Full wwPDB NMR Structure Validation Report (i)

Mar 8, 2026 – 04:12 PM UTC

PDB ID	:	2H5M / pdb_00002h5m
Title	:	NMR Solution Structure of a GCN5-like putative N-acetyltransferase from Staphylococcus aureus complexed with acetyl-CoA. Northeast Structural Genomics Consortium Target ZR31
Authors	:	Cort, J.R.; Ramelot, T.A.; Acton, T.B.; Ma, L.; Xiao, R.B.; Montelione, G.T.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2006-05-26

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

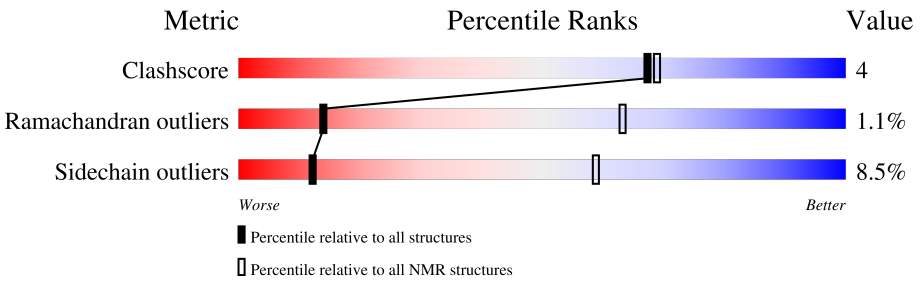
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	102	77% · 19%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:5-A:44, A:51-A:93 (83)	0.71	1

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 5 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1688 atoms, of which 819 are hydrogens and 0 are deuteriums.

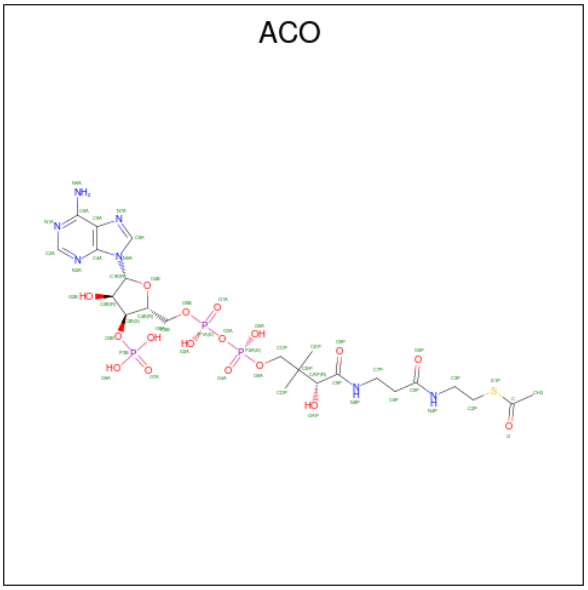
- Molecule 1 is a protein called Acetyltransferase, GNAT family.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	102	1603	507	785	146	162	3	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	LEU	-	expression tag	UNP Q5HD32
A	96	GLU	-	expression tag	UNP Q5HD32
A	97	HIS	-	expression tag	UNP Q5HD32
A	98	HIS	-	expression tag	UNP Q5HD32
A	99	HIS	-	expression tag	UNP Q5HD32
A	100	HIS	-	expression tag	UNP Q5HD32
A	101	HIS	-	expression tag	UNP Q5HD32
A	102	HIS	-	expression tag	UNP Q5HD32

- Molecule 2 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						
			Total	C	H	N	O	P	S
2	A	1	85	23	34	7	17	3	1

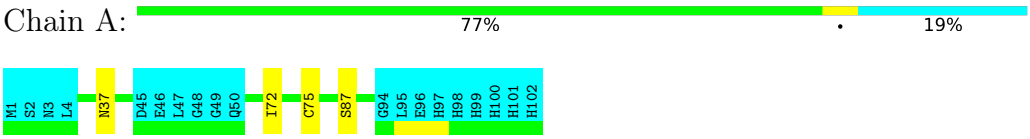
4 Residue-property plots (i)

