Full wwPDB NMR Structure Validation Report (i)

Oct 10, 2021 – 12:32 PM EDT

PDB ID	:	2KGA
Title	:	NMR Solution Structures of hexanoyl ACP (a non natural intermediate) from the actinorhodin polyketide synthase in Streptomyces coelicolor
Authors	:	Crump, M.P.; Evans, S.E.; Williams, C.
Deposited on	:	2009-03-07

This is a Full wwPDB NMR Structure 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

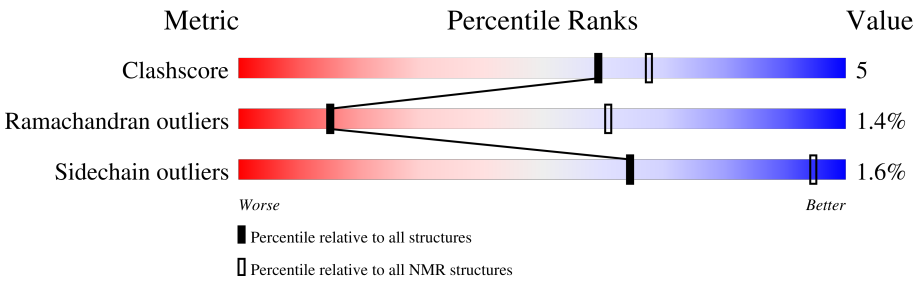
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	86	73% 8% 19%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:4-A:18, A:28-A:82 (70)	0.42	16

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 5, 7, 8, 9, 10, 11, 13, 14, 15, 16, 17, 18, 19, 20
2	3, 6
Single-model clusters	12

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1335 atoms, of which 660 are hydrogens and 0 are deuteriums.

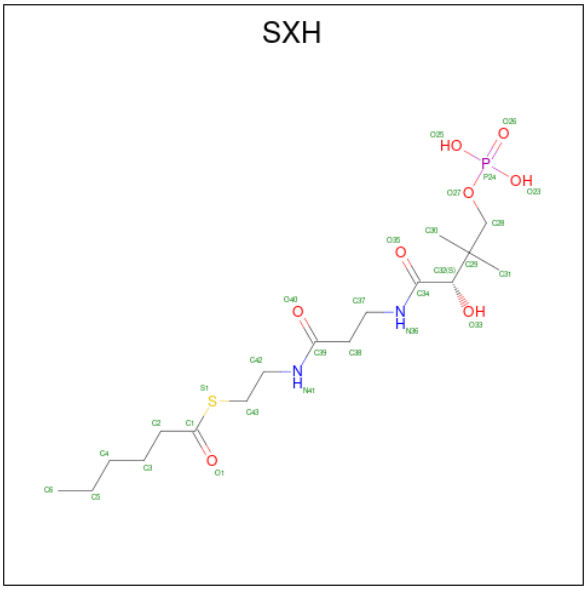
- Molecule 1 is a protein called Actinorhodin polyketide synthase acyl carrier protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	86	1276	397	629	108	140	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	SER	CYS	engineered mutation	UNP Q02054

- Molecule 2 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] hexanethioate (three-letter code: SXH) (formula: $C_{17}H_{33}N_2O_8PS$).



Mol	Chain	Residues	Atoms						
			Total	C	H	N	O	P	S
2	A	1	59	17	31	2	7	1	1

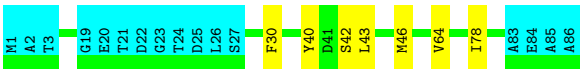
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

Chain A: 73% 8% 19%



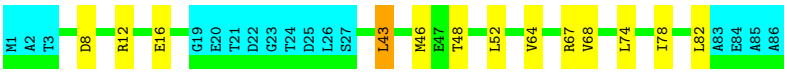
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

Chain A: 66% 14% • 19%



4.2.2 Score per residue for model 2

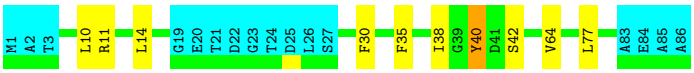
• Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

Chain A: 66% 14% • 19%

4.2.3 Score per residue for model 3

- Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

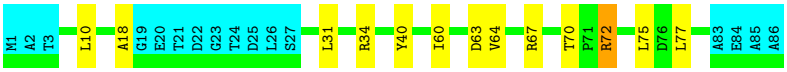
Chain A: 70% 10% • 19%



4.2.4 Score per residue for model 4

- Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

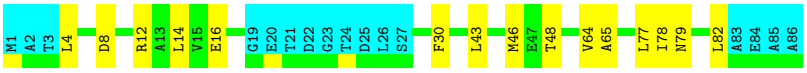
Chain A: 66% 14% • 19%



4.2.5 Score per residue for model 5

- Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

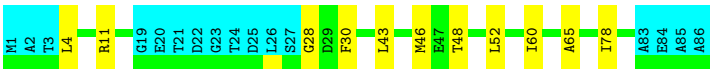
Chain A: 64% 17% 19%



4.2.6 Score per residue for model 6

- Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

Chain A: 69% 13% 19%



4.2.7 Score per residue for model 7

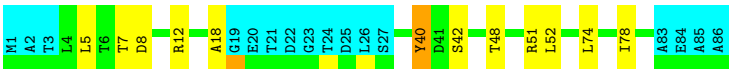
- Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

