Full wwPDB EM Validation Report ⓘ

Apr 7, 2024 – 12:06 AM JST

PDB ID	:	8J8K
EMDB ID	:	EMD-36072
Title	:	Membrane bound PRTase, C3 symmetry, acceptor bound
Authors	:	Wu, F.Y.; Gao, S.; Zhang, L.; Rao, Z.H.
Deposited on	:	2023-05-01
Resolution	:	3.36 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:

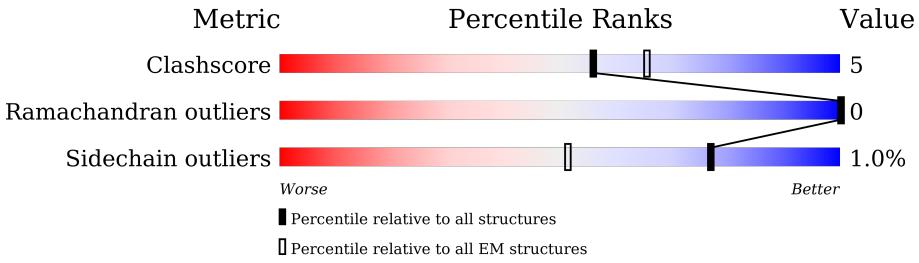
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.36 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	302	82% 12% 6%
1	B	302	84% 11% 6%
1	C	302	83% 11% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6489 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 Decaprenyl-phosphate phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	285	Total	C	N	O	S	0	0
			2133	1405	351	367	10		
1	B	285	Total	C	N	O	S	0	0
			2133	1405	351	367	10		
1	C	285	Total	C	N	O	S	0	0
			2133	1405	351	367	10		

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P9WFR5
A	2	SER	-	expression tag	UNP P9WFR5
A	3	GLU	-	expression tag	UNP P9WFR5
A	4	ASP	-	expression tag	UNP P9WFR5
A	5	VAL	-	expression tag	UNP P9WFR5
A	6	VAL	-	expression tag	UNP P9WFR5
A	7	THR	-	expression tag	UNP P9WFR5
A	8	GLN	-	expression tag	UNP P9WFR5
A	9	PRO	-	expression tag	UNP P9WFR5
A	10	PRO	-	expression tag	UNP P9WFR5
A	11	ALA	-	expression tag	UNP P9WFR5
A	12	ASN	-	expression tag	UNP P9WFR5
A	13	LEU	-	expression tag	UNP P9WFR5
A	14	VAL	-	expression tag	UNP P9WFR5
A	15	ALA	-	expression tag	UNP P9WFR5
A	16	GLY	-	expression tag	UNP P9WFR5
A	17	VAL	-	expression tag	UNP P9WFR5
A	79	ALA	GLU	engineered mutation	UNP P9WFR5
A	81	ALA	ASP	engineered mutation	UNP P9WFR5
A	82	ALA	ARG	engineered mutation	UNP P9WFR5
A	83	ALA	GLU	engineered mutation	UNP P9WFR5
A	84	ALA	HIS	engineered mutation	UNP P9WFR5
A	85	ALA	PRO	engineered mutation	UNP P9WFR5
A	86	ALA	THR	engineered mutation	UNP P9WFR5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ALA	LYS	engineered mutation	UNP P9WFR5
A	88	ALA	ARG	engineered mutation	UNP P9WFR5
A	89	ALA	PHE	engineered mutation	UNP P9WFR5
A	90	ALA	ARG	engineered mutation	UNP P9WFR5
A	91	ALA	PRO	engineered mutation	UNP P9WFR5
A	92	ALA	ILE	engineered mutation	UNP P9WFR5
B	1	MET	-	initiating methionine	UNP P9WFR5
B	2	SER	-	expression tag	UNP P9WFR5
B	3	GLU	-	expression tag	UNP P9WFR5
B	4	ASP	-	expression tag	UNP P9WFR5
B	5	VAL	-	expression tag	UNP P9WFR5
B	6	VAL	-	expression tag	UNP P9WFR5
B	7	THR	-	expression tag	UNP P9WFR5
B	8	GLN	-	expression tag	UNP P9WFR5
B	9	PRO	-	expression tag	UNP P9WFR5
B	10	PRO	-	expression tag	UNP P9WFR5
B	11	ALA	-	expression tag	UNP P9WFR5
B	12	ASN	-	expression tag	UNP P9WFR5
B	13	LEU	-	expression tag	UNP P9WFR5
B	14	VAL	-	expression tag	UNP P9WFR5
B	15	ALA	-	expression tag	UNP P9WFR5
B	16	GLY	-	expression tag	UNP P9WFR5
B	17	VAL	-	expression tag	UNP P9WFR5
B	79	ALA	GLU	engineered mutation	UNP P9WFR5
B	81	ALA	ASP	engineered mutation	UNP P9WFR5
B	82	ALA	ARG	engineered mutation	UNP P9WFR5
B	83	ALA	GLU	engineered mutation	UNP P9WFR5
B	84	ALA	HIS	engineered mutation	UNP P9WFR5
B	85	ALA	PRO	engineered mutation	UNP P9WFR5
B	86	ALA	THR	engineered mutation	UNP P9WFR5
B	87	ALA	LYS	engineered mutation	UNP P9WFR5
B	88	ALA	ARG	engineered mutation	UNP P9WFR5
B	89	ALA	PHE	engineered mutation	UNP P9WFR5
B	90	ALA	ARG	engineered mutation	UNP P9WFR5
B	91	ALA	PRO	engineered mutation	UNP P9WFR5
B	92	ALA	ILE	engineered mutation	UNP P9WFR5
C	1	MET	-	initiating methionine	UNP P9WFR5
C	2	SER	-	expression tag	UNP P9WFR5
C	3	GLU	-	expression tag	UNP P9WFR5
C	4	ASP	-	expression tag	UNP P9WFR5
C	5	VAL	-	expression tag	UNP P9WFR5
C	6	VAL	-	expression tag	UNP P9WFR5

