



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:39 AM GMT

PDB ID : 2NQX  
Title : Crystal Structure of bovine lactoperoxidase with iodide ions at 2.9A resolution  
Authors : Singh, A.K.; Kaur, P.; Singh, N.; Bhushan, A.; Sharma, S.; Singh, T.P.  
Deposited on : 2006-11-01  
Resolution : 2.95 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](mailto: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.

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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

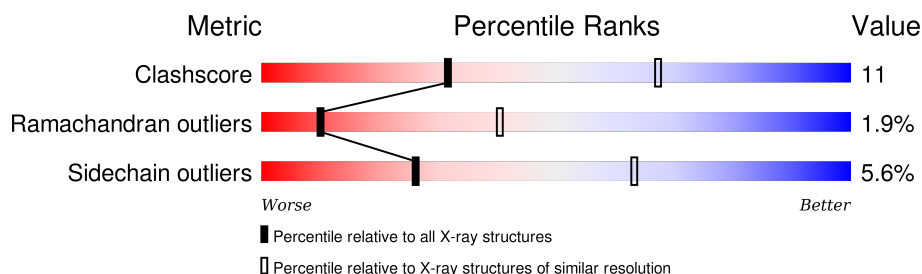
# 1 Overall quality at a glance

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  $\geq 3$ , 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	595	

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
8	OSM	A	710	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5114 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 Lactoperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4770	3037	847	860	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		
2	A	3	Total	C	N	O	0	0
			39	22	2	15		

- 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
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

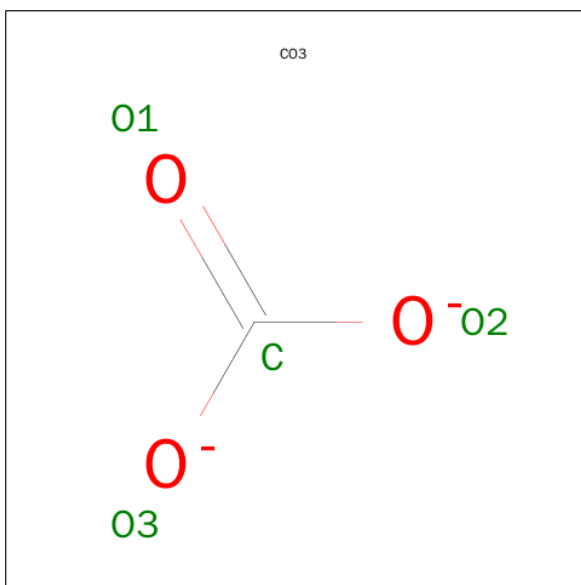
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	I	0	0
			7	7		

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



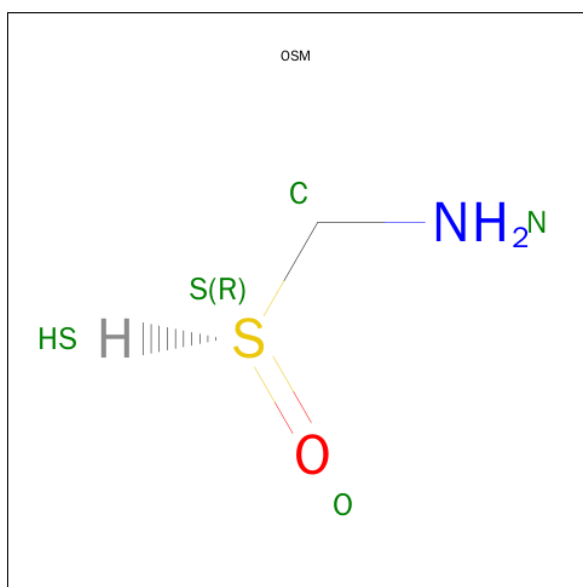
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O		0	0
			4	1	3			

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 8 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula:  $CH_5NOS$ ).



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

- Molecule 9 is water.