Chain A: 73% 8% 19%

4.2.8 Score per residue for model 8

- Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

Chain A: 67% 13% • 19%



4.2.9 Score per residue for model 9

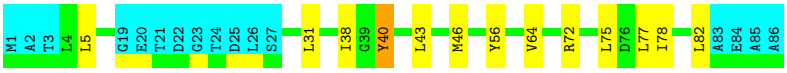
- Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

Chain A: 65% 16% 19%

4.2.10 Score per residue for model 10

- Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

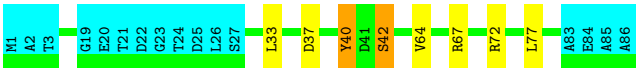
Chain A: 66% 14% • 19%



4.2.11 Score per residue for model 11

- Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

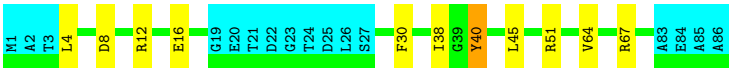
Chain A: 72% 7% • 19%



4.2.12 Score per residue for model 12

- Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

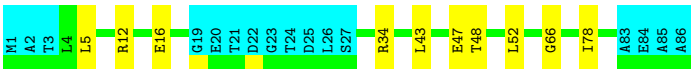
Chain A: 69% 12% • 19%



4.2.13 Score per residue for model 13

• Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

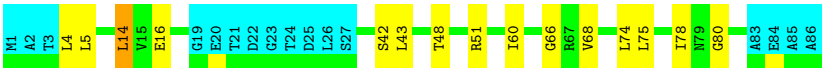
Chain A: 70% 12% 19%



4.2.14 Score per residue for model 14

• Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

Chain A: 64% 16% • 19%



4.2.15 Score per residue for model 15

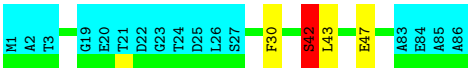
• Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

Chain A: 66% 14% • 19%

4.2.16 Score per residue for model 16 (medoid)

• Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

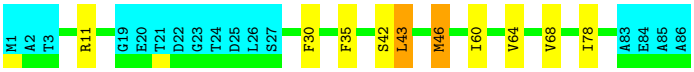
Chain A: 77% • • 19%



4.2.17 Score per residue for model 17

• Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

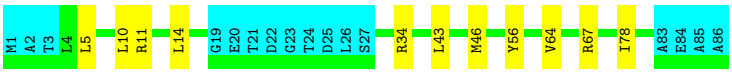
Chain A: 70% 9% • 19%



4.2.18 Score per residue for model 18

- Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

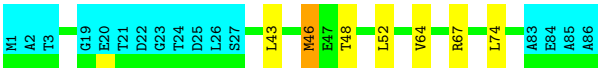
Chain A: 69% 13% 19%



4.2.19 Score per residue for model 19

- Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

Chain A: 73% 7% • 19%



4.2.20 Score per residue for model 20

- Molecule 1: Actinorhodin polyketide synthase acyl carrier protein

Chain A: 65% 16% 19%

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
ARIA	structure solution	1.2
ARIA	refinement	1.2

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

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 (average) 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	0.71±0.07	0±1/547 (0.1± 0.1%)	0.66±0.03	0±0/743 (0.0± 0.0%)
All	All	0.71	9/10940 (0.1%)	0.66	0/14860 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.5±0.8
All	All	0	9

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	40	TYR	CE2-CZ	-10.60	1.24	1.38	3	3
1	A	40	TYR	CE1-CZ	9.35	1.50	1.38	15	3
1	A	56	TYR	CE1-CZ	-7.36	1.28	1.38	10	1
1	A	56	TYR	CE2-CZ	7.06	1.47	1.38	10	1
1	A	42	SER	CB-OG	5.23	1.49	1.42	16	1

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	72	ARG	Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	40	TYR	Sidechain	2
1	A	55	ARG	Sidechain	1
1	A	34	ARG	Sidechain	1
1	A	51	ARG	Sidechain	1
1	A	11	ARG	Sidechain	1
1	A	56	TYR	Sidechain	1

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	541	535	535	5±1
2	A	28	31	31	1±1
All	All	11380	11320	11320	109

