



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2016 – 07:38 PM EDT

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 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
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) : rb-20027107

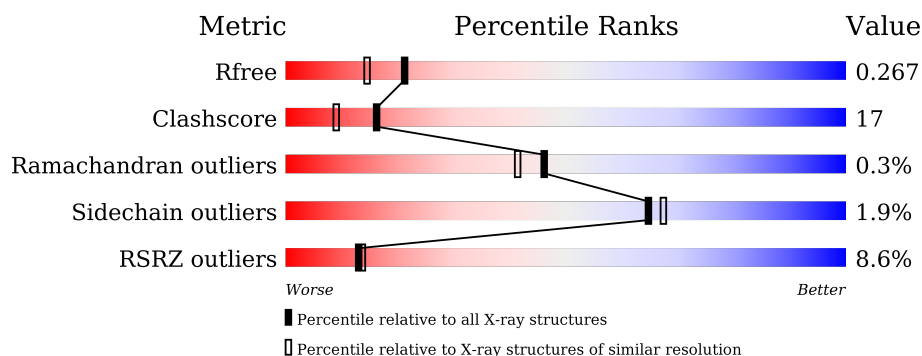
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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	595	<div> <div>9%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PEG	A	603	-	-	-	X
11	GOL	A	621	-	X	X	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	IOD	A	612	-	-	X	-
9	PZA	A	597	-	-	X	X
9	PZA	A	598	-	-	X	X



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.

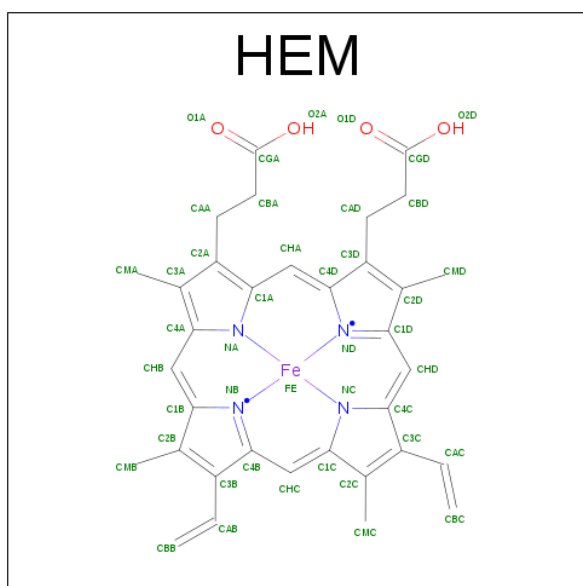
- Molecule 1 is a protein called Lactoperoxidase.

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).

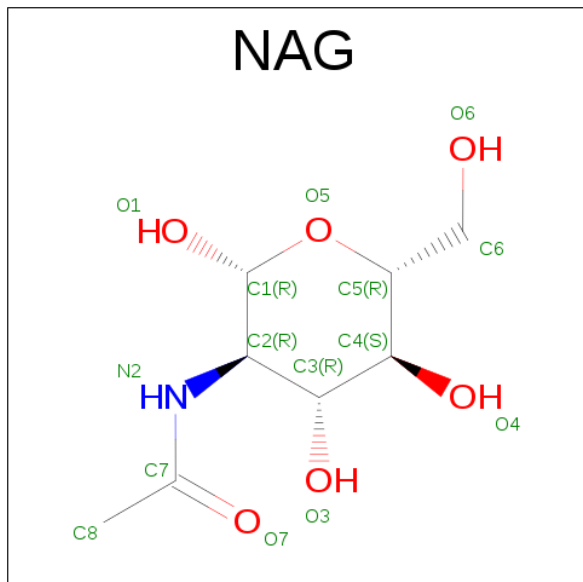
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0

- 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 43	C 34	Fe 1	N 4	O 4	0	0

- 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		

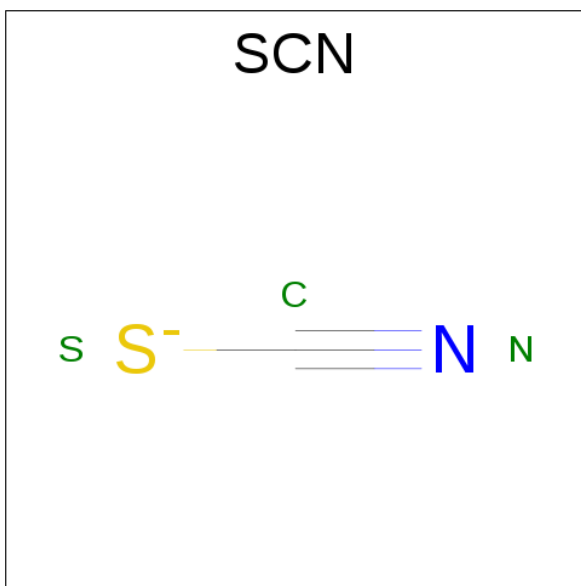
- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

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).

