



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:01 PM GMT

PDB ID : 3R4X  
Title : Crystal structure of bovine lactoperoxidase complexed with pyrazine-2-carboxamide at 2 Å resolution  
Authors : Pandey, N.; Singh, R.P.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2011-03-18  
Resolution : 2.01 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>

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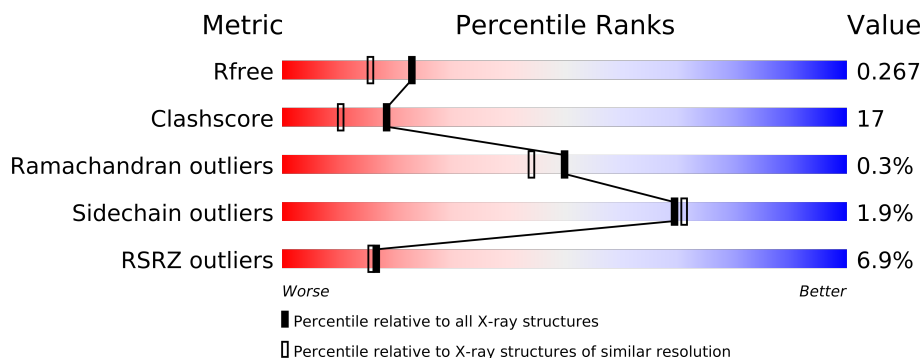
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.01 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	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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
10	PEG	A	603	-	X
11	GOL	A	621	X	X
4	NAG	A	596	-	X
4	NAG	A	604	-	X
9	PZA	A	597	-	X
9	PZA	A	598	-	X

## 2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 5468 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.

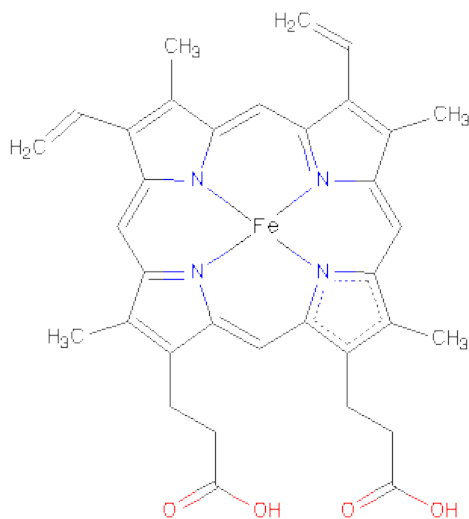
- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4774	3037	847	863	1	26			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

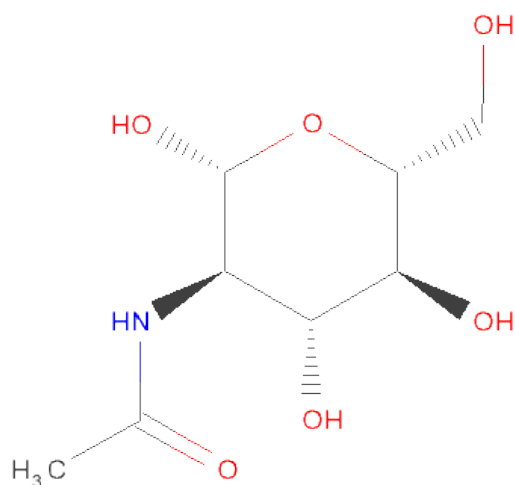
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

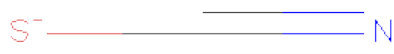
- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	I	0	0
			11	11		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

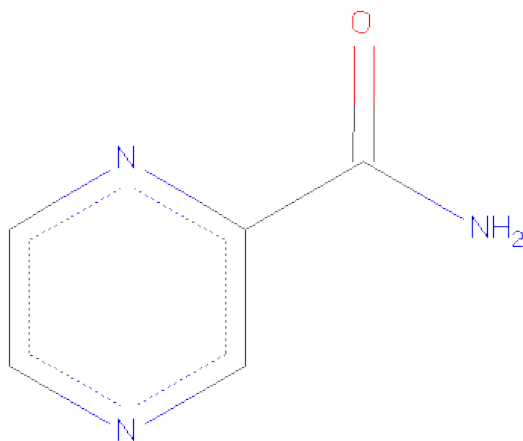
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



