Full wwPDB EM Validation Report ⓘ

Jan 8, 2024 – 04:13 PM JST

PDB ID	:	8K9R
EMDB ID	:	EMD-36996
Title	:	Cryo EM structure of the products-bound PGAP1(Bst1)-H443N from Chaetomium thermophilum
Authors	:	Li, T.; Hong, J.; Qu, Q.; Li, D.
Deposited on	:	2023-08-01
Resolution	:	2.68 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:

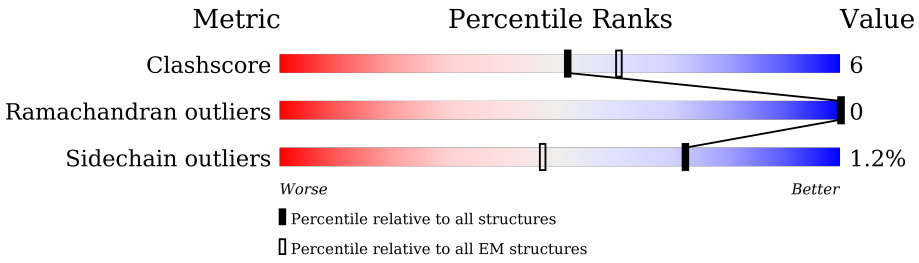
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.68 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%

Mol	Chain	Length	Quality of chain
1	A	1447	57% 9% 34%
2	B	272	· 99%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7684 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 GPI inositol-deacylase,MCherry protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	958	7487	4856	1264	1334	33	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP G0S652
A	0	GLY	-	expression tag	UNP G0S652
A	1	SER	-	expression tag	UNP G0S652
A	443	ASN	HIS	engineered mutation	UNP G0S652
A	1185	GLY	-	linker	UNP G0S652
A	1186	THR	-	linker	UNP G0S652
A	1187	LEU	-	linker	UNP G0S652
A	1188	GLU	-	linker	UNP G0S652
A	1189	VAL	-	linker	UNP G0S652
A	1190	LEU	-	linker	UNP G0S652
A	1191	PHE	-	linker	UNP G0S652
A	1192	GLN	-	linker	UNP G0S652
A	1193	GLY	-	linker	UNP G0S652
A	1194	PRO	-	linker	UNP G0S652
A	1195	LYS	-	linker	UNP G0S652
A	1196	LEU	-	linker	UNP G0S652
A	1197	GLU	-	linker	UNP G0S652
A	1198	PHE	-	linker	UNP G0S652
A	1345	SER	TRP	engineered mutation	UNP A0A366VY15
A	1363	VAL	ILE	engineered mutation	UNP A0A366VY15
A	1365	TYR	GLN	engineered mutation	UNP A0A366VY15
A	1399	ARG	ILE	engineered mutation	UNP A0A366VY15
A	1434	SER	-	expression tag	UNP A0A366VY15
A	1435	ALA	-	expression tag	UNP A0A366VY15
A	1436	HIS	-	expression tag	UNP A0A366VY15
A	1437	HIS	-	expression tag	UNP A0A366VY15
A	1438	HIS	-	expression tag	UNP A0A366VY15
A	1439	HIS	-	expression tag	UNP A0A366VY15

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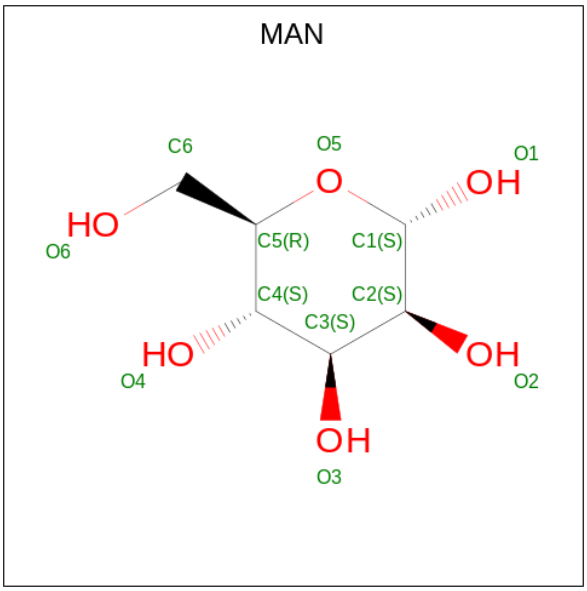
Chain	Residue	Modelled	Actual	Comment	Reference
A	1440	HIS	-	expression tag	UNP A0A366VY15
A	1441	HIS	-	expression tag	UNP A0A366VY15
A	1442	HIS	-	expression tag	UNP A0A366VY15
A	1443	HIS	-	expression tag	UNP A0A366VY15
A	1444	HIS	-	expression tag	UNP A0A366VY15
A	1445	HIS	-	expression tag	UNP A0A366VY15

- Molecule 2 is a protein called Green fluorescent protein,Complement decay-accelerating factor.

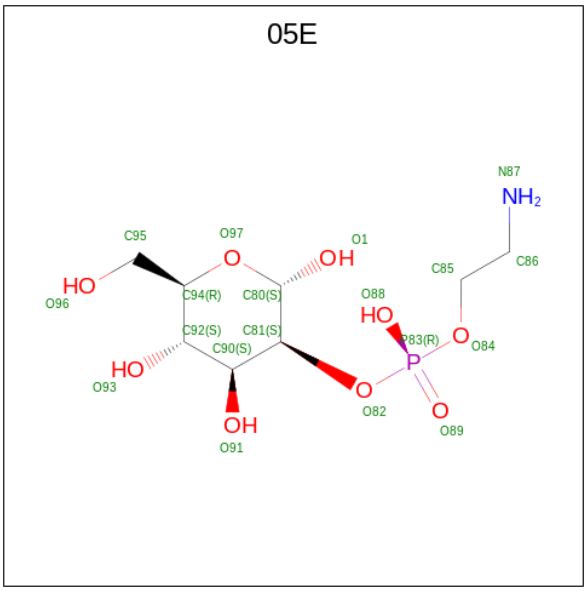
Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	4	Total	C	N	O	0	0
			24	13	4	7		

- Molecule 3 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



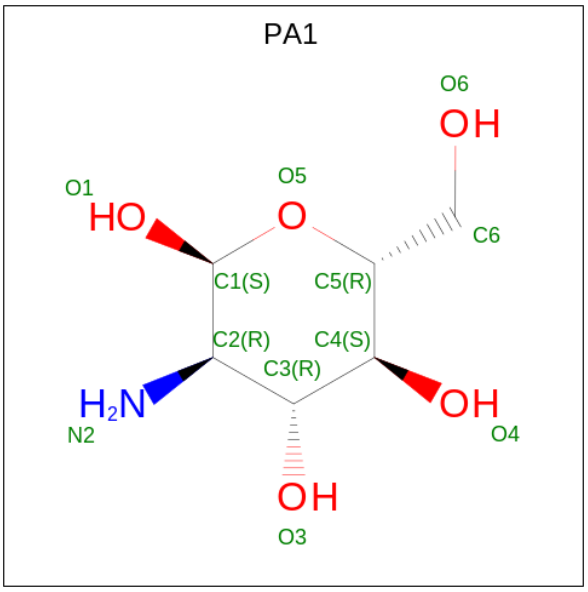
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			11	6	5	
3	A	1	Total	C	O	0
			11	6	5	