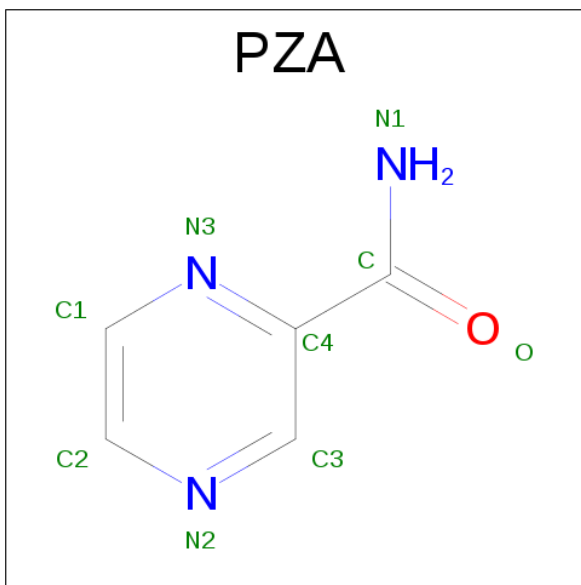
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

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



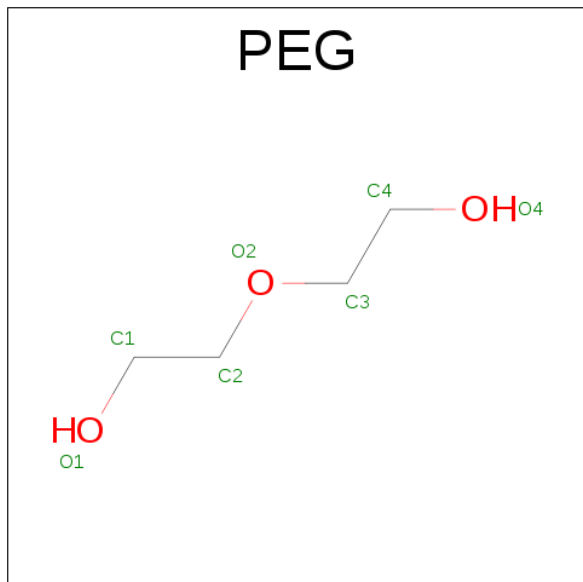
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	S	0	0
			3	1	1	1		

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



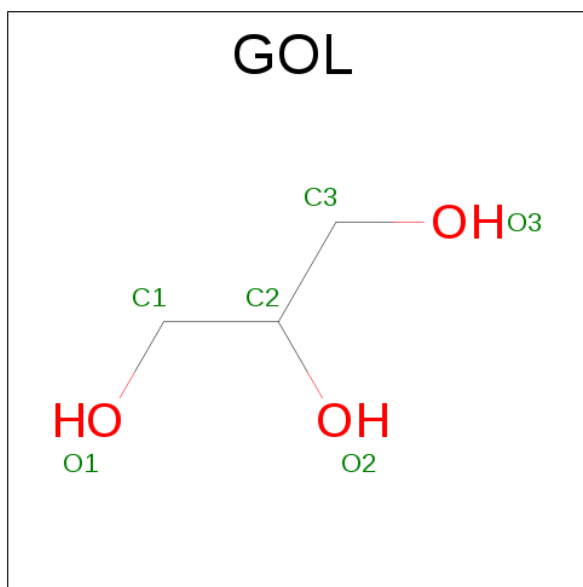
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			9	5	3	1		
9	A	1	Total	C	N	O	0	0
			9	5	3	1		