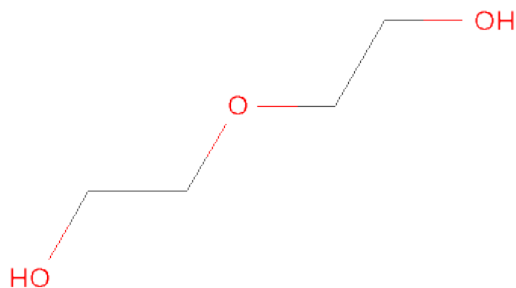
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 9 is PYRAZINE-2-CARBOXAMIDE (three-letter code: PZA) (formula: C<sub>5</sub>H<sub>5</sub>N<sub>3</sub>O).



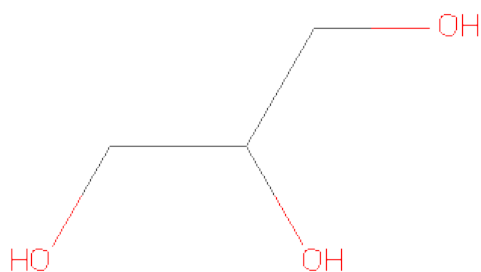
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			9	5	3	1		
9	A	1	Total	C	N	O	0	0
			9	5	3	1		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



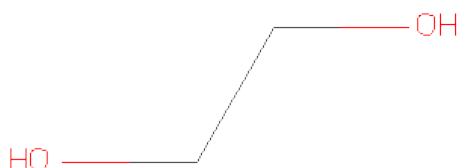
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		
10	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

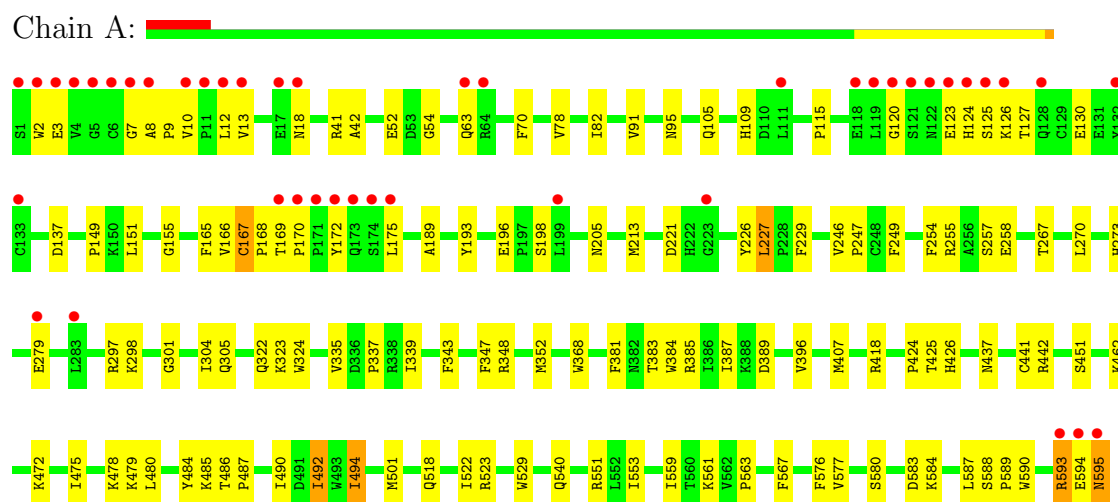
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	499	Total	O	0	0
			499	499		

### 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 ( $RSRZ > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	53.92Å 79.72Å 77.00Å 90.00° 102.22° 90.00°	Depositor
Resolution (Å)	75.26 – 2.01 43.96 – 2.01	Depositor EDS
% Data completeness (in resolution range)	97.8 (75.26-2.01) 97.8 (43.96-2.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.89 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.210 , 0.256 0.229 , 0.267	Depositor DCC
$R_{free}$ test set	2104 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.908	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 41626 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5468	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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: GOL, ZN, SCN, NAG, SEP, CA, EDO, HEM, PEG, PZA, 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	0.74	0/4891	0.85	2/6634 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	227	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	4774	0	4687	150	0
2	A	1	0	0	0	0
3	A	43	0	30	7	0
4	A	28	0	26	4	0
5	A	56	0	50	1	0
6	A	11	0	0	4	0
7	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	3	0	0	0	0
9	A	18	0	10	18	0
10	A	14	0	20	4	0
11	A	12	0	14	6	0
12	A	8	0	12	1	0
13	A	499	0	0	21	0
All	All	5468	0	4849	165	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 17.

