Full wwPDB EM Validation Report ⓘ

Nov 9, 2022 – 10:59 AM EST

PDB ID	:	6PEQ
EMDB ID	:	EMD-20330
Title	:	GluA2 in complex with its auxiliary subunit CNIH3 - map LBD-TMD-C3 - with antagonist ZK200775 -without NTD
Authors	:	Nakagawa, T.
Deposited on	:	2019-06-20
Resolution	:	2.97 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:

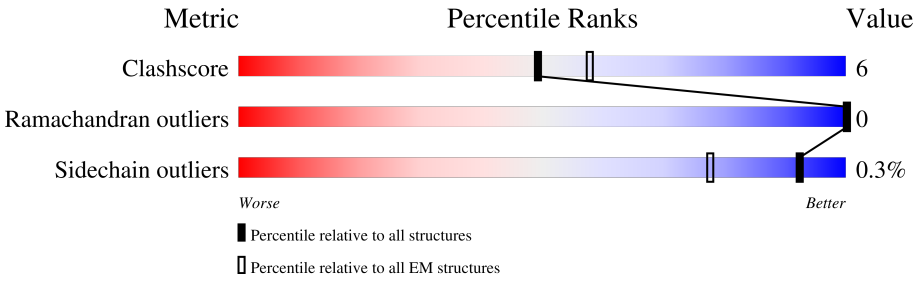
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.97 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	889	5% 36% 7% 57%
1	B	889	5% 38% · 58%
1	C	889	5% 36% 6% 57%
1	D	889	5% 38% · 58%
2	E	174	26% 66% 10% 24%
2	F	174	24% 61% 16% 23%
2	G	174	26% 65% 11% 24%
2	H	174	23% 61% 16% 23%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 32485 atoms, of which 16159 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	380	Total	C	H	N	O	S	0	0
			5559	1836	2733	456	516	18		
1	B	376	Total	C	H	N	O	S	0	0
			5558	1825	2752	455	508	18		
1	C	380	Total	C	H	N	O	S	0	0
			5559	1836	2733	456	516	18		
1	D	376	Total	C	H	N	O	S	0	0
			5558	1825	2752	455	508	18		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	586	ARG	GLN	conflict	UNP P19491
A	848	ASP	-	expression tag	UNP P19491
A	849	TYR	-	expression tag	UNP P19491
A	850	LYS	-	expression tag	UNP P19491
A	851	ASP	-	expression tag	UNP P19491
A	852	ASP	-	expression tag	UNP P19491
A	853	ASP	-	expression tag	UNP P19491
A	854	ASP	-	expression tag	UNP P19491
A	855	LYS	-	expression tag	UNP P19491
A	856	GLU	-	expression tag	UNP P19491
A	857	GLY	-	expression tag	UNP P19491
A	858	TYR	-	expression tag	UNP P19491
A	859	ASN	-	expression tag	UNP P19491
A	860	VAL	-	expression tag	UNP P19491
A	861	TYR	-	expression tag	UNP P19491
A	862	GLY	-	expression tag	UNP P19491
A	863	ILE	-	expression tag	UNP P19491
A	864	GLU	-	expression tag	UNP P19491
A	865	SER	-	expression tag	UNP P19491
A	866	VAL	-	expression tag	UNP P19491
A	867	LYS	-	expression tag	UNP P19491
A	868	ILE	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	586	ARG	GLN	conflict	UNP P19491
B	848	ASP	-	expression tag	UNP P19491
B	849	TYR	-	expression tag	UNP P19491
B	850	LYS	-	expression tag	UNP P19491
B	851	ASP	-	expression tag	UNP P19491
B	852	ASP	-	expression tag	UNP P19491
B	853	ASP	-	expression tag	UNP P19491
B	854	ASP	-	expression tag	UNP P19491
B	855	LYS	-	expression tag	UNP P19491
B	856	GLU	-	expression tag	UNP P19491
B	857	GLY	-	expression tag	UNP P19491
B	858	TYR	-	expression tag	UNP P19491
B	859	ASN	-	expression tag	UNP P19491
B	860	VAL	-	expression tag	UNP P19491
B	861	TYR	-	expression tag	UNP P19491
B	862	GLY	-	expression tag	UNP P19491
B	863	ILE	-	expression tag	UNP P19491
B	864	GLU	-	expression tag	UNP P19491
B	865	SER	-	expression tag	UNP P19491
B	866	VAL	-	expression tag	UNP P19491
B	867	LYS	-	expression tag	UNP P19491
B	868	ILE	-	expression tag	UNP P19491
C	586	ARG	GLN	conflict	UNP P19491
C	848	ASP	-	expression tag	UNP P19491
C	849	TYR	-	expression tag	UNP P19491
C	850	LYS	-	expression tag	UNP P19491
C	851	ASP	-	expression tag	UNP P19491
C	852	ASP	-	expression tag	UNP P19491
C	853	ASP	-	expression tag	UNP P19491
C	854	ASP	-	expression tag	UNP P19491
C	855	LYS	-	expression tag	UNP P19491
C	856	GLU	-	expression tag	UNP P19491
C	857	GLY	-	expression tag	UNP P19491
C	858	TYR	-	expression tag	UNP P19491
C	859	ASN	-	expression tag	UNP P19491
C	860	VAL	-	expression tag	UNP P19491
C	861	TYR	-	expression tag	UNP P19491
C	862	GLY	-	expression tag	UNP P19491
C	863	ILE	-	expression tag	UNP P19491
C	864	GLU	-	expression tag	UNP P19491
C	865	SER	-	expression tag	UNP P19491
C	866	VAL	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	867	LYS	-	expression tag	UNP P19491
C	868	ILE	-	expression tag	UNP P19491
D	586	ARG	GLN	conflict	UNP P19491
D	848	ASP	-	expression tag	UNP P19491
D	849	TYR	-	expression tag	UNP P19491
D	850	LYS	-	expression tag	UNP P19491
D	851	ASP	-	expression tag	UNP P19491
D	852	ASP	-	expression tag	UNP P19491
D	853	ASP	-	expression tag	UNP P19491
D	854	ASP	-	expression tag	UNP P19491
D	855	LYS	-	expression tag	UNP P19491
D	856	GLU	-	expression tag	UNP P19491
D	857	GLY	-	expression tag	UNP P19491
D	858	TYR	-	expression tag	UNP P19491
D	859	ASN	-	expression tag	UNP P19491
D	860	VAL	-	expression tag	UNP P19491
D	861	TYR	-	expression tag	UNP P19491
D	862	GLY	-	expression tag	UNP P19491
D	863	ILE	-	expression tag	UNP P19491
D	864	GLU	-	expression tag	UNP P19491
D	865	SER	-	expression tag	UNP P19491
D	866	VAL	-	expression tag	UNP P19491
D	867	LYS	-	expression tag	UNP P19491
D	868	ILE	-	expression tag	UNP P19491

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	132	Total	C	H	N	O	S	0	0
			2118	740	1035	162	169	12		
2	F	134	Total	C	H	N	O	S	0	0
			2185	758	1073	166	176	12		
2	G	132	Total	C	H	N	O	S	0	0
			2129	740	1046	162	169	12		
2	H	134	Total	C	H	N	O	S	0	0
			2185	758	1073	166	176	12		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	161	GLY	-	expression tag	UNP Q6ZWS4
E	162	GLY	-	expression tag	UNP Q6ZWS4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	163	ARG	-	expression tag	UNP Q6ZWS4
E	164	GLY	-	expression tag	UNP Q6ZWS4
E	165	GLY	-	expression tag	UNP Q6ZWS4
E	166	THR	-	expression tag	UNP Q6ZWS4
E	167	GLU	-	expression tag	UNP Q6ZWS4
E	168	THR	-	expression tag	UNP Q6ZWS4
E	169	SER	-	expression tag	UNP Q6ZWS4
E	170	GLN	-	expression tag	UNP Q6ZWS4
E	171	VAL	-	expression tag	UNP Q6ZWS4
E	172	ALA	-	expression tag	UNP Q6ZWS4
E	173	PRO	-	expression tag	UNP Q6ZWS4
E	174	ALA	-	expression tag	UNP Q6ZWS4
F	161	GLY	-	expression tag	UNP Q6ZWS4
F	162	GLY	-	expression tag	UNP Q6ZWS4
F	163	ARG	-	expression tag	UNP Q6ZWS4
F	164	GLY	-	expression tag	UNP Q6ZWS4
F	165	GLY	-	expression tag	UNP Q6ZWS4
F	166	THR	-	expression tag	UNP Q6ZWS4
F	167	GLU	-	expression tag	UNP Q6ZWS4
F	168	THR	-	expression tag	UNP Q6ZWS4
F	169	SER	-	expression tag	UNP Q6ZWS4
F	170	GLN	-	expression tag	UNP Q6ZWS4
F	171	VAL	-	expression tag	UNP Q6ZWS4
F	172	ALA	-	expression tag	UNP Q6ZWS4
F	173	PRO	-	expression tag	UNP Q6ZWS4
F	174	ALA	-	expression tag	UNP Q6ZWS4
G	161	GLY	-	expression tag	UNP Q6ZWS4
G	162	GLY	-	expression tag	UNP Q6ZWS4
G	163	ARG	-	expression tag	UNP Q6ZWS4
G	164	GLY	-	expression tag	UNP Q6ZWS4
G	165	GLY	-	expression tag	UNP Q6ZWS4
G	166	THR	-	expression tag	UNP Q6ZWS4
G	167	GLU	-	expression tag	UNP Q6ZWS4
G	168	THR	-	expression tag	UNP Q6ZWS4
G	169	SER	-	expression tag	UNP Q6ZWS4
G	170	GLN	-	expression tag	UNP Q6ZWS4
G	171	VAL	-	expression tag	UNP Q6ZWS4
G	172	ALA	-	expression tag	UNP Q6ZWS4
G	173	PRO	-	expression tag	UNP Q6ZWS4
G	174	ALA	-	expression tag	UNP Q6ZWS4
H	161	GLY	-	expression tag	UNP Q6ZWS4
H	162	GLY	-	expression tag	UNP Q6ZWS4

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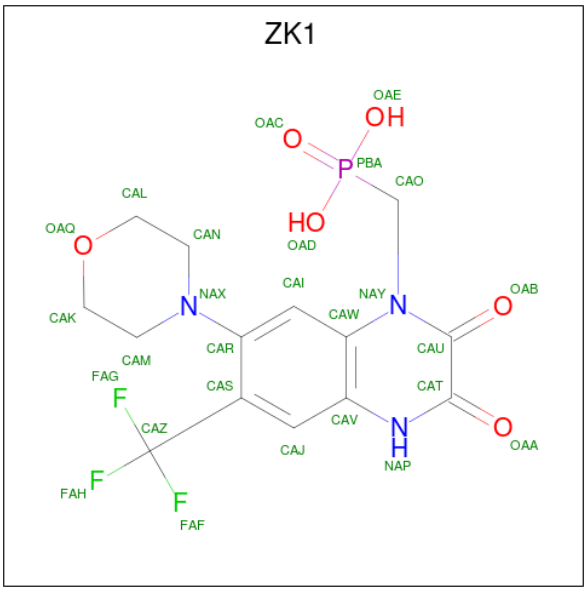
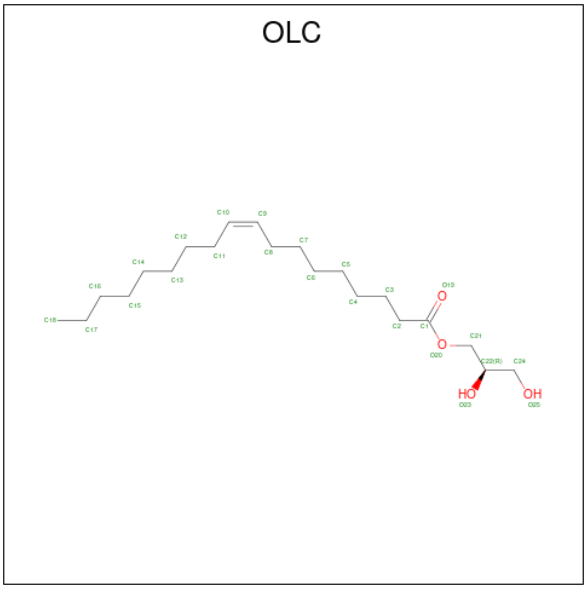
Chain	Residue	Modelled	Actual	Comment	Reference
H	163	ARG	-	expression tag	UNP Q6ZWS4
H	164	GLY	-	expression tag	UNP Q6ZWS4
H	165	GLY	-	expression tag	UNP Q6ZWS4
H	166	THR	-	expression tag	UNP Q6ZWS4
H	167	GLU	-	expression tag	UNP Q6ZWS4
H	168	THR	-	expression tag	UNP Q6ZWS4
H	169	SER	-	expression tag	UNP Q6ZWS4
H	170	GLN	-	expression tag	UNP Q6ZWS4
H	171	VAL	-	expression tag	UNP Q6ZWS4
H	172	ALA	-	expression tag	UNP Q6ZWS4
H	173	PRO	-	expression tag	UNP Q6ZWS4
H	174	ALA	-	expression tag	UNP Q6ZWS4

- Molecule 3 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: $C_{14}H_{15}F_3N_3O_6P$) (labeled as "Ligand of Interest" by depositor).



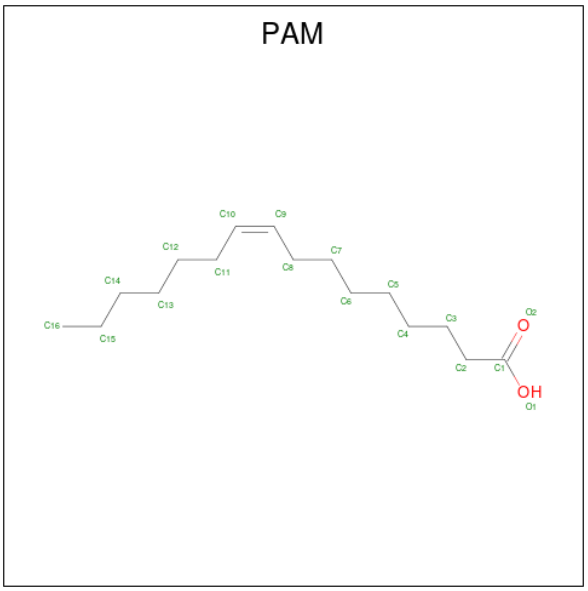
Mol	Chain	Residues	Atoms							AltConf
3	A	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	
3	B	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	
3	C	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	
3	D	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$) (labeled as "Ligand of Interest" by depositor).



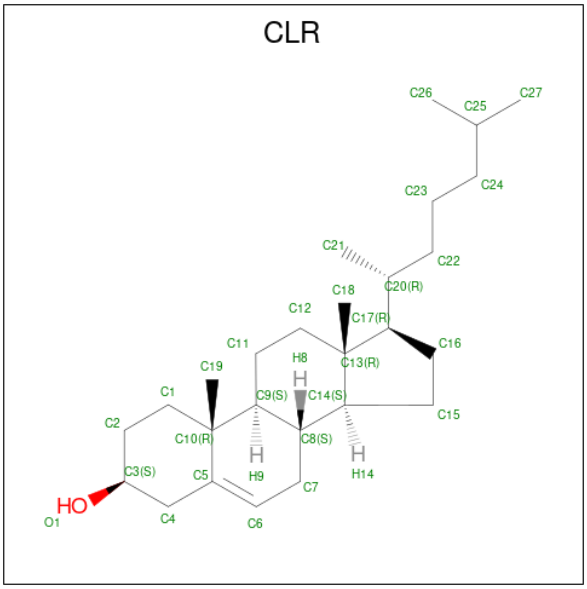
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			65	21	40	4	
4	B	1	Total	C	H	O	0
			130	42	80	8	
4	B	1	Total	C	H	O	0
			130	42	80	8	
4	C	1	Total	C	H	O	0
			130	42	80	8	
4	C	1	Total	C	H	O	0
			130	42	80	8	
4	D	1	Total	C	H	O	0
			195	63	120	12	
4	D	1	Total	C	H	O	0
			195	63	120	12	
4	D	1	Total	C	H	O	0
			195	63	120	12	

- Molecule 5 is PALMITOLEIC ACID (three-letter code: PAM) (formula: $C_{16}H_{30}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	H	O	0
			141	48	87	6	
5	A	1	Total	C	H	O	0
			141	48	87	6	
5	A	1	Total	C	H	O	0
			141	48	87	6	
5	B	1	Total	C	H	O	0
			141	48	87	6	
5	B	1	Total	C	H	O	0
			141	48	87	6	
5	B	1	Total	C	H	O	0
			141	48	87	6	
5	F	1	Total	C	H	O	0
			47	16	29	2	
5	H	1	Total	C	H	O	0
			47	16	29	2	
5	C	1	Total	C	H	O	0
			141	48	87	6	
5	C	1	Total	C	H	O	0
			141	48	87	6	
5	C	1	Total	C	H	O	0
			141	48	87	6	
5	D	1	Total	C	H	O	0
			141	48	87	6	
5	D	1	Total	C	H	O	0
			141	48	87	6	
5	D	1	Total	C	H	O	0
			141	48	87	6	

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



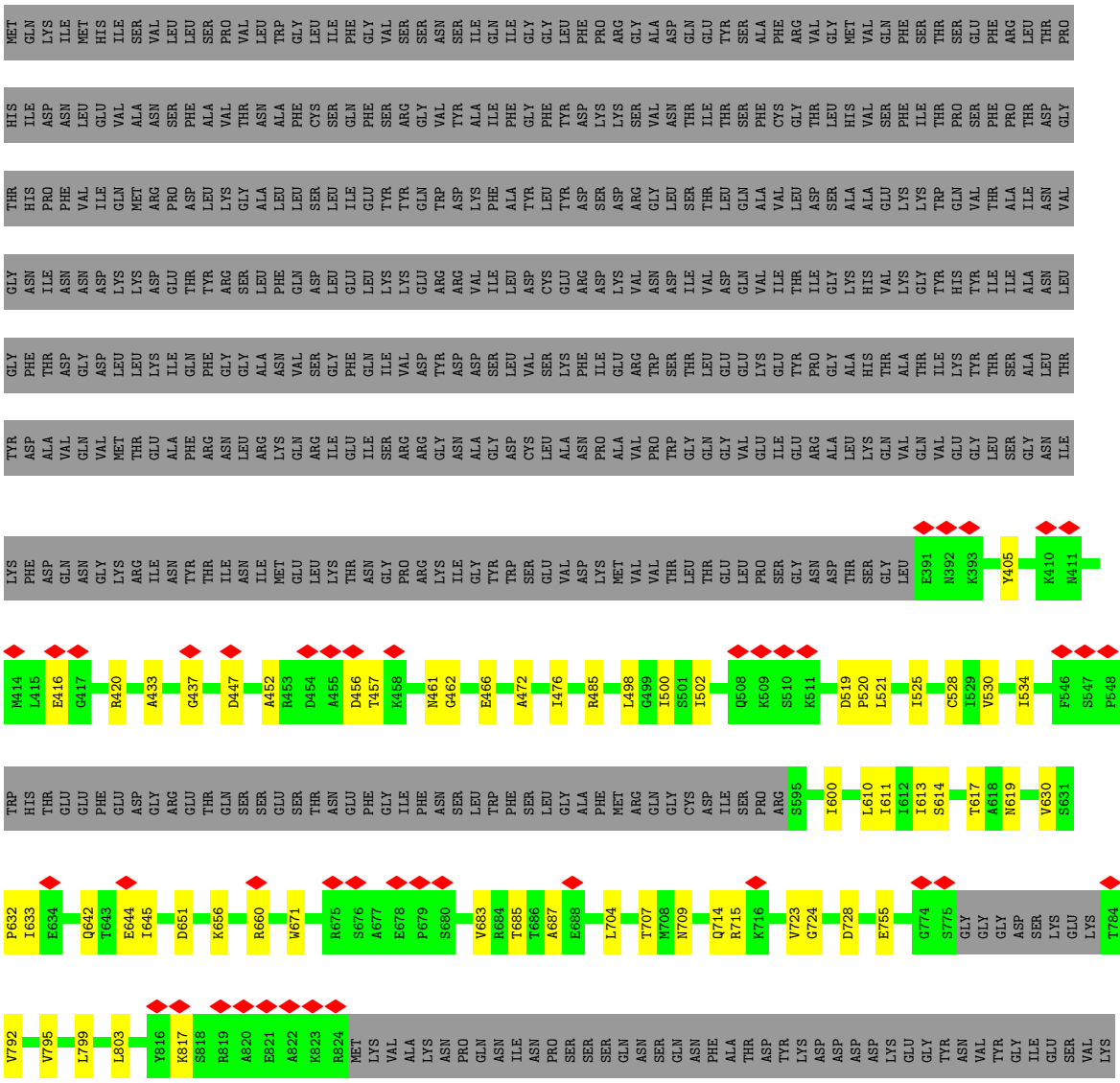
Mol	Chain	Residues	Atoms				AltConf
6	E	1	Total	C	H	O	0
			74	27	46	1	
6	F	1	Total	C	H	O	0
			74	27	46	1	
6	G	1	Total	C	H	O	0
			74	27	46	1	
6	H	1	Total	C	H	O	0
			74	27	46	1	