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: Acetyltransferase, GNAT family

Chain A:



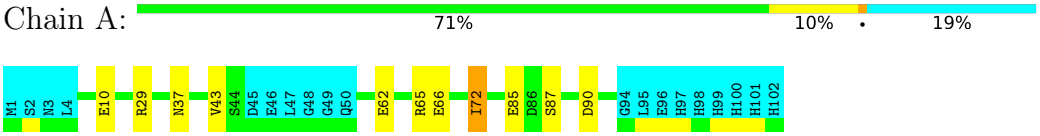
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Acetyltransferase, GNAT family

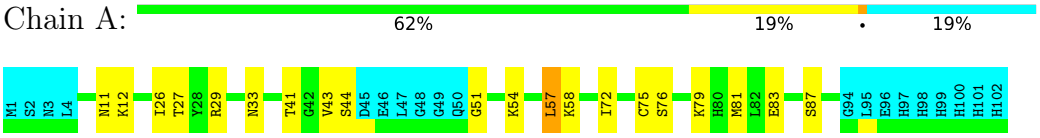
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Acetyltransferase, GNAT family

Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Acetyltransferase, GNAT family

Chain A: 71% 10% • 19%

M1 S2 N3 L4 K7 T27 Y28 R29 N37 D45 E46 L47 G48 G49 Q50 E62 I72 C75 S76 F77 A78 K79 H80 M81 Y92 L93 G94 L95 E96 H97 H98 H99 H100 H101 H102

4.2.4 Score per residue for model 4

- Molecule 1: Acetyltransferase, GNAT family

Chain A: 68% 14% 19%

M1 S2 N3 L4 E5 D18 A24 I36 G42 V43 S44 D45 E46 L47 G48 G49 Q50 E62 H63 E66 C75 S76 F77 S87 L93 G94 L95 E96 H97 H98 H99 H100 H101 H102

4.2.5 Score per residue for model 5

- Molecule 1: Acetyltransferase, GNAT family

Chain A: 68% 11% • 19%

M1 S2 N3 L4 E10 N11 N37 T41 G42 V43 S44 D45 E46 L47 G48 G49 Q50 E62 E66 I72 S76 F77 E83 S87 Y88 Q89 D90 V91 G94 L95 E96 H97 H98 H99 H100 H101 H102

4.2.6 Score per residue for model 6

- Molecule 1: Acetyltransferase, GNAT family

Chain A: 70% 11% • 19%

M1 S2 N3 L4 A24 N37 T41 G42 D45 E46 L47 G48 G49 Q50 K58 E62 E66 I72 L82 E85 D86 Y92 L93 G94 L95 E96 H97 H98 H99 H100 H101 H102

4.2.7 Score per residue for model 7

- Molecule 1: Acetyltransferase, GNAT family

Chain A: 69% 12% • 19%

M1 S2 N3 L4 E5 N20 N33 I38 S44 D45 E46 L47 G48 G49 Q50 K54 K58 I72 C75 S76 S87 V91 Y92 L93 G94 L95 E96 H97 H98 H99 H100 H101 H102

4.2.8 Score per residue for model 8

- Molecule 1: Acetyltransferase, GNAT family

Chain A: 76% 5% 19%

M1 S2 N3 L4 E5 D45 E46 L47 G48 G49 Q50 K58 C75 K79 E83 G94 L95 E96 H97 H98 H99 H100 H101 H102

4.2.9 Score per residue for model 9

- Molecule 1: Acetyltransferase, GNAT family

Chain A: 70% 12% 19%

M1 S2 N3 L4 N11 A24 T27 N37 H40 T41 G42 V43 S44 D45 E46 L47 G48 G49 Q50 C75 S76 F77 S87 G94 L95 E96 H97 H98 H99 H100 H101 H102