- Molecule 4 is 2-azanylethyl [(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-2,4,5-tris(oxidanyl)oxan-3-yl] hydrogen phosphate (three-letter code: 05E) (formula: $C_8H_{18}NO_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			18	8	1	8	1	

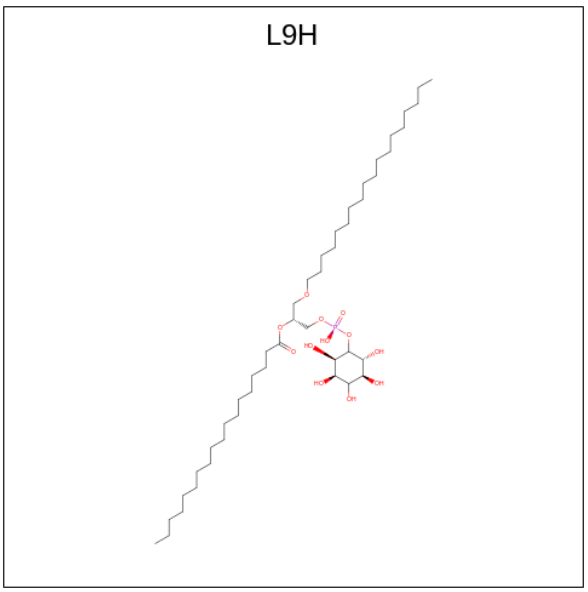
- Molecule 5 is 2-amino-2-deoxy-alpha-D-glucopyranose (three-letter code: PA1) (formula: $C_6H_{13}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			11	6	1	4	

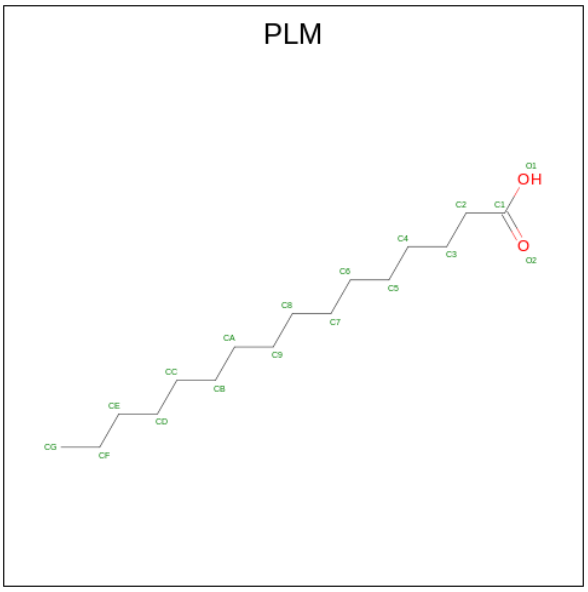
- Molecule 6 is [(2 {R})-1-octadecoxy-3-[oxidanyl-[(2 {R},3 {R},5 {S},6 {R})-2,3,4,5,6-pentakis(oxidanyl)cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] octadecanoate (three-letter code:

L9H) (formula: $C_{45}H_{89}O_{12}P$) (labeled as "Ligand of Interest" by depositor).



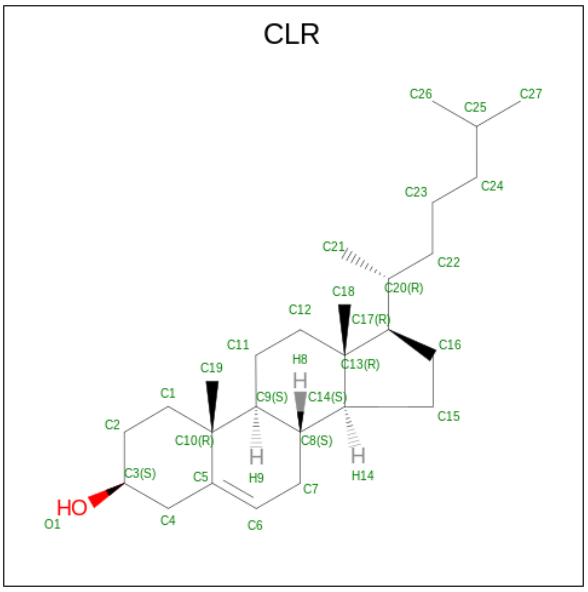
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	O	P	0
			58	45	12	1	

- Molecule 7 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



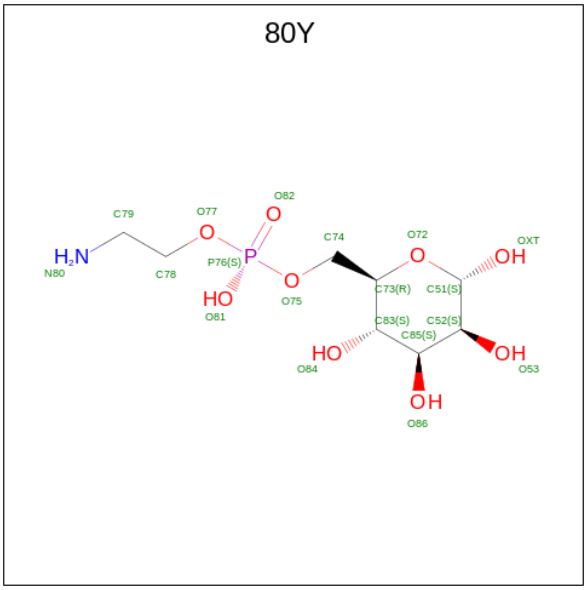
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			18	16	2	

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	A	1	28	27	1	0

- Molecule 9 is 2-azanylethyl [(2R,3S,4S,5S,6S)-3,4,5,6-tetrakis(oxidanyl)oxan-2-yl]methyl hydrogen phosphate (three-letter code: 80Y) (formula: $C_8H_{18}NO_9P$) (labeled as "Ligand of Interest" by depositor).



