



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:49 PM GMT

PDB ID : 1CPO
Title : CHLOROPEROXIDASE
Authors : Sundaramoorthy, M.; Poulos, T.L.
Deposited on : 1996-02-10
Resolution : 1.90 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

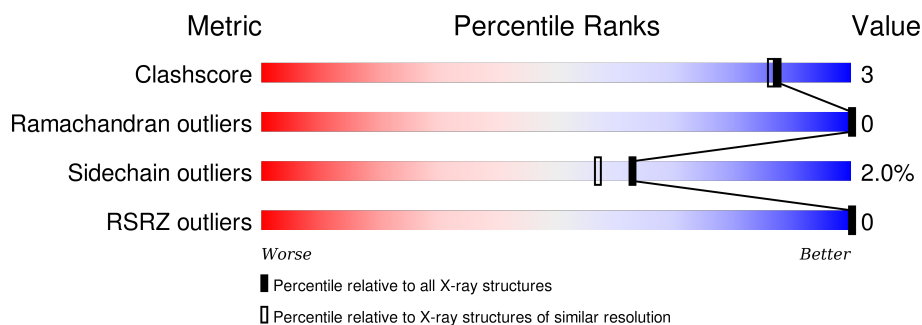
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	299	

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
3	NAG	A	593(A)	X	-	-	-
3	XYS	A	593(D)	X	-	-	-
3	XYS	A	593(E)	X	-	-	-
4	NAG	A	716(A)	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MAN	A	750	-	-	-	X
5	MAN	A	751	-	-	-	X
6	XYS	A	748	X	-	-	-
7	ARB	A	775(B)	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 2784 atoms, of which 1 is hydrogen 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 CHLOROPEROXIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	299	Total	C	H	N	O	S	0	1	0
			2323	1473	1	384	459	6			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

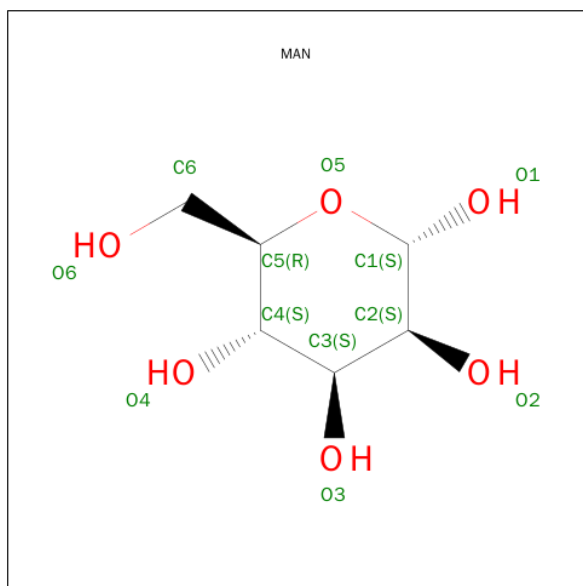
- Molecule 3 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	6	Total	C	N	O	0	0
			68	38	2	28		

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

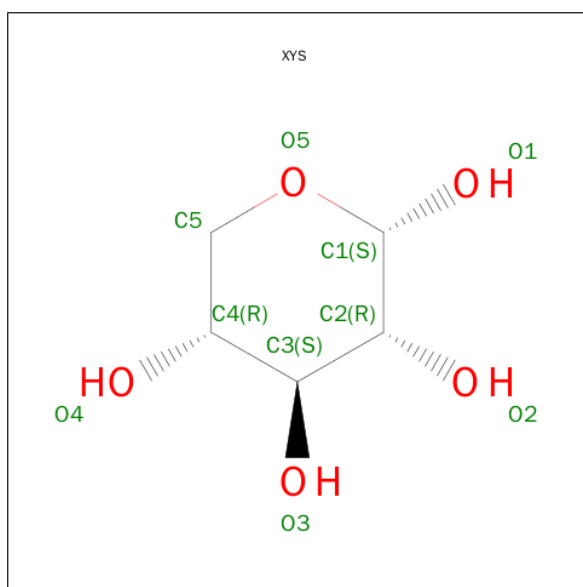
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	2	Total	C	N	O	
			28	16	2	10	
						0	0

