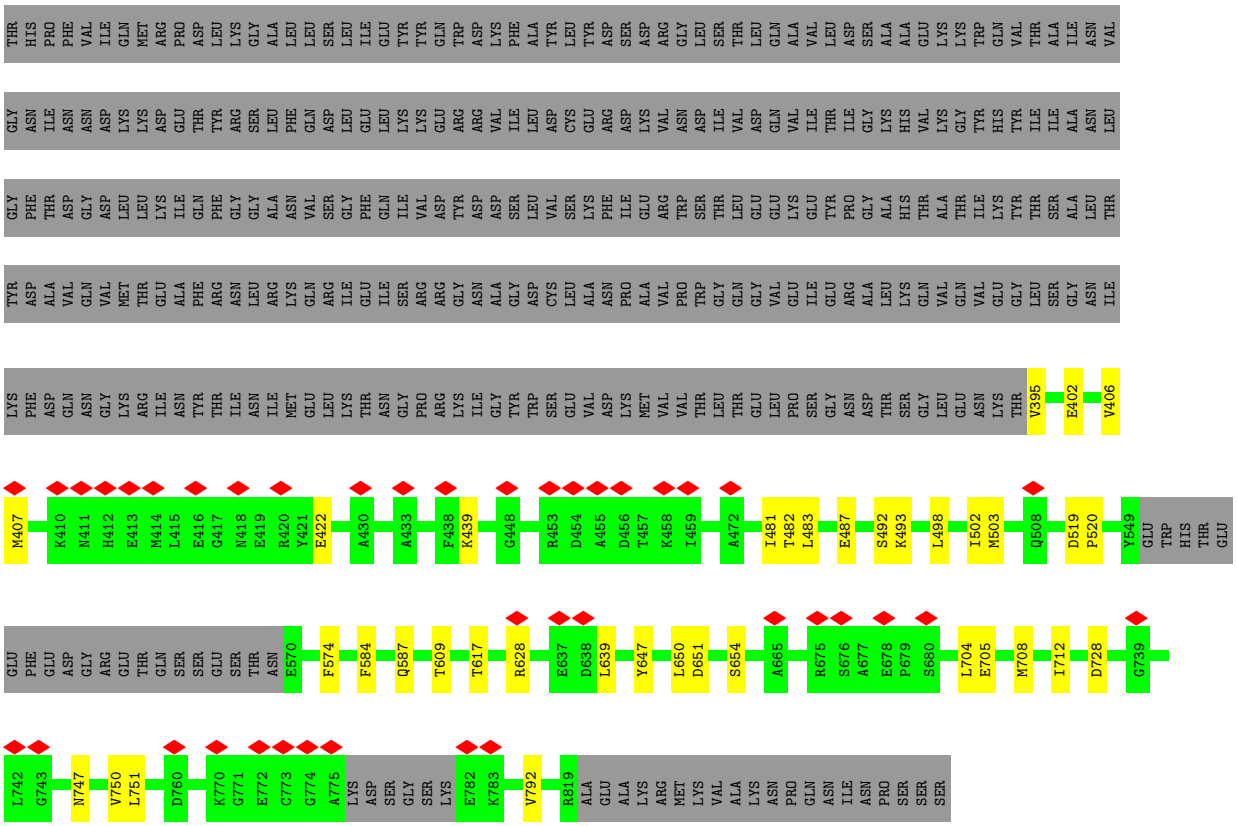
Chain C:



• Molecule 2: Isoform Flip of Glutamate receptor 2

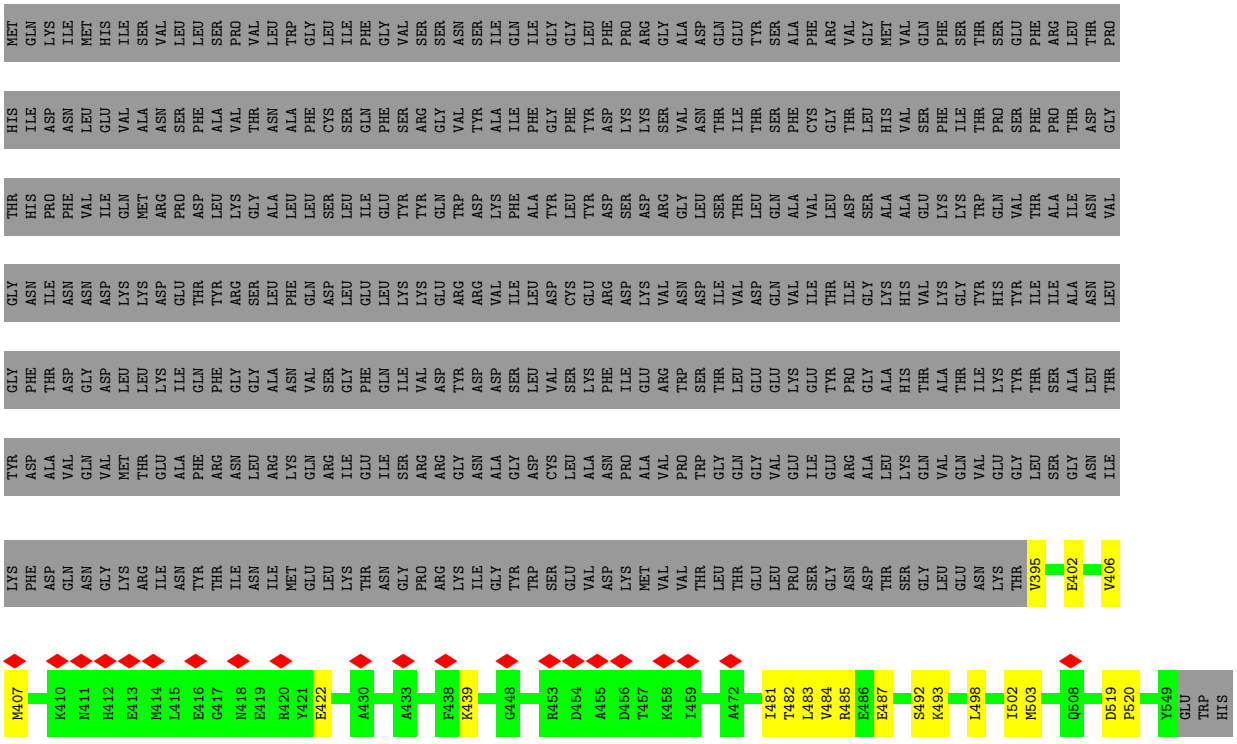
Chain B:

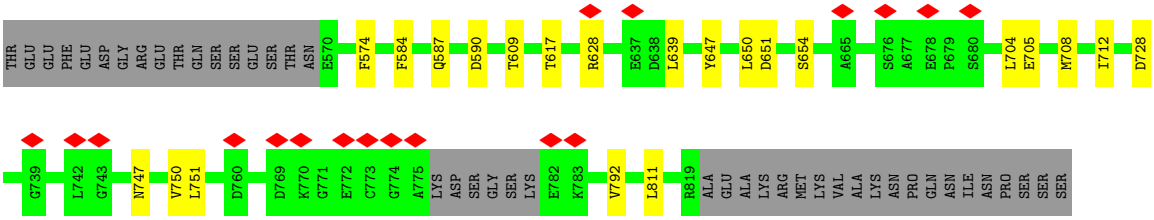




• Molecule 2: Isoform Flip of Glutamate receptor 2

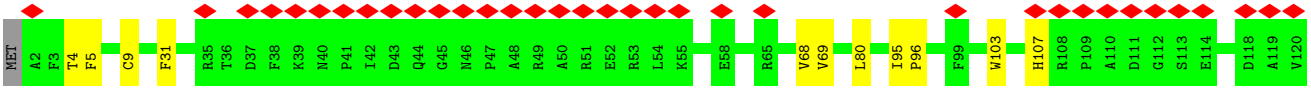
Chain D:

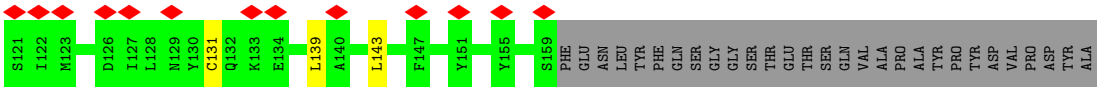




• Molecule 3: Protein cornichon homolog 2

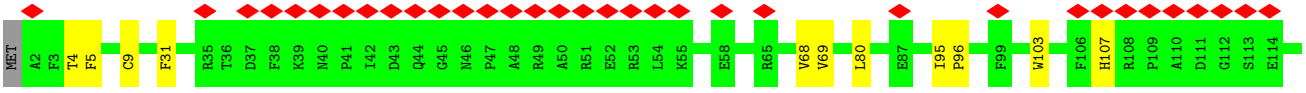
Chain G:

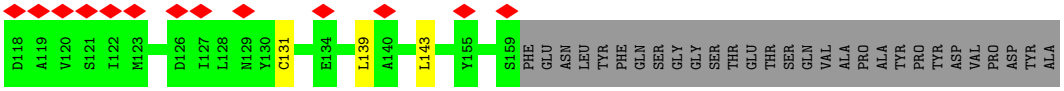




• Molecule 3: Protein cornichon homolog 2

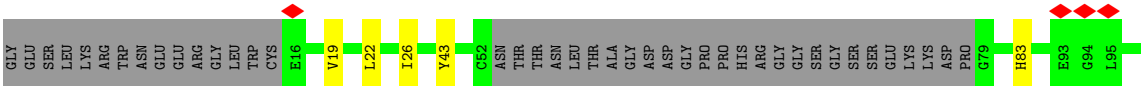
Chain E:

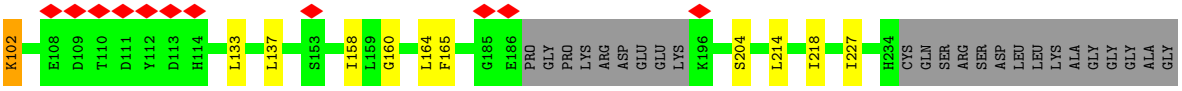


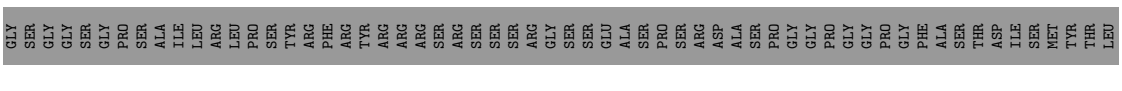


• Molecule 4: Voltage-dependent calcium channel gamma-8 subunit

Chain I:

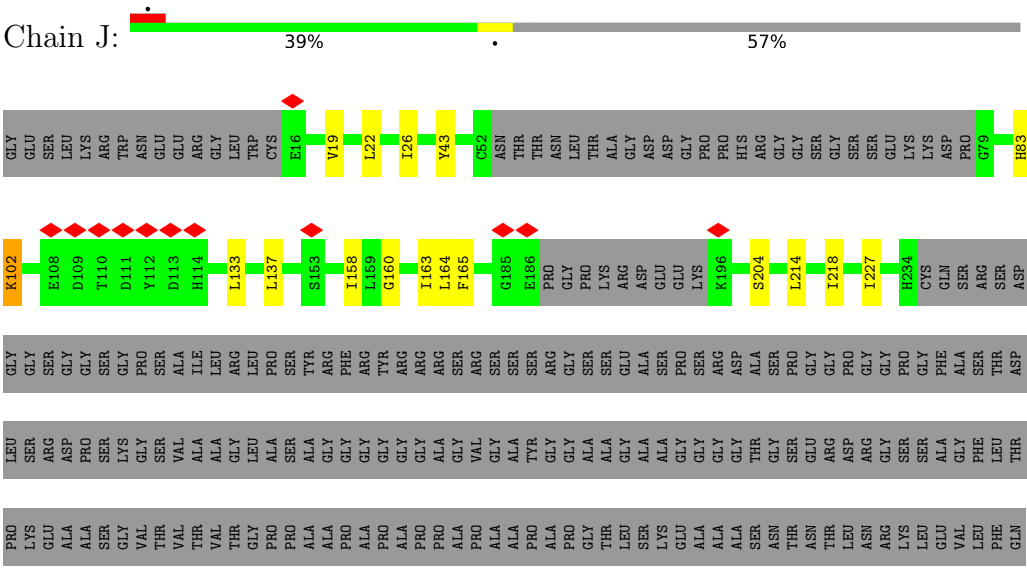






• Molecule 4: Voltage-dependent calcium channel gamma-8 subunit

Chain J:


39%
57%
GLY GLU SER LEU LYS ARG TRP ASN GLU GLU ARG GLY LEU TRP CYS E16 V19 L22 I26 Y43 C52 ASN THR THR ASN LEU THR ALA GLY ASP ASP GLY PRO PRO HIS ARG GLY GLY SER GLY SER SER GLU LYS LYS ASP PRO G79 H83 E93 G94 L95
K102 E108 D109 T110 D111 Y112 D113 H114 L133 L137 S153 I158 L159 G160 I163 L164 F165 G185 E186 PRO GLY PRO LYS ARG ASP GLU GLU LYS K196 S204 L214 I218 I227 H234 CYS GLN SER ARG SER ASP LEU LEU LYS ALA GLY GLY GLY ALA
GLY GLY SER GLY GLY SER GLY PRO SER ALA ILE LEU ARG LEU PRO SER TYR ARG PHE ARG TYR ARG ARG ARG SER ARG SER SER SER ARG GLY SER SER GLU ALA SER PRO SER ARG ASP ALA SER PRO GLY GLY PRO GLY GLY PRO GLY PHE ALA SER THR ASP ILE SER MET TYR THR
LEU SER ARG ASP PRO SER LYS GLY SER VAL ALA ALA ALA GLY LEU ALA SER ALA GLY GLY GLY GLY GLY ALA GLY VAL GLY ALA TYR GLY GLY ALA ALA ALA GLY ALA ALA GLY GLY GLY GLY GLY THR GLY SER GLU ARG ASP ARG GLY SER SER ALA GLY PHE LEU THR LEU HIS ASN ALA PHE
PRO LYS GLU ALA ALA SER GLY VAL THR VAL THR VAL THR GLY PRO PRO ALA ALA ALA PRO ALA PRO ALA PRO ALA PRO ALA ALA PRO ALA PRO ALA PRO ALA PRO GLY THR LEU SER LYS GLU ALA ALA ALA SER ASN THR ASN THR LEU ASN ARG LYS LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	120052	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CYZ, PC1

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	0.40	0/2870	0.43	0/3937
1	C	0.40	0/2870	0.44	0/3937
2	B	0.39	0/2942	0.44	0/4005
2	D	0.39	0/2942	0.44	0/4005
3	E	0.29	0/1263	0.40	0/1727
3	G	0.29	0/1263	0.40	0/1727
4	I	0.40	0/1346	0.53	1/1833 (0.1%)
4	J	0.40	0/1346	0.53	1/1833 (0.1%)
All	All	0.38	0/16842	0.45	2/23004 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	102	LYS	CD-CE-NZ	-11.02	86.35	111.70
4	J	102	LYS	CD-CE-NZ	-11.00	86.41	111.70