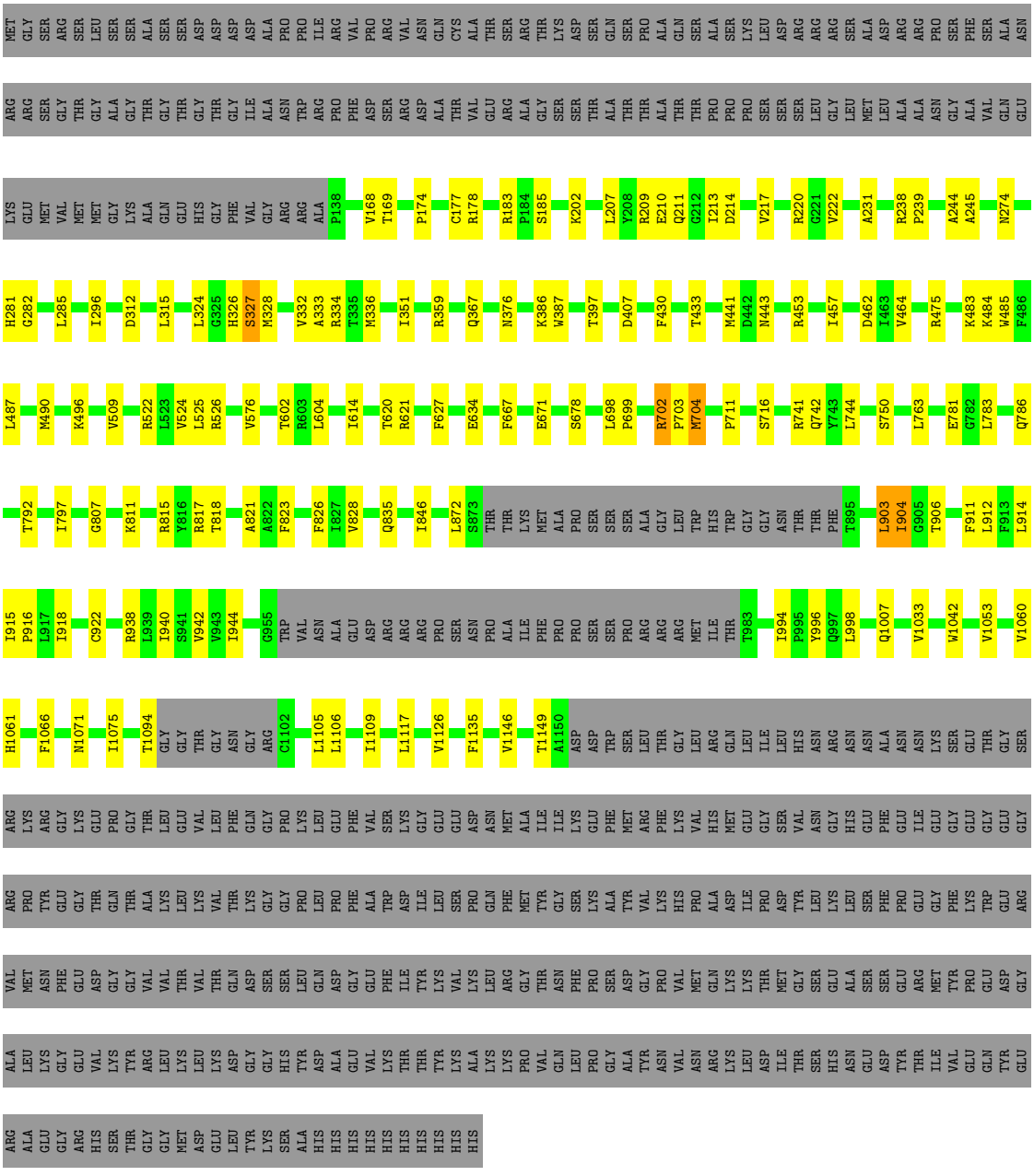
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	B	1	18	8	1	8	1	0

3 Residue-property plots (i)

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

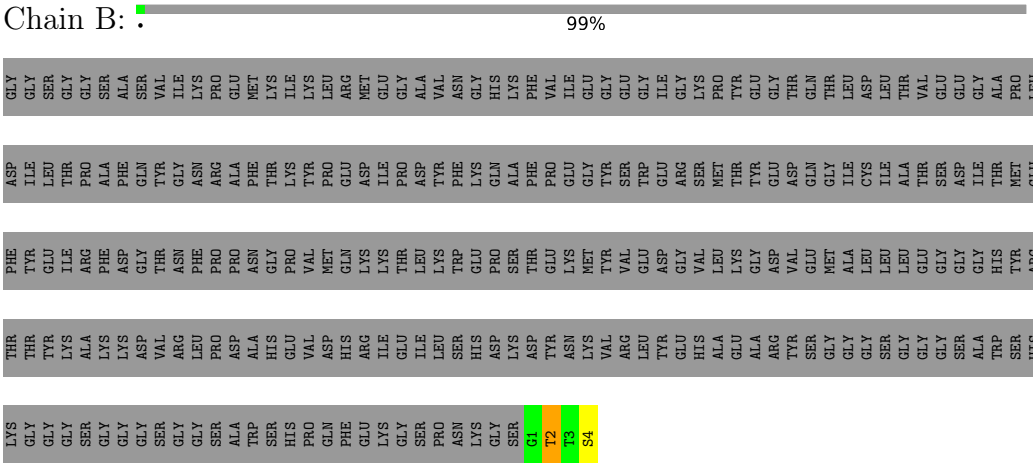
- Molecule 1: GPI inositol-deacylase,MCherry protein

Chain A:



• Molecule 2: Green fluorescent protein,Complement decay-accelerating factor

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	179980	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)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 05E, 80Y, L9H, PLM, PA1, CLR, MAN

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	0.43	0/7686	0.48	0/10499
2	B	0.52	0/23	0.69	0/30
All	All	0.43	0/7709	0.49	0/10529

