



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:09 AM GMT

PDB ID : 3HDL
Title : Crystal Structure of Highly Glycosylated Peroxidase from Royal Palm Tree
Authors : Watanabe, L.; Moura, P.R.; Bleicher, L.; Nascimento, A.S.; Zamorano, L.S.; Calvete, J.J.; Bursakov, S.; Roig, M.G.; Shnyrov, V.L.; Polikarpov, I.
Deposited on : 2009-05-07
Resolution : 1.85 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

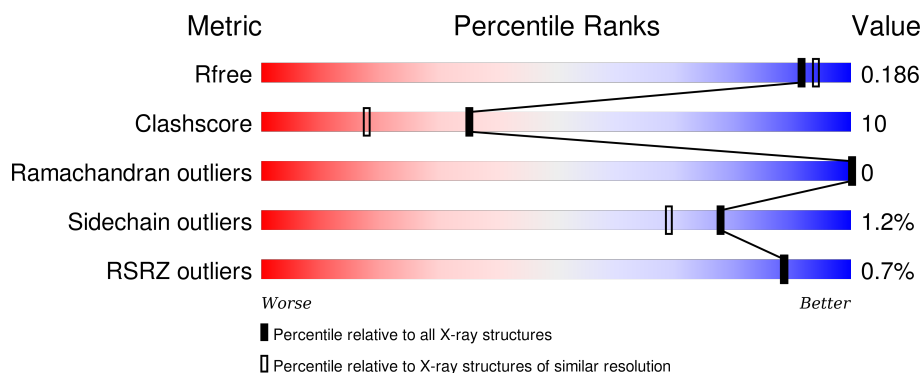
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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))
R_{free}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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.

Mol	Chain	Length	Quality of chain
1	A	304	<div> <div></div> <div>89%</div> <div>11%</div> </div>

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
10	MAN	A	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	NAG	A	1200	X	-	-	-
13	NAG	A	901	X	-	-	-
5	SO4	A	314	-	-	-	X
7	EDO	A	320	-	-	-	X
7	EDO	A	324	-	-	-	X
7	EDO	A	329	-	-	-	X
7	EDO	A	330	-	-	-	X
7	EDO	A	332	-	-	X	-
7	EDO	A	335	-	-	-	X
8	MAN	A	1005	X	-	-	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 3394 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 Royal Palm Tree Peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	12	0
			2288	1425	392	454	17			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

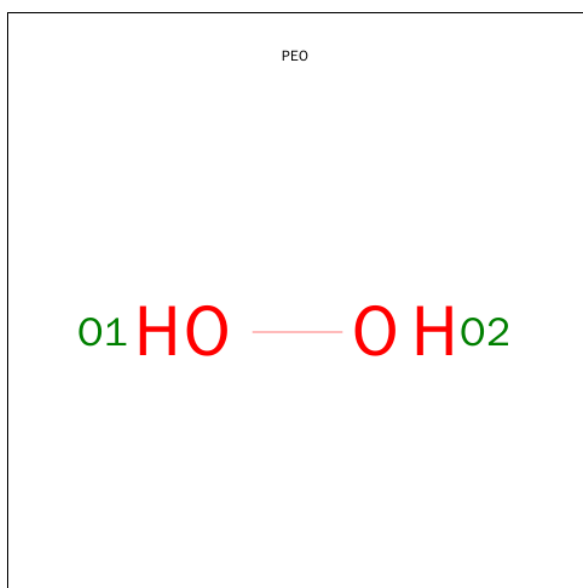


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

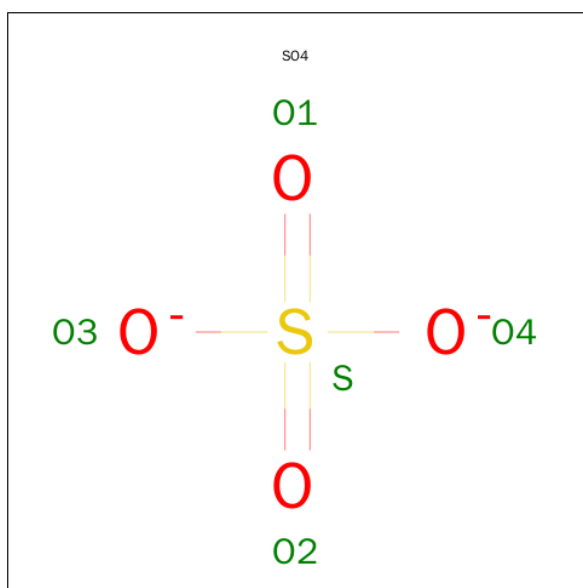
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O		0	0
			2	2			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