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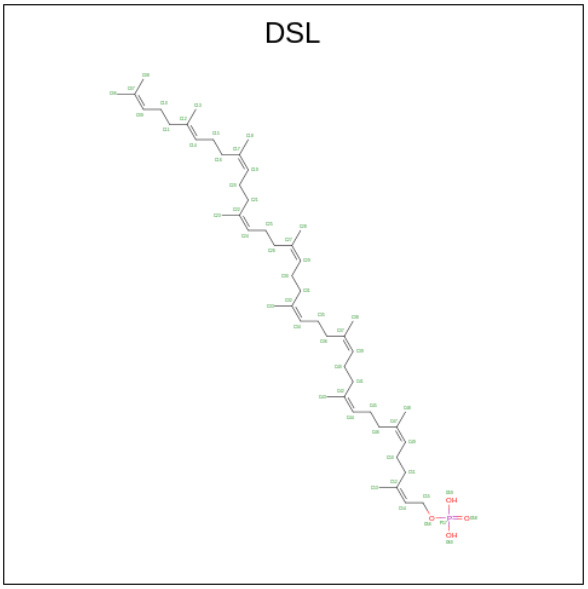
Chain	Residue	Modelled	Actual	Comment	Reference
C	7	THR	-	expression tag	UNP P9WFR5
C	8	GLN	-	expression tag	UNP P9WFR5
C	9	PRO	-	expression tag	UNP P9WFR5
C	10	PRO	-	expression tag	UNP P9WFR5
C	11	ALA	-	expression tag	UNP P9WFR5
C	12	ASN	-	expression tag	UNP P9WFR5
C	13	LEU	-	expression tag	UNP P9WFR5
C	14	VAL	-	expression tag	UNP P9WFR5
C	15	ALA	-	expression tag	UNP P9WFR5
C	16	GLY	-	expression tag	UNP P9WFR5
C	17	VAL	-	expression tag	UNP P9WFR5
C	79	ALA	GLU	engineered mutation	UNP P9WFR5
C	81	ALA	ASP	engineered mutation	UNP P9WFR5
C	82	ALA	ARG	engineered mutation	UNP P9WFR5
C	83	ALA	GLU	engineered mutation	UNP P9WFR5
C	84	ALA	HIS	engineered mutation	UNP P9WFR5
C	85	ALA	PRO	engineered mutation	UNP P9WFR5
C	86	ALA	THR	engineered mutation	UNP P9WFR5
C	87	ALA	LYS	engineered mutation	UNP P9WFR5
C	88	ALA	ARG	engineered mutation	UNP P9WFR5
C	89	ALA	PHE	engineered mutation	UNP P9WFR5
C	90	ALA	ARG	engineered mutation	UNP P9WFR5
C	91	ALA	PRO	engineered mutation	UNP P9WFR5
C	92	ALA	ILE	engineered mutation	UNP P9WFR5