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	2803	0	2471	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2803	0	2471	34	0
2	B	2878	0	2715	25	0
2	D	2878	0	2715	28	0
3	E	1222	0	1149	9	0
3	G	1222	0	1149	9	0
4	I	1322	0	1296	11	0
4	J	1322	0	1296	12	0
5	A	24	0	10	2	0
5	B	24	0	10	1	0
5	C	24	0	10	2	0
5	D	24	0	10	1	0
6	A	114	0	189	1	0
6	B	99	0	162	2	0
6	C	114	0	189	0	0
6	D	81	0	134	2	0
6	E	18	0	28	0	0
6	I	40	0	70	0	0
6	J	40	0	70	0	0
7	A	9	0	5	1	0
7	B	9	0	5	1	0
7	C	9	0	5	1	0
7	D	9	0	5	1	0
All	All	17088	0	16164	160	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 (160) 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:705:GLU:OE1	2:B:705:GLU:N	2.09	0.85
2:D:705:GLU:N	2:D:705:GLU:OE1	2.10	0.84
2:B:654:SER:N	7:B:1407:GLU:O	2.15	0.79
2:D:654:SER:N	7:D:1406:GLU:O	2.15	0.78
2:D:395:VAL:N	2:D:439:LYS:O	2.18	0.76
5:D:1401:CYZ:CL	5:D:1401:CYZ:N3	2.56	0.76
2:B:395:VAL:N	2:B:439:LYS:O	2.18	0.76
5:B:1401:CYZ:N3	5:B:1401:CYZ:CL	2.56	0.74
5:A:1401:CYZ:N3	5:A:1401:CYZ:CL	2.59	0.72
5:C:1401:CYZ:N3	5:C:1401:CYZ:CL	2.59	0.72
4:J:43:TYR:O	4:J:204:SER:OG	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:ILE:HD11	1:C:629:ILE:HG21	1.74	0.69
1:A:500:ILE:HD11	1:A:629:ILE:HG21	1.75	0.68
1:A:568:GLY:O	1:A:572:SER:OG	2.11	0.65
1:C:745:ALA:O	1:C:749:LEU:HD23	1.97	0.65
1:A:745:ALA:O	1:A:749:LEU:HD23	1.97	0.65
1:C:710:GLN:NE2	1:C:763:TRP:O	2.23	0.64
4:I:43:TYR:O	4:I:204:SER:OG	2.07	0.63
1:A:710:GLN:NE2	1:A:763:TRP:O	2.29	0.62
1:A:643:TYR:HB3	1:A:697:ALA:HB3	1.83	0.61
1:C:643:TYR:HB3	1:C:697:ALA:HB3	1.83	0.60
1:C:568:GLY:O	1:C:572:SER:OG	2.11	0.60
1:A:397:LEU:O	1:A:397:LEU:HD23	2.03	0.59
1:C:397:LEU:HD23	1:C:397:LEU:O	2.03	0.58
1:A:541:ARG:O	4:J:227:ILE:HD11	2.04	0.57
1:A:749:LEU:HD13	1:A:754:VAL:HG11	1.88	0.55
4:I:83:HIS:O	4:I:83:HIS:ND1	2.39	0.55
4:J:83:HIS:ND1	4:J:83:HIS:O	2.39	0.55
1:C:749:LEU:HD13	1:C:754:VAL:HG11	1.88	0.55
1:C:642:ALA:O	1:C:697:ALA:N	2.41	0.54
1:A:495:GLY:O	1:A:702:SER:N	2.40	0.54
1:C:495:GLY:O	1:C:702:SER:N	2.40	0.54
1:C:472:VAL:HG23	1:C:472:VAL:O	2.09	0.52
1:A:642:ALA:O	1:A:697:ALA:N	2.41	0.52
1:A:472:VAL:O	1:A:472:VAL:HG23	2.09	0.52
4:J:158:ILE:H	4:J:158:ILE:HD12	1.75	0.51
1:C:749:LEU:CD1	1:C:754:VAL:HG11	2.40	0.51
4:I:214:LEU:O	4:I:218:ILE:HG12	2.11	0.51
4:J:214:LEU:O	4:J:218:ILE:HG12	2.11	0.51
1:A:610:SER:HB3	2:D:617:THR:HG23	1.93	0.51
1:C:655:PHE:CZ	1:C:699:LEU:HD23	2.45	0.51
1:A:749:LEU:CD1	1:A:754:VAL:HG11	2.40	0.51
1:C:429:ALA:O	1:C:433:GLY:N	2.30	0.51
1:A:655:PHE:CZ	1:A:699:LEU:HD23	2.46	0.50
4:I:158:ILE:H	4:I:158:ILE:HD12	1.75	0.50
2:B:617:THR:HG23	1:C:610:SER:HB3	1.94	0.50
4:J:163:ILE:CD1	2:D:811:LEU:HD21	2.42	0.50
2:D:481:ILE:HG22	2:D:482:THR:N	2.27	0.50
2:B:481:ILE:HG22	2:B:482:THR:N	2.27	0.49
2:D:747:ASN:O	2:D:751:LEU:HD13	2.13	0.49
1:C:784:SER:OG	1:C:787:ASN:OD1	2.29	0.49
2:B:747:ASN:O	2:B:751:LEU:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:SER:OG	1:C:546:GLU:OE1	2.32	0.48
2:B:728:ASP:N	2:B:728:ASP:OD1	2.47	0.48
1:A:429:ALA:O	1:A:433:GLY:N	2.30	0.48
1:A:784:SER:OG	1:A:787:ASN:OD1	2.30	0.48
2:D:728:ASP:N	2:D:728:ASP:OD1	2.47	0.48
1:A:543:SER:OG	1:A:546:GLU:OE1	2.32	0.47
7:A:1408:GLU:N	7:A:1408:GLU:OE2	2.47	0.47
2:D:590:ASP:OD1	2:D:590:ASP:N	2.45	0.47
1:A:654:PHE:O	1:A:658:SER:N	2.48	0.47
1:C:654:PHE:O	1:C:658:SER:N	2.48	0.47
4:J:158:ILE:HD12	4:J:158:ILE:N	2.30	0.47
4:J:160:GLY:O	4:J:164:LEU:HG	2.15	0.47
2:D:402:GLU:O	2:D:406:VAL:N	2.48	0.47
2:D:483:LEU:O	2:D:487:GLU:HG3	2.15	0.47
4:I:160:GLY:O	4:I:164:LEU:HG	2.15	0.47
2:B:483:LEU:O	2:B:487:GLU:HG3	2.15	0.46
4:I:158:ILE:HD12	4:I:158:ILE:N	2.30	0.46
1:C:479:LEU:HA	2:D:751:LEU:HD23	1.97	0.46
3:G:95:ILE:N	3:G:96:PRO:HD2	2.30	0.46
3:E:80:LEU:HD23	3:E:80:LEU:O	2.15	0.46
3:G:4:THR:HG22	3:G:5:PHE:N	2.32	0.45
1:A:425:ALA:HB2	1:A:472:VAL:HG21	1.99	0.45
1:A:479:LEU:HA	2:B:751:LEU:HD23	1.98	0.45
3:G:80:LEU:O	3:G:80:LEU:HD23	2.15	0.45
7:C:1408:GLU:N	7:C:1408:GLU:OE2	2.49	0.45
3:E:4:THR:HG22	3:E:5:PHE:N	2.32	0.45
3:E:95:ILE:N	3:E:96:PRO:HD2	2.30	0.45
3:E:95:ILE:HG13	3:E:96:PRO:HD3	1.99	0.45
2:B:587:GLN:NE2	1:C:582:GLN:OE1	2.50	0.45
1:C:655:PHE:CE2	1:C:699:LEU:HD23	2.52	0.45
1:A:494:LEU:HD11	1:A:726:LYS:HB2	1.99	0.44
3:G:95:ILE:HG13	3:G:96:PRO:HD3	1.99	0.44
1:C:494:LEU:HD11	1:C:726:LYS:HB2	1.99	0.44
2:D:747:ASN:O	2:D:750:VAL:HG22	2.17	0.44
1:C:425:ALA:HB2	1:C:472:VAL:HG21	1.99	0.44
2:B:492:SER:OG	2:B:493:LYS:N	2.51	0.44
2:D:639:LEU:HD21	2:D:647:TYR:CD1	2.53	0.44
4:I:165:PHE:CD2	4:I:218:ILE:HG22	2.53	0.44
1:A:655:PHE:CE2	1:A:699:LEU:HD23	2.52	0.44
4:J:165:PHE:CD2	4:J:218:ILE:HG22	2.53	0.44
2:D:492:SER:OG	2:D:493:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:574:PHE:CE1	6:D:1405:PC1:H3I1	2.52	0.44
1:C:617:ALA:O	1:C:621:THR:HG22	2.18	0.44
1:C:679:VAL:HG22	1:C:680:ARG:N	2.33	0.43
1:A:617:ALA:O	1:A:621:THR:HG22	2.18	0.43
2:B:498:LEU:HD23	2:B:498:LEU:N	2.33	0.43
2:B:574:PHE:CE1	6:B:1406:PC1:H3I1	2.52	0.43
1:A:750:SER:OG	5:A:1401:CYZ:N2	2.49	0.43
2:B:747:ASN:O	2:B:750:VAL:HG22	2.17	0.43
2:D:498:LEU:HD23	2:D:498:LEU:N	2.33	0.43
1:C:750:SER:OG	5:C:1401:CYZ:N2	2.50	0.43
2:B:639:LEU:HD21	2:B:647:TYR:CD1	2.53	0.43
4:I:19:VAL:HG22	4:I:19:VAL:O	2.19	0.43
4:I:227:ILE:HD11	1:C:541:ARG:O	2.18	0.43
1:A:582:GLN:OE1	2:D:587:GLN:NE2	2.52	0.42
1:A:679:VAL:HG22	1:A:680:ARG:N	2.33	0.42
1:A:500:ILE:HD11	1:A:629:ILE:CG2	2.47	0.42
2:B:792:VAL:O	2:B:792:VAL:HG13	2.19	0.42
4:J:19:VAL:HG22	4:J:19:VAL:O	2.19	0.42
3:E:68:VAL:HG13	3:E:69:VAL:N	2.35	0.42
1:A:515:ASP:N	1:A:516:PRO:CD	2.83	0.42
1:A:740:GLY:N	1:A:741:PRO:CD	2.83	0.42
1:C:754:VAL:HG13	1:C:755:LEU:N	2.35	0.42
4:J:22:LEU:O	4:J:26:ILE:HG12	2.20	0.42
2:B:402:GLU:O	2:B:406:VAL:N	2.48	0.42
2:B:407:MET:N	2:B:422:GLU:O	2.45	0.42
2:B:519:ASP:N	2:B:520:PRO:CD	2.83	0.42
3:G:68:VAL:HG13	3:G:69:VAL:N	2.35	0.42
4:I:22:LEU:O	4:I:26:ILE:HG12	2.19	0.42
1:C:500:ILE:HD11	1:C:629:ILE:CG2	2.47	0.42
2:B:502:ILE:HG22	2:B:503:MET:N	2.35	0.42
1:C:515:ASP:N	1:C:516:PRO:CD	2.83	0.42
2:D:792:VAL:O	2:D:792:VAL:HG13	2.19	0.42
2:B:650:LEU:HD23	2:B:651:ASP:O	2.20	0.42
1:C:481:ARG:O	1:C:485:ILE:HG22	2.20	0.42
1:A:754:VAL:HG13	1:A:755:LEU:N	2.35	0.42
1:C:740:GLY:N	1:C:741:PRO:CD	2.83	0.42
1:A:580:PHE:HA	1:A:605:THR:OG1	2.20	0.41
3:G:103:TRP:O	3:G:107:HIS:HB2	2.21	0.41
1:A:401:TYR:O	1:A:421:CYS:N	2.48	0.41
2:D:708:MET:O	2:D:712:ILE:HG12	2.21	0.41
1:A:723:LEU:HD12	1:A:723:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:502:ILE:HG22	2:D:503:MET:N	2.35	0.41
2:D:519:ASP:N	2:D:520:PRO:CD	2.83	0.41
2:B:704:LEU:HD12	2:B:705:GLU:O	2.20	0.41
1:C:723:LEU:HD12	1:C:723:LEU:N	2.36	0.41
2:D:407:MET:N	2:D:422:GLU:O	2.44	0.41
2:D:650:LEU:HD23	2:D:651:ASP:O	2.20	0.41
1:C:580:PHE:HA	1:C:605:THR:OG1	2.20	0.41
3:G:139:LEU:O	3:G:143:LEU:HD23	2.20	0.41
3:E:139:LEU:O	3:E:143:LEU:HD23	2.20	0.41
4:J:133:LEU:O	4:J:137:LEU:HG	2.21	0.41
3:G:5:PHE:CE1	3:G:9:CYS:SG	3.14	0.41
3:G:31:PHE:HE2	3:G:131:CYS:CB	2.34	0.41
4:I:133:LEU:O	4:I:137:LEU:HG	2.21	0.41
2:D:484:VAL:HG23	2:D:485:ARG:N	2.36	0.41
3:E:103:TRP:O	3:E:107:HIS:HB2	2.21	0.41
2:D:584:PHE:HA	2:D:609:THR:OG1	2.21	0.41
3:E:5:PHE:CE1	3:E:9:CYS:SG	3.14	0.40
1:A:808:ILE:HG21	6:A:1404:PC1:H271	2.03	0.40
2:B:574:PHE:CD1	6:B:1406:PC1:H3I1	2.56	0.40
2:D:574:PHE:CD1	6:D:1405:PC1:H3I1	2.56	0.40
3:E:31:PHE:HE2	3:E:131:CYS:CB	2.34	0.40
2:D:704:LEU:HD12	2:D:705:GLU:O	2.20	0.40
1:A:481:ARG:O	1:A:485:ILE:HG22	2.20	0.40
1:C:401:TYR:O	1:C:421:CYS:N	2.47	0.40
2:B:584:PHE:HA	2:B:609:THR:OG1	2.21	0.40
2:B:708:MET:O	2:B:712:ILE:HG12	2.20	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	400/915 (44%)	380 (95%)	20 (5%)	0	100	100
1	C	400/915 (44%)	380 (95%)	20 (5%)	0	100	100
2	B	393/860 (46%)	373 (95%)	20 (5%)	0	100	100
2	D	393/860 (46%)	373 (95%)	20 (5%)	0	100	100
3	E	156/188 (83%)	154 (99%)	2 (1%)	0	100	100
3	G	156/188 (83%)	154 (99%)	2 (1%)	0	100	100
4	I	178/423 (42%)	173 (97%)	5 (3%)	0	100	100
4	J	178/423 (42%)	172 (97%)	6 (3%)	0	100	100
All	All	2254/4772 (47%)	2159 (96%)	95 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/778 (30%)	235 (100%)	0	100	100
1	C	235/778 (30%)	235 (100%)	0	100	100
2	B	270/737 (37%)	269 (100%)	1 (0%)	91	97
2	D	270/737 (37%)	269 (100%)	1 (0%)	91	97
3	E	114/166 (69%)	114 (100%)	0	100	100
3	G	114/166 (69%)	114 (100%)	0	100	100
4	I	124/309 (40%)	123 (99%)	1 (1%)	81	91
4	J	124/309 (40%)	123 (99%)	1 (1%)	81	91
All	All	1486/3980 (37%)	1482 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	628	ARG
4	I	102	LYS

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Mol	Chain	Res	Type
4	J	102	LYS
2	D	628	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

34 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PC1	C	1406	-	19,19,53	0.78	1 (5%)	19,19,61	1.01	0
6	PC1	E	1901	-	17,17,53	0.81	1 (5%)	17,17,61	1.09	0
6	PC1	C	1407	-	19,19,53	0.75	1 (5%)	19,19,61	1.10	0
6	PC1	C	1403	-	17,17,53	0.82	1 (5%)	17,17,61	1.11	1 (5%)
6	PC1	C	1404	-	17,17,53	0.81	1 (5%)	17,17,61	1.09	1 (5%)
6	PC1	J	1902	-	19,19,53	0.76	1 (5%)	19,19,61	1.06	0
6	PC1	B	1403	-	19,19,53	0.76	1 (5%)	19,19,61	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PC1	B	1402	-	15,15,53	1.71	2 (13%)	15,15,61	1.00	0
6	PC1	A	1406	-	19,19,53	0.79	1 (5%)	19,19,61	1.02	0
6	PC1	A	1404	-	17,17,53	0.82	1 (5%)	17,17,61	1.09	1 (5%)
7	GLU	A	1408	-	7,8,9	0.86	0	4,9,11	1.02	0
6	PC1	C	1402	-	17,17,53	0.81	1 (5%)	17,17,61	1.08	1 (5%)
7	GLU	D	1406	-	7,8,9	0.86	0	4,9,11	0.99	0
6	PC1	A	1402	-	17,17,53	0.80	1 (5%)	17,17,61	1.09	1 (5%)
6	PC1	D	1403	-	19,19,53	0.75	1 (5%)	19,19,61	1.05	0
6	PC1	A	1403	-	17,17,53	0.81	1 (5%)	17,17,61	1.10	1 (5%)
6	PC1	D	1404	-	19,19,53	0.79	1 (5%)	19,19,61	0.97	0
5	CYZ	B	1401	-	26,27,27	7.59	18 (69%)	38,44,44	3.36	13 (34%)
6	PC1	D	1402	-	15,15,53	1.70	2 (13%)	15,15,61	1.00	0
6	PC1	B	1405	-	17,17,53	0.81	1 (5%)	17,17,61	1.09	0
6	PC1	B	1406	-	24,24,53	0.78	2 (8%)	25,25,61	1.03	1 (4%)
5	CYZ	A	1401	-	26,27,27	7.59	18 (69%)	38,44,44	3.44	16 (42%)
6	PC1	A	1405	-	19,19,53	0.77	1 (5%)	19,19,61	0.99	0
5	CYZ	D	1401	-	26,27,27	7.60	18 (69%)	38,44,44	3.36	13 (34%)
6	PC1	J	1901	-	19,19,53	0.76	1 (5%)	19,19,61	1.09	1 (5%)
6	PC1	D	1405	-	24,24,53	0.78	2 (8%)	25,25,61	1.04	1 (4%)
7	GLU	B	1407	-	7,8,9	0.85	0	4,9,11	1.00	0
5	CYZ	C	1401	-	26,27,27	7.59	18 (69%)	38,44,44	3.45	15 (39%)
7	GLU	C	1408	-	7,8,9	0.85	0	4,9,11	1.02	0
6	PC1	I	1802	-	19,19,53	0.76	1 (5%)	19,19,61	1.10	1 (5%)
6	PC1	C	1405	-	19,19,53	0.77	1 (5%)	19,19,61	0.99	0
6	PC1	B	1404	-	19,19,53	0.79	1 (5%)	19,19,61	0.97	0
6	PC1	I	1801	-	19,19,53	0.76	1 (5%)	19,19,61	1.06	0
6	PC1	A	1407	-	19,19,53	0.76	1 (5%)	19,19,61	1.09	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	PC1	C	1406	-	-	6/17/17/57	-
6	PC1	E	1901	-	-	7/15/15/57	-
6	PC1	C	1407	-	-	6/17/17/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PC1	C	1403	-	-	3/15/15/57	-
6	PC1	C	1404	-	-	5/15/15/57	-
6	PC1	J	1902	-	-	5/17/17/57	-
6	PC1	B	1403	-	-	10/17/17/57	-
6	PC1	B	1402	-	-	7/13/13/57	-
6	PC1	A	1406	-	-	6/17/17/57	-
6	PC1	A	1404	-	-	5/15/15/57	-
7	GLU	A	1408	-	-	3/6/7/9	-
6	PC1	C	1402	-	-	6/15/15/57	-
7	GLU	D	1406	-	-	2/6/7/9	-
6	PC1	A	1402	-	-	6/15/15/57	-
6	PC1	D	1403	-	-	10/17/17/57	-
6	PC1	A	1403	-	-	3/15/15/57	-
6	PC1	D	1404	-	-	3/17/17/57	-
5	CYZ	B	1401	-	-	6/6/42/42	0/5/4/4
6	PC1	D	1402	-	-	7/13/13/57	-
6	PC1	B	1405	-	-	7/15/15/57	-
6	PC1	B	1406	-	-	6/24/24/57	-
5	CYZ	A	1401	-	-	6/6/42/42	0/5/4/4
6	PC1	A	1405	-	-	10/17/17/57	-
5	CYZ	D	1401	-	-	6/6/42/42	0/5/4/4
6	PC1	J	1901	-	-	10/17/17/57	-
6	PC1	D	1405	-	-	6/24/24/57	-
7	GLU	B	1407	-	-	2/6/7/9	-
5	CYZ	C	1401	-	-	6/6/42/42	0/5/4/4
7	GLU	C	1408	-	-	3/6/7/9	-
6	PC1	I	1802	-	-	10/17/17/57	-
6	PC1	C	1405	-	-	10/17/17/57	-
6	PC1	B	1404	-	-	3/17/17/57	-
6	PC1	I	1801	-	-	5/17/17/57	-
6	PC1	A	1407	-	-	6/17/17/57	-

