



wwPDB EM Model Validation Summary Report ⓘ

Apr 20, 2020 – 02:09 PM EDT

PDB ID : 6LCP
EMDB ID : EMD-0872
Title : Cryo-EM structure of Dnf1 from Chaetomium thermophilum in the E2P state
Authors : He, Y.; Xu, J.; Wu, X.; Li, L.
Deposited on : 2019-11-19
Resolution : 3.48 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

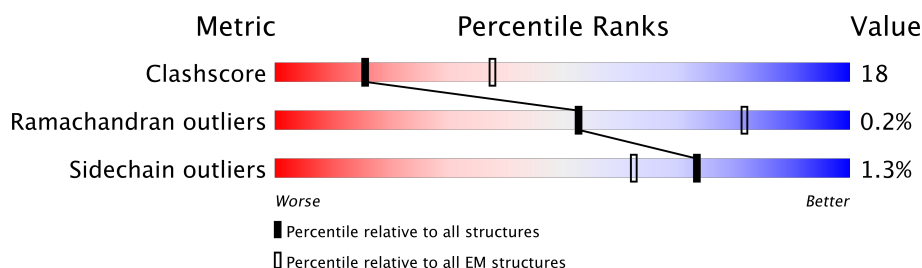
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.48 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1555	
2	B	407	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BEF	A	2002	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12421 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 Phospholipid-transporting ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1140	Total	C	N	O	S	0	0
			9082	5832	1535	1664	51		

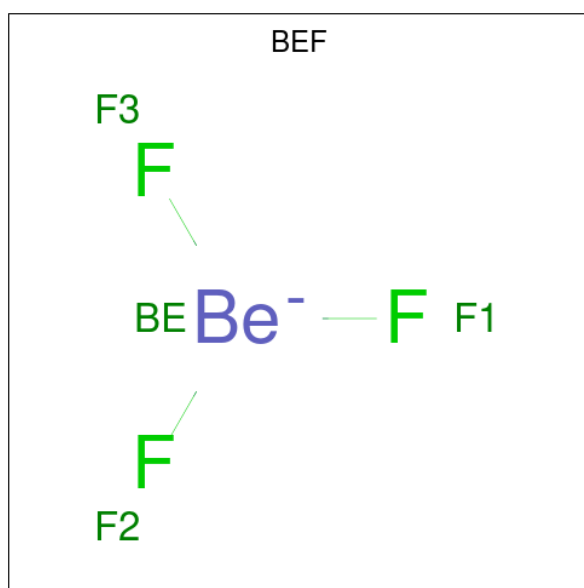
- Molecule 2 is a protein called Cdc50.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	376	Total	C	N	O	S	0	0
			3061	1979	512	558	12		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

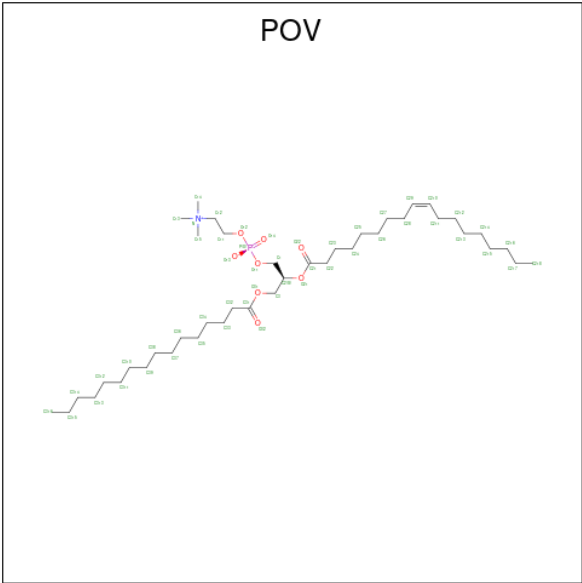
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