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 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:VAL:HG11	1:A:77:LEU:HG	0.88	1.45	10	6
1:A:42:SER:HB2	2:A:87:SXH:H28	0.64	1.67	16	2
1:A:11:ARG:HB2	1:A:30:PHE:CE1	0.62	2.29	17	3
1:A:31:LEU:HG	1:A:72:ARG:HB2	0.59	1.73	10	1
1:A:11:ARG:HD3	1:A:28:GLY:H	0.57	1.59	6	1
2:A:87:SXH:H3	2:A:87:SXH:H31B	0.56	1.77	19	1
1:A:66:GLY:HA2	2:A:87:SXH:H4A	0.55	1.78	14	1
1:A:43:LEU:O	1:A:46:MET:HG3	0.55	2.02	5	6
1:A:78:ILE:O	1:A:82:LEU:HG	0.53	2.03	10	5
1:A:5:LEU:HD23	1:A:75:LEU:HD12	0.53	1.80	14	2
1:A:68:VAL:HG21	1:A:74:LEU:HD23	0.53	1.81	7	4
1:A:48:THR:O	1:A:52:LEU:HG	0.52	2.04	19	6
1:A:64:VAL:O	1:A:67:ARG:HG2	0.52	2.04	19	5
1:A:31:LEU:O	1:A:70:THR:HB	0.51	2.06	4	1
1:A:8:ASP:O	1:A:12:ARG:HG2	0.51	2.06	7	1
1:A:45:LEU:HG	2:A:87:SXH:H6	0.51	1.83	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ASP:O	1:A:12:ARG:HG3	0.51	2.06	8	4
1:A:64:VAL:O	1:A:68:VAL:HG23	0.50	2.06	17	1
1:A:18:ALA:HB3	1:A:40:TYR:CE1	0.50	2.42	4	2
1:A:16:GLU:HB3	1:A:51:ARG:NH1	0.49	2.22	12	1
1:A:60:ILE:HD11	1:A:78:ILE:HD11	0.48	1.85	6	3
1:A:15:VAL:HA	1:A:18:ALA:O	0.48	2.08	9	1
1:A:5:LEU:HD13	1:A:78:ILE:HG21	0.48	1.86	8	2
1:A:52:LEU:HD11	1:A:74:LEU:HD11	0.48	1.85	19	1
1:A:60:ILE:HG23	1:A:77:LEU:HD21	0.47	1.87	4	1
1:A:52:LEU:HD13	1:A:74:LEU:HD11	0.47	1.87	1	1
1:A:10:LEU:O	1:A:14:LEU:HD23	0.47	2.10	18	3
1:A:64:VAL:HA	1:A:67:ARG:HG2	0.46	1.86	11	3
1:A:12:ARG:O	1:A:16:GLU:HG3	0.46	2.10	13	4
1:A:33:LEU:HB3	1:A:37:ASP:HB2	0.45	1.88	2	2
1:A:43:LEU:O	1:A:46:MET:HG2	0.45	2.10	1	2
1:A:64:VAL:CG1	1:A:77:LEU:HG	0.45	2.37	2	2
1:A:16:GLU:HB2	1:A:51:ARG:NH1	0.45	2.27	20	2
1:A:35:PHE:CE2	1:A:68:VAL:HG12	0.45	2.47	17	1
1:A:35:PHE:O	1:A:40:TYR:HB2	0.44	2.13	3	1
1:A:68:VAL:HG21	1:A:74:LEU:HB2	0.44	1.88	1	1
1:A:10:LEU:O	1:A:14:LEU:HG	0.44	2.13	3	1
1:A:65:ALA:HB1	2:A:87:SXH:H3A	0.43	1.91	5	1
1:A:42:SER:HB2	2:A:87:SXH:C28	0.43	2.43	16	2
1:A:66:GLY:HA2	2:A:87:SXH:H6A	0.43	1.90	13	1
1:A:43:LEU:O	1:A:47:GLU:HG3	0.43	2.13	9	2
1:A:65:ALA:HB2	2:A:87:SXH:H4	0.43	1.90	6	1
1:A:38:ILE:HG13	1:A:40:TYR:HB2	0.43	1.90	10	2
1:A:14:LEU:HD13	1:A:48:THR:HG21	0.43	1.91	14	1
1:A:14:LEU:HD23	1:A:48:THR:HG21	0.42	1.90	5	1
1:A:74:LEU:O	1:A:78:ILE:HG12	0.42	2.14	8	1
1:A:14:LEU:HG	1:A:30:PHE:CE2	0.42	2.49	15	1
1:A:62:ASP:HB3	2:A:87:SXH:S1	0.42	2.54	9	1
1:A:10:LEU:HD22	1:A:75:LEU:HB2	0.42	1.92	4	1
1:A:31:LEU:HB3	1:A:72:ARG:HB2	0.41	1.92	4	1
1:A:43:LEU:O	1:A:47:GLU:HG2	0.41	2.16	16	1
1:A:35:PHE:HE2	1:A:68:VAL:HG12	0.41	1.75	17	1
1:A:34:ARG:HD3	1:A:69:ASP:OD2	0.41	2.15	2	1
1:A:5:LEU:HD22	1:A:78:ILE:HG21	0.41	1.92	13	2
1:A:34:ARG:HG2	1:A:69:ASP:OD2	0.41	2.15	9	1
1:A:52:LEU:CD1	1:A:74:LEU:HD11	0.41	2.46	1	1
1:A:34:ARG:HD2	1:A:34:ARG:N	0.40	2.30	18	1