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1401	CYZ	C2-C3	-18.94	0.99	1.51
5	A	1401	CYZ	C2-C3	-18.92	0.99	1.51
5	B	1401	CYZ	C2-C3	-18.75	1.00	1.51
5	D	1401	CYZ	C2-C3	-18.74	1.00	1.51
5	A	1401	CYZ	C2-C1	-15.57	1.21	1.55
5	C	1401	CYZ	C2-C1	-15.55	1.21	1.55
5	D	1401	CYZ	C2-C1	-15.48	1.21	1.55
5	B	1401	CYZ	C2-C1	-15.47	1.21	1.55
5	C	1401	CYZ	C7-C2	-11.78	1.27	1.54
5	B	1401	CYZ	C7-C2	-11.77	1.27	1.54
5	A	1401	CYZ	C7-C2	-11.76	1.27	1.54
5	D	1401	CYZ	C7-C2	-11.76	1.27	1.54
5	D	1401	CYZ	C10-N2	10.76	1.59	1.39
5	B	1401	CYZ	C10-N2	10.74	1.59	1.39
5	A	1401	CYZ	C10-N2	10.49	1.58	1.39
5	C	1401	CYZ	C10-N2	10.46	1.58	1.39
5	D	1401	CYZ	O1-S1	10.20	1.55	1.43
5	A	1401	CYZ	O1-S1	10.18	1.55	1.43
5	B	1401	CYZ	O1-S1	10.16	1.55	1.43
5	C	1401	CYZ	O1-S1	10.16	1.55	1.43
5	D	1401	CYZ	C9-S1	-9.56	1.67	1.75
5	B	1401	CYZ	C9-S1	-9.48	1.67	1.75
5	C	1401	CYZ	C9-S1	-9.36	1.67	1.75
5	A	1401	CYZ	C9-S1	-9.34	1.67	1.75
5	C	1401	CYZ	C5-C4	-9.07	1.07	1.50
5	A	1401	CYZ	C5-C4	-9.05	1.07	1.50
5	D	1401	CYZ	C5-C4	-9.01	1.07	1.50
5	B	1401	CYZ	C5-C4	-9.01	1.07	1.50
5	A	1401	CYZ	C6-C1	-8.54	1.30	1.53
5	C	1401	CYZ	C6-C1	-8.52	1.30	1.53
5	B	1401	CYZ	C6-C1	-8.50	1.30	1.53
5	D	1401	CYZ	C6-C1	-8.50	1.30	1.53
5	A	1401	CYZ	C4-C3	8.48	1.57	1.32
5	D	1401	CYZ	C4-C3	8.47	1.57	1.32
5	C	1401	CYZ	C4-C3	8.46	1.57	1.32
5	B	1401	CYZ	C4-C3	8.46	1.57	1.32
5	A	1401	CYZ	S2-N3	7.14	1.74	1.60
5	D	1401	CYZ	S2-N3	7.14	1.74	1.60
5	B	1401	CYZ	S2-N3	7.11	1.74	1.60
5	C	1401	CYZ	S2-N3	7.09	1.74	1.60
5	D	1401	CYZ	C6-C5	-6.97	1.12	1.51
5	A	1401	CYZ	C6-C5	-6.96	1.12	1.51
5	B	1401	CYZ	C6-C5	-6.96	1.12	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1401	CYZ	C6-C5	-6.95	1.12	1.51
5	D	1401	CYZ	C8-N2	6.87	1.54	1.46
5	B	1401	CYZ	C8-N2	6.87	1.54	1.46
5	A	1401	CYZ	C8-N2	6.68	1.54	1.46
5	C	1401	CYZ	C8-N2	6.66	1.54	1.46
6	B	1402	PC1	O22-C21	5.41	1.40	1.22
6	D	1402	PC1	O22-C21	5.40	1.40	1.22
5	D	1401	CYZ	C12-S2	5.03	1.83	1.77
5	C	1401	CYZ	C12-S2	4.99	1.83	1.77
5	B	1401	CYZ	C12-S2	4.99	1.83	1.77
5	A	1401	CYZ	C12-S2	4.94	1.83	1.77
5	C	1401	CYZ	C10-C9	-4.66	1.33	1.40
5	A	1401	CYZ	C10-C9	-4.64	1.33	1.40
5	B	1401	CYZ	C10-C9	-4.39	1.34	1.40
5	D	1401	CYZ	C10-C9	-4.38	1.34	1.40
6	B	1402	PC1	O21-C21	-3.58	1.18	1.30
5	C	1401	CYZ	C8-N1	-3.57	1.42	1.46
6	D	1402	PC1	O21-C21	-3.57	1.18	1.30
5	B	1401	CYZ	C8-N1	-3.52	1.42	1.46
5	A	1401	CYZ	C8-N1	-3.48	1.42	1.46
5	D	1401	CYZ	C8-N1	-3.44	1.42	1.46
5	A	1401	CYZ	O3-S2	3.07	1.49	1.43
5	B	1401	CYZ	O3-S2	3.05	1.49	1.43
5	C	1401	CYZ	O3-S2	3.03	1.49	1.43
5	D	1401	CYZ	O3-S2	3.00	1.49	1.43
6	C	1407	PC1	O21-C21	2.86	1.40	1.30
6	A	1407	PC1	O21-C21	2.86	1.40	1.30
6	A	1406	PC1	O21-C21	2.86	1.40	1.30
6	E	1901	PC1	O21-C21	2.85	1.40	1.30
6	C	1403	PC1	O21-C21	2.85	1.40	1.30
6	A	1402	PC1	O21-C21	2.85	1.40	1.30
6	C	1406	PC1	O21-C21	2.85	1.40	1.30
6	A	1404	PC1	O21-C21	2.85	1.40	1.30
6	A	1403	PC1	O21-C21	2.84	1.40	1.30
6	B	1405	PC1	O21-C21	2.84	1.40	1.30
6	C	1404	PC1	O21-C21	2.83	1.40	1.30
6	B	1404	PC1	O21-C21	2.83	1.40	1.30
6	C	1402	PC1	O21-C21	2.83	1.40	1.30
6	I	1801	PC1	O21-C21	2.83	1.40	1.30
6	D	1404	PC1	O21-C21	2.83	1.40	1.30
6	A	1405	PC1	O21-C21	2.82	1.40	1.30
6	J	1902	PC1	O21-C21	2.82	1.40	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1405	PC1	O21-C21	2.81	1.40	1.30
6	I	1802	PC1	O21-C21	2.81	1.40	1.30
6	J	1901	PC1	O21-C21	2.80	1.40	1.30
6	B	1403	PC1	O21-C21	2.78	1.40	1.30
6	D	1403	PC1	O21-C21	2.77	1.40	1.30
5	C	1401	CYZ	C14-C13	-2.51	1.34	1.38
5	A	1401	CYZ	C14-C13	-2.49	1.34	1.38
6	B	1406	PC1	O31-C31	2.38	1.40	1.33
6	D	1405	PC1	O31-C31	2.36	1.40	1.33
5	B	1401	CYZ	C14-C13	-2.32	1.34	1.38
5	D	1401	CYZ	C14-C13	-2.32	1.34	1.38
5	B	1401	CYZ	C7-C5	2.21	1.64	1.51
5	D	1401	CYZ	C7-C5	2.20	1.64	1.51
5	C	1401	CYZ	C7-C5	2.14	1.64	1.51
5	A	1401	CYZ	C7-C5	2.14	1.64	1.51
6	D	1405	PC1	O31-C3	-2.14	1.40	1.45
6	B	1406	PC1	O31-C3	-2.12	1.40	1.45

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1401	CYZ	C9-S1-N1	11.77	118.45	103.43
5	A	1401	CYZ	C9-S1-N1	11.75	118.42	103.43
5	D	1401	CYZ	C9-S1-N1	11.22	117.75	103.43
5	B	1401	CYZ	C9-S1-N1	11.19	117.71	103.43
5	B	1401	CYZ	O4-S2-O3	-10.79	101.03	118.76
5	D	1401	CYZ	O4-S2-O3	-10.76	101.08	118.76
5	C	1401	CYZ	O4-S2-O3	-10.73	101.12	118.76
5	A	1401	CYZ	O4-S2-O3	-10.73	101.12	118.76
5	C	1401	CYZ	O2-S1-O1	-7.94	110.36	118.46
5	A	1401	CYZ	O2-S1-O1	-7.93	110.37	118.46
5	D	1401	CYZ	O2-S1-O1	-7.42	110.89	118.46
5	B	1401	CYZ	O2-S1-O1	-7.38	110.93	118.46
5	D	1401	CYZ	C1-C2-C3	4.42	114.08	106.92
5	B	1401	CYZ	C1-C2-C3	4.42	114.07	106.92
5	A	1401	CYZ	C1-C2-C3	4.39	114.02	106.92
5	C	1401	CYZ	C1-C2-C3	4.37	113.99	106.92
5	A	1401	CYZ	C6-C1-C2	3.44	110.31	104.22
5	B	1401	CYZ	C6-C1-C2	3.42	110.29	104.22
5	C	1401	CYZ	C6-C1-C2	3.42	110.29	104.22
5	D	1401	CYZ	C6-C1-C2	3.42	110.28	104.22
5	B	1401	CYZ	C13-C12-S2	-3.26	119.36	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1401	CYZ	C13-C12-S2	-3.26	119.36	123.49
5	C	1401	CYZ	O3-S2-C12	3.25	112.05	107.29
5	A	1401	CYZ	C13-C12-S2	-3.24	119.37	123.49
5	C	1401	CYZ	C13-C12-S2	-3.24	119.38	123.49
5	A	1401	CYZ	O3-S2-C12	3.22	112.00	107.29
5	D	1401	CYZ	O3-S2-C12	3.14	111.88	107.29
5	B	1401	CYZ	O3-S2-C12	3.12	111.86	107.29
5	C	1401	CYZ	O3-S2-N3	2.95	111.74	107.36
5	A	1401	CYZ	O3-S2-N3	2.90	111.66	107.36
5	B	1401	CYZ	O3-S2-N3	2.85	111.59	107.36
5	D	1401	CYZ	O3-S2-N3	2.84	111.58	107.36
5	B	1401	CYZ	C2-C1-C8	-2.81	110.81	114.81
5	D	1401	CYZ	C2-C1-C8	-2.78	110.86	114.81
5	D	1401	CYZ	C12-C13-CL	-2.76	119.47	121.49
5	B	1401	CYZ	O4-S2-N3	2.76	111.45	107.36
5	B	1401	CYZ	C12-C13-CL	-2.75	119.48	121.49
5	D	1401	CYZ	O4-S2-N3	2.72	111.39	107.36
5	C	1401	CYZ	C12-C13-CL	-2.67	119.54	121.49
5	A	1401	CYZ	O4-S2-C12	2.64	111.16	107.29
6	D	1405	PC1	O31-C31-C32	2.61	120.11	111.91
6	B	1406	PC1	O31-C31-C32	2.61	120.10	111.91
5	C	1401	CYZ	O4-S2-C12	2.60	111.10	107.29
5	D	1401	CYZ	O4-S2-C12	2.55	111.02	107.29
5	B	1401	CYZ	O4-S2-C12	2.55	111.02	107.29
5	A	1401	CYZ	O4-S2-N3	2.46	111.01	107.36
5	A	1401	CYZ	C12-C13-CL	-2.46	119.69	121.49
5	A	1401	CYZ	C2-C1-C8	-2.42	111.38	114.81
5	C	1401	CYZ	O4-S2-N3	2.41	110.93	107.36
5	C	1401	CYZ	C2-C1-C8	-2.35	111.47	114.81
5	C	1401	CYZ	C11-C9-S1	2.32	121.72	119.82
5	C	1401	CYZ	C6-C1-C8	-2.29	108.53	114.40
5	A	1401	CYZ	C11-C9-S1	2.28	121.69	119.82
6	J	1901	PC1	C23-C22-C21	-2.27	108.75	114.47
6	I	1802	PC1	C23-C22-C21	-2.26	108.77	114.47
5	A	1401	CYZ	C6-C1-C8	-2.24	108.68	114.40
5	B	1401	CYZ	C6-C1-C8	-2.12	108.97	114.40
5	D	1401	CYZ	C6-C1-C8	-2.12	108.97	114.40
6	C	1403	PC1	C23-C22-C21	-2.08	109.22	114.47
6	A	1402	PC1	C23-C22-C21	-2.07	109.25	114.47
6	C	1404	PC1	C23-C22-C21	-2.07	109.26	114.47
6	C	1402	PC1	C23-C22-C21	-2.07	109.26	114.47
6	A	1403	PC1	C23-C22-C21	-2.06	109.28	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1404	PC1	C23-C22-C21	-2.04	109.32	114.47
5	A	1401	CYZ	O2-S1-C9	-2.04	106.78	109.29
5	A	1401	CYZ	C11-C12-S2	2.02	120.75	118.34
5	C	1401	CYZ	O2-S1-C9	-2.00	106.82	109.29

There are no chirality outliers.