- Molecule 5 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O		
			11	6	5	0	0
5	A	1	Total	C	O		
			11	6	5	0	0
5	A	1	Total	C	O		
			11	6	5	0	0
5	A	1	Total	C	O		
			11	6	5	0	0
5	A	1	Total	C	O		
			11	6	5	0	0
5	A	1	Total	C	O		
			11	6	5	0	0
5	A	1	Total	C	O		
			11	6	5	0	0
5	A	1	Total	C	O		
			11	6	5	0	0

- Molecule 6 is SUGAR (XYLOPYRANOSE) (three-letter code: XY5) (formula: $C_5H_{10}O_5$).



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

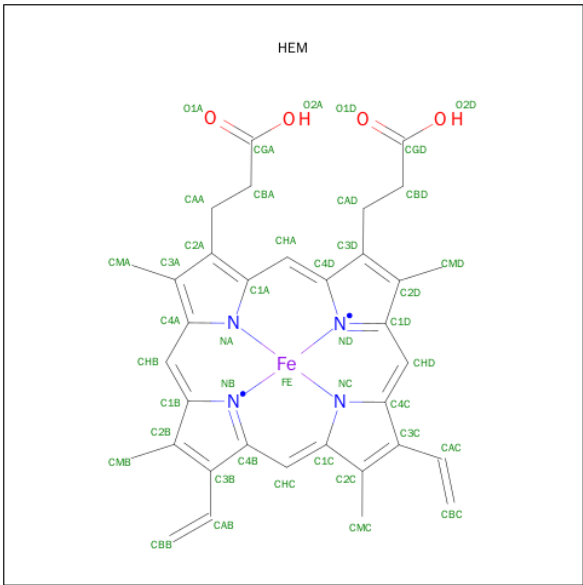
- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	2	Total	C	O	0	0
			20	11	9		

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	179	Total	O	0	0
			179	179		

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: CHLOROPEROXIDASE

Chain A:  92% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.77Å 71.36Å 91.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.90 49.49 – 1.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-1.90) 88.3 (49.49-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.88Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , 0.224 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 28124 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2784	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.36% 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: YYS, NAG, MN, ARB, BMA, HEM, PCA, 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	0.37	0/2392	0.60	0/3280

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
3	A	3	0
4	A	1	0
All	All	4	0

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	593(A)	NAG	C1
3	A	593(D)	YYS	C2
3	A	593(E)	YYS	C2
4	A	716(A)	NAG	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	2322	1	2137	13	0
2	A	14	0	13	1	0
3	A	68	0	57	0	0
4	A	28	0	25	0	0
5	A	99	0	90	1	0
6	A	9	0	8	0	0
7	A	20	0	17	0	0
8	A	1	0	0	0	0
9	A	43	0	30	0	0
10	A	179	0	0	0	0
All	All	2783	1	2377	13	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 3.

All (13) 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:27:ALA:HB2	1:A:94:LEU:HB3	1.83	0.59
1:A:0:PCA:HB3	1:A:297:ASN:HD22	1.67	0.59
1:A:253:PRO:HG2	1:A:256:LEU:HD13	1.89	0.53
1:A:1:GLU:HG2	1:A:16:PRO:HB3	1.91	0.53
1:A:80:GLU:HA	1:A:85:SER:O	2.10	0.52
1:A:27:ALA:HB1	1:A:28:PRO:HD2	1.91	0.50
1:A:10:TYR:O	2:A:512:NAG:H82	2.16	0.45
1:A:253:PRO:HB3	5:A:751:MAN:O4	2.17	0.45
1:A:147:HIS:HA	1:A:205:VAL:O	2.15	0.45
1:A:1:GLU:H	1:A:297:ASN:ND2	2.16	0.43
1:A:219:PHE:HA	1:A:220:PRO:HD3	1.78	0.42
1:A:53:LEU:HA	1:A:53:LEU:HD12	1.95	0.41
1:A:240:ALA:O	1:A:244:VAL:HG23	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	298/299 (100%)	288 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	252/251 (100%)	247 (98%)	5 (2%)	63	57