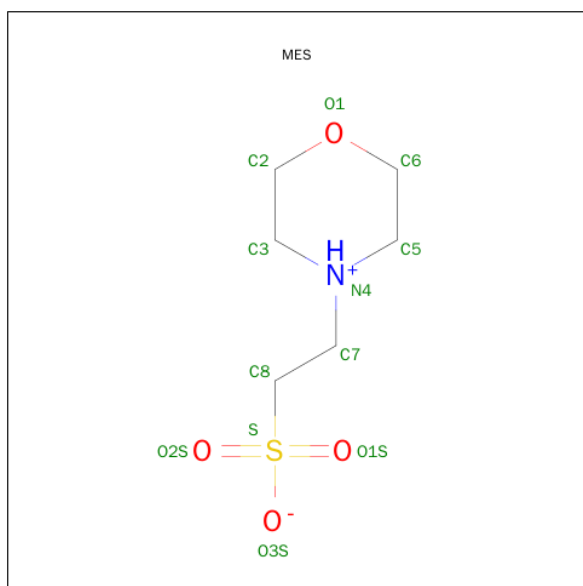
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

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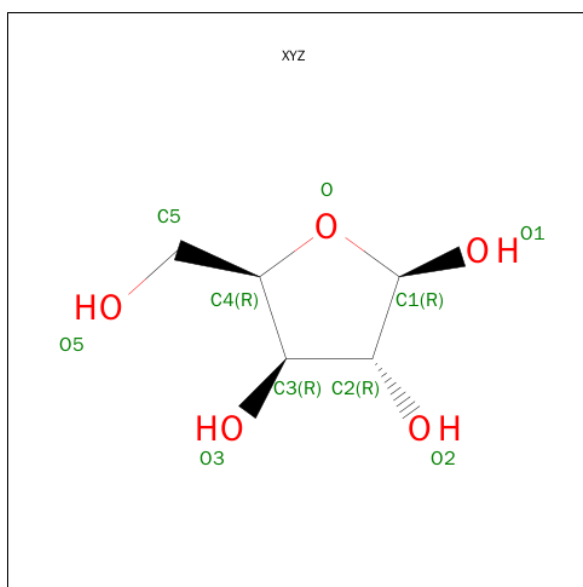
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	6	Total	C	N	O	0	0
			71	40	2	29		
8	A	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 9 is BETA-D-XYLOFURANOSE (three-letter code: XYZ) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			9	5	4		

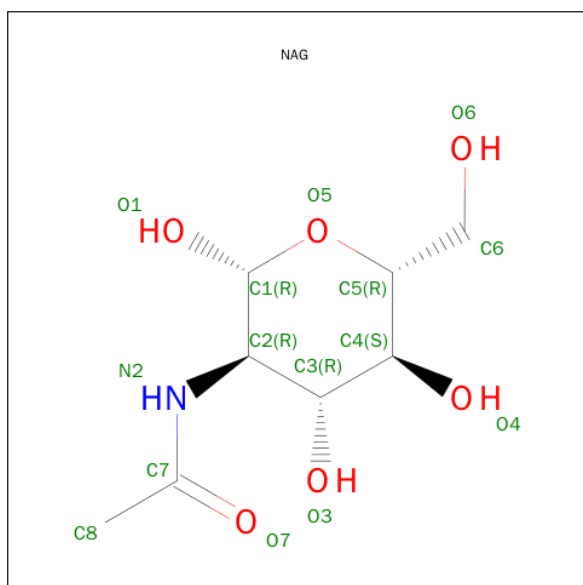
- Molecule 10 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 11 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	3	Total	C	N	O	0	0
			38	22	2	14		
11	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 12 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	N	O	0	0
			14	8	1	5		
12	A	1	Total	C	N	O	0	0
			14	8	1	5		
12	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 13 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	2	Total	C	N	O	0	0
			28	16	2	10		

