



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:47 AM GMT

PDB ID : 3RKE  
Title : Crystal Structure of goat Lactoperoxidase complexed with a tightly bound inhibitor, 4-aminophenyl-4H-imidazole-1-ylmethanone at 2.3 Å resolution  
Authors : Dube, D.; Singh, R.P.; Sinha, M.; Singh, A.K.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2011-04-18  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

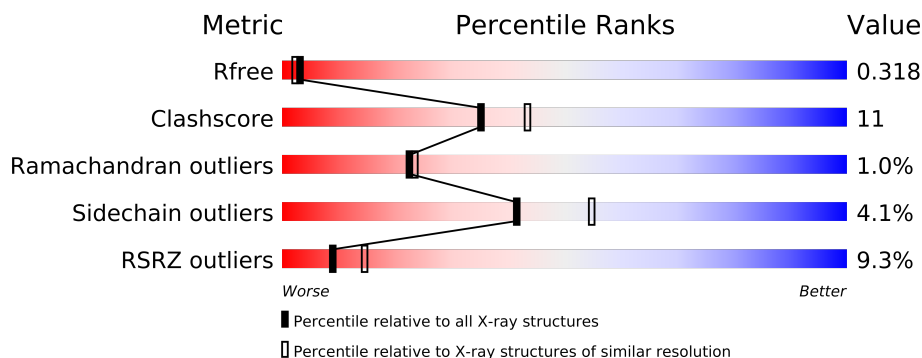
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	595	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	596	-	X
6	IOD	A	600	-	X
6	IOD	A	604	-	X
6	IOD	A	606	-	X
8	MZZ	A	610	X	-

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 5174 atoms, of which 0 are hydrogen and 0 are deuterium.

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	P	S	0	0	0
			4757	3021	844	865	1	26			

- 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		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

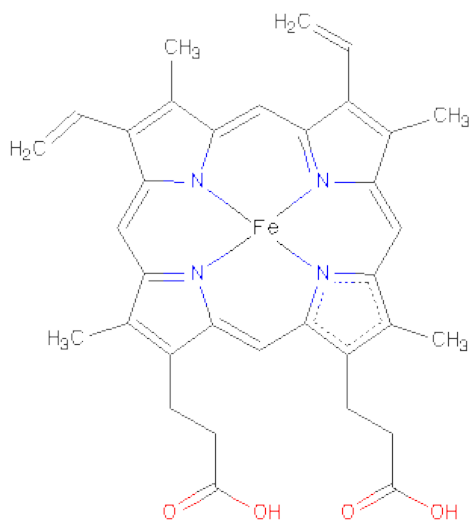
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

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

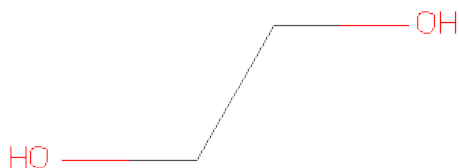


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

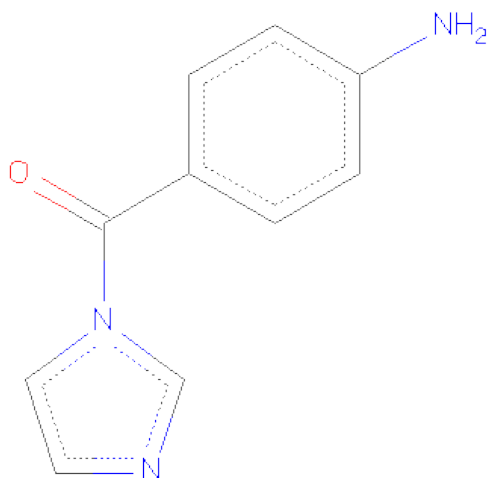
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	I	0	0
			9	9		

- 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		

- Molecule 8 is (4-AMINOPHENYL)-IMIDAZOL-1-YL-METHANONE (three-letter code: MZZ) (formula: C<sub>10</sub>H<sub>9</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	10	3	1		

