



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:27 AM GMT

PDB ID : 3ERH
Title : First structural evidence of substrate specificity in mammalian peroxidases: Crystal structures of substrate complexes with lactoperoxidases from two different species
Authors : Sheikh, I.A.; Singh, N.; Singh, A.K.; Sinha, M.; Singh, S.B.; Bhushan, A.; Kaur, P.; Srinivasan, A.; Sharma, S.; Singh, T.P.
Deposited on : 2008-10-02
Resolution : 2.40 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
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 (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

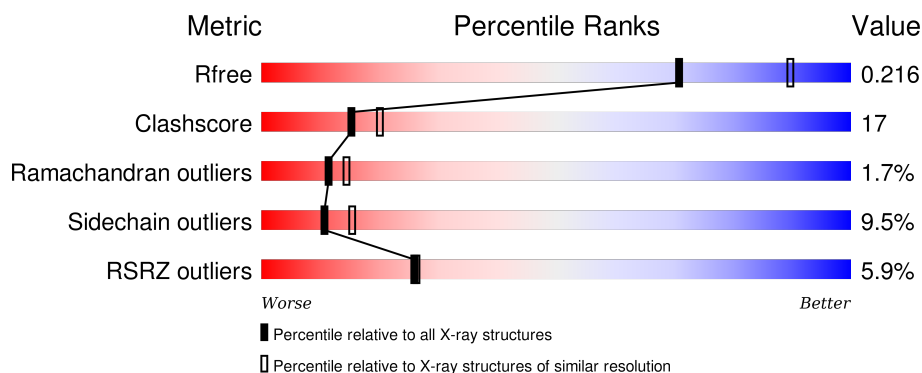
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 ≥ 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>6%</div> <div>71%</div> <div>23%</div> <div>5%</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
5	IOD	A	611	-	-	X	-

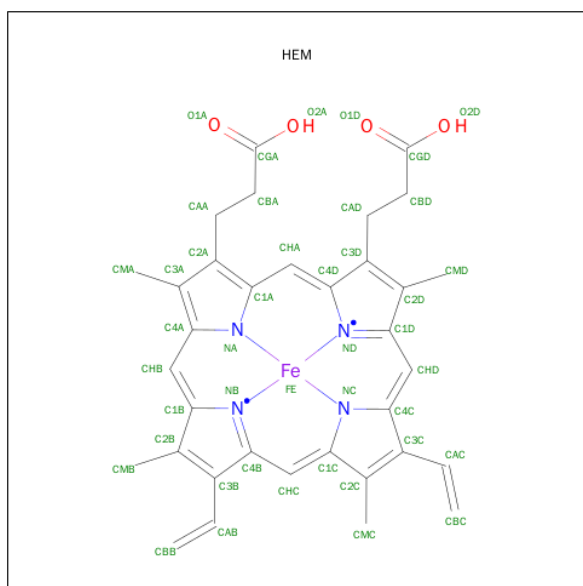
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In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues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

- Molecule 1 is a protein called Lactoperoxidase.

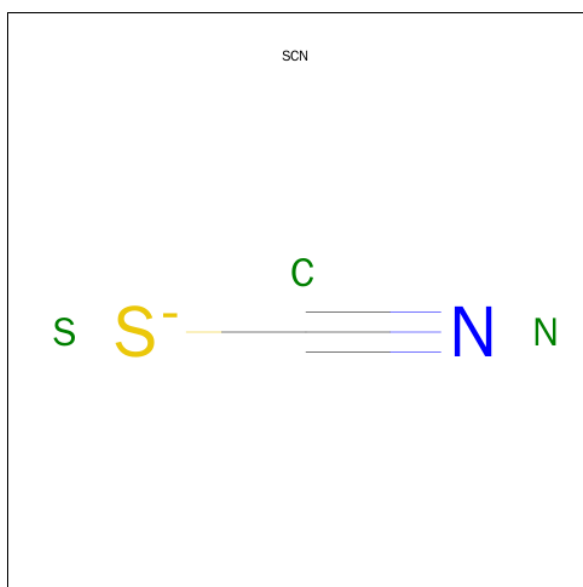
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4778	3040	847	864	1	26			