- Molecule 2 is MONO-TRANS, OCTA-CIS DECAPRENYL-PHOSPHATE (three-letter code: DSL) (formula: $C_{50}H_{83}O_4P$) (labeled as "Ligand of Interest" by depositor).



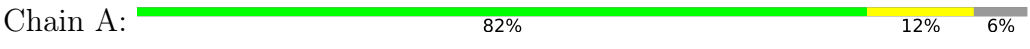
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			30	25	4	1	
2	B	1	Total	C	O	P	0
			30	25	4	1	
2	C	1	Total	C	O	P	0
			30	25	4	1	

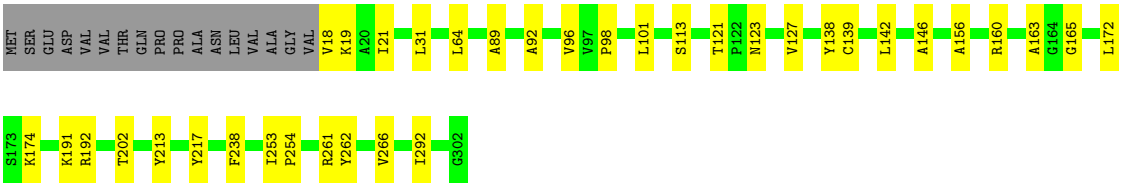
3 Residue-property plots (i)

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. 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: Decaprenyl-phosphate phosphoribosyltransferase

Chain A:



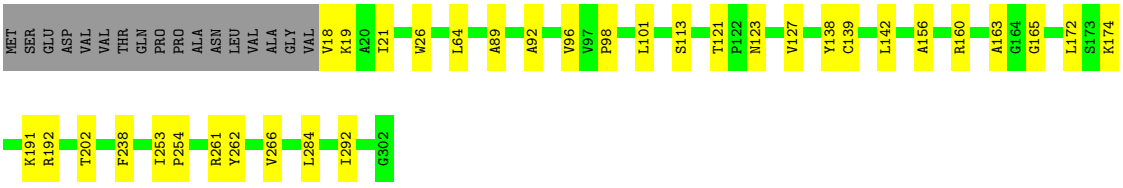


• Molecule 1: Decaprenyl-phosphate phosphoribosyltransferase

Chain B:

• Molecule 1: Decaprenyl-phosphate phosphoribosyltransferase

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	272777	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF amplitude correction was performed following 3D reconstruction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
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: DSL

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	0.33	0/2181	0.47	0/2980
1	B	0.33	0/2181	0.47	0/2980
1	C	0.33	0/2181	0.47	0/2980
All	All	0.33	0/6543	0.47	0/8940

