



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:16 PM GMT

PDB ID : 4OEK  
Title : Crystal Structure of the Complex of goat Lactoperoxidase with Phenylethylamine at 2.47 Å Resolution  
Authors : Kumar, M.; Singh, R.P.; Sinha, M.; Bhushan, A.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2014-01-13  
Resolution : 2.47 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

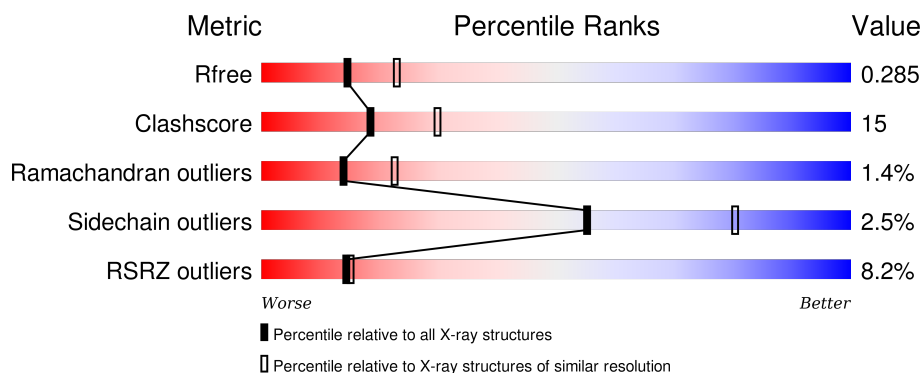
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.47 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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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>8%</div> <div>73%</div> <div>24%</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
6	IOD	A	615	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	IOD	A	620	-	-	X	-
7	SCN	A	621	-	-	-	X
8	EDO	A	622	-	-	-	X
8	EDO	A	623	-	-	-	X
9	PEA	A	627	-	-	X	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5166 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	595	4757	3021	844	865	1	26	0	0	0

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

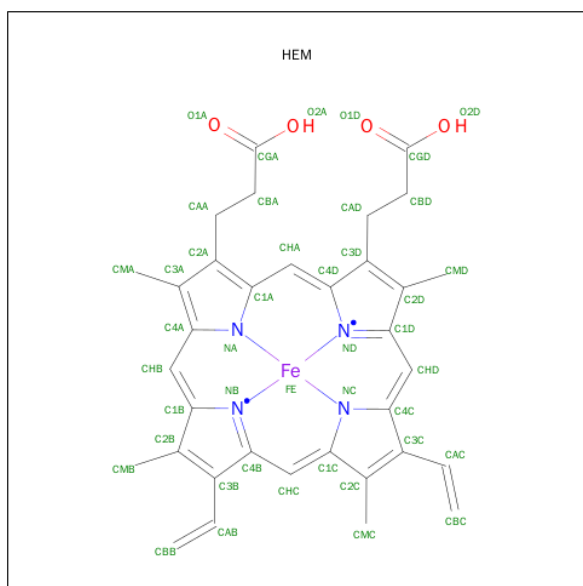


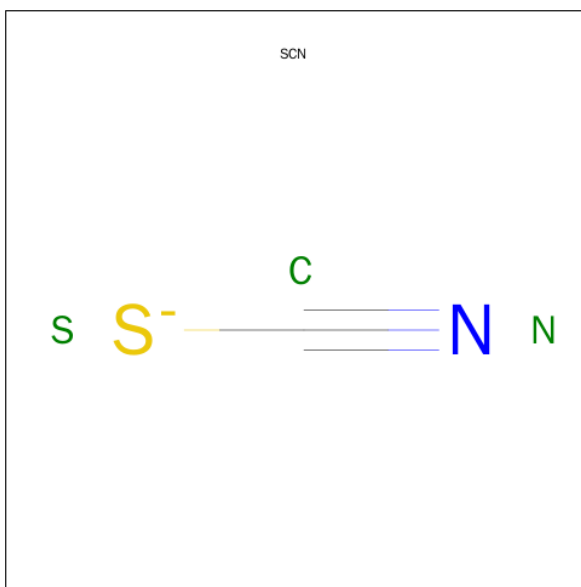
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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		