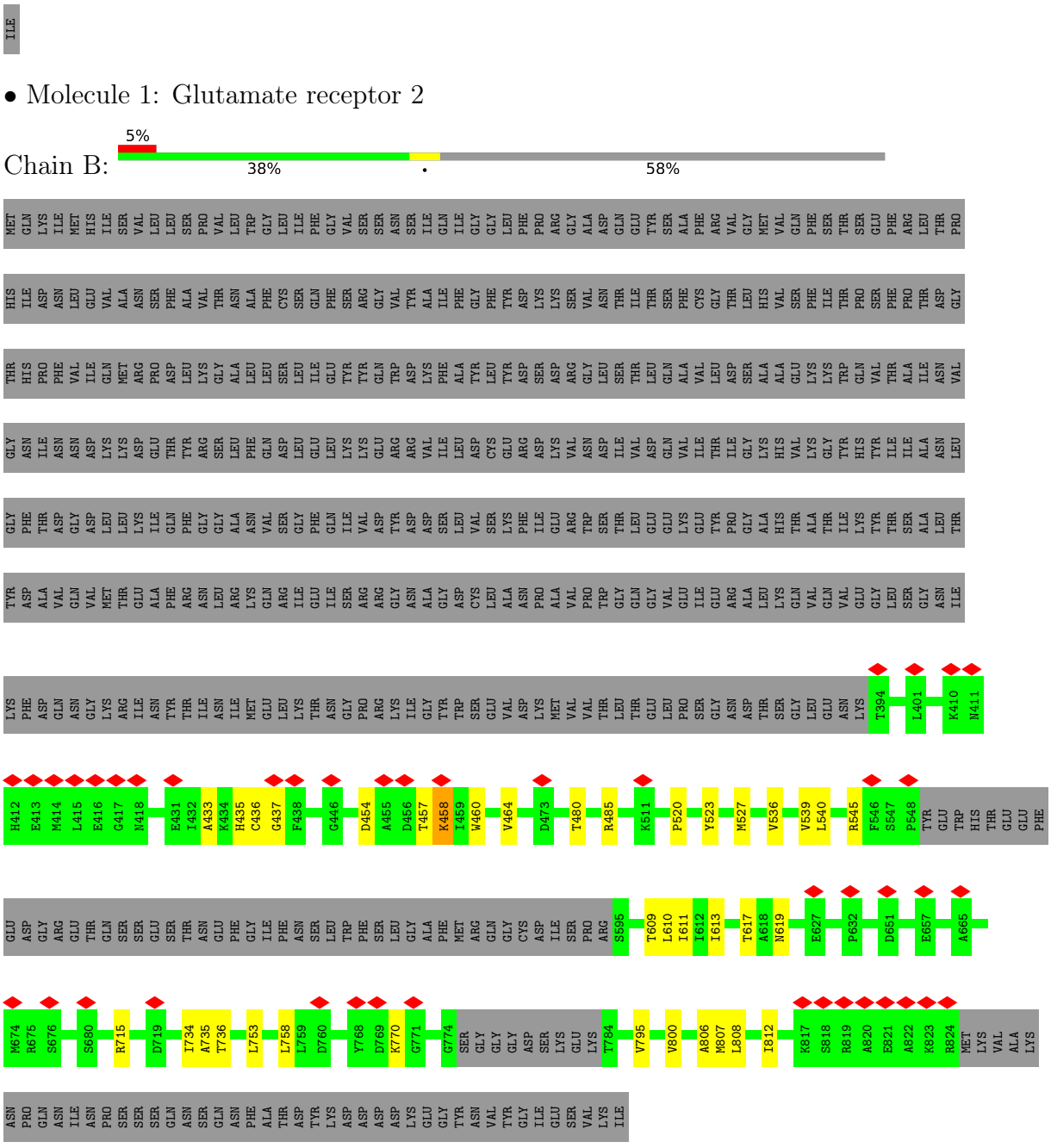
3 Residue-property plots (i)

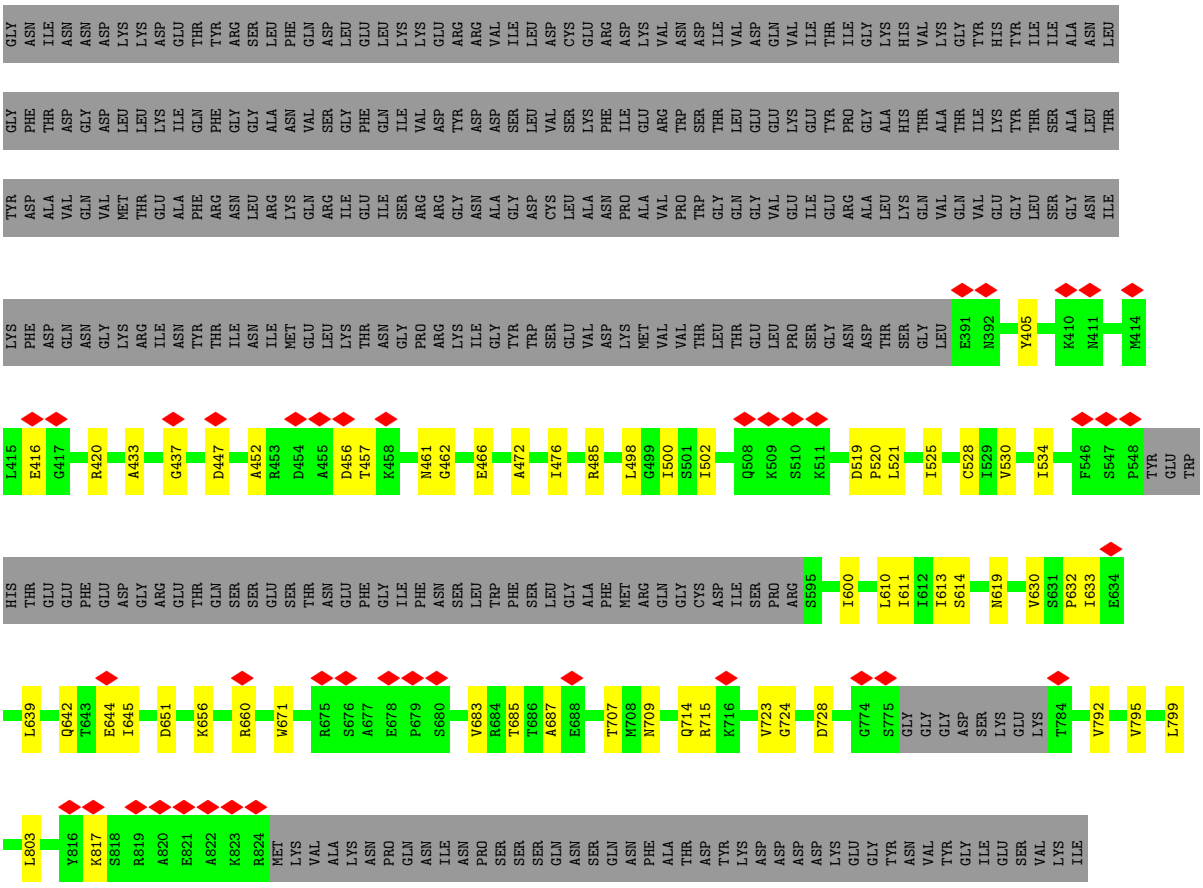
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Glutamate receptor 2

Chain A:

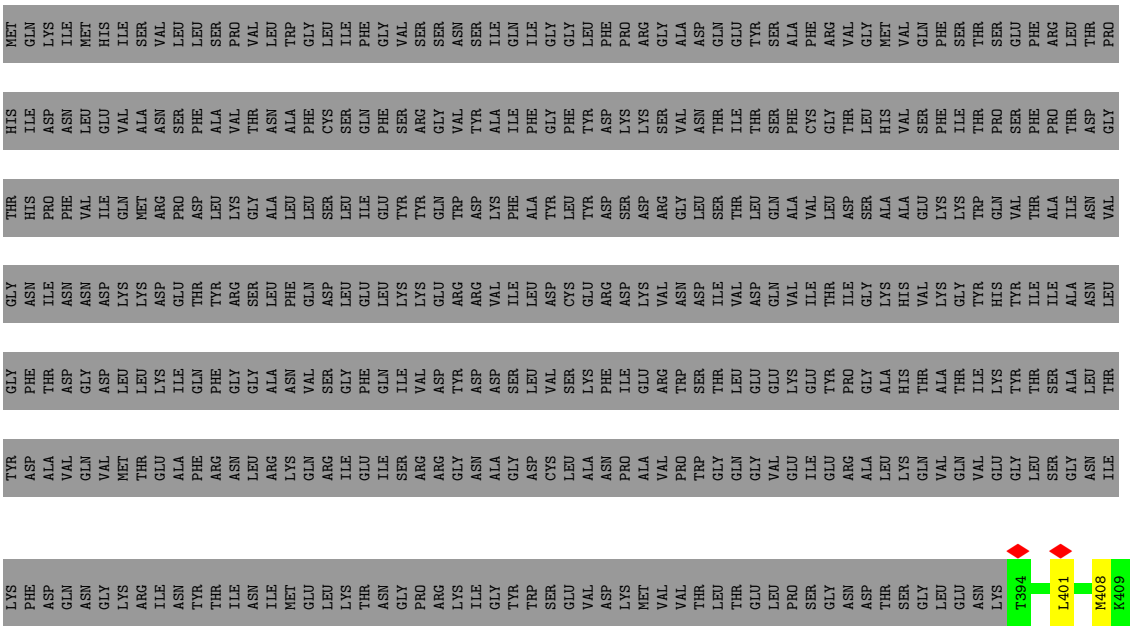


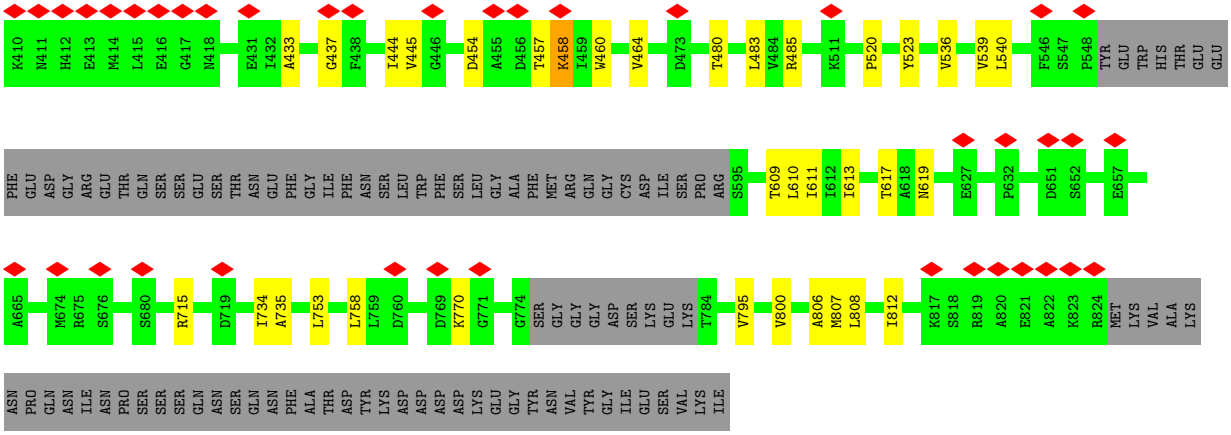

ILE
• Molecule 1: Glutamate receptor 2
Chain B:
5%
38%
58%
T394
L401
K410
N411
H412
E413
M414
L415
E416
G417
N418
E431
I432
A433
K434
H435
C436
G437
F438
G446
D454
A455
D456
T457
K458
I459
W460
V464
D473
T480
R485
K511
P520
Y523
M527
V536
V539
L540
R545
F546
S547
P548
S595
T609
L610
I611
I612
I613
T617
A618
N619
E627
P632
D651
E657
A665
M674
R675
S676
S680
R715
D719
I734
A735
T736
L753
L758
L759
D760
Y768
D769
K770
G771
G774
T784
V795
V800
A806
M807
L808
I812
K817
S818
R819
A820
E821
A822
K823
R824
• Molecule 1: Glutamate receptor 2
Chain C:
5%
36%
6%
57%



• Molecule 1: Glutamate receptor 2

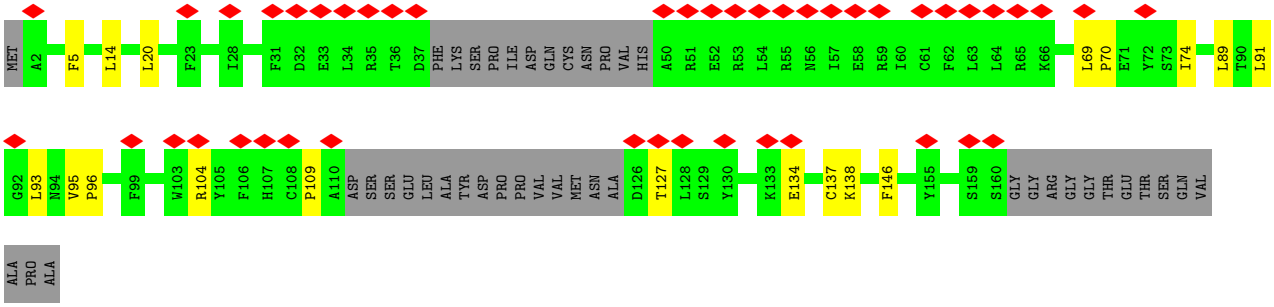
Chain D:





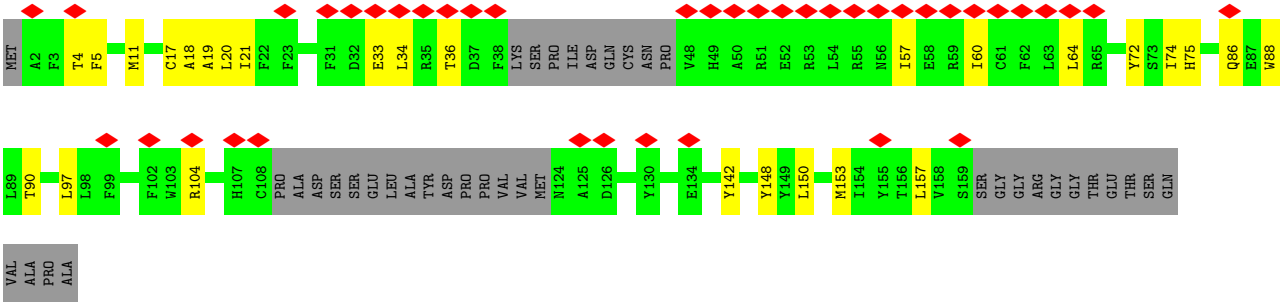
• Molecule 2: Protein cornichon homolog 3

Chain E:



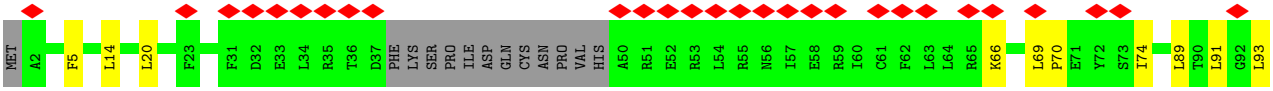
• Molecule 2: Protein cornichon homolog 3

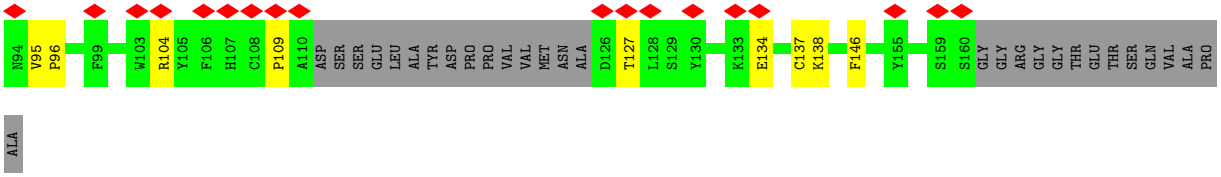
Chain F:



• Molecule 2: Protein cornichon homolog 3

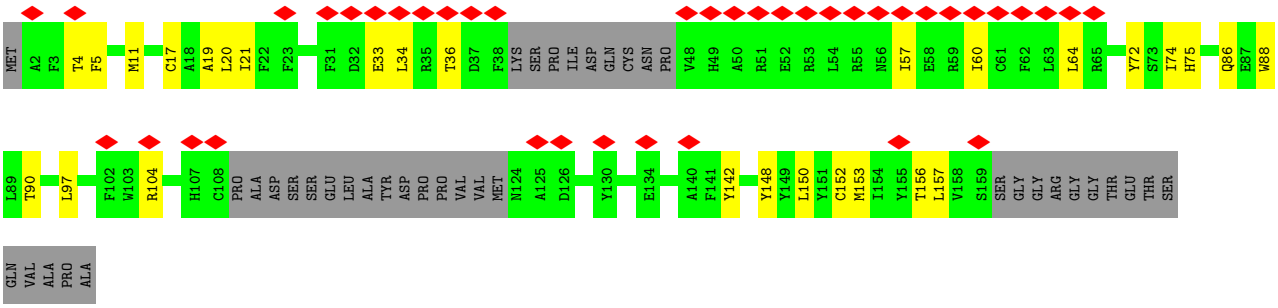
Chain G:





• Molecule 2: Protein cornichon homolog 3

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	188982	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 ($e^-/Å^2$)	58.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0299	Depositor
Map size (Å)	383.76, 383.76, 383.76	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066, 1.066, 1.066	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZK1, OLC, CLR, PAM

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	0.28	0/2885	0.40	0/3919
1	B	0.28	0/2865	0.41	0/3889
1	C	0.28	0/2885	0.40	0/3919
1	D	0.28	0/2865	0.41	0/3889
2	E	0.27	0/1120	0.35	0/1523
2	F	0.29	0/1149	0.38	0/1561
2	G	0.27	0/1120	0.35	0/1523
2	H	0.29	0/1149	0.38	0/1561
All	All	0.28	0/16038	0.39	0/21784

