



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:36 PM GMT

PDB ID : 4CUO
Title : Banyan peroxidase with glycosylation
Authors : Palm, G.J.; Sharma, A.; Hinrichs, W.
Deposited on : 2014-03-20
Resolution : 1.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

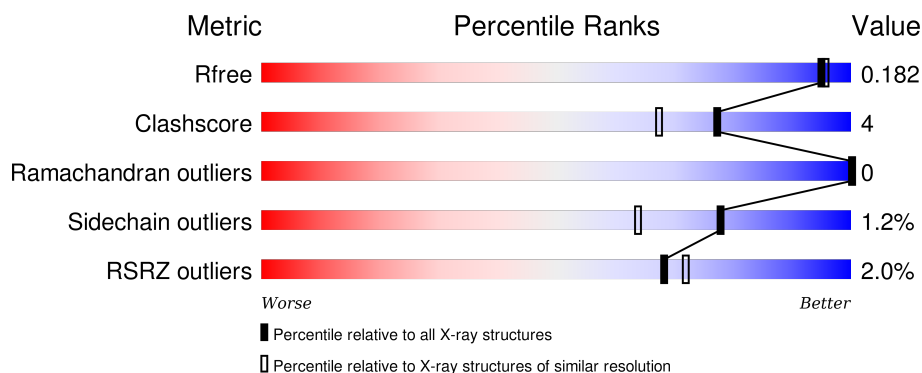
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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	4802 (1.70-1.66)
Clashscore	102246	5317 (1.70-1.66)
Ramachandran outliers	100387	5225 (1.70-1.66)
Sidechain outliers	100360	5224 (1.70-1.66)
RSRZ outliers	91569	4813 (1.70-1.66)

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	306	<div> <div>2%</div> <div>91%</div> <div>8%</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	SO4	A	1332	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CO3	A	1338	-	-	-	X
5	NAG	A	1317	-	-	-	X
6	NAG	A	1320	X	-	-	-
6	NAG	A	1324	X	-	-	X

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 2989 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 BANYAN PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	11	0
			2360	1466	405	478	11			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			24	14	1	9		

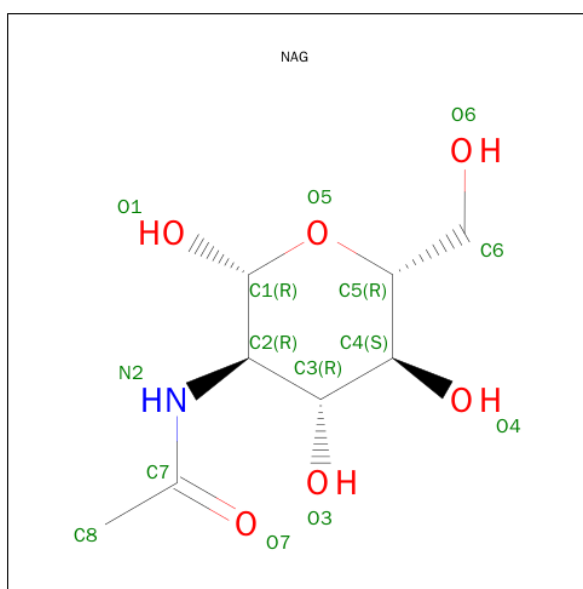
- Molecule 4 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	7	Total	C	N	O	0	0
			80	45	2	33		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			38	22	2	14		
5	A	3	Total	C	N	O	0	1
			39	22	2	15		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