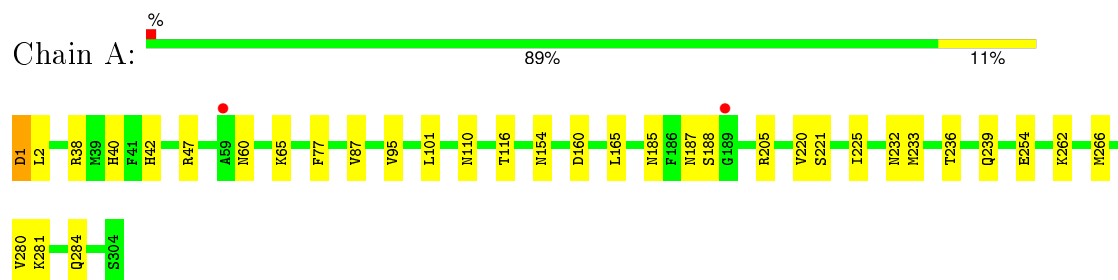
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	586	Total	O	0	0
			586	586		

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.

- Molecule 1: Royal Palm Tree Peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.82Å 117.82Å 93.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.78 – 1.85 44.78 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.78-1.85) 99.8 (44.78-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.176 , 0.187 0.177 , 0.186	Depositor DCC
R_{free} test set	3241 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.4	EDS
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 63971 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3394	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: NAG, CA, EDO, PEO, FUC, MES, HEM, MAN, XYZ, SO4

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	0.26	0/2357	0.44	0/3215

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
8	A	1	0
10	A	1	0
13	A	1	0
All	All	3	0

There are no bond length outliers.

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	503	MAN	C1
13	A	901	NAG	C1
8	A	1005	MAN	C1

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	2288	0	2270	40	0
2	A	43	0	30	4	0
3	A	2	0	0	0	0
4	A	2	0	0	1	0
5	A	40	0	0	0	0
6	A	12	0	12	2	0
7	A	64	0	96	21	0
8	A	142	0	121	0	0
9	A	9	0	8	1	0
10	A	60	0	52	2	0
11	A	76	0	68	0	0
12	A	42	0	39	4	0
13	A	28	0	25	0	0
14	A	586	0	0	20	4
All	All	3394	0	2721	54	4

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 10.

The worst 5 of 54 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)
9:A:406:XYZ:H51	14:A:570:HOH:O	1.63	0.98
1:A:116:THR:OG1	14:A:367:HOH:O	1.90	0.88
1:A:47:ARG:HH12	7:A:326:EDO:H21	1.38	0.88
1:A:232:ASN:HD21	7:A:322:EDO:H12	1.40	0.87
12:A:1100:NAG:H2	14:A:554:HOH:O	1.80	0.82

All (4) 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)
14:A:575:HOH:O	14:A:580:HOH:O[3_564]	1.71	0.49
14:A:518:HOH:O	14:A:582:HOH:O[6_555]	1.81	0.39
14:A:913:HOH:O	14:A:915:HOH:O[2_665]	1.89	0.31
14:A:488:HOH:O	14:A:492:HOH:O[3_564]	2.13	0.07

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	314/304 (103%)	311 (99%)	3 (1%)	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 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	256/244 (105%)	252 (98%)	4 (2%)	70	57

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	101[A]	LEU
1	A	101[B]	LEU
1	A	110	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	110	ASN
1	A	118	GLN
1	A	137	GLN

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Mol	Chain	Res	Type
1	A	187	ASN

