WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 11:57 pm GMT

PDB ID	:	1L9H
Title	:	Crystal structure of bovine rhodopsin at 2.6 angstroms RESOLUTION
Authors	:	Okada, T.; Fujiyoshi, Y.; Silow, M.; Navarro, J.; Landau, E.M.; Shichida, Y.
Deposited on	:	2002-03-23
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
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:

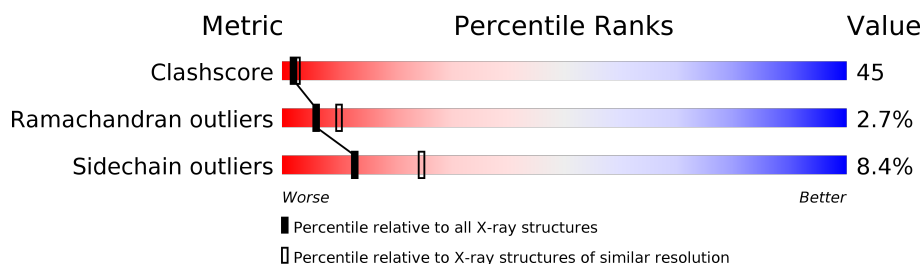|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Clashscore		45
Ramachandran outliers		2.7%
Sidechain outliers		8.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	349	38% 51% 8% ••
1	B	349	31% 48% 7% 13%

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
2	MAN	A	503	X	-	-	-
2	NAG	A	504	X	-	-	-
2	NAG	A	505	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	604	X	-	-	-
3	NAG	B	605	-	-	X	-
4	NAG	A	704	X	-	-	-
4	NAG	B	804	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 5584 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2685	1783	413	463	26			
1	B	302	Total	C	N	O	S	0	0	0
			2398	1603	366	404	25			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			41	22	2	17		

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	4	Total	C	N	O	0	0
			53	28	2	23		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			29	16	2	11		
4	B	2	Total	C	N	O	0	0
			29	16	2	11		

- Molecule 5 is SUGAR (B-NONYLGLUCOSIDE) (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).
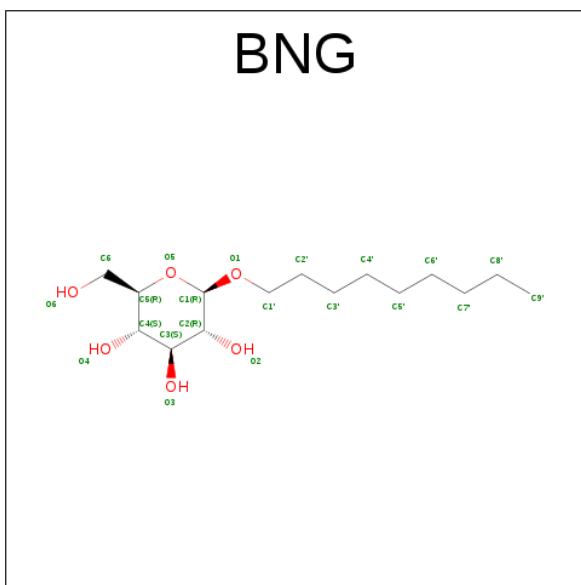
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 21	C 15	O 6	0	0
5	A	1	Total 21	C 15	O 6	0	0
5	B	1	Total 21	C 15	O 6	0	0
5	A	1	Total 21	C 15	O 6	0	0
5	A	1	Total 21	C 15	O 6	0	0
5	A	1	Total 21	C 15	O 6	0	0
5	B	1	Total 21	C 15	O 6	0	0

- Molecule 6 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total 3	Hg 3	0	0
6	A	3	Total 3	Hg 3	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	3	Total 3	Zn 3	0	0
7	A	4	Total 4	Zn 4	0	0

- Molecule 8 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).
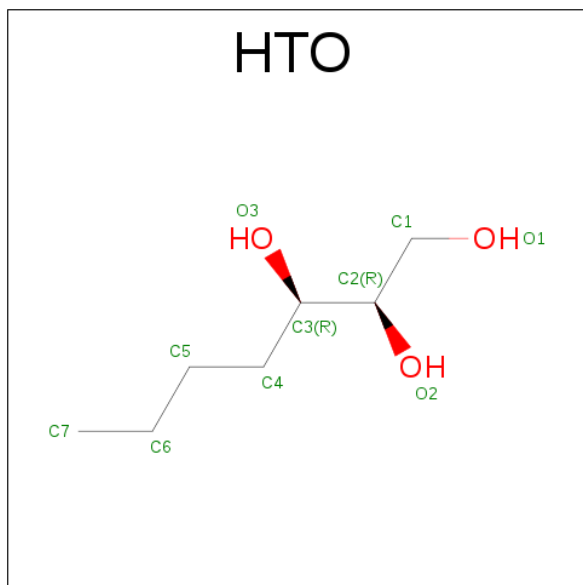
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 10	C 7	O 3	0	0
8	A	1	Total 10	C 7	O 3	0	0
8	A	1	Total 10	C 7	O 3	0	0
8	A	1	Total 10	C 7	O 3	0	0

- Molecule 9 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).