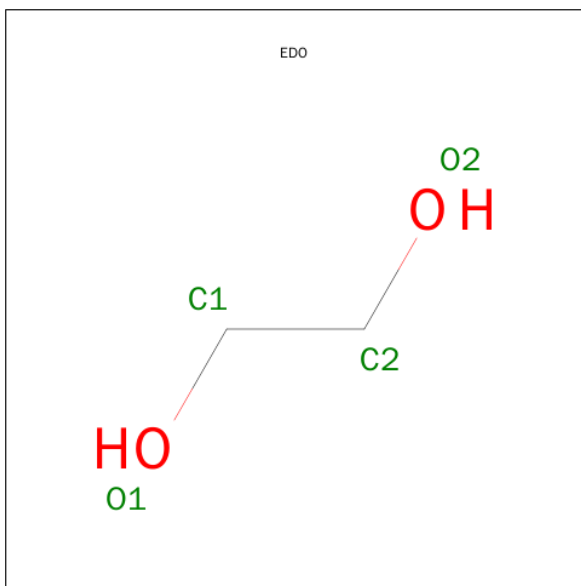
- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



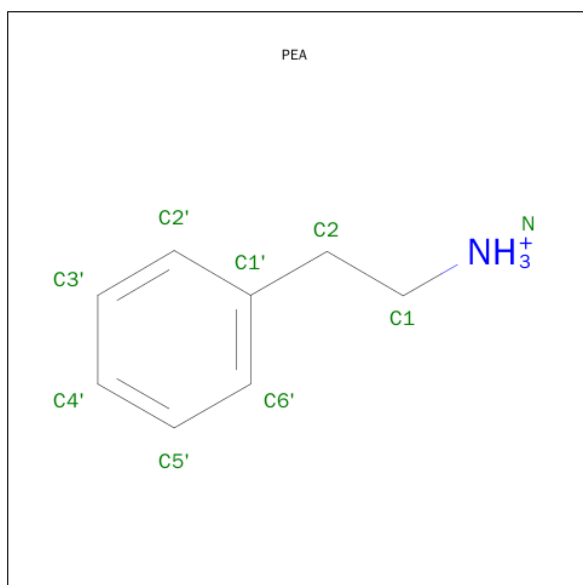
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 9 is 2-PHENYLETHYLAMINE (three-letter code: PEA) (formula: C<sub>8</sub>H<sub>12</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	N	0	0
			9	8	1		

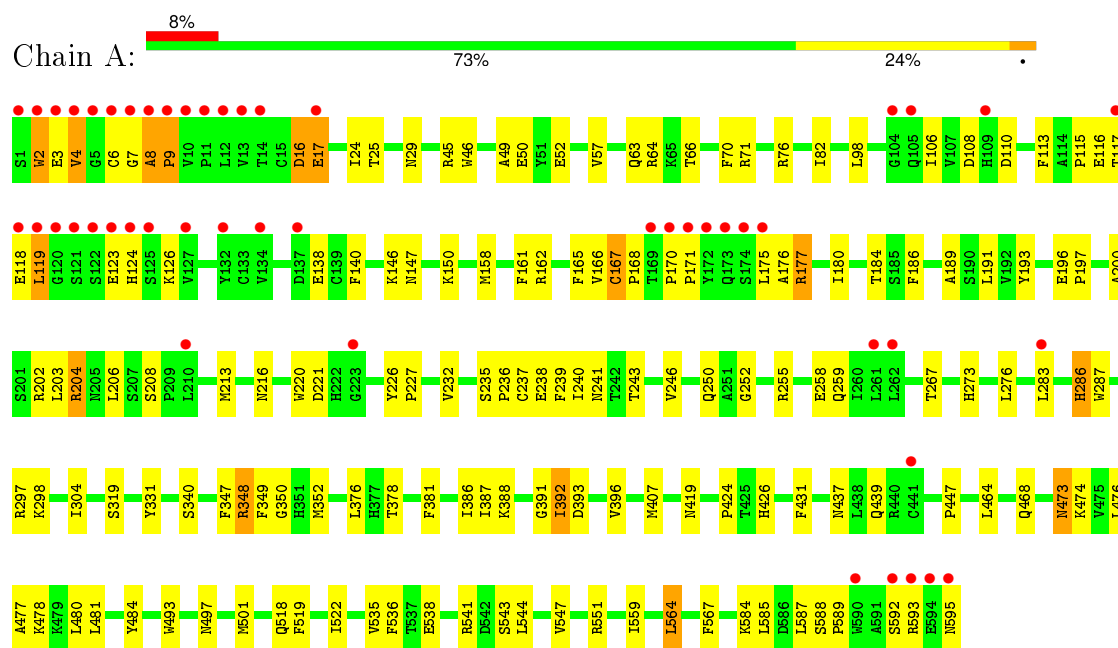
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	250	Total	O	0	0
			250	250		

### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	53.17Å 79.89Å 75.28Å 90.00° 101.80° 90.00°	Depositor
Resolution (Å)	73.69 – 2.47 39.95 – 2.47	Depositor EDS
% Data completeness (in resolution range)	88.0 (73.69-2.47) 88.0 (39.95-2.47)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.43 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.204 , 0.281 0.208 , 0.285	Depositor DCC
$R_{free}$ test set	995 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 33.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 19573 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5166	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: SCN, NAG, SEP, CA, EDO, HEM, IOD, PEA

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	0.71	3/4875 (0.1%)	0.76	3/6621 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	ILE	C-N	8.39	1.53	1.34
1	A	241	ASN	C-N	-5.13	1.22	1.34
1	A	220	TRP	CD2-CE2	5.01	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	204	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	348	ARG	NE-CZ-NH1	5.13	122.86	120.30

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	4757	0	4643	144	0
2	A	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	25	1	0
4	A	43	0	30	15	0
5	A	1	0	0	0	0
6	A	13	0	0	7	0
7	A	3	0	0	0	0
8	A	20	0	30	3	0
9	A	9	0	12	13	0
10	A	250	0	0	11	0
All	All	5166	0	4779	150	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 15.

All (150) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:OE2	4:A:606:HEM:CMB	1.73	1.36
1:A:108:ASP:OD2	4:A:606:HEM:CMD	1.76	1.32
6:A:616:IOD:I	10:A:719:HOH:O	2.36	1.13
1:A:258:GLU:OE2	4:A:606:HEM:HMB1	0.91	1.07
1:A:108:ASP:OD2	4:A:606:HEM:HMD1	0.82	0.99
1:A:108:ASP:CG	4:A:606:HEM:HMD1	1.86	0.94
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.57	0.87
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.09	0.82
3:A:604:NAG:O6	10:A:761:HOH:O	1.99	0.80
1:A:538:GLU:HG2	1:A:541:ARG:NH2	1.98	0.79
6:A:615:IOD:I	10:A:813:HOH:O	2.73	0.76
1:A:258:GLU:HG3	9:A:627:PEA:H6'	1.69	0.73
4:A:606:HEM:C4A	9:A:627:PEA:H12	2.25	0.72
1:A:255:ARG:HG2	9:A:627:PEA:H2'	1.70	0.72
1:A:258:GLU:CD	4:A:606:HEM:CMB	2.59	0.69
1:A:258:GLU:CD	4:A:606:HEM:HMB1	2.03	0.69
4:A:606:HEM:C3A	9:A:627:PEA:H12	2.28	0.68
1:A:473:ASN:ND2	1:A:476:LEU:H	1.92	0.68
1:A:538:GLU:HG2	1:A:541:ARG:HH22	1.57	0.67
1:A:258:GLU:HG3	9:A:627:PEA:H21	1.77	0.65
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.79	0.64
1:A:63:GLN:O	1:A:71:ARG:NH1	2.32	0.62
1:A:52:GLU:CG	1:A:57:VAL:HG12	2.29	0.62
1:A:123:GLU:HB3	1:A:126:LYS:HB2	1.81	0.62
1:A:255:ARG:CG	9:A:627:PEA:H22	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:CYS:CB	1:A:168:PRO:CD	2.79	0.61
1:A:203:LEU:HB3	1:A:213:MET:CE	2.30	0.61
1:A:255:ARG:HB3	9:A:627:PEA:H22	1.82	0.60
1:A:2:TRP:CD1	1:A:175:LEU:HD13	2.36	0.60