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 ⓘ

25 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	$\# Z > 2$
8	NAG	A	1000	1,8	14,14,15	0.45	0	15,19,21	0.99	1 (6%)
8	NAG	A	1001	8	14,14,15	0.47	0	15,19,21	0.86	1 (6%)
8	FUC	A	1002	8	10,10,11	0.61	0	14,14,16	0.78	0
8	MAN	A	1003	8	11,11,12	0.72	0	14,15,17	1.44	3 (21%)
8	MAN	A	1004	8	11,11,12	0.55	0	14,15,17	0.61	0
8	MAN	A	1005	8	11,11,12	0.65	0	14,15,17	1.24	2 (14%)
8	NAG	A	400	1,8	14,14,15	0.50	0	15,19,21	0.72	0
8	NAG	A	401	8	14,14,15	0.46	0	15,19,21	0.77	0
8	FUC	A	402	8	10,10,11	0.59	0	14,14,16	0.74	0
8	MAN	A	403	8	11,11,12	0.68	0	14,15,17	0.61	0
8	MAN	A	404	8	11,11,12	0.55	0	14,15,17	0.65	0
8	MAN	A	405	8	11,11,12	0.60	0	14,15,17	0.88	0
10	NAG	A	500	1,10	14,14,15	0.42	0	15,19,21	1.10	1 (6%)
10	NAG	A	501	10	14,14,15	0.47	0	15,19,21	0.77	0
10	FUC	A	502	10	10,10,11	0.57	0	14,14,16	0.74	1 (7%)
10	MAN	A	503	10	11,11,12	0.59	0	14,15,17	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	A	504	10	11,11,12	0.61	0	14,15,17	1.27	3 (21%)
11	NAG	A	600	1,11	14,14,15	0.46	0	15,19,21	1.13	1 (6%)
11	NAG	A	601	11	14,14,15	0.48	0	15,19,21	0.79	0
11	FUC	A	602	11	10,10,11	0.59	0	14,14,16	0.84	1 (7%)
11	NAG	A	800	1,11	14,14,15	0.51	0	15,19,21	0.64	0
11	NAG	A	801	11	14,14,15	0.44	0	15,19,21	0.94	1 (6%)
11	FUC	A	802	11	10,10,11	0.57	0	14,14,16	0.80	1 (7%)
13	NAG	A	900	1,13	14,14,15	0.50	0	15,19,21	0.67	0
13	NAG	A	901	13	14,14,15	0.44	0	15,19,21	0.80	1 (6%)

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
8	NAG	A	1000	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	1001	8	-	0/6/23/26	0/1/1/1
8	FUC	A	1002	8	-	0/0/17/20	0/1/1/1
8	MAN	A	1003	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1004	8	-	0/2/19/22	1/1/1/1
8	MAN	A	1005	8	1/1/4/5	0/2/19/22	0/1/1/1
8	NAG	A	400	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	401	8	-	0/6/23/26	0/1/1/1
8	FUC	A	402	8	-	0/0/17/20	0/1/1/1
8	MAN	A	403	8	-	0/2/19/22	0/1/1/1
8	MAN	A	404	8	-	0/2/19/22	1/1/1/1
8	MAN	A	405	8	-	0/2/19/22	0/1/1/1
10	NAG	A	500	1,10	-	0/6/23/26	0/1/1/1
10	NAG	A	501	10	-	0/6/23/26	0/1/1/1
10	FUC	A	502	10	-	0/0/17/20	0/1/1/1
10	MAN	A	503	10	1/1/4/5	0/2/19/22	0/1/1/1
10	MAN	A	504	10	-	0/2/19/22	0/1/1/1
11	NAG	A	600	1,11	-	0/6/23/26	0/1/1/1
11	NAG	A	601	11	-	2/6/23/26	0/1/1/1
11	FUC	A	602	11	-	0/0/17/20	0/1/1/1
11	NAG	A	800	1,11	-	0/6/23/26	0/1/1/1
11	NAG	A	801	11	-	0/6/23/26	0/1/1/1
11	FUC	A	802	11	-	0/0/17/20	0/1/1/1
13	NAG	A	900	1,13	-	0/6/23/26	0/1/1/1
13	NAG	A	901	13	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
8	A	1005	MAN	O5-C1-C2	-2.48	106.83	110.86
10	A	504	MAN	O5-C1-C2	-2.12	107.42	110.86
13	A	901	NAG	C1-O5-C5	2.10	114.91	112.25
11	A	602	FUC	O5-C5-C6	2.15	109.68	106.13
10	A	502	FUC	O5-C5-C6	2.19	109.75	106.13

