



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 11:21 AM GMT

PDB ID : 3GCJ  
Title : Mode of ligand binding and assignment of subsites in mammalian peroxidases: crystal structure of lactoperoxidase complexes with acetyl salicylic acid, salicylhydroxamic acid and benzylhydroxamic acid  
Authors : Singh, A.K.; Singh, N.; Sinha, M.; Kaur, P.; Srinivasan, A.; Sharma, S.; Singh, T.P.  
Deposited on : 2009-02-22  
Resolution : 2.34 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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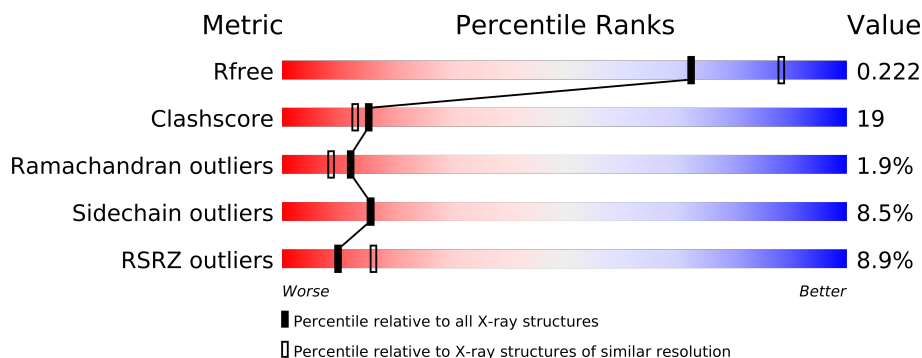
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.34 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	4049 (2.38-2.30)
Clashscore	79885	1094 (2.36-2.32)
Ramachandran outliers	78287	1080 (2.36-2.32)
Sidechain outliers	78261	1081 (2.36-2.32)
RSRZ outliers	66119	4050 (2.38-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	595	

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

Mol	Type	Chain	Res	Geometry	Electron density
8	SHA	A	617	-	X

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 5326 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
			Total	C	N	O	P	S			
1	A	595	4775	3037	847	864	1	26	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

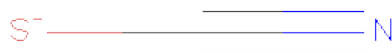
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total I 8 8	0	0

- Molecule 5 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

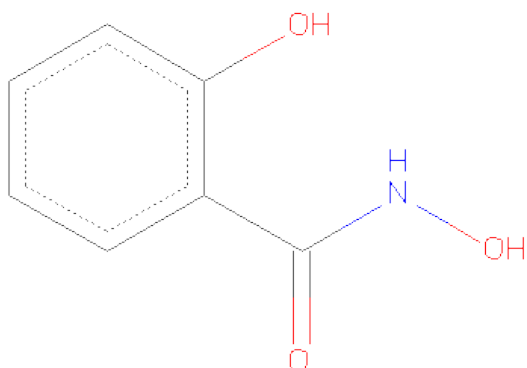
- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total C N O 39 22 2 15	0	0
6	A	3	Total C N O 39 22 2 15	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 8 is SALICYLHYDROXAMIC ACID (three-letter code: SHA) (formula:  $C_7H_7NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			11	7	1	3		