All (202) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1401	CYZ	C11-C12-S2-O4
5	A	1401	CYZ	C11-C12-S2-N3
5	A	1401	CYZ	C13-C12-S2-O3
5	A	1401	CYZ	C13-C12-S2-O4
5	A	1401	CYZ	C13-C12-S2-N3
5	B	1401	CYZ	C11-C12-S2-O3
5	B	1401	CYZ	C11-C12-S2-N3
5	B	1401	CYZ	C13-C12-S2-O3
5	B	1401	CYZ	C13-C12-S2-O4
5	B	1401	CYZ	C13-C12-S2-N3
5	C	1401	CYZ	C11-C12-S2-O4
5	C	1401	CYZ	C11-C12-S2-N3
5	C	1401	CYZ	C13-C12-S2-O3
5	C	1401	CYZ	C13-C12-S2-O4
5	C	1401	CYZ	C13-C12-S2-N3
5	D	1401	CYZ	C11-C12-S2-O3
5	D	1401	CYZ	C11-C12-S2-N3
5	D	1401	CYZ	C13-C12-S2-O3
5	D	1401	CYZ	C13-C12-S2-O4
5	D	1401	CYZ	C13-C12-S2-N3
6	B	1406	PC1	C1-C2-C3-O31
6	D	1405	PC1	C1-C2-C3-O31
7	A	1408	GLU	O-C-CA-CB
7	C	1408	GLU	O-C-CA-CB
6	B	1406	PC1	O21-C2-C3-O31
6	D	1405	PC1	O21-C2-C3-O31
6	B	1406	PC1	C32-C31-O31-C3
6	D	1405	PC1	C32-C31-O31-C3
5	B	1401	CYZ	C11-C12-S2-O4
5	D	1401	CYZ	C11-C12-S2-O4
6	B	1406	PC1	C31-C32-C33-C34
6	D	1405	PC1	C31-C32-C33-C34
6	B	1406	PC1	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
6	D	1405	PC1	C37-C38-C39-C3A
6	B	1406	PC1	O32-C31-O31-C3
6	D	1405	PC1	O32-C31-O31-C3
5	A	1401	CYZ	C11-C12-S2-O3
5	C	1401	CYZ	C11-C12-S2-O3
6	A	1405	PC1	C2B-C2C-C2D-C2E
6	C	1405	PC1	C2B-C2C-C2D-C2E
6	J	1901	PC1	C29-C2A-C2B-C2C
6	A	1405	PC1	C26-C27-C28-C29
6	I	1802	PC1	C29-C2A-C2B-C2C
6	C	1405	PC1	C26-C27-C28-C29
6	I	1802	PC1	C2E-C2F-C2G-C2H
6	J	1901	PC1	C2E-C2F-C2G-C2H
6	B	1405	PC1	C26-C27-C28-C29
6	E	1901	PC1	C26-C27-C28-C29
6	A	1407	PC1	C2E-C2F-C2G-C2H
6	B	1405	PC1	C23-C24-C25-C26
6	C	1407	PC1	C2E-C2F-C2G-C2H
6	E	1901	PC1	C23-C24-C25-C26
6	A	1403	PC1	C27-C28-C29-C2A
6	C	1403	PC1	C27-C28-C29-C2A
6	J	1901	PC1	C21-C22-C23-C24
6	A	1404	PC1	C28-C29-C2A-C2B
6	B	1402	PC1	C29-C2A-C2B-C2C
6	D	1402	PC1	C29-C2A-C2B-C2C
6	A	1402	PC1	C2B-C2C-C2D-C2E
6	C	1402	PC1	C2B-C2C-C2D-C2E
6	C	1404	PC1	C28-C29-C2A-C2B
6	D	1402	PC1	C25-C26-C27-C28
6	B	1402	PC1	C25-C26-C27-C28
6	B	1403	PC1	C27-C28-C29-C2A
6	I	1801	PC1	C29-C2A-C2B-C2C
6	J	1902	PC1	C29-C2A-C2B-C2C
6	D	1403	PC1	C27-C28-C29-C2A
6	I	1802	PC1	C21-C22-C23-C24
6	A	1402	PC1	C26-C27-C28-C29
6	A	1404	PC1	C24-C25-C26-C27
6	C	1402	PC1	C26-C27-C28-C29
6	C	1404	PC1	C24-C25-C26-C27
6	I	1801	PC1	C26-C27-C28-C29
6	J	1902	PC1	C26-C27-C28-C29
6	B	1402	PC1	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
6	D	1402	PC1	C24-C25-C26-C27
6	B	1403	PC1	C25-C26-C27-C28
6	D	1403	PC1	C25-C26-C27-C28
6	B	1404	PC1	C21-C22-C23-C24
6	D	1404	PC1	C21-C22-C23-C24
6	A	1402	PC1	C25-C26-C27-C28
6	A	1403	PC1	C26-C27-C28-C29
6	C	1402	PC1	C25-C26-C27-C28
6	C	1403	PC1	C26-C27-C28-C29
6	C	1406	PC1	C29-C2A-C2B-C2C
6	B	1403	PC1	C26-C27-C28-C29
6	A	1406	PC1	C29-C2A-C2B-C2C
6	D	1403	PC1	C26-C27-C28-C29
6	C	1406	PC1	C22-C23-C24-C25
6	A	1406	PC1	C22-C23-C24-C25
6	J	1901	PC1	C2F-C2G-C2H-C2I
6	I	1802	PC1	C2F-C2G-C2H-C2I
6	C	1405	PC1	C2A-C2B-C2C-C2D
6	A	1405	PC1	C2A-C2B-C2C-C2D
6	B	1404	PC1	C22-C23-C24-C25
6	D	1404	PC1	C22-C23-C24-C25
6	J	1902	PC1	C2F-C2G-C2H-C2I
6	I	1801	PC1	C2F-C2G-C2H-C2I
6	A	1407	PC1	C26-C27-C28-C29
6	C	1407	PC1	C26-C27-C28-C29
6	I	1802	PC1	C27-C28-C29-C2A
6	J	1901	PC1	C27-C28-C29-C2A
6	C	1403	PC1	C29-C2A-C2B-C2C
6	B	1404	PC1	C23-C24-C25-C26
6	D	1404	PC1	C23-C24-C25-C26
6	A	1403	PC1	C29-C2A-C2B-C2C
6	A	1406	PC1	C21-C22-C23-C24
6	C	1406	PC1	C21-C22-C23-C24
6	B	1402	PC1	C2B-C2C-C2D-C2E
6	D	1402	PC1	C2B-C2C-C2D-C2E
6	C	1406	PC1	C24-C25-C26-C27
6	A	1406	PC1	C24-C25-C26-C27
6	D	1402	PC1	C26-C27-C28-C29
6	B	1402	PC1	C26-C27-C28-C29
6	C	1405	PC1	C28-C29-C2A-C2B
6	A	1405	PC1	C28-C29-C2A-C2B
6	B	1405	PC1	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
6	E	1901	PC1	C25-C26-C27-C28
6	A	1404	PC1	C22-C23-C24-C25
6	C	1404	PC1	C22-C23-C24-C25
6	A	1402	PC1	C2A-C2B-C2C-C2D
6	A	1406	PC1	C28-C29-C2A-C2B
6	C	1402	PC1	C2A-C2B-C2C-C2D
6	A	1405	PC1	C25-C26-C27-C28
6	C	1405	PC1	C25-C26-C27-C28
6	C	1406	PC1	C28-C29-C2A-C2B
6	B	1403	PC1	C23-C24-C25-C26
6	D	1403	PC1	C23-C24-C25-C26
6	C	1407	PC1	C28-C29-C2A-C2B
6	J	1901	PC1	C28-C29-C2A-C2B
6	I	1802	PC1	C28-C29-C2A-C2B
6	A	1407	PC1	C28-C29-C2A-C2B
6	C	1404	PC1	C29-C2A-C2B-C2C
6	A	1404	PC1	C29-C2A-C2B-C2C
6	A	1407	PC1	C25-C26-C27-C28
6	B	1403	PC1	C2F-C2G-C2H-C2I
6	D	1403	PC1	C2E-C2F-C2G-C2H
6	D	1403	PC1	C2F-C2G-C2H-C2I
6	B	1403	PC1	C2E-C2F-C2G-C2H
6	B	1405	PC1	O21-C21-C22-C23
6	E	1901	PC1	O21-C21-C22-C23
6	J	1901	PC1	C25-C26-C27-C28
6	B	1405	PC1	O22-C21-C22-C23
6	E	1901	PC1	O22-C21-C22-C23
6	B	1403	PC1	O21-C21-C22-C23
6	I	1801	PC1	O21-C21-C22-C23
6	J	1902	PC1	O21-C21-C22-C23
6	D	1403	PC1	O21-C21-C22-C23
6	C	1407	PC1	C25-C26-C27-C28
6	I	1801	PC1	O22-C21-C22-C23
6	J	1902	PC1	O22-C21-C22-C23
6	I	1802	PC1	C25-C26-C27-C28
6	B	1403	PC1	C28-C29-C2A-C2B
6	D	1403	PC1	C28-C29-C2A-C2B
6	B	1403	PC1	O22-C21-C22-C23
6	D	1403	PC1	O22-C21-C22-C23
7	B	1407	GLU	OE2-CD-CG-CB
7	D	1406	GLU	OE2-CD-CG-CB
6	C	1407	PC1	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
6	I	1802	PC1	O21-C21-C22-C23
6	J	1901	PC1	O21-C21-C22-C23
6	A	1402	PC1	O21-C21-C22-C23
6	B	1402	PC1	O21-C21-C22-C23
6	C	1405	PC1	O21-C21-C22-C23
6	A	1405	PC1	O21-C21-C22-C23
6	C	1402	PC1	O21-C21-C22-C23
6	D	1402	PC1	O21-C21-C22-C23
6	I	1802	PC1	O22-C21-C22-C23
6	J	1901	PC1	O22-C21-C22-C23
6	A	1407	PC1	C2C-C2D-C2E-C2F
6	I	1802	PC1	C23-C24-C25-C26
6	C	1405	PC1	C23-C24-C25-C26
6	C	1405	PC1	O22-C21-C22-C23
7	A	1408	GLU	OE2-CD-CG-CB
6	B	1405	PC1	C27-C28-C29-C2A
6	E	1901	PC1	C27-C28-C29-C2A
6	A	1405	PC1	O22-C21-C22-C23
6	A	1405	PC1	C23-C24-C25-C26
6	A	1402	PC1	O22-C21-C22-C23
6	C	1402	PC1	O22-C21-C22-C23
7	C	1408	GLU	OE2-CD-CG-CB
7	B	1407	GLU	OE1-CD-CG-CB
7	D	1406	GLU	OE1-CD-CG-CB
6	J	1901	PC1	C23-C24-C25-C26
6	E	1901	PC1	C2B-C2C-C2D-C2E
6	B	1405	PC1	C2B-C2C-C2D-C2E
6	C	1405	PC1	C2C-C2D-C2E-C2F
6	B	1402	PC1	O22-C21-C22-C23
6	D	1403	PC1	C29-C2A-C2B-C2C
6	B	1403	PC1	C29-C2A-C2B-C2C
6	D	1402	PC1	O22-C21-C22-C23
7	A	1408	GLU	OE1-CD-CG-CB
7	C	1408	GLU	OE1-CD-CG-CB
6	C	1405	PC1	C24-C25-C26-C27
6	C	1404	PC1	C26-C27-C28-C29
6	A	1405	PC1	C2C-C2D-C2E-C2F
6	C	1406	PC1	C2D-C2E-C2F-C2G
6	A	1406	PC1	C27-C28-C29-C2A
6	C	1407	PC1	C2B-C2C-C2D-C2E
6	A	1407	PC1	C2B-C2C-C2D-C2E
6	A	1405	PC1	C24-C25-C26-C27

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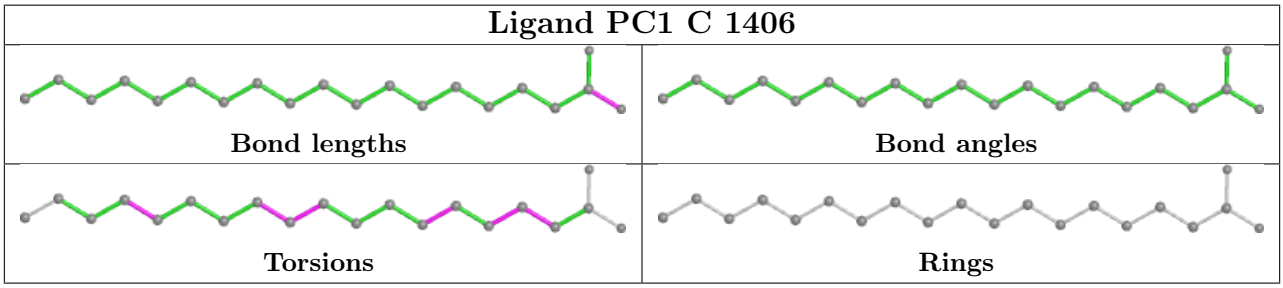
Mol	Chain	Res	Type	Atoms
6	A	1404	PC1	C26-C27-C28-C29

There are no ring outliers.

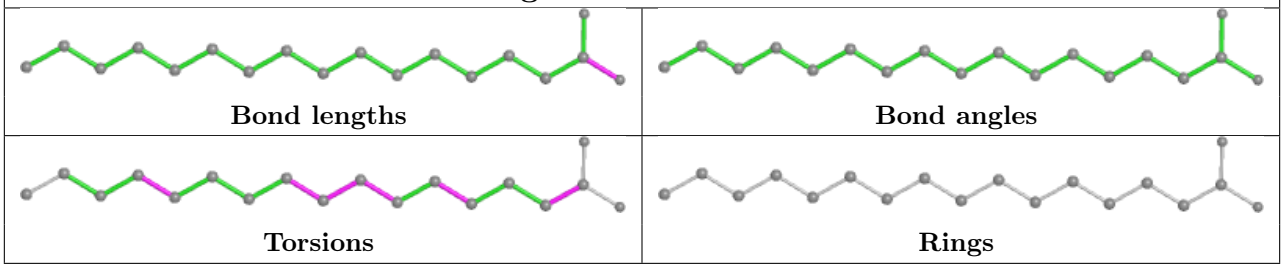
11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1404	PC1	1	0
7	A	1408	GLU	1	0
7	D	1406	GLU	1	0
5	B	1401	CYZ	1	0
6	B	1406	PC1	2	0
5	A	1401	CYZ	2	0
5	D	1401	CYZ	1	0
6	D	1405	PC1	2	0
7	B	1407	GLU	1	0
5	C	1401	CYZ	2	0
7	C	1408	GLU	1	0

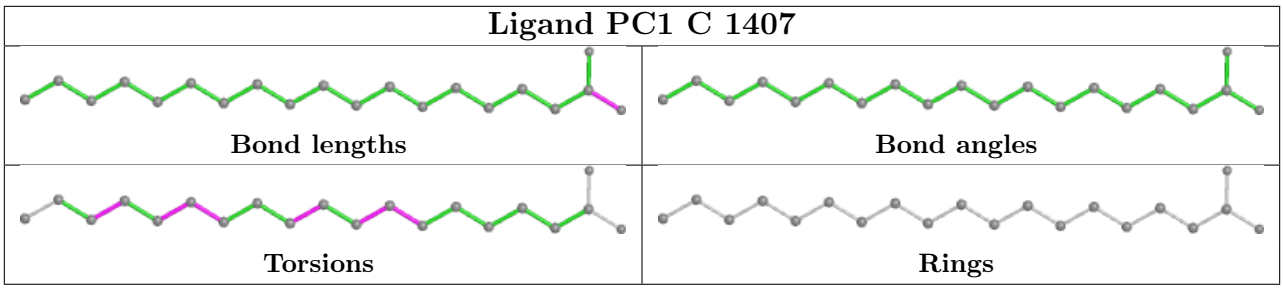
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