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



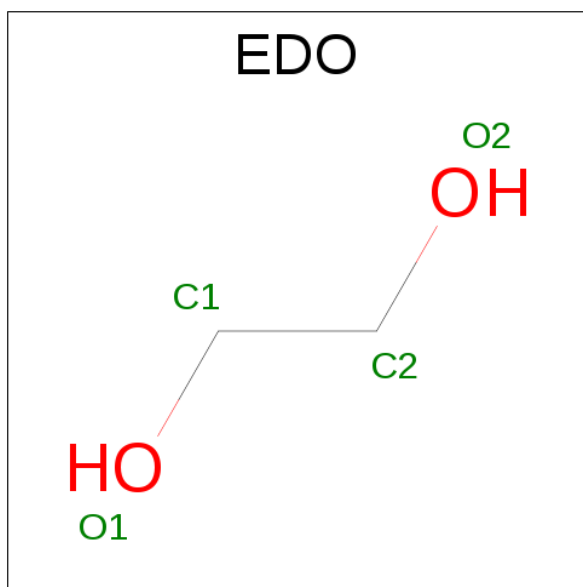
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		
10	A	1	Total	C	O	0	0
			7	4	3		

- 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.

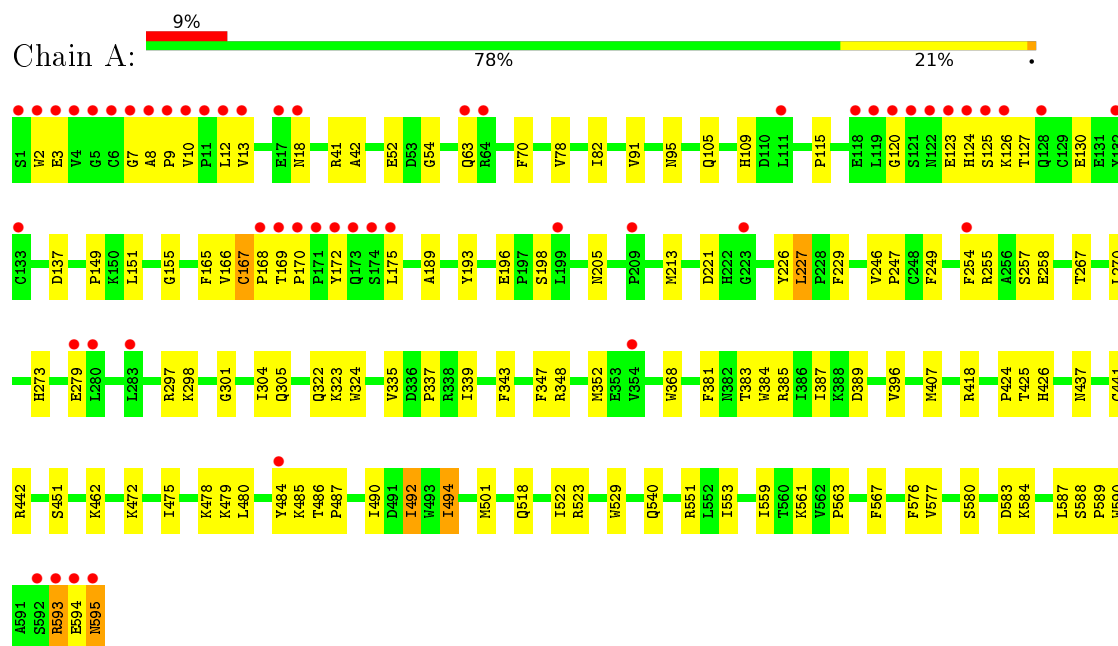
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	499	Total	O	0	0
			499	499		



### 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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	53.92Å 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 0.228 , 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 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	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.

<sup>2</sup>Theoretical 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: 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( $^{\circ}$ )	Ideal( $^{\circ}$ )
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 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	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
8	A	3	0	0	0	0
9	A	18	0	10	18	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 17.