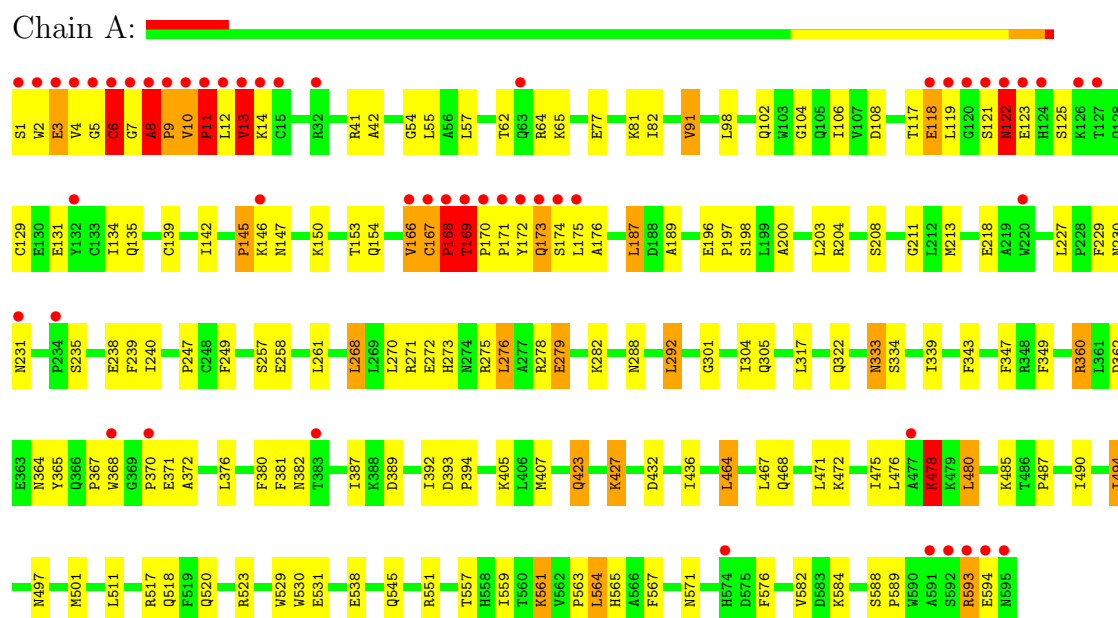
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	351	Total	O	0	0
			351	351		

### 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, $\alpha$ , $\beta$ , $\gamma$	54.62Å 80.55Å 77.80Å 90.00° 102.55° 90.00°	Depositor
Resolution (Å)	19.47 – 2.34 19.88 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.47-2.34) 98.5 (19.88-2.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.33Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.204 , 0.212 0.186 , 0.222	Depositor DCC
$R_{free}$ test set	871 reflections (3.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 27439 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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: SCN, NAG, SEP, CA, SHA, HEM, IOD, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.50	1/4892 (0.0%)	0.79	12/6634 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	PRO	N-CA	5.52	1.56	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	PRO	CA-N-CD	-8.55	99.53	111.50
1	A	11	PRO	N-CA-C	8.21	133.44	112.10
1	A	168	PRO	CA-C-N	-8.18	99.21	117.20
1	A	173	GLN	N-CA-C	7.52	131.31	111.00
1	A	5	GLY	N-CA-C	7.06	130.76	113.10
1	A	168	PRO	N-CA-C	6.85	129.90	112.10
1	A	13	VAL	CB-CA-C	-6.77	98.55	111.40
1	A	6	CYS	CA-CB-SG	6.04	124.88	114.00
1	A	8	ALA	C-N-CD	-5.81	107.82	120.60
1	A	168	PRO	O-C-N	5.64	131.72	122.70
1	A	122	ASN	N-CA-C	-5.58	95.93	111.00
1	A	593	ARG	CD-NE-CZ	5.49	131.28	123.60



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	478	LYS	Peptide

## 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	4775	0	4687	177	0
2	A	43	0	30	6	0
3	A	1	0	0	0	0
4	A	8	0	0	2	0
5	A	3	0	0	0	0
6	A	78	0	68	2	0
7	A	56	0	50	3	0
8	A	11	0	7	0	0
9	A	351	0	0	44	0
All	All	5326	0	4842	185	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 19.