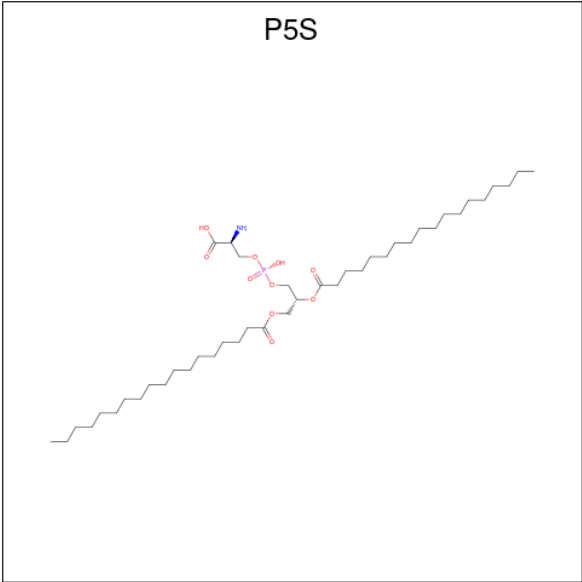
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	Be	F	0
			4	1	3	

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



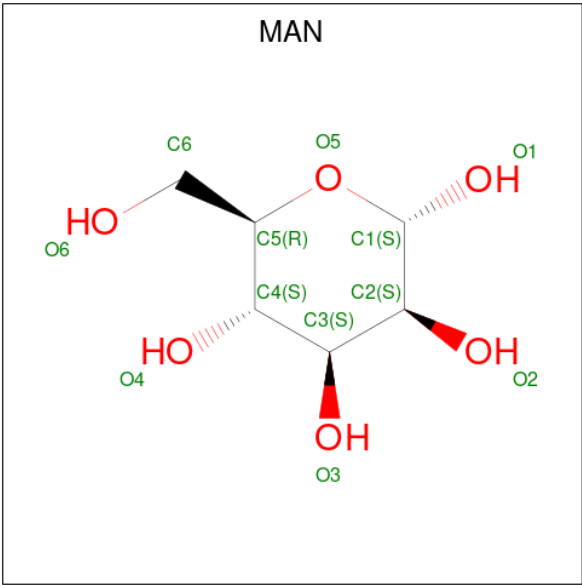
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			66	46	2	16	2	
5	A	1	Total	C	N	O	P	0
			66	46	2	16	2	

- Molecule 6 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-se rine (three-letter code: P5S) (formula: C₄₂H₈₂NO₁₀P).



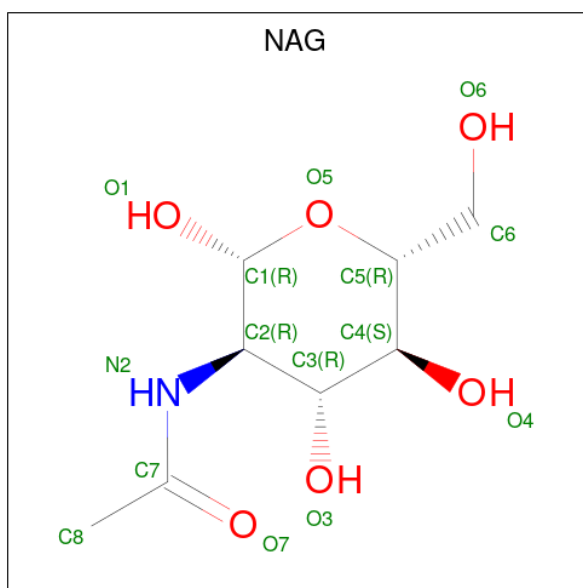
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	40	28	1	10	1	0

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



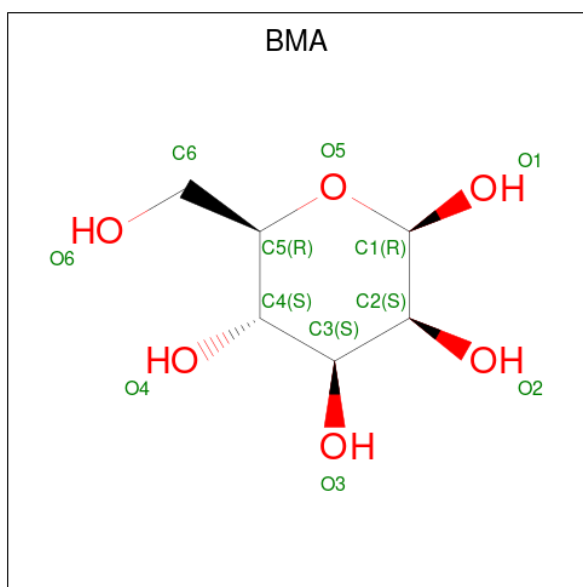
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	A	1	22	12	10	0
			22	12	10	
7	B	1	11	6	5	0
			11	6	5	