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	72	LEU
1	A	103	PHE
1	A	223	LEU
1	A	281	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	284	ASN
1	A	290	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	297	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	PCA	A	0	1	7,8,9	1.69	1 (14%)	9,10,12	1.59	1 (11%)

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	PCA	A	0	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	0	PCA	CD-N	4.11	1.47	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	0	PCA	OE-CD-CG	-3.07	119.96	126.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	0	PCA	1	0

5.5 Carbohydrates [i](#)

10 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	593(A)	1,3	14,14,15	0.48	0	15,19,21	1.04	0
3	NAG	A	593(B)	3	14,14,15	0.54	0	15,19,21	1.21	2 (13%)
3	BMA	A	593(C)	3	11,11,12	0.73	0	14,15,17	0.81	1 (7%)
3	XYS	A	593(D)	3	9,9,10	1.74	1 (11%)	12,12,14	1.60	3 (25%)
3	XYS	A	593(E)	3	9,9,10	1.37	1 (11%)	12,12,14	1.69	2 (16%)
3	MAN	A	593(F)	3	11,11,12	1.15	1 (9%)	14,15,17	1.20	2 (14%)
4	NAG	A	716(A)	1,4	14,14,15	0.95	0	15,19,21	1.07	1 (6%)
4	NAG	A	716(B)	4	14,14,15	0.65	0	15,19,21	1.23	1 (6%)
7	MAN	A	775(A)	1,7	11,11,12	1.00	0	14,15,17	1.48	2 (14%)
7	ARB	A	775(B)	7	9,9,10	0.90	0	12,12,14	2.40	5 (41%)

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	593(A)	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	593(B)	3	-	0/6/23/26	0/1/1/1
3	BMA	A	593(C)	3	-	0/2/19/22	0/1/1/1
3	XYS	A	593(D)	3	1/1/3/4	0/0/14/17	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XYS	A	593(E)	3	1/1/3/4	0/0/14/17	0/1/1/1
3	MAN	A	593(F)	3	-	0/2/19/22	0/1/1/1
4	NAG	A	716(A)	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	716(B)	4	-	0/6/23/26	0/1/1/1
7	MAN	A	775(A)	1,7	-	0/2/19/22	0/1/1/1
7	ARB	A	775(B)	7	-	0/0/14/17	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	593(E)	XYS	C4-C3	2.47	1.55	1.52
3	A	593(F)	MAN	C4-C5	2.55	1.58	1.53
3	A	593(D)	XYS	C4-C3	4.04	1.58	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	775(B)	ARB	O3-C3-C2	-3.17	104.27	110.00
3	A	593(B)	NAG	C3-C2-N2	-2.89	103.65	110.56
7	A	775(B)	ARB	O2-C2-C3	-2.66	104.76	110.12
7	A	775(A)	MAN	C1-C2-C3	-2.15	107.00	109.54
3	A	593(F)	MAN	O4-C4-C3	-2.00	105.82	110.34
3	A	593(D)	XYS	C5-C4-C3	2.18	112.11	109.54
3	A	593(B)	NAG	C1-O5-C5	2.40	115.29	112.25
3	A	593(C)	BMA	C1-O5-C5	2.41	115.31	112.25
3	A	593(E)	XYS	O2-C2-C1	2.47	114.16	109.21
7	A	775(B)	ARB	C1-C2-C3	2.88	112.95	109.54
4	A	716(B)	NAG	C1-O5-C5	2.96	116.00	112.25
3	A	593(F)	MAN	C1-O5-C5	2.96	116.01	112.25
3	A	593(D)	XYS	C1-C2-C3	3.05	113.15	109.54
7	A	775(A)	MAN	O3-C3-C2	3.48	116.28	110.00
4	A	716(A)	NAG	C1-O5-C5	3.54	116.74	112.25
3	A	593(D)	XYS	C5-O5-C1	3.58	117.34	111.57
7	A	775(B)	ARB	O2-C2-C1	3.67	116.56	109.21
7	A	775(B)	ARB	C5-O5-C1	4.12	118.22	111.57
3	A	593(E)	XYS	C5-O5-C1	4.38	118.64	111.57