All (165) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:12:LEU:HD23	1:A:13:VAL:N	1.40	1.36
1:A:10:VAL:HG11	1:A:41:ARG:CZ	1.65	1.26
4:A:596:NAG:O7	11:A:621:GOL:H11	1.39	1.20
1:A:424:PRO:O	1:A:425:THR:HG22	1.37	1.19
1:A:593:ARG:HG2	1:A:593:ARG:HH11	0.96	1.11
1:A:123:GLU:HG3	1:A:125:SER:H	1.00	1.08
1:A:167:CYS:CB	1:A:168:PRO:CD	2.31	1.08
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.28	1.07
1:A:105:GLN:HE21	9:A:597:PZA:H2	1.02	1.02
1:A:167:CYS:HB3	1:A:168:PRO:CD	1.91	1.00
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.46	0.97
1:A:167:CYS:CB	1:A:168:PRO:HD2	1.92	0.96
1:A:169:THR:HB	1:A:170:PRO:HD3	1.48	0.95
1:A:593:ARG:HG2	1:A:593:ARG:NH1	1.71	0.93
1:A:123:GLU:HG3	1:A:125:SER:N	1.83	0.93
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.70	0.90
9:A:597:PZA:H5	9:A:598:PZA:C	2.02	0.90
1:A:10:VAL:CG1	1:A:41:ARG:CZ	2.52	0.87
1:A:593:ARG:CG	1:A:593:ARG:HH11	1.85	0.87
1:A:168:PRO:HG3	1:A:172:TYR:HD1	1.38	0.86
1:A:54:GLY:HA2	13:A:936:HOH:O	1.74	0.85
1:A:12:LEU:HD23	1:A:13:VAL:H	1.41	0.85
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.57	0.85
1:A:279:GLU:HG2	1:A:587:LEU:HD12	1.57	0.85
1:A:12:LEU:CD2	1:A:13:VAL:N	2.34	0.84
1:A:255:ARG:HA	9:A:598:PZA:N2	1.94	0.82
1:A:9:PRO:CD	1:A:167:CYS:HA	2.10	0.81
1:A:12:LEU:C	1:A:12:LEU:HD23	2.00	0.81
1:A:424:PRO:O	1:A:425:THR:CG2	2.28	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:462:LYS:HD2	13:A:974:HOH:O	1.83	0.78
1:A:10:VAL:HG11	1:A:41:ARG:NH2	2.00	0.77
1:A:105:GLN:NE2	9:A:597:PZA:H2	1.82	0.75
1:A:124:HIS:HB2	1:A:127:THR:HB	1.68	0.75
1:A:10:VAL:CG1	1:A:41:ARG:NH2	2.50	0.74
1:A:168:PRO:HG3	1:A:172:TYR:CD1	2.21	0.74
1:A:339:ILE:HD13	1:A:522:ILE:HD11	1.71	0.72
1:A:9:PRO:HG2	1:A:167:CYS:O	1.92	0.70
1:A:95:ASN:HD22	11:A:621:GOL:H12	1.57	0.69
1:A:109:HIS:NE2	9:A:597:PZA:C	2.56	0.69
1:A:396:VAL:HG11	1:A:553:ILE:HD12	1.74	0.69
1:A:105:GLN:HG3	9:A:597:PZA:N1	2.08	0.68
1:A:12:LEU:HD23	1:A:13:VAL:CA	2.23	0.68
1:A:9:PRO:HG2	1:A:167:CYS:CA	2.24	0.68
1:A:10:VAL:HG11	1:A:41:ARG:NH1	2.08	0.67
1:A:494:ILE:O	1:A:494:ILE:HD13	1.94	0.67
1:A:127:THR:HA	13:A:1122:HOH:O	1.95	0.67
1:A:227:LEU:HD22	1:A:270:LEU:HD22	1.75	0.67
1:A:105:GLN:HG3	9:A:597:PZA:H1	1.62	0.65
1:A:258:GLU:HB2	9:A:598:PZA:H4	1.77	0.65
1:A:12:LEU:C	1:A:12:LEU:CD2	2.66	0.64
6:A:614:IOD:I	13:A:1014:HOH:O	2.85	0.64
1:A:418:ARG:HH22	10:A:603:PEG:C4	2.11	0.64
1:A:105:GLN:NE2	9:A:597:PZA:H4	2.13	0.63
1:A:475:ILE:HG22	1:A:479:LYS:HE3	1.81	0.62
1:A:9:PRO:HD2	1:A:167:CYS:HA	1.81	0.62
1:A:78:VAL:HG21	1:A:484:TYR:OH	2.00	0.61