- Molecule 8 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			112	64	8	40	
8	B	1	Total	C	N	O	0
			112	64	8	40	
8	B	1	Total	C	N	O	0
			112	64	8	40	
8	B	1	Total	C	N	O	0
			112	64	8	40	
8	B	1	Total	C	N	O	0
			112	64	8	40	
8	B	1	Total	C	N	O	0
			112	64	8	40	
8	B	1	Total	C	N	O	0
			112	64	8	40	

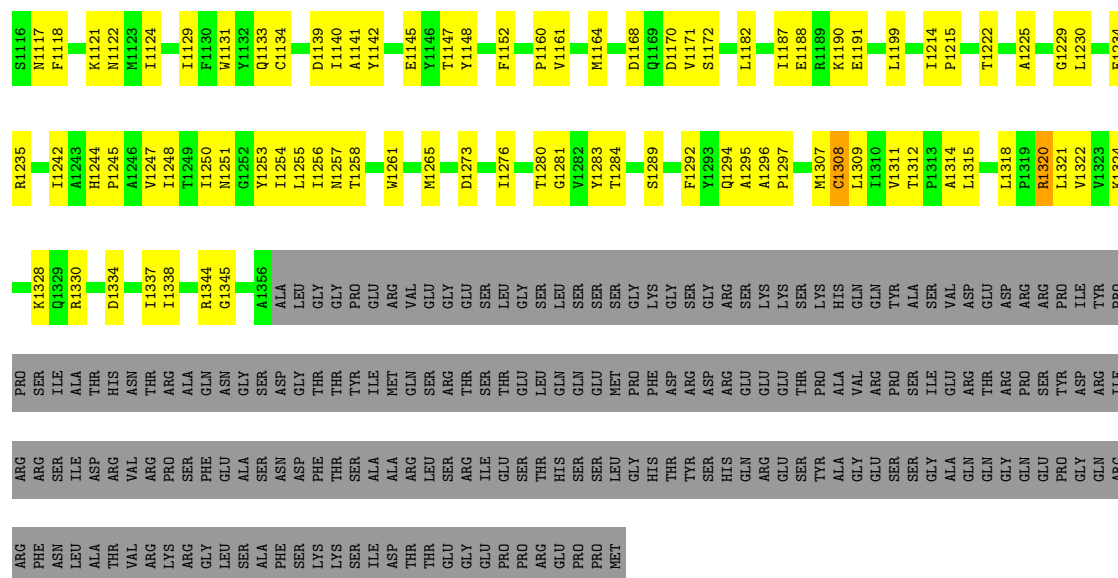
- Molecule 9 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



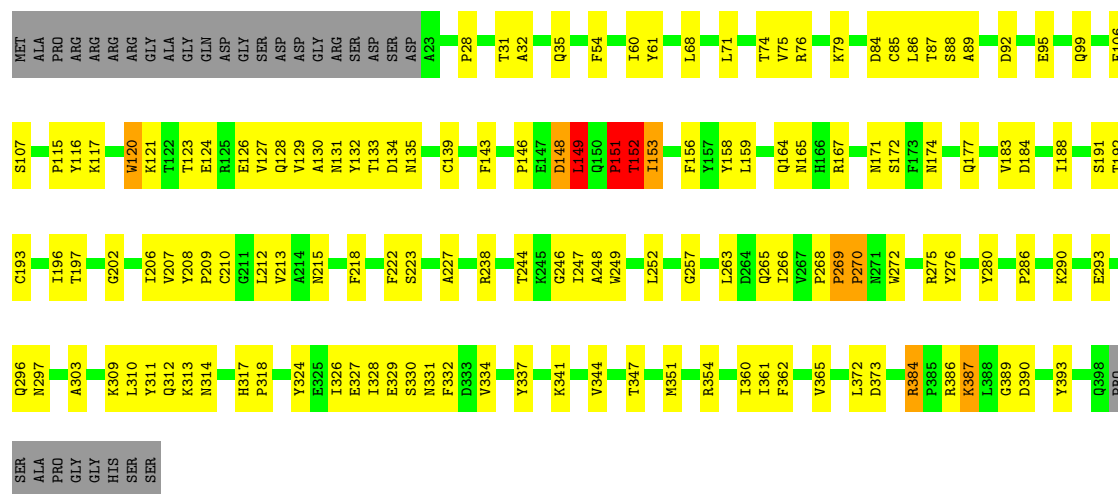
Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	C	O	0
			22	12	10	
9	B	1	Total	C	O	0
			22	12	10	