PLM
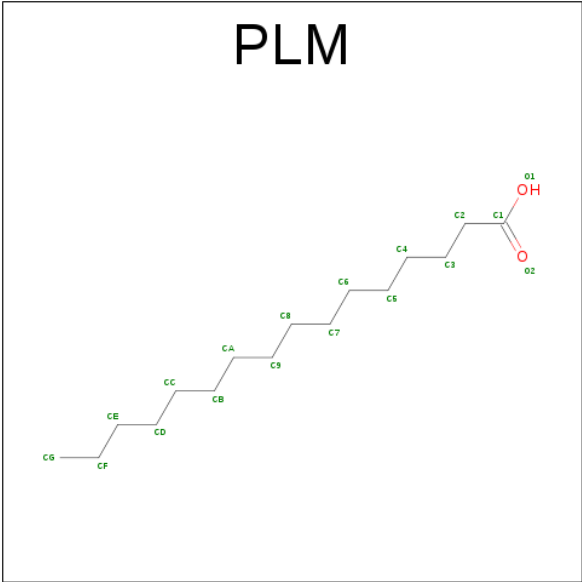
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C 16 16	0	0
9	A	1	Total C 16 16	0	0
9	A	1	Total C O 17 16 1	0	0
9	A	1	Total C O 17 16 1	0	0
9	B	1	Total C O 17 16 1	0	0

- Molecule 10 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).

RET
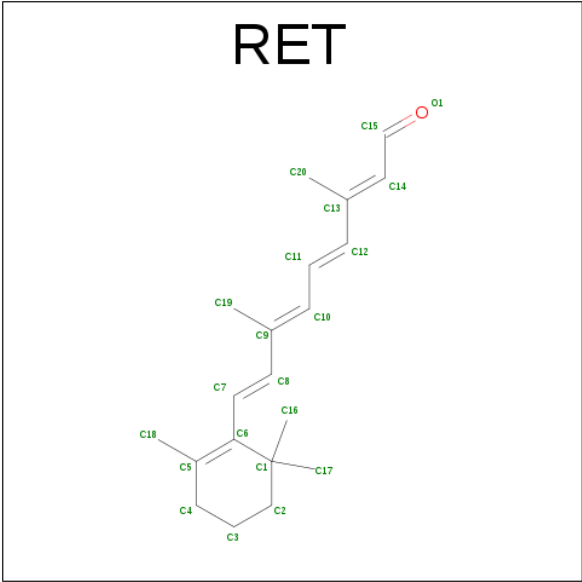
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total 20	C 20	0	0
10	B	1	Total 20	C 20	0	0

• Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	13	Total 13	O 13	0	0
11	B	13	Total 13	O 13	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

Note EDS was not executed.