1:A:567:PHE:HB2	6:A:615:IOD:I	2.72	0.60
1:A:203:LEU:HB3	1:A:213:MET:HE1	1.84	0.60
1:A:158:MET:HE1	1:A:431:PHE:HA	1.84	0.59
1:A:175:LEU:HD12	1:A:176:ALA:H	1.67	0.59
1:A:146:LYS:O	1:A:147:ASN:HB2	2.03	0.59
1:A:108:ASP:CG	4:A:606:HEM:CMD	2.60	0.59
1:A:258:GLU:CG	9:A:627:PEA:H6'	2.33	0.58
1:A:298:LYS:NZ	1:A:535:VAL:O	2.28	0.58
1:A:239:PHE:HB2	10:A:852:HOH:O	2.03	0.57
1:A:387:ILE:HG22	1:A:388:LYS:HG3	1.86	0.57
1:A:8:ALA:H	1:A:9:PRO:HD3	1.70	0.56
1:A:2:TRP:HB3	10:A:875:HOH:O	2.06	0.56
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.86	0.56
1:A:258:GLU:HG3	9:A:627:PEA:C6'	2.35	0.56
1:A:9:PRO:HG2	10:A:924:HOH:O	2.06	0.56
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.36	0.56
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.53	0.55
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.88	0.55
1:A:197:PRO:HA	8:A:624:EDO:H12	1.89	0.55
1:A:200:ALA:O	1:A:204:ARG:HG3	2.05	0.55
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.42	0.55
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.88	0.54
1:A:170:PRO:HB2	1:A:171:PRO:HD2	1.89	0.53
1:A:119:LEU:HD12	1:A:138:GLU:HG3	1.90	0.53
1:A:407:MET:HG3	10:A:723:HOH:O	2.08	0.53
1:A:237:CYS:HA	1:A:381:PHE:O	2.08	0.53
1:A:206:LEU:C	10:A:861:HOH:O	2.47	0.53
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.91	0.53
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.44	0.52
1:A:16:ASP:OD1	1:A:16:ASP:C	2.47	0.52
1:A:66:THR:HB	1:A:70:PHE:N	2.25	0.51
1:A:63:GLN:HG3	1:A:71:ARG:HH12	1.74	0.51
1:A:7:GLY:O	1:A:8:ALA:HB2	2.10	0.51
1:A:386:ILE:CG2	1:A:392:ILE:HD13	2.40	0.50
1:A:518:GLN:O	1:A:522:ILE:HG23	2.11	0.50
1:A:25:THR:O	1:A:184:THR:HG22	2.10	0.50
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:CE2	1:A:115:PRO:HB3	2.48	0.49
4:A:606:HEM:HBC2	4:A:606:HEM:HMC1	1.93	0.49
1:A:45:ARG:CZ	1:A:49:ALA:HB2	2.42	0.49
1:A:255:ARG:CB	9:A:627:PEA:H22	2.42	0.49
1:A:287:TRP:CZ2	1:A:592:SER:HB2	2.48	0.49
1:A:165:PHE:CG	1:A:177:ARG:HD2	2.48	0.49
1:A:544:LEU:O	1:A:547:VAL:HG22	2.12	0.49
1:A:64:ARG:NH2	10:A:920:HOH:O	2.39	0.48
1:A:255:ARG:HG2	9:A:627:PEA:H22	1.95	0.48
1:A:393:ASP:HB3	1:A:559:ILE:HD11	1.94	0.47
1:A:376:LEU:HD13	10:A:942:HOH:O	2.13	0.47
1:A:216:ASN:HB2	1:A:227:PRO:O	2.14	0.47
1:A:246:VAL:HG22	8:A:625:EDO:H11	1.95	0.47
1:A:349:PHE:CD1	1:A:349:PHE:C	2.87	0.47
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.50	0.47
1:A:52:GLU:HG2	1:A:57:VAL:HG12	1.96	0.46
1:A:82:ILE:HD13	1:A:480:LEU:HD23	1.97	0.46
1:A:258:GLU:OE2	4:A:606:HEM:HMB2	1.98	0.46
1:A:140:PHE:CE2	1:A:439:GLN:HG3	2.50	0.46
1:A:276:LEU:HD21	1:A:585:LEU:HD23	1.96	0.46
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.45	0.46
1:A:473:ASN:HD22	1:A:473:ASN:C	2.18	0.46
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.29	0.46
1:A:464:LEU:HA	1:A:481:LEU:HD12	1.98	0.46