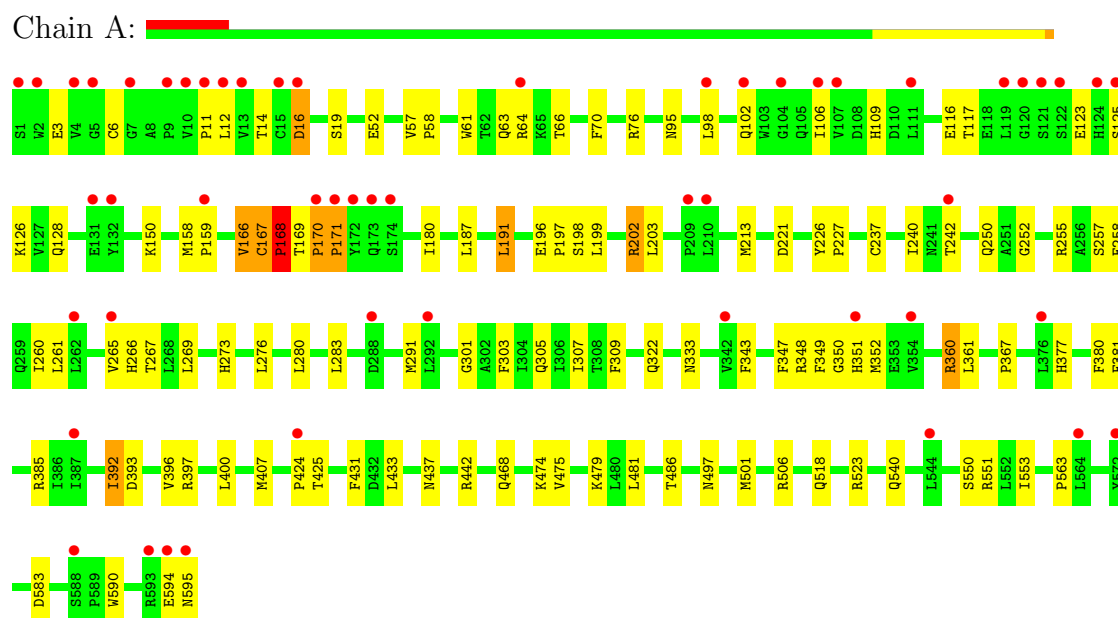
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	290	Total 290	O 290	0	0

### 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: Lactoperoxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.98Å 80.53Å 76.16Å 90.00° 103.07° 90.00°	Depositor
Resolution (Å)	44.03 – 2.30 44.03 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (44.03-2.30) 97.4 (44.03-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.245 , 0.263 0.239 , 0.318	Depositor DCC
$R_{free}$ test set	1392 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.894	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 38.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 27726 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5174	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SEP, CA, EDO, MZZ, HEM, IOD

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	0.58	0/4875	0.68	1/6621 (0.0%)

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	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	486	THR	N-CA-CB	5.38	120.52	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	442	ARG	Sidechain