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	2133	0	2206	26	0
1	B	2133	0	2206	22	0
1	C	2133	0	2206	23	0
2	A	30	0	38	2	0
2	B	30	0	38	2	0
2	C	30	0	38	2	0
All	All	6489	0	6732	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (69) 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:202:THR:HG22	1:A:202:THR:O	1.82	0.79
1:C:202:THR:HG22	1:C:202:THR:O	1.82	0.78
1:B:202:THR:O	1:B:202:THR:HG22	1.82	0.77
1:A:138:TYR:HA	1:A:142:LEU:HB2	1.74	0.69
1:C:138:TYR:HA	1:C:142:LEU:HB2	1.74	0.69
1:B:138:TYR:HA	1:B:142:LEU:HB2	1.74	0.68
1:A:174:LYS:HD3	1:B:238:PHE:HB3	1.75	0.67
1:A:121:THR:HG22	1:A:123:ASN:H	1.62	0.65
1:C:121:THR:HG22	1:C:123:ASN:H	1.62	0.63
1:B:121:THR:HG22	1:B:123:ASN:H	1.62	0.62
1:A:64:LEU:HB2	1:A:113:SER:HB2	1.82	0.62
1:C:64:LEU:HB2	1:C:113:SER:HB2	1.82	0.61
1:B:64:LEU:HB2	1:B:113:SER:HB2	1.82	0.61
1:C:127:VAL:HG11	1:C:163:ALA:HB2	1.86	0.58
1:A:127:VAL:HG11	1:A:163:ALA:HB2	1.86	0.58
1:B:127:VAL:HG11	1:B:163:ALA:HB2	1.86	0.57
1:B:191:LYS:NZ	2:B:401:DSL:H551	2.22	0.54
1:A:191:LYS:NZ	2:A:401:DSL:H551	2.23	0.54
1:B:174:LYS:HD3	1:C:238:PHE:HB3	1.89	0.54
1:B:262:TYR:O	1:B:266:VAL:HG23	2.08	0.54
1:A:262:TYR:O	1:A:266:VAL:HG23	2.08	0.54
1:A:253:ILE:HB	1:A:254:PRO:HD3	1.90	0.53
1:C:253:ILE:HB	1:C:254:PRO:HD3	1.90	0.53
1:C:202:THR:O	1:C:202:THR:CG2	2.53	0.53
1:C:262:TYR:O	1:C:266:VAL:HG23	2.08	0.53
1:B:253:ILE:HB	1:B:254:PRO:HD3	1.90	0.52
1:A:174:LYS:HD3	1:B:238:PHE:CB	2.40	0.52
1:C:191:LYS:NZ	2:C:401:DSL:H551	2.25	0.52
1:B:202:THR:O	1:B:202:THR:CG2	2.53	0.51
1:C:165:GLY:HA3	1:C:172:LEU:HD21	1.94	0.49
1:A:165:GLY:HA3	1:A:172:LEU:HD21	1.95	0.49
1:B:165:GLY:HA3	1:B:172:LEU:HD21	1.95	0.49
1:A:238:PHE:HB3	1:C:174:LYS:HD3	1.95	0.48
1:A:202:THR:O	1:A:202:THR:CG2	2.53	0.48
1:B:156:ALA:O	1:B:160:ARG:NH1	2.48	0.47
1:C:156:ALA:O	1:C:160:ARG:NH1	2.48	0.46
1:A:146:ALA:O	1:A:213:TYR:OH	2.20	0.46
1:A:156:ALA:O	1:A:160:ARG:NH1	2.48	0.45
1:C:138:TYR:HD1	1:C:139:CYS:HG	1.63	0.45
1:A:138:TYR:HD1	1:A:139:CYS:HG	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LYS:HD2	1:B:191:LYS:C	2.38	0.44
1:A:217:TYR:CZ	1:B:264:VAL:HG23	2.53	0.43
1:A:292:ILE:HD13	1:A:292:ILE:HA	1.89	0.43
1:C:191:LYS:HD2	1:C:191:LYS:C	2.38	0.43
1:C:98:PRO:HD2	1:C:101:LEU:HD12	2.00	0.43
1:C:18:VAL:O	1:C:21:ILE:HG12	2.19	0.43
1:A:18:VAL:O	1:A:21:ILE:HG12	2.19	0.43
1:A:98:PRO:HD2	1:A:101:LEU:HD12	2.00	0.43
1:A:191:LYS:HD2	1:A:191:LYS:C	2.38	0.42
1:A:19:LYS:HD3	1:A:19:LYS:HA	1.76	0.42
1:C:89:ALA:HB1	1:C:96:VAL:HG22	2.01	0.42
1:C:292:ILE:HD13	1:C:292:ILE:HA	1.89	0.42
1:B:18:VAL:O	1:B:21:ILE:HG12	2.19	0.42
1:B:89:ALA:HB1	1:B:96:VAL:HG22	2.01	0.42
1:B:124:LEU:HD12	1:B:124:LEU:HA	1.83	0.42
1:A:89:ALA:HB1	1:A:96:VAL:HG22	2.01	0.42
2:A:401:DSL:H511	2:A:401:DSL:H481	2.02	0.42
1:B:98:PRO:HD2	1:B:101:LEU:HD12	2.01	0.42
1:C:284:LEU:HD12	1:C:284:LEU:HA	1.91	0.41
1:C:89:ALA:HB3	1:C:92:ALA:O	2.21	0.41
1:A:89:ALA:HB3	1:A:92:ALA:O	2.21	0.41
1:B:89:ALA:HB3	1:B:92:ALA:O	2.21	0.41
2:C:401:DSL:H481	2:C:401:DSL:H511	2.02	0.41
1:A:31:LEU:HD12	1:A:31:LEU:HA	1.89	0.40
1:C:19:LYS:HD3	1:C:19:LYS:HA	1.76	0.40
1:A:18:VAL:HG13	1:A:19:LYS:N	2.36	0.40
2:B:401:DSL:H481	2:B:401:DSL:H511	2.02	0.40
1:C:21:ILE:HD12	1:C:26:TRP:CH2	2.57	0.40
1:B:18:VAL:HG13	1:B:19:LYS:N	2.36	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	283/302 (94%)	266 (94%)	17 (6%)	0	100	100
1	B	283/302 (94%)	266 (94%)	17 (6%)	0	100	100
1	C	283/302 (94%)	266 (94%)	17 (6%)	0	100	100
All	All	849/906 (94%)	798 (94%)	51 (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	208/222 (94%)	206 (99%)	2 (1%)	76	87
1	B	208/222 (94%)	206 (99%)	2 (1%)	76	87
1	C	208/222 (94%)	206 (99%)	2 (1%)	76	87
All	All	624/666 (94%)	618 (99%)	6 (1%)	77	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	ARG
1	A	261	ARG
1	B	192	ARG
1	B	261	ARG
1	C	192	ARG
1	C	261	ARG