1:A:169:THR:N	1:A:170:PRO:CD	2.63	0.61
1:A:82:ILE:HD13	1:A:480:LEU:HD23	1.83	0.61
9:A:597:PZA:H5	9:A:598:PZA:N1	2.16	0.60
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.36	0.60
1:A:165:PHE:CZ	1:A:169:THR:O	2.54	0.60
1:A:559:ILE:HG23	6:A:607:IOD:I	2.73	0.59
1:A:63:GLN:CD	1:A:63:GLN:H	2.06	0.58
1:A:105:GLN:HE21	9:A:597:PZA:H4	1.69	0.58
1:A:407:MET:HB3	1:A:501:MET:HE3	1.86	0.57
1:A:492:ILE:O	1:A:492:ILE:HD13	2.05	0.57
1:A:168:PRO:HB2	1:A:170:PRO:O	2.06	0.56
1:A:18:ASN:ND2	13:A:1008:HOH:O	2.37	0.56
1:A:594:GLU:O	1:A:595:ASN:HB2	2.06	0.56
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.41	0.55
1:A:10:VAL:HG12	1:A:41:ARG:NH2	2.21	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:105:GLN:CG	9:A:597:PZA:N1	2.70	0.55
1:A:580:SER:HA	11:A:622:GOL:O2	2.07	0.55
1:A:339:ILE:CD1	1:A:522:ILE:HD11	2.35	0.54
1:A:9:PRO:CG	1:A:167:CYS:HA	2.36	0.54
1:A:82:ILE:HD13	1:A:480:LEU:CD2	2.38	0.54
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.43	0.54
1:A:492:ILE:C	1:A:492:ILE:HD13	2.28	0.54
4:A:596:NAG:O7	11:A:621:GOL:C1	2.33	0.53
1:A:472:LYS:HE3	12:A:624:EDO:H21	1.89	0.53
1:A:169:THR:HB	1:A:170:PRO:CD	2.31	0.53
3:A:605:HEM:HMC2	3:A:605:HEM:HBC2	1.91	0.53
1:A:551:ARG:HD3	1:A:583:ASP:O	2.09	0.53
1:A:149:PRO:HB2	10:A:603:PEG:H22	1.91	0.52
1:A:518:GLN:O	1:A:522:ILE:HG12	2.10	0.52
1:A:383:THR:HG22	1:A:387:ILE:HD12	1.91	0.52
1:A:169:THR:N	1:A:170:PRO:HD2	2.24	0.52
1:A:258:GLU:HG3	9:A:598:PZA:N1	2.25	0.52
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.45	0.52
3:A:605:HEM:NC	9:A:597:PZA:N1	2.58	0.51
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.57	0.51
1:A:451:SER:HA	13:A:1042:HOH:O	2.08	0.51
1:A:426:HIS:HE1	13:A:1057:HOH:O	1.92	0.51
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.07	0.51
1:A:323:LYS:HD3	1:A:324:TRP:CE2	2.46	0.51
1:A:227:LEU:HD21	1:A:267:THR:HA	1.92	0.51
6:A:612:IOD:I	13:A:1072:HOH:O	2.88	0.51
1:A:9:PRO:HG2	1:A:167:CYS:C	2.32	0.50
1:A:109:HIS:NE2	9:A:597:PZA:C4	2.74	0.50
3:A:605:HEM:HBD2	13:A:886:HOH:O	2.10	0.50
1:A:384:TRP:CZ2	5:A:601:NAG:H2	2.45	0.50
1:A:42:ALA:HB2	1:A:166:VAL:HG11	1.93	0.50
1:A:584:LYS:HE3	11:A:622:GOL:H11	1.93	0.49
1:A:407:MET:HB3	1:A:501:MET:CE	2.42	0.49
1:A:63:GLN:N	1:A:63:GLN:CD	2.66	0.49
1:A:70:PHE:CG	1:A:485:LYS:HB2	2.48	0.49
1:A:82:ILE:CD1	1:A:480:LEU:HD23	2.42	0.48
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.94	0.48
1:A:249:PHE:CE1	1:A:383:THR:HG23	2.49	0.48
1:A:301:GLY:O	1:A:305:GLN:HG3	2.14	0.48
1:A:52:GLU:HG2	13:A:981:HOH:O	2.14	0.47
1:A:487:PRO:HA	1:A:490:ILE:HD12	1.96	0.47