- 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
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	I	0	0
			7	7		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	398	Total	O	0	0
			398	398		

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, α , β , γ	54.21Å 80.54Å 77.88Å 90.00° 102.64° 90.00°	Depositor
Resolution (Å)	19.46 – 2.40 19.46 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.46-2.40) 98.8 (19.46-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.41Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.180 , 0.195 0.188 , 0.216	Depositor DCC
R_{free} test set	1289 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 46.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 25355 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5378	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SCN, NAG, SEP, CA, BMA, 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	3/4896 (0.1%)	0.86	15/6640 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	PRO	N-CA	10.37	1.64	1.47
1	A	222	HIS	C-N	-5.34	1.23	1.33
1	A	367	PRO	CA-C	-5.25	1.42	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	CYS	O-C-N	-10.95	100.29	121.10
1	A	168	PRO	N-CA-C	10.39	139.11	112.10
1	A	167	CYS	CA-C-N	8.63	141.26	117.10
1	A	168	PRO	C-N-CA	8.37	142.63	121.70
1	A	172	TYR	N-CA-C	7.74	131.89	111.00
1	A	504	ARG	CD-NE-CZ	6.94	133.32	123.60
1	A	171	PRO	N-CA-C	6.64	129.36	112.10
1	A	172	TYR	C-N-CA	6.26	137.35	121.70
1	A	173	GLN	N-CA-C	6.26	127.89	111.00
1	A	169	THR	N-CA-CB	5.50	120.74	110.30
1	A	424	PRO	CA-N-CD	-5.28	104.11	111.50
1	A	123	GLU	N-CA-C	5.16	124.92	111.00
1	A	222	HIS	CB-CA-C	-5.13	100.14	110.40
1	A	6	CYS	C-N-CA	-5.06	111.67	122.30
1	A	167	CYS	N-CA-C	-5.04	97.38	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	4778	0	4685	153	0
2	A	43	0	30	5	0
3	A	6	0	0	1	0
4	A	1	0	0	0	0
5	A	7	0	0	3	0
6	A	56	0	50	4	0
7	A	39	0	34	3	0
8	A	50	0	43	9	0
9	A	398	0	0	46	0
All	All	5378	0	4842	171	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 (171) 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:504:ARG:NH2	5:A:611:IOD:I	2.64	1.01
1:A:584:LYS:HD2	9:A:819:HOH:O	1.59	1.00
1:A:197:PRO:HD2	1:A:198:SEP:O3P	1.62	1.00
1:A:156:LYS:HD2	9:A:750:HOH:O	1.64	0.95
8:A:624:NAG:H3	9:A:986:HOH:O	1.64	0.95
1:A:127:THR:HG23	1:A:131:GLU:HG3	1.51	0.92
1:A:481:MET:SD	1:A:487:PRO:HD3	2.10	0.89
1:A:2:TRP:HB3	1:A:175:LEU:HG	1.57	0.86