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
2	DSL	C	401	-	29,29,54	0.37	0	35,36,66	0.38	0
2	DSL	B	401	-	29,29,54	0.38	0	35,36,66	0.38	0
2	DSL	A	401	-	29,29,54	0.38	0	35,36,66	0.38	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
2	DSL	C	401	-	-	18/31/31/61	-
2	DSL	B	401	-	-	18/31/31/61	-
2	DSL	A	401	-	-	18/31/31/61	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	DSL	C46-C47-C49-C50
2	A	401	DSL	C51-C52-C54-C55
2	A	401	DSL	C53-C52-C54-C55
2	A	401	DSL	C54-C55-O56-P57
2	B	401	DSL	C46-C47-C49-C50
2	B	401	DSL	C51-C52-C54-C55
2	B	401	DSL	C53-C52-C54-C55
2	B	401	DSL	C54-C55-O56-P57
2	C	401	DSL	C46-C47-C49-C50
2	C	401	DSL	C51-C52-C54-C55
2	C	401	DSL	C53-C52-C54-C55
2	C	401	DSL	C54-C55-O56-P57
2	A	401	DSL	C48-C47-C49-C50
2	B	401	DSL	C48-C47-C49-C50
2	C	401	DSL	C48-C47-C49-C50
2	A	401	DSL	C40-C41-C42-C43
2	B	401	DSL	C40-C41-C42-C43
2	C	401	DSL	C40-C41-C42-C43
2	A	401	DSL	C40-C41-C42-C44
2	B	401	DSL	C40-C41-C42-C44
2	C	401	DSL	C40-C41-C42-C44
2	A	401	DSL	C38-C37-C39-C40
2	A	401	DSL	C43-C42-C44-C45
2	B	401	DSL	C38-C37-C39-C40
2	B	401	DSL	C43-C42-C44-C45
2	C	401	DSL	C38-C37-C39-C40
2	C	401	DSL	C43-C42-C44-C45
2	A	401	DSL	C41-C42-C44-C45
2	B	401	DSL	C41-C42-C44-C45
2	C	401	DSL	C41-C42-C44-C45
2	A	401	DSL	C45-C46-C47-C48
2	B	401	DSL	C45-C46-C47-C48
2	C	401	DSL	C45-C46-C47-C48
2	A	401	DSL	C50-C51-C52-C53
2	B	401	DSL	C50-C51-C52-C53
2	C	401	DSL	C50-C51-C52-C53
2	A	401	DSL	C35-C36-C37-C38
2	B	401	DSL	C35-C36-C37-C38
2	C	401	DSL	C35-C36-C37-C38
2	A	401	DSL	C50-C51-C52-C54
2	B	401	DSL	C50-C51-C52-C54
2	C	401	DSL	C50-C51-C52-C54
2	A	401	DSL	C45-C46-C47-C49