All (185) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:561:LYS:HG3	9:A:923:HOH:O	1.38	1.17
1:A:171:PRO:HA	9:A:948:HOH:O	1.52	1.08
1:A:170:PRO:HA	9:A:946:HOH:O	1.55	1.07
1:A:10:VAL:HG11	1:A:41:ARG:NE	1.72	1.05
1:A:196:GLU:HB3	1:A:198:SEP:O2P	1.58	1.03
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.42	1.02
1:A:134:ILE:HA	9:A:943:HOH:O	1.62	0.95
1:A:147:ASN:HB2	9:A:944:HOH:O	1.68	0.91
1:A:129:CYS:HB2	9:A:922:HOH:O	1.71	0.89
1:A:169:THR:HG22	1:A:170:PRO:HD3	1.56	0.88
1:A:13:VAL:HG21	9:A:702:HOH:O	1.73	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.04	0.88
1:A:432:ASP:O	1:A:436:ILE:HD13	1.73	0.88
1:A:487:PRO:HA	1:A:490:ILE:HD13	1.57	0.85
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.07	0.82
1:A:168:PRO:HB3	1:A:170:PRO:HD2	1.64	0.80
1:A:150:LYS:HZ2	1:A:154:GLN:HE22	1.30	0.78
1:A:121:SER:O	1:A:122:ASN:HB2	1.84	0.77
1:A:485:LYS:CE	9:A:942:HOH:O	2.33	0.77
1:A:102:GLN:O	1:A:106:ILE:HD13	1.85	0.77
1:A:282:LYS:HE2	9:A:967:HOH:O	1.83	0.76
1:A:123:GLU:HG3	1:A:125:SER:H	1.51	0.76
1:A:571:ASN:HB3	9:A:961:HOH:O	1.86	0.75
1:A:10:VAL:HG11	1:A:41:ARG:HE	1.48	0.74
1:A:231:ASN:HB3	9:A:965:HOH:O	1.86	0.73
1:A:167:CYS:CB	1:A:168:PRO:CD	2.66	0.73
2:A:605:HEM:HMB1	2:A:605:HEM:HBB2	1.71	0.72
1:A:282:LYS:CE	9:A:967:HOH:O	2.39	0.71
1:A:3:GLU:HG2	1:A:175:LEU:HD13	1.73	0.71
1:A:517:ARG:NH1	9:A:939:HOH:O	2.24	0.70
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.72	0.70
1:A:282:LYS:NZ	1:A:282:LYS:HB2	2.07	0.70
1:A:123:GLU:HG3	1:A:125:SER:HB3	1.74	0.70
1:A:235:SER:OG	1:A:238:GLU:HG2	1.92	0.70
1:A:561:LYS:HE3	9:A:847:HOH:O	1.92	0.69
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.73	0.69
1:A:485:LYS:NZ	9:A:942:HOH:O	2.26	0.69
1:A:360:ARG:NH1	1:A:372:ALA:HA	2.08	0.68
1:A:150:LYS:NZ	1:A:154:GLN:HE22	1.91	0.68
1:A:557:THR:HB	1:A:559:ILE:HD13	1.76	0.67
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.31	0.66
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.30	0.66
1:A:55:LEU:HD22	1:A:174:SER:O	1.96	0.65
1:A:119:LEU:CD2	9:A:946:HOH:O	2.45	0.64
1:A:494:ILE:O	1:A:494:ILE:HD13	1.96	0.64
1:A:2:TRP:O	1:A:4:VAL:N	2.29	0.64
1:A:8:ALA:HB1	9:A:822:HOH:O	1.96	0.64
1:A:333:ASN:HD22	1:A:334:SER:N	1.95	0.64
1:A:123:GLU:CG	1:A:125:SER:HB3	2.27	0.63
1:A:2:TRP:O	1:A:4:VAL:HG22	1.99	0.63
1:A:557:THR:CB	1:A:559:ILE:HD13	2.29	0.63
1:A:65:LYS:NZ	9:A:925:HOH:O	2.28	0.62
1:A:240:ILE:HD11	1:A:382:ASN:HA	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:567:PHE:HB2	4:A:614:IOD:I	2.70	0.62
1:A:168:PRO:HB3	1:A:170:PRO:CD	2.29	0.61
1:A:485:LYS:HE2	9:A:942:HOH:O	1.95	0.61
1:A:211:GLY:N	9:A:956:HOH:O	2.27	0.60
1:A:81:LYS:HE2	9:A:940:HOH:O	2.01	0.60
1:A:423:GLN:HA	1:A:423:GLN:HE21	1.66	0.59
1:A:230:ASN:OD1	1:A:231:ASN:N	2.34	0.59
1:A:593:ARG:HD2	9:A:952:HOH:O	2.01	0.59
1:A:301:GLY:O	1:A:305:GLN:HG3	2.03	0.59