• Molecule 1: rhodopsin
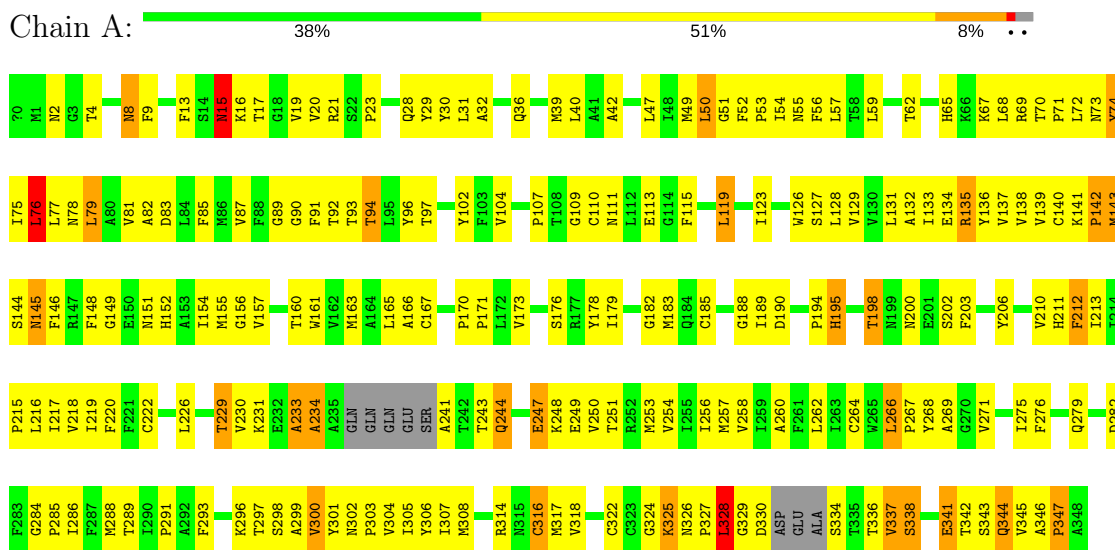
• Molecule 1: rhodopsin
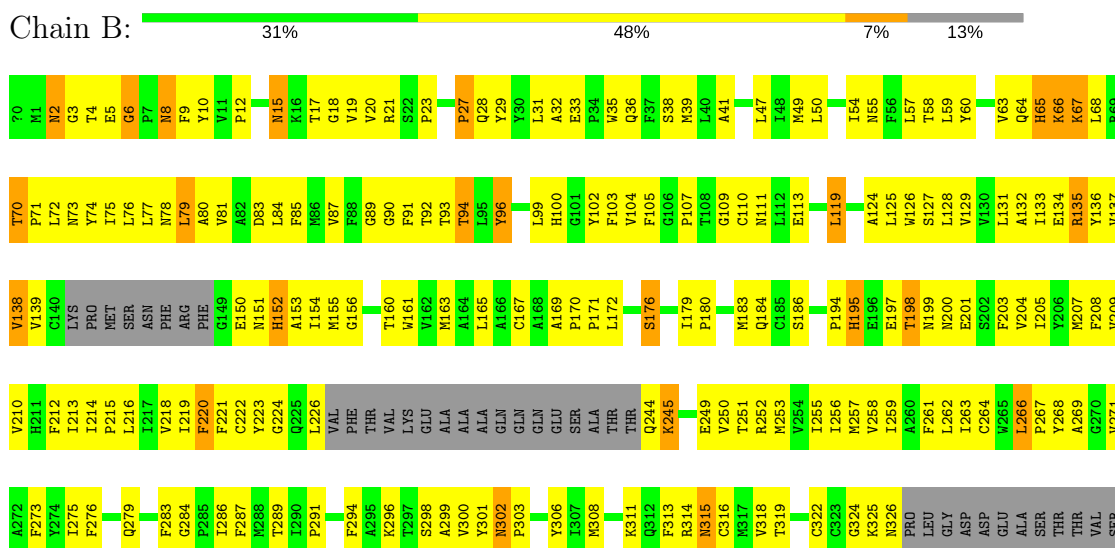
LYS THR GLU THR SER GLN VAL ALA PRO ALA

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	96.75Å 96.75Å 149.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	71.0 (30.00-2.60)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.188 , 0.225	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5584	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG, ACE, HTO, RET, PLM, BNG, HG, 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	0.68	2/2765 (0.1%)	0.76	6/3767 (0.2%)
1	B	0.68	0/2472	0.77	6/3368 (0.2%)
All	All	0.68	2/5237 (0.0%)	0.76	12/7135 (0.2%)

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 outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	A	2	0
3	B	1	0
4	A	1	0
4	B	1	0
All	All	5	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	ASN	CG-ND2	7.93	1.52	1.32
1	A	15	ASN	CA-CB	5.82	1.68	1.53

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	ASN	CB-CA-C	-11.05	88.31	110.40
1	A	15	ASN	CB-CG-ND2	-11.00	90.29	116.70
1	B	15	ASN	N-CA-CB	7.56	124.21	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ASN	CB-CA-C	-6.83	96.73	110.40
1	B	296	LYS	CD-CE-NZ	6.79	127.31	111.70

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	503	MAN	C1
2	A	504	NAG	C1
4	A	704	NAG	C1
3	B	604	NAG	C1
4	B	804	NAG	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ASN	Sidechain
1	B	96	TYR	Sidechain

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	2685	0	2657	263	0
1	B	2398	0	2369	242	0
2	A	41	0	36	11	0
3	B	53	0	45	7	0
4	A	29	0	26	6	0
4	B	29	0	26	1	0
5	A	105	0	150	11	0
5	B	42	0	60	7	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	4	0	0	0	0
7	B	3	0	0	0	0
8	A	40	0	64	4	0
9	A	50	0	89	3	0
9	B	33	0	58	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	20	0	27	1	0
10	B	20	0	27	3	0
11	A	13	0	0	2	0
11	B	13	0	0	5	0
All	All	5584	0	5634	496	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 45.

The worst 5 of 496 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:B:2:ASN:HD21	4:B:805:NAG:C1	1.13	1.56
1:A:2:ASN:HD21	4:A:705:NAG:C1	1.29	1.41
1:A:15:ASN:HD21	2:A:505:NAG:C1	1.29	1.40
1:A:65:HIS:HB3	1:A:337:VAL:HG22	1.26	1.12
1:A:75:ILE:HG21	1:A:131:LEU:HD21	1.32	1.10

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 X-ray entries followed by that with respect to entries of similar resolution.

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	335/349 (96%)	284 (85%)	37 (11%)	14 (4%)	3	4
1	B	296/349 (85%)	253 (86%)	40 (14%)	3 (1%)	18	37
All	All	631/698 (90%)	537 (85%)	77 (12%)	17 (3%)	6	10

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	LYS
1	A	328	LEU
1	A	347	PRO
1	A	142	PRO
1	A	195	HIS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	289/296 (98%)	266 (92%)	23 (8%)	14	27
1	B	257/296 (87%)	234 (91%)	23 (9%)	11	22
All	All	546/592 (92%)	500 (92%)	46 (8%)	13	25

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	GLU
1	B	64	GLN
1	B	300	VAL
1	A	343	SER
1	B	8	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	A	344	GLN
1	B	64	GLN
1	A	302	ASN
1	B	8	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

11 carbohydrates 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	MAN	A	503	2	12,12,12	0.56	0	17,17,17	0.62	0
2	NAG	A	504	2	15,15,15	0.56	0	21,21,21	1.08	2 (9%)
2	NAG	A	505	1,2	14,14,15	0.67	0	15,19,21	0.77	0
4	NAG	A	704	4	15,15,15	0.72	0	21,21,21	1.07	2 (9%)
4	NAG	A	705	1,4	14,14,15	0.52	0	15,19,21	0.85	0
3	MAN	B	602	3	12,12,12	0.55	0	17,17,17	0.58	0
3	MAN	B	603	3	12,12,12	0.70	0	17,17,17	0.64	0
3	NAG	B	604	3	15,15,15	0.42	0	21,21,21	1.61	1 (4%)
3	NAG	B	605	1,3	14,14,15	0.46	0	15,19,21	0.89	0
4	NAG	B	804	4	15,15,15	0.69	0	21,21,21	0.82	0
4	NAG	B	805	1,4	14,14,15	0.65	0	15,19,21	0.76	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	MAN	A	503	2	1/1/5/5	0/2/22/22	0/1/1/1
2	NAG	A	504	2	1/1/6/7	0/6/26/26	0/1/1/1
2	NAG	A	505	1,2	-	0/6/23/26	0/1/1/1
4	NAG	A	704	4	1/1/6/7	0/6/26/26	0/1/1/1
4	NAG	A	705	1,4	-	1/6/23/26	0/1/1/1
3	MAN	B	602	3	-	0/2/22/22	0/1/1/1
3	MAN	B	603	3	-	0/2/22/22	0/1/1/1
3	NAG	B	604	3	1/1/6/7	0/6/26/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	605	1,3	-	0/6/23/26	0/1/1/1
4	NAG	B	804	4	1/1/6/7	0/6/26/26	0/1/1/1
4	NAG	B	805	1,4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	504	NAG	C1-C2-N2	-2.63	107.68	110.73
4	A	704	NAG	O5-C1-C2	2.04	111.56	109.52
4	A	704	NAG	C4-C3-C2	2.20	113.58	110.33
2	A	504	NAG	C4-C3-C2	2.37	113.84	110.33
3	B	604	NAG	C2-N2-C7	7.01	140.95	123.19

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	604	NAG	C1
2	A	503	MAN	C1
4	B	804	NAG	C1
2	A	504	NAG	C1
4	A	704	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	805	NAG	O7-C7-N2-C2
4	A	705	NAG	O7-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	MAN	3	0
2	A	504	NAG	4	0
2	A	505	NAG	8	0
4	A	705	NAG	6	0
3	B	604	NAG	2	0
3	B	605	NAG	7	0
4	B	805	NAG	1	0