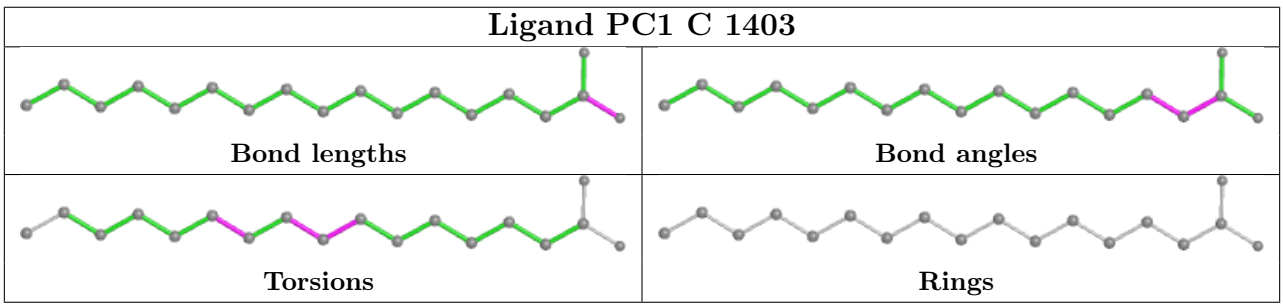
Ligand PC1 E 1901



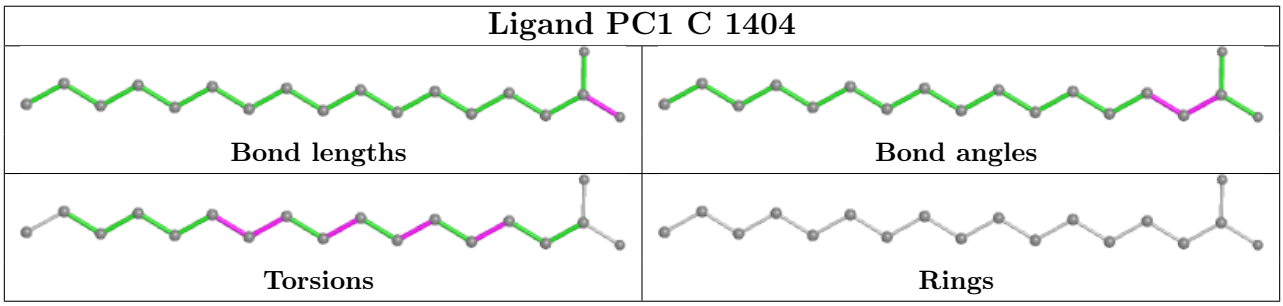
Ligand PC1 C 1407



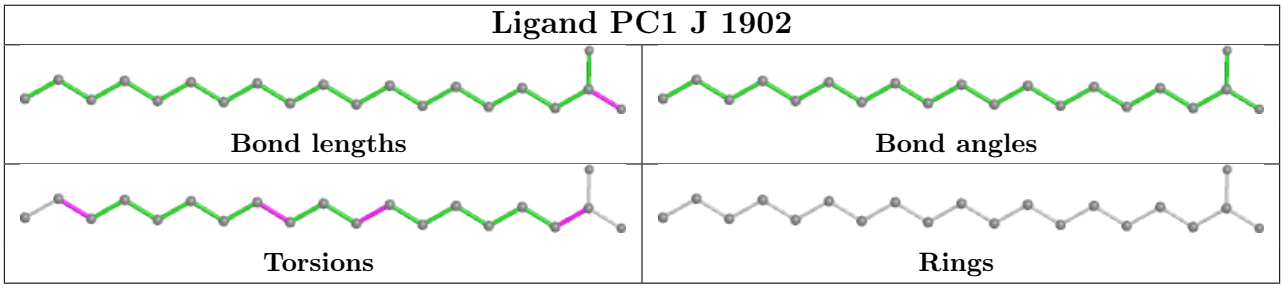
Ligand PC1 C 1403



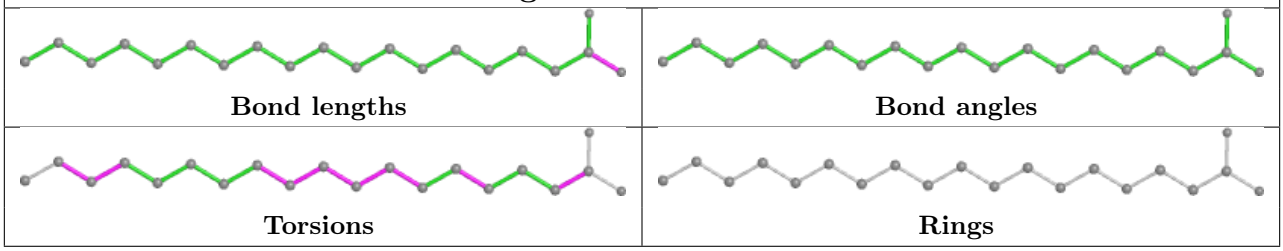
Ligand PC1 C 1404



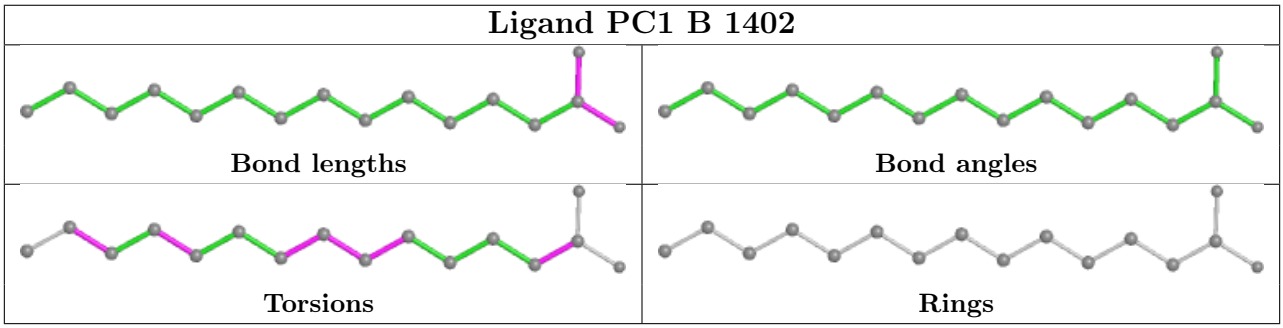
Ligand PC1 J 1902



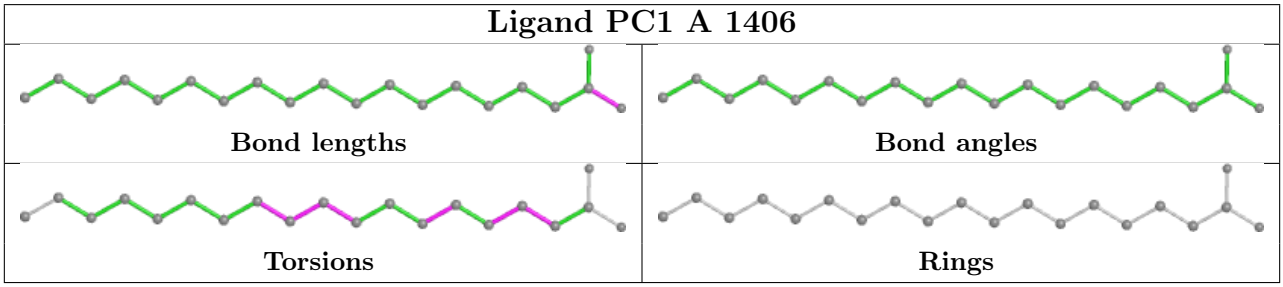
Ligand PC1 B 1403



Ligand PC1 B 1402



Ligand PC1 A 1406



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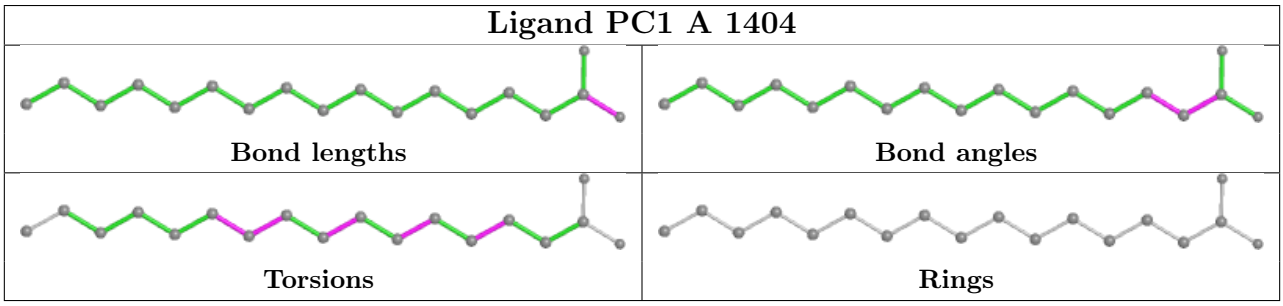
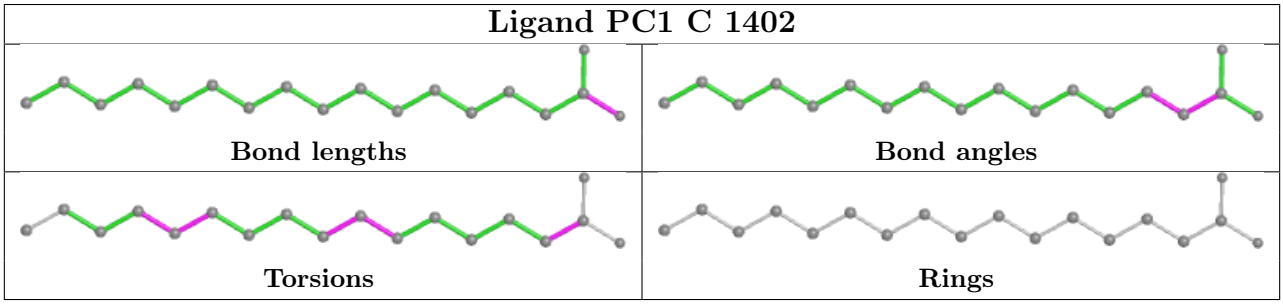
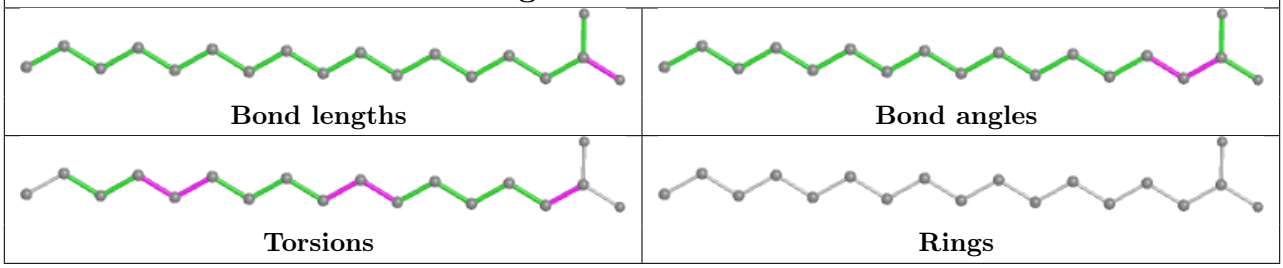


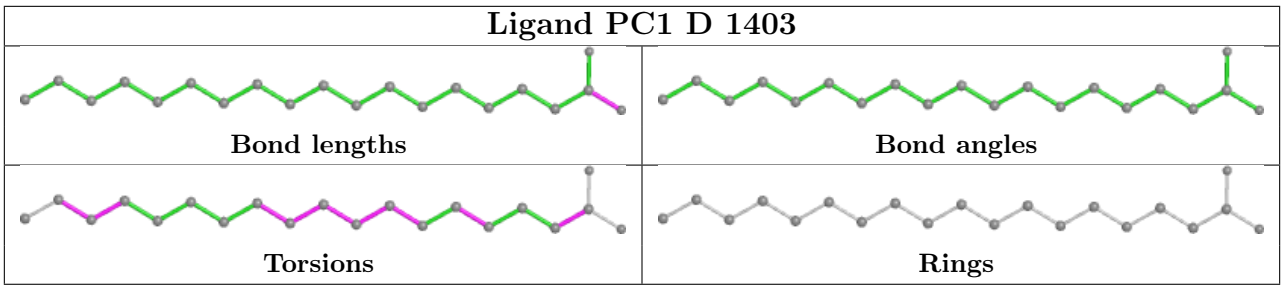
Ligand PC1 C 1402



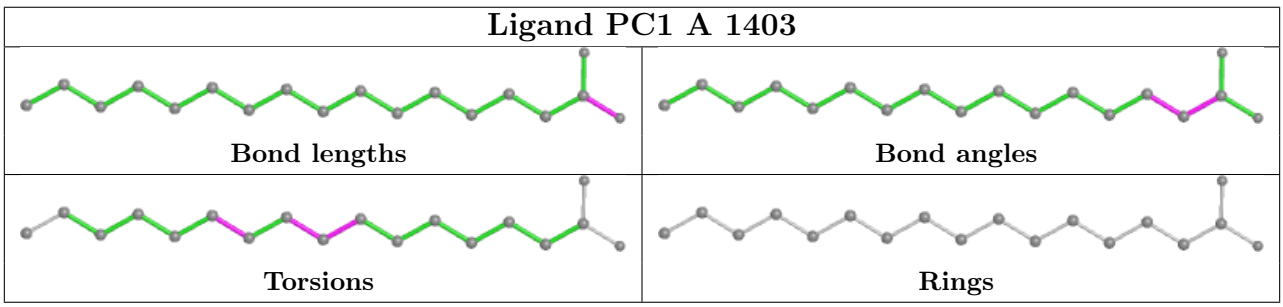
Ligand PC1 A 1402



Ligand PC1 D 1403



Ligand PC1 A 1403



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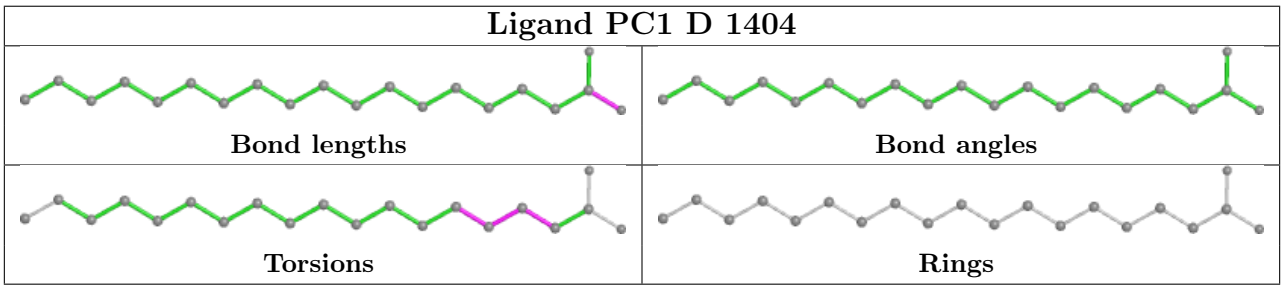
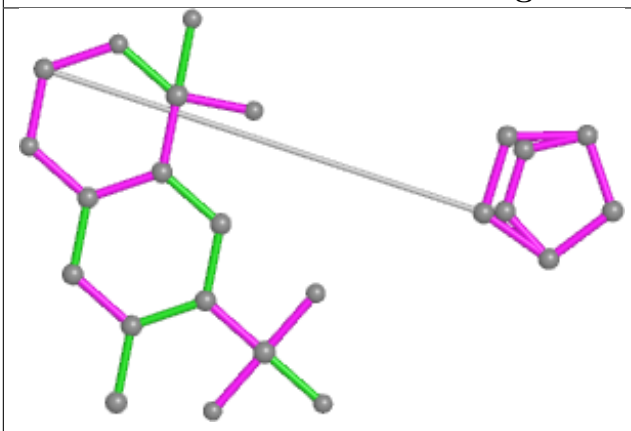
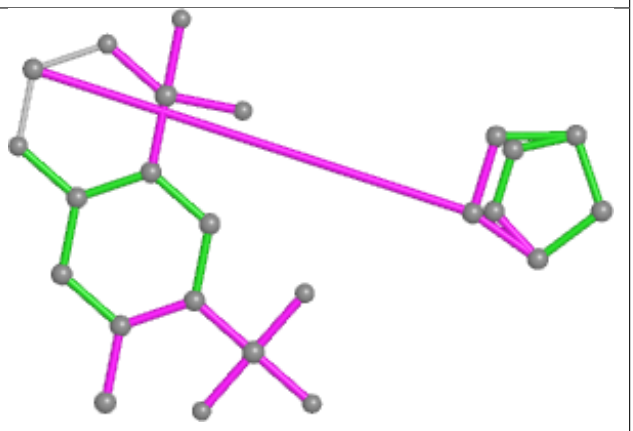