1:A:288:ASN:O	1:A:292:LEU:HD22	2.03	0.58
1:A:3:GLU:HG2	1:A:175:LEU:HD22	1.83	0.58
1:A:333:ASN:HD22	1:A:333:ASN:C	2.05	0.58
1:A:571:ASN:CA	9:A:961:HOH:O	2.51	0.58
1:A:200:ALA:O	1:A:204:ARG:HG3	2.03	0.58
1:A:571:ASN:CB	9:A:961:HOH:O	2.47	0.57
1:A:362:ASP:OD1	1:A:362:ASP:C	2.44	0.56
1:A:169:THR:HG22	1:A:170:PRO:CD	2.33	0.56
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.41	0.56
1:A:42:ALA:HB2	1:A:166:VAL:HG11	1.87	0.56
1:A:249:PHE:CZ	1:A:387:ILE:HD11	2.40	0.56
1:A:173:GLN:HG2	9:A:921:HOH:O	2.06	0.56
1:A:257:SER:O	1:A:381:PHE:HA	2.06	0.55
1:A:494:ILE:C	1:A:494:ILE:HD13	2.27	0.55
1:A:393:ASP:HB2	9:A:734:HOH:O	2.07	0.55
1:A:282:LYS:NZ	9:A:967:HOH:O	2.40	0.55
1:A:3:GLU:CG	1:A:175:LEU:HD22	2.37	0.55
1:A:169:THR:CG2	1:A:170:PRO:HD3	2.35	0.55
1:A:370:PRO:HG2	1:A:371:GLU:HG3	1.90	0.55
2:A:605:HEM:HMC2	2:A:605:HEM:HBC2	1.88	0.54
1:A:565:HIS:HB3	4:A:614:IOD:I	2.77	0.54
1:A:169:THR:H	1:A:170:PRO:CD	2.20	0.54
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.89	0.54
1:A:559:ILE:N	1:A:559:ILE:HD12	2.22	0.54
1:A:571:ASN:HA	9:A:961:HOH:O	2.07	0.54
1:A:102:GLN:HE21	1:A:106:ILE:CD1	2.21	0.54
1:A:3:GLU:HG2	1:A:175:LEU:CD1	2.38	0.53
1:A:487:PRO:HA	1:A:490:ILE:CD1	2.33	0.53
1:A:62:THR:HG22	1:A:64:ARG:HG2	1.91	0.53
1:A:360:ARG:NH1	1:A:371:GLU:O	2.40	0.52
1:A:322:GLN:HB2	9:A:933:HOH:O	2.08	0.52
1:A:139:CYS:HB2	9:A:922:HOH:O	2.10	0.52
1:A:322:GLN:HG3	9:A:933:HOH:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.41	0.52
1:A:218:GLU:HA	9:A:958:HOH:O	2.09	0.51
1:A:82:ILE:HD13	1:A:480:LEU:HD13	1.91	0.51
1:A:490:ILE:HD12	1:A:490:ILE:N	2.26	0.50
1:A:9:PRO:HD3	1:A:167:CYS:O	2.11	0.50
1:A:142:ILE:CD1	1:A:436:ILE:HD12	2.42	0.50
1:A:2:TRP:CG	1:A:3:GLU:N	2.80	0.50
1:A:487:PRO:CA	1:A:490:ILE:HD13	2.34	0.50
1:A:8:ALA:HB3	1:A:9:PRO:CD	2.42	0.49
1:A:551:ARG:HD2	1:A:582:VAL:HG12	1.94	0.49
1:A:368:TRP:CH2	1:A:389:ASP:O	2.65	0.49
1:A:339:ILE:HD13	1:A:518:GLN:CD	2.32	0.49
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.47	0.49
1:A:82:ILE:HD13	1:A:480:LEU:CD1	2.42	0.49
1:A:467:LEU:HG	1:A:471:LEU:HD22	1.95	0.49
1:A:239:PHE:CZ	1:A:427:LYS:HB3	2.48	0.48
1:A:588:SER:OG	1:A:589:PRO:HD3	2.13	0.48
1:A:108:ASP:OD2	2:A:605:HEM:HHD	2.13	0.48
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.94	0.48
1:A:104:GLY:HA3	2:A:605:HEM:CBC	2.44	0.48
1:A:197:PRO:HD2	1:A:198:SEP:O2P	2.13	0.48
1:A:175:LEU:HG	1:A:176:ALA:N	2.28	0.48
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.49	0.48
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.96	0.48
1:A:322:GLN:CB	9:A:933:HOH:O	2.62	0.47
1:A:258:GLU:HG2	1:A:258:GLU:O	2.14	0.47
1:A:150:LYS:NZ	1:A:154:GLN:NE2	2.60	0.47
7:A:600:NAG:N2	9:A:941:HOH:O	2.36	0.47
1:A:545:GLN:HB2	9:A:930:HOH:O	2.14	0.47
1:A:119:LEU:HD12	1:A:119:LEU:N	2.29	0.47
6:A:602:NAG:H4	6:A:603:MAN:H2	1.58	0.47