6.3 Torsion angles (i)

6.3.1 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 NMR 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	70/86 (81%)	66±1 (95±2%)	3±1 (4±1%)	1±1 (1±1%)	15 61
All	All	1400/1720 (81%)	1323 (94%)	57 (4%)	20 (1%)	15 61

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	30	PHE	7
1	A	42	SER	6
1	A	4	LEU	5
1	A	38	ILE	2

6.3.2 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 NMR 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	58/68 (85%)	57±1 (98±1%)	1±1 (2±1%)	64 94
All	All	1160/1360 (85%)	1142 (98%)	18 (2%)	64 94

All 9 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	43	LEU	3
1	A	46	MET	3
1	A	40	TYR	3
1	A	79	ASN	2
1	A	34	ARG	2
1	A	42	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	63	ASP	1
1	A	7	THR	1
1	A	14	LEU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	SXH	A	87	1	21,27,28	1.02±0.09	1±1 (6±3%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	SXH	A	87	1	26,34,37	0.98±0.07	2±1 (6±2%)

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	SXH	A	87	1	-	0±0,32,34,35	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	87	SXH	O1-C1	3.16	1.26	1.21	7	13
2	A	87	SXH	C2-C1	2.56	1.53	1.50	10	3
2	A	87	SXH	C43-S1	2.47	1.71	1.81	4	13

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	87	SXH	O1-C1-C2	2.82	120.66	123.99	18	19
2	A	87	SXH	C2-C1-S1	2.66	116.55	113.46	13	1
2	A	87	SXH	C37-C38-C39	2.42	116.39	112.36	7	12
2	A	87	SXH	C30-C29-C32	2.08	112.43	108.82	20	2

There are no chirality outliers.

All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

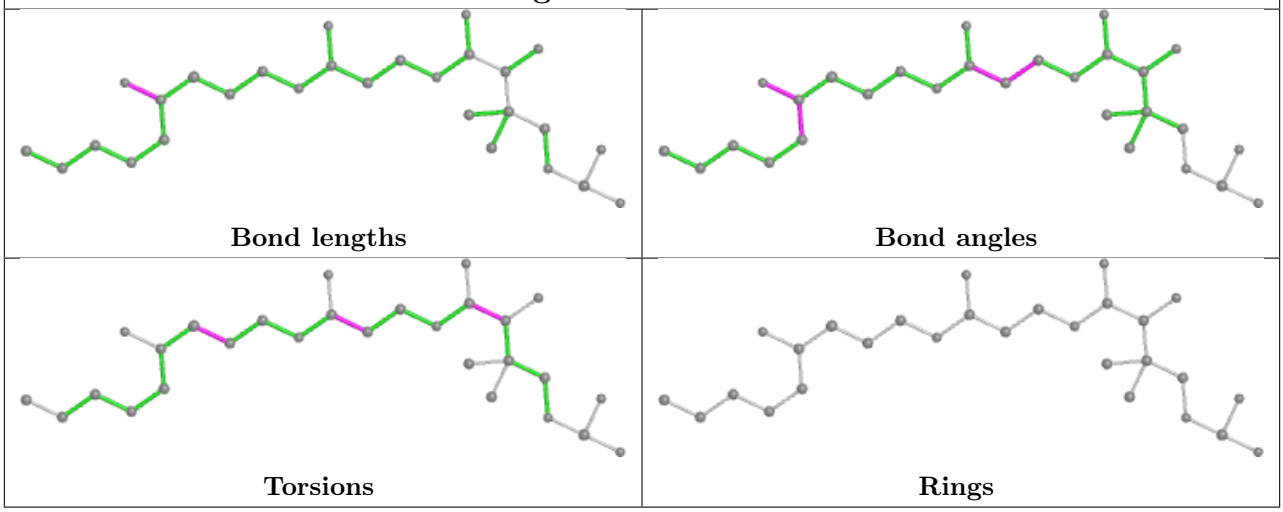
Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	87	SXH	O1-C1-S1-C43	4
2	A	87	SXH	C2-C1-S1-C43	4

There are no ring outliers.

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 SXH A 87



6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided