



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:05 AM GMT

PDB ID : 2PED
Title : Crystallographic model of 9-cis-rhodopsin
Authors : Nakamichi, H.; Okada, T.
Deposited on : 2007-04-02
Resolution : 2.95 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

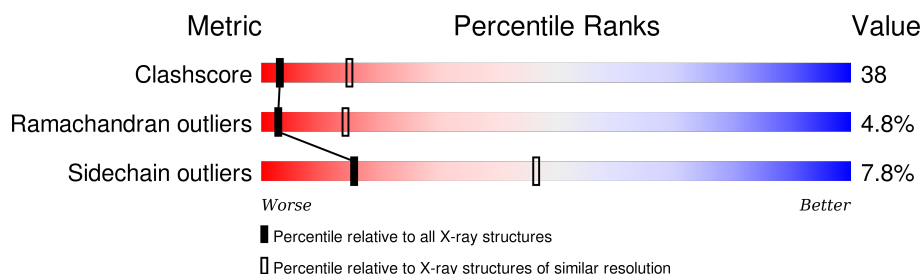
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

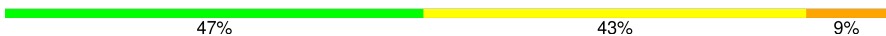
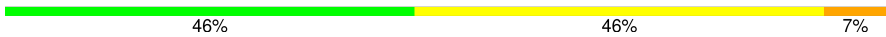
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)

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 $\leq 5\%$. 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	
1	B	349	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 5990 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	349	Total	C	N	O	S	0	0	0
			2749	1818	424	481	26			
1	B	349	Total	C	N	O	S	0	0	0
			2749	1818	424	481	26			

- 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
			39	22	2	15		

- 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
			50	28	2	20		

- 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
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

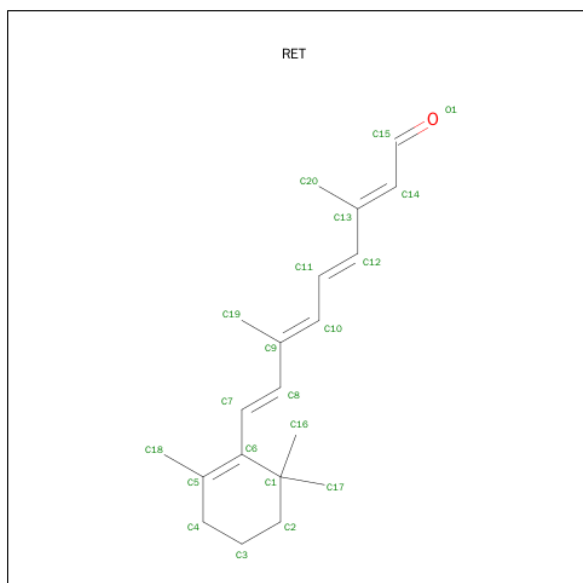
- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O).



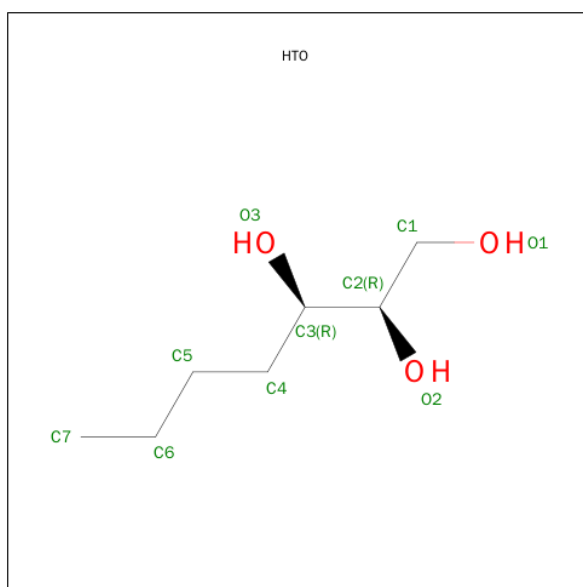
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	C	0	0
			20	20		
7	B	1	Total	C	0	0
			20	20		

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



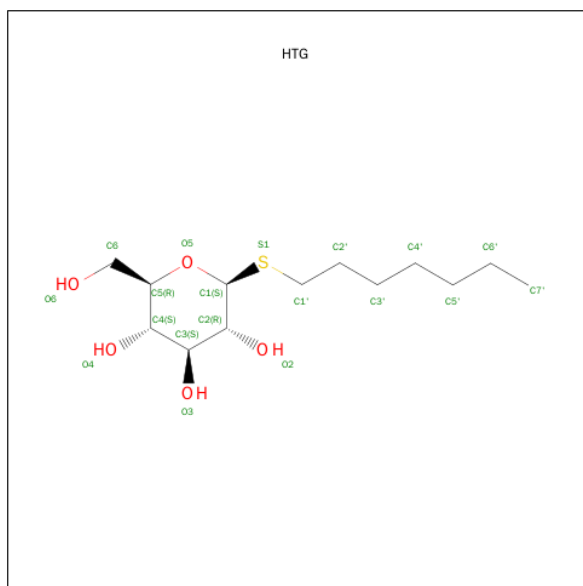
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			17	16	1		
8	A	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C		0	0
			16	16			
8	A	1	Total	C		0	0
			16	16			

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	O	S	0	0
			19	13	5	1		
10	A	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O	S	0	0
			19	13	5	1		
10	B	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 11 is water.

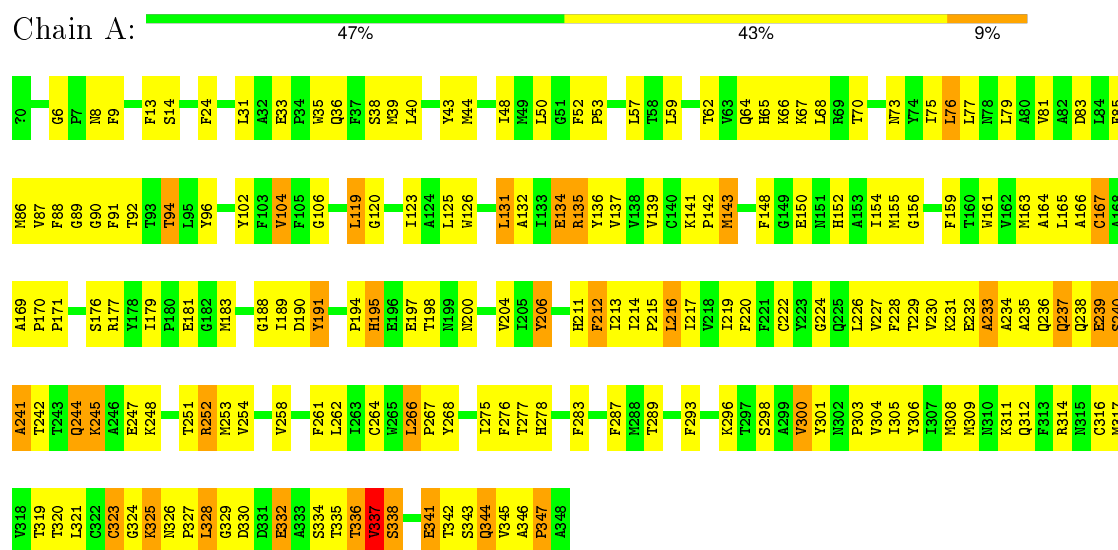
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	58	Total	O	0	0
			58	58		
11	B	50	Total	O	0	0
			50	50		

3 Residue-property plots

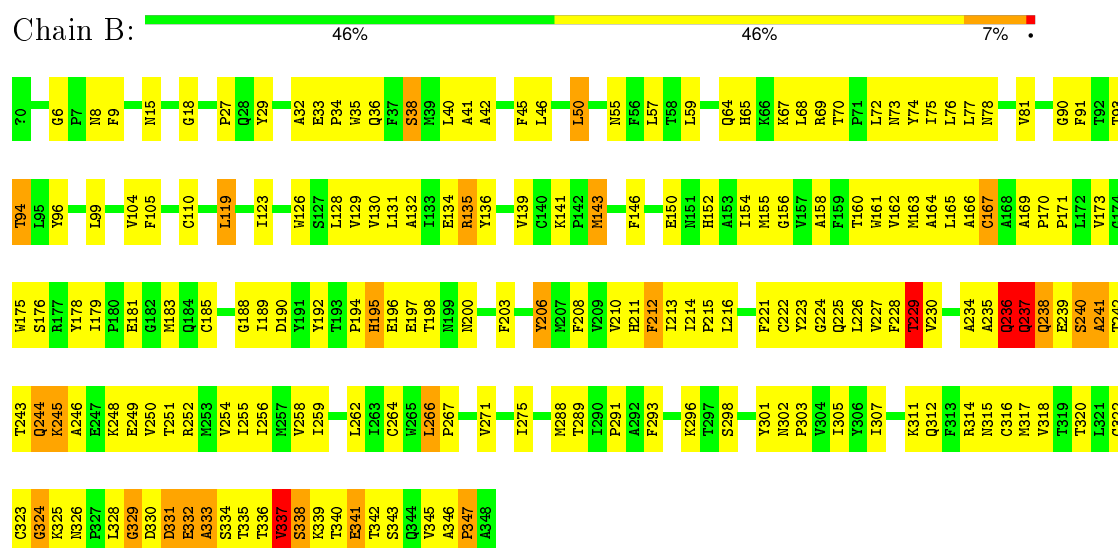
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	95.96 Å 95.96 Å 150.84 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.95	Depositor
% Data completeness (in resolution range)	94.3 (50.00-2.95)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5990	wwPDB-VP
Average B, all atoms (Å ²)	71.0	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: HTG, ZN, BMA, NAG, ACE, HTO, RET, PLM, 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	0.61	0/2831	0.69	1/3859 (0.0%)
1	B	0.56	0/2831	0.66	1/3859 (0.0%)
All	All	0.59	0/5662	0.67	2/7718 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	LYS	CD-CE-NZ	5.64	124.68	111.70
1	B	296	LYS	CD-CE-NZ	5.02	123.24	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	2749	0	2706	203	1
1	B	2749	0	2707	254	0
2	A	39	0	34	3	0
3	B	50	0	43	1	0
4	A	28	0	25	0	0
4	B	28	0	25	0	0
5	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	3	0	0	0	0
6	A	4	0	0	0	0
6	B	3	0	0	0	0
7	A	20	0	27	2	0
7	B	20	0	27	2	0
8	A	50	0	89	1	0
8	B	50	0	89	3	0
9	B	10	0	16	0	0
10	A	38	0	52	3	0
10	B	38	0	52	1	1
11	A	58	0	0	2	0
11	B	50	0	0	10	0
All	All	5990	0	5892	448	1

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 38.

The worst 5 of 448 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:65:HIS:HB3	1:A:337:VAL:HG22	1.38	1.03
1:B:67:LYS:H	1:B:337:VAL:HG21	1.23	1.01
1:A:345:VAL:HG12	1:A:347:PRO:HD3	1.43	1.01
1:B:341:GLU:HG3	1:B:342:THR:H	1.27	0.97
1:B:245:LYS:HA	1:B:245:LYS:HE3	1.47	0.95

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLN:NE2	10:B:1509:HTG:O6[3_655]	2.16	0.04

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	347/349 (99%)	293 (84%)	38 (11%)	16 (5%)	3	15
1	B	347/349 (99%)	291 (84%)	39 (11%)	17 (5%)	3	14
All	All	694/698 (99%)	584 (84%)	77 (11%)	33 (5%)	3	14

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	THR
1	A	240	SER
1	A	241	ALA
1	A	328	LEU
1	B	229	THR

5.3.2 Protein sidechains ⓘ

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	296/296 (100%)	270 (91%)	26 (9%)	12	40
1	B	296/296 (100%)	276 (93%)	20 (7%)	20	54
All	All	592/592 (100%)	546 (92%)	46 (8%)	16	46

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

Mol	Chain	Res	Type
1	A	300	VAL
1	A	344	GLN
1	B	264	CYS
1	A	332	GLU
1	A	337	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	ASN
1	B	8	ASN
1	B	244	GLN
1	A	237	GLN
1	B	237	GLN

5.3.3 RNA ⓘ

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	11,11,12	0.61	0	14,15,17	0.69	0
2	NAG	A	504	2	14,14,15	0.61	0	15,19,21	0.76	0
2	NAG	A	505	1,2	14,14,15	0.56	0	15,19,21	0.90	1 (6%)
4	NAG	A	704	4	14,14,15	0.51	0	15,19,21	0.79	1 (6%)
4	NAG	A	705	1,4	14,14,15	0.54	0	15,19,21	1.01	1 (6%)
3	BMA	B	602	3	11,11,12	0.73	0	14,15,17	0.73	1 (7%)
3	BMA	B	603	3	11,11,12	0.61	0	14,15,17	0.52	0
3	NAG	B	604	3	14,14,15	0.51	0	15,19,21	1.09	1 (6%)
3	NAG	B	605	1,3	14,14,15	0.56	0	15,19,21	0.70	0
4	NAG	B	804	4	14,14,15	0.55	0	15,19,21	0.84	1 (6%)
4	NAG	B	805	1,4	14,14,15	0.60	0	15,19,21	0.78	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	-	0/2/19/22	0/1/1/1
2	NAG	A	504	2	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1,2	-	0/6/23/26	0/1/1/1
4	NAG	A	704	4	-	0/6/23/26	0/1/1/1
4	NAG	A	705	1,4	-	1/6/23/26	0/1/1/1
3	BMA	B	602	3	-	0/2/19/22	0/1/1/1
3	BMA	B	603	3	-	0/2/19/22	0/1/1/1
3	NAG	B	604	3	-	0/6/23/26	0/1/1/1
3	NAG	B	605	1,3	-	0/6/23/26	0/1/1/1
4	NAG	B	804	4	-	0/6/23/26	0/1/1/1
4	NAG	B	805	1,4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	604	NAG	C2-N2-C7	-3.45	118.61	123.04
4	A	705	NAG	C2-N2-C7	-2.68	119.59	123.04
2	A	505	NAG	C2-N2-C7	-2.54	119.78	123.04
4	A	704	NAG	C2-N2-C7	-2.40	119.95	123.04
4	B	804	NAG	C2-N2-C7	-2.31	120.07	123.04