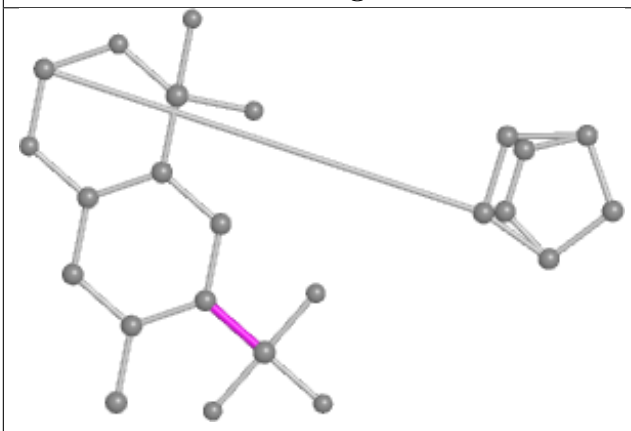
Ligand CYZ B 1401



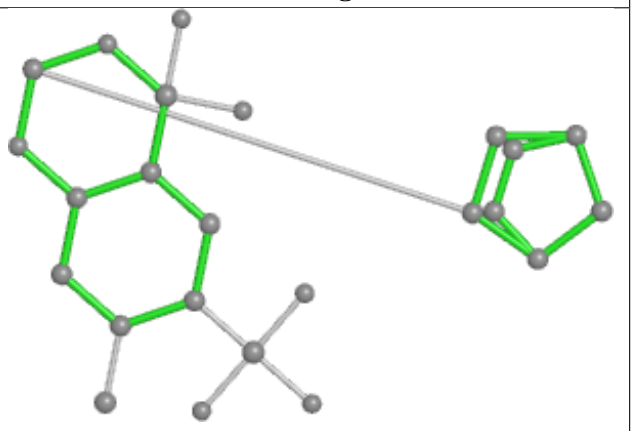
Bond lengths



Bond angles

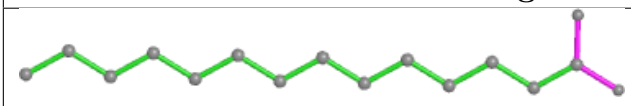


Torsions

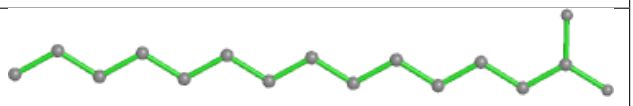


Rings

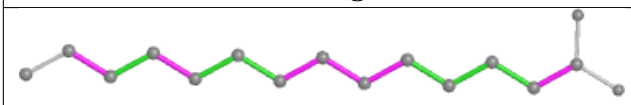
Ligand PC1 D 1402



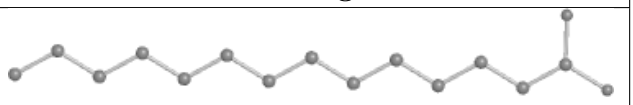
Bond lengths



Bond angles

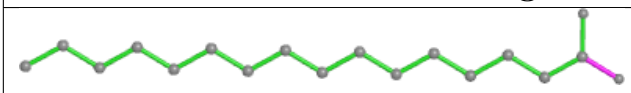


Torsions

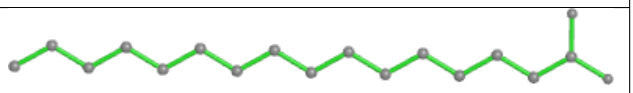


Rings

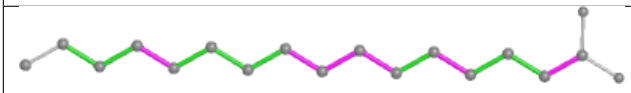
Ligand PC1 B 1405



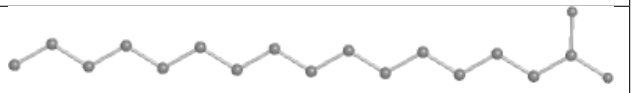
Bond lengths



Bond angles

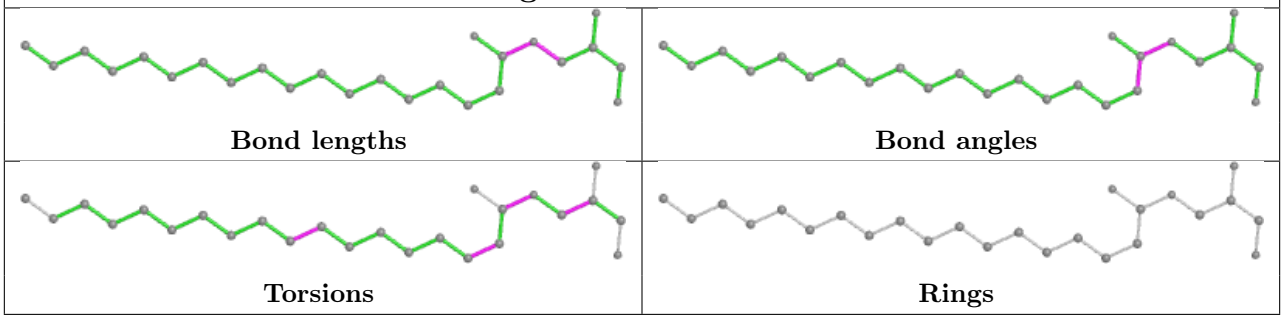


Torsions

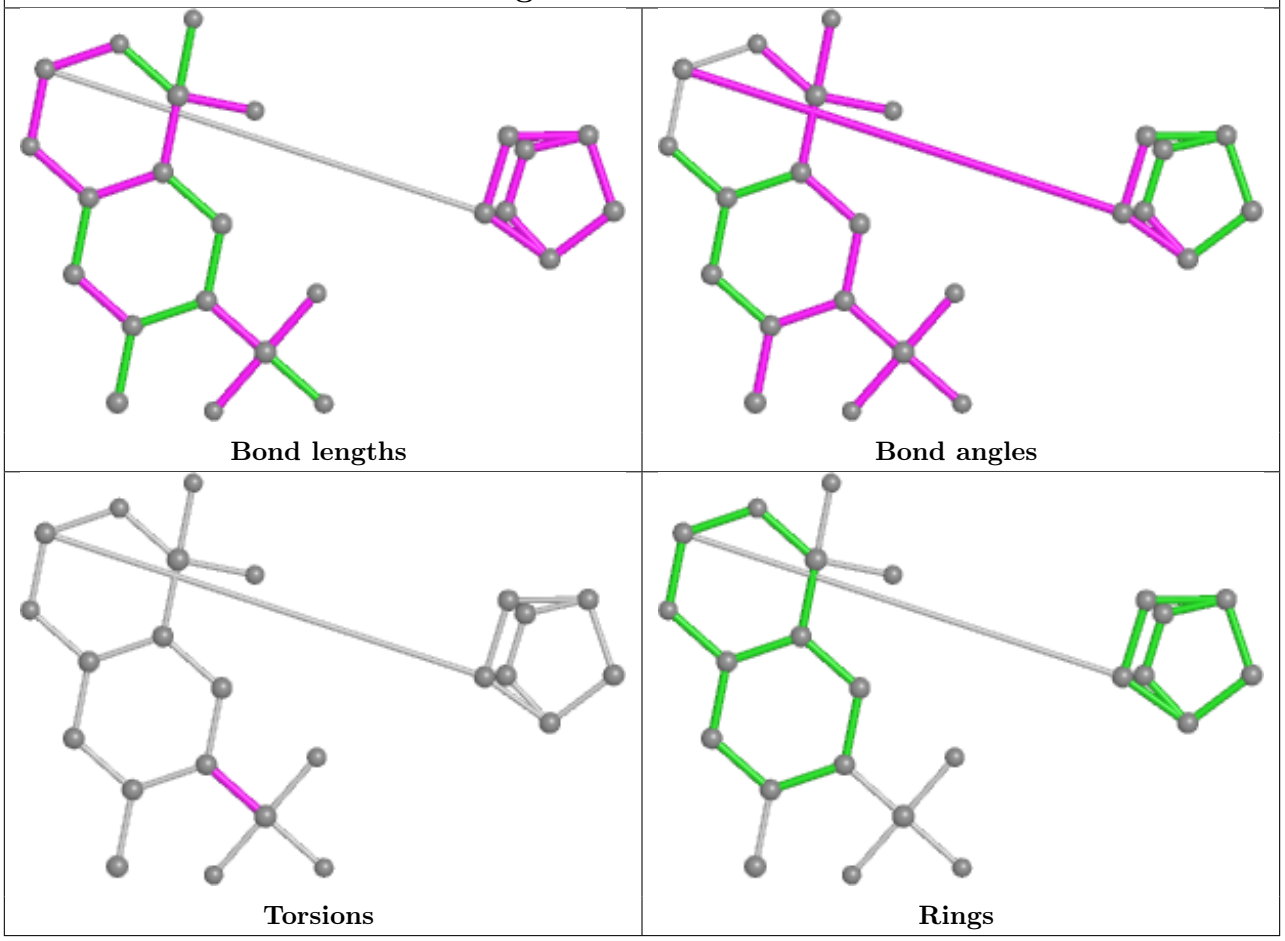


Rings

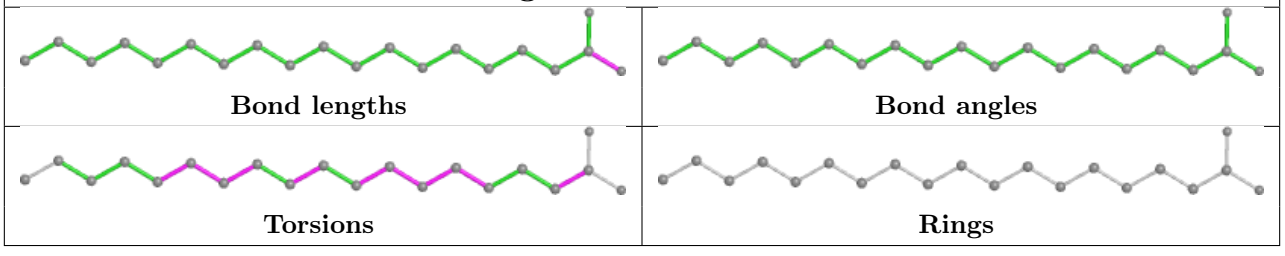
Ligand PC1 B 1406



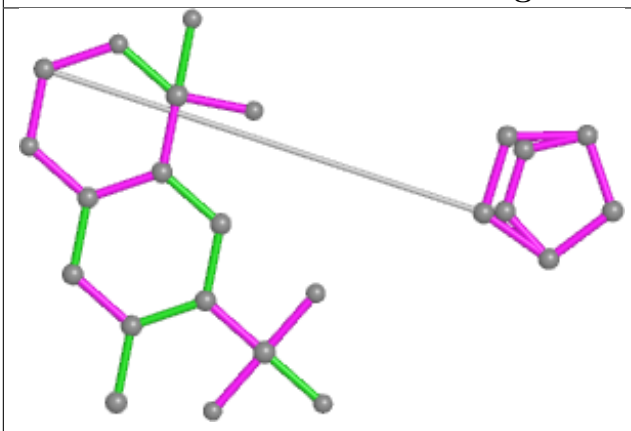
Ligand CYZ A 1401



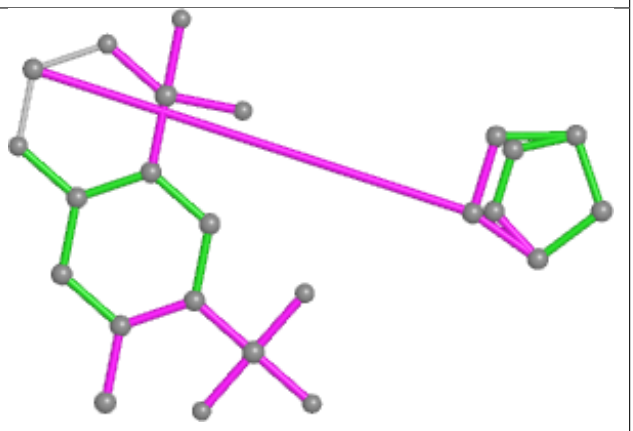
Ligand PC1 A 1405



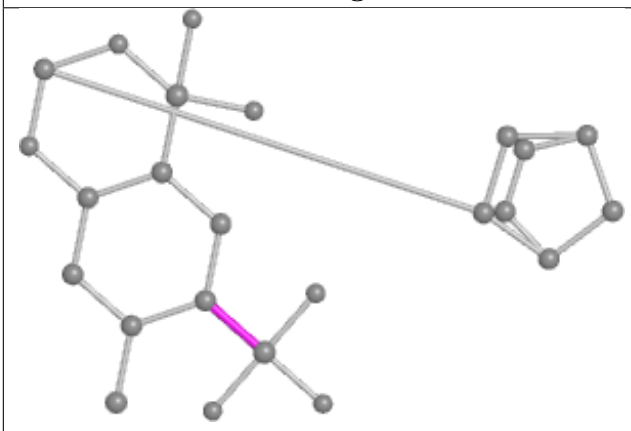
Ligand CYZ D 1401



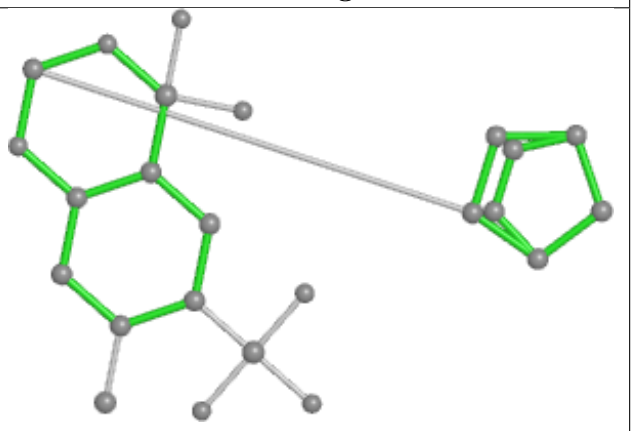
Bond lengths



Bond angles

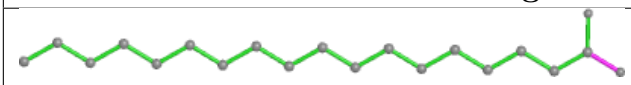


Torsions

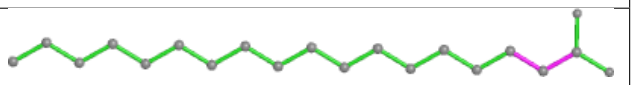


Rings

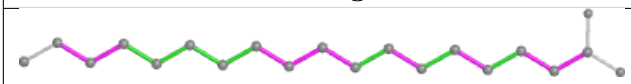
Ligand PC1 J 1901



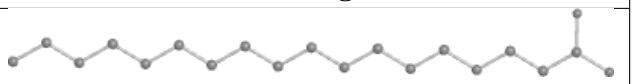
Bond lengths



Bond angles

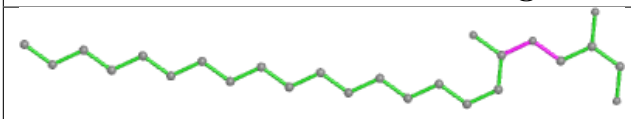


Torsions

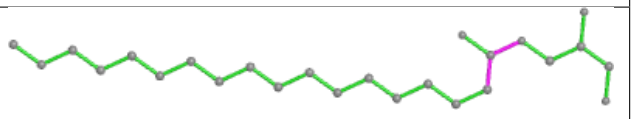


Rings

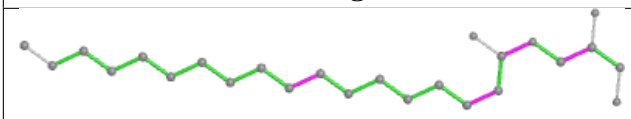
Ligand PC1 D 1405



Bond lengths



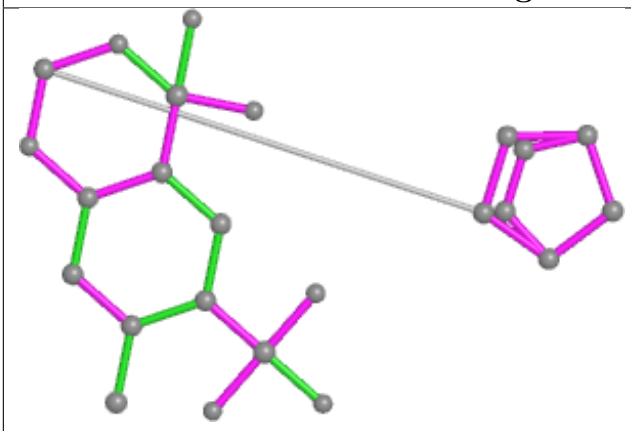
Bond angles



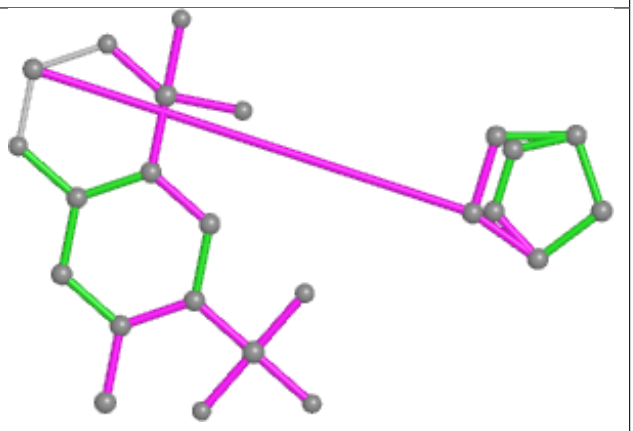
Torsions

Rings

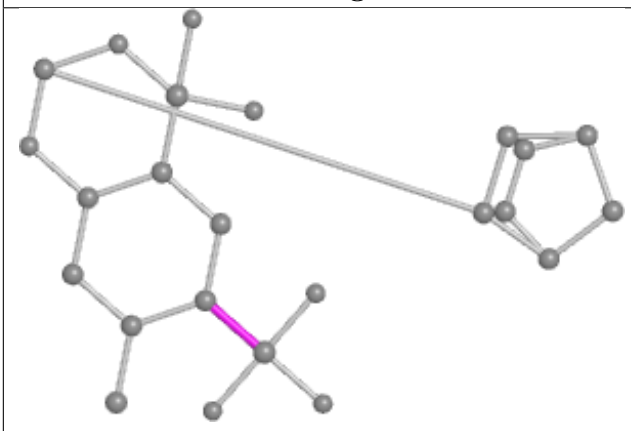
Ligand CYZ C 1401



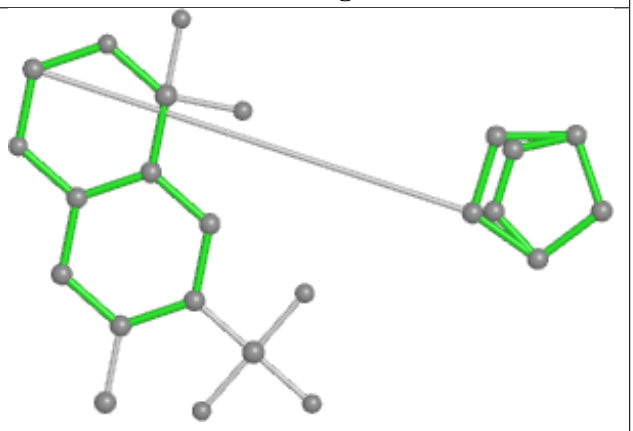
Bond lengths



Bond angles

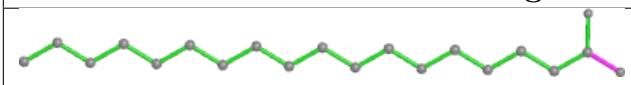


Torsions



Rings

Ligand PC1 I 1802



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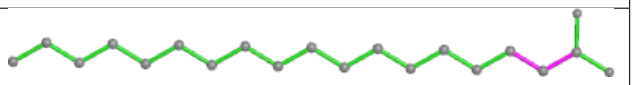
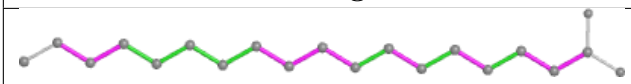
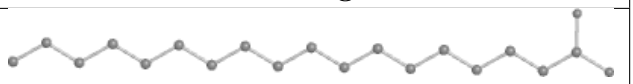