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4757	0	4645	96	0
2	A	28	0	26	0	0
3	A	28	0	25	0	0
4	A	1	0	0	0	0
5	A	43	0	30	8	0
6	A	9	0	0	1	0
7	A	4	0	6	2	0
8	A	14	0	9	14	0
9	A	290	0	0	0	0
All	All	5174	0	4741	102	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (102) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.29	1.14
1:A:202:ARG:HH11	1:A:202:ARG:HG3	1.10	1.08
1:A:167:CYS:CB	1:A:168:PRO:HD2	1.85	1.06
1:A:360:ARG:NH1	1:A:360:ARG:HG3	1.63	1.05
1:A:360:ARG:HH11	1:A:360:ARG:HG3	0.87	1.03
1:A:196:GLU:HB3	1:A:198:SEP:O2P	1.67	0.94
1:A:167:CYS:HB3	1:A:168:PRO:CD	1.98	0.93
1:A:360:ARG:HH11	1:A:360:ARG:CG	1.79	0.92
1:A:202:ARG:NH1	1:A:202:ARG:HG3	1.86	0.87
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.09	0.87
1:A:3:GLU:HB3	1:A:6:CYS:HB2	1.59	0.84
1:A:227:PRO:HD3	1:A:267:THR:HG23	1.60	0.84
1:A:198:SEP:O	1:A:202:ARG:HG2	1.78	0.83
1:A:52:GLU:HB3	1:A:57:VAL:HG12	1.60	0.83
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.28	0.82
1:A:125:SER:HA	1:A:128:GLN:HB3	1.61	0.82
1:A:202:ARG:CG	1:A:202:ARG:HH11	1.94	0.78
1:A:261:LEU:O	1:A:265:VAL:HG23	1.83	0.78
1:A:167:CYS:CB	1:A:168:PRO:CD	2.56	0.76
1:A:407:MET:HB3	1:A:501:MET:CE	2.18	0.73
1:A:102:GLN:HG2	1:A:265:VAL:HG21	1.73	0.71
1:A:301:GLY:O	1:A:305:GLN:HG3	1.88	0.71
5:A:1001:HEM:C2A	8:A:610:MZZ:H2	2.26	0.70
1:A:594:GLU:HG3	1:A:595:ASN:HD22	1.56	0.70
1:A:102:GLN:CG	1:A:265:VAL:HG21	2.22	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.29	0.67
1:A:187:LEU:HB3	1:A:305:GLN:HE21	1.60	0.66
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.72	0.66
1:A:255:ARG:HA	8:A:610:MZZ:H20	1.78	0.64
1:A:203:LEU:HD23	1:A:250:GLN:HE21	1.63	0.63
1:A:63:GLN:HG3	1:A:64:ARG:H	1.64	0.63
1:A:258:GLU:HB2	8:A:610:MZZ:H5	1.81	0.62
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.84	0.60
1:A:106:ILE:HG23	1:A:191:LEU:HD21	1.84	0.60
1:A:424:PRO:O	6:A:604:IOD:I	2.90	0.59
1:A:237:CYS:HA	1:A:381:PHE:O	2.02	0.59
1:A:52:GLU:CB	1:A:57:VAL:HG12	2.30	0.59
1:A:197:PRO:HD2	1:A:198:SEP:O2P	2.04	0.58
1:A:392:ILE:HG23	1:A:396:VAL:CG2	2.34	0.57
1:A:258:GLU:CB	8:A:610:MZZ:H5	2.37	0.54
5:A:1001:HEM:C1A	8:A:610:MZZ:H2	2.42	0.53
5:A:1001:HEM:C2A	8:A:610:MZZ:C2	2.91	0.53
1:A:199:LEU:HA	1:A:202:ARG:HG3	1.92	0.52
1:A:255:ARG:HA	8:A:610:MZZ:C20	2.39	0.52
1:A:117:THR:HG23	1:A:117:THR:O	2.10	0.52
1:A:198:SEP:O	1:A:202:ARG:CG	2.55	0.51
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.45	0.51
1:A:257:SER:O	1:A:381:PHE:HA	2.11	0.50
1:A:240:ILE:HG12	1:A:381:PHE:O	2.12	0.50
1:A:255:ARG:CB	8:A:610:MZZ:H20	2.42	0.49
1:A:166:VAL:HG13	1:A:167:CYS:N	2.28	0.49
1:A:66:THR:HB	1:A:70:PHE:N	2.28	0.49
1:A:424:PRO:HG2	8:A:610:MZZ:H17	1.95	0.48
1:A:242:THR:HG22	1:A:242:THR:O	2.14	0.48
1:A:169:THR:N	1:A:170:PRO:CD	2.76	0.48
1:A:255:ARG:CA	8:A:610:MZZ:H20	2.43	0.48
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.49	0.48
1:A:106:ILE:HD11	1:A:265:VAL:HB	1.95	0.48
1:A:102:GLN:HG3	1:A:265:VAL:HG21	1.95	0.47
1:A:392:ILE:HG23	1:A:396:VAL:HG23	1.96	0.47
1:A:400:LEU:HD21	1:A:553:ILE:CD1	2.44	0.47
1:A:551:ARG:HD3	1:A:583:ASP:O	2.15	0.47
1:A:123:GLU:HB3	1:A:126:LYS:HG3	1.97	0.47
1:A:159:PRO:HD2	1:A:431:PHE:CE2	2.50	0.47
1:A:255:ARG:HG2	8:A:610:MZZ:H20	1.97	0.46
1:A:360:ARG:CG	1:A:360:ARG:NH1	2.47	0.46
5:A:1001:HEM:C3A	8:A:610:MZZ:C2	2.99	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:350:GLY:HA3	5:A:1001:HEM:CBC	2.45	0.46
5:A:1001:HEM:NA	8:A:610:MZZ:N7	2.64	0.45
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.98	0.45
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.51	0.45
1:A:361:LEU:O	1:A:397:ARG:HD2	2.16	0.45
1:A:276:LEU:O	1:A:280:LEU:HG	2.17	0.45
1:A:16:ASP:HB3	1:A:19:SER:HB2	1.98	0.44
1:A:166:VAL:HG23	1:A:180:ILE:HG12	1.99	0.44
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.47	0.44
1:A:303:PHE:O	1:A:307:ILE:HG12	2.18	0.44
1:A:506:ARG:NH2	7:A:598:EDO:H22	2.33	0.44
1:A:102:GLN:HG2	1:A:265:VAL:CG2	2.45	0.44
1:A:109:HIS:NE2	8:A:610:MZZ:N7	2.65	0.43
5:A:1001:HEM:HMC2	5:A:1001:HEM:HBC2	2.00	0.43
1:A:199:LEU:HA	1:A:202:ARG:CG	2.48	0.43
1:A:203:LEU:HD11	1:A:252:GLY:HA2	2.02	0.42
1:A:63:GLN:HG3	1:A:64:ARG:N	2.33	0.42
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.84	0.42
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.55	0.42
1:A:58:PRO:HG2	1:A:61:TRP:HB2	2.01	0.42
1:A:196:GLU:CB	1:A:198:SEP:O2P	2.55	0.41
1:A:203:LEU:CD2	1:A:250:GLN:HE21	2.31	0.41
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.90	0.41
1:A:221:ASP:HB2	1:A:226:TYR:CE2	2.56	0.41
1:A:540:GLN:HG2	1:A:590:TRP:CE2	2.56	0.41
1:A:98:LEU:HD12	1:A:98:LEU:HA	1.87	0.41
1:A:400:LEU:HD13	1:A:563:PRO:HD3	2.03	0.41
1:A:305:GLN:O	1:A:309:PHE:HB2	2.20	0.40
1:A:191:LEU:O	1:A:266:HIS:HE1	2.04	0.40
1:A:348:ARG:NH2	5:A:1001:HEM:HAD1	2.37	0.40
1:A:95:ASN:HD22	7:A:598:EDO:H21	1.87	0.40
1:A:76:ARG:HH21	1:A:150:LYS:HG3	1.87	0.40
1:A:475:VAL:O	1:A:479:LYS:HG3	2.22	0.40
1:A:260:ILE:CD1	1:A:385:ARG:HB2	2.52	0.40
1:A:150:LYS:HD2	1:A:158:MET:HE2	2.03	0.40