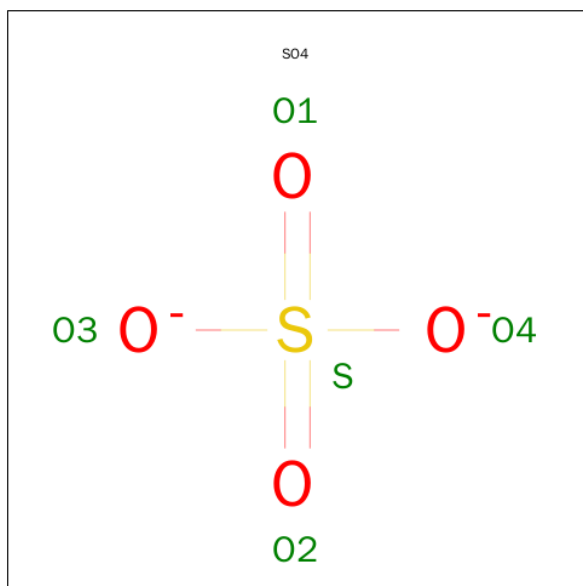
- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

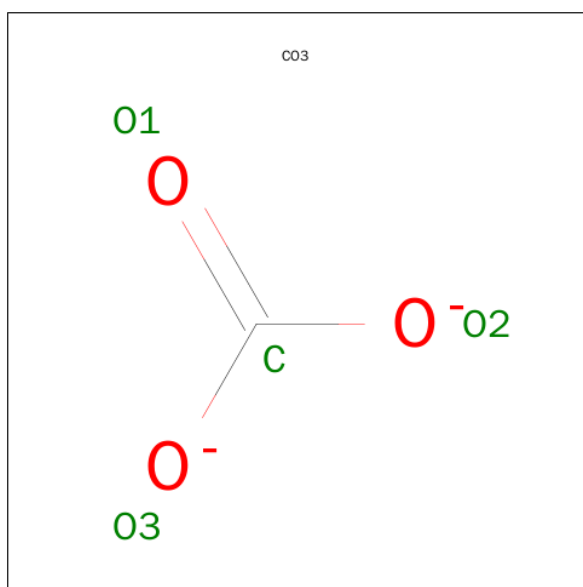
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total Cl 3 3	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 11 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			4	1	3		
11	A	1	Total	C	O	0	0
			4	1	3		
11	A	1	Total	C	O	0	0
			4	1	3		
11	A	1	Total	C	O	0	0
			4	1	3		

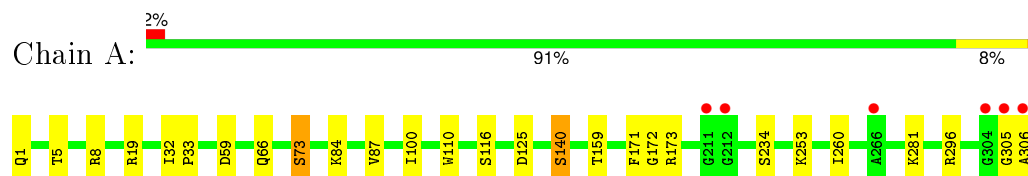
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	321	Total	O	0	5
			326	326		

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: BANYAN PEROXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.11Å 73.11Å 164.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.32 – 1.67 19.78 – 1.67	Depositor EDS
% Data completeness (in resolution range)	99.6 (63.32-1.67) 99.7 (19.78-1.67)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.157 , 0.180 0.159 , 0.182	Depositor DCC
R_{free} test set	3032 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.3	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 60287 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2989	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: SO4, CO3, BMA, NAG, CL, SNN, NA, CA, XYS, FUC, HEM, 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	1.07	2/2418 (0.1%)	1.00	4/3290 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	SER	CB-OG	-6.54	1.33	1.42
1	A	140	SER	CB-OG	-5.19	1.35	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	125	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	173	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	296	ARG	NE-CZ-NH2	5.58	123.09	120.30

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	2360	0	2290	18	0
2	A	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	24	0	22	1	0
4	A	80	0	68	1	0
5	A	77	0	63	0	0
6	A	42	0	39	2	0
7	A	2	0	0	0	0
8	A	1	0	0	0	0
9	A	3	0	0	0	0
10	A	15	0	0	0	0
11	A	16	0	0	1	0
12	A	326	0	0	5	0
All	All	2989	0	2512	19	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 4.