10:A:619:PEG:H41	13:A:900:HOH:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:123:GLU:HG2	1:A:125:SER:HB3	1.97	0.47
4:A:596:NAG:H4	13:A:1056:HOH:O	2.15	0.46
1:A:63:GLN:NE2	13:A:1019:HOH:O	2.47	0.46
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.51	0.46
1:A:368:TRP:CE3	1:A:368:TRP:O	2.69	0.46
1:A:385:ARG:O	1:A:389:ASP:HB3	2.15	0.46
4:A:596:NAG:H2	11:A:621:GOL:H31	1.97	0.46
1:A:494:ILE:C	1:A:494:ILE:HD13	2.36	0.46
1:A:9:PRO:CG	1:A:167:CYS:O	2.61	0.45
1:A:540:GLN:HG2	1:A:590:TRP:CE2	2.51	0.45
1:A:205:ASN:HA	13:A:1068:HOH:O	2.16	0.45
1:A:561:LYS:HA	1:A:577:VAL:O	2.17	0.44
1:A:246:VAL:HG11	1:A:387:ILE:HD12	1.99	0.44
1:A:249:PHE:CZ	1:A:383:THR:HG23	2.52	0.44
1:A:8:ALA:N	1:A:9:PRO:CD	2.80	0.44
1:A:257:SER:O	1:A:381:PHE:HA	2.18	0.44
1:A:123:GLU:HG2	1:A:125:SER:CB	2.48	0.44
1:A:279:GLU:CG	1:A:587:LEU:HD12	2.38	0.44
1:A:418:ARG:HH22	10:A:603:PEG:H42	1.82	0.44
3:A:605:HEM:HBB2	3:A:605:HEM:CMB	2.48	0.43
3:A:605:HEM:C1A	9:A:597:PZA:N3	2.87	0.43
1:A:298:LYS:HG3	13:A:1061:HOH:O	2.18	0.43
1:A:123:GLU:CG	1:A:125:SER:CB	2.96	0.43
1:A:175:LEU:HD12	13:A:1106:HOH:O	2.18	0.43
1:A:424:PRO:C	1:A:425:THR:HG22	2.22	0.43
1:A:254:PHE:CE2	9:A:598:PZA:C1	3.02	0.43
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.54	0.43
1:A:227:LEU:CD2	1:A:270:LEU:HD22	2.45	0.43
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.54	0.43
1:A:567:PHE:HB2	6:A:612:IOD:I	2.89	0.43
1:A:396:VAL:CG1	1:A:553:ILE:HD12	2.46	0.42
1:A:335:VAL:O	1:A:337:PRO:HD3	2.19	0.42
1:A:9:PRO:CG	1:A:167:CYS:CA	2.94	0.42
1:A:540:GLN:HG2	1:A:590:TRP:CZ2	2.54	0.42
1:A:193:TYR:OH	1:A:297:ARG:HA	2.20	0.42
3:A:605:HEM:ND	9:A:597:PZA:O	2.53	0.42
1:A:120:GLY:HA3	1:A:126:LYS:HG3	2.02	0.42
1:A:368:TRP:HE3	1:A:368:TRP:O	2.02	0.42
1:A:123:GLU:CG	1:A:125:SER:HB3	2.50	0.41
1:A:478:LYS:HE2	13:A:978:HOH:O	2.21	0.41
1:A:2:TRP:HA	13:A:773:HOH:O	2.20	0.41
1:A:352:MET:CB	1:A:407:MET:HG2	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:130:GLU:OE1	1:A:426:HIS:ND1	2.51	0.41
1:A:487:PRO:HA	1:A:490:ILE:CD1	2.50	0.41
1:A:322:GLN:HG2	13:A:687:HOH:O	2.20	0.41
1:A:151:LEU:HD12	1:A:155:GLY:O	2.21	0.41
1:A:189:ALA:HB2	1:A:304:ILE:HD12	2.02	0.41
1:A:78:VAL:HG13	1:A:82:ILE:HD12	2.03	0.40
1:A:229:PHE:HZ	1:A:387:ILE:HD13	1.86	0.40
1:A:115:PRO:HG2	13:A:1037:HOH:O	2.21	0.40
1:A:105:GLN:HG3	3:A:605:HEM:C1C	2.56	0.40
1:A:130:GLU:HB2	13:A:1057:HOH:O	2.22	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%)	569 (96%)	21 (4%)	2 (0%)	50 44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	7	GLY