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	592/595 (100%)	543 (92%)	43 (7%)	6 (1%)	22 23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	171	PRO
1	A	11	PRO
1	A	170	PRO
1	A	367	PRO
1	A	168	PRO

### 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	516/516 (100%)	495 (96%)	21 (4%)	41 55

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	14	THR
1	A	16	ASP
1	A	116	GLU
1	A	166	VAL
1	A	168	PRO
1	A	191	LEU
1	A	202	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	283	LEU
1	A	291	MET
1	A	322	GLN
1	A	333	ASN
1	A	347	PHE
1	A	352	MET
1	A	360	ARG
1	A	392	ILE
1	A	393	ASP
1	A	425	THR
1	A	481	LEU
1	A	523	ARG
1	A	550	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	217	GLN
1	A	250	GLN
1	A	305	GLN
1	A	333	ASN
1	A	403	ASN
1	A	497	ASN
1	A	570	ASN
1	A	574	HIS
1	A	595	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	SEP	A	198	1	9,9,10	6.82	3 (33%)	10,12,14	2.36	4 (40%)

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	SEP	A	198	1	-	0/6/8/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	O-C	19.83	1.25	1.11
1	A	198	SEP	CA-C	3.82	1.55	1.48
1	A	198	SEP	P-O1P	2.29	1.58	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O3P-P-OG	4.35	118.67	106.65
1	A	198	SEP	C-CA-N	-3.77	110.07	113.83
1	A	198	SEP	O3P-P-O1P	-2.83	101.19	110.44
1	A	198	SEP	O2P-P-OG	-2.10	100.85	106.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