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	1005	MAN	C1
10	A	503	MAN	C1
13	A	901	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	601	NAG	O7-C7-N2-C2
11	A	601	NAG	C8-C7-N2-C2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	404	MAN	C1-C2-C3-C4-C5-O5
8	A	1004	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	504	MAN	2	0

5.6 Ligand geometry

Of 33 ligands modelled in this entry, 2 are monoatomic - leaving 31 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	$\# Z > 2$
12	NAG	A	1100	1	14,14,15	0.44	0	15,19,21	1.47	3 (20%)
12	NAG	A	1200	1	14,14,15	0.50	0	15,19,21	0.69	0
2	HEM	A	305	1,4	30,50,50	2.07	8 (26%)	24,82,82	2.51	13 (54%)
4	PEO	A	309	2	1,1,1	0.06	0	0,0,0	0.00	-
5	SO4	A	311	-	4,4,4	0.21	0	6,6,6	0.10	0
5	SO4	A	312	-	4,4,4	0.22	0	6,6,6	0.19	0
5	SO4	A	313	-	4,4,4	0.21	0	6,6,6	0.10	0
5	SO4	A	314	-	4,4,4	0.24	0	6,6,6	0.18	0
5	SO4	A	315	-	4,4,4	0.22	0	6,6,6	0.13	0
5	SO4	A	316	-	4,4,4	0.17	0	6,6,6	0.07	0
5	SO4	A	317	-	4,4,4	0.21	0	6,6,6	0.15	0
5	SO4	A	318	-	4,4,4	0.21	0	6,6,6	0.14	0
6	MES	A	319	-	11,12,12	0.55	0	14,16,16	2.82	5 (35%)
7	EDO	A	320	-	3,3,3	0.31	0	2,2,2	0.94	0
7	EDO	A	321	-	3,3,3	0.40	0	2,2,2	0.53	0
7	EDO	A	322	-	3,3,3	0.46	0	2,2,2	0.42	0
7	EDO	A	323	-	3,3,3	0.47	0	2,2,2	0.48	0
7	EDO	A	324	-	3,3,3	0.46	0	2,2,2	0.51	0
7	EDO	A	326	-	3,3,3	0.47	0	2,2,2	0.43	0
7	EDO	A	327	-	3,3,3	0.45	0	2,2,2	0.53	0
7	EDO	A	328	-	3,3,3	0.47	0	2,2,2	0.46	0
7	EDO	A	329	-	3,3,3	0.45	0	2,2,2	0.51	0
7	EDO	A	330	-	3,3,3	0.48	0	2,2,2	0.39	0
7	EDO	A	331	-	3,3,3	0.49	0	2,2,2	0.37	0
7	EDO	A	332	-	3,3,3	0.43	0	2,2,2	0.50	0
7	EDO	A	333	-	3,3,3	0.51	0	2,2,2	0.33	0
7	EDO	A	334	-	3,3,3	0.47	0	2,2,2	0.40	0
7	EDO	A	335	-	3,3,3	0.47	0	2,2,2	0.41	0
7	EDO	A	336	-	3,3,3	0.45	0	2,2,2	0.40	0
9	XYZ	A	406	-	9,9,10	0.43	0	12,12,14	1.23	1 (8%)
12	NAG	A	700	1	14,14,15	0.46	0	15,19,21	0.90	2 (13%)