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.75	0.85
1:A:115:PRO:HD2	9:A:965:HOH:O	1.77	0.84
1:A:106:ILE:HD11	1:A:265:ALA:HB1	1.60	0.84
1:A:175:LEU:HD22	1:A:176:ALA:H	1.44	0.83
1:A:82:ILE:HD11	1:A:479:LYS:HB2	1.60	0.83
1:A:63:GLN:HB3	9:A:941:HOH:O	1.79	0.82
8:A:625:NAG:H61	9:A:943:HOH:O	1.79	0.81
1:A:9:PRO:HG2	1:A:41:ARG:CZ	2.11	0.80
1:A:175:LEU:CD2	1:A:176:ALA:H	1.94	0.80
1:A:547:PHE:HE2	1:A:585:LEU:HD22	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:O	1:A:11:PRO:HD3	1.81	0.79
2:A:605:HEM:HMC2	2:A:605:HEM:HBC2	1.65	0.79
1:A:580:SER:HB2	9:A:921:HOH:O	1.84	0.76
1:A:169:THR:HB	1:A:170:PRO:HD3	1.68	0.76
8:A:625:NAG:H62	8:A:626:BMA:O5	1.85	0.76
8:A:627:MAN:H2	9:A:1001:HOH:O	1.87	0.73
1:A:472:LYS:HE3	9:A:985:HOH:O	1.91	0.71
1:A:127:THR:HG23	1:A:131:GLU:CG	2.20	0.71
1:A:565:HIS:CE1	6:A:618:NAG:H81	2.25	0.71
1:A:170:PRO:HB3	1:A:171:PRO:HD2	1.73	0.70
1:A:166:VAL:HG12	1:A:180:ILE:HG12	1.74	0.69
1:A:503:GLU:HG3	9:A:794:HOH:O	1.93	0.68
1:A:172:TYR:HB3	9:A:827:HOH:O	1.93	0.68
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.29	0.68
1:A:174:SER:HA	9:A:936:HOH:O	1.93	0.67
8:A:625:NAG:H2	9:A:806:HOH:O	1.95	0.67
1:A:504:ARG:NE	5:A:611:IOD:I	2.97	0.66
1:A:175:LEU:HD22	1:A:176:ALA:N	2.08	0.66
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.78	0.66
1:A:565:HIS:ND1	6:A:618:NAG:H81	2.11	0.65
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.62	0.64
1:A:8:ALA:N	1:A:9:PRO:HD2	2.13	0.64
1:A:588:SER:OG	1:A:589:PRO:HD3	1.99	0.63
1:A:504:ARG:CZ	5:A:611:IOD:I	3.16	0.63
6:A:620:NAG:H4	9:A:808:HOH:O	1.98	0.63
1:A:123:GLU:HG3	1:A:125:SER:HB3	1.81	0.63
1:A:465:LYS:HD2	9:A:748:HOH:O	1.99	0.63
1:A:407:MET:HB3	1:A:501:MET:CE	2.29	0.62
1:A:127:THR:CG2	1:A:131:GLU:HG3	2.28	0.62
1:A:8:ALA:N	1:A:9:PRO:CD	2.62	0.62
1:A:242:THR:HG21	9:A:928:HOH:O	1.99	0.62
1:A:13:VAL:HA	9:A:754:HOH:O	2.01	0.61
1:A:106:ILE:HD11	1:A:265:ALA:CB	2.30	0.60
1:A:257:SER:O	1:A:381:PHE:HA	2.02	0.60
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.84	0.60
1:A:564:LEU:HB3	1:A:565:HIS:HD2	1.66	0.59
8:A:626:BMA:H3	9:A:699:HOH:O	2.02	0.59
1:A:282:LYS:HD3	9:A:927:HOH:O	2.02	0.59
1:A:284:ASN:HA	1:A:286:HIS:CE1	2.38	0.59
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.36	0.58
1:A:93:ASP:O	1:A:403:LYS:HD3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:TYR:CD1	1:A:523:ARG:HD3	2.39	0.58
1:A:504:ARG:HD2	9:A:803:HOH:O	2.05	0.57