2 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	602	1,3	12,14,15	0.76	1 (8%)	15,19,21	0.85	0
3	NAG	A	603	3	12,14,15	0.61	0	15,19,21	1.40	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	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	603	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NAG	O5-C5	-2.10	1.41	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	NAG	O5-C5-C4	2.66	114.03	110.65
3	A	603	NAG	C3-C4-C5	2.57	114.79	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 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
5	HEM	A	1001	1	49,50,50	2.43	13 (26%)	46,82,82	1.70	8 (17%)
2	NAG	A	596	1	12,14,15	0.52	0	15,19,21	2.00	2 (13%)
7	EDO	A	598	-	3,3,3	0.29	0	2,2,2	1.23	0
2	NAG	A	599	1	12,14,15	0.61	0	15,19,21	0.94	0
8	MZZ	A	610	-	15,15,15	6.53	12 (80%)	20,20,20	3.96	11 (55%)

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
5	HEM	A	1001	1	-	0/14/114/114	0/0/8/8
2	NAG	A	596	1	-	0/6/23/26	0/1/1/1
7	EDO	A	598	-	-	0/1/1/1	0/0/0/0
2	NAG	A	599	1	-	0/6/23/26	0/1/1/1
8	MZZ	A	610	-	-	0/4/8/8	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	610	MZZ	O12-C8	18.83	1.41	1.21
8	A	610	MZZ	C17-N9	-8.26	1.27	1.39
8	A	610	MZZ	C20-N9	-7.42	1.25	1.36
5	A	1001	HEM	C2B-C1B	7.20	1.46	1.44
8	A	610	MZZ	C6-C1	-6.38	1.24	1.39
8	A	610	MZZ	C1-N7	5.57	1.59	1.38
5	A	1001	HEM	C3B-C2B	-5.52	1.34	1.43
5	A	1001	HEM	C4A-C3A	5.42	1.46	1.40
8	A	610	MZZ	C3-C4	-5.28	1.30	1.39
5	A	1001	HEM	C3B-CAB	4.95	1.56	1.40
5	A	1001	HEM	C3C-C2C	-4.79	1.35	1.43
5	A	1001	HEM	C3D-C4D	4.68	1.45	1.44
5	A	1001	HEM	C3D-C2D	4.66	1.51	1.43
5	A	1001	HEM	C3C-CAC	4.56	1.54	1.40
8	A	610	MZZ	C3-C2	-4.04	1.31	1.38
8	A	610	MZZ	C5-C4	-3.32	1.33	1.39
8	A	610	MZZ	C2-C1	-3.21	1.32	1.39
8	A	610	MZZ	C6-C5	-3.18	1.32	1.38
5	A	1001	HEM	FE-NB	2.99	2.08	1.97
5	A	1001	HEM	FE-ND	2.66	2.07	1.97
5	A	1001	HEM	CMC-C2C	2.61	1.55	1.47