- Molecule 1: Phospholipid-transporting ATPase





- Molecule 2: Cdc50



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	249694	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (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: MG, BMA, NAG, POV, BEF, P5S, 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	0.39	0/9281	0.52	2/12589 (0.0%)
2	B	0.38	0/3154	0.55	3/4300 (0.1%)
All	All	0.39	0/12435	0.53	5/16889 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	151	PRO	CA-C-N	-5.92	104.18	117.20
1	A	1320	ARG	CB-CA-C	-5.68	99.03	110.40
1	A	527	GLY	N-CA-C	5.62	127.16	113.10
2	B	149	LEU	CA-CB-CG	5.50	127.94	115.30
2	B	151	PRO	C-N-CA	5.46	135.35	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9082	0	9056	328	0
2	B	3061	0	2980	122	0
3	A	1	0	0	0	0
4	A	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	66	0	80	2	0
6	A	40	0	46	5	0
7	A	22	0	19	5	0
7	B	11	0	10	0	0
8	B	112	0	99	8	0
9	B	22	0	19	3	0
All	All	12421	0	12309	435	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 18.

The worst 5 of 435 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:114:ARG:NH2	1:A:476:ILE:CD1	1.79	1.44
1:A:114:ARG:NH2	1:A:476:ILE:HD11	1.45	1.20
7:A:2006:MAN:H5	9:B:507:BMA:O6	1.51	1.11
1:A:114:ARG:NH2	1:A:476:ILE:HD12	1.49	1.05
1:A:114:ARG:HH22	1:A:476:ILE:CD1	1.68	1.02

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	1132/1555 (73%)	1026 (91%)	106 (9%)	0	100	100
2	B	374/407 (92%)	329 (88%)	42 (11%)	3 (1%)	21	62
All	All	1506/1962 (77%)	1355 (90%)	148 (10%)	3 (0%)	53	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	270	PRO
2	B	152	THR
2	B	269	PRO

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	973/1329 (73%)	964 (99%)	9 (1%)	81	92
2	B	335/357 (94%)	327 (98%)	8 (2%)	52	79
All	All	1308/1686 (78%)	1291 (99%)	17 (1%)	73	88