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Mol	Chain	Res	Type	Atoms
2	B	401	DSL	C45-C46-C47-C49
2	C	401	DSL	C45-C46-C47-C49
2	A	401	DSL	C36-C37-C39-C40
2	A	401	DSL	C35-C36-C37-C39
2	B	401	DSL	C35-C36-C37-C39
2	C	401	DSL	C35-C36-C37-C39
2	B	401	DSL	C36-C37-C39-C40
2	C	401	DSL	C36-C37-C39-C40
2	A	401	DSL	C47-C49-C50-C51
2	B	401	DSL	C47-C49-C50-C51
2	C	401	DSL	C47-C49-C50-C51

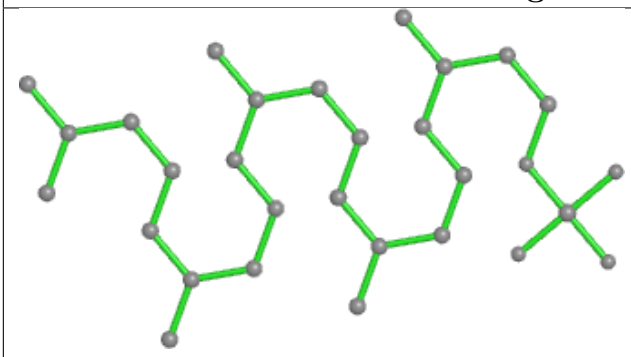
There are no ring outliers.

3 monomers are involved in 6 short contacts:

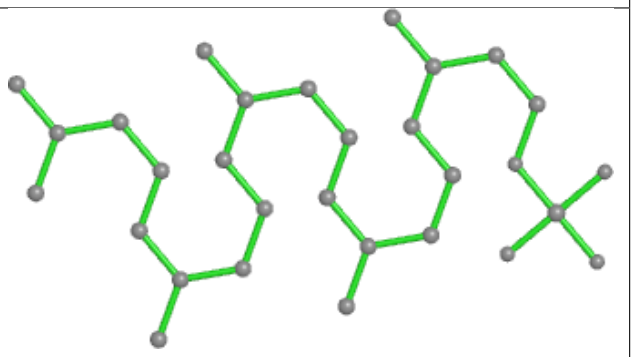
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	DSL	2	0
2	B	401	DSL	2	0
2	A	401	DSL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