All (165) 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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HG12	1:A:41:ARG:NH2	2.21	0.55
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:229:PHE:CD1	1:A:247:PRO:HG2	2.43	0.54
1:A:82:ILE:HD13	1:A:480:LEU:CD2	2.38	0.54
1:A:492:ILE:C	1:A:492:ILE:HD13	2.28	0.54
1:A:472:LYS:HE3	12:A:624:EDO:H21	1.89	0.53
4:A:596:NAG:O7	11:A:621:GOL:C1	2.33	0.53
1:A:169:THR:HB	1:A:170:PRO:CD	2.31	0.53
3:A:605:HEM:HBC2	3:A:605:HEM:HMC2	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
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.57	0.51
3:A:605:HEM:NC	9:A:597:PZA:N1	2.58	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:42:ALA:HB2	1:A:166:VAL:HG11	1.93	0.50
1:A:384:TRP:CZ2	5:A:601:NAG:H2	2.45	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:487:PRO:HA	1:A:490:ILE:HD12	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLU:HG2	13:A:981:HOH:O	2.14	0.47
10:A:619:PEG:H41	13:A:900:HOH:O	2.14	0.47
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:368:TRP:CE3	1:A:368:TRP:O	2.69	0.46
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.51	0.46
1:A:63:GLN:NE2	13:A:1019:HOH:O	2.47	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:205:ASN:HA	13:A:1068:HOH:O	2.16	0.45
1:A:540:GLN:HG2	1:A:590:TRP:CE2	2.51	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:257:SER:O	1:A:381:PHE:HA	2.18	0.44
1:A:8:ALA:N	1:A:9:PRO:CD	2.80	0.44
1:A:123:GLU:HG2	1:A:125:SER:CB	2.48	0.44
1:A:418:ARG:HH22	10:A:603:PEG:H42	1.82	0.44
1:A:279:GLU:CG	1:A:587:LEU:HD12	2.38	0.44
3:A:605:HEM:HBB2	3:A:605:HEM:CMB	2.48	0.43
1:A:298:LYS:HG3	13:A:1061:HOH:O	2.18	0.43
3:A:605:HEM:C1A	9:A:597:PZA:N3	2.87	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:227:LEU:CD2	1:A:270:LEU:HD22	2.45	0.43
1:A:424:PRO:C	1:A:425:THR:HG22	2.22	0.43
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.54	0.43
1:A:254:PHE:CE2	9:A:598:PZA:C1	3.02	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:335:VAL:O	1:A:337:PRO:HD3	2.19	0.42
1:A:396:VAL:CG1	1:A:553:ILE:HD12	2.46	0.42
1:A:9:PRO:CG	1:A:167:CYS:CA	2.94	0.42
1:A:193:TYR:OH	1:A:297:ARG:HA	2.20	0.42
1:A:540:GLN:HG2	1:A:590:TRP:CZ2	2.54	0.42
1:A:120:GLY:HA3	1:A:126:LYS:HG3	2.02	0.42
3:A:605:HEM:ND	9:A:597:PZA:O	2.53	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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:TRP:HA	13:A:773:HOH:O	2.20	0.41
1:A:478:LYS:HE2	13:A:978:HOH:O	2.21	0.41
1:A:130:GLU:OE1	1:A:426:HIS:ND1	2.51	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:322:GLN:HG2	13:A:687:HOH:O	2.20	0.41
1:A:352:MET:CB	1:A:407:MET:HG2	2.51	0.41
1:A:487:PRO:HA	1:A:490:ILE:CD1	2.50	0.41
1:A:229:PHE:HZ	1:A:387:ILE:HD13	1.86	0.40
1:A:78:VAL:HG13	1:A:82:ILE:HD12	2.03	0.40
1:A:115:PRO:HG2	13:A:1037:HOH:O	2.21	0.40
1:A:130:GLU:HB2	13:A:1057:HOH:O	2.22	0.40
1:A:105:GLN:HG3	3:A:605:HEM:C1C	2.56	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	592/595 (100%)	569 (96%)	21 (4%)	2 (0%)	46	41

All (2) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar



resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/517 (100%)	507 (98%)	10 (2%)	65	67

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 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	SEP	A	198	1	7,9,10	1.73	1 (14%)	8,12,14	1.42	1 (12%)

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	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	3.40	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-CB-CA	2.51	110.44	108.26

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	198	SEP	1	0

## 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	14,14,15	0.47	0	15,19,21	0.74	0
5	NAG	A	600	5	14,14,15	1.05	1 (7%)	15,19,21	1.46	4 (26%)
5	NAG	A	601	1,5	14,14,15	0.63	0	15,19,21	0.77	0
5	NAG	A	602	5	14,14,15	0.42	0	15,19,21	2.29	3 (20%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	NAG	C8-C7	2.53	1.55	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	NAG	C4-C3-C2	-2.93	106.79	111.34
5	A	600	NAG	O5-C5-C4	-2.43	106.10	110.13
5	A	600	NAG	C1-O5-C5	-2.37	108.65	112.14
5	A	600	NAG	C2-N2-C7	2.10	125.84	123.11
5	A	600	NAG	C4-C3-C2	2.88	115.81	111.34
5	A	602	NAG	O5-C5-C4	4.12	116.96	110.13
5	A	602	NAG	C1-O5-C5	6.37	121.50	112.14