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	7487	0	7480	88	0
2	B	24	0	24	2	0
3	A	22	0	19	0	0
4	A	18	0	0	0	0
5	A	11	0	10	1	0
6	A	58	0	0	0	0
7	A	18	0	31	4	0
8	A	28	0	46	1	0
9	B	18	0	0	0	0
All	All	7684	0	7610	89	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 (89) 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)
1:A:698:LEU:HB3	1:A:702:ARG:HD3	1.69	0.73
1:A:178:ARG:NH2	1:A:634:GLU:OE2	2.23	0.71
1:A:698:LEU:CB	1:A:702:ARG:HD3	2.22	0.69
1:A:324:LEU:HD22	1:A:351:ILE:HB	1.74	0.67
1:A:741:ARG:NH1	1:A:786:GLN:OE1	2.31	0.63
1:A:238:ARG:HB3	1:A:239:PRO:HD3	1.81	0.62
1:A:1146:VAL:O	1:A:1149:THR:HG22	1.99	0.62
1:A:244:ALA:HB2	1:A:457:ILE:HD12	1.83	0.59
1:A:522:ARG:NH1	1:A:671:GLU:OE2	2.35	0.58
1:A:818:THR:HA	7:A:1506:PLM:HD1	1.86	0.57
1:A:716:SER:OG	1:A:815:ARG:NH2	2.38	0.56
1:A:334:ARG:HH22	1:A:376:ASN:HA	1.69	0.56
1:A:183:ARG:HB3	1:A:211:GLN:CD	2.28	0.54
8:A:1507:CLR:H161	8:A:1507:CLR:H242	1.89	0.54
1:A:821:ALA:HB2	7:A:1506:PLM:HD2	1.90	0.53
1:A:285:LEU:HD12	1:A:332:VAL:HG22	1.91	0.53
1:A:509:VAL:O	1:A:602:THR:N	2.42	0.52
1:A:526:ARG:NH1	1:A:792:THR:OG1	2.41	0.52
1:A:1066:PHE:HB3	1:A:1071:ASN:OD1	2.09	0.52
1:A:213:ILE:HG21	1:A:245:ALA:HB1	1.92	0.52
1:A:281:HIS:ND1	1:A:1053:VAL:HG11	2.24	0.52
1:A:462:ASP:OD2	1:A:485:TRP:NE1	2.39	0.51
1:A:835:GLN:NE2	1:A:846:ILE:O	2.40	0.51
1:A:1117:LEU:HD13	1:A:1135:PHE:CD2	2.46	0.51
1:A:312:ASP:HB2	1:A:315:LEU:HG	1.92	0.51
1:A:678:SER:HB3	1:A:703:PRO:HG2	1.94	0.50
1:A:742:GLN:HE21	1:A:783:LEU:HD11	1.76	0.50
1:A:483:LYS:HG2	1:A:487:LEU:HD12	1.92	0.50
1:A:359:ARG:HH21	1:A:1126:VAL:HG12	1.77	0.49
1:A:397:THR:HG23	1:A:475:ARG:HG2	1.94	0.49
1:A:174:PRO:HB2	1:A:627:PHE:HZ	1.77	0.49
1:A:324:LEU:CD2	1:A:351:ILE:HB	2.42	0.49
1:A:994:ILE:HD12	1:A:998:LEU:HD23	1.95	0.49
1:A:702:ARG:NH1	1:A:797:ILE:HG22	2.27	0.49
1:A:823:PHE:HD2	1:A:922:CYS:SG	2.36	0.49
1:A:326:HIS:NE2	1:A:443:ASN:O	2.45	0.49
1:A:742:GLN:NE2	1:A:783:LEU:HD11	2.28	0.48
1:A:239:PRO:O	1:A:453:ARG:HD2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:SER:HB3	1:A:209:ARG:O	2.14	0.48
1:A:698:LEU:HB2	1:A:702:ARG:HD3	1.96	0.48
1:A:994:ILE:HG23	1:A:998:LEU:HD23	1.96	0.48
1:A:209:ARG:HA	1:A:214:ASP:OD2	2.15	0.47
1:A:699:PRO:O	1:A:702:ARG:HB2	2.14	0.47
1:A:823:PHE:O	1:A:826:PHE:HB3	2.15	0.47
1:A:490:MET:HG3	1:A:614:ILE:HD13	1.96	0.47
1:A:183:ARG:HG2	2:B:2:THR:HB	1.97	0.47
1:A:328:MET:O	1:A:332:VAL:HG23	2.15	0.46
1:A:217:VAL:O	1:A:217:VAL:HG13	2.16	0.46
1:A:744:LEU:HD11	1:A:763:LEU:HD12	1.96	0.46
1:A:296:ILE:HD12	1:A:336:MET:HE1	1.98	0.46
1:A:168:VAL:HG23	1:A:169:THR:HG23	1.99	0.45
1:A:386:LYS:HD2	1:A:387:TRP:CZ3	2.52	0.45
1:A:704:MET:HE3	1:A:704:MET:HB3	1.71	0.45
1:A:183:ARG:HB2	1:A:210:GLU:OE2	2.16	0.45
1:A:282:GLY:HA3	1:A:367:GLN:HB3	1.98	0.44
1:A:238:ARG:NH1	2:B:4:SER:O	2.51	0.44
1:A:333:ALA:O	1:A:336:MET:HB2	2.17	0.44
1:A:1060:VAL:O	1:A:1061:HIS:HB2	2.18	0.44
1:A:903:LEU:HB3	1:A:904:ILE:H	1.70	0.43
1:A:576:VAL:HA	1:A:604:LEU:HD23	2.00	0.43
1:A:807:GLY:O	1:A:811:LYS:HG2	2.18	0.43
1:A:823:PHE:CD2	1:A:918:ILE:HG22	2.53	0.43
1:A:496:LYS:HA	1:A:496:LYS:HD3	1.81	0.43
1:A:940:ILE:O	1:A:944:ILE:HG12	2.18	0.43
1:A:1105:LEU:O	1:A:1109:ILE:HG13	2.19	0.43
1:A:359:ARG:HH11	1:A:359:ARG:HG3	1.84	0.43
1:A:872:LEU:HD11	1:A:912:LEU:HD11	2.00	0.43
1:A:430:PHE:O	1:A:433:THR:HG22	2.19	0.43
1:A:711:PRO:HB3	1:A:781:GLU:HG3	2.01	0.42
1:A:202:LYS:O	1:A:274:ASN:ND2	2.53	0.42
1:A:911:PHE:HB3	1:A:914:LEU:HD12	2.00	0.42
1:A:525:LEU:O	1:A:667:PHE:HA	2.19	0.42
1:A:1094:THR:HG21	1:A:1106:LEU:HB2	2.01	0.42
1:A:327:SER:HB3	1:A:328:MET:H	1.66	0.42
1:A:828:VAL:HG21	1:A:1042:TRP:CD1	2.55	0.42
1:A:207:LEU:HD23	1:A:217:VAL:HG23	2.02	0.41
1:A:407:ASP:OD1	1:A:443:ASN:HB2	2.21	0.41
1:A:484:LYS:HA	1:A:484:LYS:HD3	1.79	0.41
1:A:938:ARG:O	1:A:942:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:GLN:NE2	1:A:1033:VAL:HG13	2.35	0.41
1:A:818:THR:HA	7:A:1506:PLM:CD	2.51	0.41
1:A:177:CYS:SG	1:A:441:MET:HG2	2.61	0.41
1:A:433:THR:HB	1:A:750:SER:H	1.85	0.41
1:A:522:ARG:HG3	1:A:524:VAL:HG23	2.02	0.41
1:A:915:ILE:HB	1:A:916:PRO:HD3	2.01	0.41
1:A:231:ALA:O	5:A:1504:PA1:N2	2.54	0.40
1:A:817:ARG:O	7:A:1506:PLM:HD1	2.21	0.40
1:A:222:VAL:HG21	1:A:464:VAL:HB	2.04	0.40
1:A:996:TYR:HB2	1:A:1075:ILE:HB	2.04	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	950/1447 (66%)	924 (97%)	26 (3%)	0	100	100
2	B	2/272 (1%)	2 (100%)	0	0	100	100
All	All	952/1719 (55%)	926 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	822/1249 (66%)	813 (99%)	9 (1%)	73 89
2	B	3/219 (1%)	2 (67%)	1 (33%)	0 0
All	All	825/1468 (56%)	815 (99%)	10 (1%)	72 87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	ARG
1	A	327	SER
1	A	620	THR
1	A	621	ARG
1	A	702	ARG
1	A	704	MET
1	A	903	LEU
1	A	904	ILE
1	A	906	THR
2	B	2	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	L9H	A	1505	5	58,58,58	0.39	0	67,69,69	0.52	1 (1%)
8	CLR	A	1507	-	31,31,31	0.32	0	48,48,48	0.62	0
3	MAN	A	1501	9	11,11,12	0.45	0	15,15,17	0.83	0
7	PLM	A	1506	-	17,17,17	0.52	0	17,17,17	0.49	0
9	80Y	B	101	2,3	18,18,19	0.64	0	24,25,27	1.01	1 (4%)
4	05E	A	1503	5,3	18,18,19	0.68	0	22,25,27	0.88	1 (4%)
5	PA1	A	1504	4,6	11,11,12	0.79	0	12,15,17	1.46	2 (16%)
3	MAN	A	1502	9,4	11,11,12	0.59	0	15,15,17	1.05	2 (13%)