1:A:286:HIS:N	1:A:286:HIS:ND1	2.60	0.46
1:A:593:ARG:HA	1:A:593:ARG:NH1	2.31	0.46
1:A:8:ALA:HB3	1:A:167:CYS:O	2.16	0.45
1:A:197:PRO:HD2	6:A:620:IOD:I	2.86	0.45
1:A:162:ARG:CZ	1:A:177:ARG:NH2	2.80	0.45
1:A:113:PHE:CE1	1:A:255:ARG:HD3	2.51	0.45
1:A:350:GLY:HA3	4:A:606:HEM:CBC	2.45	0.45
1:A:193:TYR:OH	1:A:297:ARG:HA	2.16	0.45
1:A:119:LEU:HD12	1:A:138:GLU:CG	2.47	0.45
1:A:117:THR:HG22	1:A:119:LEU:H	1.82	0.45
1:A:468:GLN:HG2	1:A:477:ALA:HB3	1.98	0.45
1:A:474:LYS:O	1:A:478:LYS:HG3	2.17	0.45
1:A:352:MET:CB	1:A:407:MET:HG2	2.46	0.44
1:A:98:LEU:HD22	10:A:745:HOH:O	2.17	0.44
1:A:407:MET:HB3	1:A:501:MET:CE	2.48	0.44
1:A:76:ARG:HH22	1:A:419:ASN:ND2	2.16	0.44
1:A:276:LEU:CD2	1:A:587:LEU:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:THR:HG22	8:A:622:EDO:H12	1.98	0.44
1:A:481:LEU:HA	1:A:484:TYR:O	2.17	0.44
1:A:203:LEU:HD11	1:A:252:GLY:HA2	1.99	0.44
1:A:519:PHE:HA	1:A:522:ILE:HG12	2.00	0.44
1:A:165:PHE:CD2	1:A:177:ARG:HD2	2.52	0.44
1:A:259:GLN:HG2	4:A:606:HEM:CBB	2.48	0.44
1:A:8:ALA:N	1:A:9:PRO:HD3	2.32	0.44
1:A:29:ASN:CB	1:A:186:PHE:CZ	3.01	0.44
1:A:7:GLY:O	1:A:8:ALA:CB	2.66	0.43
1:A:258:GLU:HG3	9:A:627:PEA:C2	2.45	0.43
1:A:236:PRO:HB3	6:A:618:IOD:I	2.89	0.43
1:A:117:THR:HG22	1:A:119:LEU:N	2.34	0.43
1:A:202:ARG:HE	1:A:250:GLN:CD	2.22	0.43
1:A:227:PRO:HD3	1:A:267:THR:HG23	2.01	0.43
1:A:258:GLU:OE2	4:A:606:HEM:C2B	2.62	0.42
1:A:392:ILE:O	1:A:396:VAL:HG23	2.19	0.42
1:A:221:ASP:OD1	1:A:391:GLY:HA3	2.20	0.42
1:A:3:GLU:O	1:A:4:VAL:C	2.58	0.42
1:A:407:MET:HB3	1:A:501:MET:HE3	2.02	0.42
1:A:232:VAL:O	1:A:232:VAL:HG23	2.19	0.42
1:A:146:LYS:O	1:A:147:ASN:CB	2.66	0.42
1:A:352:MET:CE	1:A:493:TRP:CZ2	3.02	0.42
1:A:24:ILE:HA	1:A:24:ILE:HD13	1.80	0.42
1:A:202:ARG:HG2	1:A:250:GLN:OE1	2.20	0.42
1:A:235:SER:HB3	1:A:238:GLU:OE2	2.20	0.41
1:A:116:GLU:HG2	1:A:161:PHE:O	2.19	0.41
1:A:158:MET:HE1	1:A:431:PHE:CA	2.49	0.41
1:A:196:GLU:HB3	6:A:620:IOD:I	2.90	0.41
1:A:16:ASP:O	1:A:17:GLU:CB	2.69	0.41
1:A:50:GLU:OE2	1:A:447:PRO:HB3	2.20	0.41
1:A:283:LEU:HD13	1:A:587:LEU:O	2.20	0.41
1:A:150:LYS:HE2	1:A:419:ASN:HD22	1.85	0.41
1:A:424:PRO:C	1:A:426:HIS:H	2.24	0.41
1:A:331:TYR:HE2	6:A:619:IOD:I	2.74	0.41
1:A:298:LYS:HG2	1:A:536:PHE:CZ	2.56	0.41
1:A:29:ASN:HB3	1:A:186:PHE:CZ	2.56	0.41
1:A:595:ASN:HD22	1:A:595:ASN:N	2.19	0.41
1:A:239:PHE:C	1:A:239:PHE:CD2	2.93	0.41
1:A:564:LEU:HA	1:A:564:LEU:HD12	1.90	0.41
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.86	0.40
1:A:193:TYR:O	1:A:200:ALA:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:HB3	9:A:627:PEA:C2	2.49	0.40
1:A:166:VAL:CG1	1:A:180:ILE:HG12	2.52	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%)	546 (92%)	38 (6%)	8 (1%)	14 22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	119	LEU
1	A	167	CYS
1	A	2	TRP
1	A	17	GLU
1	A	9	PRO
1	A	319	SER
1	A	4	VAL