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	955	GLU
1	A	1308	CYS
2	B	152	THR
1	A	953	SER
2	B	153	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	698	ASN
1	A	717	HIS
2	B	271	ASN
1	A	704	GLN
1	A	974	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	B	509	2	14,14,15	0.24	0	17,19,21	0.36	0
8	NAG	B	502	8,2	14,14,15	0.24	0	17,19,21	0.37	0
9	BMA	B	504	8	11,11,12	0.55	0	15,15,17	0.92	0
6	P5S	A	2005	-	36,39,53	1.09	2 (5%)	38,46,60	1.20	3 (7%)
8	NAG	B	501	2	14,14,15	0.58	0	17,19,21	0.67	1 (5%)
5	POV	A	2004	-	32,32,51	1.18	2 (6%)	38,40,59	1.10	2 (5%)
8	NAG	B	505	8,2	14,14,15	0.22	0	17,19,21	0.94	1 (5%)
7	MAN	B	508	9	11,11,12	0.24	0	15,15,17	0.59	0
7	MAN	A	2006	7	11,11,12	0.24	0	15,15,17	0.57	0
9	BMA	B	507	8,7	11,11,12	0.22	0	15,15,17	0.63	0
5	POV	A	2003	-	32,32,51	1.18	2 (6%)	38,40,59	1.20	3 (7%)
7	MAN	A	2007	7	11,11,12	0.24	0	15,15,17	0.58	0
8	NAG	B	503	9,8	14,14,15	0.18	0	17,19,21	0.56	0
8	NAG	B	510	8,2	14,14,15	0.28	0	17,19,21	0.57	0
8	NAG	B	511	8	14,14,15	0.28	0	17,19,21	0.59	0
4	BEF	A	2002	-	0,3,3	0.00	-	-	-	-
8	NAG	B	506	9,8	14,14,15	0.26	0	17,19,21	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	509	2	-	0/6/23/26	0/1/1/1
8	NAG	B	502	8,2	-	0/6/23/26	0/1/1/1
9	BMA	B	504	8	-	2/2/19/22	0/1/1/1
6	P5S	A	2005	-	-	9/41/45/59	-
8	NAG	B	501	2	-	3/6/23/26	0/1/1/1
5	POV	A	2004	-	-	9/36/36/55	-
8	NAG	B	505	8,2	-	0/6/23/26	0/1/1/1
7	MAN	B	508	9	-	0/2/19/22	0/1/1/1
7	MAN	A	2006	7	-	0/2/19/22	0/1/1/1
9	BMA	B	507	8,7	-	0/2/19/22	0/1/1/1
5	POV	A	2003	-	-	12/36/36/55	-
7	MAN	A	2007	7	-	1/2/19/22	0/1/1/1
8	NAG	B	503	9,8	-	2/6/23/26	0/1/1/1
8	NAG	B	510	8,2	-	1/6/23/26	0/1/1/1
8	NAG	B	511	8	-	0/6/23/26	0/1/1/1
8	NAG	B	506	9,8	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2003	POV	O31-C31	4.28	1.45	1.33
6	A	2005	P5S	O19-C17	4.17	1.45	1.33
6	A	2005	P5S	O37-C38	4.14	1.46	1.34
5	A	2004	POV	O31-C31	4.12	1.45	1.33
5	A	2004	POV	O21-C21	4.02	1.45	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2005	P5S	O37-C38-C39	4.11	120.37	111.50
5	A	2004	POV	O21-C21-C22	3.91	119.93	111.50
5	A	2003	POV	O21-C21-C22	3.65	119.37	111.50
8	B	505	NAG	C1-O5-C5	3.20	116.53	112.19
5	A	2003	POV	O31-C31-C32	2.78	120.64	111.91