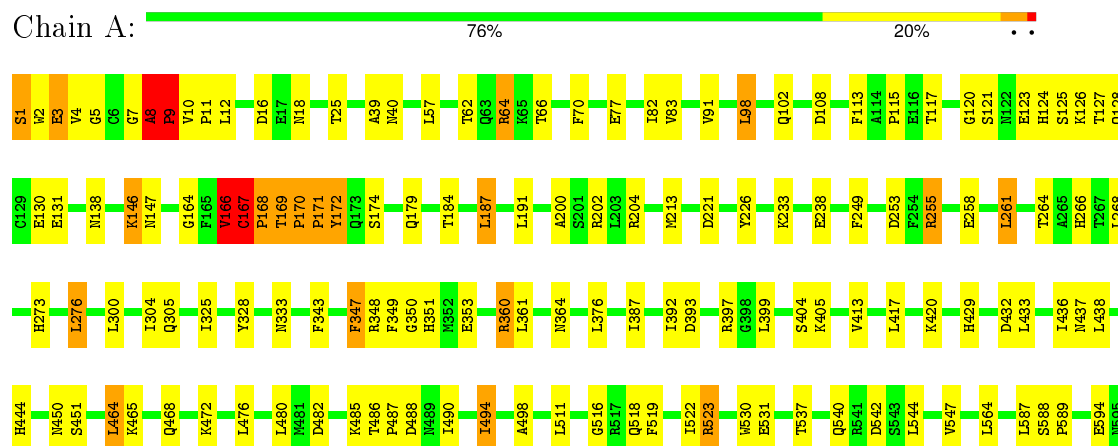
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	151	Total	O	0	0
			151	151		

### 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: Lactoperoxidase



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.53 Å   80.55 Å   78.03 Å 90.00°   103.74°   90.00°	Depositor
Resolution (Å)	25.00 – 2.95	Depositor
% Data completeness (in resolution range)	98.5 (25.00-2.95)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.196 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, NAG, CA, OSM, HEM, IOD, 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	0.40	0/4898	0.67	12/6645 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	VAL	CA-CB-CG2	-12.08	92.78	110.90
1	A	167	CYS	CA-CB-SG	-9.96	96.07	114.00
1	A	166	VAL	N-CA-CB	9.76	132.98	111.50
1	A	1	SER	O-C-N	-8.71	108.77	122.70
1	A	8	ALA	CB-CA-C	7.77	121.76	110.10
1	A	18	ASN	N-CA-CB	7.20	123.56	110.60
1	A	166	VAL	C-N-CA	6.79	138.69	121.70
1	A	486	THR	N-CA-CB	6.77	123.17	110.30
1	A	2	TRP	N-CA-C	6.26	127.91	111.00
1	A	138	ASN	N-CA-C	5.55	125.99	111.00
1	A	172	TYR	N-CA-C	5.40	125.58	111.00
1	A	167	CYS	CB-CA-C	-5.07	100.26	110.40

All (1) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
1	A	166	VAL	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	SER	Mainchain
1	A	166	VAL	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4770	0	4690	99	0
2	A	78	0	68	0	0
3	A	56	0	50	0	0
4	A	1	0	0	0	0
5	A	7	0	0	2	0
6	A	4	0	0	0	0
7	A	43	0	30	10	0
8	A	4	0	5	2	0
9	A	151	0	0	1	0
All	All	5114	0	4843	103	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 11.