### 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	516/516 (100%)	503 (98%)	13 (2%)	55 80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	16	ASP
1	A	118	GLU
1	A	124	HIS
1	A	177	ARG
1	A	208	SER
1	A	243	THR
1	A	286	HIS
1	A	347	PHE
1	A	392	ILE
1	A	473	ASN
1	A	543	SER
1	A	564	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	147	ASN
1	A	245	HIS
1	A	377	HIS
1	A	419	ASN
1	A	437	ASN
1	A	468	GLN
1	A	473	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 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	8,9,10	0.80	0	8,12,14	2.66	5 (62%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	198	SEP	OG-P-O1P	-2.59	100.55	107.14
1	A	198	SEP	O3P-P-OG	-2.47	99.45	106.56
1	A	198	SEP	O2P-P-OG	3.49	116.61	106.56
1	A	198	SEP	O3P-P-O1P	3.68	122.42	110.58
1	A	198	SEP	OG-CB-CA	4.18	111.84	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	603	1,3	14,14,15	1.08	1 (7%)	15,19,21	2.26	6 (40%)
3	NAG	A	604	3	14,14,15	0.92	1 (7%)	15,19,21	1.16	1 (6%)

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	603	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	604	3	-	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)
3	A	603	NAG	O5-C1	-2.67	1.39	1.43
3	A	604	NAG	C1-C2	2.79	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	NAG	C3-C4-C5	-4.36	102.60	110.20
3	A	603	NAG	O3-C3-C2	-2.45	104.27	109.11
3	A	603	NAG	O6-C6-C5	-2.08	104.46	111.33
3	A	604	NAG	O3-C3-C2	2.13	113.34	109.11
3	A	603	NAG	O7-C7-N2	2.55	127.06	121.86
3	A	603	NAG	C4-C3-C2	3.28	116.33	111.23
3	A	603	NAG	C2-N2-C7	4.80	129.21	123.04