### 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	517/517 (100%)	507 (98%)	10 (2%)	69 71

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	91	VAL
1	A	137	ASP
1	A	347	PHE
1	A	441	CYS
1	A	486	THR
1	A	492	ILE
1	A	494	ILE
1	A	593	ARG
1	A	595	ASN

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	102	GLN
1	A	105	GLN
1	A	259	GLN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	570	ASN
1	A	571	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	6.28	3 (33%)	10,12,14	1.09	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
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	18.07	1.23	1.11
1	A	198	SEP	CA-C	3.33	1.54	1.48
1	A	198	SEP	P-O1P	3.08	1.61	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

4 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
5	NAG	A	599	1,5	12,14,15	0.56	0	15,19,21	0.85	0
5	NAG	A	600	5	12,14,15	1.11	2 (16%)	15,19,21	1.91	3 (20%)
5	NAG	A	601	1,5	12,14,15	0.68	0	15,19,21	0.96	1 (6%)
5	NAG	A	602	5	12,14,15	0.46	0	15,19,21	1.85	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
5	NAG	A	599	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	600	5	-	0/6/23/26	0/1/1/1
5	NAG	A	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	602	5	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	NAG	C8-C7	2.51	1.55	1.50
5	A	600	NAG	O5-C5	-2.28	1.41	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	NAG	O5-C5-C4	4.97	116.96	110.65
5	A	600	NAG	C3-C2-N2	-4.42	105.02	111.76
5	A	600	NAG	O5-C5-C4	-3.59	106.10	110.65
5	A	600	NAG	O5-C5-C6	3.21	110.35	106.98
5	A	602	NAG	O5-C5-C6	3.06	110.19	106.98
5	A	601	NAG	O5-C5-C6	2.45	109.55	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