1:A:561:LYS:HG3	9:A:813:HOH:O	2.05	0.57
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.39	0.57
1:A:129:CYS:HB2	9:A:698:HOH:O	2.04	0.57
1:A:9:PRO:CG	1:A:41:ARG:NE	2.68	0.57
1:A:146:LYS:O	1:A:147:ASN:HB2	2.05	0.56
1:A:120:GLY:HA3	9:A:786:HOH:O	2.06	0.56
1:A:169:THR:CB	1:A:170:PRO:CD	2.82	0.56
1:A:169:THR:HB	1:A:170:PRO:CD	2.36	0.56
1:A:538:GLU:HB3	9:A:981:HOH:O	2.05	0.55
1:A:197:PRO:CD	1:A:198:SEP:O3P	2.48	0.55
1:A:165:PHE:CE1	1:A:177:ARG:NH2	2.75	0.55
1:A:9:PRO:HG3	1:A:41:ARG:HD3	1.89	0.55
1:A:11:PRO:O	1:A:13:VAL:HG22	2.06	0.55
2:A:605:HEM:HBC2	2:A:605:HEM:CMC	2.36	0.55
1:A:200:ALA:O	1:A:204:ARG:HG3	2.07	0.55
1:A:165:PHE:O	1:A:180:ILE:HD11	2.07	0.54
1:A:322:GLN:HG3	9:A:755:HOH:O	2.06	0.54
1:A:360:ARG:O	1:A:361:LEU:HD23	2.07	0.54
1:A:362:ASP:O	1:A:365:TYR:N	2.35	0.54
1:A:175:LEU:CD2	1:A:176:ALA:N	2.67	0.54
1:A:16:ASP:HB3	1:A:19:SER:HB2	1.90	0.53
1:A:572:TYR:CZ	1:A:573:PRO:HB3	2.43	0.53
1:A:408:ASN:HB2	9:A:768:HOH:O	2.08	0.53
1:A:481:MET:SD	1:A:487:PRO:CD	2.94	0.52
1:A:10:VAL:HG12	9:A:817:HOH:O	2.10	0.52
1:A:272:GLU:HG3	1:A:276:LEU:HD22	1.92	0.51
1:A:8:ALA:HB3	9:A:798:HOH:O	2.10	0.51
1:A:172:TYR:N	1:A:172:TYR:CD2	2.72	0.51
1:A:301:GLY:O	1:A:305:GLN:HG3	2.10	0.51
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.22	0.51
1:A:407:MET:HB3	1:A:501:MET:HE3	1.93	0.51
1:A:557:THR:OG1	1:A:559:ILE:HG12	2.11	0.51
1:A:588:SER:N	1:A:589:PRO:CD	2.75	0.50
1:A:407:MET:HB3	1:A:501:MET:HE1	1.93	0.50
1:A:221:ASP:O	1:A:222:HIS:HB2	2.11	0.50
1:A:281:LYS:HD2	1:A:285:PRO:HA	1.94	0.50
1:A:381:PHE:CZ	1:A:424:PRO:HG3	2.47	0.50
1:A:360:ARG:NH1	1:A:371:GLU:O	2.44	0.50
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:622:NAG:H3	9:A:840:HOH:O	2.12	0.50
1:A:9:PRO:HG2	1:A:41:ARG:NE	2.26	0.49
1:A:286:HIS:N	1:A:286:HIS:ND1	2.46	0.49
1:A:397:ARG:HG2	1:A:559:ILE:HD12	1.94	0.49
1:A:242:THR:O	1:A:245:ARG:NH2	2.46	0.49
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.48	0.48
8:A:627:MAN:H5	9:A:942:HOH:O	2.13	0.48
1:A:9:PRO:HG3	1:A:41:ARG:CD	2.43	0.48
1:A:572:TYR:CE2	1:A:573:PRO:HB3	2.49	0.48
1:A:467:LEU:HG	1:A:471:LEU:HD22	1.94	0.47
1:A:118:GLU:CB	9:A:834:HOH:O	2.61	0.47
1:A:205:ASN:C	1:A:205:ASN:OD1	2.52	0.47
1:A:118:GLU:HG3	9:A:770:HOH:O	2.14	0.47
1:A:165:PHE:CZ	1:A:169:THR:O	2.67	0.47
1:A:349:PHE:CA	1:A:497:ASN:HD21	2.26	0.47
1:A:175:LEU:HD13	9:A:708:HOH:O	2.14	0.47
1:A:503:GLU:HB2	9:A:742:HOH:O	2.15	0.47