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	L9H	A	1505	5	-	20/52/76/76	0/1/1/1
8	CLR	A	1507	-	-	5/10/68/68	0/4/4/4
3	MAN	A	1501	9	-	0/2/19/22	1/1/1/1
7	PLM	A	1506	-	-	7/15/15/15	-
9	80Y	B	101	2,3	-	10/11/28/31	0/1/1/1
4	05E	A	1503	5,3	-	4/12/29/32	0/1/1/1
5	PA1	A	1504	4,6	-	2/2/19/22	0/1/1/1
3	MAN	A	1502	9,4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	101	80Y	O53-C52-C85	-3.94	102.25	110.14
5	A	1504	PA1	C1-O5-C5	3.68	117.18	112.19
5	A	1504	PA1	C4-C3-C2	-2.95	106.38	111.37
6	A	1505	L9H	O10-C9-C7	-2.93	103.57	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1502	MAN	O2-C2-C3	-2.44	105.25	110.14
3	A	1502	MAN	O2-C2-C1	-2.43	104.18	109.15
4	A	1503	05E	C80-O97-C94	2.11	115.05	112.19

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1503	05E	O84-C85-C86-N87
4	A	1503	05E	C85-O84-P83-O88
9	B	101	80Y	O72-C73-C74-O75
9	B	101	80Y	C83-C73-C74-O75
9	B	101	80Y	C74-O75-P76-O77
9	B	101	80Y	C74-O75-P76-O81
9	B	101	80Y	C74-O75-P76-O82
6	A	1505	L9H	CD6-CD7-CD8-CD9
6	A	1505	L9H	CD8-CD9-CE0-CE1
5	A	1504	PA1	O5-C5-C6-O6
8	A	1507	CLR	C17-C20-C22-C23
5	A	1504	PA1	C4-C5-C6-O6
8	A	1507	CLR	C21-C20-C22-C23
8	A	1507	CLR	C20-C22-C23-C24
9	B	101	80Y	C78-O77-P76-O75
6	A	1505	L9H	CB1-CB2-CB3-CB4
6	A	1505	L9H	CD3-CD4-CD5-CD6
6	A	1505	L9H	CD5-CD6-CD7-CD8
6	A	1505	L9H	CD7-CD8-CD9-CE0
7	A	1506	PLM	C7-C8-C9-CA
6	A	1505	L9H	CB8-CB9-CC0-CC1
9	B	101	80Y	O77-C78-C79-N80
6	A	1505	L9H	OD1-CD2-CD3-CD4
6	A	1505	L9H	CE2-CE3-CE4-CE5
7	A	1506	PLM	C3-C4-C5-C6
8	A	1507	CLR	C23-C24-C25-C27
6	A	1505	L9H	CC4-CC5-CC6-CC7
6	A	1505	L9H	CC0-CC1-CC2-CC3
6	A	1505	L9H	CD4-CD5-CD6-CD7
7	A	1506	PLM	CD-CE-CF-CG
6	A	1505	L9H	CE5-CE6-CE7-CE8
7	A	1506	PLM	C9-CA-CB-CC
6	A	1505	L9H	CB6-CB7-CB8-CB9
9	B	101	80Y	C73-C74-O75-P76

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Mol	Chain	Res	Type	Atoms
4	A	1503	05E	C85-O84-P83-O82
8	A	1507	CLR	C23-C24-C25-C26
6	A	1505	L9H	CE6-CE7-CE8-CE9
6	A	1505	L9H	CB4-CB5-CB6-CB7
6	A	1505	L9H	CA9-CD0-OD1-CD2
7	A	1506	PLM	C6-C7-C8-C9
4	A	1503	05E	C85-O84-P83-O89
9	B	101	80Y	C78-O77-P76-O81
9	B	101	80Y	C78-O77-P76-O82
6	A	1505	L9H	OA7-CA8-CA9-CD0
6	A	1505	L9H	OA7-CA8-CA9-OB0
6	A	1505	L9H	CC3-CC4-CC5-CC6
7	A	1506	PLM	C5-C6-C7-C8
7	A	1506	PLM	CA-CB-CC-CD

All (1) ring outliers are listed below:

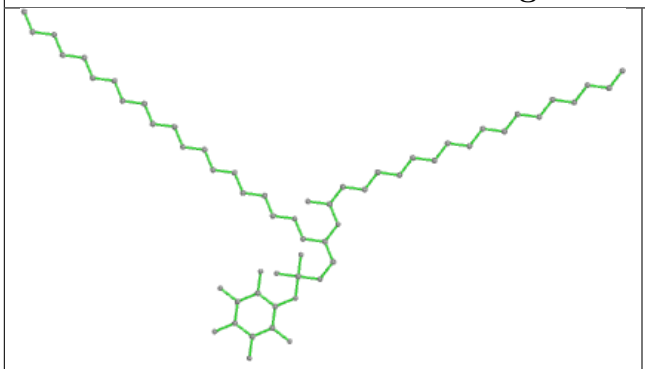
Mol	Chain	Res	Type	Atoms
3	A	1501	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 6 short contacts:

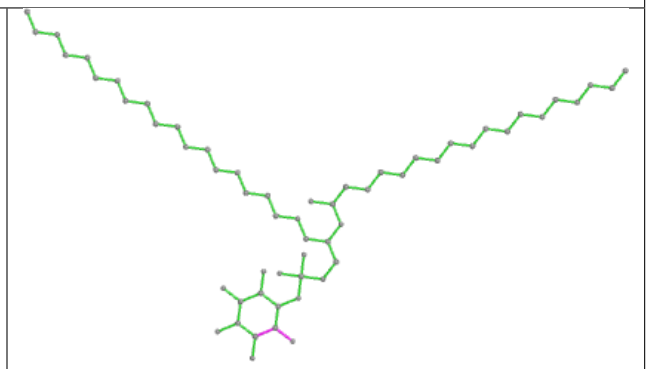
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1507	CLR	1	0
7	A	1506	PLM	4	0
5	A	1504	PA1	1	0

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.