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2004	POV	C1-O11-P-O12

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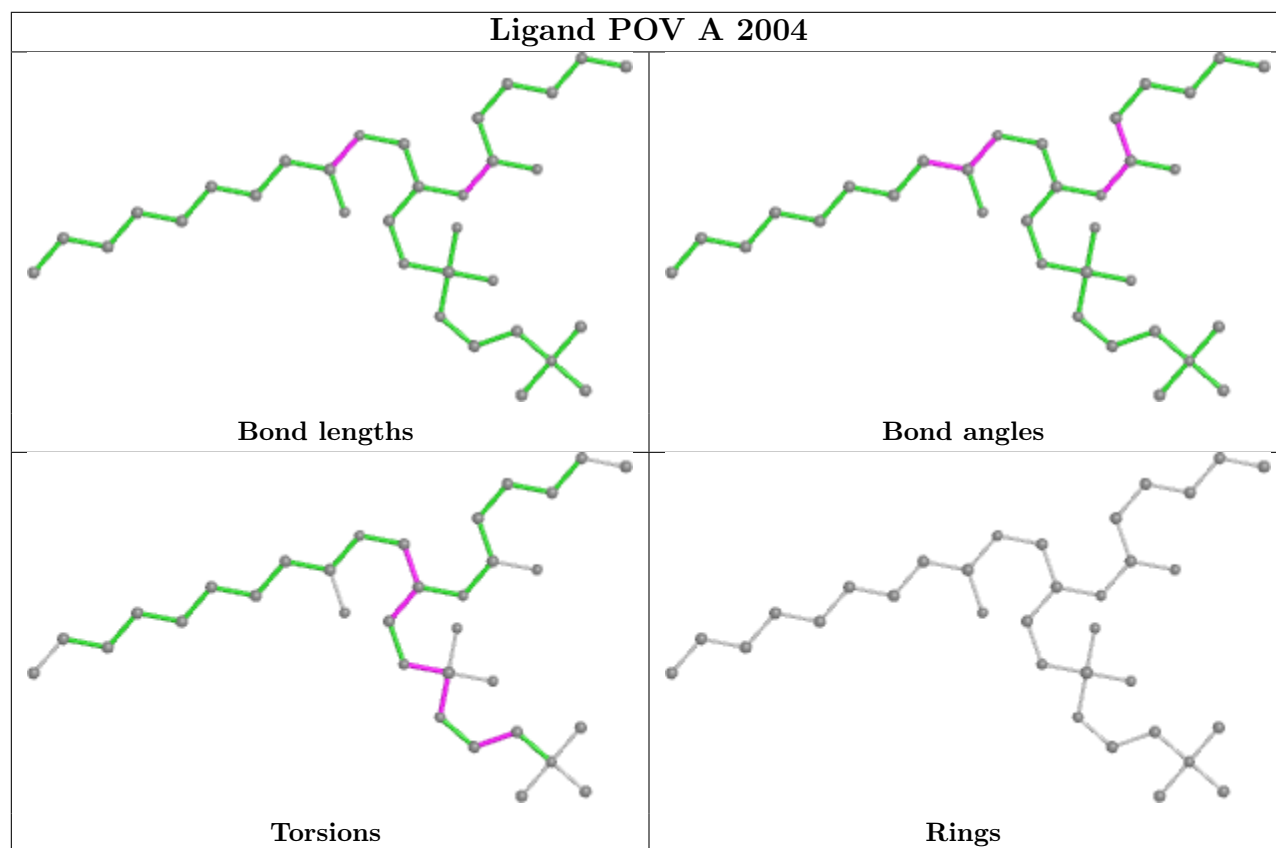
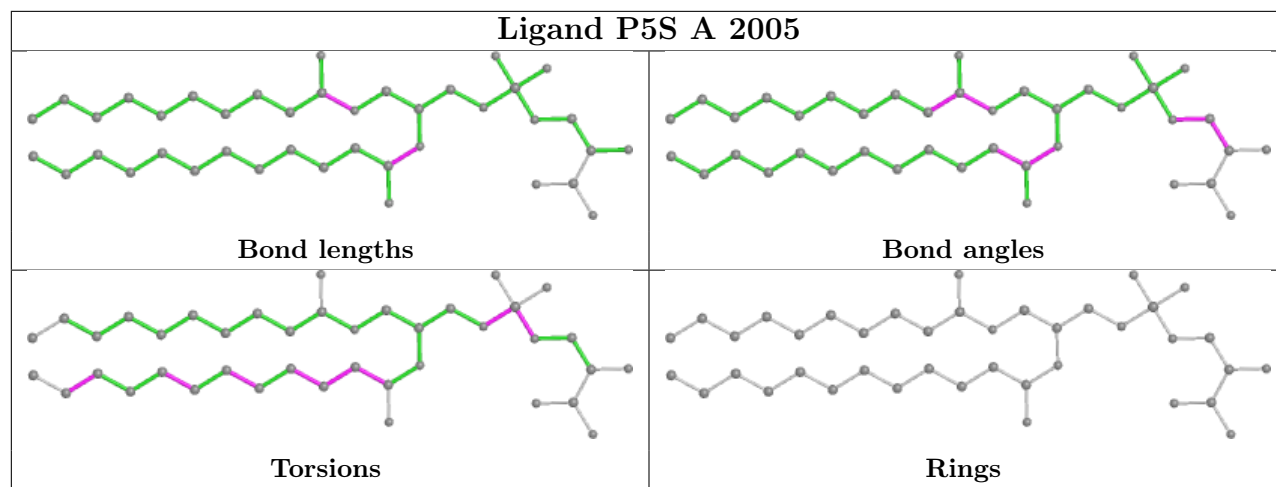
Mol	Chain	Res	Type	Atoms
5	A	2004	POV	C11-O12-P-O13
5	A	2004	POV	O12-C11-C12-N
5	A	2003	POV	C11-O12-P-O14
5	A	2003	POV	C22-C21-O21-C2