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
12	NAG	A	1100	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	A	1200	1	1/1/5/7	0/6/23/26	0/1/1/1
2	HEM	A	305	1,4	-	0/10/54/54	0/0/8/8
4	PEO	A	309	2	-	0/0/0/0	0/0/0/0
5	SO4	A	311	-	-	0/0/0/0	0/0/0/0
5	SO4	A	312	-	-	0/0/0/0	0/0/0/0
5	SO4	A	313	-	-	0/0/0/0	0/0/0/0
5	SO4	A	314	-	-	0/0/0/0	0/0/0/0
5	SO4	A	315	-	-	0/0/0/0	0/0/0/0
5	SO4	A	316	-	-	0/0/0/0	0/0/0/0
5	SO4	A	317	-	-	0/0/0/0	0/0/0/0
5	SO4	A	318	-	-	0/0/0/0	0/0/0/0
6	MES	A	319	-	-	0/6/14/14	0/1/1/1
7	EDO	A	320	-	-	0/1/1/1	0/0/0/0
7	EDO	A	321	-	-	0/1/1/1	0/0/0/0
7	EDO	A	322	-	-	0/1/1/1	0/0/0/0
7	EDO	A	323	-	-	0/1/1/1	0/0/0/0
7	EDO	A	324	-	-	0/1/1/1	0/0/0/0
7	EDO	A	326	-	-	0/1/1/1	0/0/0/0
7	EDO	A	327	-	-	0/1/1/1	0/0/0/0
7	EDO	A	328	-	-	0/1/1/1	0/0/0/0
7	EDO	A	329	-	-	0/1/1/1	0/0/0/0
7	EDO	A	330	-	-	0/1/1/1	0/0/0/0
7	EDO	A	331	-	-	0/1/1/1	0/0/0/0
7	EDO	A	332	-	-	0/1/1/1	0/0/0/0
7	EDO	A	333	-	-	0/1/1/1	0/0/0/0
7	EDO	A	334	-	-	0/1/1/1	0/0/0/0
7	EDO	A	335	-	-	0/1/1/1	0/0/0/0
7	EDO	A	336	-	-	0/1/1/1	0/0/0/0
9	XYZ	A	406	-	-	0/2/15/18	0/1/1/1
12	NAG	A	700	1	-	2/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	305	HEM	C3B-C4B	-6.55	1.46	1.51
2	A	305	HEM	C3D-C4D	-4.97	1.45	1.51
2	A	305	HEM	C2C-C1C	-3.49	1.45	1.52
2	A	305	HEM	C2D-C1D	-2.10	1.45	1.51
2	A	305	HEM	C2B-C1B	-2.00	1.45	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	305	HEM	CBD-CAD-C3D	-4.01	101.89	113.55
2	A	305	HEM	C3B-CAB-CBB	-3.15	119.63	124.46
2	A	305	HEM	CAA-CBA-CGA	-2.70	107.80	112.75
2	A	305	HEM	C3B-C4B-NB	-2.14	107.54	111.63
2	A	305	HEM	CAA-C2A-C1A	-2.13	124.70	127.01

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	1200	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	700	NAG	O7-C7-N2-C2
12	A	700	NAG	C8-C7-N2-C2

There are no ring outliers.