Bond angles

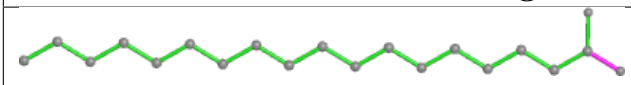


Torsions

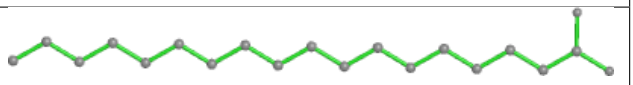


Rings

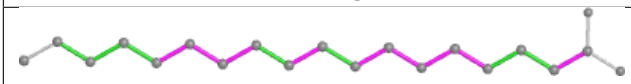
Ligand PC1 C 1405



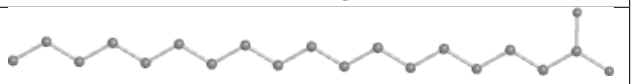
Bond lengths



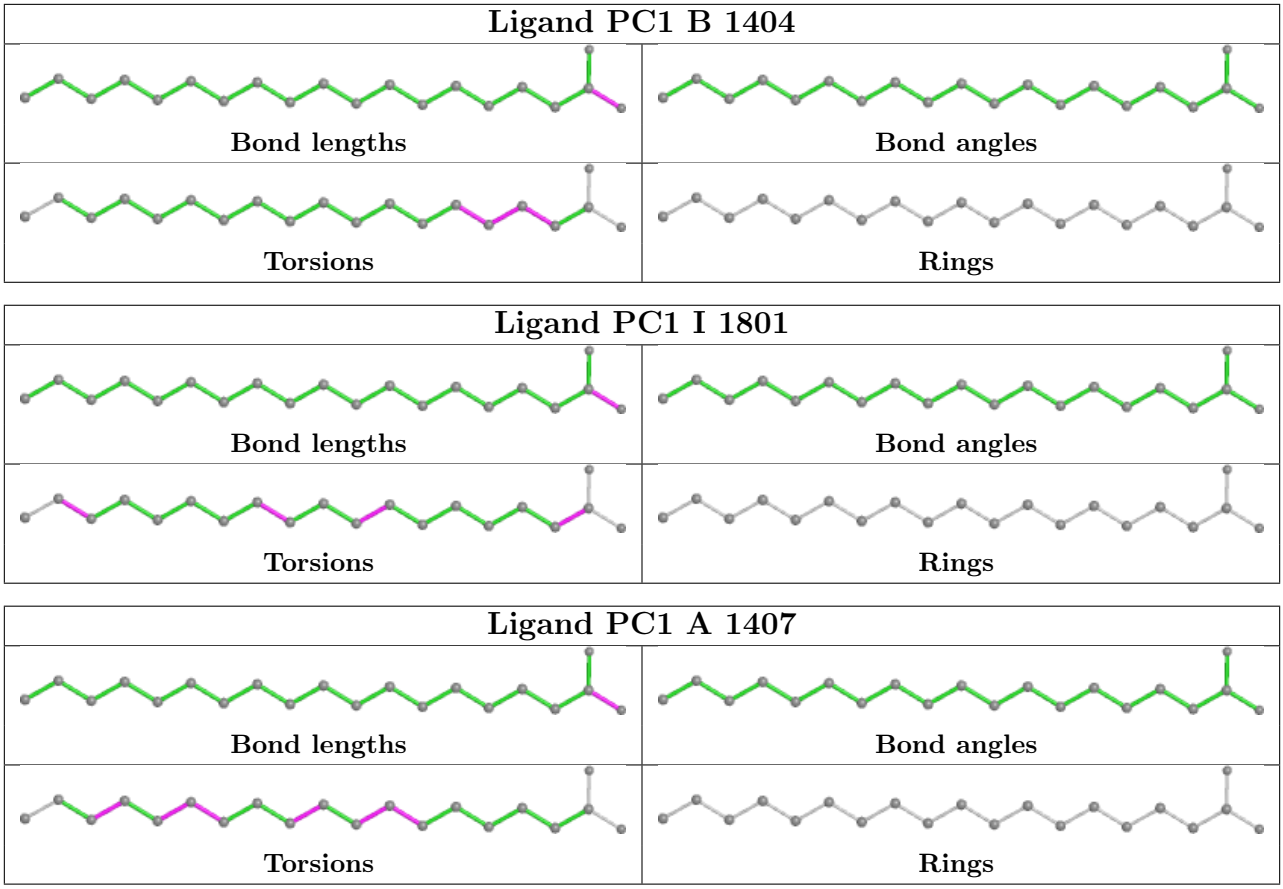
Bond angles



Torsions



Rings



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.

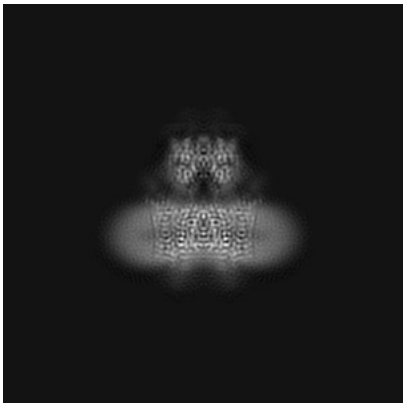
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12806. These allow visual inspection of the internal detail of the map and identification of artifacts.

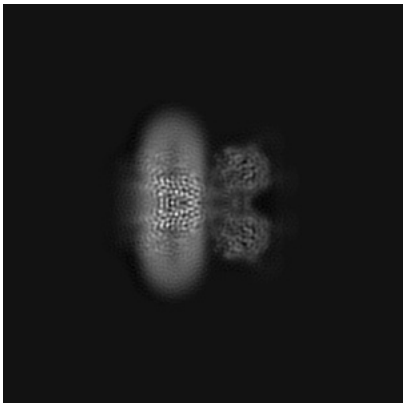
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

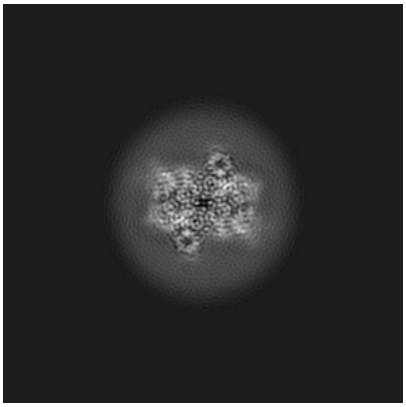
6.1.1 Primary map



X



Y

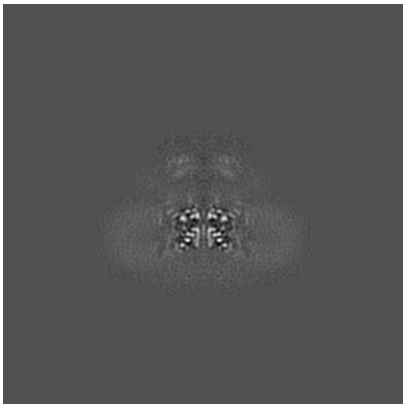


Z

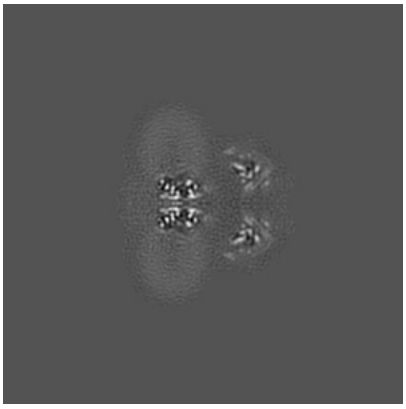
The images above show the map projected in three orthogonal directions.

6.2 Central slices

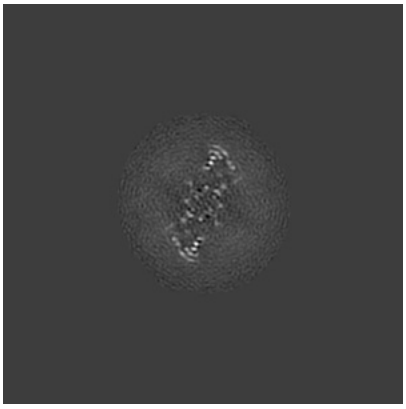
6.2.1 Primary map



X Index: 160



Y Index: 160

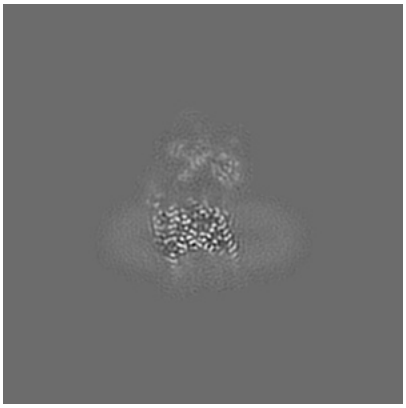


Z Index: 160

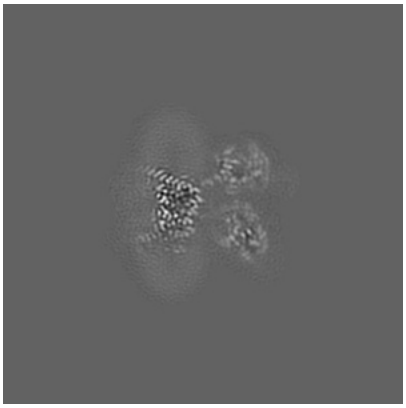
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

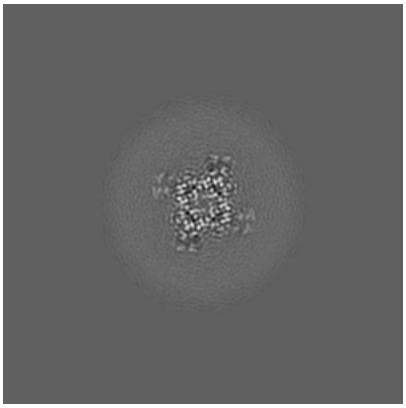
6.3.1 Primary map



X Index: 147



Y Index: 174

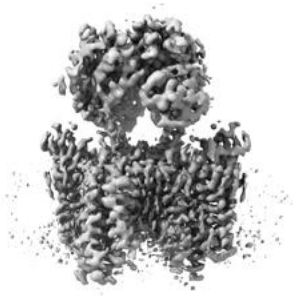


Z Index: 127

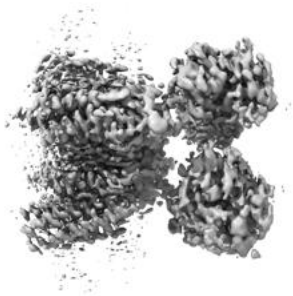
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

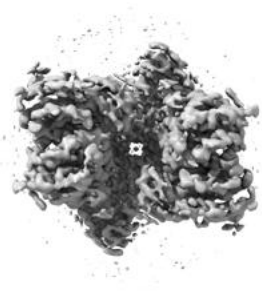
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

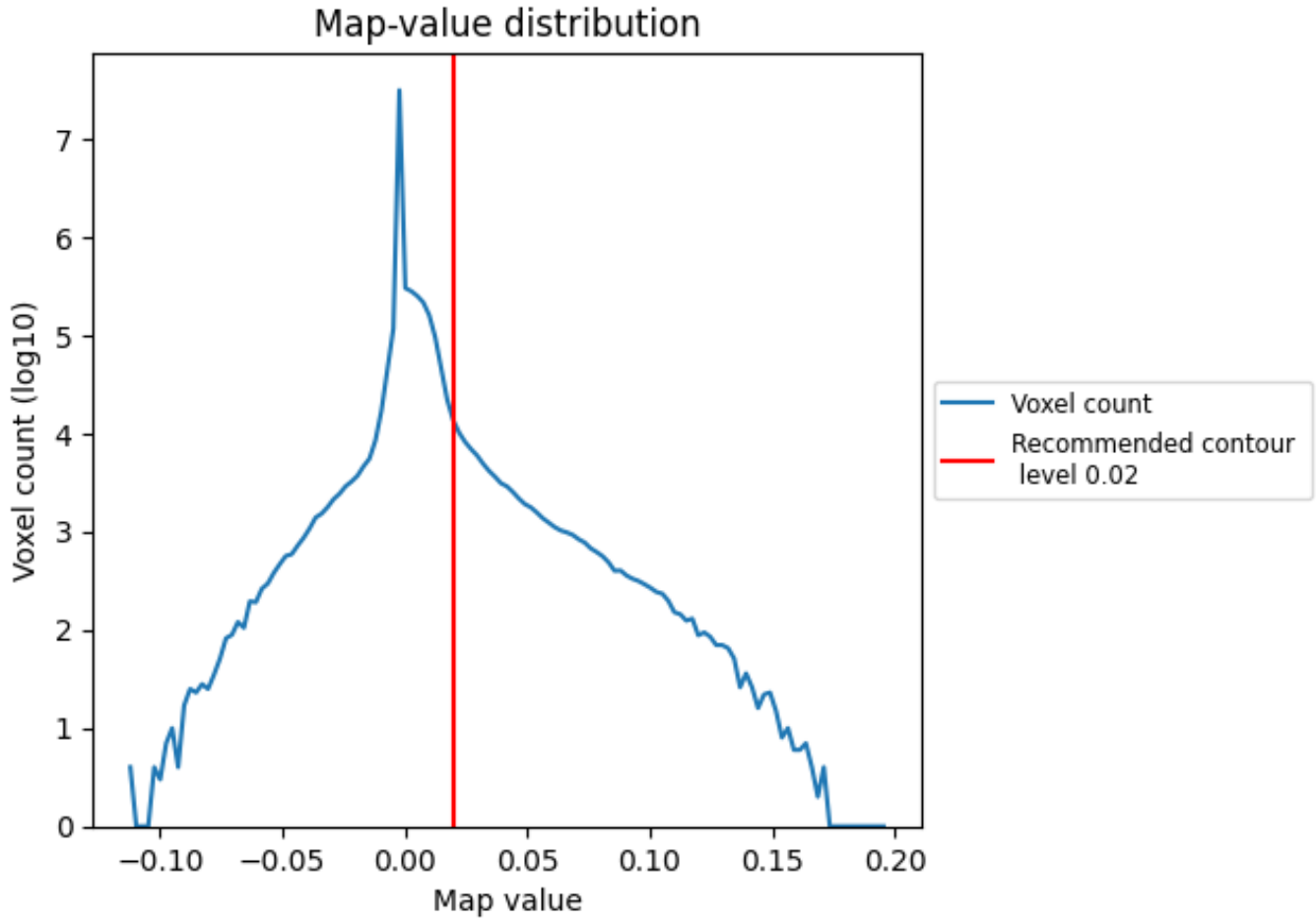
6.5 Mask visualisation (i)

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

7 Map analysis

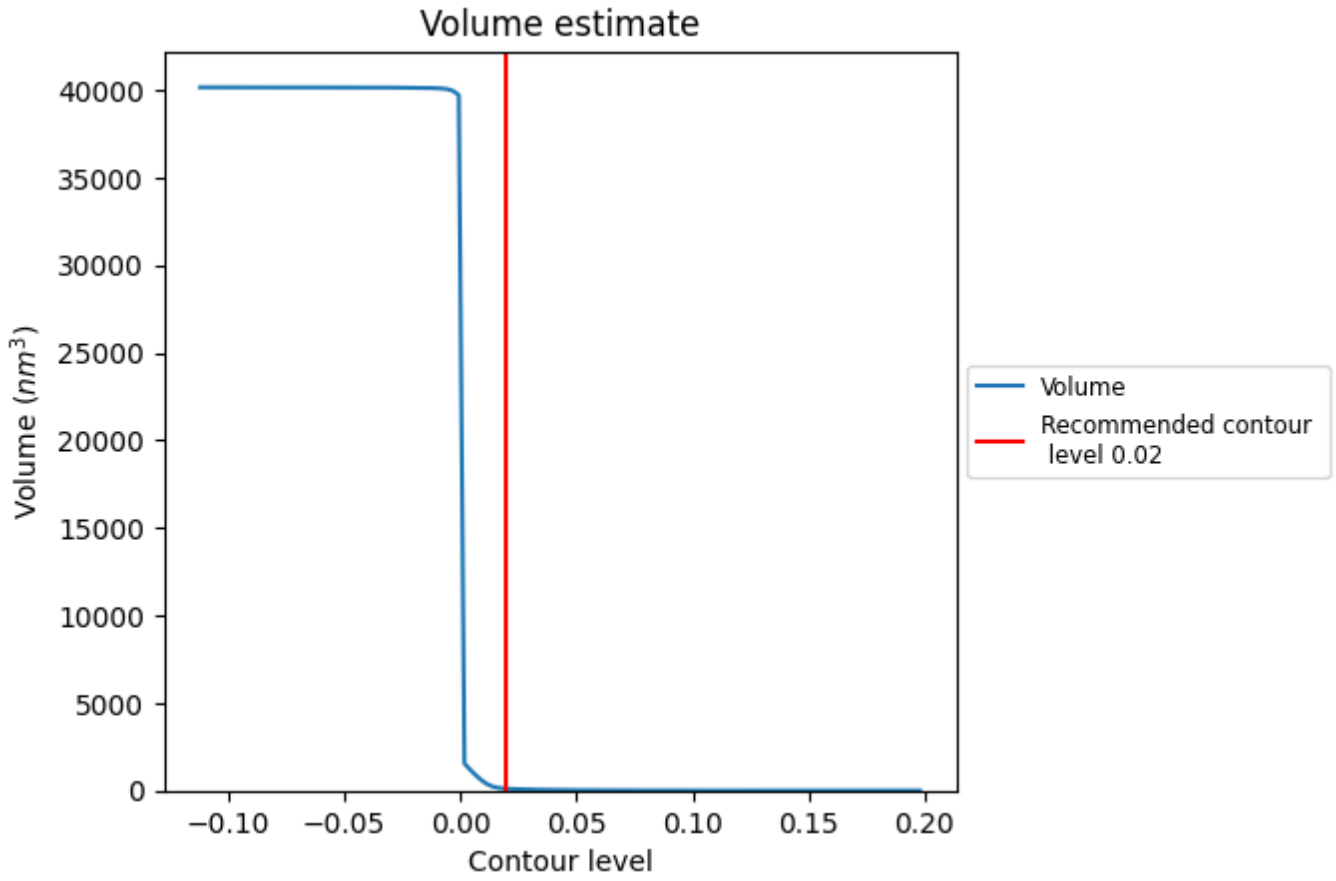
This section contains the results of statistical analysis of the map.