4.2.10 Score per residue for model 10

- Molecule 1: Acetyltransferase, GNAT family

Chain A: 72% 9% • 19%

M1 S2 N3 L4 E5 E35 I36 N37 D45 E46 L47 G48 G49 Q50 K70 I71 I72 C75 S76 E85 D86 S87 L93 G94 L95 E96 H97 H98 H99 H100 H101 H102

4.2.11 Score per residue for model 11

- Molecule 1: Acetyltransferase, GNAT family

Chain A: 72% 10% 19%

M1 S2 N3 L4 E10 I15 R29 N37 I38 D39 S44 D45 E46 L47 G48 G49 Q50 L56 I72 S76 S87 G94 L95 E96 H97 H98 H99 H100 H101 H102

4.2.12 Score per residue for model 12

- Molecule 1: Acetyltransferase, GNAT family

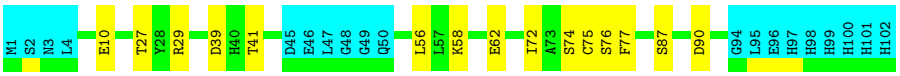
Chain A: 67% 15% 19%

M1 S2 N3 L4 N11 K12 I26 T27 Y28 N37 T41 G42 V43 S44 D45 E46 L47 G48 G49 Q50 H63 E66 I71 I72 A73 S74 E85 D86 S87 Y92 L93 G94 L95 E96 H97 H98 H99 H100 H101 H102

4.2.13 Score per residue for model 13

- Molecule 1: Acetyltransferase, GNAT family

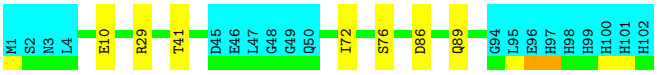
Chain A: 67% 15% 19%



4.2.14 Score per residue for model 14

- Molecule 1: Acetyltransferase, GNAT family

Chain A: 75% 7% 19%



4.2.15 Score per residue for model 15

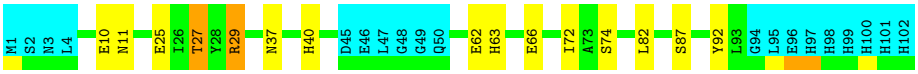
- Molecule 1: Acetyltransferase, GNAT family

Chain A: 74% 8% 19%

4.2.16 Score per residue for model 16

- Molecule 1: Acetyltransferase, GNAT family

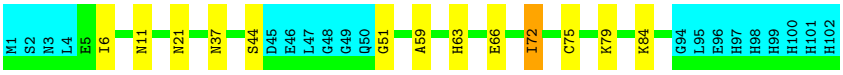
Chain A: 67% 13% • 19%



4.2.17 Score per residue for model 17

- Molecule 1: Acetyltransferase, GNAT family

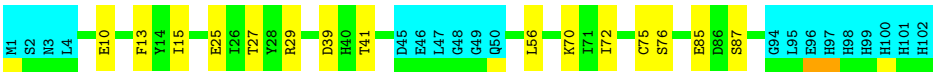
Chain A: 69% 12% • 19%



4.2.18 Score per residue for model 18

- Molecule 1: Acetyltransferase, GNAT family

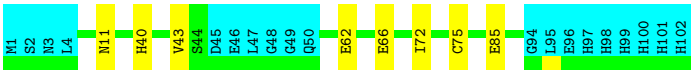
Chain A: 67% 15% 19%



4.2.19 Score per residue for model 19

- Molecule 1: Acetyltransferase, GNAT family

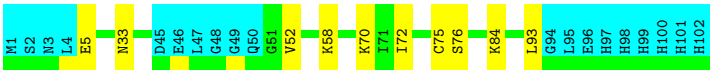
Chain A: 74% 8% 19%



4.2.20 Score per residue for model 20

- Molecule 1: Acetyltransferase, GNAT family

Chain A: 72% 10% 19%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Refinement was conducted with HADDOCK. Starting structures were the 1R57 ensemble, which is the protein in the absence of ligand.*