All (103) 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:258:GLU:OE2	7:A:709:HEM:HMB3	1.68	0.94
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.20	0.88
1:A:258:GLU:HG3	8:A:710:OSM:HS	1.37	0.87
1:A:170:PRO:HB2	1:A:171:PRO:CD	2.06	0.86
1:A:487:PRO:HA	1:A:490:ILE:HD13	1.57	0.86
1:A:487:PRO:HA	1:A:490:ILE:CD1	2.04	0.85
1:A:8:ALA:CB	1:A:9:PRO:HD2	2.08	0.84
1:A:123:GLU:OE2	1:A:125:SER:HB3	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:HG2	1:A:167:CYS:O	1.81	0.81
1:A:8:ALA:HB1	1:A:9:PRO:CD	2.14	0.78
1:A:8:ALA:O	1:A:10:VAL:HG22	1.84	0.77
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.67	0.77
1:A:8:ALA:CB	1:A:9:PRO:CD	2.65	0.75
7:A:709:HEM:HBB2	7:A:709:HEM:HMB1	1.68	0.74
1:A:170:PRO:CB	1:A:171:PRO:CD	2.65	0.74
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.25	0.67
1:A:169:THR:H	1:A:170:PRO:CD	2.08	0.67
1:A:170:PRO:HB2	1:A:171:PRO:HD2	1.75	0.66
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.29	0.66
1:A:258:GLU:HG3	8:A:710:OSM:S	2.35	0.66
7:A:709:HEM:HBC2	7:A:709:HEM:HMC2	1.77	0.66
1:A:253:ASP:OD2	1:A:255:ARG:HD3	1.97	0.65
1:A:544:LEU:O	1:A:547:VAL:HG22	1.98	0.64
1:A:351:HIS:HD1	1:A:437:ASN:ND2	1.95	0.63
1:A:8:ALA:HB3	1:A:9:PRO:HD2	1.79	0.63
1:A:82:ILE:HG21	1:A:494:ILE:HD11	1.83	0.60
1:A:125:SER:HA	1:A:128:GLN:HB3	1.85	0.59
1:A:108:ASP:OD2	7:A:709:HEM:HMD1	2.04	0.58
1:A:328:TYR:HD1	1:A:523:ARG:HD3	1.68	0.57
1:A:328:TYR:CD1	1:A:523:ARG:HD3	2.40	0.57
1:A:519:PHE:CD1	1:A:522:ILE:HD11	2.40	0.56
1:A:8:ALA:HB1	1:A:9:PRO:HD2	1.81	0.56
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.42	0.55
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.36	0.55
1:A:249:PHE:CZ	1:A:387:ILE:HD11	2.43	0.53
1:A:8:ALA:O	1:A:9:PRO:C	2.46	0.53
1:A:258:GLU:CD	7:A:709:HEM:HMB3	2.30	0.52
1:A:464:LEU:O	1:A:468:GLN:HG3	2.09	0.52
1:A:5:GLY:O	1:A:7:GLY:N	2.42	0.52
1:A:117:THR:HG22	1:A:164:GLY:HA2	1.90	0.52
1:A:123:GLU:HG2	1:A:125:SER:H	1.76	0.50
1:A:102:GLN:OE1	1:A:261:LEU:HB3	2.11	0.50
1:A:537:THR:OG1	1:A:540:GLN:HG3	2.10	0.50
1:A:200:ALA:O	1:A:204:ARG:HG3	2.12	0.49
1:A:450:ASN:HD21	1:A:487:PRO:HB2	1.76	0.49
1:A:300:LEU:O	1:A:304:ILE:HG12	2.12	0.49
1:A:8:ALA:HB1	1:A:9:PRO:HD3	1.92	0.49
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.47	0.49
1:A:113:PHE:O	1:A:115:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASP:CG	7:A:709:HEM:HMD1	2.34	0.48