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	2826	2733	2758	42	0
1	B	2806	2752	2751	32	0
1	C	2826	2733	2758	40	0
1	D	2806	2752	2751	30	0
2	E	1083	1035	1045	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1112	1073	1071	24	0
2	G	1083	1046	1045	15	0
2	H	1112	1073	1071	22	0
3	A	27	13	13	1	0
3	B	27	13	13	1	0
3	C	27	13	13	1	0
3	D	27	13	13	1	0
4	A	25	40	40	1	0
4	B	50	80	80	0	0
4	C	50	80	80	0	0
4	D	75	120	120	1	0
5	A	54	87	87	0	0
5	B	54	87	87	5	0
5	C	54	87	87	0	0
5	D	54	87	87	2	0
5	F	18	29	29	0	0
5	H	18	29	29	0	0
6	E	28	46	46	1	0
6	F	28	46	46	4	0
6	G	28	46	46	0	0
6	H	28	46	46	1	0
All	All	16326	16159	16212	199	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (199) 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:E:20:LEU:HD21	2:E:74:ILE:HD11	1.60	0.84
2:G:20:LEU:HD21	2:G:74:ILE:HD11	1.60	0.82
1:C:651:ASP:N	1:C:683:VAL:O	2.18	0.77
1:A:651:ASP:N	1:A:683:VAL:O	2.18	0.76
4:A:902:OLC:O25	4:A:902:OLC:O20	2.06	0.73
2:E:20:LEU:HD21	2:E:74:ILE:CD1	2.20	0.72
1:A:803:LEU:HD12	1:D:539:VAL:HG21	1.71	0.72
6:E:201:CLR:H183	6:E:201:CLR:H212	1.70	0.72
2:G:20:LEU:HD21	2:G:74:ILE:CD1	2.20	0.71
1:A:714:GLN:O	1:A:715:ARG:NH1	2.23	0.71
1:C:714:GLN:O	1:C:715:ARG:NH1	2.23	0.70
1:B:800:VAL:HG21	2:F:11:MET:SD	2.32	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:ALA:HB2	1:D:807:MET:SD	2.33	0.69
1:C:632:PRO:O	1:C:633:ILE:HG23	1.94	0.68
1:A:632:PRO:O	1:A:633:ILE:HG23	1.94	0.68
1:B:539:VAL:HG21	1:C:803:LEU:HD12	1.75	0.68
1:B:480:THR:O	1:B:485:ARG:NH1	2.27	0.67
1:D:480:THR:O	1:D:485:ARG:NH1	2.27	0.67
1:B:807:MET:SD	2:F:19:ALA:HB2	2.34	0.67
1:C:520:PRO:O	1:C:619:ASN:ND2	2.28	0.67
1:A:520:PRO:O	1:A:619:ASN:ND2	2.28	0.66
2:H:11:MET:SD	1:D:800:VAL:HG21	2.37	0.65
2:H:20:LEU:HD21	2:H:142:TYR:CE2	2.32	0.64
2:F:20:LEU:HD21	2:F:142:TYR:CZ	2.33	0.64
2:H:20:LEU:HD21	2:H:142:TYR:CZ	2.33	0.64
1:C:416:GLU:O	1:C:420:ARG:N	2.32	0.63
2:F:20:LEU:HD21	2:F:142:TYR:CE2	2.32	0.63
1:C:502:ILE:O	1:C:709:ASN:ND2	2.33	0.62
1:A:416:GLU:O	1:A:420:ARG:N	2.32	0.61
1:A:476:ILE:HG22	1:A:476:ILE:O	2.00	0.61
1:A:502:ILE:O	1:A:709:ASN:ND2	2.33	0.61
1:C:476:ILE:O	1:C:476:ILE:HG22	2.00	0.60
1:C:600:ILE:HD11	1:D:806:ALA:HA	1.83	0.60
1:A:600:ILE:HD11	1:B:806:ALA:HA	1.84	0.59
1:B:613:ILE:O	1:B:617:THR:HG23	2.04	0.58
1:D:433:ALA:O	1:D:437:GLY:N	2.34	0.58
1:B:433:ALA:O	1:B:437:GLY:N	2.34	0.58
1:B:485:ARG:NH1	3:B:901:ZK1:OAA	2.36	0.58
1:D:613:ILE:O	1:D:617:THR:HG23	2.03	0.58
1:A:611:ILE:HG21	1:B:795:VAL:HG21	1.86	0.57
6:H:201:CLR:H212	6:H:201:CLR:H183	1.86	0.57
1:B:520:PRO:O	1:B:619:ASN:ND2	2.38	0.57
1:A:613:ILE:HG22	1:D:610:LEU:CD1	2.35	0.56
2:F:90:THR:HG22	2:F:148:TYR:HE2	1.70	0.56
1:C:611:ILE:HG21	1:D:795:VAL:HG21	1.87	0.56
1:D:485:ARG:NH1	3:D:901:ZK1:OAA	2.36	0.56
2:F:153:MET:O	2:F:157:LEU:N	2.39	0.56
2:H:153:MET:O	2:H:157:LEU:N	2.39	0.56
1:C:405:TYR:OH	1:C:707:THR:HG21	2.06	0.56
1:A:405:TYR:OH	1:A:707:THR:HG21	2.06	0.55
1:B:545:ARG:NH1	2:G:66:LYS:O	2.38	0.55
2:G:20:LEU:HD11	2:G:74:ILE:HD12	1.89	0.55
2:H:90:THR:HG22	2:H:148:TYR:HE2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:ILE:N	1:C:728:ASP:OD1	2.38	0.54
1:D:520:PRO:O	1:D:619:ASN:ND2	2.38	0.54
1:A:500:ILE:N	1:A:728:ASP:OD1	2.38	0.54
2:E:20:LEU:HD11	2:E:74:ILE:HD12	1.89	0.54
1:B:610:LEU:CD1	1:C:613:ILE:HG22	2.38	0.53
1:C:466:GLU:O	1:C:472:ALA:N	2.42	0.53
2:H:5:PHE:HD1	1:C:528:CYS:HG	1.55	0.53
1:A:466:GLU:O	1:A:472:ALA:N	2.42	0.52
2:E:20:LEU:HD11	2:E:74:ILE:CD1	2.40	0.52
2:G:20:LEU:HD11	2:G:74:ILE:CD1	2.40	0.52
2:F:20:LEU:HD22	2:F:74:ILE:HD11	1.91	0.52
2:F:17:CYS:O	2:F:21:ILE:HG12	2.10	0.52
2:G:91:LEU:O	2:G:95:VAL:HG13	2.10	0.52
2:H:20:LEU:HD22	2:H:74:ILE:HD11	1.91	0.51
1:D:753:LEU:HD22	1:D:758:LEU:HD22	1.93	0.51
2:H:17:CYS:O	2:H:21:ILE:HG12	2.10	0.51
1:A:660:ARG:HG2	1:A:671:TRP:CZ2	2.46	0.51
1:A:799:LEU:O	1:A:803:LEU:HD23	2.11	0.51
1:C:723:VAL:HG23	1:C:724:GLY:N	2.26	0.51
2:F:90:THR:HG22	2:F:148:TYR:CE2	2.46	0.51
1:A:630:VAL:HG23	1:A:630:VAL:O	2.11	0.50
2:E:91:LEU:O	2:E:95:VAL:HG13	2.10	0.50
1:A:521:LEU:HD12	1:A:525:ILE:HG21	1.92	0.50
1:A:528:CYS:HG	2:F:5:PHE:HD1	1.58	0.50
1:B:611:ILE:HG21	1:C:795:VAL:HG21	1.93	0.50
1:B:753:LEU:HD22	1:B:758:LEU:HD22	1.93	0.50
1:B:536:VAL:O	1:B:540:LEU:HD23	2.12	0.50
1:C:521:LEU:HD12	1:C:525:ILE:HG21	1.92	0.50
1:C:660:ARG:HG2	1:C:671:TRP:CZ2	2.46	0.50
1:C:799:LEU:O	1:C:803:LEU:HD23	2.11	0.50
1:D:536:VAL:O	1:D:540:LEU:HD23	2.12	0.50
2:G:109:PRO:HB2	2:G:127:THR:HG23	1.94	0.50
1:A:723:VAL:HG23	1:A:724:GLY:N	2.26	0.50
2:H:90:THR:HG22	2:H:148:TYR:CE2	2.46	0.50
1:C:630:VAL:O	1:C:630:VAL:HG23	2.12	0.50
1:C:660:ARG:HG2	1:C:671:TRP:CE2	2.47	0.50
1:A:660:ARG:HG2	1:A:671:TRP:CE2	2.47	0.50
2:H:150:LEU:O	2:H:153:MET:HG2	2.12	0.50
1:C:433:ALA:O	1:C:437:GLY:N	2.43	0.49
1:A:723:VAL:HG23	1:A:724:GLY:H	1.78	0.49
2:E:109:PRO:HB2	2:E:127:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:157:LEU:HD21	6:F:201:CLR:H22	1.93	0.49
1:C:723:VAL:HG23	1:C:724:GLY:H	1.78	0.48
2:F:34:LEU:HD22	2:F:57:ILE:HD12	1.96	0.48
4:D:902:OLC:O25	5:D:905:PAM:O2	2.25	0.48
1:A:614:SER:CB	1:B:617:THR:HG22	2.43	0.48
2:F:150:LEU:O	2:F:153:MET:HG2	2.12	0.48
1:A:456:ASP:OD1	1:A:457:THR:N	2.46	0.48
2:H:34:LEU:HD22	2:H:57:ILE:HD12	1.96	0.47
1:A:433:ALA:O	1:A:437:GLY:N	2.43	0.47
2:H:33:GLU:O	2:H:36:THR:OG1	2.29	0.47
2:G:5:PHE:O	2:G:5:PHE:CG	2.68	0.47
1:C:614:SER:CB	1:D:617:THR:HG22	2.43	0.47
2:F:60:ILE:O	2:F:64:LEU:HD13	2.15	0.47
2:F:33:GLU:O	2:F:36:THR:OG1	2.29	0.46
2:F:72:TYR:OH	2:F:104:ARG:NH1	2.48	0.46
2:G:127:THR:HG22	2:G:127:THR:O	2.15	0.46
1:A:795:VAL:HG21	1:D:611:ILE:HG21	1.96	0.46
2:E:89:LEU:O	2:E:93:LEU:HD23	2.16	0.46
1:C:642:GLN:OE1	1:C:644:GLU:N	2.49	0.46
2:E:95:VAL:N	2:E:96:PRO:CD	2.79	0.46
2:F:157:LEU:HD21	6:F:201:CLR:C2	2.46	0.46
2:H:4:THR:O	2:H:5:PHE:HB3	2.15	0.46
1:C:456:ASP:OD1	1:C:457:THR:N	2.46	0.46
2:E:127:THR:O	2:E:127:THR:HG22	2.15	0.46
2:G:95:VAL:N	2:G:96:PRO:CD	2.79	0.46
2:H:60:ILE:O	2:H:64:LEU:HD13	2.15	0.46
1:C:452:ALA:N	1:C:461:ASN:OD1	2.49	0.46
2:E:5:PHE:O	2:E:5:PHE:CG	2.68	0.46
2:F:4:THR:O	2:F:5:PHE:HB3	2.15	0.46
1:A:642:GLN:OE1	1:A:644:GLU:N	2.49	0.46
1:A:792:VAL:HG12	1:A:792:VAL:O	2.16	0.46
1:A:447:ASP:OD2	1:A:462:GLY:N	2.49	0.45
1:C:600:ILE:HD11	1:D:806:ALA:CA	2.45	0.45
1:C:685:THR:HG22	1:C:687:ALA:H	1.81	0.45
2:G:89:LEU:O	2:G:93:LEU:HD23	2.16	0.45
1:B:457:THR:O	1:B:458:LYS:HG3	2.17	0.45
1:A:600:ILE:HD11	1:B:806:ALA:CA	2.47	0.45
1:A:642:GLN:OE1	1:A:645:ILE:HD12	2.17	0.45
2:F:4:THR:O	2:F:4:THR:HG22	2.17	0.45
1:A:485:ARG:NH1	3:A:901:ZK1:OAA	2.44	0.45
1:A:685:THR:HG22	1:A:687:ALA:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:GLN:OE1	1:C:645:ILE:HD12	2.17	0.45
1:D:454:ASP:O	1:D:458:LYS:N	2.48	0.45
1:A:452:ALA:N	1:A:461:ASN:OD1	2.49	0.45
2:H:5:PHE:O	2:H:5:PHE:CG	2.69	0.45
2:H:72:TYR:OH	2:H:104:ARG:NH1	2.48	0.45
2:G:14:LEU:HD11	2:G:146:PHE:CZ	2.52	0.44
2:F:57:ILE:O	2:F:60:ILE:HG22	2.18	0.44
2:H:57:ILE:O	2:H:60:ILE:HG22	2.18	0.44
1:C:792:VAL:O	1:C:792:VAL:HG12	2.16	0.44
1:B:454:ASP:O	1:B:458:LYS:N	2.48	0.44
2:F:5:PHE:O	2:F:5:PHE:CG	2.69	0.44
1:A:610:LEU:HD13	1:B:613:ILE:HG12	1.99	0.44
1:D:808:LEU:O	1:D:812:ILE:HG23	2.18	0.44
1:A:519:ASP:N	1:A:520:PRO:CD	2.81	0.44
5:B:906:PAM:H121	6:F:201:CLR:H6	2.00	0.44
2:G:137:CYS:SG	2:G:138:LYS:N	2.91	0.43
1:B:715:ARG:NH2	1:B:770:LYS:O	2.51	0.43
5:B:906:PAM:C12	6:F:201:CLR:H6	2.48	0.43
1:D:457:THR:O	1:D:458:LYS:HG3	2.17	0.43
1:D:715:ARG:NH2	1:D:770:LYS:O	2.51	0.43
2:E:14:LEU:HD11	2:E:146:PHE:CZ	2.52	0.43
2:E:137:CYS:SG	2:E:138:LYS:N	2.91	0.43
1:B:523:TYR:HB3	5:B:904:PAM:H61	2.00	0.43
1:D:523:TYR:HB3	5:D:905:PAM:H51	1.99	0.43
1:C:530:VAL:O	1:C:534:ILE:HG23	2.19	0.43
1:A:530:VAL:O	1:A:534:ILE:HG23	2.19	0.43
1:B:808:LEU:O	1:B:812:ILE:HG23	2.18	0.43
2:H:4:THR:O	2:H:4:THR:HG22	2.17	0.43
1:C:519:ASP:N	1:C:520:PRO:CD	2.81	0.43
1:B:609:THR:O	1:B:613:ILE:HD12	2.18	0.43
1:D:609:THR:O	1:D:613:ILE:HD12	2.19	0.43
1:C:447:ASP:OD2	1:C:462:GLY:N	2.49	0.42
1:D:460:TRP:CE3	1:D:464:VAL:HG11	2.54	0.42
1:A:656:LYS:O	1:A:660:ARG:HG3	2.19	0.42
1:C:498:LEU:HD23	1:C:498:LEU:N	2.34	0.42
1:C:656:LYS:O	1:C:660:ARG:HG3	2.19	0.42
1:B:460:TRP:CE3	1:B:464:VAL:HG11	2.54	0.42
1:B:807:MET:HE1	2:F:18:ALA:HB3	2.01	0.42
1:A:755:GLU:OE2	1:D:483:LEU:N	2.46	0.42
1:B:734:ILE:HG22	1:B:735:ALA:N	2.35	0.42
1:D:734:ILE:HG22	1:D:735:ALA:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:TYR:HB3	5:B:904:PAM:C5	2.50	0.42
2:H:86:GLN:O	2:H:88:TRP:NE1	2.53	0.41
1:A:498:LEU:N	1:A:498:LEU:HD23	2.34	0.41
1:A:617:THR:HG23	1:D:617:THR:OG1	2.20	0.41
1:C:633:ILE:HG21	1:C:639:LEU:HD21	2.02	0.41
2:G:104:ARG:NH1	2:G:134:GLU:OE2	2.54	0.41
1:B:435:HIS:CE1	1:B:436:CYS:HG	2.39	0.41
1:C:610:LEU:HD13	1:D:613:ILE:HG12	2.02	0.41
2:E:104:ARG:NH1	2:E:134:GLU:OE2	2.54	0.41
1:C:485:ARG:NH1	3:C:901:ZK1:OAA	2.44	0.41
1:D:458:LYS:O	1:D:458:LYS:HD2	2.21	0.41
1:B:527:MET:CG	5:B:904:PAM:H42	2.51	0.41
2:E:69:LEU:N	2:E:70:PRO:CD	2.84	0.41
2:G:69:LEU:N	2:G:70:PRO:CD	2.84	0.41
2:F:86:GLN:O	2:F:88:TRP:NE1	2.53	0.40
1:D:444:ILE:HG22	1:D:445:VAL:N	2.36	0.40
2:H:75:HIS:CE1	2:H:97:LEU:HD22	2.56	0.40
2:H:152:CYS:O	2:H:156:THR:N	2.54	0.40
1:A:704:LEU:HD23	1:A:704:LEU:N	2.36	0.40
2:F:75:HIS:CE1	2:F:97:LEU:HD22	2.56	0.40
1:B:458:LYS:HD2	1:B:458:LYS:O	2.20	0.40
1:B:735:ALA:O	1:B:736:THR:OG1	2.37	0.40
1:D:401:LEU:HD21	1:D:408:MET:SD	2.61	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	374/889 (42%)	353 (94%)	21 (6%)	0	100	100
1	B	370/889 (42%)	349 (94%)	21 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	374/889 (42%)	352 (94%)	22 (6%)	0	100	100
1	D	370/889 (42%)	348 (94%)	22 (6%)	0	100	100
2	E	126/174 (72%)	125 (99%)	1 (1%)	0	100	100
2	F	128/174 (74%)	115 (90%)	13 (10%)	0	100	100
2	G	126/174 (72%)	124 (98%)	2 (2%)	0	100	100
2	H	128/174 (74%)	117 (91%)	11 (9%)	0	100	100
All	All	1996/4252 (47%)	1883 (94%)	113 (6%)	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	284/761 (37%)	283 (100%)	1 (0%)	91	97
1	B	282/761 (37%)	281 (100%)	1 (0%)	91	97
1	C	284/761 (37%)	283 (100%)	1 (0%)	91	97
1	D	282/761 (37%)	281 (100%)	1 (0%)	91	97
2	E	110/153 (72%)	110 (100%)	0	100	100
2	F	114/153 (74%)	114 (100%)	0	100	100
2	G	110/153 (72%)	110 (100%)	0	100	100
2	H	114/153 (74%)	114 (100%)	0	100	100
All	All	1580/3656 (43%)	1576 (100%)	4 (0%)	92	97

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

Mol	Chain	Res	Type
1	A	817	LYS
1	B	458	LYS
1	C	817	LYS
1	D	458	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	508	GLN
1	D	508	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

30 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	$\#\|Z\| > 2$
4	OLC	A	902	-	24,24,24	1.38	4 (16%)	25,25,25	0.99	2 (8%)
5	PAM	D	905	-	17,17,17	0.81	0	17,17,17	0.70	0
5	PAM	H	202	-	17,17,17	0.78	0	17,17,17	0.69	0
5	PAM	D	906	-	17,17,17	0.89	0	17,17,17	0.64	0
5	PAM	C	905	-	17,17,17	0.84	0	17,17,17	0.72	0
5	PAM	A	903	-	17,17,17	0.84	0	17,17,17	0.74	0
5	PAM	F	202	-	17,17,17	0.82	0	17,17,17	0.72	0
5	PAM	B	906	-	17,17,17	0.83	0	17,17,17	0.76	0
5	PAM	A	904	-	17,17,17	0.83	0	17,17,17	0.71	0
3	ZK1	A	901	-	28,29,29	3.60	8 (28%)	42,45,45	1.52	7 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CLR	E	201	-	31,31,31	1.06	3 (9%)	48,48,48	1.53	5 (10%)
5	PAM	A	905	-	17,17,17	0.84	0	17,17,17	0.70	0
5	PAM	D	907	-	17,17,17	0.79	0	17,17,17	0.73	0
4	OLC	B	902	-	24,24,24	1.41	4 (16%)	25,25,25	1.01	2 (8%)
4	OLC	C	902	-	24,24,24	1.37	4 (16%)	25,25,25	0.96	2 (8%)
5	PAM	B	905	-	17,17,17	0.85	0	17,17,17	0.72	0
4	OLC	D	903	-	24,24,24	1.36	4 (16%)	25,25,25	0.98	2 (8%)
5	PAM	C	904	-	17,17,17	0.83	0	17,17,17	0.73	0
5	PAM	B	904	-	17,17,17	0.73	0	17,17,17	0.68	0
6	CLR	H	201	-	31,31,31	1.04	3 (9%)	48,48,48	1.70	9 (18%)
3	ZK1	D	901	-	28,29,29	3.61	8 (28%)	42,45,45	1.54	8 (19%)
4	OLC	C	903	-	24,24,24	1.32	3 (12%)	25,25,25	1.00	2 (8%)
3	ZK1	B	901	-	28,29,29	3.60	8 (28%)	42,45,45	1.54	7 (16%)
6	CLR	G	201	-	31,31,31	0.98	2 (6%)	48,48,48	1.59	8 (16%)
6	CLR	F	201	-	31,31,31	1.03	2 (6%)	48,48,48	1.65	9 (18%)
4	OLC	B	903	-	24,24,24	1.36	4 (16%)	25,25,25	1.00	2 (8%)
4	OLC	D	902	-	24,24,24	1.39	4 (16%)	25,25,25	0.97	2 (8%)
4	OLC	D	904	-	24,24,24	1.35	4 (16%)	25,25,25	0.98	2 (8%)
5	PAM	C	906	-	17,17,17	0.86	0	17,17,17	0.75	0
3	ZK1	C	901	-	28,29,29	3.59	8 (28%)	42,45,45	1.52	7 (16%)

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
4	OLC	A	902	-	-	16/24/24/24	-
5	PAM	D	905	-	-	7/15/15/15	-
5	PAM	H	202	-	-	9/15/15/15	-
5	PAM	D	906	-	-	5/15/15/15	-
5	PAM	C	905	-	-	6/15/15/15	-
5	PAM	A	903	-	-	9/15/15/15	-
5	PAM	F	202	-	-	8/15/15/15	-
5	PAM	B	906	-	-	8/15/15/15	-
5	PAM	A	904	-	-	8/15/15/15	-
3	ZK1	A	901	-	-	7/13/23/23	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLR	E	201	-	-	3/10/68/68	0/4/4/4
5	PAM	A	905	-	-	7/15/15/15	-
5	PAM	D	907	-	-	6/15/15/15	-
4	OLC	B	902	-	-	15/24/24/24	-
4	OLC	C	902	-	-	16/24/24/24	-
5	PAM	B	905	-	-	9/15/15/15	-
4	OLC	D	903	-	-	11/24/24/24	-
5	PAM	C	904	-	-	5/15/15/15	-
5	PAM	B	904	-	-	8/15/15/15	-
6	CLR	H	201	-	-	4/10/68/68	0/4/4/4
3	ZK1	D	901	-	-	7/13/23/23	0/3/3/3
4	OLC	C	903	-	-	12/24/24/24	-
3	ZK1	B	901	-	-	7/13/23/23	0/3/3/3
6	CLR	G	201	-	-	0/10/68/68	0/4/4/4
6	CLR	F	201	-	-	0/10/68/68	0/4/4/4
4	OLC	B	903	-	-	10/24/24/24	-
4	OLC	D	902	-	-	17/24/24/24	-
4	OLC	D	904	-	-	15/24/24/24	-
5	PAM	C	906	-	-	7/15/15/15	-
3	ZK1	C	901	-	-	7/13/23/23	0/3/3/3

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	ZK1	OAA-CAT	8.71	1.40	1.23
3	C	901	ZK1	OAA-CAT	8.69	1.40	1.23
3	D	901	ZK1	OAA-CAT	8.66	1.40	1.23
3	B	901	ZK1	OAA-CAT	8.62	1.40	1.23
3	D	901	ZK1	OAB-CAU	8.11	1.40	1.23
3	C	901	ZK1	OAB-CAU	8.09	1.40	1.23
3	B	901	ZK1	OAB-CAU	8.06	1.40	1.23
3	A	901	ZK1	OAB-CAU	8.04	1.40	1.23
3	B	901	ZK1	CAJ-CAV	7.43	1.51	1.39
3	D	901	ZK1	CAJ-CAV	7.36	1.51	1.39
3	A	901	ZK1	CAJ-CAV	7.31	1.50	1.39
3	C	901	ZK1	CAJ-CAV	7.29	1.50	1.39
3	C	901	ZK1	CAI-CAW	6.90	1.50	1.39
3	D	901	ZK1	CAI-CAW	6.88	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	ZK1	CAI-CAW	6.87	1.50	1.39
3	B	901	ZK1	CAI-CAW	6.85	1.50	1.39
3	B	901	ZK1	CAV-NAP	5.36	1.49	1.39
3	A	901	ZK1	CAV-NAP	5.36	1.49	1.39
3	D	901	ZK1	CAV-NAP	5.35	1.49	1.39
3	C	901	ZK1	CAV-NAP	5.31	1.49	1.39
3	D	901	ZK1	CAV-CAW	-4.97	1.35	1.40
3	B	901	ZK1	CAV-CAW	-4.97	1.35	1.40
3	A	901	ZK1	CAV-CAW	-4.87	1.35	1.40
3	C	901	ZK1	CAV-CAW	-4.84	1.35	1.40
3	A	901	ZK1	CAW-NAY	4.50	1.49	1.41
3	C	901	ZK1	CAW-NAY	4.47	1.49	1.41
3	D	901	ZK1	CAW-NAY	4.47	1.49	1.41
3	B	901	ZK1	CAW-NAY	4.46	1.49	1.41
3	D	901	ZK1	CAT-NAP	4.45	1.42	1.35
3	B	901	ZK1	CAT-NAP	4.44	1.42	1.35
3	A	901	ZK1	CAT-NAP	4.42	1.41	1.35
3	C	901	ZK1	CAT-NAP	4.40	1.41	1.35
4	B	902	OLC	C21-C22	3.43	1.63	1.51
4	D	902	OLC	C21-C22	3.23	1.62	1.51
4	C	902	OLC	C21-C22	3.21	1.62	1.51
4	D	903	OLC	C21-C22	3.18	1.62	1.51
4	D	904	OLC	C21-C22	3.14	1.62	1.51
4	A	902	OLC	C21-C22	3.09	1.62	1.51
4	B	903	OLC	C21-C22	3.08	1.62	1.51
4	C	903	OLC	C21-C22	3.02	1.61	1.51
6	E	201	CLR	C20-C17	2.80	1.59	1.54
6	H	201	CLR	C8-C9	2.77	1.58	1.53
6	G	201	CLR	C8-C9	2.66	1.58	1.53
6	H	201	CLR	C20-C17	2.60	1.59	1.54
4	B	902	OLC	C24-C22	2.48	1.61	1.51
6	E	201	CLR	C8-C9	2.48	1.58	1.53
4	C	902	OLC	O20-C1	2.36	1.40	1.33
6	F	201	CLR	C8-C9	2.36	1.58	1.53
4	D	902	OLC	C24-C22	2.30	1.61	1.51
4	C	902	OLC	C24-C22	2.29	1.61	1.51
4	B	903	OLC	C24-C22	2.28	1.61	1.51
4	A	902	OLC	C24-C22	2.26	1.61	1.51
4	D	903	OLC	C24-C22	2.25	1.61	1.51
6	H	201	CLR	C4-C3	2.25	1.56	1.52
6	E	201	CLR	C4-C3	2.25	1.56	1.52
4	C	903	OLC	C24-C22	2.23	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	201	CLR	C20-C17	2.23	1.58	1.54
4	B	902	OLC	O20-C1	2.22	1.39	1.33
4	D	904	OLC	C24-C22	2.22	1.60	1.51
4	D	904	OLC	O20-C1	2.21	1.39	1.33
4	A	902	OLC	O20-C1	2.21	1.39	1.33
4	B	903	OLC	O20-C1	2.20	1.39	1.33
4	B	902	OLC	C2-C1	2.20	1.57	1.50
4	D	902	OLC	O20-C1	2.18	1.39	1.33
4	D	903	OLC	O20-C1	2.17	1.39	1.33
4	B	903	OLC	C2-C1	2.17	1.57	1.50
4	D	902	OLC	C2-C1	2.16	1.57	1.50
4	A	902	OLC	C2-C1	2.16	1.57	1.50
4	C	903	OLC	O20-C1	2.13	1.39	1.33
4	C	902	OLC	C2-C1	2.13	1.56	1.50
4	D	903	OLC	C2-C1	2.10	1.56	1.50
6	F	201	CLR	C20-C17	2.05	1.58	1.54
4	D	904	OLC	C2-C1	2.02	1.56	1.50