1:A:385:ARG:O	1:A:389:ASP:HB3	2.15	0.47
1:A:462:LYS:HG3	9:A:790:HOH:O	2.14	0.46
1:A:313:LEU:HB2	1:A:314:PRO:CD	2.45	0.46
1:A:333:ASN:HD22	1:A:334:SER:N	2.13	0.46
1:A:82:ILE:HG21	1:A:494:ILE:HD11	1.96	0.46
1:A:123:GLU:OE1	1:A:123:GLU:N	2.48	0.46
1:A:347:PHE:HB3	2:A:605:HEM:HMD3	1.98	0.46
1:A:175:LEU:HA	9:A:883:HOH:O	2.15	0.46
1:A:57:LEU:HA	1:A:58:PRO:HD3	1.83	0.46
1:A:27:ASP:O	1:A:28:CYS:HB2	2.16	0.46
1:A:175:LEU:HD23	1:A:176:ALA:H	1.77	0.45
1:A:349:PHE:HA	1:A:497:ASN:ND2	2.29	0.45
1:A:362:ASP:OD1	1:A:362:ASP:C	2.55	0.45
7:A:622:NAG:H4	7:A:623:MAN:H2	1.32	0.45
1:A:574:HIS:HB3	9:A:886:HOH:O	2.15	0.45
1:A:2:TRP:CB	1:A:175:LEU:HG	2.39	0.45
2:A:605:HEM:HMC2	2:A:605:HEM:CBC	2.42	0.45
1:A:581:THR:HG22	1:A:581:THR:O	2.17	0.45
1:A:544:LEU:HD23	1:A:547:PHE:CZ	2.52	0.45
1:A:63:GLN:HG3	9:A:917:HOH:O	2.16	0.44
1:A:259:GLN:OE1	1:A:261:LEU:HB2	2.16	0.44
1:A:202:ARG:HD2	1:A:250:LEU:HD21	1.98	0.44
1:A:7:GLY:C	1:A:9:PRO:HD2	2.37	0.44
1:A:165:PHE:CD1	1:A:165:PHE:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:THR:HG23	1:A:392:ILE:HB	1.99	0.44
7:A:623:MAN:H4	9:A:910:HOH:O	2.17	0.44
8:A:625:NAG:H62	8:A:626:BMA:C5	2.48	0.44
2:A:605:HEM:HBB2	2:A:605:HEM:CMB	2.48	0.43
6:A:620:NAG:H3	9:A:829:HOH:O	2.19	0.43
1:A:572:TYR:HA	1:A:573:PRO:HA	1.82	0.43
1:A:231:ASN:HA	9:A:686:HOH:O	2.18	0.43
1:A:45:ARG:CZ	1:A:49:ALA:HB2	2.49	0.43
1:A:118:GLU:HB2	9:A:834:HOH:O	2.18	0.42
1:A:55:LEU:HD21	9:A:1005:HOH:O	2.19	0.42
1:A:165:PHE:HZ	9:A:939:HOH:O	2.02	0.42
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.17	0.42
1:A:313:LEU:HB2	1:A:314:PRO:HD3	2.00	0.42
1:A:362:ASP:N	1:A:366:GLN:O	2.43	0.42
1:A:258:GLU:OE1	1:A:259:GLN:HG2	2.20	0.42
1:A:519:PHE:CD1	1:A:522:ILE:HD11	2.55	0.42
1:A:24:ILE:HA	1:A:24:ILE:HD13	1.92	0.42
1:A:258:GLU:HG3	3:A:608:SCN:S	2.59	0.42
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.89	0.41
1:A:14:LYS:HE2	1:A:14:LYS:HB3	1.86	0.41
8:A:625:NAG:H62	8:A:626:BMA:C6	2.51	0.41
1:A:364:ASN:O	1:A:365:TYR:HB2	2.21	0.41
1:A:32:ARG:NH1	9:A:1014:HOH:O	2.53	0.41
1:A:63:GLN:HB2	9:A:773:HOH:O	2.20	0.41
1:A:381:PHE:CE2	1:A:424:PRO:HD3	2.55	0.41
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.93	0.40
1:A:33:SER:HA	1:A:34:PRO:HD2	1.89	0.40
1:A:196:GLU:HA	1:A:197:PRO:HD3	1.85	0.40
1:A:82:ILE:CD1	1:A:479:LYS:HB2	2.42	0.40
1:A:361:LEU:HA	1:A:366:GLN:O	2.21	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%)	552 (93%)	30 (5%)	10 (2%)	11	14