All (19) 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:87[B]:VAL:HG21	1:A:100:ILE:HD11	1.69	0.74
1:A:253:LYS:HG2	12:A:2254:HOH:O	1.90	0.71
1:A:260:ILE:HD11	6:A:1325:NAG:H82	1.72	0.71
1:A:305[B]:GLY:O	1:A:306[B]:ALA:HB2	1.93	0.69
4:A:1314:XY5:H51	12:A:2312:HOH:O	1.96	0.65
1:A:5:THR:HB	1:A:8:ARG:HD3	1.91	0.52
1:A:305[B]:GLY:O	1:A:306[B]:ALA:CB	2.58	0.52
1:A:59[A]:ASP:HB2	1:A:306[A]:ALA:CB	2.41	0.51
1:A:159:THR:HG21	6:A:1325:NAG:C1	2.46	0.46
1:A:19:ARG:NH1	11:A:1335:CO3:O2	2.50	0.45
1:A:32:ILE:CG2	1:A:33:PRO:HD3	2.47	0.44
1:A:73:SER:HB2	12:A:2100:HOH:O	2.18	0.43
1:A:234[B]:SER:OG	12:A:2243:HOH:O	2.20	0.43
1:A:281[B]:LYS:NZ	12:A:2189:HOH:O	2.17	0.43
1:A:110:TRP:CD1	1:A:116:SER:HB3	2.53	0.42
1:A:172:GLY:HA3	2:A:1307:HEM:HAD1	2.00	0.42
1:A:84:LYS:HA	1:A:87[B]:VAL:HG22	2.03	0.41
1:A:253:LYS:HA	1:A:253:LYS:HD3	1.97	0.41
1:A:66:GLN:HB3	3:A:1308:NAG:H82	2.03	0.41

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	311/306 (102%)	306 (98%)	5 (2%)	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	268/260 (103%)	265 (99%)	3 (1%)	80	67

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	140	SER
1	A	171	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	23	GLN
1	A	47	ASN
1	A	136	GLN
1	A	155	GLN

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Mol	Chain	Res	Type
1	A	210	GLN
1	A	239	GLN
1	A	273	ASN
1	A	284	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	SNN	A	290	1	7,8,8	7.40	2 (28%)	7,11,11	9.50	5 (71%)

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
1	SNN	A	290	1	-	0/0/12/12	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	SNN	C2-N1	11.71	1.52	1.37
1	A	290	SNN	C5-N1	15.52	1.60	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	SNN	C5-N1-C2	-16.55	97.08	113.76
1	A	290	SNN	O2-C2-N1	-5.96	117.62	124.83
1	A	290	SNN	O5-C5-N1	-2.26	122.13	125.13
1	A	290	SNN	C4-C5-N1	10.97	113.46	108.27
1	A	290	SNN	C3-C2-N1	13.91	118.12	107.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