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	201	CLR	C19-C10-C9	-5.11	105.58	111.68
6	F	201	CLR	C19-C10-C9	-4.80	105.96	111.68
6	H	201	CLR	C19-C10-C9	-4.63	106.16	111.68
6	G	201	CLR	C17-C13-C14	4.59	105.51	100.07
6	G	201	CLR	C19-C10-C9	-4.53	106.28	111.68
6	F	201	CLR	C17-C13-C14	4.48	105.38	100.07
6	H	201	CLR	C17-C13-C14	4.47	105.37	100.07
3	B	901	ZK1	CAV-NAP-CAT	-4.13	119.54	124.80
3	D	901	ZK1	CAV-NAP-CAT	-4.11	119.57	124.80
6	H	201	CLR	C19-C10-C5	4.11	114.99	108.34
3	A	901	ZK1	CAV-NAP-CAT	-4.05	119.65	124.80
3	C	901	ZK1	CAV-NAP-CAT	-4.01	119.70	124.80
6	F	201	CLR	C11-C9-C10	3.86	118.17	113.08
6	E	201	CLR	C17-C13-C14	3.84	104.62	100.07
6	G	201	CLR	C19-C10-C5	3.79	114.47	108.34
3	B	901	ZK1	CAO-NAY-CAU	3.70	120.12	116.51
3	D	901	ZK1	CAO-NAY-CAU	3.70	120.11	116.51
3	A	901	ZK1	CAO-NAY-CAU	3.58	120.00	116.51
6	E	201	CLR	C19-C10-C5	3.53	114.05	108.34
3	C	901	ZK1	CAO-NAY-CAU	3.53	119.94	116.51
6	F	201	CLR	C19-C10-C5	3.34	113.75	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	902	OLC	O20-C1-C2	3.25	122.12	111.91
6	G	201	CLR	C11-C9-C10	3.17	117.26	113.08
4	C	903	OLC	O20-C1-C2	3.16	121.82	111.91
4	B	903	OLC	O20-C1-C2	3.11	121.68	111.91
4	A	902	OLC	O20-C1-C2	3.07	121.53	111.91
4	D	904	OLC	O20-C1-C2	3.05	121.48	111.91
4	D	902	OLC	O20-C1-C2	3.04	121.44	111.91
4	C	902	OLC	O20-C1-C2	3.03	121.40	111.91
4	D	903	OLC	O20-C1-C2	2.99	121.31	111.91
6	E	201	CLR	C11-C9-C10	2.99	117.02	113.08
6	H	201	CLR	C11-C9-C10	2.91	116.92	113.08
6	F	201	CLR	C9-C10-C5	2.80	114.05	109.65
6	H	201	CLR	C16-C17-C13	-2.79	100.48	103.84
6	H	201	CLR	C3-C4-C5	2.65	116.53	112.03
3	A	901	ZK1	CAN-NAX-CAR	-2.64	110.02	116.27
3	C	901	ZK1	CAN-NAX-CAR	-2.63	110.03	116.27
6	H	201	CLR	C14-C8-C9	2.61	112.58	109.09
3	D	901	ZK1	CAW-NAY-CAU	-2.59	119.59	122.79
3	C	901	ZK1	CAW-NAY-CAU	-2.58	119.60	122.79
3	B	901	ZK1	CAW-NAY-CAU	-2.57	119.60	122.79
4	B	902	OLC	O20-C1-O19	-2.55	117.14	123.59
6	E	201	CLR	C16-C17-C13	-2.52	100.80	103.84
3	D	901	ZK1	CAN-NAX-CAR	-2.51	110.31	116.27
3	A	901	ZK1	CAW-NAY-CAU	-2.51	119.68	122.79
4	C	903	OLC	O20-C1-O19	-2.50	117.27	123.59
4	A	902	OLC	O20-C1-O19	-2.48	117.32	123.59
3	B	901	ZK1	CAN-NAX-CAR	-2.48	110.39	116.27
4	B	903	OLC	O20-C1-O19	-2.48	117.33	123.59
4	D	904	OLC	O20-C1-O19	-2.46	117.38	123.59
4	D	903	OLC	O20-C1-O19	-2.43	117.47	123.59
4	D	902	OLC	O20-C1-O19	-2.41	117.50	123.59
3	B	901	ZK1	CAM-NAX-CAR	-2.40	110.58	116.27
3	D	901	ZK1	CAM-NAX-CAR	-2.39	110.62	116.27
3	B	901	ZK1	CAU-CAT-NAP	2.34	119.90	117.49
4	C	902	OLC	O20-C1-O19	-2.33	117.71	123.59
6	F	201	CLR	C11-C9-C8	-2.32	108.41	111.75
3	D	901	ZK1	CAU-CAT-NAP	2.32	119.88	117.49
6	H	201	CLR	C10-C9-C8	-2.31	109.27	112.73
6	F	201	CLR	C13-C17-C20	-2.30	115.89	119.49
6	H	201	CLR	C22-C20-C17	2.30	115.03	110.28
3	A	901	ZK1	CAM-NAX-CAR	-2.25	110.93	116.27
3	C	901	ZK1	CAM-NAX-CAR	-2.24	110.96	116.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	901	ZK1	CAT-CAU-NAY	2.21	119.86	117.32
6	F	201	CLR	C22-C20-C17	2.19	114.80	110.28
3	A	901	ZK1	CAT-CAU-NAY	2.16	119.80	117.32
3	A	901	ZK1	CAU-CAT-NAP	2.15	119.70	117.49
6	G	201	CLR	C22-C20-C17	2.14	114.71	110.28
6	G	201	CLR	C13-C17-C20	-2.13	116.15	119.49
3	C	901	ZK1	CAU-CAT-NAP	2.10	119.65	117.49
6	F	201	CLR	C3-C4-C5	2.08	115.55	112.03
3	D	901	ZK1	CAT-CAU-NAY	2.07	119.69	117.32
6	G	201	CLR	C16-C17-C13	-2.05	101.37	103.84
3	B	901	ZK1	CAT-CAU-NAY	2.04	119.66	117.32
6	G	201	CLR	C10-C9-C8	-2.04	109.67	112.73
3	D	901	ZK1	FAH-CAZ-CAS	-2.02	109.18	112.70

There are no chirality outliers.

All (249) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ZK1	NAY-CAO-PBA-OAE
3	B	901	ZK1	NAY-CAO-PBA-OAD
3	C	901	ZK1	NAY-CAO-PBA-OAD
3	C	901	ZK1	NAY-CAO-PBA-OAE
3	D	901	ZK1	NAY-CAO-PBA-OAD
4	A	902	OLC	O23-C22-C24-O25
4	B	902	OLC	C21-C22-C24-O25
4	B	902	OLC	O23-C22-C24-O25
4	B	903	OLC	C21-C22-C24-O25
4	B	903	OLC	C2-C1-O20-C21
4	B	903	OLC	O19-C1-O20-C21
4	D	903	OLC	C11-C10-C9-C8
4	D	904	OLC	C21-C22-C24-O25
5	A	904	PAM	C11-C10-C9-C8
5	H	202	PAM	C11-C10-C9-C8
4	D	903	OLC	O19-C1-O20-C21
4	D	903	OLC	C2-C1-O20-C21
4	B	902	OLC	O19-C1-O20-C21
4	A	902	OLC	C11-C10-C9-C8
4	C	902	OLC	C11-C10-C9-C8
4	D	904	OLC	C11-C10-C9-C8
5	A	903	PAM	C11-C10-C9-C8
5	F	202	PAM	C11-C10-C9-C8
5	C	904	PAM	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
4	B	902	OLC	C2-C1-O20-C21
4	C	903	OLC	C2-C1-O20-C21
4	C	903	OLC	O19-C1-O20-C21
4	A	902	OLC	C12-C13-C14-C15
6	H	201	CLR	C21-C20-C22-C23
4	D	904	OLC	C2-C1-O20-C21
4	C	902	OLC	C1-C2-C3-C4
4	A	902	OLC	C14-C15-C16-C17
4	A	902	OLC	O20-C21-C22-C24
4	C	902	OLC	O20-C21-C22-C24
6	H	201	CLR	C17-C20-C22-C23
6	E	201	CLR	C13-C17-C20-C21
4	C	902	OLC	O23-C22-C24-O25
4	A	902	OLC	C1-C2-C3-C4
5	B	904	PAM	C1-C2-C3-C4
5	C	906	PAM	C3-C4-C5-C6
5	B	905	PAM	C3-C4-C5-C6
5	B	906	PAM	C3-C4-C5-C6
4	D	904	OLC	O19-C1-O20-C21
6	E	201	CLR	C16-C17-C20-C22
4	A	902	OLC	C6-C7-C8-C9
6	H	201	CLR	C22-C23-C24-C25
4	A	902	OLC	O20-C21-C22-O23
4	C	902	OLC	O20-C21-C22-O23
4	D	902	OLC	O20-C21-C22-O23
4	D	903	OLC	O20-C21-C22-O23
5	C	906	PAM	C5-C6-C7-C8
5	A	904	PAM	C5-C6-C7-C8
5	B	904	PAM	C5-C6-C7-C8
5	C	905	PAM	C4-C5-C6-C7
5	D	907	PAM	C2-C3-C4-C5
4	D	903	OLC	O20-C21-C22-C24
4	B	902	OLC	C3-C4-C5-C6
4	D	902	OLC	C2-C3-C4-C5
4	C	903	OLC	C13-C14-C15-C16
5	B	905	PAM	C11-C12-C13-C14
4	D	902	OLC	C11-C10-C9-C8
5	C	904	PAM	C3-C4-C5-C6
5	F	202	PAM	C2-C3-C4-C5
4	D	902	OLC	C4-C5-C6-C7
4	D	904	OLC	C13-C14-C15-C16
5	D	907	PAM	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	B	902	OLC	C12-C13-C14-C15
5	A	904	PAM	C11-C12-C13-C14
5	C	904	PAM	C12-C13-C14-C15
4	A	902	OLC	C21-C22-C24-O25
4	C	902	OLC	C21-C22-C24-O25
4	C	903	OLC	C21-C22-C24-O25
4	D	903	OLC	C21-C22-C24-O25
5	A	905	PAM	C11-C12-C13-C14
5	D	906	PAM	C1-C2-C3-C4
4	D	904	OLC	C3-C4-C5-C6
5	C	904	PAM	C5-C6-C7-C8
5	A	905	PAM	C4-C5-C6-C7
5	C	905	PAM	C3-C4-C5-C6
4	B	903	OLC	C12-C13-C14-C15
5	A	903	PAM	C3-C4-C5-C6
5	A	905	PAM	C3-C4-C5-C6
4	C	902	OLC	C2-C3-C4-C5
4	B	903	OLC	O23-C22-C24-O25
4	D	904	OLC	O23-C22-C24-O25
4	B	903	OLC	C2-C3-C4-C5
4	D	902	OLC	C6-C7-C8-C9
5	B	904	PAM	C10-C11-C12-C13
4	C	902	OLC	C3-C4-C5-C6
5	H	202	PAM	C3-C4-C5-C6
5	C	905	PAM	C5-C6-C7-C8
4	B	903	OLC	C5-C6-C7-C8
4	D	902	OLC	C5-C6-C7-C8
5	B	906	PAM	C4-C5-C6-C7
4	A	902	OLC	C2-C1-O20-C21
4	C	903	OLC	O20-C21-C22-O23
5	A	903	PAM	C5-C6-C7-C8
4	B	903	OLC	C11-C10-C9-C8
5	B	906	PAM	C11-C10-C9-C8
5	A	903	PAM	C6-C7-C8-C9
5	C	906	PAM	C6-C7-C8-C9
5	D	905	PAM	C6-C7-C8-C9
4	C	903	OLC	O20-C21-C22-C24
3	C	901	ZK1	CAI-CAR-NAX-CAN
4	B	902	OLC	C14-C15-C16-C17
5	D	905	PAM	C2-C3-C4-C5
4	A	902	OLC	O19-C1-O20-C21
3	A	901	ZK1	CAI-CAR-NAX-CAN

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Mol	Chain	Res	Type	Atoms
4	D	902	OLC	C3-C4-C5-C6
5	H	202	PAM	C4-C5-C6-C7
5	C	906	PAM	C12-C13-C14-C15
6	E	201	CLR	C16-C17-C20-C21
4	D	902	OLC	C11-C12-C13-C14
5	A	904	PAM	C6-C7-C8-C9
5	F	202	PAM	C6-C7-C8-C9
4	C	903	OLC	C2-C3-C4-C5
5	B	904	PAM	C11-C12-C13-C14
5	C	905	PAM	C11-C10-C9-C8
5	D	905	PAM	C11-C10-C9-C8
5	A	904	PAM	C13-C14-C15-C16
5	B	905	PAM	C12-C13-C14-C15
4	C	903	OLC	O23-C22-C24-O25
4	C	902	OLC	C10-C11-C12-C13
4	D	904	OLC	C10-C11-C12-C13
5	B	905	PAM	C6-C7-C8-C9
4	A	902	OLC	C4-C5-C6-C7
4	C	902	OLC	C4-C5-C6-C7
3	B	901	ZK1	CAI-CAR-NAX-CAN
3	D	901	ZK1	CAI-CAR-NAX-CAN
4	A	902	OLC	C2-C3-C4-C5
4	D	902	OLC	C15-C16-C17-C18
5	A	903	PAM	C11-C12-C13-C14
5	B	906	PAM	C12-C13-C14-C15
4	D	903	OLC	C4-C5-C6-C7
4	D	904	OLC	C4-C5-C6-C7
5	F	202	PAM	C11-C12-C13-C14
5	D	907	PAM	C4-C5-C6-C7
3	B	901	ZK1	CAI-CAR-NAX-CAM
3	D	901	ZK1	CAI-CAR-NAX-CAM
4	C	903	OLC	C11-C10-C9-C8
4	D	902	OLC	C13-C14-C15-C16
4	C	903	OLC	C3-C4-C5-C6
5	B	905	PAM	C13-C14-C15-C16
5	F	202	PAM	C4-C5-C6-C7
4	C	903	OLC	C12-C13-C14-C15
4	B	902	OLC	C5-C6-C7-C8
4	D	902	OLC	C1-C2-C3-C4
3	A	901	ZK1	CAS-CAR-NAX-CAN
3	B	901	ZK1	CAS-CAR-NAX-CAM
3	D	901	ZK1	CAS-CAR-NAX-CAM

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Mol	Chain	Res	Type	Atoms
4	D	903	OLC	C3-C4-C5-C6
5	B	905	PAM	C5-C6-C7-C8
5	D	906	PAM	C11-C12-C13-C14
5	A	905	PAM	C1-C2-C3-C4
4	A	902	OLC	C13-C14-C15-C16
4	B	902	OLC	C11-C12-C13-C14
5	A	903	PAM	C13-C14-C15-C16
5	A	904	PAM	C2-C3-C4-C5
5	B	905	PAM	C4-C5-C6-C7
3	C	901	ZK1	CAI-CAR-NAX-CAM
4	C	902	OLC	C15-C16-C17-C18
5	C	904	PAM	C6-C7-C8-C9
3	A	901	ZK1	CAI-CAR-NAX-CAM
5	B	904	PAM	C13-C14-C15-C16
3	B	901	ZK1	CAS-CAR-NAX-CAN
3	C	901	ZK1	CAS-CAR-NAX-CAN
3	D	901	ZK1	CAS-CAR-NAX-CAN
3	A	901	ZK1	NAY-CAO-PBA-OAD
3	B	901	ZK1	NAY-CAO-PBA-OAE
4	D	903	OLC	O23-C22-C24-O25
4	D	904	OLC	C12-C13-C14-C15
4	C	902	OLC	C6-C7-C8-C9
5	F	202	PAM	C5-C6-C7-C8
5	H	202	PAM	C1-C2-C3-C4
5	H	202	PAM	C11-C12-C13-C14
3	A	901	ZK1	NAY-CAO-PBA-OAC
3	B	901	ZK1	NAY-CAO-PBA-OAC
3	C	901	ZK1	NAY-CAO-PBA-OAC
3	D	901	ZK1	NAY-CAO-PBA-OAC
4	C	902	OLC	C11-C12-C13-C14
5	C	905	PAM	C12-C13-C14-C15
5	B	906	PAM	C13-C14-C15-C16
5	C	906	PAM	C13-C14-C15-C16
4	D	903	OLC	O20-C1-C2-C3
5	D	905	PAM	C12-C13-C14-C15
4	B	902	OLC	C6-C7-C8-C9
4	A	902	OLC	C9-C10-C11-C12
5	A	905	PAM	C5-C6-C7-C8
4	D	902	OLC	O20-C1-C2-C3
4	A	902	OLC	C5-C6-C7-C8
5	B	904	PAM	C7-C8-C9-C10
4	D	904	OLC	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
4	C	903	OLC	C1-C2-C3-C4
5	D	906	PAM	C2-C3-C4-C5
4	D	902	OLC	C2-C1-O20-C21
4	D	902	OLC	O19-C1-O20-C21
5	D	907	PAM	C11-C10-C9-C8
5	C	905	PAM	C6-C7-C8-C9
4	B	902	OLC	C13-C14-C15-C16
5	H	202	PAM	C6-C7-C8-C9
5	H	202	PAM	C10-C11-C12-C13
5	B	904	PAM	O2-C1-C2-C3
5	A	903	PAM	O2-C1-C2-C3
5	F	202	PAM	O1-C1-C2-C3
4	C	902	OLC	C13-C14-C15-C16
5	A	903	PAM	O1-C1-C2-C3
5	B	906	PAM	O1-C1-C2-C3
5	B	906	PAM	O2-C1-C2-C3
5	A	903	PAM	C12-C13-C14-C15
3	C	901	ZK1	CAS-CAR-NAX-CAM
4	B	902	OLC	O20-C21-C22-C24
4	D	904	OLC	O20-C21-C22-C24
4	D	904	OLC	C7-C8-C9-C10
6	H	201	CLR	C20-C22-C23-C24
5	B	904	PAM	O1-C1-C2-C3
4	B	903	OLC	C4-C5-C6-C7
5	A	904	PAM	O1-C1-C2-C3
5	D	905	PAM	C11-C12-C13-C14
5	A	905	PAM	C11-C10-C9-C8
5	F	202	PAM	O2-C1-C2-C3
4	D	902	OLC	C12-C13-C14-C15
5	B	905	PAM	C1-C2-C3-C4
4	B	902	OLC	O20-C1-C2-C3
5	A	904	PAM	O2-C1-C2-C3
4	D	904	OLC	C5-C6-C7-C8
4	D	903	OLC	C2-C3-C4-C5
4	C	902	OLC	C9-C10-C11-C12
5	D	906	PAM	C7-C8-C9-C10
5	H	202	PAM	O1-C1-C2-C3
5	D	907	PAM	O2-C1-C2-C3
5	C	906	PAM	C7-C8-C9-C10
4	C	902	OLC	O20-C1-C2-C3
5	A	905	PAM	C7-C8-C9-C10
4	D	902	OLC	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
5	B	905	PAM	C9-C10-C11-C12
5	B	906	PAM	C9-C10-C11-C12
5	D	905	PAM	C9-C10-C11-C12
5	H	202	PAM	O2-C1-C2-C3
5	D	907	PAM	O1-C1-C2-C3
3	A	901	ZK1	CAS-CAR-NAX-CAM
4	D	904	OLC	C9-C10-C11-C12
3	D	901	ZK1	NAY-CAO-PBA-OAE
4	B	902	OLC	C9-C10-C11-C12
4	B	903	OLC	C9-C10-C11-C12
5	C	906	PAM	C9-C10-C11-C12
4	D	902	OLC	O20-C21-C22-C24
5	D	905	PAM	C5-C6-C7-C8
4	B	902	OLC	C7-C8-C9-C10
5	D	906	PAM	C12-C13-C14-C15

There are no ring outliers.

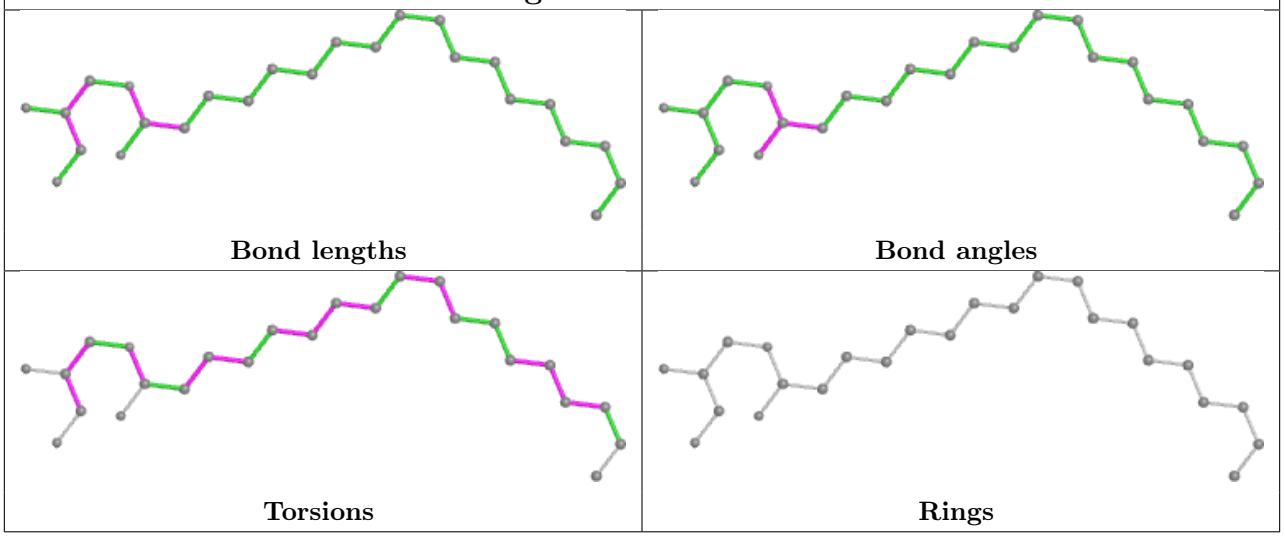
12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	OLC	1	0
5	D	905	PAM	2	0
5	B	906	PAM	2	0
3	A	901	ZK1	1	0
6	E	201	CLR	1	0
5	B	904	PAM	3	0
6	H	201	CLR	1	0
3	D	901	ZK1	1	0
3	B	901	ZK1	1	0
6	F	201	CLR	4	0
4	D	902	OLC	1	0
3	C	901	ZK1	1	0

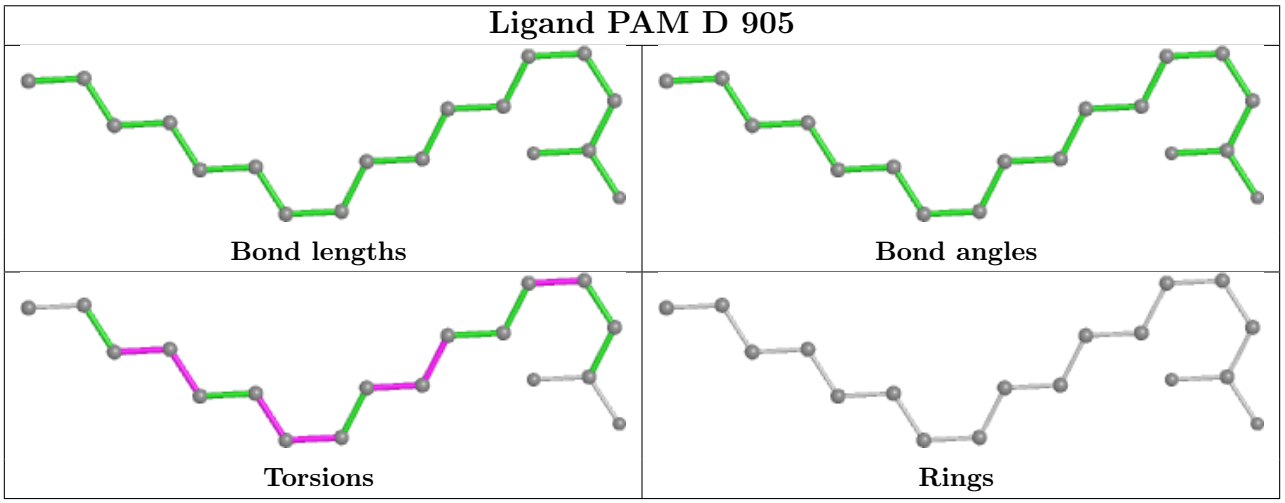
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