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
5	A	601	NAG	1	0

## 5.6 Ligand geometry [i](#)

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	14,14,15	0.76	1 (7%)	15,19,21	1.34	1 (6%)
9	PZA	A	597	3	9,9,9	0.50	0	11,11,11	1.97	5 (45%)
9	PZA	A	598	-	9,9,9	0.39	0	11,11,11	1.94	4 (36%)
10	PEG	A	603	-	6,6,6	1.55	1 (16%)	5,5,5	1.01	1 (20%)
4	NAG	A	604	1	14,14,15	0.43	0	15,19,21	0.77	0
3	HEM	A	605	1,9	24,50,50	2.27	9 (37%)	16,82,82	1.97	6 (37%)
10	PEG	A	619	-	6,6,6	1.40	1 (16%)	5,5,5	0.95	0
8	SCN	A	620	-	2,2,2	2.73	1 (50%)	1,1,1	0.03	0
11	GOL	A	621	-	5,5,5	3.44	2 (40%)	5,5,5	2.32	4 (80%)
11	GOL	A	622	-	5,5,5	1.02	0	5,5,5	0.99	1 (20%)
12	EDO	A	623	-	3,3,3	0.85	0	2,2,2	0.94	0
12	EDO	A	624	-	3,3,3	0.40	0	2,2,2	0.49	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	-	0/4/4/4	0/1/1/1
9	PZA	A	598	-	-	0/4/4/4	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	-	0/6/54/54	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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	621	GOL	O2-C2	-7.14	1.22	1.43
3	A	605	HEM	C4D-ND	-4.28	1.31	1.36
10	A	603	PEG	C2-C1	-3.09	1.32	1.49
10	A	619	PEG	C2-C1	-2.58	1.35	1.49
3	A	605	HEM	C3B-C2B	-2.09	1.37	1.40
3	A	605	HEM	C4B-CHC	-2.05	1.34	1.40
3	A	605	HEM	C1A-CHA	-2.03	1.34	1.40
3	A	605	HEM	C1D-CHD	2.03	1.45	1.40
4	A	596	NAG	C8-C7	2.29	1.55	1.50
11	A	621	GOL	O1-C1	2.39	1.52	1.42
3	A	605	HEM	CMC-C2C	3.18	1.58	1.51
3	A	605	HEM	C3C-CAC	3.63	1.55	1.47
8	A	620	SCN	C-S	3.81	1.86	1.63
3	A	605	HEM	C3D-C2D	4.71	1.51	1.37
3	A	605	HEM	C3B-CAB	5.19	1.58	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	597	PZA	C4-C3-N2	-2.89	118.53	122.05
3	A	605	HEM	CMD-C2D-C3D	-2.84	119.30	125.24
9	A	597	PZA	C2-C1-N3	-2.63	118.94	122.23
3	A	605	HEM	CBD-CAD-C3D	-2.63	107.86	112.47
3	A	605	HEM	CBA-CAA-C2A	-2.40	108.28	112.49
11	A	621	GOL	C3-C2-C1	-2.32	101.28	111.06
3	A	605	HEM	C3B-CAB-CBB	-2.21	121.96	126.40
3	A	605	HEM	CAD-C3D-C2D	-2.17	122.81	129.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	622	GOL	O2-C2-C3	-2.01	98.81	108.47
11	A	621	GOL	O1-C1-C2	-2.01	99.81	109.97
10	A	603	PEG	O2-C2-C1	2.01	118.67	110.25
9	A	598	PZA	C3-C4-C	2.03	121.82	119.74
9	A	598	PZA	C2-N2-C3	2.10	120.68	116.82
9	A	597	PZA	C2-N2-C3	2.30	121.05	116.82
9	A	597	PZA	C1-N3-C4	2.49	120.25	116.93
9	A	598	PZA	C1-N3-C4	2.55	120.32	116.93
11	A	621	GOL	O2-C2-C3	2.76	121.70	108.47
11	A	621	GOL	O2-C2-C1	2.88	122.30	108.47
9	A	597	PZA	C4-C-N1	3.36	119.45	116.22
9	A	598	PZA	C4-C-N1	3.50	119.58	116.22
4	A	596	NAG	C1-O5-C5	3.87	117.83	112.14
3	A	605	HEM	CMD-C2D-C1D	5.19	137.15	128.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	596	NAG	4	0
9	A	597	PZA	14	0
9	A	598	PZA	6	0
10	A	603	PEG	3	0
3	A	605	HEM	7	0
10	A	619	PEG	1	0
11	A	621	GOL	4	0
11	A	622	GOL	2	0
12	A	624	EDO	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, 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	594/595 (99%)	0.48	51 (8%) 13 14	15, 31, 57, 94	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	14.7
1	A	172	TYR	10.7
1	A	121	SER	9.8
1	A	12	LEU	9.6
1	A	171	PRO	8.8
1	A	119	LEU	8.5
1	A	11	PRO	8.2
1	A	173	GLN	7.6
1	A	120	GLY	7.5
1	A	13	VAL	7.1
1	A	7	GLY	6.7
1	A	4	VAL	6.6
1	A	122	ASN	6.3
1	A	10	VAL	6.0
1	A	6	CYS	5.8
1	A	170	PRO	5.6
1	A	283	LEU	5.6
1	A	1	SER	5.6
1	A	8	ALA	5.4
1	A	124	HIS	5.4
1	A	123	GLU	5.2
1	A	593	ARG	4.8
1	A	595	ASN	4.7
1	A	174	SER	4.7
1	A	169	THR	4.2
1	A	3	GLU	3.7
1	A	128	GLN	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	132	TYR	3.6
1	A	133	CYS	3.5
1	A	18	ASN	3.4
1	A	594	GLU	3.4
1	A	5	GLY	3.3
1	A	223	GLY	2.9
1	A	64	ARG	2.9
1	A	279	GLU	2.9
1	A	175	LEU	2.7
1	A	592	SER	2.5
1	A	63	GLN	2.5
1	A	17	GLU	2.5
1	A	9	PRO	2.5
1	A	125	SER	2.5
1	A	280	LEU	2.3
1	A	254	PHE	2.3
1	A	168	PRO	2.2
1	A	199	LEU	2.2
1	A	118	GLU	2.2
1	A	111	LEU	2.1
1	A	484	TYR	2.1
1	A	354	VAL	2.1
1	A	209	PRO	2.1
1	A	126	LYS	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	A	198	10/11	0.85	0.23	-	39,40,41,41	0