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	593(A)	NAG	C1
4	A	716(A)	NAG	C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
3	A	593(D)	XYS	C2
3	A	593(E)	XYS	C2

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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$
9	HEM	A	396	1,8	30,50,50	2.72	9 (30%)	24,82,82	2.39	10 (41%)
2	NAG	A	512	1	14,14,15	0.71	0	15,19,21	1.28	1 (6%)
5	MAN	A	738	1	11,11,12	0.67	0	14,15,17	0.99	0
5	MAN	A	739	1	11,11,12	0.78	0	14,15,17	1.42	2 (14%)
5	MAN	A	741	1	11,11,12	0.70	0	14,15,17	1.31	1 (7%)
5	MAN	A	742	1	11,11,12	0.79	0	14,15,17	1.77	1 (7%)
6	XYS	A	748	1	9,9,10	1.45	1 (11%)	12,12,14	1.69	3 (25%)
5	MAN	A	750	1	11,11,12	0.88	0	14,15,17	1.15	1 (7%)
5	MAN	A	751	1	11,11,12	0.92	0	14,15,17	1.34	2 (14%)
5	MAN	A	752	1	11,11,12	0.80	0	14,15,17	1.38	2 (14%)
5	MAN	A	783	1	11,11,12	1.32	1 (9%)	14,15,17	1.74	4 (28%)
5	MAN	A	793	1	11,11,12	0.86	0	14,15,17	1.15	1 (7%)

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
9	HEM	A	396	1,8	-	0/10/54/54	0/0/8/8
2	NAG	A	512	1	-	0/6/23/26	0/1/1/1
5	MAN	A	738	1	-	0/2/19/22	0/1/1/1
5	MAN	A	739	1	-	0/2/19/22	0/1/1/1
5	MAN	A	741	1	-	0/2/19/22	0/1/1/1
5	MAN	A	742	1	-	0/2/19/22	0/1/1/1
6	XYS	A	748	1	1/1/3/4	0/0/14/17	0/1/1/1
5	MAN	A	750	1	-	0/2/19/22	0/1/1/1
5	MAN	A	751	1	-	0/2/19/22	0/1/1/1
5	MAN	A	752	1	-	0/2/19/22	0/1/1/1
5	MAN	A	783	1	-	0/2/19/22	0/1/1/1
5	MAN	A	793	1	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	396	HEM	C2D-C3D	-6.20	1.35	1.54
9	A	396	HEM	C3B-CAB	-5.88	1.40	1.51
9	A	396	HEM	C3C-CAC	-5.88	1.40	1.51
9	A	396	HEM	C3B-C4B	-5.72	1.46	1.51
9	A	396	HEM	C3D-C4D	-4.68	1.45	1.51
9	A	396	HEM	C2C-C1C	-4.02	1.45	1.52
6	A	748	XYS	O5-C5	2.04	1.46	1.42
9	A	396	HEM	C1C-NC	2.10	1.38	1.36
9	A	396	HEM	C4C-NC	2.21	1.38	1.36
9	A	396	HEM	CBC-CAC	2.67	1.44	1.29
5	A	783	MAN	C2-C3	3.25	1.57	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	783	MAN	C3-C4-C5	-2.20	106.36	110.20
6	A	748	XYS	O2-C2-C3	-2.19	105.72	110.12
5	A	793	MAN	O3-C3-C2	-2.19	106.05	110.00
9	A	396	HEM	CAA-C2A-C1A	-2.09	124.73	127.01
9	A	396	HEM	C3B-CAB-CBB	2.11	127.69	124.46
5	A	752	MAN	O2-C2-C1	2.15	113.52	109.21
5	A	751	MAN	C1-C2-C3	2.24	112.19	109.54
5	A	783	MAN	O4-C4-C5	2.33	115.42	109.24
9	A	396	HEM	C3B-C4B-CHC	2.36	126.49	123.16
6	A	748	XYS	C5-O5-C1	2.60	115.76	111.57
5	A	783	MAN	C1-C2-C3	2.68	112.71	109.54
5	A	752	MAN	C1-O5-C5	2.86	115.88	112.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	396	HEM	C3C-CAC-CBC	2.89	128.88	124.46
9	A	396	HEM	CMD-C2D-C3D	2.89	127.14	114.35
5	A	739	MAN	C1-O5-C5	3.05	116.11	112.25
5	A	751	MAN	C1-O5-C5	3.14	116.23	112.25
5	A	739	MAN	C1-C2-C3	3.15	113.27	109.54
9	A	396	HEM	C2D-C3D-C4D	3.40	107.26	101.50
5	A	783	MAN	C1-O5-C5	3.44	116.61	112.25
2	A	512	NAG	C1-O5-C5	3.49	116.67	112.25
5	A	750	MAN	C1-O5-C5	3.53	116.73	112.25
6	A	748	XYS	C1-C2-C3	3.74	113.97	109.54
9	A	396	HEM	CAD-C3D-C4D	3.83	125.99	112.47
5	A	741	MAN	C1-O5-C5	4.16	117.53	112.25
9	A	396	HEM	CMB-C2B-C3B	4.41	127.54	116.53
9	A	396	HEM	CAD-C3D-C2D	4.69	126.71	113.22
9	A	396	HEM	CMC-C2C-C3C	5.33	129.84	116.53
5	A	742	MAN	C1-O5-C5	5.80	119.61	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	748	XYS	C2