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
3	A	604	NAG	1	0

## 5.6 Ligand geometry

Of 25 ligands modelled in this entry, 14 are monoatomic - leaving 11 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$
2	NAG	A	601	1	14,14,15	1.11	2 (14%)	15,19,21	1.73	1 (6%)
2	NAG	A	602	1	14,14,15	1.15	0	15,19,21	1.85	5 (33%)
2	NAG	A	605	1	14,14,15	0.44	0	15,19,21	2.35	3 (20%)
4	HEM	A	606	1,10	30,50,50	2.88	14 (46%)	24,82,82	2.76	11 (45%)
7	SCN	A	621	-	2,2,2	1.54	1 (50%)	1,1,1	0.23	0
8	EDO	A	622	-	3,3,3	0.12	0	2,2,2	0.99	0
8	EDO	A	623	-	3,3,3	0.63	0	2,2,2	0.35	0
8	EDO	A	624	-	3,3,3	0.59	0	2,2,2	0.19	0
8	EDO	A	625	-	3,3,3	0.28	0	2,2,2	1.06	0
8	EDO	A	626	-	3,3,3	0.59	0	2,2,2	0.12	0
9	PEA	A	627	-	9,9,9	1.00	1 (11%)	10,10,10	1.18	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	605	1	-	0/6/23/26	0/1/1/1
4	HEM	A	606	1,10	-	0/10/54/54	0/0/8/8
7	SCN	A	621	-	-	0/0/0/0	0/0/0/0
8	EDO	A	622	-	-	0/1/1/1	0/0/0/0
8	EDO	A	623	-	-	0/1/1/1	0/0/0/0
8	EDO	A	624	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	A	625	-	-	0/1/1/1	0/0/0/0
8	EDO	A	626	-	-	0/1/1/1	0/0/0/0
9	PEA	A	627	-	-	0/3/3/3	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	606	HEM	C3B-C4B	-4.60	1.47	1.51
4	A	606	HEM	C2D-C3D	-3.34	1.44	1.54
4	A	606	HEM	C3D-C4D	-2.68	1.48	1.51
2	A	601	NAG	O5-C1	-2.66	1.39	1.43
4	A	606	HEM	CAD-C3D	-2.35	1.49	1.54
9	A	627	PEA	C2'-C1'	-2.28	1.34	1.38
7	A	621	SCN	C-S	-2.16	1.49	1.63
2	A	601	NAG	C2-N2	-2.04	1.42	1.46
4	A	606	HEM	CHD-C1D	2.26	1.45	1.38
4	A	606	HEM	C4A-CHB	2.31	1.46	1.39
4	A	606	HEM	FE-ND	2.45	2.10	1.97
4	A	606	HEM	CHC-C4B	2.55	1.46	1.38
4	A	606	HEM	FE-NB	2.75	2.12	1.97
4	A	606	HEM	C2A-C3A	3.22	1.47	1.37
4	A	606	HEM	CHD-C4C	3.47	1.44	1.36
4	A	606	HEM	CHC-C1C	4.41	1.46	1.36
4	A	606	HEM	C4C-NC	7.02	1.44	1.36
4	A	606	HEM	C1C-NC	8.11	1.46	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAG	C2-N2-C7	-5.98	115.36	123.04
2	A	602	NAG	C2-N2-C7	-3.94	117.97	123.04
4	A	606	HEM	CBA-CAA-C2A	-2.73	107.63	112.53
4	A	606	HEM	CBD-CAD-C3D	-2.69	105.73	113.55
2	A	602	NAG	O3-C3-C2	-2.59	103.98	109.11
2	A	602	NAG	C3-C2-N2	-2.57	104.40	110.56
2	A	602	NAG	C3-C4-C5	-2.55	105.75	110.20
4	A	606	HEM	C3B-C4B-CHC	-2.45	119.71	123.16
9	A	627	PEA	C2-C1-N	-2.29	106.73	111.45
4	A	606	HEM	C2C-C1C-CHC	-2.07	120.54	123.68
2	A	605	NAG	O3-C3-C2	2.06	113.19	109.11
2	A	602	NAG	C1-O5-C5	2.17	115.00	112.25
4	A	606	HEM	C3B-C4B-NB	2.32	116.06	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	NAG	O5-C5-C6	3.03	113.92	107.35
4	A	606	HEM	CMD-C2D-C3D	3.16	128.35	114.35
4	A	606	HEM	C2C-C1C-NC	3.45	116.02	110.21
4	A	606	HEM	CAD-C3D-C4D	4.79	129.35	112.47
4	A	606	HEM	CAD-C3D-C2D	5.42	128.80	113.22
4	A	606	HEM	CMB-C2B-C3B	5.84	131.10	116.53
4	A	606	HEM	CMC-C2C-C3C	5.86	131.15	116.53
2	A	605	NAG	C2-N2-C7	7.18	132.26	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	606	HEM	15	0
8	A	622	EDO	1	0
8	A	624	EDO	1	0
8	A	625	EDO	1	0
9	A	627	PEA	13	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%)	0.36	49 (8%) 14 15	24, 40, 83, 111	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	10.3
1	A	1	SER	9.9
1	A	174	SER	8.4
1	A	121	SER	7.6
1	A	13	VAL	7.5
1	A	12	LEU	7.2
1	A	120	GLY	6.9
1	A	173	GLN	6.8
1	A	8	ALA	6.5
1	A	172	TYR	6.4
1	A	122	SER	6.4
1	A	595	ASN	6.4
1	A	125	SER	5.8
1	A	9	PRO	5.5
1	A	7	GLY	5.2
1	A	119	LEU	5.1
1	A	11	PRO	5.0
1	A	593	ARG	4.9
1	A	5	GLY	4.9
1	A	124	HIS	4.5
1	A	4	VAL	4.5
1	A	127	VAL	4.5
1	A	592	SER	4.3
1	A	118	GLU	4.1
1	A	6	CYS	4.0
1	A	223	GLY	3.9
1	A	10	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	3.7
1	A	283	LEU	3.4
1	A	117	THR	3.3
1	A	262	LEU	3.2
1	A	170	PRO	3.1
1	A	175	LEU	3.0
1	A	169	THR	2.7
1	A	594	GLU	2.6
1	A	261	LEU	2.6
1	A	109	HIS	2.5
1	A	132	TYR	2.5
1	A	210	LEU	2.5
1	A	105	GLN	2.4
1	A	3	GLU	2.3
1	A	123	GLU	2.3
1	A	134	VAL	2.2
1	A	590	TRP	2.2
1	A	441	CYS	2.2
1	A	17	GLU	2.2
1	A	104	GLY	2.1
1	A	137	ASP	2.1
1	A	14	THR	2.1