## 6.3 Carbohydrates [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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	A	601	14/15	0.77	0.17	0.85	38,40,43,47	0
5	NAG	A	599	14/15	0.84	0.15	0.23	39,44,46,50	0
5	NAG	A	602	14/15	0.73	0.24	-	51,55,56,56	0
5	NAG	A	600	14/15	0.71	0.41	-	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	PZA	A	597	9/9	0.64	0.42	10.42	28,29,30,31	0
9	PZA	A	598	9/9	0.74	0.39	5.19	27,27,27,28	9
11	GOL	A	621	6/6	0.83	0.26	4.17	45,46,47,49	0
10	PEG	A	603	7/7	0.80	0.19	2.91	33,35,36,37	0
11	GOL	A	622	6/6	0.70	0.18	1.52	58,58,59,60	0
10	PEG	A	619	7/7	0.78	0.14	0.80	50,51,51,51	0
8	SCN	A	620	3/3	0.83	0.19	0.38	30,30,30,30	0
12	EDO	A	623	4/4	0.95	0.17	0.35	41,42,42,43	0
3	HEM	A	605	43/43	0.97	0.16	0.02	14,18,22,24	0
2	CA	A	606	1/1	0.99	0.11	-0.76	22,22,22,22	0
6	IOD	A	607	1/1	0.95	0.05	-2.28	51,51,51,51	0
6	IOD	A	615	1/1	1.00	0.04	-2.60	26,26,26,26	0
6	IOD	A	609	1/1	0.97	0.03	-2.88	57,57,57,57	0
6	IOD	A	616	1/1	0.99	0.07	-3.69	36,36,36,36	0
6	IOD	A	610	1/1	0.99	0.03	-3.89	58,58,58,58	0
6	IOD	A	617	1/1	0.99	0.07	-	53,53,53,53	0
6	IOD	A	608	1/1	0.99	0.03	-	40,40,40,40	0
7	ZN	A	618	1/1	0.98	0.04	-	44,44,44,44	0
6	IOD	A	614	1/1	0.94	0.06	-	55,55,55,55	1
6	IOD	A	613	1/1	0.97	0.07	-	64,64,64,64	1
12	EDO	A	624	4/4	0.87	0.13	-	30,31,32,34	0
6	IOD	A	611	1/1	0.98	0.09	-	63,63,63,63	0
4	NAG	A	596	14/15	0.69	0.32	-	47,50,52,52	0
4	NAG	A	604	14/15	0.62	0.30	-	39,39,40,40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	IOD	A	612	1/1	0.96	0.05	-	52,52,52,52	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.