Of 25 ligands modelled in this entry, 13 are 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
4	NAG	A	596	1	12,14,15	0.85	1 (8%)	15,19,21	0.93	1 (6%)
9	PZA	A	597	3	9,9,9	0.46	0	11,11,11	2.23	5 (45%)
9	PZA	A	598	-	9,9,9	0.36	0	11,11,11	2.12	4 (36%)
10	PEG	A	603	-	6,6,6	1.57	1 (16%)	5,5,5	0.85	0
4	NAG	A	604	1	12,14,15	0.68	0	15,19,21	0.97	2 (13%)
3	HEM	A	605	1,9	49,50,50	3.15	20 (40%)	46,82,82	1.87	12 (26%)
10	PEG	A	619	-	6,6,6	1.43	1 (16%)	5,5,5	0.81	0
8	SCN	A	620	-	2,2,2	2.55	1 (50%)	1,1,1	0.03	0
11	GOL	A	621	-	5,5,5	3.26	2 (40%)	5,5,5	2.41	4 (80%)
11	GOL	A	622	-	5,5,5	0.96	0	5,5,5	1.02	1 (20%)
12	EDO	A	623	-	3,3,3	0.86	0	2,2,2	0.90	0
12	EDO	A	624	-	3,3,3	0.39	0	2,2,2	0.46	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
4	NAG	A	596	1	-	0/6/23/26	0/1/1/1
9	PZA	A	597	3	-	4/4/4/4	0/1/1/1
9	PZA	A	598	-	-	4/4/4/4	0/1/1/1
10	PEG	A	603	-	-	0/4/4/4	0/0/0/0
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
3	HEM	A	605	1,9	-	0/14/114/114	0/0/8/8
10	PEG	A	619	-	-	0/4/4/4	0/0/0/0
8	SCN	A	620	-	-	0/0/0/0	0/0/0/0
11	GOL	A	621	-	-	0/4/4/4	0/0/0/0
11	GOL	A	622	-	-	0/4/4/4	0/0/0/0
12	EDO	A	623	-	-	0/1/1/1	0/0/0/0
12	EDO	A	624	-	-	0/1/1/1	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	HEM	C2B-C1B	-10.96	1.41	1.44
3	A	605	HEM	C2D-C1D	-7.12	1.42	1.44
11	A	621	GOL	O2-C2	-6.72	1.22	1.43
3	A	605	HEM	C3B-CAB	5.82	1.58	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	HEM	C4A-C3A	5.67	1.47	1.40
3	A	605	HEM	C1A-C2A	5.18	1.52	1.43
3	A	605	HEM	C3C-CAC	4.74	1.55	1.40
3	A	605	HEM	CHD-C4C	4.60	1.44	1.36
3	A	605	HEM	C3D-C2D	4.50	1.51	1.43
3	A	605	HEM	C4D-ND	-4.12	1.31	1.39
3	A	605	HEM	FE-NB	3.85	2.11	1.97
3	A	605	HEM	CMC-C2C	3.60	1.58	1.47
8	A	620	SCN	C-S	3.56	1.86	1.63
3	A	605	HEM	C3B-C2B	-3.46	1.37	1.43
3	A	605	HEM	CHB-C1B	3.36	1.40	1.35
3	A	605	HEM	C3D-C4D	-3.29	1.43	1.44
10	A	603	PEG	C2-C1	-3.14	1.32	1.49
3	A	605	HEM	C3C-C2C	-3.00	1.38	1.43
3	A	605	HEM	CHD-C1D	2.67	1.45	1.39
10	A	619	PEG	C2-C1	-2.63	1.35	1.49
3	A	605	HEM	FE-ND	2.61	2.07	1.97
3	A	605	HEM	C3B-C4B	-2.58	1.41	1.44
11	A	621	GOL	O1-C1	2.39	1.52	1.42
3	A	605	HEM	C1B-NB	-2.39	1.34	1.39
4	A	596	NAG	C8-C7	2.26	1.55	1.50
3	A	605	HEM	CHC-C1C	2.21	1.40	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	HEM	CAD-C3D-C4D	5.71	134.80	124.53
3	A	605	HEM	C3B-C4B-NB	-4.18	111.01	114.00
9	A	598	PZA	C4-C-N1	4.16	119.58	115.96
9	A	597	PZA	C4-C3-N2	-4.15	118.53	122.14
9	A	597	PZA	C4-C-N1	4.01	119.45	115.96
11	A	621	GOL	O2-C2-C1	3.09	122.30	108.22
3	A	605	HEM	C4D-ND-C1D	3.05	108.28	105.16
3	A	605	HEM	CBD-CAD-C3D	-2.98	107.86	114.37
3	A	605	HEM	C4C-NC-C1C	-2.97	102.45	105.53
11	A	621	GOL	O2-C2-C3	2.96	121.70	108.22
9	A	598	PZA	C4-C3-N2	-2.88	119.64	122.14
3	A	605	HEM	CMD-C2D-C3D	-2.78	119.30	125.60
3	A	605	HEM	C4A-CHB-C1B	2.76	131.11	127.47
3	A	605	HEM	CHC-C4B-NB	-2.76	122.29	124.58
4	A	604	NAG	O5-C5-C6	2.62	109.73	106.98
9	A	597	PZA	C2-C1-N3	-2.56	118.94	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	HEM	CBA-CAA-C2A	-2.50	108.28	112.69
3	A	605	HEM	C3A-C4A-NA	2.41	111.23	109.41
9	A	598	PZA	C1-N3-C4	2.39	120.32	116.96
3	A	605	HEM	CHC-C1C-NC	-2.36	122.68	124.73
9	A	597	PZA	C2-N2-C3	2.34	121.05	116.85
9	A	597	PZA	C1-N3-C4	2.34	120.25	116.96
11	A	621	GOL	C3-C2-C1	-2.26	101.28	111.26
4	A	596	NAG	O5-C5-C4	2.18	113.42	110.65
9	A	598	PZA	C2-N2-C3	2.14	120.68	116.85
3	A	605	HEM	CHD-C1D-ND	2.11	126.34	124.58
4	A	604	NAG	O5-C5-C4	-2.08	108.02	110.65
11	A	622	GOL	O2-C2-C3	-2.07	98.81	108.22
11	A	621	GOL	O1-C1-C2	-2.03	99.81	109.71