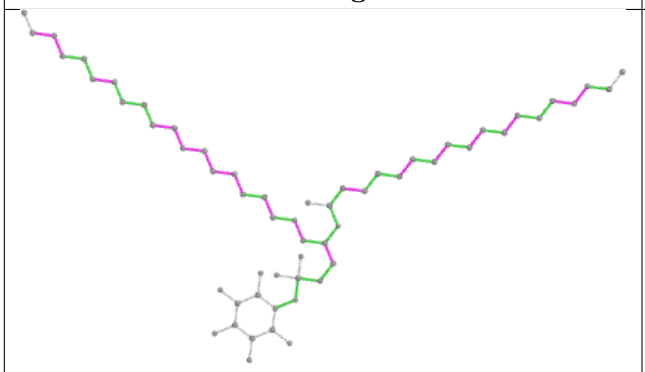
Ligand L9H A 1505



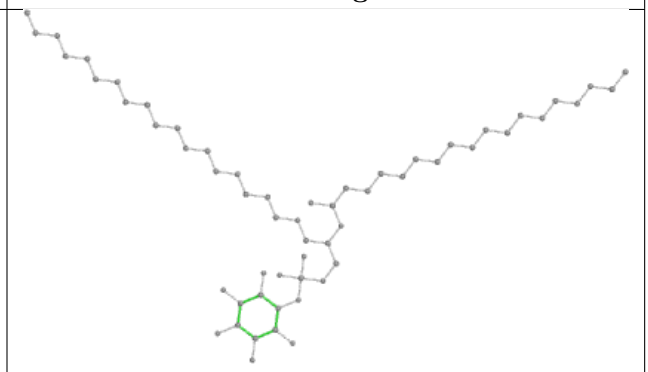
Bond lengths



Bond angles

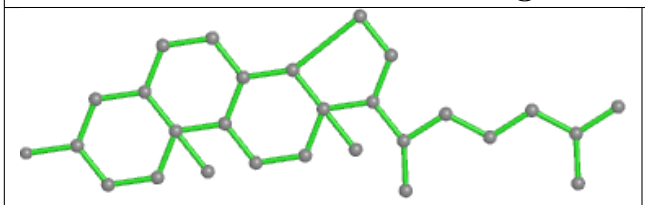


Torsions

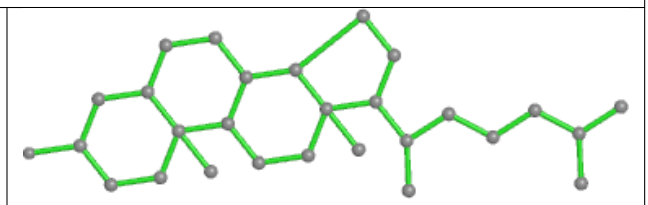


Rings

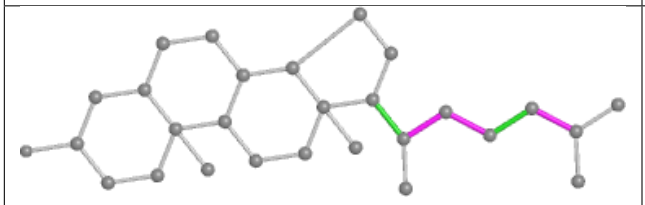
Ligand CLR A 1507



Bond lengths



Bond angles



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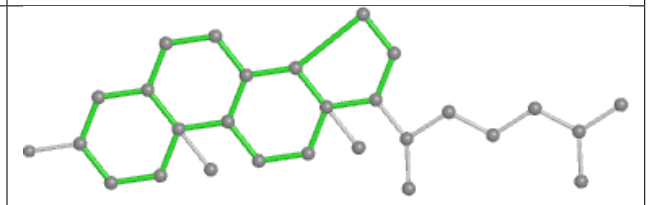
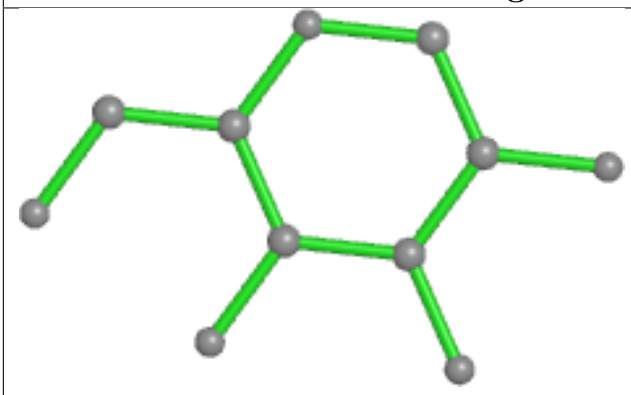
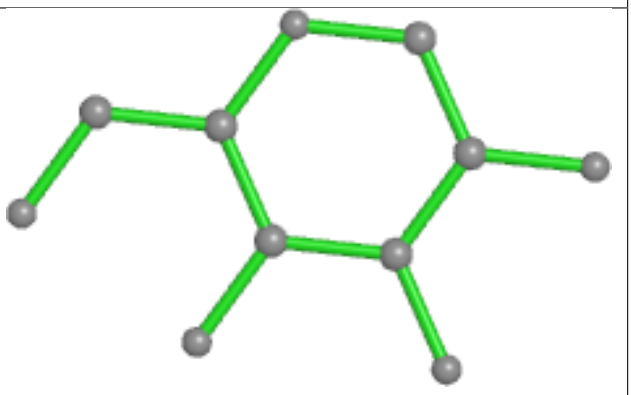