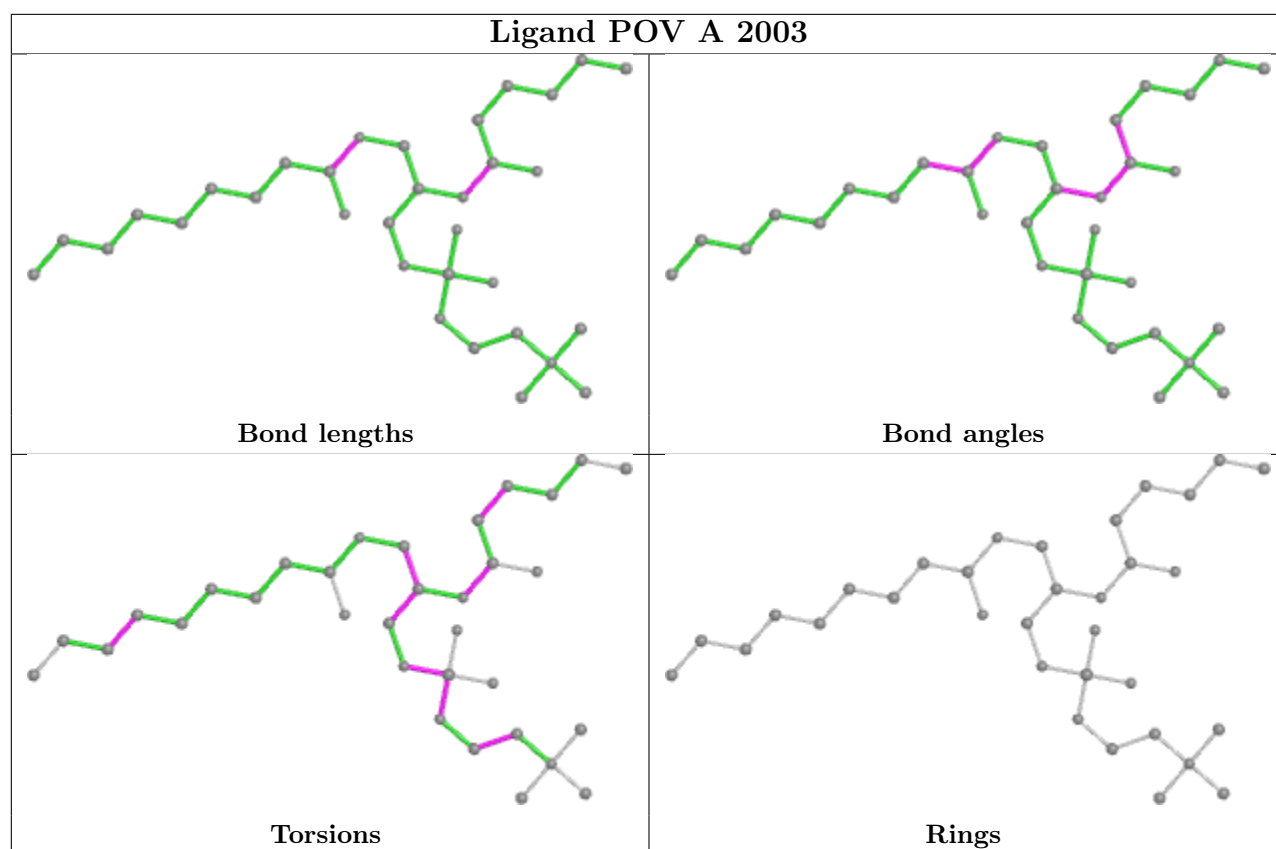
There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2005	P5S	5	0
8	B	501	NAG	3	0
5	A	2004	POV	1	0
8	B	505	NAG	3	0
7	A	2006	MAN	4	0
9	B	507	BMA	3	0
5	A	2003	POV	1	0
7	A	2007	MAN	2	0
8	B	503	NAG	1	0
8	B	510	NAG	1	0
8	B	506	NAG	1	0

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





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.