1:A:8:ALA:CB	1:A:9:PRO:CD	2.93	0.47
1:A:135:GLN:N	9:A:943:HOH:O	2.41	0.47
1:A:169:THR:N	1:A:170:PRO:CD	2.77	0.47
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.82	0.47
1:A:588:SER:N	1:A:589:PRO:CD	2.78	0.47
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.96	0.46
1:A:393:ASP:N	1:A:394:PRO:CD	2.78	0.46
1:A:407:MET:HB3	1:A:501:MET:CE	2.46	0.46
7:A:599:NAG:H61	7:A:600:NAG:C1	2.45	0.46
1:A:275:ARG:O	1:A:279:GLU:HB2	2.16	0.46
1:A:54:GLY:HA2	9:A:814:HOH:O	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.51	0.46
1:A:3:GLU:HG2	1:A:175:LEU:CD2	2.45	0.45
1:A:557:THR:HB	1:A:559:ILE:CD1	2.45	0.45
1:A:175:LEU:HD12	9:A:706:HOH:O	2.16	0.45
1:A:231:ASN:CB	9:A:965:HOH:O	2.57	0.45
1:A:211:GLY:CA	9:A:956:HOH:O	2.63	0.45
1:A:490:ILE:N	1:A:490:ILE:CD1	2.80	0.45
1:A:119:LEU:HD21	1:A:169:THR:HG23	1.99	0.45
1:A:464:LEU:HD21	1:A:478:LYS:HB2	1.98	0.45
1:A:231:ASN:HA	9:A:742:HOH:O	2.17	0.45
1:A:8:ALA:CB	1:A:9:PRO:HD3	2.47	0.45
1:A:249:PHE:HZ	1:A:387:ILE:HD11	1.79	0.45
1:A:173:GLN:CG	9:A:921:HOH:O	2.61	0.45
1:A:258:GLU:O	1:A:380:PHE:HA	2.17	0.45
2:A:605:HEM:HBB2	2:A:605:HEM:CMB	2.43	0.44
1:A:407:MET:HB3	1:A:501:MET:HE1	1.99	0.44
1:A:387:ILE:N	1:A:387:ILE:HD12	2.33	0.44
1:A:360:ARG:HH11	1:A:372:ALA:HA	1.80	0.44
1:A:271:ARG:NH1	1:A:392:ILE:HD11	2.33	0.44
1:A:10:VAL:HG12	1:A:11:PRO:HD2	1.99	0.44
1:A:272:GLU:O	1:A:276:LEU:HB2	2.18	0.44
1:A:118:GLU:HB3	1:A:119:LEU:H	1.68	0.44
1:A:123:GLU:HG2	1:A:125:SER:HB3	1.99	0.44
1:A:2:TRP:CD1	1:A:3:GLU:N	2.80	0.43
1:A:557:THR:OG1	1:A:559:ILE:HD13	2.17	0.43
1:A:10:VAL:HG11	1:A:41:ARG:CZ	2.44	0.43
1:A:364:ASN:O	1:A:365:TYR:HB2	2.18	0.43
1:A:387:ILE:H	1:A:387:ILE:HD12	1.82	0.43
1:A:123:GLU:HG3	1:A:125:SER:CB	2.47	0.43
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.54	0.42
1:A:231:ASN:O	1:A:231:ASN:OD1	2.37	0.42
1:A:10:VAL:CB	1:A:11:PRO:HD2	2.50	0.42
1:A:9:PRO:CD	1:A:167:CYS:O	2.68	0.42
1:A:14:LYS:HE2	1:A:14:LYS:HB3	1.67	0.42
6:A:601:NAG:H61	6:A:602:NAG:C1	2.49	0.42
1:A:282:LYS:HB2	1:A:282:LYS:HZ3	1.80	0.42
1:A:272:GLU:HG3	1:A:276:LEU:HD22	2.03	0.41
1:A:91:VAL:HG13	1:A:405:LYS:HG3	2.02	0.41
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.95	0.41
1:A:393:ASP:CB	1:A:394:PRO:HD3	2.51	0.41
1:A:476:LEU:C	1:A:478:LYS:H	2.23	0.41
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:211:GLY:HA2	9:A:956:HOH:O	2.20	0.41
1:A:172:TYR:CE2	9:A:945:HOH:O	2.58	0.41
1:A:282:LYS:HZ2	1:A:282:LYS:HB2	1.83	0.40
7:A:616:NAG:N2	7:A:616:NAG:H5	2.36	0.40
1:A:108:ASP:OD2	2:A:605:HEM:CHD	2.69	0.40
1:A:468:GLN:O	1:A:472:LYS:N	2.54	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%)	560 (95%)	21 (4%)	11 (2%)	12 9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	12	LEU
1	A	122	ASN
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	166	VAL
1	A	3	GLU
1	A	6	CYS
1	A	7	GLY
1	A	8	ALA