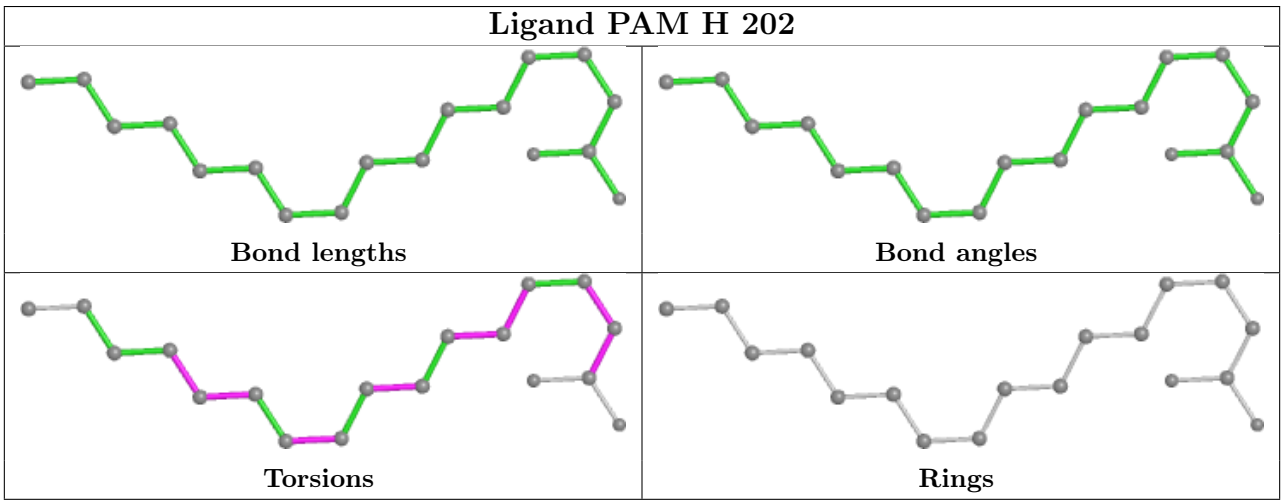
Ligand OLC A 902



Ligand PAM D 905

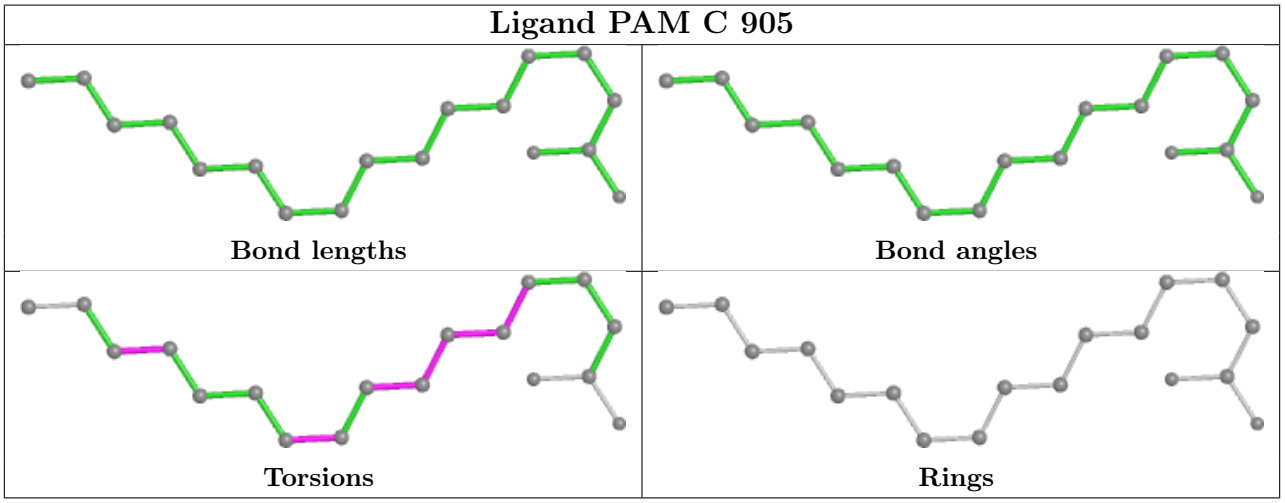


Ligand PAM H 202

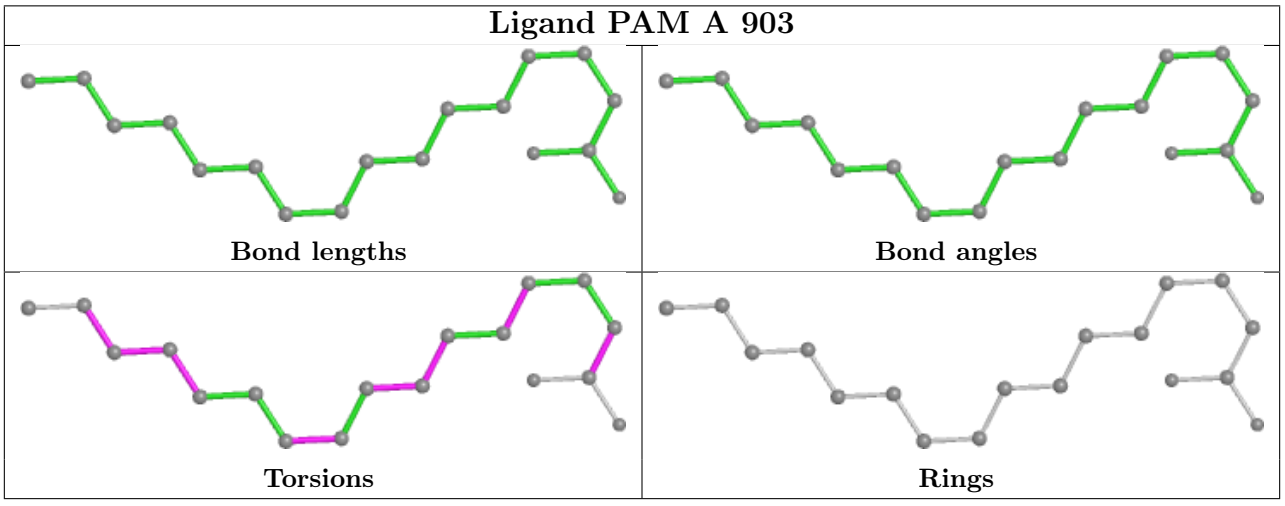


Ligand PAM D 906

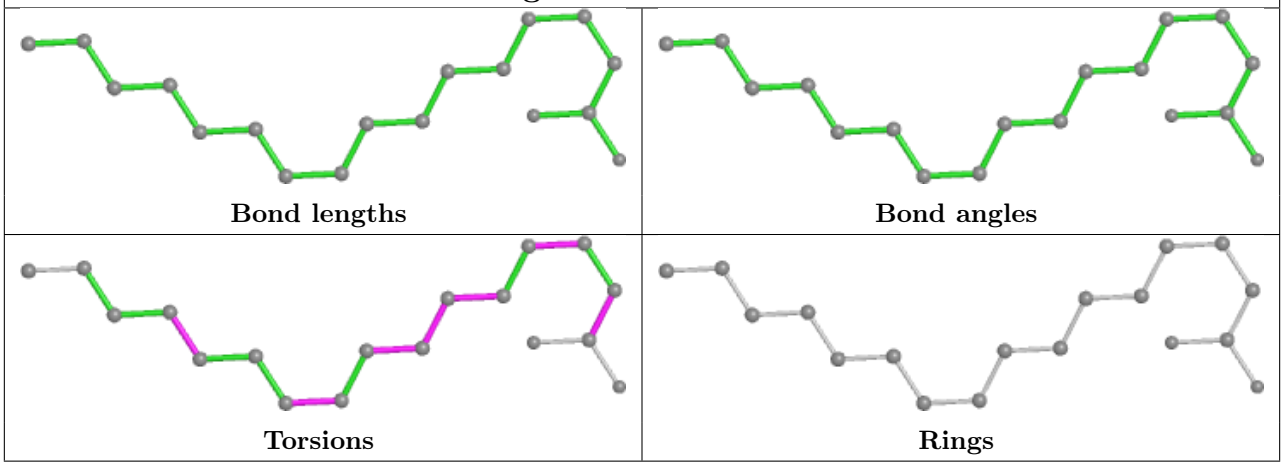
Ligand PAM C 905



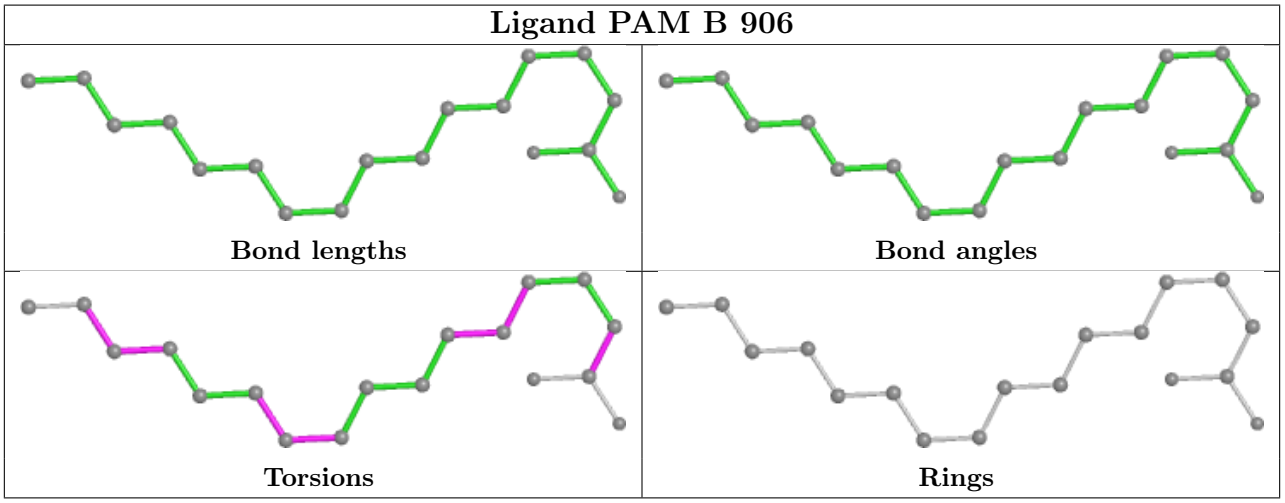
Ligand PAM A 903



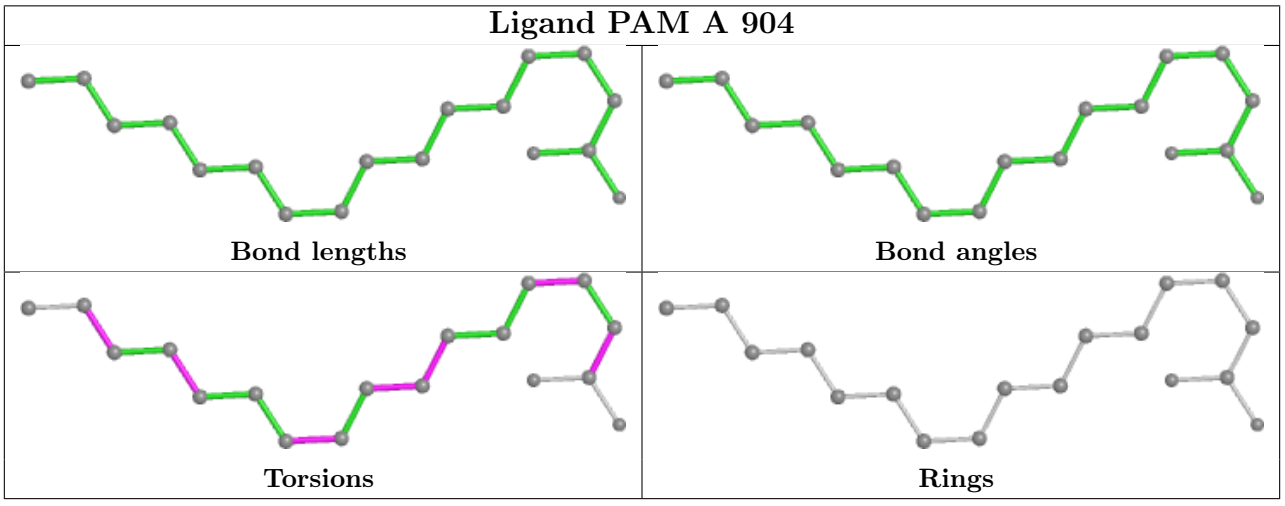
Ligand PAM F 202



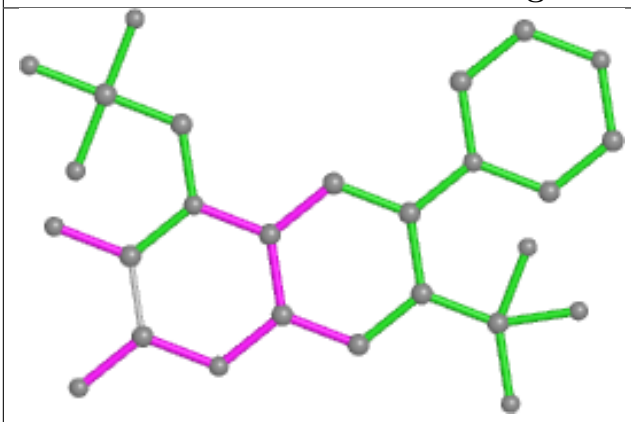
Ligand PAM B 906



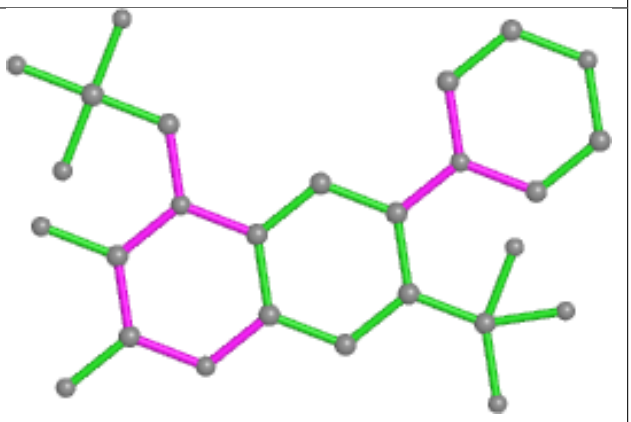
Ligand PAM A 904



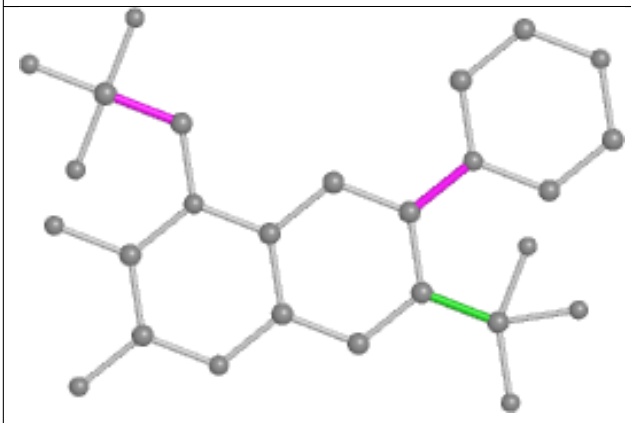
Ligand ZK1 A 901



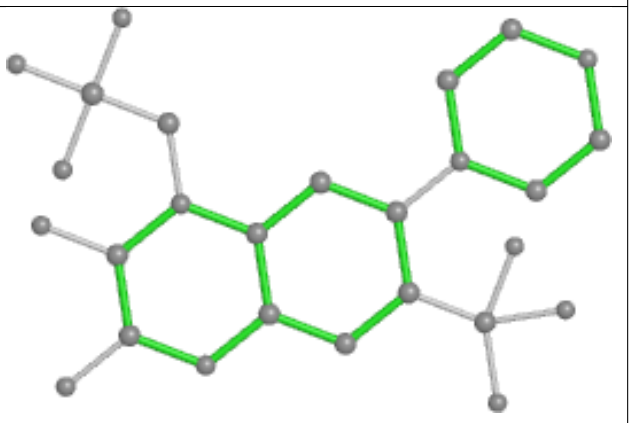
Bond lengths



Bond angles

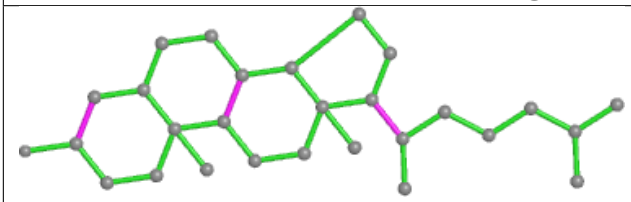


Torsions

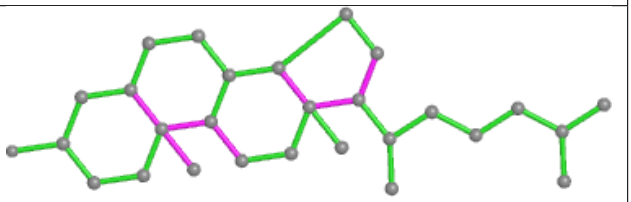


Rings

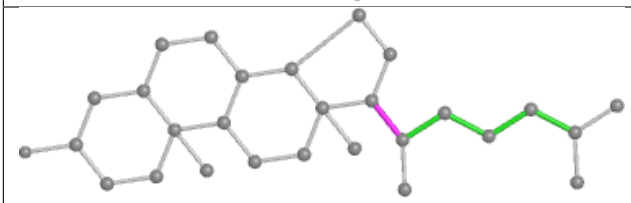
Ligand CLR E 201



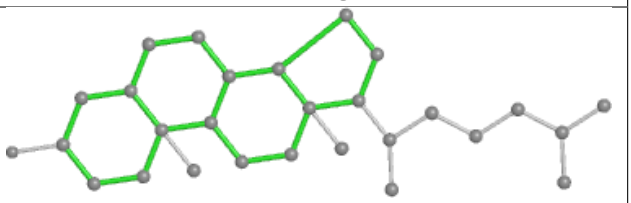
Bond lengths



Bond angles

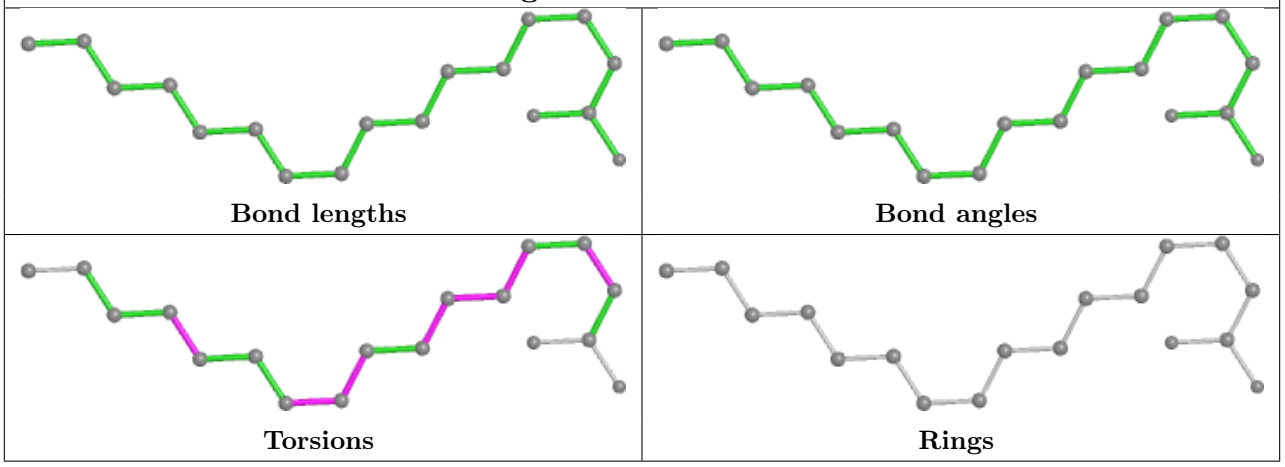


Torsions

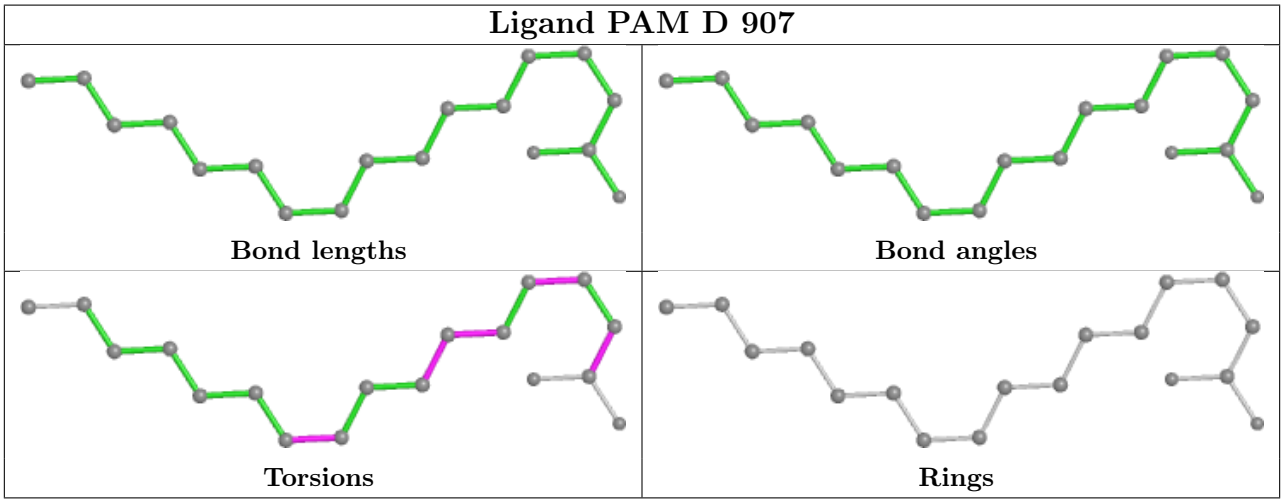


Rings

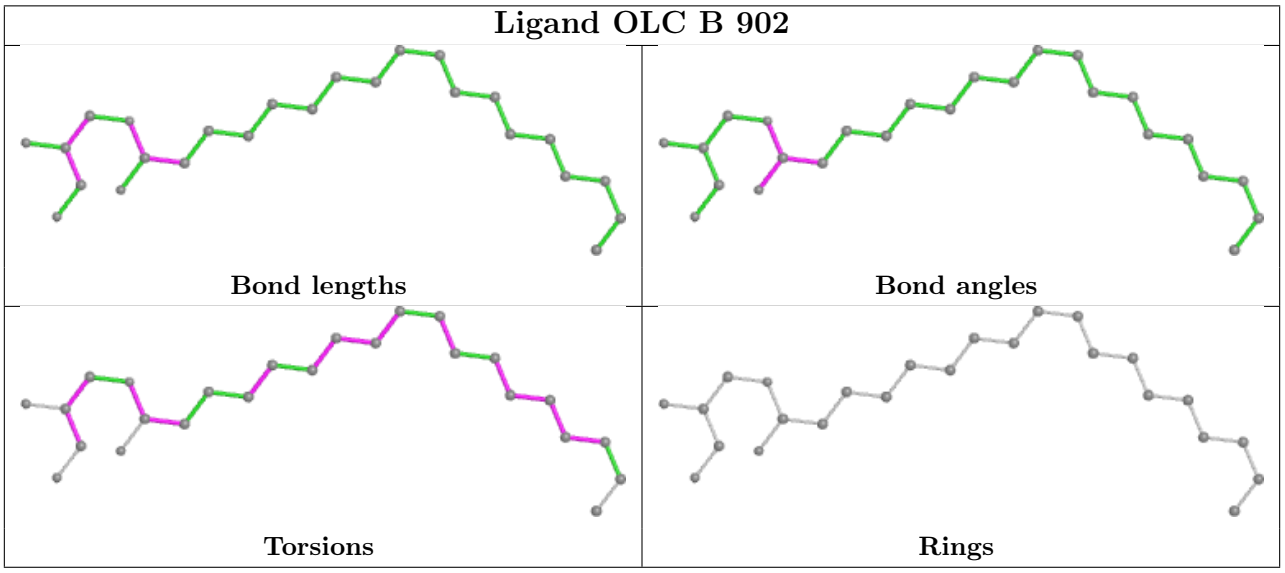
Ligand PAM A 905



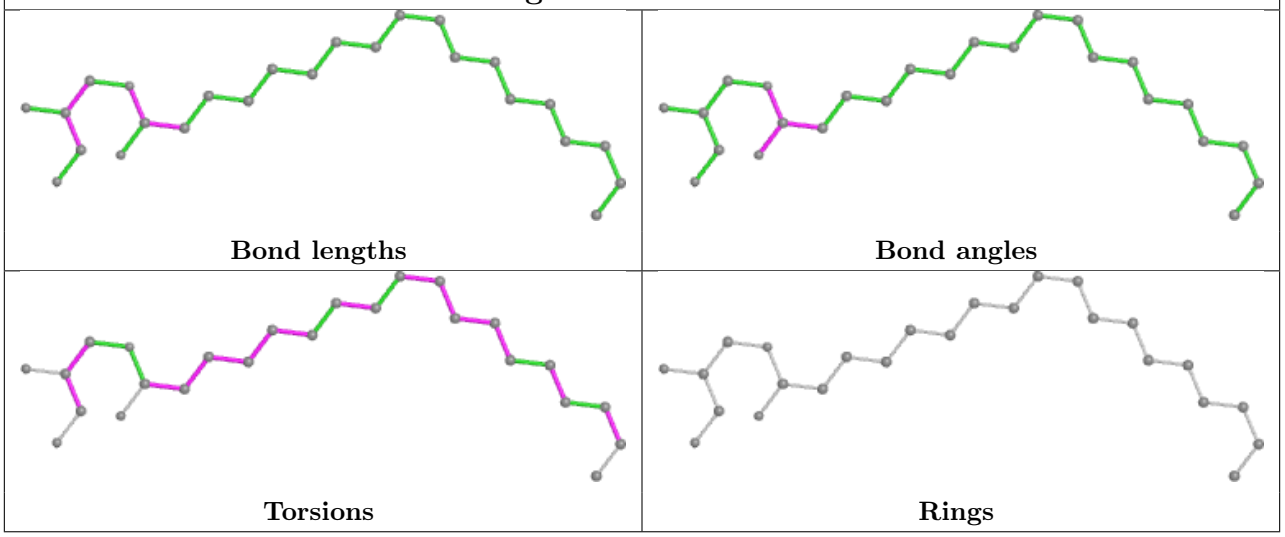
Ligand PAM D 907



Ligand OLC B 902



Ligand OLC C 902



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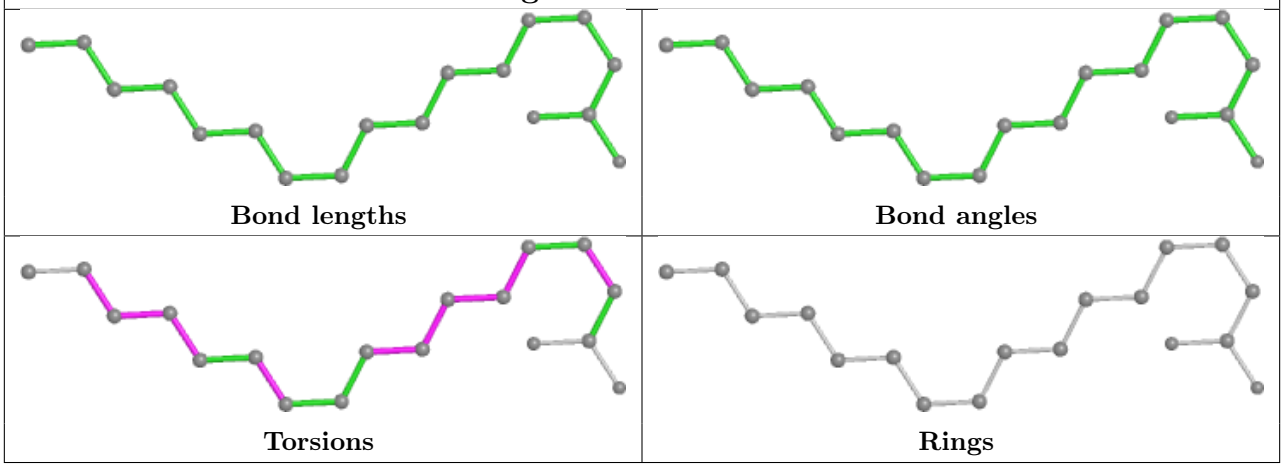

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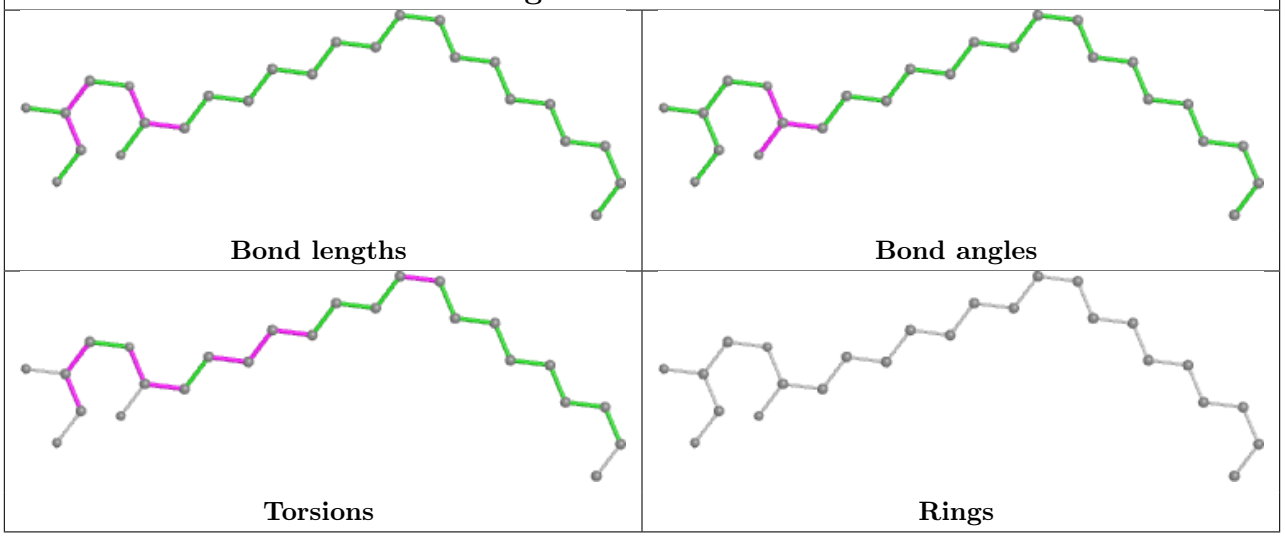
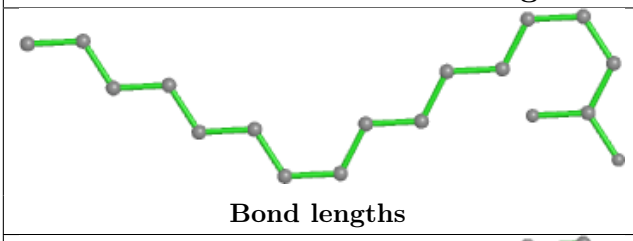
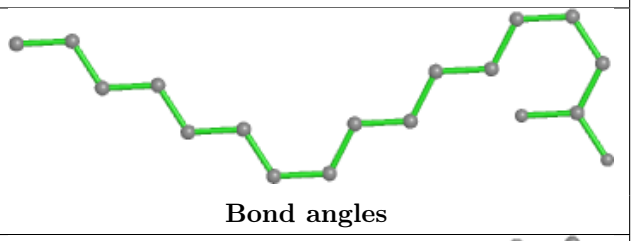
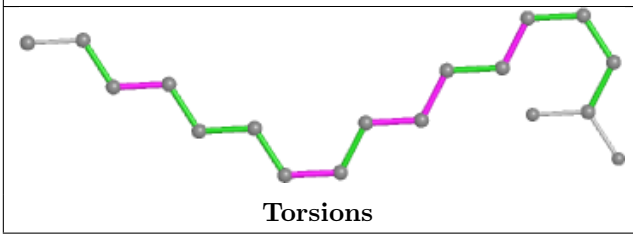