## 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	A	198	10/11	0.79	0.25	-	44,50,54,61	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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	603	14/15	0.91	0.14	-0.47	49,52,55,56	0
3	NAG	A	604	14/15	0.74	0.35	-	52,56,59,60	14

## 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( $\text{\AA}^2$ )	Q<0.9
8	EDO	A	622	4/4	0.90	0.40	10.66	22,22,24,28	0
8	EDO	A	623	4/4	0.76	0.24	2.70	34,39,42,43	0
9	PEA	A	627	9/9	0.80	0.39	2.61	27,32,37,37	0
7	SCN	A	621	3/3	0.86	0.21	2.26	42,42,43,49	0
8	EDO	A	625	4/4	0.90	0.26	0.98	32,34,36,37	0
8	EDO	A	624	4/4	0.92	0.18	0.80	35,36,36,37	0
8	EDO	A	626	4/4	0.84	0.28	0.58	34,35,38,38	0
4	HEM	A	606	43/43	0.96	0.21	0.26	21,24,25,27	0
2	NAG	A	602	14/15	0.93	0.15	-0.44	46,49,51,52	0
6	IOD	A	614	1/1	0.99	0.09	-0.78	47,47,47,47	1
6	IOD	A	611	1/1	1.00	0.04	-1.99	43,43,43,43	0
6	IOD	A	610	1/1	0.98	0.06	-2.05	44,44,44,44	0
6	IOD	A	609	1/1	0.99	0.04	-2.52	43,43,43,43	1
6	IOD	A	617	1/1	0.98	0.04	-2.76	40,40,40,40	1
5	CA	A	607	1/1	1.00	0.07	-3.37	27,27,27,27	0
6	IOD	A	608	1/1	1.00	0.05	-4.27	34,34,34,34	0
6	IOD	A	620	1/1	0.99	0.05	-4.36	45,45,45,45	0
6	IOD	A	613	1/1	0.99	0.02	-4.47	38,38,38,38	0
6	IOD	A	618	1/1	1.00	0.03	-5.69	45,45,45,45	1
6	IOD	A	619	1/1	0.96	0.17	-	54,54,54,54	1
6	IOD	A	616	1/1	0.98	0.12	-	48,48,48,48	1
6	IOD	A	612	1/1	0.95	0.17	-	53,53,53,53	1
2	NAG	A	601	14/15	0.84	0.32	-	45,48,51,51	0
6	IOD	A	615	1/1	0.98	0.15	-	51,51,51,51	1
2	NAG	A	605	14/15	0.66	0.26	-	51,55,57,57	14



## 6.5 Other polymers

There are no such residues in this entry.