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	NAG	3	0
2	A	505	NAG	3	0
3	B	605	NAG	1	0

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 13 are monoatomic - leaving 13 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
7	RET	A	1296	1	19,20,21	1.52	2 (10%)	27,27,28	1.34	4 (14%)
8	PLM	A	1322	1	16,16,17	0.49	0	14,15,17	0.47	0
8	PLM	A	1323	1	16,16,17	0.48	0	14,15,17	0.48	0
8	PLM	A	1410	-	15,15,17	1.76	3 (20%)	14,14,17	3.30	5 (35%)
10	HTG	A	1507	-	19,19,19	2.84	7 (36%)	22,24,24	2.58	1 (4%)
10	HTG	A	1508	-	19,19,19	2.39	8 (42%)	22,24,24	3.52	3 (13%)
7	RET	B	1296	1	19,20,21	1.70	2 (10%)	27,27,28	1.26	2 (7%)
8	PLM	B	1322	1	16,16,17	0.47	0	14,15,17	0.40	0
8	PLM	B	1323	1	16,16,17	0.59	0	14,15,17	0.48	0
9	HTO	B	1401	-	9,9,9	1.69	1 (11%)	8,10,10	1.18	1 (12%)
8	PLM	B	1407	-	15,15,17	1.70	3 (20%)	14,14,17	3.32	6 (42%)
10	HTG	B	1506	-	19,19,19	2.74	7 (36%)	22,24,24	2.76	2 (9%)
10	HTG	B	1509	-	19,19,19	2.87	8 (42%)	22,24,24	3.07	2 (9%)

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
7	RET	A	1296	1	-	0/13/30/31	0/1/1/1
8	PLM	A	1322	1	-	0/13/14/15	0/0/0/0
8	PLM	A	1323	1	-	0/13/14/15	0/0/0/0
8	PLM	A	1410	-	-	0/13/13/15	0/0/0/0
10	HTG	A	1507	-	-	0/10/30/30	0/1/1/1
10	HTG	A	1508	-	-	0/10/30/30	0/1/1/1
7	RET	B	1296	1	-	0/13/30/31	0/1/1/1
8	PLM	B	1322	1	-	0/13/14/15	0/0/0/0
8	PLM	B	1323	1	-	0/13/14/15	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HTO	B	1401	-	-	0/10/10/10	0/0/0/0
8	PLM	B	1407	-	-	0/13/13/15	0/0/0/0
10	HTG	B	1506	-	-	0/10/30/30	0/1/1/1
10	HTG	B	1509	-	-	0/10/30/30	0/1/1/1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1410	PLM	CC-CB	-4.64	1.24	1.51
8	B	1407	PLM	CC-CB	-4.47	1.25	1.51
8	A	1410	PLM	CB-CA	-3.26	1.32	1.51
8	B	1407	PLM	CB-CA	-3.23	1.32	1.51
8	A	1410	PLM	CD-CC	-2.92	1.34	1.51

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1508	HTG	O5-C1-C2	-2.42	106.90	110.19
9	B	1401	HTO	O3-C3-C4	-2.34	104.14	109.35
7	A	1296	RET	C1-C6-C5	-2.06	119.64	122.66
10	B	1506	HTG	O5-C5-C6	2.02	111.46	106.36
8	B	1407	PLM	C9-C8-C7	2.07	125.24	114.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1296	RET	2	0
8	A	1410	PLM	1	0
10	A	1508	HTG	3	0
7	B	1296	RET	2	0
8	B	1322	PLM	2	0
8	B	1323	PLM	1	0
10	B	1509	HTG	1	1

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.