Rings

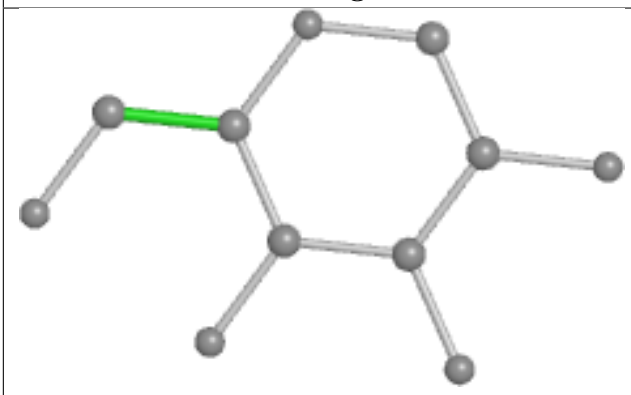
Ligand MAN A 1501



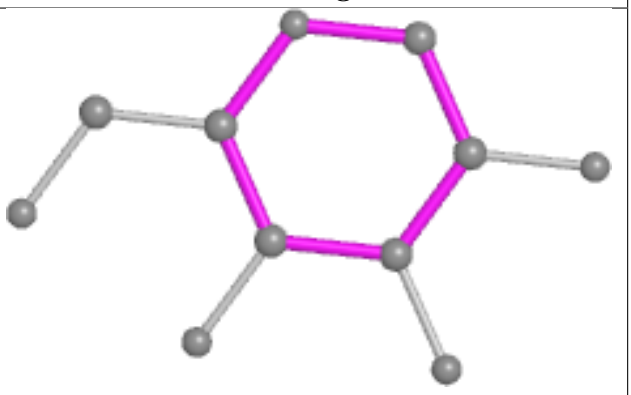
Bond lengths



Bond angles

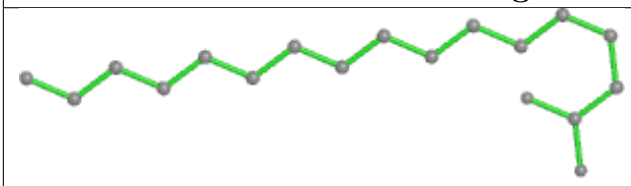


Torsions

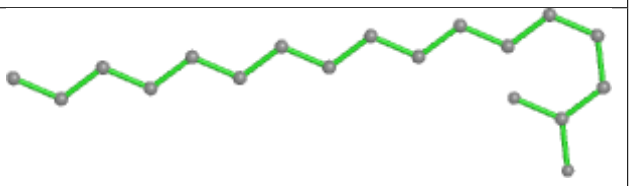


Rings

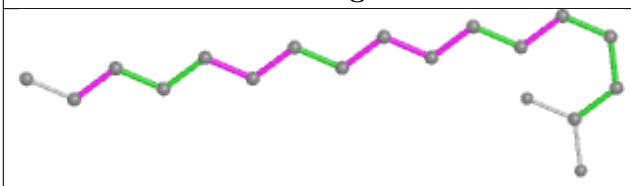
Ligand PLM A 1506



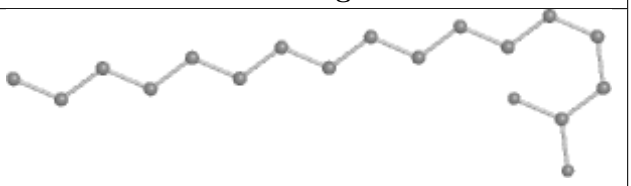
Bond lengths



Bond angles

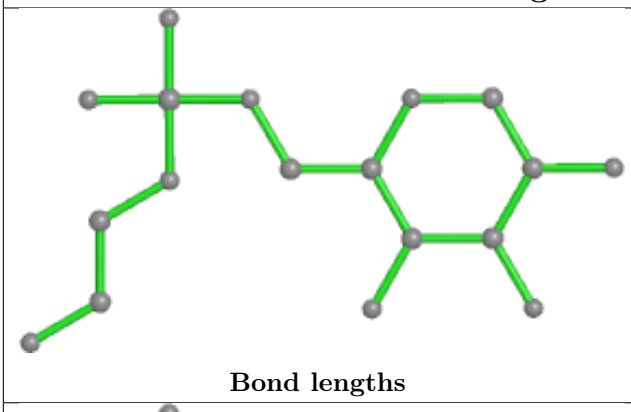


Torsions



Rings

Ligand 80Y B 101



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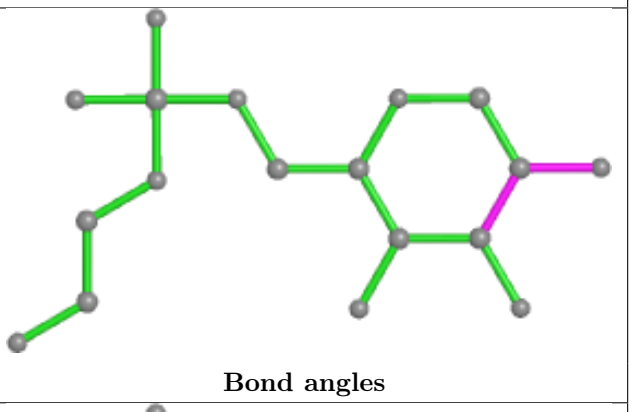
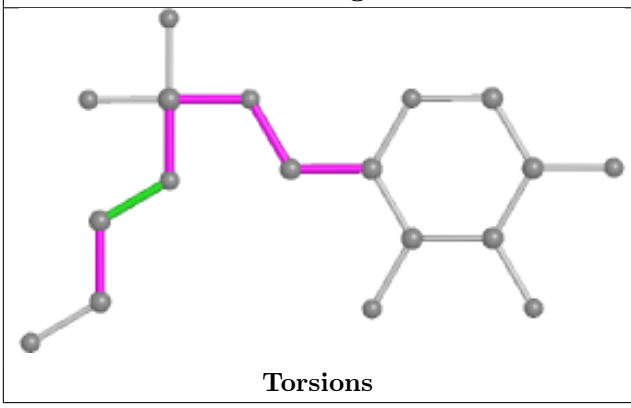


Bond angles



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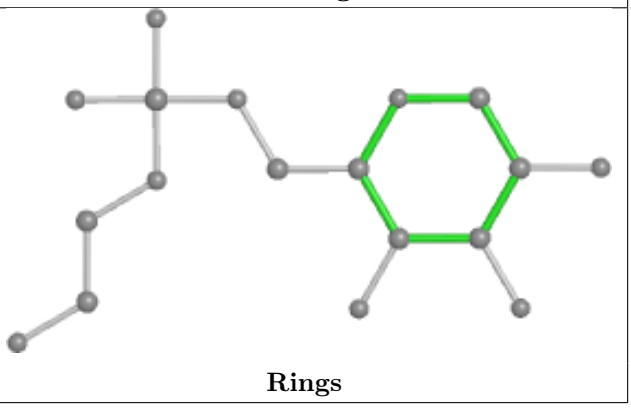
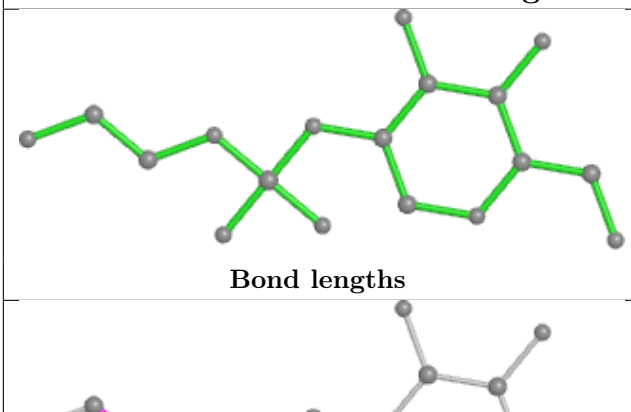


Rings

Ligand 05E A 1503



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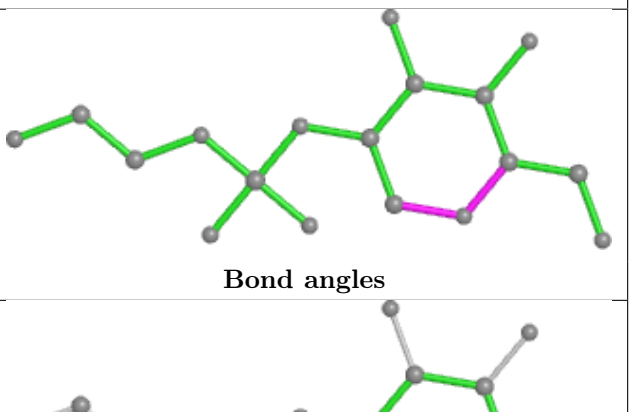

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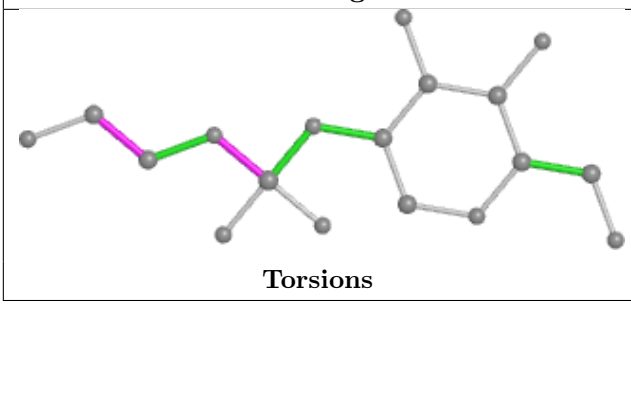