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	597	PZA	C3-C4-C-N1
9	A	597	PZA	N3-C4-C-N1
9	A	597	PZA	O-C-C4-N3
9	A	597	PZA	O-C-C4-C3
9	A	598	PZA	C3-C4-C-N1
9	A	598	PZA	O-C-C4-C3
9	A	598	PZA	O-C-C4-N3
9	A	598	PZA	N3-C4-C-N1

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%)	0.47	43 (7%) 15 14	15, 31, 57, 94	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	12.2
1	A	12	LEU	9.3
1	A	172	TYR	9.3
1	A	121	SER	8.5
1	A	119	LEU	8.4
1	A	171	PRO	7.3
1	A	11	PRO	7.1
1	A	4	VAL	6.7
1	A	120	GLY	6.5
1	A	13	VAL	6.2
1	A	173	GLN	6.2
1	A	122	ASN	6.1
1	A	10	VAL	5.9
1	A	124	HIS	5.3
1	A	170	PRO	4.9
1	A	7	GLY	4.8
1	A	174	SER	4.7
1	A	123	GLU	4.7
1	A	1	SER	4.3
1	A	6	CYS	4.3
1	A	595	ASN	4.2
1	A	8	ALA	4.1
1	A	283	LEU	4.1
1	A	593	ARG	4.1
1	A	169	THR	3.8
1	A	128	GLN	3.4
1	A	64	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	3	GLU	3.1
1	A	5	GLY	3.1
1	A	18	ASN	3.1
1	A	594	GLU	3.0
1	A	17	GLU	2.6
1	A	132	TYR	2.6
1	A	279	GLU	2.6
1	A	133	CYS	2.6
1	A	63	GLN	2.5
1	A	223	GLY	2.5
1	A	175	LEU	2.4
1	A	126	LYS	2.3
1	A	125	SER	2.3
1	A	199	LEU	2.1
1	A	118	GLU	2.1
1	A	111	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	0.24	2.15	39,40,41,41	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
5	NAG	A	602	14/15	0.22	7.68	51,55,56,56	0
5	NAG	A	601	14/15	0.17	0.95	38,40,43,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	599	14/15	0.14	0.35	39,44,46,50	0
5	NAG	A	600	14/15	0.42	-	54,57,58,58	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( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	604	14/15	0.28	21.49	39,39,40,40	0
9	PZA	A	597	9/9	0.41	10.39	28,29,30,31	0
9	PZA	A	598	9/9	0.39	5.56	27,27,27,28	9
4	NAG	A	596	14/15	0.31	3.93	47,50,52,52	0
11	GOL	A	621	6/6	0.26	3.74	45,46,47,49	0
10	PEG	A	603	7/7	0.18	3.17	33,35,36,37	0
8	SCN	A	620	3/3	0.21	0.98	30,30,30,30	0
11	GOL	A	622	6/6	0.17	0.78	58,58,59,60	0
10	PEG	A	619	7/7	0.14	0.50	50,51,51,51	0
12	EDO	A	623	4/4	0.17	0.31	41,42,42,43	0
3	HEM	A	605	43/43	0.17	0.29	14,18,22,24	0
12	EDO	A	624	4/4	0.13	-0.55	30,31,32,34	0
6	IOD	A	611	1/1	0.09	-0.57	63,63,63,63	0
2	CA	A	606	1/1	0.12	-0.72	22,22,22,22	0
6	IOD	A	614	1/1	0.06	-1.82	55,55,55,55	1
6	IOD	A	613	1/1	0.07	-1.94	64,64,64,64	1
6	IOD	A	607	1/1	0.05	-2.11	51,51,51,51	0
6	IOD	A	615	1/1	0.04	-2.82	26,26,26,26	0
6	IOD	A	616	1/1	0.06	-3.20	36,36,36,36	0
6	IOD	A	612	1/1	0.05	-3.28	52,52,52,52	1
6	IOD	A	609	1/1	0.03	-3.58	57,57,57,57	0
6	IOD	A	617	1/1	0.08	-3.87	53,53,53,53	0
6	IOD	A	610	1/1	0.03	-4.17	58,58,58,58	0
6	IOD	A	608	1/1	0.03	-4.37	40,40,40,40	0
7	ZN	A	618	1/1	0.04	-4.49	44,44,44,44	0



## 6.5 Other polymers ⓘ

There are no such residues in this entry.