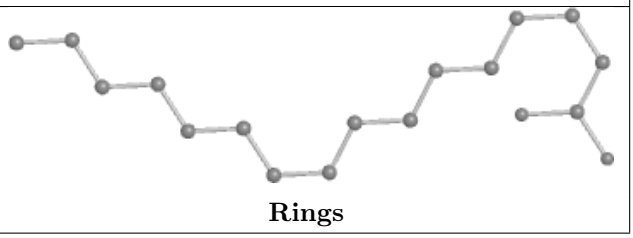


Ligand PAM C 904

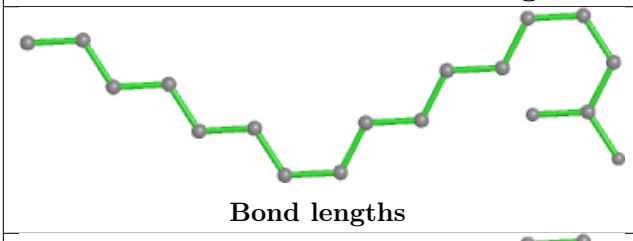

Bond lengths


Bond angles


Torsions


Rings

Ligand PAM B 904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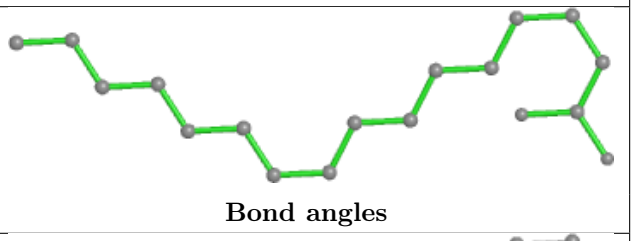
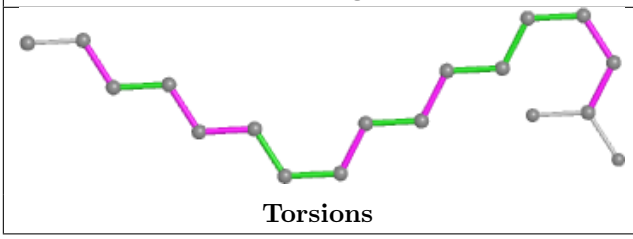

Bond angles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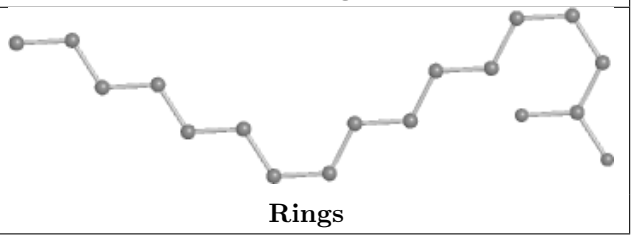
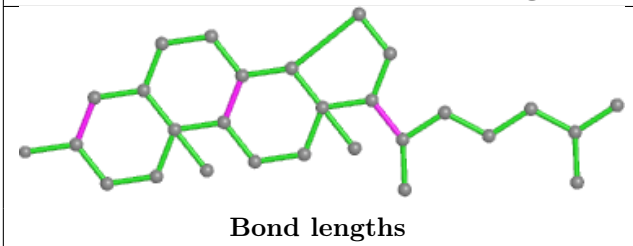

Rings

Ligand CLR H 201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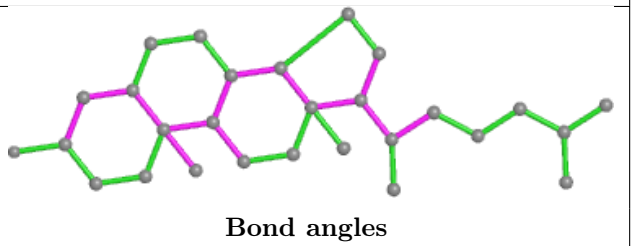
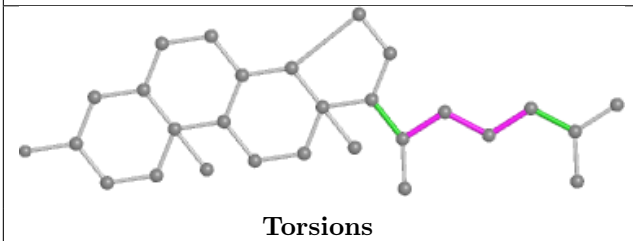

Bond angles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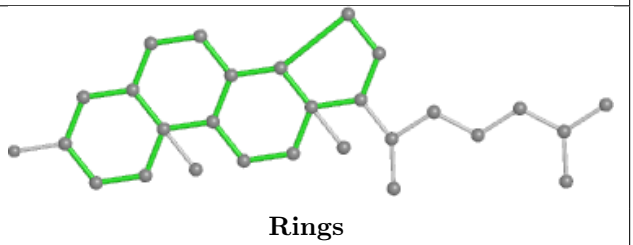
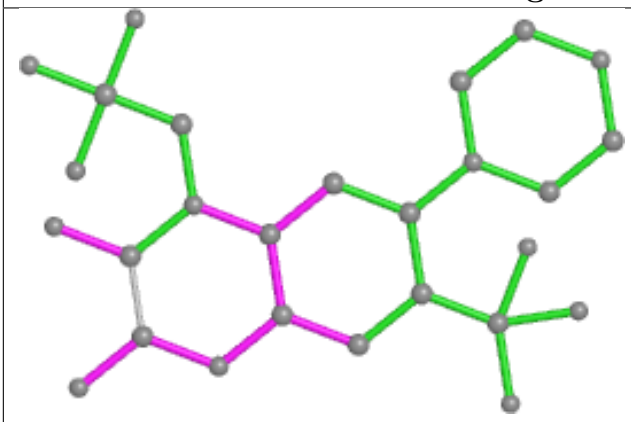

Rings

Ligand ZK1 D 901



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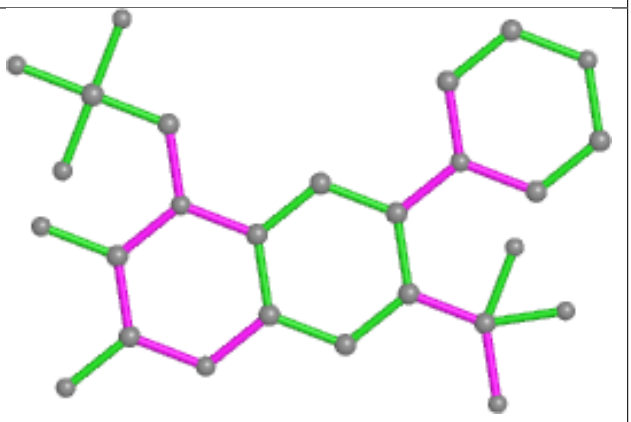
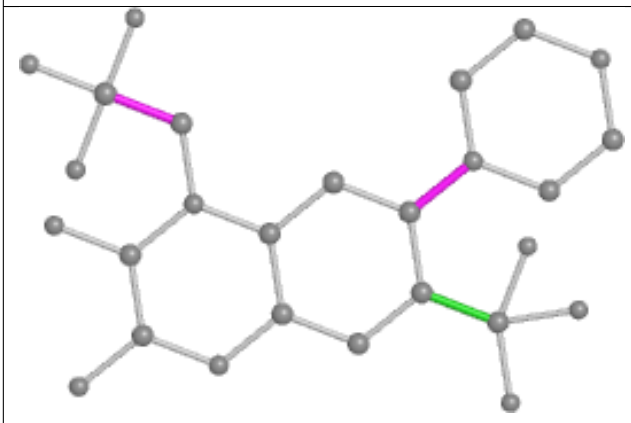
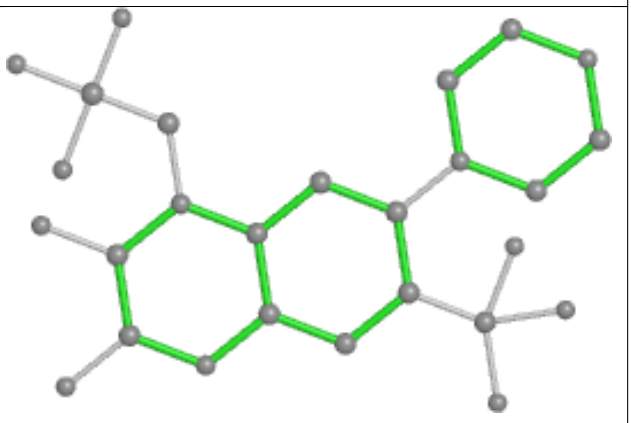


Bond angles

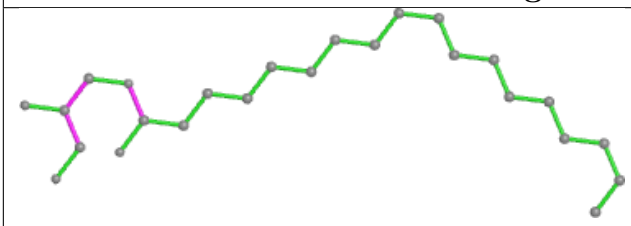


Torsions

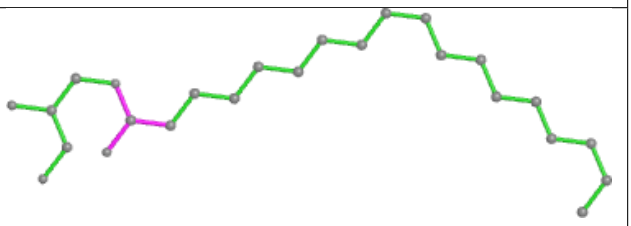


Rings

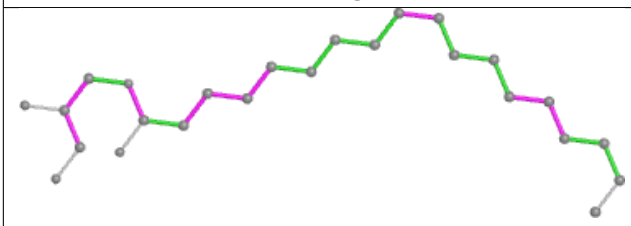
Ligand OLC C 903



Bond lengths



Bond angles



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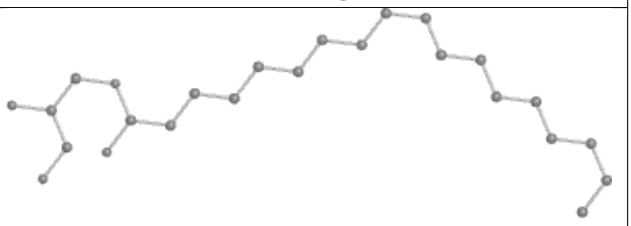
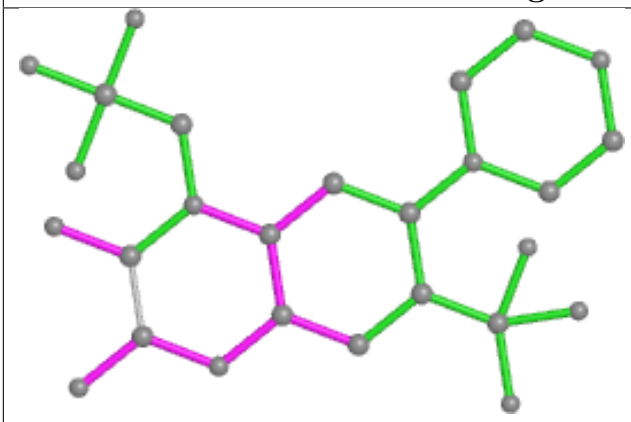


Rings

Ligand ZK1 B 901



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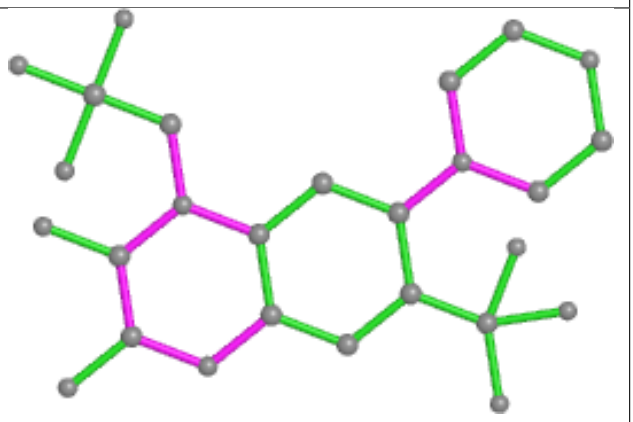
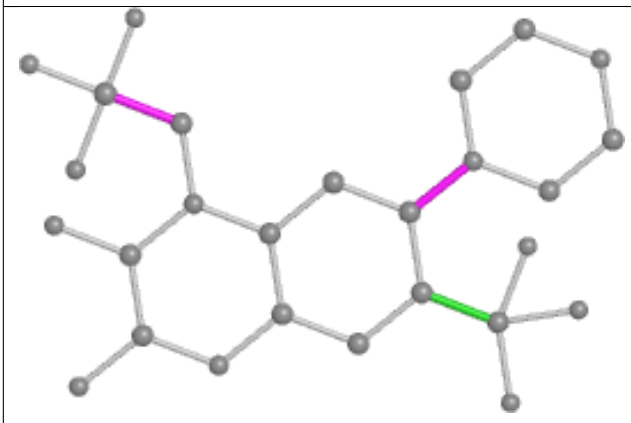