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
HADDOCK	refinement	1.3

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: ACO

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	664	649	646	3±2
2	A	51	34	34	3±2
All	All	14300	13660	13600	105

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:103:ACO:H141	2:A:103:ACO:O9P	0.76	1.81	13	7
2:A:103:ACO:H131	2:A:103:ACO:N8P	0.68	2.04	7	8
1:A:43:VAL:HB	2:A:103:ACO:H142	0.59	1.73	19	6
1:A:70:LYS:HB3	1:A:93:LEU:HD22	0.57	1.75	20	2
1:A:40:HIS:HA	1:A:75:CYS:SG	0.56	2.40	19	1
1:A:93:LEU:H	1:A:93:LEU:HD23	0.55	1.61	10	2
2:A:103:ACO:O9P	2:A:103:ACO:CEP	0.55	2.54	13	2
1:A:77:PHE:CD1	2:A:103:ACO:H132	0.55	2.36	9	1
2:A:103:ACO:O2B	2:A:103:ACO:P3B	0.53	2.67	9	2
1:A:37:ASN:HA	1:A:72:ILE:O	0.52	2.03	6	8
2:A:103:ACO:C5P	2:A:103:ACO:C9P	0.52	2.87	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:103:ACO:O4B	2:A:103:ACO:P1A	0.52	2.66	12	1
1:A:24:ALA:HA	1:A:42:GLY:O	0.52	2.05	4	3
1:A:27:THR:OG1	1:A:40:HIS:HB2	0.51	2.06	9	1
1:A:57:LEU:HD13	1:A:81:MET:HG2	0.50	1.84	2	1
2:A:103:ACO:C4B	2:A:103:ACO:O7A	0.50	2.60	20	1
2:A:103:ACO:N8P	2:A:103:ACO:CDP	0.50	2.74	7	6
1:A:39:ASP:O	1:A:75:CYS:HB2	0.49	2.06	13	1
1:A:77:PHE:CE2	2:A:103:ACO:H143	0.48	2.44	3	2
2:A:103:ACO:H131	2:A:103:ACO:C6P	0.48	2.38	5	2
1:A:65:ARG:HD3	1:A:90:ASP:OD2	0.48	2.08	1	1
1:A:77:PHE:CZ	2:A:103:ACO:H143	0.48	2.44	13	1
1:A:79:LYS:O	1:A:83:GLU:HG3	0.48	2.08	2	2
2:A:103:ACO:H131	2:A:103:ACO:C7P	0.47	2.38	7	3
2:A:103:ACO:O9P	2:A:103:ACO:N4P	0.47	2.47	19	1
1:A:62:GLU:O	1:A:66:GLU:HG3	0.47	2.10	19	6
1:A:6:ILE:HD13	1:A:59:ALA:HB2	0.47	1.86	17	1
2:A:103:ACO:H131	2:A:103:ACO:H61	0.46	1.87	5	1
1:A:11:ASN:HB2	1:A:29:ARG:NH2	0.45	2.26	16	1
1:A:63:HIS:HA	1:A:66:GLU:OE1	0.45	2.12	4	5
1:A:38:ILE:HG22	1:A:75:CYS:SG	0.45	2.52	7	1
1:A:77:PHE:CG	2:A:103:ACO:H143	0.45	2.47	5	1
2:A:103:ACO:O9P	2:A:103:ACO:H131	0.45	2.11	19	1
1:A:15:ILE:HG13	1:A:56:LEU:HD21	0.44	1.89	18	2
1:A:27:THR:OG1	1:A:40:HIS:HB3	0.43	2.13	16	1
2:A:103:ACO:O5P	2:A:103:ACO:HH33	0.43	2.13	10	1
1:A:58:LYS:HG2	1:A:62:GLU:OE2	0.43	2.14	13	1
1:A:12:LYS:HB2	1:A:26:ILE:O	0.43	2.14	2	2
1:A:58:LYS:O	1:A:62:GLU:HB2	0.43	2.14	6	1
1:A:54:LYS:HE3	1:A:81:MET:SD	0.42	2.53	2	1
2:A:103:ACO:O4B	2:A:103:ACO:O1A	0.42	2.38	13	1
1:A:79:LYS:HG2	1:A:92:TYR:OH	0.42	2.15	3	1
2:A:103:ACO:O5P	2:A:103:ACO:H131	0.42	2.14	2	1
1:A:28:TYR:HA	1:A:37:ASN:O	0.42	2.15	12	1
1:A:83:GLU:HA	1:A:89:GLN:NE2	0.41	2.31	5	1
1:A:82:LEU:HD13	1:A:92:TYR:CD1	0.41	2.50	16	2
1:A:13:PHE:HB3	1:A:56:LEU:HD22	0.41	1.93	18	1
1:A:70:LYS:N	1:A:70:LYS:HD2	0.40	2.30	18	1
2:A:103:ACO:O2A	2:A:103:ACO:O4B	0.40	2.39	5	1
1:A:71:ILE:O	1:A:92:TYR:HA	0.40	2.15	12	1
1:A:39:ASP:C	1:A:75:CYS:HB2	0.40	2.41	18	1
2:A:103:ACO:O2A	2:A:103:ACO:C8A	0.40	2.70	4	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	83/102 (81%)	77±1 (93±1%)	5±1 (6±1%)	1±1 (1±1%)	14 63
All	All	1660/2040 (81%)	1543 (93%)	99 (6%)	18 (1%)	14 63