16 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
3	NAG	A	1308	1,3	14,14,15	0.68	0	15,19,21	2.35	3 (20%)
3	FUC	A	1309	3	10,10,11	0.62	0	14,14,16	0.82	1 (7%)
4	NAG	A	1310	1,4	14,14,15	0.82	0	15,19,21	1.45	2 (13%)
4	FUC	A	1311	4	10,10,11	1.26	1 (10%)	14,14,16	1.25	1 (7%)
4	NAG	A	1312	4	14,14,15	0.85	0	15,19,21	1.30	2 (13%)
4	BMA	A	1313	4	11,11,12	1.06	1 (9%)	14,15,17	1.17	1 (7%)
4	XYS	A	1314	4	9,9,10	1.68	2 (22%)	12,12,14	2.29	4 (33%)
4	MAN	A	1315	4	11,11,12	0.62	0	14,15,17	1.83	3 (21%)
4	MAN	A	1316	4	11,11,12	0.82	1 (9%)	14,15,17	1.82	4 (28%)
5	NAG	A	1317	1,5	14,14,15	0.78	0	15,19,21	1.20	2 (13%)
5	FUC	A	1318	5	10,10,11	0.76	0	14,14,16	1.37	3 (21%)
5	NAG	A	1319	5	14,14,15	0.54	0	15,19,21	0.99	0
5	NAG	A	1321[A]	-	14,14,15	0.78	0	15,19,21	1.25	2 (13%)
5	NAG	A	1321[B]	-	14,14,15	0.78	0	15,19,21	1.28	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUC	A	1322	5	10,10,11	0.61	0	14,14,16	1.06	0
5	NAG	A	1323	5	14,14,15	0.49	0	15,19,21	1.93	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
3	NAG	A	1308	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	1309	3	-	0/0/17/20	0/1/1/1
4	NAG	A	1310	1,4	-	0/6/23/26	0/1/1/1
4	FUC	A	1311	4	-	0/0/17/20	0/1/1/1
4	NAG	A	1312	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1313	4	-	0/2/19/22	0/1/1/1
4	XYS	A	1314	4	-	0/0/14/17	0/1/1/1
4	MAN	A	1315	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1316	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1317	1,5	-	0/6/23/26	0/1/1/1
5	FUC	A	1318	5	-	0/0/17/20	0/1/1/1
5	NAG	A	1319	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1321[A]	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1321[B]	-	-	0/6/23/26	0/1/1/1
5	FUC	A	1322	5	-	0/0/17/20	0/1/1/1
5	NAG	A	1323	5	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1316	MAN	C2-C3	2.27	1.55	1.52
4	A	1313	BMA	O2-C2	2.87	1.49	1.43
4	A	1311	FUC	C2-C3	2.91	1.56	1.52
4	A	1314	XYS	O5-C1	3.15	1.49	1.42
4	A	1314	XYS	C2-C3	3.22	1.56	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1308	NAG	C2-N2-C7	-6.42	114.79	123.04
4	A	1310	NAG	C2-N2-C7	-3.65	118.36	123.04
4	A	1310	NAG	O3-C3-C4	-2.99	103.61	110.34
5	A	1321[A]	NAG	C4-C3-C2	-2.68	107.07	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1321[B]	NAG	C4-C3-C2	-2.68	107.07	111.23
5	A	1321[A]	NAG	C3-C4-C5	-2.64	105.60	110.20
5	A	1321[B]	NAG	C3-C4-C5	-2.64	105.60	110.20
4	A	1316	MAN	C1-C2-C3	-2.63	106.43	109.54
4	A	1311	FUC	C1-C2-C3	-2.51	106.58	109.54
4	A	1313	BMA	C1-C2-C3	-2.50	106.59	109.54
4	A	1314	XYS	C5-O5-C1	-2.33	107.81	111.57
5	A	1317	NAG	O6-C6-C5	-2.19	104.10	111.33
3	A	1308	NAG	O3-C3-C4	-2.09	105.64	110.34
4	A	1312	NAG	O4-C4-C3	-2.07	105.68	110.34
4	A	1315	MAN	C1-C2-C3	-2.05	107.11	109.54
5	A	1317	NAG	C1-O5-C5	2.12	114.94	112.25
4	A	1316	MAN	O5-C5-C6	2.20	112.11	107.35
5	A	1318	FUC	O5-C5-C4	2.20	113.35	109.53
3	A	1309	FUC	O5-C5-C6	2.35	110.01	106.13
4	A	1314	XYS	O3-C3-C2	2.35	114.25	110.00
5	A	1318	FUC	O5-C5-C6	2.37	110.05	106.13
4	A	1315	MAN	O2-C2-C1	2.74	114.71	109.21
5	A	1318	FUC	C1-O5-C5	2.80	116.70	112.38
4	A	1314	XYS	C4-C3-C2	3.00	114.20	111.24
4	A	1316	MAN	C1-O5-C5	3.19	116.30	112.25
4	A	1312	NAG	C1-O5-C5	3.32	116.46	112.25
4	A	1316	MAN	O2-C2-C3	3.48	117.11	110.12
5	A	1323	NAG	C2-N2-C7	3.85	127.98	123.04
4	A	1315	MAN	C1-O5-C5	4.77	118.30	112.25
5	A	1323	NAG	C1-O5-C5	4.77	118.30	112.25
3	A	1308	NAG	C1-O5-C5	4.96	118.54	112.25
4	A	1314	XYS	C1-C2-C3	5.56	116.12	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1308	NAG	1	0
4	A	1314	XYS	1	0