Bond angles



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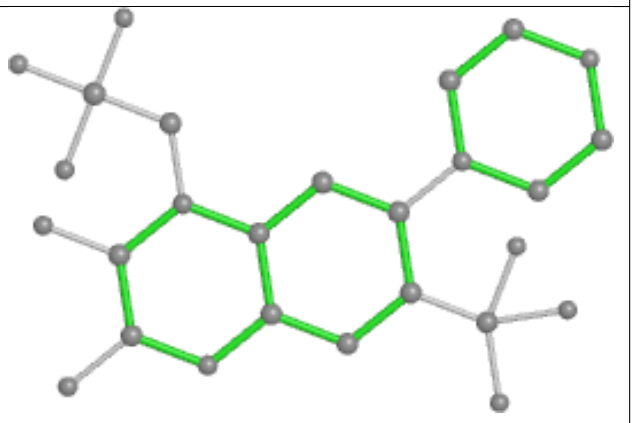
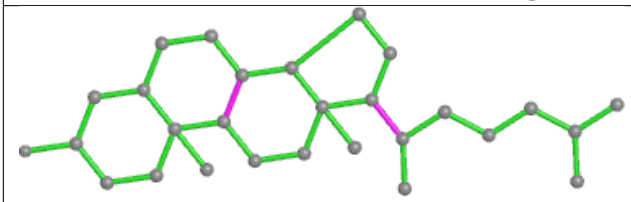


Rings

Ligand CLR G 201



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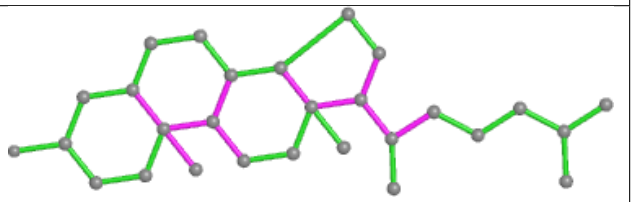
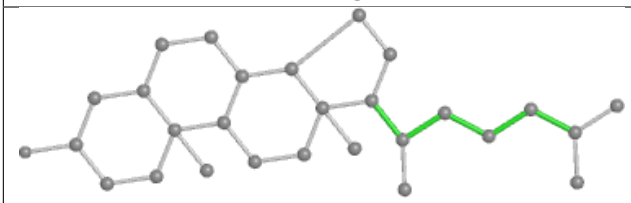
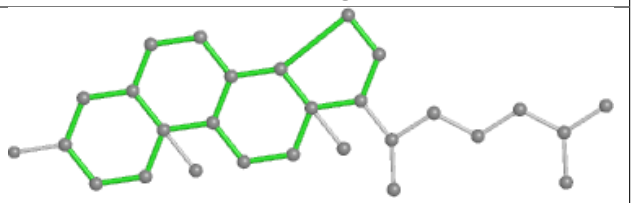


Bond angles

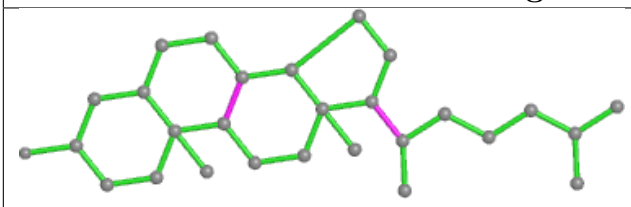


Torsions



Rings

Ligand CLR F 201



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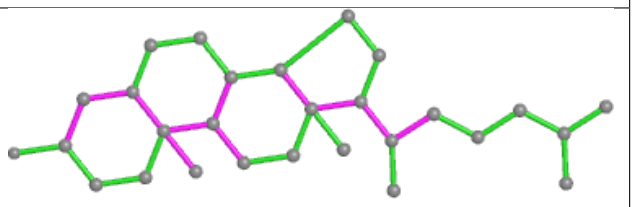
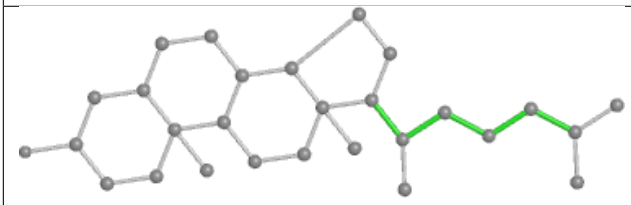


Bond angles



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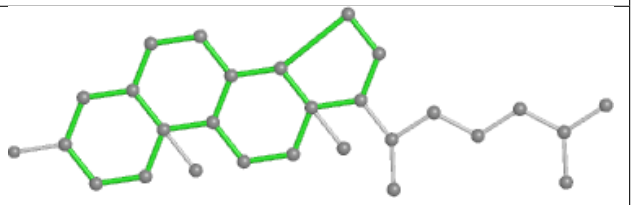
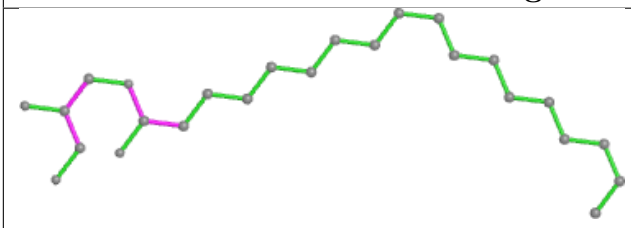


Rings

Ligand OLC B 903



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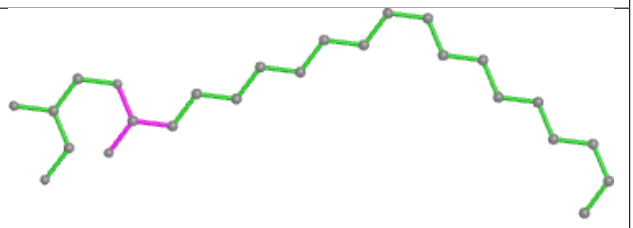
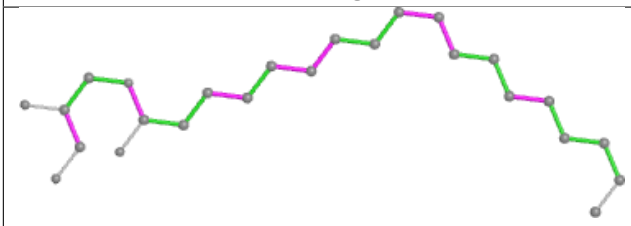


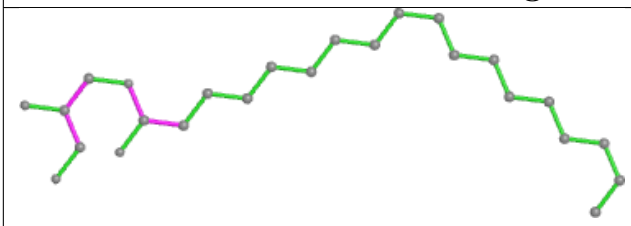
Bond angles



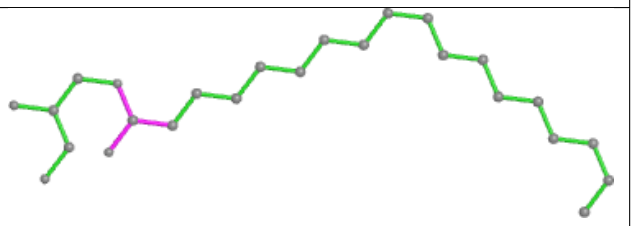
Torsions

Rings

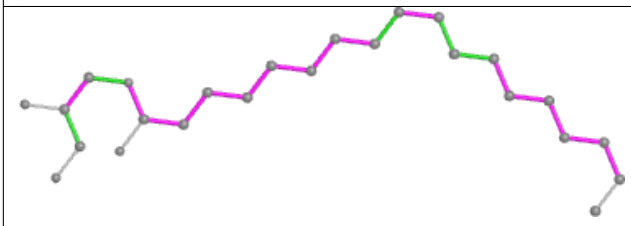
Ligand OLC D 902



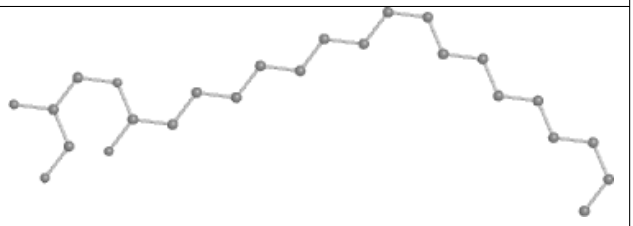
Bond lengths



Bond angles

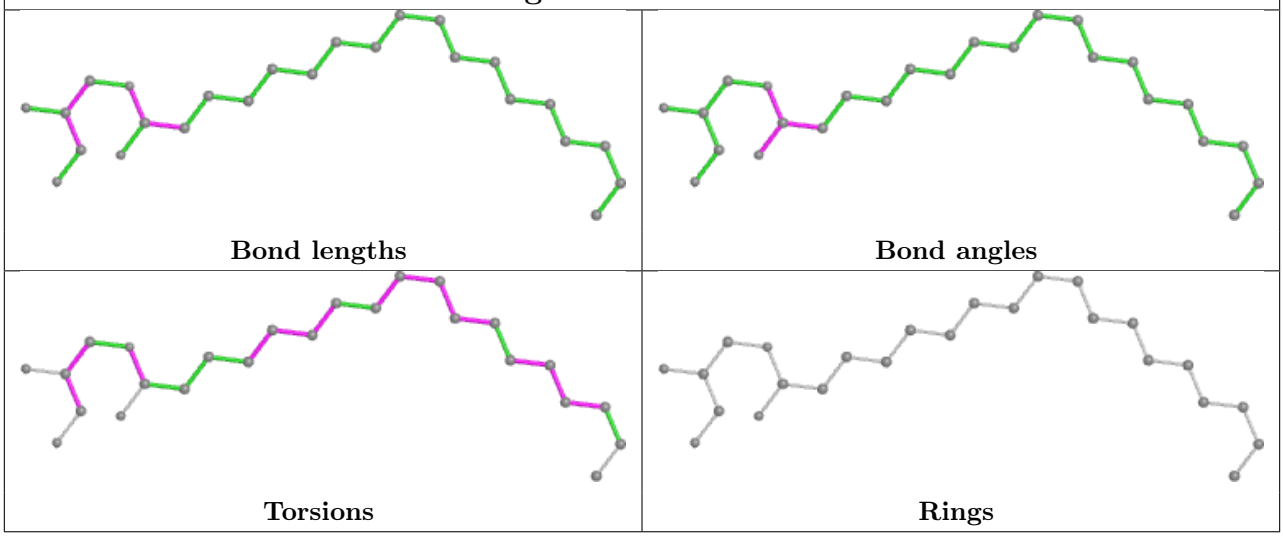


Torsions

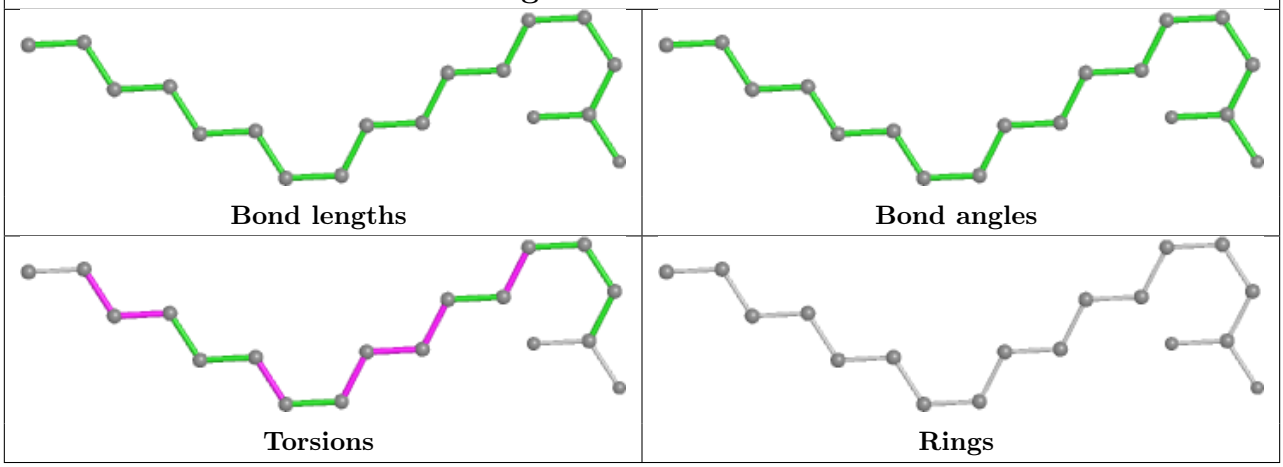


Rings

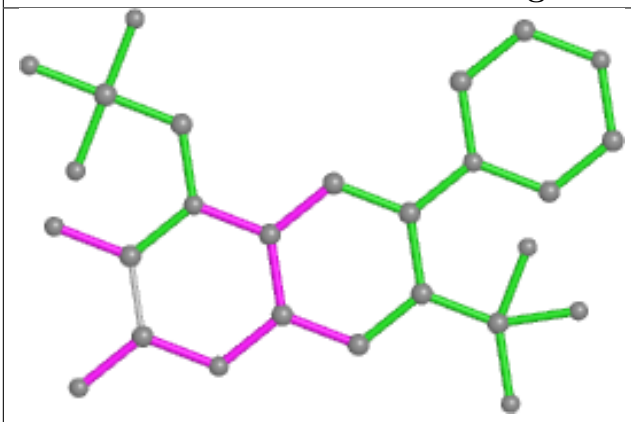
Ligand OLC D 904



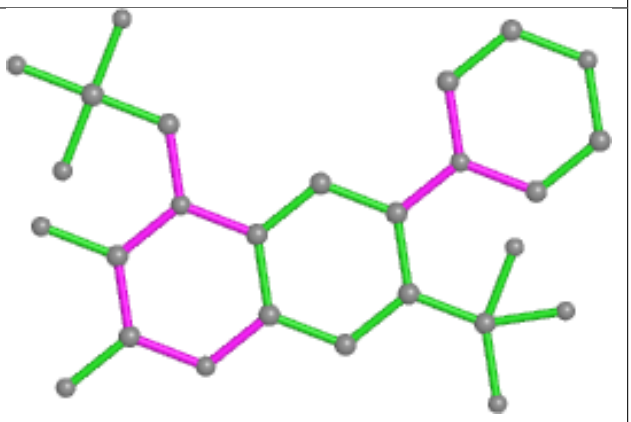
Ligand PAM C 906



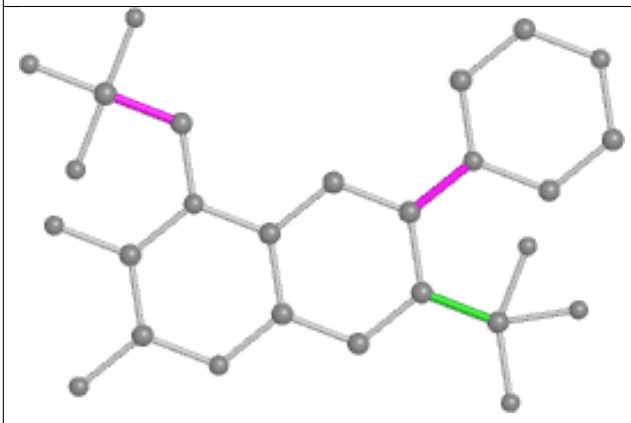
Ligand ZK1 C 901



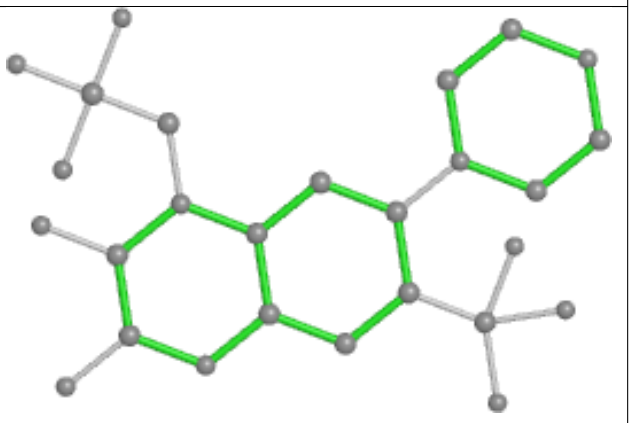
Bond lengths



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.

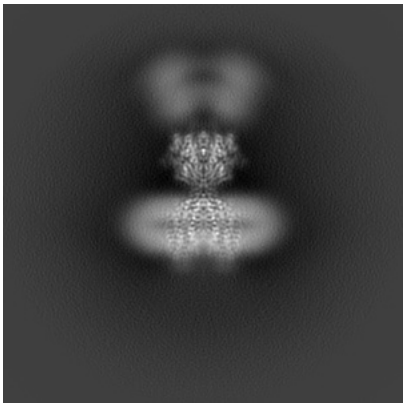
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20330. These allow visual inspection of the internal detail of the map and identification of artifacts.

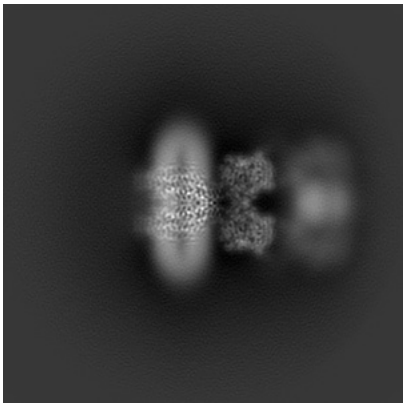
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

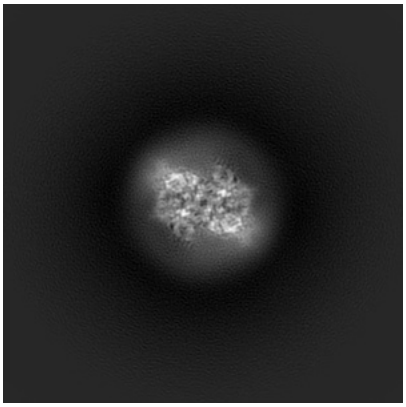
6.1.1 Primary map



X



Y

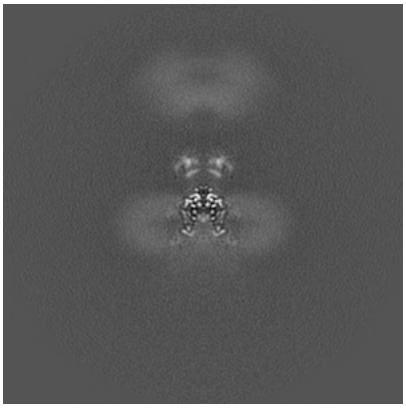


Z

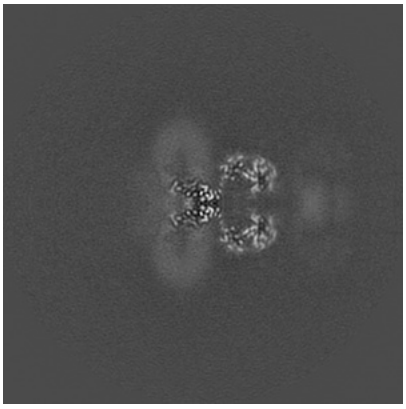
The images above show the map projected in three orthogonal directions.

6.2 Central slices

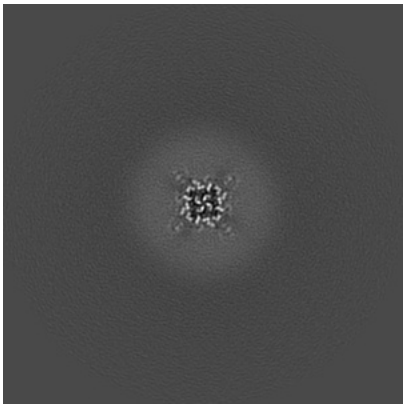
6.2.1 Primary map



X Index: 180



Y Index: 180

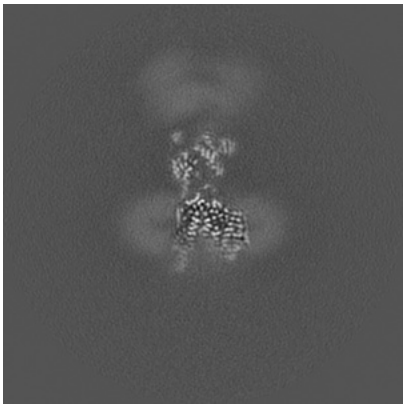


Z Index: 180

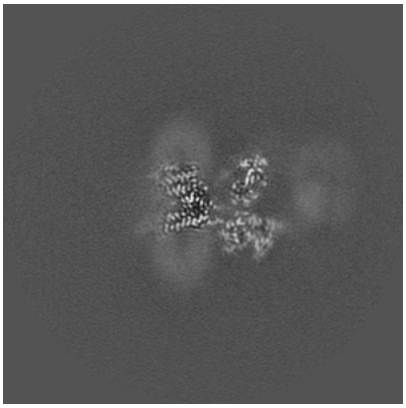
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

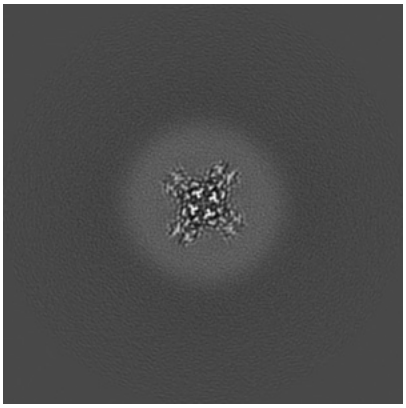
6.3.1 Primary map



X Index: 193



Y Index: 170



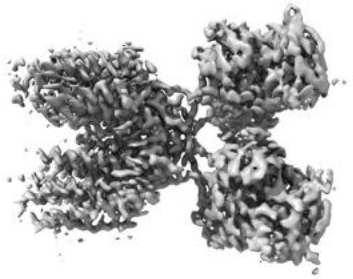
Z Index: 170

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

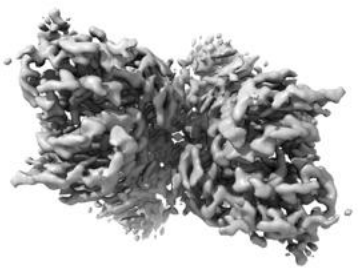
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0299. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