17 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1100	NAG	3	0
2	A	305	HEM	4	0
4	A	309	PEO	1	0
6	A	319	MES	2	0
7	A	320	EDO	2	0
7	A	321	EDO	3	0
7	A	322	EDO	1	0
7	A	323	EDO	1	0
7	A	324	EDO	2	0
7	A	326	EDO	2	0
7	A	327	EDO	1	0
7	A	330	EDO	2	0
7	A	332	EDO	4	0
7	A	335	EDO	1	0
7	A	336	EDO	2	0
9	A	406	XYZ	1	0
12	A	700	NAG	1	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	304/304 (100%)	-0.19	2 (0%) 89 88	21, 28, 42, 63	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	GLY	2.9
1	A	59	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	NAG	A	401	14/15	0.89	0.24	-	37,46,53,57	0
8	MAN	A	1004	11/12	0.84	0.33	-	72,84,95,105	0
8	MAN	A	1003	11/12	0.88	0.37	-	85,101,107,109	0
8	MAN	A	404	11/12	0.88	0.47	-	78,98,108,108	0
8	NAG	A	1000	14/15	0.94	0.12	-	33,38,48,53	0
8	MAN	A	1005	11/12	0.90	0.48	-	109,111,115,116	0
8	NAG	A	1001	14/15	0.89	0.23	-	44,51,65,66	0
8	FUC	A	402	10/11	0.96	0.16	-	34,47,49,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	MAN	A	405	11/12	0.65	0.49	-	103,109,116,117	0
11	NAG	A	801	14/15	0.88	0.47	-	102,108,117,120	0
11	NAG	A	800	14/15	0.92	0.27	-	49,70,85,86	0
8	FUC	A	1002	10/11	0.94	0.22	-	49,58,63,65	0
11	FUC	A	602	10/11	0.85	0.33	-	62,79,83,85	0
10	MAN	A	503	11/12	0.78	0.45	-	68,78,88,89	0
10	FUC	A	502	10/11	0.87	0.23	-	74,83,86,94	0
13	NAG	A	901	14/15	0.84	0.38	-	91,96,102,103	0
11	FUC	A	802	10/11	0.89	0.36	-	89,94,99,101	0
10	NAG	A	501	14/15	0.95	0.21	-	51,60,69,85	0
10	MAN	A	504	11/12	0.81	0.32	-	54,66,92,97	0
10	NAG	A	500	14/15	0.90	0.20	-	52,59,74,91	0
8	NAG	A	400	14/15	0.96	0.11	-	30,37,47,48	0
13	NAG	A	900	14/15	0.84	0.34	-	54,65,76,80	0
11	NAG	A	600	14/15	0.88	0.18	-	37,60,71,73	0
8	MAN	A	403	11/12	0.85	0.34	-	59,82,94,99	0
11	NAG	A	601	14/15	0.83	0.25	-	75,80,87,92	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	EDO	A	320	4/4	0.94	0.23	7.10	30,32,34,49	0
7	EDO	A	329	4/4	0.92	0.17	5.26	49,51,62,65	0
7	EDO	A	324	4/4	0.78	0.24	4.74	52,57,57,58	0
7	EDO	A	330	4/4	0.75	0.25	4.14	45,66,71,73	0
5	SO4	A	314	5/5	0.99	0.11	3.05	30,42,49,65	0
7	EDO	A	335	4/4	0.90	0.14	2.43	37,45,54,60	0
7	EDO	A	333	4/4	0.91	0.10	1.91	29,40,48,49	0
7	EDO	A	328	4/4	0.95	0.14	1.72	37,41,53,65	0
3	CA	A	307	1/1	0.99	0.12	1.40	27,27,27,27	0
6	MES	A	319	12/12	0.96	0.16	1.07	33,36,46,48	0
3	CA	A	306	1/1	1.00	0.10	0.99	25,25,25,25	0
7	EDO	A	322	4/4	0.93	0.14	0.59	45,47,50,67	0
7	EDO	A	334	4/4	0.92	0.10	0.26	45,52,55,67	0
2	HEM	A	305	43/43	0.98	0.13	0.20	18,23,26,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	A	312	5/5	0.99	0.08	-1.40	34,40,44,53	0
7	EDO	A	331	4/4	0.96	0.08	-1.44	30,37,43,49	0
12	NAG	A	1100	14/15	0.65	0.40	-	81,102,111,119	0
5	SO4	A	315	5/5	0.97	0.11	-	51,55,60,81	0
4	PEO	A	309	2/2	0.98	0.13	-	27,27,27,31	1
7	EDO	A	323	4/4	0.49	0.26	-	78,83,84,86	0
9	XYZ	A	406	9/10	0.88	0.38	-	94,98,103,108	0
7	EDO	A	327	4/4	0.85	0.16	-	62,63,67,68	0
5	SO4	A	311	5/5	0.87	0.30	-	116,117,118,123	0
7	EDO	A	321	4/4	0.97	0.29	-	35,43,46,54	0
7	EDO	A	326	4/4	0.81	0.12	-	59,67,71,73	0
7	EDO	A	332	4/4	0.96	0.14	-	55,57,66,66	0
5	SO4	A	316	5/5	0.90	0.32	-	96,106,109,112	0
12	NAG	A	700	14/15	0.78	0.19	-	64,95,107,110	0
12	NAG	A	1200	14/15	0.73	0.38	-	91,108,116,124	0
5	SO4	A	317	5/5	0.84	0.39	-	116,120,122,126	0
7	EDO	A	336	4/4	0.94	0.22	-	38,50,57,60	0
5	SO4	A	313	5/5	0.96	0.27	-	74,87,96,102	0
5	SO4	A	318	5/5	0.94	0.15	-	113,114,116,117	0

6.5 Other polymers [i](#)

There are no such residues in this entry.