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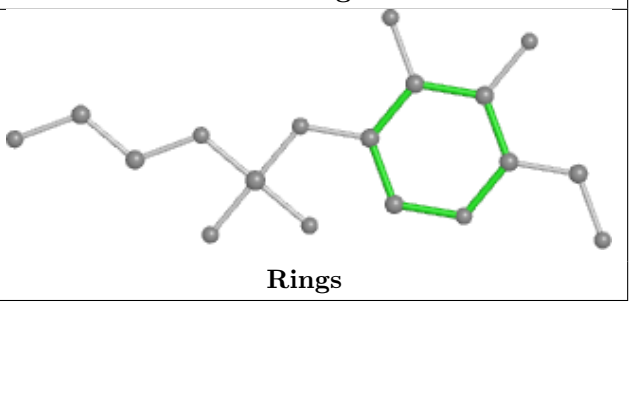
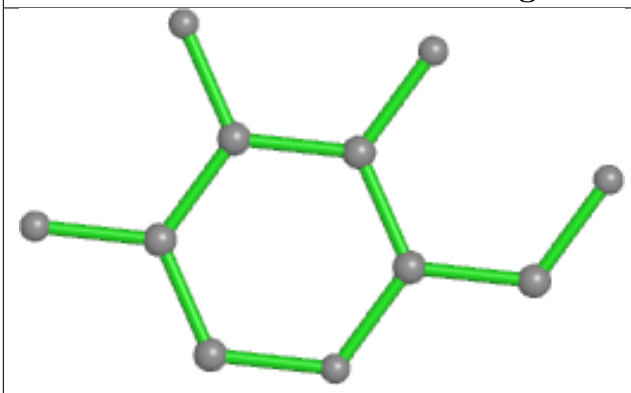
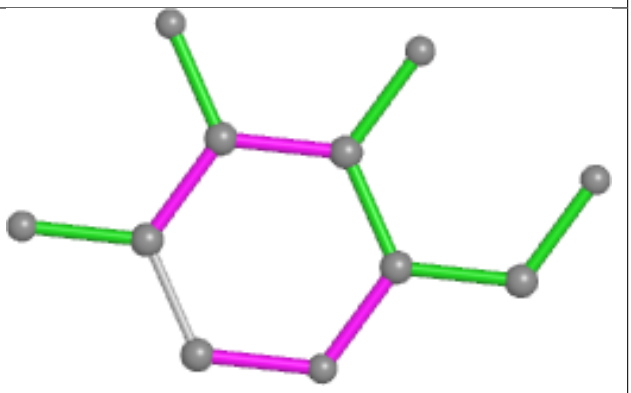


Rings

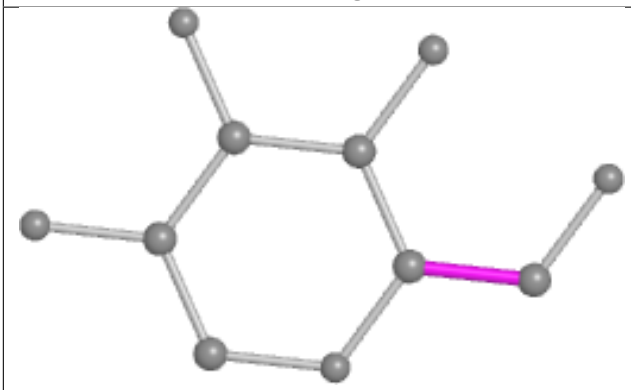
Ligand PA1 A 1504



Bond lengths



Bond angles



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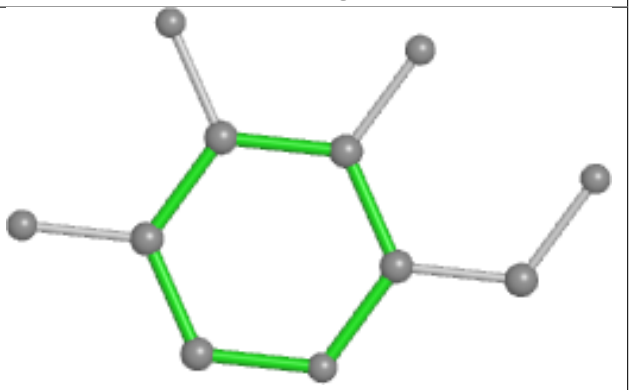
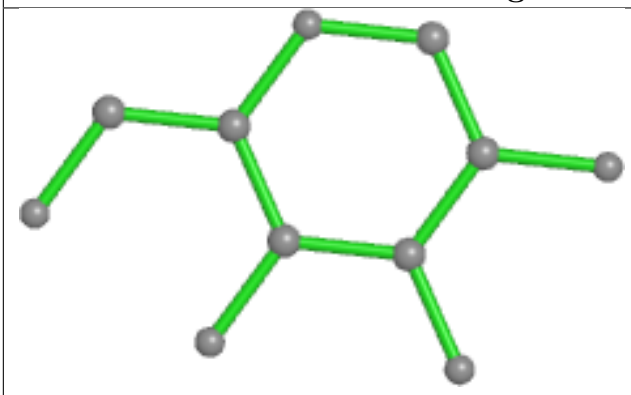
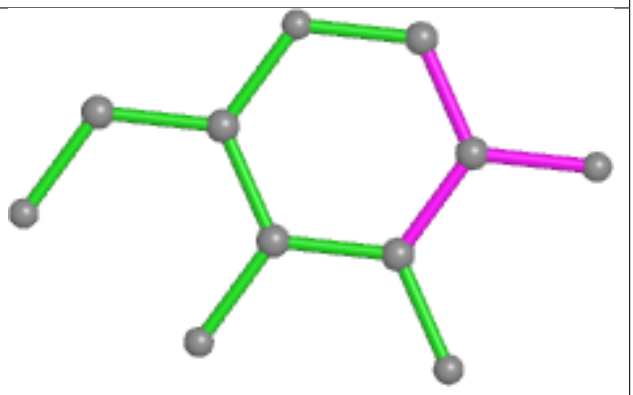


Rings

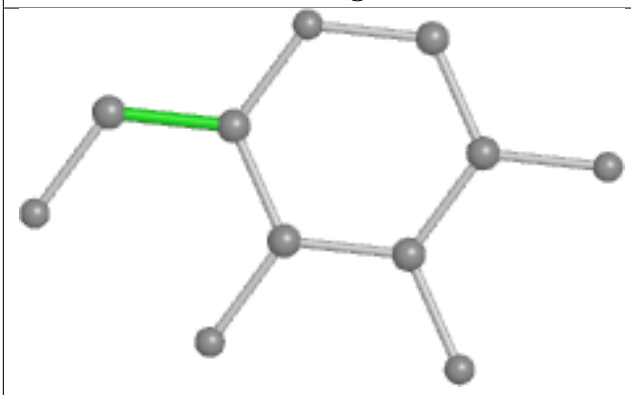
Ligand MAN A 1502



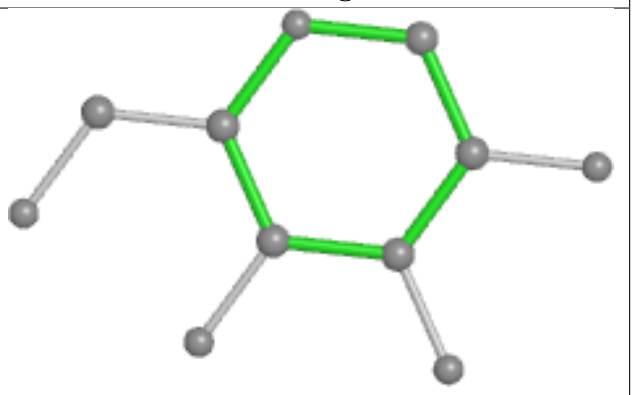
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.