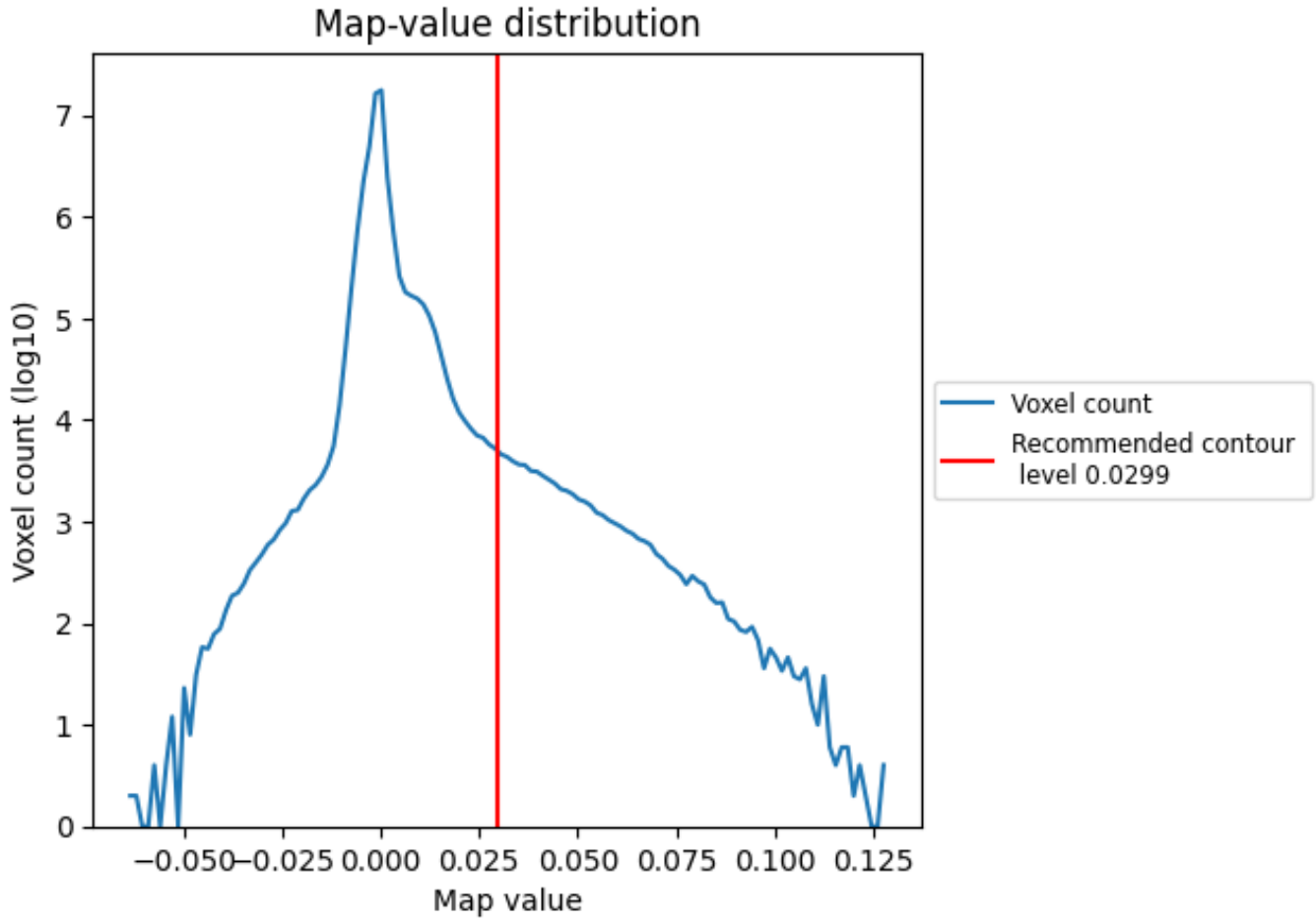
6.5 Mask visualisation (i)

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

7 Map analysis

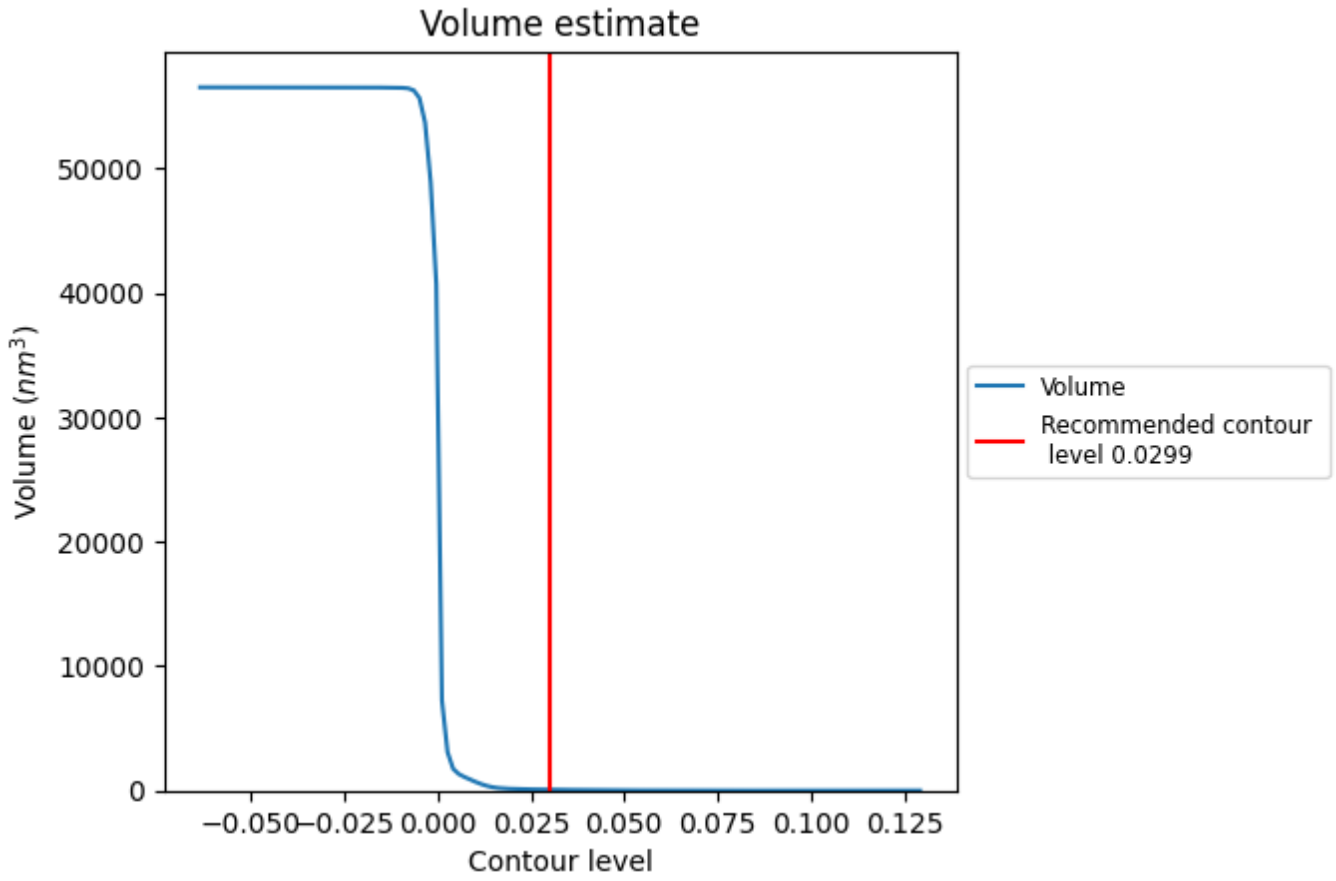
This section contains the results of statistical analysis of the map.

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.

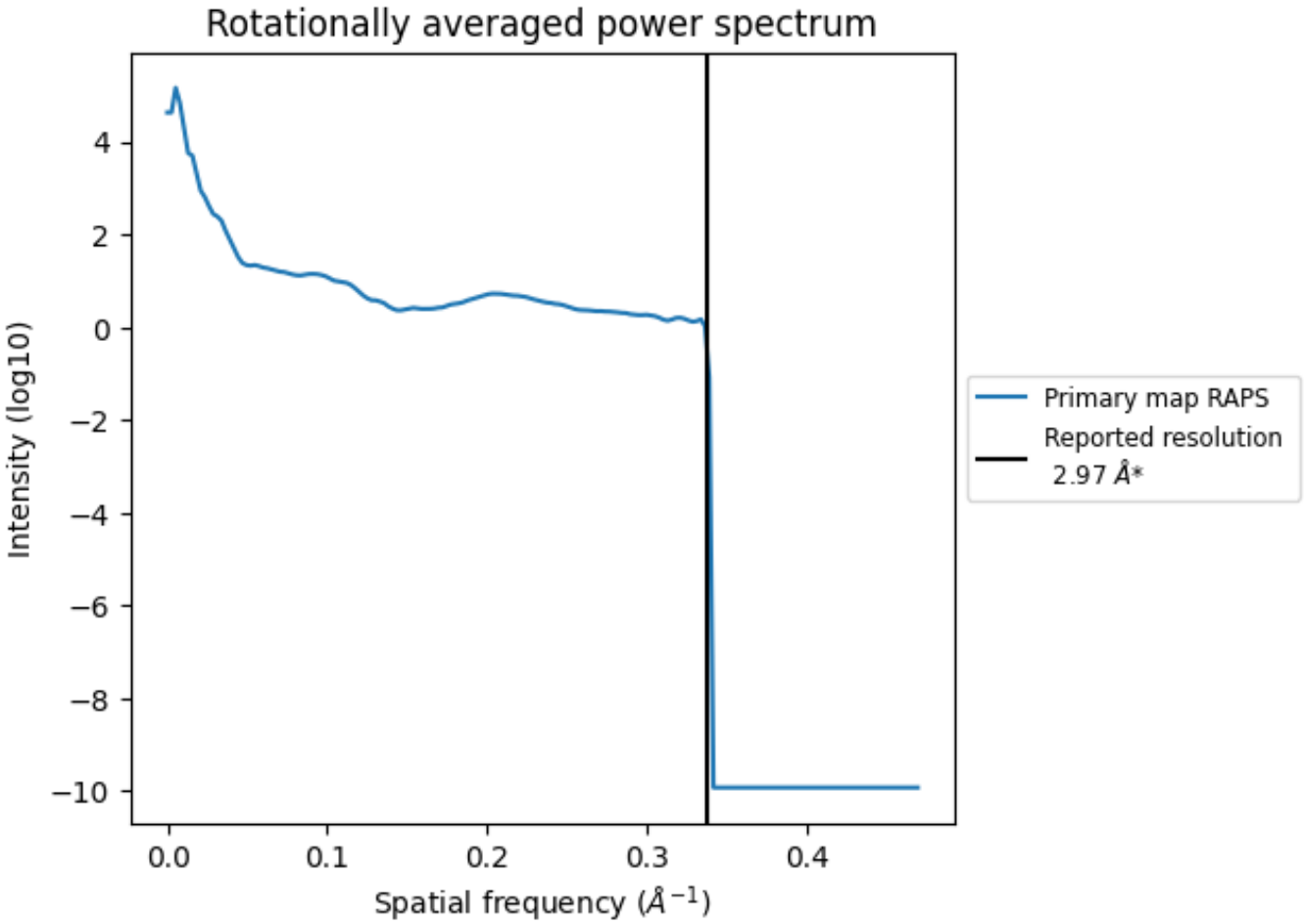
7.2 Volume estimate



The volume at the recommended contour level is 73 nm^3; this corresponds to an approximate mass of 66 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)

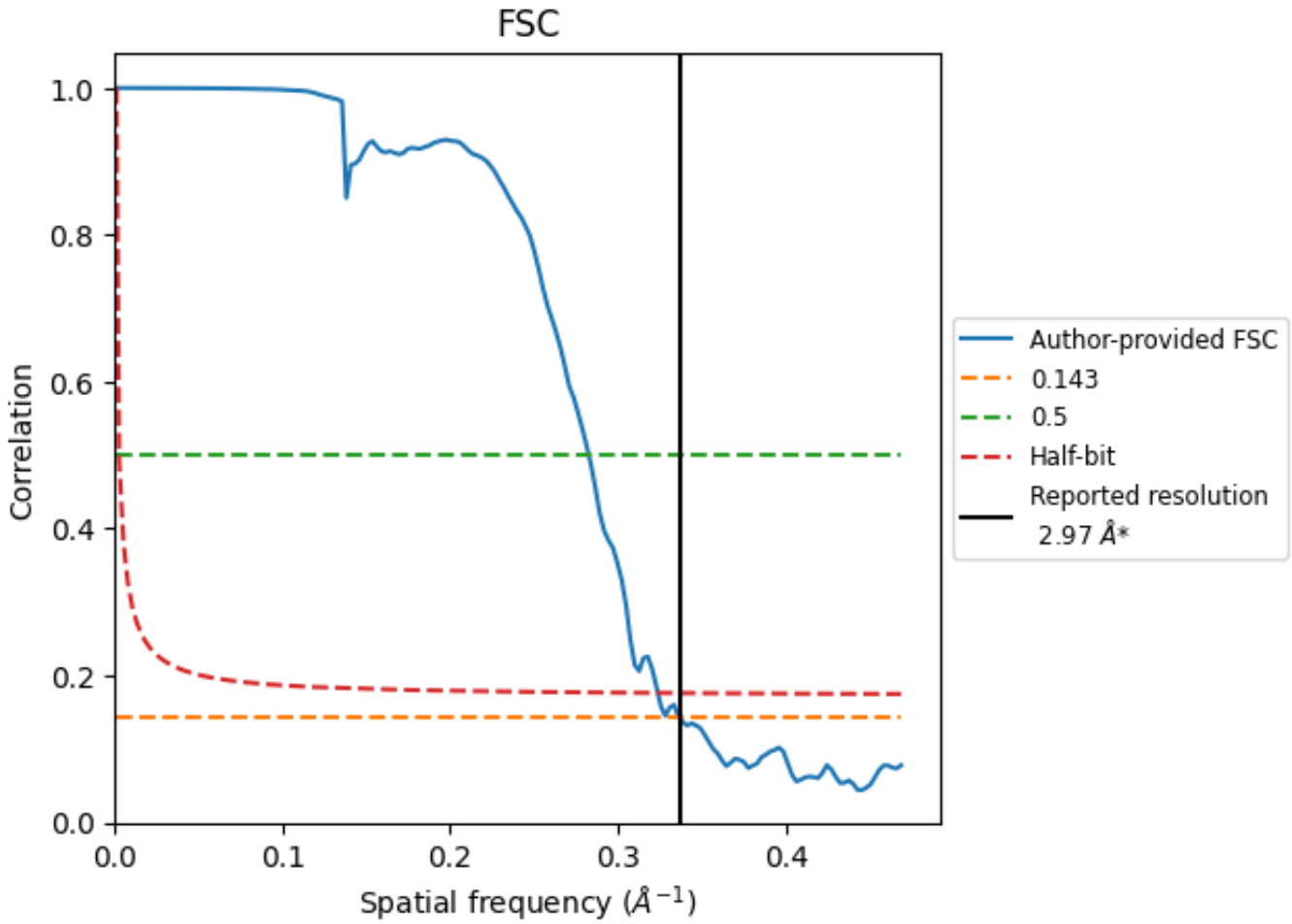


*Reported resolution corresponds to spatial frequency of 0.337 Å^{-1}

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 0.337 Å^{-1}

8.2 Resolution estimates (i)

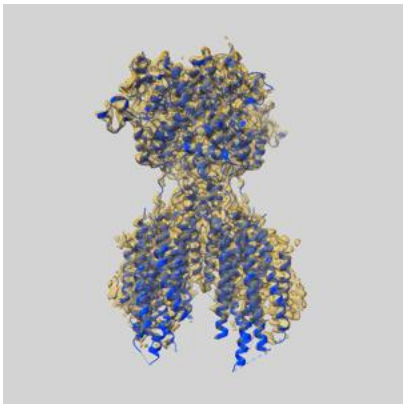
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.97	3.54	3.09
Unmasked-calculated*	-	-	-

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

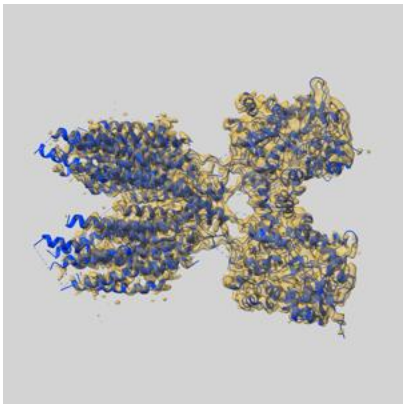
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20330 and PDB model 6PEQ. Per-residue inclusion information can be found in section 3 on page 11.

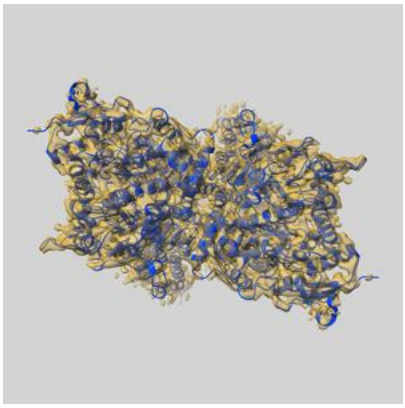
9.1 Map-model overlay



X



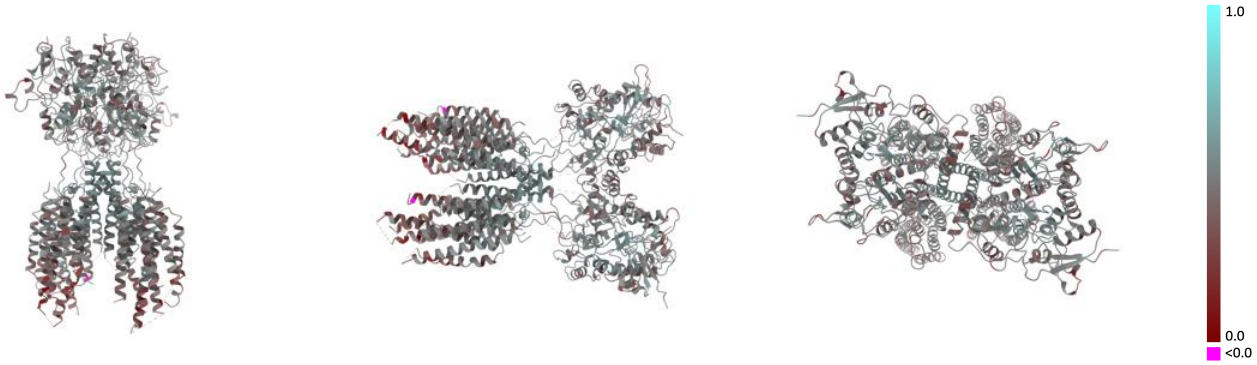
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0299 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.

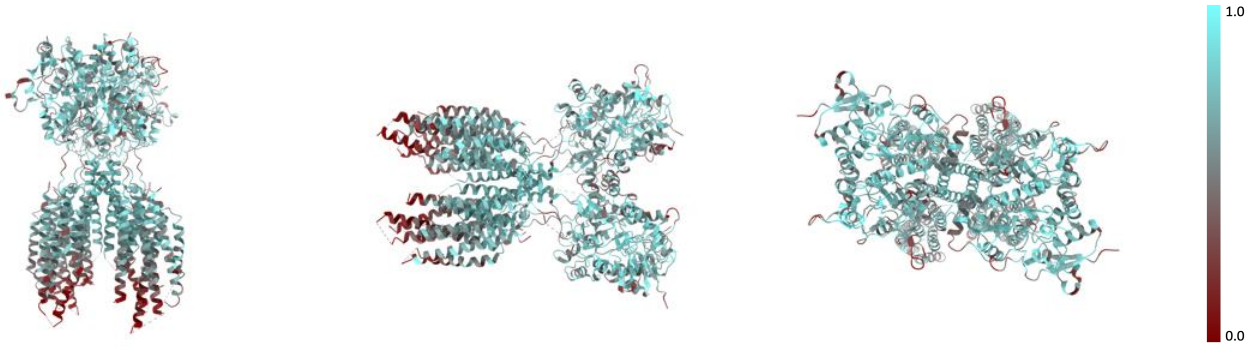
9.2 Q-score mapped to coordinate model (i)



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.

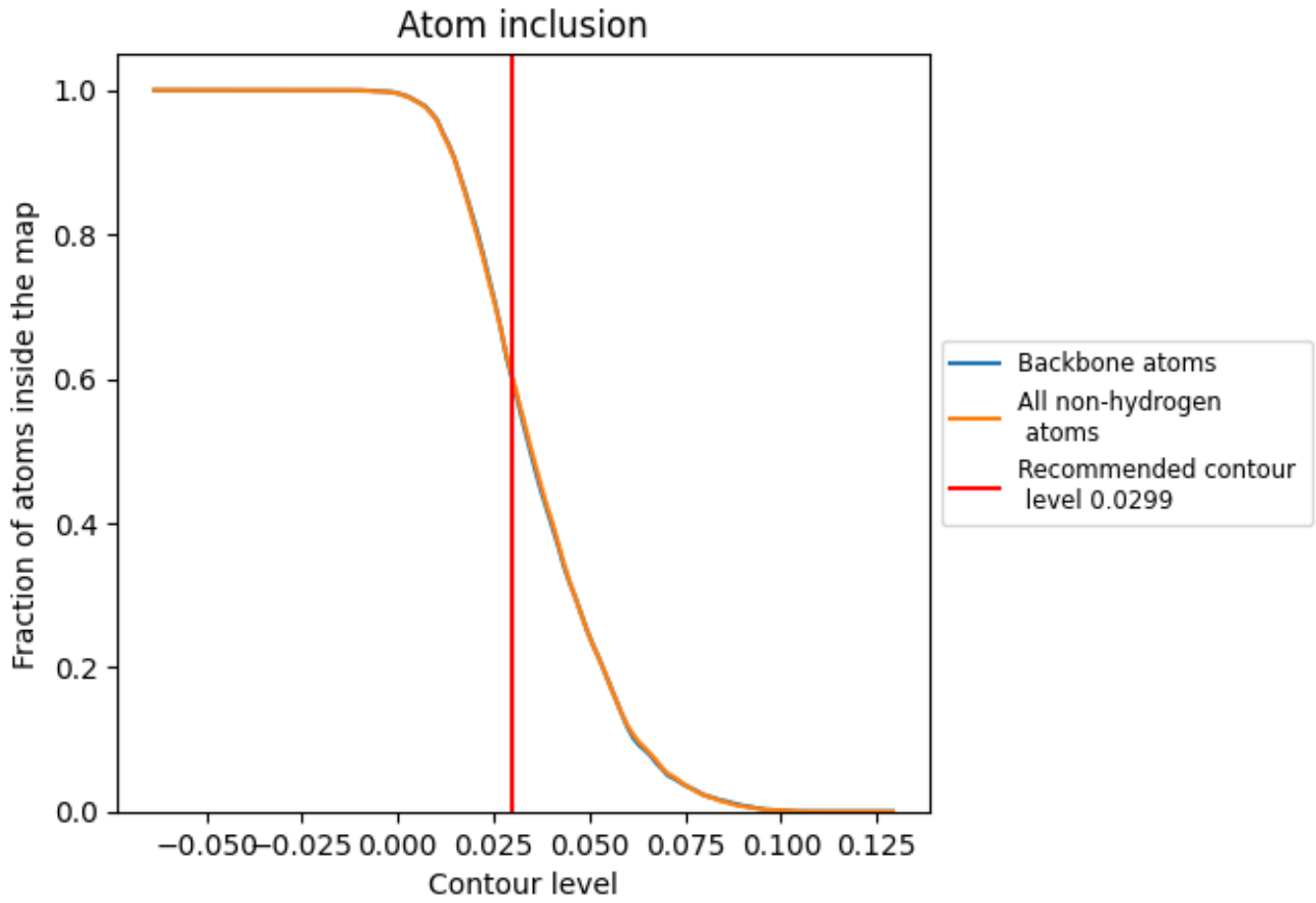
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0299).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 60% 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 (0.0299) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6022	0.4620
A	0.6638	0.4810
B	0.6498	0.4810
C	0.6605	0.4820
D	0.6484	0.4810
E	0.4601	0.4110
F	0.5158	0.4110
G	0.4711	0.4170
H	0.5150	0.4110