### 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%)	473 (92%)	44 (8%)	15	16

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	6	CYS
1	A	9	PRO
1	A	10	VAL
1	A	13	VAL
1	A	57	LEU
1	A	91	VAL
1	A	98	LEU
1	A	117	THR
1	A	118	GLU
1	A	122	ASN
1	A	131	GLU
1	A	145	PRO
1	A	146	LYS
1	A	153	THR
1	A	169	THR
1	A	187	LEU
1	A	203	LEU
1	A	208	SER
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	278	ARG
1	A	279	GLU
1	A	292	LEU
1	A	317	LEU
1	A	333	ASN
1	A	347	PHE
1	A	360	ARG
1	A	367	PRO
1	A	376	LEU
1	A	423	GLN
1	A	427	LYS
1	A	464	LEU
1	A	475	ILE
1	A	478	LYS

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Mol	Chain	Res	Type
1	A	480	LEU
1	A	494	ILE
1	A	511	LEU
1	A	520	GLN
1	A	538	GLU
1	A	561	LYS
1	A	564	LEU
1	A	594	GLU

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

Mol	Chain	Res	Type
1	A	154	GLN
1	A	222	HIS
1	A	333	ASN
1	A	364	ASN
1	A	423	GLN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	520	GLN
1	A	558	HIS
1	A	570	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	6.84	4 (44%)	10,12,14	2.48	4 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	198	1	-	0/6/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	O-C	19.74	1.25	1.11
1	A	198	SEP	CA-C	3.95	1.55	1.48
1	A	198	SEP	P-O1P	2.74	1.60	1.51
1	A	198	SEP	P-OG	2.19	1.67	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	C-CA-N	-4.66	109.18	113.83
1	A	198	SEP	P-OG-CB	3.96	129.63	118.19
1	A	198	SEP	O3P-P-OG	3.46	116.20	106.65
1	A	198	SEP	O2P-P-OG	2.19	112.69	106.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