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	10	GLU	8
1	A	5	GLU	5
1	A	33	ASN	3
1	A	51	GLY	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	72/88 (82%)	66±2 (91±3%)	6±2 (9±3%)	12 59
All	All	1440/1760 (82%)	1317 (91%)	123 (9%)	12 59

All 34 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	72	ILE	15
1	A	87	SER	12
1	A	75	CYS	10
1	A	76	SER	10
1	A	29	ARG	9
1	A	41	THR	8

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Mol	Chain	Res	Type	Models (Total)
1	A	85	GLU	6
1	A	11	ASN	6
1	A	44	SER	6
1	A	27	THR	5
1	A	58	LYS	4
1	A	74	SER	3
1	A	62	GLU	2
1	A	37	ASN	2
1	A	89	GLN	2
1	A	91	VAL	2
1	A	86	ASP	2
1	A	25	GLU	2
1	A	84	LYS	2
1	A	57	LEU	1
1	A	7	LYS	1
1	A	81	MET	1
1	A	18	ASP	1
1	A	36	ILE	1
1	A	20	ASN	1
1	A	54	LYS	1
1	A	93	LEU	1
1	A	35	GLU	1
1	A	39	ASP	1
1	A	56	LEU	1
1	A	90	ASP	1
1	A	21	ASN	1
1	A	79	LYS	1
1	A	52	VAL	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 oligosaccharides 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	ACO	A	103	-	51,53,53	1.49±0.01	9±0 (17±0%)

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	ACO	A	103	-	73,79,79	1.54±0.01	11±1 (15±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	ACO	A	103	-	-	0±0,51,67,67	0±0,3,3,3

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	103	ACO	O-C	4.45	1.43	1.21	6	20
2	A	103	ACO	P3B-O7A	3.69	1.62	1.50	14	20
2	A	103	ACO	C2A-N3A	3.47	1.40	1.33	17	20
2	A	103	ACO	C2A-N1A	3.25	1.39	1.33	10	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	103	ACO	C5A-N7A	3.16	1.33	1.39	8	20
2	A	103	ACO	C5A-C4A	2.65	1.34	1.39	4	20
2	A	103	ACO	C8A-N9A	2.59	1.33	1.37	9	20
2	A	103	ACO	C5A-C6A	2.44	1.34	1.41	17	20
2	A	103	ACO	C4A-N9A	2.28	1.32	1.37	9	19
2	A	103	ACO	P2A-O3A	2.12	1.61	1.59	17	2