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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
2	HEM	A	1307	1	30,50,50	2.40	8 (26%)	24,82,82	2.42	9 (37%)
6	NAG	A	1320	1	14,14,15	0.62	0	15,19,21	1.24	3 (20%)
6	NAG	A	1324	1	14,14,15	0.74	1 (7%)	15,19,21	1.22	1 (6%)
6	NAG	A	1325	1	14,14,15	0.89	1 (7%)	15,19,21	2.65	5 (33%)
10	SO4	A	1332	-	4,4,4	0.83	0	6,6,6	0.43	0
10	SO4	A	1333	-	4,4,4	0.41	0	6,6,6	0.71	0
10	SO4	A	1334	-	4,4,4	0.65	0	6,6,6	0.22	0
11	CO3	A	1335	-	0,3,3	0.00	-	0,3,3	0.00	-
11	CO3	A	1336	-	0,3,3	0.00	-	0,3,3	0.00	-
11	CO3	A	1337	-	0,3,3	0.00	-	0,3,3	0.00	-
11	CO3	A	1338	-	0,3,3	0.00	-	0,3,3	0.00	-

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	HEM	A	1307	1	-	0/10/54/54	0/0/8/8
6	NAG	A	1320	1	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	A	1324	1	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	A	1325	1	-	0/6/23/26	0/1/1/1
10	SO4	A	1332	-	-	0/0/0/0	0/0/0/0
10	SO4	A	1333	-	-	0/0/0/0	0/0/0/0
10	SO4	A	1334	-	-	0/0/0/0	0/0/0/0
11	CO3	A	1335	-	-	0/0/0/0	0/0/0/0
11	CO3	A	1336	-	-	0/0/0/0	0/0/0/0
11	CO3	A	1337	-	-	0/0/0/0	0/0/0/0
11	CO3	A	1338	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1307	HEM	C2D-C3D	-5.95	1.36	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1307	HEM	C2C-C1C	-5.59	1.42	1.52
2	A	1307	HEM	C3B-C4B	-5.23	1.47	1.51
2	A	1307	HEM	C2B-C1B	-3.34	1.40	1.51
2	A	1307	HEM	CAD-C3D	-3.21	1.47	1.54
2	A	1307	HEM	C3D-C4D	-2.54	1.48	1.51
6	A	1325	NAG	C1-C2	2.05	1.55	1.52
6	A	1324	NAG	C1-C2	2.17	1.55	1.52
2	A	1307	HEM	FE-NC	3.10	2.08	1.95
2	A	1307	HEM	C4C-NC	4.21	1.41	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1307	HEM	CBA-CAA-C2A	-3.16	106.86	112.53
2	A	1307	HEM	C3C-CAC-CBC	-3.08	119.73	124.46
2	A	1307	HEM	CBD-CAD-C3D	-2.98	104.89	113.55
6	A	1325	NAG	O7-C7-C8	-2.96	116.63	122.06
6	A	1325	NAG	C4-C3-C2	-2.80	106.88	111.23
2	A	1307	HEM	C3B-CAB-CBB	-2.17	121.14	124.46
6	A	1320	NAG	C3-C4-C5	2.09	113.84	110.20
2	A	1307	HEM	CMD-C2D-C3D	2.33	124.67	114.35
6	A	1320	NAG	O5-C5-C6	2.36	112.46	107.35
6	A	1325	NAG	C3-C2-N2	2.46	116.44	110.56
6	A	1325	NAG	C2-N2-C7	2.62	126.41	123.04
6	A	1320	NAG	C1-O5-C5	2.72	115.70	112.25
2	A	1307	HEM	CMB-C2B-C3B	2.95	123.90	116.53
2	A	1307	HEM	CAD-C3D-C4D	4.01	126.63	112.47
6	A	1324	NAG	C2-N2-C7	4.03	128.22	123.04
2	A	1307	HEM	CMC-C2C-C3C	4.89	128.75	116.53
2	A	1307	HEM	CAD-C3D-C2D	5.46	128.92	113.22
6	A	1325	NAG	C1-O5-C5	8.08	122.50	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1320	NAG	C1
6	A	1324	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1307	HEM	1	0
6	A	1325	NAG	2	0
11	A	1335	CO3	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	305/306 (99%)	-0.31	6 (1%) 68 72	26, 35, 53, 80	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305[A]	GLY	6.4
1	A	306[A]	ALA	5.6
1	A	304	GLY	4.4
1	A	211	GLY	4.2
1	A	212	GLY	3.9
1	A	266	ALA	3.5