1:A:120:GLY:HA3	1:A:123:GLU:OE1	2.13	0.48
1:A:108:ASP:OD2	7:A:709:HEM:HMD2	2.14	0.47
1:A:325:ILE:HD11	1:A:516:GLY:HA2	1.96	0.47
1:A:420:LYS:HA	1:A:429:HIS:O	2.13	0.47
1:A:348:ARG:HD3	1:A:437:ASN:OD1	2.14	0.47
1:A:169:THR:N	1:A:170:PRO:CD	2.74	0.47
1:A:170:PRO:HB3	1:A:171:PRO:HD3	1.96	0.47
1:A:350:GLY:HA3	7:A:709:HEM:CBC	2.45	0.47
1:A:25:THR:O	1:A:184:THR:HG22	2.15	0.47
1:A:77:GLU:HG3	5:A:704:IOD:I	2.85	0.46
1:A:276:LEU:HD12	1:A:587:LEU:HD11	1.96	0.46
1:A:417:LEU:HD22	1:A:433:LEU:HD22	1.98	0.45
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.83	0.45
1:A:9:PRO:O	1:A:10:VAL:HG13	2.16	0.45
1:A:146:LYS:O	1:A:147:ASN:HB2	2.17	0.45
1:A:124:HIS:O	1:A:128:GLN:N	2.47	0.45
1:A:123:GLU:HB3	1:A:126:LYS:HE2	1.97	0.45
7:A:709:HEM:HBC2	7:A:709:HEM:CMC	2.47	0.44
1:A:127:THR:HG22	1:A:131:GLU:CG	2.47	0.44
1:A:233:LYS:HE2	1:A:238:GLU:OE1	2.17	0.44
1:A:450:ASN:ND2	1:A:488:ASP:OD1	2.47	0.44
1:A:98:LEU:HD13	1:A:399:LEU:HD23	2.00	0.44
1:A:530:TRP:HZ2	5:A:707:IOD:I	2.70	0.43
1:A:62:THR:HG22	1:A:64:ARG:HG3	2.01	0.43
1:A:39:ALA:O	1:A:40:ASN:HB2	2.18	0.43
1:A:364:ASN:N	1:A:364:ASN:HD22	2.15	0.43
7:A:709:HEM:CBB	7:A:709:HEM:HMB1	2.43	0.43
1:A:66:THR:HB	1:A:70:PHE:O	2.19	0.43
1:A:393:ASP:O	1:A:397:ARG:HG3	2.19	0.43
1:A:83:VAL:HG12	1:A:413:VAL:HB	2.00	0.43
1:A:476:LEU:HD21	1:A:498:ALA:HB1	2.00	0.43
1:A:120:GLY:CA	1:A:123:GLU:OE1	2.67	0.43
1:A:187:LEU:HB3	1:A:305:GLN:HG2	2.01	0.42
1:A:465:LYS:HE3	9:A:736:HOH:O	2.18	0.42
1:A:179:GLN:HG2	1:A:444:HIS:NE2	2.34	0.42
1:A:169:THR:H	1:A:170:PRO:HD2	1.83	0.42
1:A:360:ARG:O	1:A:361:LEU:HD23	2.19	0.42
1:A:3:GLU:C	1:A:4:VAL:CG2	2.88	0.42
1:A:464:LEU:HD22	1:A:468:GLN:OE1	2.20	0.42
1:A:168:PRO:HG2	1:A:172:TYR:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HA	1:A:11:PRO:HD3	1.90	0.41
1:A:468:GLN:O	1:A:472:LYS:N	2.54	0.41
1:A:438:LEU:HD21	1:A:494:ILE:HB	2.02	0.41
1:A:482:ASP:O	1:A:485:LYS:NZ	2.53	0.41
1:A:264:THR:HG23	1:A:392:ILE:HB	2.03	0.41
1:A:187:LEU:HD13	1:A:305:GLN:HA	2.02	0.41
1:A:432:ASP:O	1:A:436:ILE:HG12	2.20	0.41
1:A:347:PHE:C	1:A:349:PHE:H	2.24	0.40
1:A:353:GLU:HA	1:A:405:LYS:O	2.21	0.40
1:A:249:PHE:HZ	1:A:387:ILE:HD11	1.86	0.40
1:A:191:LEU:O	1:A:266:HIS:HE1	2.04	0.40
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.57	0.40
1:A:588:SER:OG	1:A:589:PRO:HD3	2.22	0.40