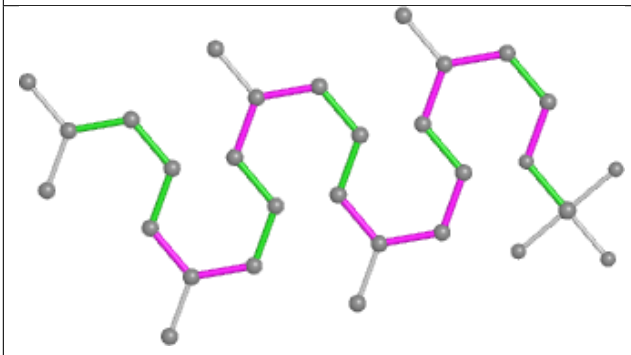
Ligand DSL C 401



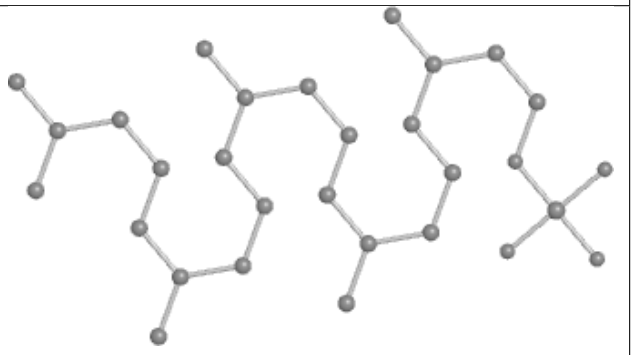
Bond lengths



Bond angles

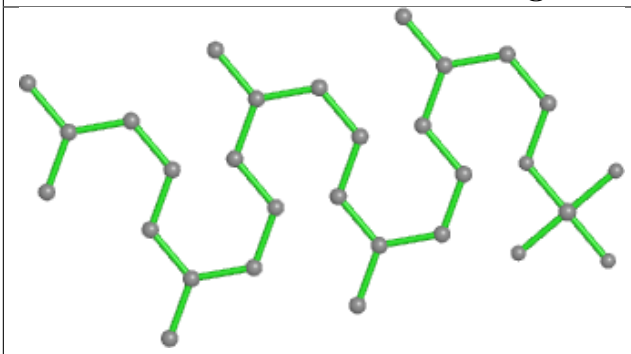


Torsions

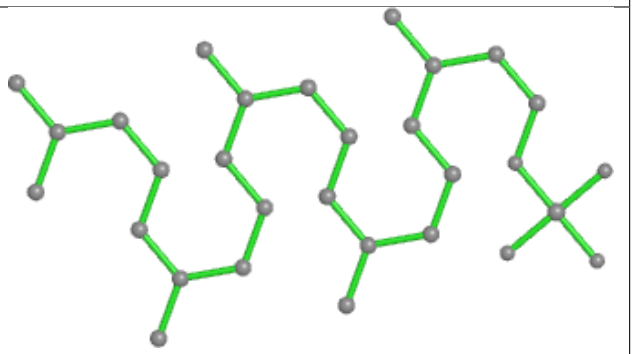


Rings

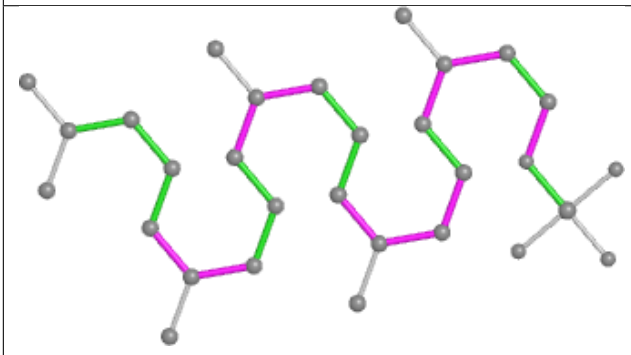
Ligand DSL B 401



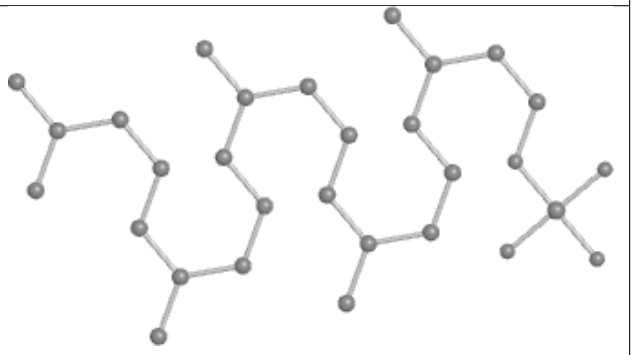