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

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
1	SNN	A	290	8/8	0.98	0.05	-	37,38,44,46	0

6.3 Carbohydrates

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
5	NAG	A	1317	14/15	0.89	0.14	7.61	60,67,79,83	0
4	FUC	A	1311	10/11	0.97	0.04	-1.00	38,39,40,41	0
3	NAG	A	1308	14/15	0.76	0.27	-	55,74,83,84	14
4	NAG	A	1310	14/15	0.97	0.05	-	35,38,45,48	0
5	FUC	A	1318	10/11	0.91	0.41	-	90,99,104,104	0
4	NAG	A	1312	14/15	0.96	0.10	-	40,42,45,46	0
4	MAN	A	1315	11/12	0.91	0.21	-	52,57,61,62	0
5	NAG	A	1321[A]	14/15	0.91	0.15	-	38,43,56,75	1
5	NAG	A	1319	14/15	0.77	0.39	-	90,100,107,110	0
4	XYS	A	1314	9/10	0.90	0.26	-	55,66,73,76	0
4	BMA	A	1313	11/12	0.95	0.12	-	42,45,50,52	0
3	FUC	A	1309	10/11	0.65	0.50	-	92,97,100,101	10
5	FUC	A	1322	10/11	0.81	0.30	-	61,73,79,80	0
5	NAG	A	1323	14/15	0.82	0.36	-	80,94,110,112	0
5	NAG	A	1321[B]	14/15	0.91	0.15	-	38,43,56,75	1
4	MAN	A	1316	11/12	0.83	0.28	-	60,70,80,82	0

6.4 Ligands [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(\AA^2)	Q<0.9
10	SO4	A	1332	5/5	0.99	0.12	8.81	44,44,47,50	0
11	CO3	A	1338	4/4	0.94	0.13	8.31	34,39,43,48	4
6	NAG	A	1324	14/15	0.72	0.36	2.58	103,118,130,131	0
11	CO3	A	1335	4/4	0.95	0.09	1.86	55,70,75,76	0
9	CL	A	1330	1/1	0.99	0.07	0.39	38,38,38,38	1
2	HEM	A	1307	43/43	0.99	0.06	-0.42	26,28,32,44	0
9	CL	A	1331	1/1	0.99	0.05	-0.99	36,36,36,36	1
8	NA	A	1328	1/1	1.00	0.04	-1.47	24,24,24,24	1
7	CA	A	1327	1/1	1.00	0.03	-1.70	34,34,34,34	1
7	CA	A	1326	1/1	0.99	0.03	-1.90	32,32,32,32	0
9	CL	A	1329	1/1	0.95	0.10	-	29,29,29,29	1
10	SO4	A	1333	5/5	0.99	0.05	-	38,39,42,44	0
10	SO4	A	1334	5/5	0.94	0.18	-	78,78,90,91	0
6	NAG	A	1325	14/15	0.41	0.41	-	63,79,86,88	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CO3	A	1336	4/4	0.93	0.12	-	73,77,78,79	0
6	NAG	A	1320	14/15	0.54	0.39	-	90,107,116,117	0
11	CO3	A	1337	4/4	0.92	0.08	-	73,77,78,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.