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 13 are monoatomic - leaving 18 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	#$|Z| > 2$
10	RET	A	1296	1	19,20,21	1.73	4 (21%)	27,27,28	1.98	10 (37%)
9	PLM	A	1322	1	16,16,17	0.50	0	15,15,17	0.64	0
9	PLM	A	1323	1	16,16,17	0.52	0	15,15,17	0.62	0
8	HTO	A	1400	-	9,9,9	2.11	3 (33%)	9,10,10	1.07	0
8	HTO	A	1401	-	9,9,9	2.18	3 (33%)	9,10,10	1.30	2 (22%)
8	HTO	A	1404	-	9,9,9	2.37	3 (33%)	9,10,10	1.06	0
8	HTO	A	1405	-	9,9,9	2.01	2 (22%)	9,10,10	1.06	0
9	PLM	A	1410	-	15,15,17	1.79	3 (20%)	14,14,17	3.28	7 (50%)
5	BNG	A	1500	-	21,21,21	2.02	6 (28%)	26,26,26	0.80	1 (3%)
5	BNG	A	1501	-	21,21,21	1.92	7 (33%)	26,26,26	0.71	0
5	BNG	A	1503	-	21,21,21	2.14	7 (33%)	26,26,26	0.81	1 (3%)
5	BNG	A	1504	-	21,21,21	1.94	7 (33%)	26,26,26	0.75	1 (3%)
5	BNG	A	1505	-	21,21,21	2.04	7 (33%)	26,26,26	0.92	1 (3%)
10	RET	B	1296	1	19,20,21	1.68	4 (21%)	27,27,28	1.99	9 (33%)
9	PLM	B	1322	1	16,16,17	0.64	0	15,15,17	0.51	0
9	PLM	B	1407	-	15,15,17	1.71	3 (20%)	14,14,17	3.27	6 (42%)
5	BNG	B	1502	-	21,21,21	2.21	7 (33%)	26,26,26	0.87	2 (7%)
5	BNG	B	1506	-	21,21,21	1.88	7 (33%)	26,26,26	0.83	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
10	RET	A	1296	1	-	0/13/30/31	0/1/1/1
9	PLM	A	1322	1	-	0/13/14/15	0/0/0/0
9	PLM	A	1323	1	-	0/13/14/15	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HTO	A	1400	-	-	0/10/10/10	0/0/0/0
8	HTO	A	1401	-	-	0/10/10/10	0/0/0/0
8	HTO	A	1404	-	-	0/10/10/10	0/0/0/0
8	HTO	A	1405	-	-	0/10/10/10	0/0/0/0
9	PLM	A	1410	-	-	0/13/13/15	0/0/0/0
5	BNG	A	1500	-	-	0/12/32/32	0/1/1/1
5	BNG	A	1501	-	-	0/12/32/32	0/1/1/1
5	BNG	A	1503	-	-	0/12/32/32	0/1/1/1
5	BNG	A	1504	-	-	0/12/32/32	0/1/1/1
5	BNG	A	1505	-	-	0/12/32/32	0/1/1/1
10	RET	B	1296	1	-	0/13/30/31	0/1/1/1
9	PLM	B	1322	1	-	0/13/14/15	0/0/0/0
9	PLM	B	1407	-	-	0/13/13/15	0/0/0/0
5	BNG	B	1502	-	-	0/12/32/32	0/1/1/1
5	BNG	B	1506	-	-	0/12/32/32	0/1/1/1

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1410	PLM	CC-CB	-4.77	1.24	1.51
9	B	1407	PLM	CC-CB	-4.57	1.25	1.51
9	A	1410	PLM	CB-CA	-3.37	1.32	1.51
9	B	1407	PLM	CB-CA	-3.26	1.33	1.51
9	A	1410	PLM	CD-CC	-2.95	1.34	1.51

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	1296	RET	C8-C7-C6	-3.57	117.26	127.25
10	A	1296	RET	C1-C6-C5	-2.84	118.59	122.59
10	A	1296	RET	C8-C7-C6	-2.77	119.50	127.25
10	B	1296	RET	C1-C6-C5	-2.40	119.22	122.59
10	A	1296	RET	C17-C1-C16	-2.26	101.58	108.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1296	RET	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1322	PLM	3	0
8	A	1401	HTO	2	0
8	A	1404	HTO	1	0
8	A	1405	HTO	1	0
5	A	1500	BNG	6	0
5	A	1501	BNG	1	0
5	A	1503	BNG	1	0
5	A	1504	BNG	1	0
5	A	1505	BNG	2	0
10	B	1296	RET	3	0
9	B	1322	PLM	1	0
9	B	1407	PLM	1	0
5	B	1506	BNG	7	0

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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.