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
2	A	512	NAG	1	0
5	A	751	MAN	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	298/299 (99%)	-0.30	0 100 100	5, 14, 31, 40	0

There are no RSRZ outliers to report.

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	PCA	A	0	8/9	0.94	0.09	-	13,14,17,17	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(Å ²)	Q<0.9
7	ARB	A	775(B)	9/10	0.76	0.21	7.38	34,38,41,43	0
3	NAG	A	593(B)	14/15	0.92	0.10	1.06	15,22,31,34	0
3	NAG	A	593(A)	14/15	0.95	0.10	0.50	13,18,21,21	0
4	NAG	A	716(A)	14/15	0.97	0.08	-0.32	7,11,17,20	0
7	MAN	A	775(A)	11/12	0.81	0.17	-	37,41,47,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BMA	A	593(C)	11/12	0.83	0.15	-	36,37,40,43	0
3	XYS	A	593(E)	9/10	0.75	0.13	-	43,45,47,50	0
4	NAG	A	716(B)	14/15	0.84	0.15	-	31,39,44,46	0
3	XYS	A	593(D)	9/10	0.75	0.24	-	48,50,51,55	0
3	MAN	A	593(F)	11/12	0.80	0.22	-	46,52,54,57	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
5	MAN	A	750	11/12	0.78	0.15	4.47	42,46,47,51	0
5	MAN	A	751	11/12	0.91	0.13	3.30	35,39,42,44	0
9	HEM	A	396	43/43	0.98	0.08	-0.05	3,6,10,21	0
5	MAN	A	739	11/12	0.95	0.10	-0.53	19,21,23,26	0
5	MAN	A	741	11/12	0.95	0.08	-0.71	12,13,18,19	0
8	MN	A	301	1/1	0.99	0.07	-1.55	14,14,14,14	0
5	MAN	A	738	11/12	0.85	0.14	-	27,36,42,43	0
2	NAG	A	512	14/15	0.80	0.14	-	41,46,50,51	0
5	MAN	A	783	11/12	0.69	0.25	-	45,53,55,55	0
5	MAN	A	752	11/12	0.82	0.14	-	31,33,38,43	0
5	MAN	A	793	11/12	0.79	0.18	-	40,46,48,52	0
5	MAN	A	742	11/12	0.88	0.14	-	33,38,42,42	0
6	XYS	A	748	9/10	0.69	0.27	-	49,53,55,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.