10 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	596	1,6	12,14,15	0.58	0	15,19,21	0.81	1 (6%)
6	NAG	A	597	6	12,14,15	0.73	0	15,19,21	0.84	0
6	MAN	A	598	6	10,11,12	0.44	0	11,15,17	0.29	0
7	NAG	A	599	1,7	12,14,15	0.52	0	15,19,21	0.95	1 (6%)
7	NAG	A	600	7	12,14,15	0.56	0	15,19,21	1.34	3 (20%)
6	NAG	A	601	1,6	12,14,15	0.53	0	15,19,21	0.94	1 (6%)
6	NAG	A	602	6	12,14,15	0.53	0	15,19,21	0.89	0
6	MAN	A	603	6	10,11,12	0.46	0	11,15,17	0.26	0
7	NAG	A	604	1,7	12,14,15	0.53	0	15,19,21	1.06	1 (6%)
7	NAG	A	616	7	12,14,15	0.51	0	15,19,21	0.61	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
6	NAG	A	596	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	597	6	-	0/6/23/26	0/1/1/1
6	MAN	A	598	6	-	0/2/19/22	0/1/1/1
7	NAG	A	599	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	600	7	-	0/6/23/26	0/1/1/1
6	NAG	A	601	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	602	6	-	0/6/23/26	0/1/1/1
6	MAN	A	603	6	-	0/2/19/22	0/1/1/1
7	NAG	A	604	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	616	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	604	NAG	C3-C2-N2	-2.57	107.85	111.76
7	A	600	NAG	O5-C5-C6	2.51	109.61	106.98
7	A	600	NAG	C2-N2-C7	-2.44	119.00	123.09
6	A	601	NAG	C3-C2-N2	-2.37	108.15	111.76
7	A	599	NAG	C3-C2-N2	-2.24	108.36	111.76
7	A	600	NAG	C6-C5-C4	2.13	118.14	113.00
6	A	596	NAG	C3-C2-N2	-2.09	108.58	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	A	605	1	49,50,50	5.81	20 (40%)	46,82,82	1.75	8 (17%)
5	SCN	A	615	-	2,2,2	2.83	1 (50%)	1,1,1	0.04	0
8	SHA	A	617	-	11,11,11	2.61	5 (45%)	14,14,14	1.31	3 (21%)

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	HEM	A	605	1	-	0/14/114/114	0/0/8/8
5	SCN	A	615	-	-	0/0/0/0	0/0/0/0
8	SHA	A	617	-	-	0/6/6/6	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C2B-C1B	22.18	1.50	1.44
2	A	605	HEM	C2D-C1D	21.71	1.50	1.44
2	A	605	HEM	C3D-C4D	19.52	1.49	1.44
2	A	605	HEM	C4A-C3A	7.13	1.49	1.40
2	A	605	HEM	C3C-CAC	5.91	1.59	1.40
2	A	605	HEM	FE-NC	5.78	2.19	1.97
2	A	605	HEM	C3B-CAB	5.46	1.57	1.40
8	A	617	SHA	C3-C2	4.58	1.49	1.39
2	A	605	HEM	CMC-C2C	4.07	1.60	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	CBA-CGA	-3.97	1.40	1.50
8	A	617	SHA	O9-N8	3.92	1.47	1.39
5	A	615	SCN	C-S	3.81	1.88	1.63
2	A	605	HEM	CMA-C3A	-3.73	1.43	1.51
2	A	605	HEM	C3B-C2B	-3.60	1.37	1.43
2	A	605	HEM	C3D-C2D	3.59	1.50	1.43
8	A	617	SHA	C2-C1	-3.58	1.33	1.39
2	A	605	HEM	CHB-C1B	3.58	1.40	1.35
2	A	605	HEM	C1A-C2A	3.37	1.49	1.43
2	A	605	HEM	FE-NA	3.24	2.06	1.92
8	A	617	SHA	C1-C7	-2.83	1.44	1.50
2	A	605	HEM	CMB-C2B	2.53	1.55	1.47
2	A	605	HEM	CAA-C2A	2.43	1.56	1.52
8	A	617	SHA	O6-C6	2.41	1.41	1.36
2	A	605	HEM	C3B-C4B	2.39	1.47	1.44
2	A	605	HEM	C1D-ND	2.22	1.43	1.37
2	A	605	HEM	CAD-CBD	2.21	1.58	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEM	CHD-C1D-ND	5.16	128.87	124.58
2	A	605	HEM	CBD-CAD-C3D	-4.48	104.60	114.37
2	A	605	HEM	C4D-ND-C1D	4.20	109.46	105.16
2	A	605	HEM	C3B-C4B-NB	-3.99	111.14	114.00
2	A	605	HEM	C2D-C1D-ND	-3.24	109.10	112.93
8	A	617	SHA	C3-C4-C5	-2.62	115.81	120.17
2	A	605	HEM	CAD-C3D-C4D	2.58	129.17	124.53
8	A	617	SHA	C1-C7-N8	2.58	119.94	115.52
2	A	605	HEM	CAA-CBA-CGA	2.07	120.13	113.47
2	A	605	HEM	C1A-C2A-C3A	-2.04	104.81	106.92
8	A	617	SHA	C4-C5-C6	2.03	122.75	120.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	595/595 (100%)	0.36	51 (8%)	11 17	15, 31, 74, 100	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	11.2
1	A	595	ASN	9.2
1	A	1	SER	8.7
1	A	8	ALA	7.9
1	A	120	GLY	7.8
1	A	174	SER	7.6
1	A	4	VAL	7.4
1	A	170	PRO	7.4
1	A	122	ASN	7.2
1	A	7	GLY	7.2
1	A	593	ARG	7.0
1	A	119	LEU	6.8
1	A	121	SER	6.0
1	A	171	PRO	5.8
1	A	172	TYR	5.4
1	A	5	GLY	5.4
1	A	173	GLN	5.2
1	A	231	ASN	5.1
1	A	167	CYS	4.7
1	A	6	CYS	4.7
1	A	13	VAL	4.5
1	A	574	HIS	4.3
1	A	12	LEU	4.0
1	A	3	GLU	3.9
1	A	594	GLU	3.8
1	A	169	THR	3.8
1	A	124	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	9	PRO	3.6
1	A	63	GLN	3.5
1	A	123	GLU	3.5
1	A	220	TRP	3.5
1	A	10	VAL	3.4
1	A	592	SER	3.3
1	A	126	LYS	3.2
1	A	234	PRO	3.1
1	A	118	GLU	2.8
1	A	370	PRO	2.7
1	A	32	ARG	2.7
1	A	14	LYS	2.6
1	A	11	PRO	2.5
1	A	591	ALA	2.4
1	A	132	TYR	2.4
1	A	175	LEU	2.4
1	A	477	ALA	2.3
1	A	146	LYS	2.3
1	A	166	VAL	2.2
1	A	15	CYS	2.2
1	A	127	THR	2.2
1	A	383	THR	2.2
1	A	168	PRO	2.1
1	A	368	TRP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	A	198	10/11	0.17	0.88	34,39,46,48	0