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	103	ACO	N3A-C2A-N1A	6.55	118.67	128.58	9	20
2	A	103	ACO	C5A-C4A-N3A	4.55	120.46	126.72	15	20
2	A	103	ACO	N9A-C8A-N7A	4.27	107.88	113.94	6	20
2	A	103	ACO	C2A-N3A-C4A	3.16	119.56	111.83	18	20
2	A	103	ACO	C5A-N7A-C8A	3.08	108.29	103.45	8	20
2	A	103	ACO	N3A-C4A-N9A	2.79	131.91	127.17	8	20
2	A	103	ACO	C4A-N9A-C8A	2.73	108.61	105.74	6	20
2	A	103	ACO	C4B-O4B-C1B	2.70	103.51	109.47	9	14
2	A	103	ACO	C5A-C6A-N6A	2.68	116.64	123.29	8	20
2	A	103	ACO	C6A-C5A-C4A	2.61	120.75	117.18	4	20
2	A	103	ACO	C4A-C5A-N7A	2.58	107.63	110.58	2	20
2	A	103	ACO	C3B-C2B-C1B	2.13	104.58	99.89	13	6

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	103	ACO	O-C-S1P-C2P	4
2	A	103	ACO	CH3-C-S1P-C2P	2
2	A	103	ACO	C6P-C5P-N4P-C3P	1

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.

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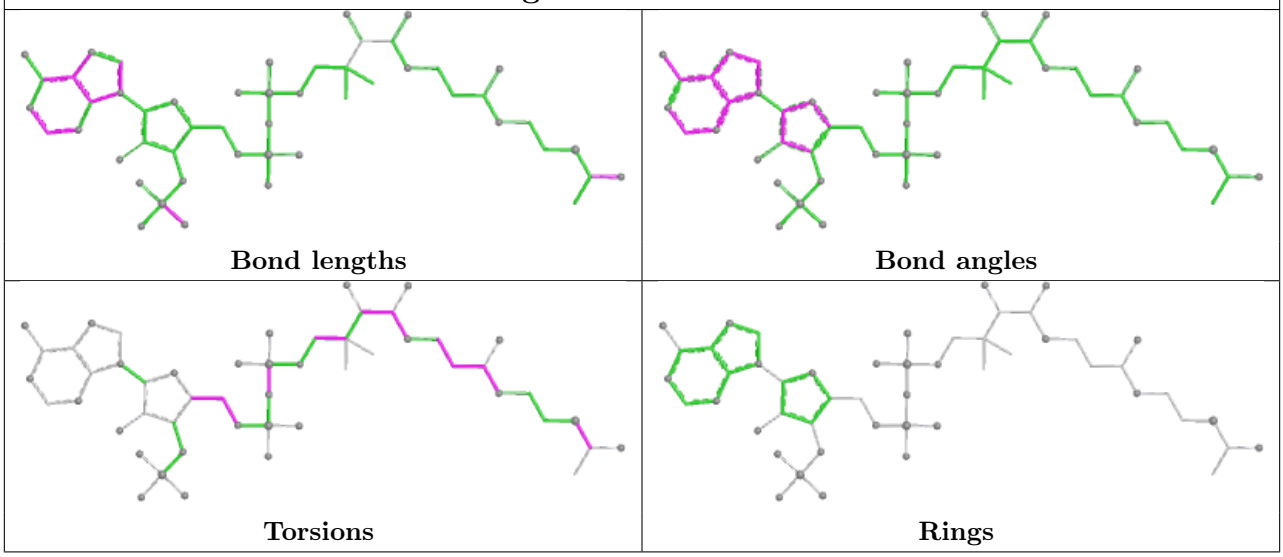

6.7 Other polymers (i)

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