Bond lengths



Bond angles

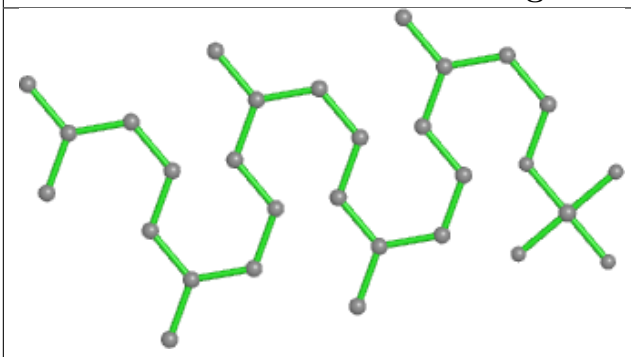


Torsions

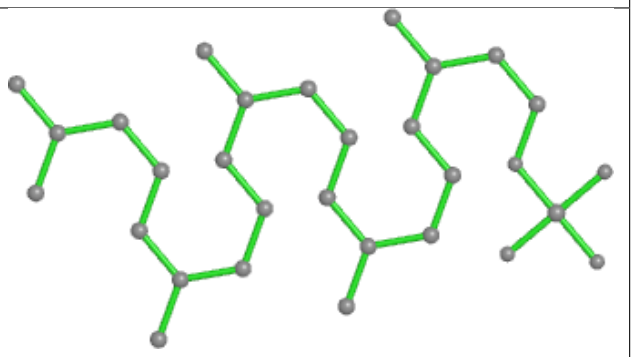


Rings

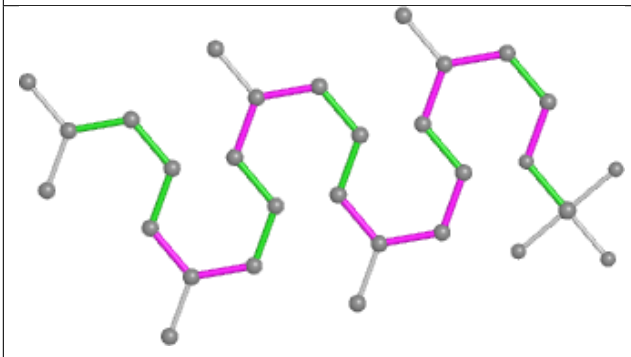
Ligand DSL A 401



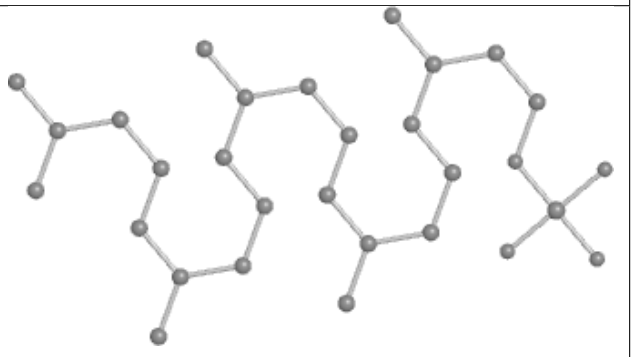
Bond lengths



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.