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.

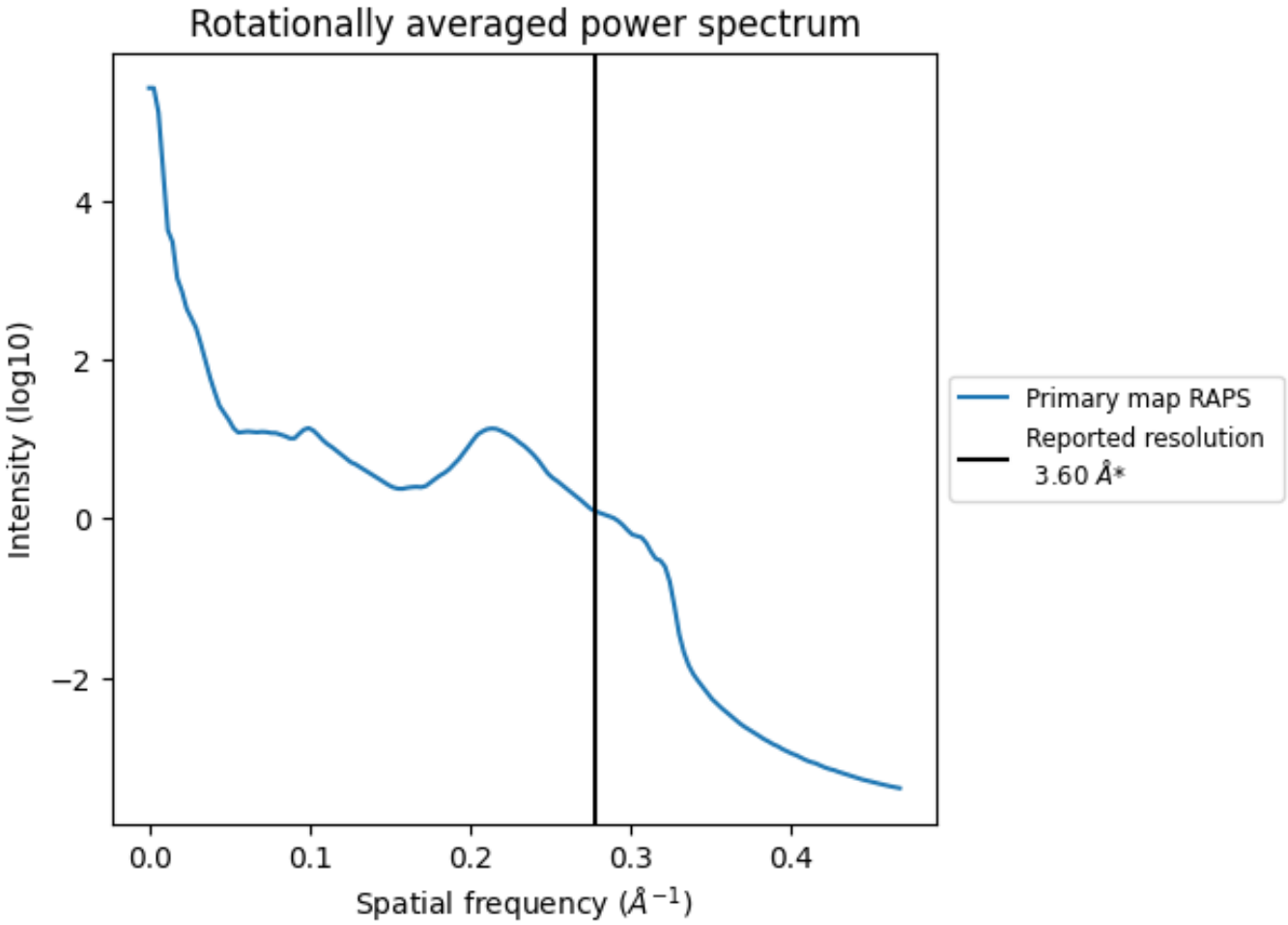
7.2 Volume estimate (i)



The volume at the recommended contour level is 108 nm^3; this corresponds to an approximate mass of 97 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)

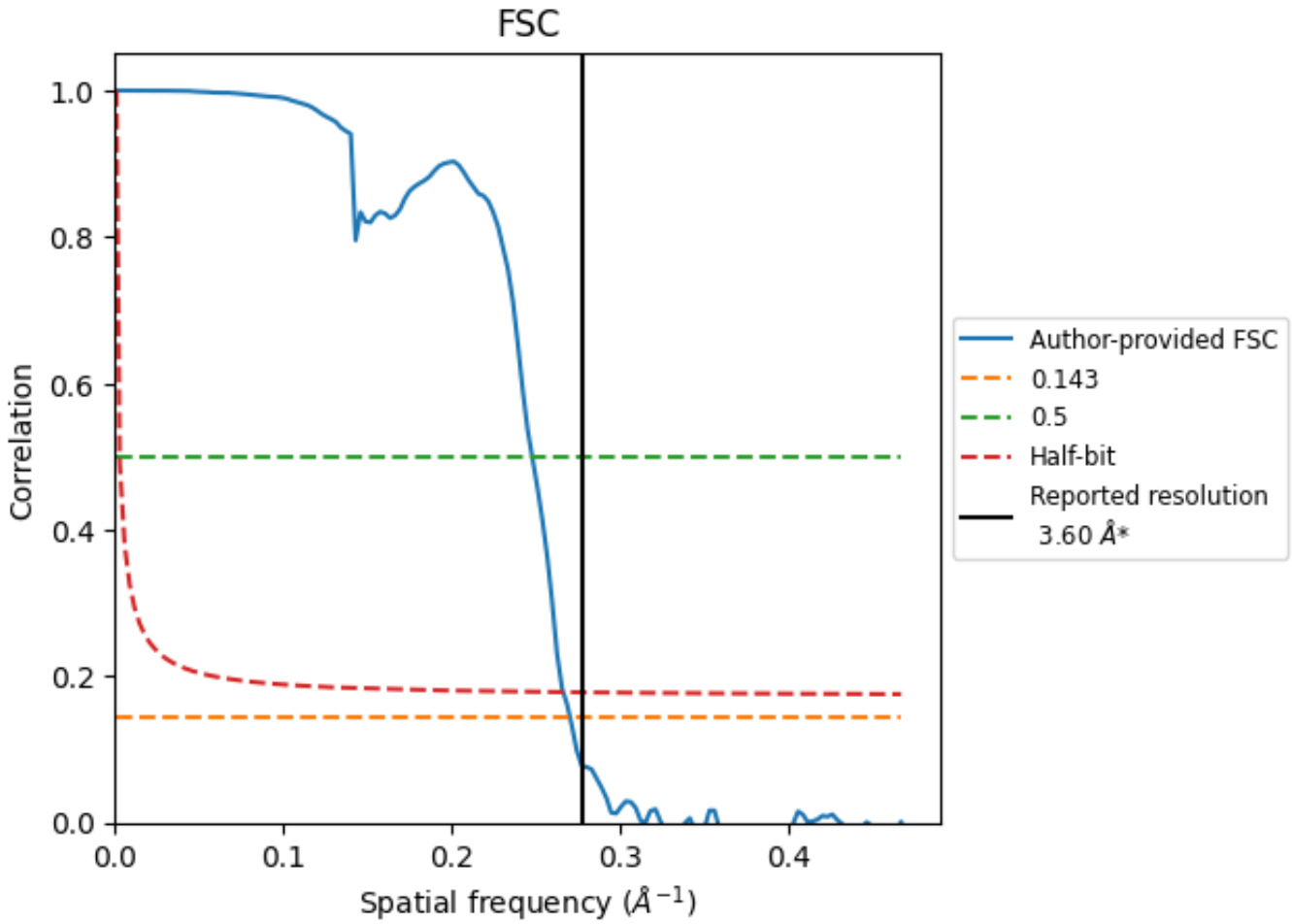


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

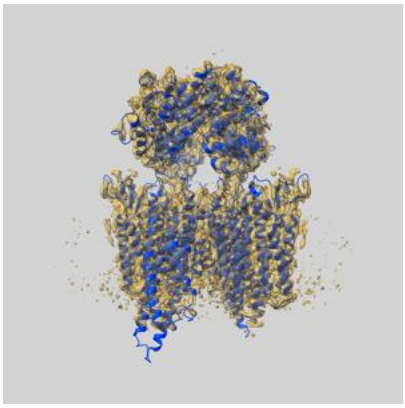
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.70	4.03	3.75
Unmasked-calculated*	-	-	-

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

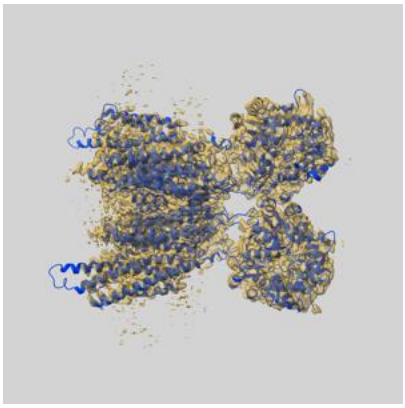
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12806 and PDB model 7OCF. Per-residue inclusion information can be found in section 3 on page 10.

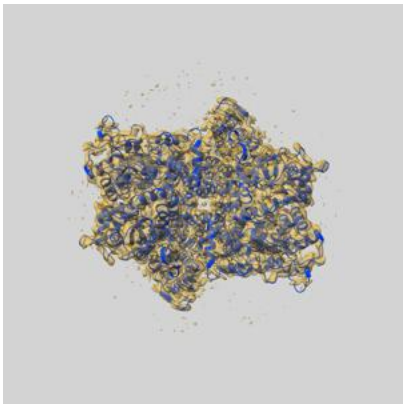
9.1 Map-model overlay



X



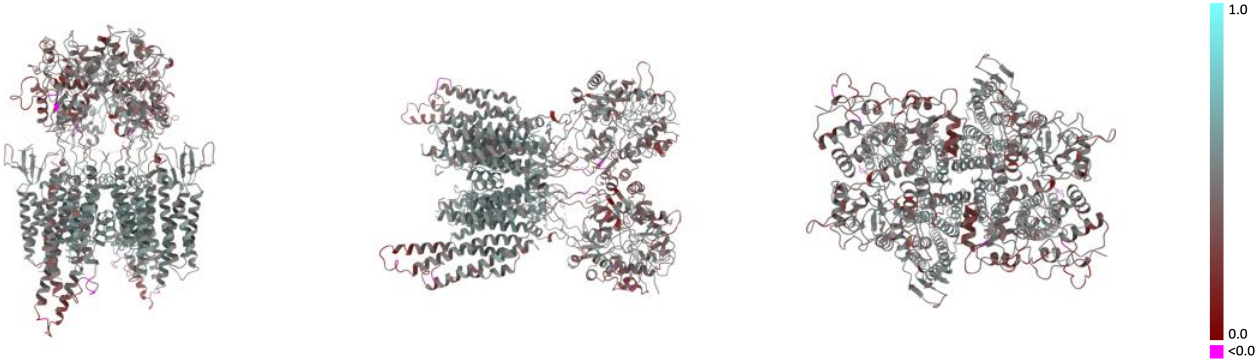
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

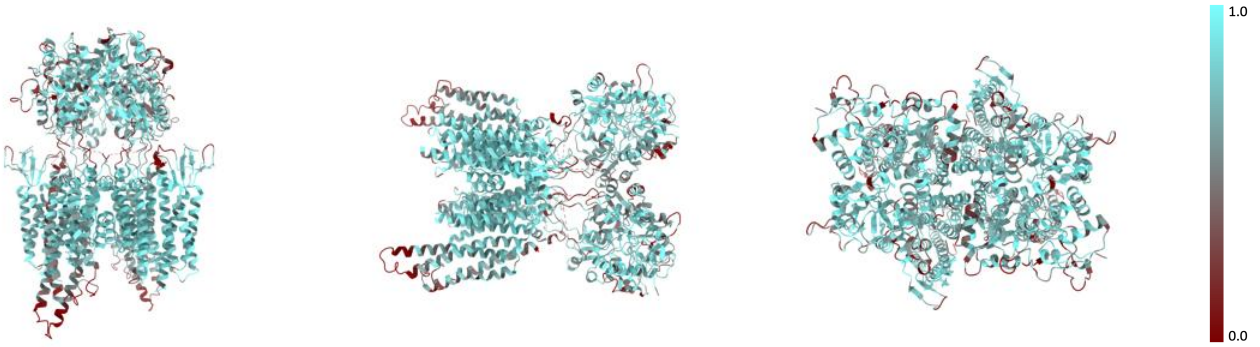
9.2 Q-score mapped to coordinate model (i)



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.

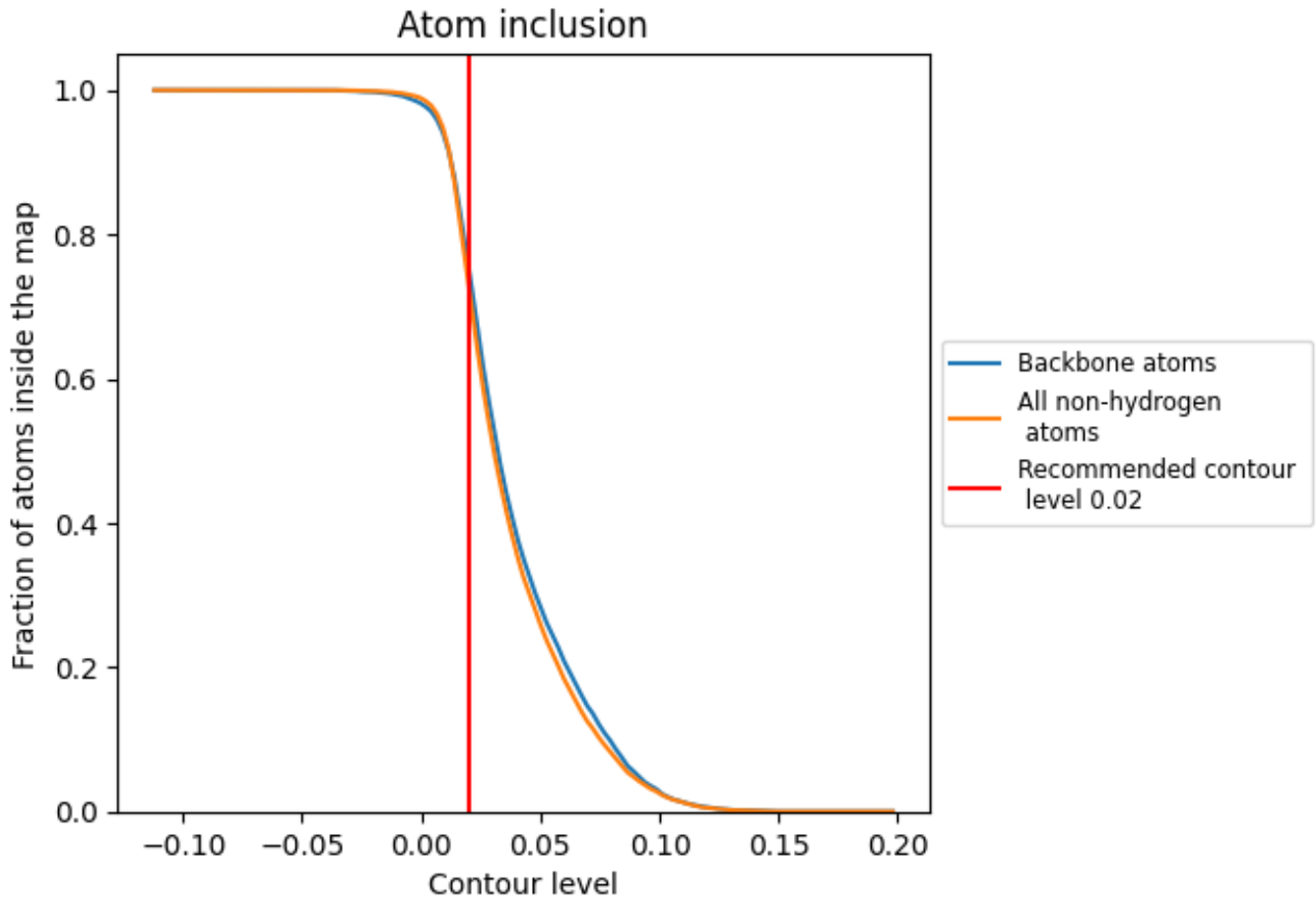
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7278	0.4650
A	0.7218	0.4520
B	0.7704	0.4800
C	0.7256	0.4520
D	0.7768	0.4820
E	0.5737	0.4310
G	0.5489	0.4250
I	0.7865	0.4880
J	0.7858	0.4880