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	610	MZZ	C20-N19	2.52	1.39	1.34
8	A	610	MZZ	C8-N9	-2.34	1.39	1.44
5	A	1001	HEM	CMB-C2B	2.23	1.54	1.47
5	A	1001	HEM	CMD-C2D	2.02	1.53	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	610	MZZ	C4-C8-N9	11.50	133.00	118.26
8	A	610	MZZ	C3-C2-C1	6.35	130.31	120.67
2	A	596	NAG	O5-C5-C4	5.97	118.23	110.65
5	A	1001	HEM	C3B-C4B-NB	-5.72	109.91	114.00
8	A	610	MZZ	C6-C1-C2	-5.28	108.97	118.20
8	A	610	MZZ	O12-C8-C4	-5.25	110.25	120.17
8	A	610	MZZ	C5-C4-C8	4.37	131.01	120.32
8	A	610	MZZ	C5-C4-C3	-4.36	112.41	118.63
5	A	1001	HEM	C4D-ND-C1D	4.19	109.45	105.16
5	A	1001	HEM	CBD-CAD-C3D	-3.93	105.80	114.37
2	A	596	NAG	C3-C4-C5	3.48	116.42	110.20
5	A	1001	HEM	C3A-C4A-NA	-2.94	107.19	109.41
8	A	610	MZZ	C5-C6-C1	2.94	125.13	120.67
8	A	610	MZZ	C6-C5-C4	2.91	124.24	120.76
8	A	610	MZZ	C17-N9-C20	2.89	113.76	108.50
5	A	1001	HEM	CBA-CAA-C2A	-2.50	108.29	112.69
8	A	610	MZZ	C6-C1-N7	2.33	125.78	120.90
5	A	1001	HEM	C4A-C3A-C2A	2.31	108.60	107.00
5	A	1001	HEM	CAD-C3D-C4D	2.06	128.24	124.53
5	A	1001	HEM	C1B-NB-C4B	2.06	107.27	105.16
8	A	610	MZZ	C2-C1-N7	2.04	125.18	120.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	595/595 (100%)	0.62	53 (8%)	10 16	24, 45, 81, 106	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	LEU	13.1
1	A	120	GLY	8.8
1	A	2	TRP	8.3
1	A	10	VAL	7.7
1	A	174	SER	7.2
1	A	595	ASN	6.6
1	A	1	SER	6.0
1	A	593	ARG	5.9
1	A	7	GLY	5.6
1	A	121	SER	5.6
1	A	173	GLN	5.4
1	A	4	VAL	5.3
1	A	124	HIS	5.3
1	A	544	LEU	4.9
1	A	210	LEU	4.7
1	A	594	GLU	4.5
1	A	122	SER	4.4
1	A	172	TYR	4.4
1	A	209	PRO	4.3
1	A	13	VAL	4.2
1	A	292	LEU	3.9
1	A	288	ASP	3.8
1	A	11	PRO	3.7
1	A	64	ARG	3.5
1	A	376	LEU	3.5
1	A	262	LEU	3.4
1	A	111	LEU	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	16	ASP	3.2
1	A	265	VAL	3.0
1	A	5	GLY	2.9
1	A	354	VAL	2.9
1	A	104	GLY	2.9
1	A	102	GLN	2.8
1	A	170	PRO	2.7
1	A	171	PRO	2.7
1	A	564	LEU	2.7
1	A	159	PRO	2.6
1	A	107	VAL	2.5
1	A	106	ILE	2.4
1	A	588	SER	2.4
1	A	242	THR	2.3
1	A	387	ILE	2.3
1	A	125	SER	2.3
1	A	9	PRO	2.2
1	A	131	GLU	2.2
1	A	132	TYR	2.2
1	A	572	TYR	2.2
1	A	15	CYS	2.2
1	A	351	HIS	2.2
1	A	98	LEU	2.1
1	A	342	VAL	2.1
1	A	424	PRO	2.0
1	A	119	LEU	2.0

## 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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	A	198	10/11	0.17	0.16	36,45,48,48	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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	603	14/15	0.31	3.76	63,65,71,72	0
3	NAG	A	602	14/15	0.09	-1.14	48,52,54,59	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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	IOD	A	600	1/1	0.28	5.33	40,40,40,40	1
2	NAG	A	596	14/15	0.29	3.23	59,64,69,70	0
6	IOD	A	606	1/1	0.24	2.78	63,63,63,63	1
6	IOD	A	604	1/1	0.26	2.28	40,40,40,40	1
6	IOD	A	597	1/1	0.22	1.96	17,17,17,17	1
8	MZZ	A	610	14/14	0.29	1.80	29,43,46,46	0
6	IOD	A	607	1/1	0.19	1.60	61,61,61,61	1
6	IOD	A	605	1/1	0.25	1.25	49,49,49,49	1
7	EDO	A	598	4/4	0.25	0.78	32,34,39,39	0
5	HEM	A	1001	43/43	0.22	0.24	21,26,32,38	0
2	NAG	A	599	14/15	0.19	-0.04	65,66,69,72	0
6	IOD	A	609	1/1	0.13	-0.50	63,63,63,63	1
6	IOD	A	608	1/1	0.13	-0.94	73,73,73,73	1
4	CA	A	1000	1/1	0.09	-1.25	34,34,34,34	0
6	IOD	A	601	1/1	0.11	-1.60	63,63,63,63	1

### 6.5 Other polymers ⓘ

There are no such residues in this entry.