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	593/595 (100%)	543 (92%)	39 (7%)	11 (2%)	10	40

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	9	PRO
1	A	12	LEU
1	A	169	THR
1	A	174	SER
1	A	3	GLU
1	A	166	VAL
1	A	170	PRO

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Mol	Chain	Res	Type
1	A	171	PRO
1	A	168	PRO
1	A	167	CYS

### 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	518/518 (100%)	489 (94%)	29 (6%)	26	63

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	16	ASP
1	A	57	LEU
1	A	64	ARG
1	A	91	VAL
1	A	98	LEU
1	A	121	SER
1	A	130	GLU
1	A	146	LYS
1	A	187	LEU
1	A	202	ARG
1	A	255	ARG
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	333	ASN
1	A	347	PHE
1	A	360	ARG
1	A	376	LEU
1	A	404	SER
1	A	451	SER
1	A	464	LEU
1	A	480	LEU

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Mol	Chain	Res	Type
1	A	494	ILE
1	A	511	LEU
1	A	523	ARG
1	A	542	ASP
1	A	564	LEU
1	A	594	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	122	ASN
1	A	147	ASN
1	A	266	HIS
1	A	333	ASN
1	A	364	ASN
1	A	423	GLN
1	A	497	ASN
1	A	520	GLN
1	A	545	GLN
1	A	570	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 ⓘ

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	$\# Z  > 2$
2	NAG	A	596	1,2	14,14,15	0.50	0	15,19,21	0.82	1 (6%)
2	NAG	A	597	2	14,14,15	0.59	0	15,19,21	1.36	1 (6%)
2	MAN	A	598	2	11,11,12	0.57	0	14,15,17	1.15	1 (7%)
3	NAG	A	599	1,3	14,14,15	0.50	0	15,19,21	0.74	0
3	NAG	A	600	3	14,14,15	0.60	0	15,19,21	1.12	2 (13%)
2	NAG	A	601	1,2	14,14,15	0.46	0	15,19,21	0.84	0
2	NAG	A	602	2	14,14,15	0.40	0	15,19,21	2.18	1 (6%)
2	MAN	A	603	2	11,11,12	0.57	0	14,15,17	1.15	1 (7%)
3	NAG	A	604	1,3	14,14,15	0.51	0	15,19,21	0.90	1 (6%)
3	NAG	A	605	3	14,14,15	0.50	0	15,19,21	0.88	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	NAG	A	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	597	2	-	0/6/23/26	0/1/1/1
2	MAN	A	598	2	-	0/2/19/22	0/1/1/1
3	NAG	A	599	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	600	3	-	0/6/23/26	0/1/1/1
2	NAG	A	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	2	-	0/6/23/26	0/1/1/1
2	MAN	A	603	2	-	0/2/19/22	0/1/1/1
3	NAG	A	604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	605	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	596	NAG	C2-N2-C7	-2.03	120.43	123.04
3	A	600	NAG	C4-C3-C2	2.26	114.75	111.23
3	A	600	NAG	C3-C4-C5	2.33	114.25	110.20
3	A	604	NAG	C4-C3-C2	2.50	115.11	111.23
2	A	603	MAN	C1-O5-C5	2.75	115.73	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	598	MAN	C1-O5-C5	3.21	116.32	112.25
2	A	597	NAG	C4-C3-C2	3.88	117.26	111.23
2	A	602	NAG	C1-O5-C5	7.75	122.09	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	$\# Z  > 2$
6	CO3	A	688	-	0,3,3	0.00	-	0,3,3	0.00	-
7	HEM	A	709	1	30,50,50	2.24	9 (30%)	24,82,82	2.16	7 (29%)
8	OSM	A	710	-	1,3,3	0.61	0	0,2,2	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
6	CO3	A	688	-	-	0/0/0/0	0/0/0/0
7	HEM	A	709	1	-	0/10/54/54	0/0/8/8
8	OSM	A	710	-	-	0/0/1/1	0/0/0/0

All (9) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	709	HEM	C3B-C4B	-7.79	1.44	1.51
7	A	709	HEM	C3D-C4D	-4.42	1.45	1.51
7	A	709	HEM	C2C-C1C	-3.71	1.45	1.52
7	A	709	HEM	C2D-C1D	-2.12	1.44	1.51
7	A	709	HEM	CAA-C2A	2.12	1.55	1.52
7	A	709	HEM	C3B-CAB	2.48	1.56	1.51
7	A	709	HEM	FE-NB	2.51	2.10	1.97
7	A	709	HEM	C3C-CAC	2.66	1.56	1.51
7	A	709	HEM	FE-NC	2.69	2.06	1.95

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	709	HEM	CBD-CAD-C3D	-2.22	107.08	113.55
7	A	709	HEM	CAA-C2A-C1A	-2.01	124.82	127.01
7	A	709	HEM	CMD-C2D-C3D	2.70	126.28	114.35
7	A	709	HEM	CMB-C2B-C3B	3.47	125.20	116.53
7	A	709	HEM	CAD-C3D-C2D	4.45	126.01	113.22
7	A	709	HEM	CAD-C3D-C4D	4.75	129.21	112.47
7	A	709	HEM	CMC-C2C-C3C	4.81	128.53	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	709	HEM	10	0
8	A	710	OSM	2	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 ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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