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	NAG	A	604	14/15	0.28	9.27	64,67,71,76	0
6	NAG	A	602	14/15	0.40	6.04	71,74,77,81	0
6	NAG	A	597	14/15	0.54	5.67	83,88,89,92	0
7	NAG	A	600	14/15	0.30	1.68	64,67,68,69	0
6	NAG	A	596	14/15	0.23	0.99	62,66,71,77	0
6	NAG	A	601	14/15	0.13	-0.29	54,56,60,66	0
7	NAG	A	599	14/15	0.15	-0.44	51,54,57,61	0
6	MAN	A	603	11/12	0.48	-	84,87,88,88	0
6	MAN	A	598	11/12	0.48	-	95,97,98,98	0
7	NAG	A	616	14/15	0.60	-	80,83,84,84	0

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	SHA	A	617	11/11	0.22	3.81	26,28,30,31	0
2	HEM	A	605	43/43	0.13	0.42	13,15,21,22	0
5	SCN	A	615	3/3	0.13	-0.50	32,32,32,36	0
3	CA	A	606	1/1	0.11	-0.65	20,20,20,20	0
4	IOD	A	609	1/1	0.08	-1.22	63,63,63,63	1
4	IOD	A	613	1/1	0.04	-1.35	56,56,56,56	0
4	IOD	A	608	1/1	0.05	-1.44	89,89,89,89	0
4	IOD	A	614	1/1	0.06	-2.23	77,77,77,77	1
4	IOD	A	611	1/1	0.07	-2.72	84,84,84,84	0
4	IOD	A	610	1/1	0.04	-3.80	67,67,67,67	0
4	IOD	A	612	1/1	0.04	-4.15	64,64,64,64	0
4	IOD	A	607	1/1	0.03	-5.98	20,20,20,20	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.