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	167	CYS
1	A	169	THR
1	A	18	ASN
1	A	168	PRO
1	A	170	PRO
1	A	171	PRO
1	A	3	GLU
1	A	9	PRO
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%)	468 (90%)	49 (10%)	11	15

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	6	CYS
1	A	13	VAL
1	A	14	LYS
1	A	36	LEU
1	A	91	VAL
1	A	98	LEU
1	A	117	THR
1	A	119	LEU

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Mol	Chain	Res	Type
1	A	122	ASN
1	A	123	GLU
1	A	130	GLU
1	A	165	PHE
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	171	PRO
1	A	172	TYR
1	A	175	LEU
1	A	187	LEU
1	A	202	ARG
1	A	203	LEU
1	A	218	GLU
1	A	231	ASN
1	A	242	THR
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	282	LYS
1	A	286	HIS
1	A	292	LEU
1	A	317	LEU
1	A	333	ASN
1	A	347	PHE
1	A	360	ARG
1	A	376	LEU
1	A	418	ARG
1	A	423	GLN
1	A	424	PRO
1	A	464	LEU
1	A	479	LYS
1	A	494	ILE
1	A	511	LEU
1	A	520	GLN
1	A	522	ILE
1	A	539	LYS
1	A	564	LEU
1	A	592	SER
1	A	594	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	135	GLN
1	A	217	GLN
1	A	322	GLN
1	A	329	GLN
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	545	GLN
1	A	565	HIS
1	A	570	ASN
1	A	574	HIS

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	1.41	1 (12%)	8,12,14	3.62	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	OG-CB	2.97	1.57	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O3P-P-OG	-4.02	94.98	106.56
1	A	198	SEP	O3P-P-O1P	-2.07	103.91	110.58
1	A	198	SEP	OG-CB-CA	3.08	110.90	108.27
1	A	198	SEP	O3P-P-O2P	3.36	120.18	107.38
1	A	198	SEP	OG-P-O1P	7.71	126.77	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	3	0

5.5 Carbohydrates ⓘ

11 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	617	1,6	14,14,15	0.98	1 (7%)	15,19,21	2.34	4 (26%)
6	NAG	A	618	6	14,14,15	0.65	0	15,19,21	2.50	8 (53%)
6	NAG	A	619	1,6	14,14,15	0.97	1 (7%)	15,19,21	1.31	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	620	6	14,14,15	1.26	1 (7%)	15,19,21	2.81	6 (40%)
7	NAG	A	621	1,7	14,14,15	1.27	2 (14%)	15,19,21	1.37	3 (20%)
7	NAG	A	622	7	14,14,15	1.15	1 (7%)	15,19,21	2.32	1 (6%)
7	MAN	A	623	7	11,11,12	0.76	0	14,15,17	2.71	3 (21%)
8	NAG	A	624	1,8	14,14,15	0.84	0	15,19,21	2.36	6 (40%)
8	NAG	A	625	8	14,14,15	0.82	1 (7%)	15,19,21	1.76	4 (26%)
8	BMA	A	626	8	11,11,12	0.62	0	14,15,17	1.74	2 (14%)
8	MAN	A	627	8	11,11,12	0.53	0	14,15,17	1.29	1 (7%)

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	617	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	618	6	-	0/6/23/26	0/1/1/1
6	NAG	A	619	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	620	6	-	0/6/23/26	0/1/1/1
7	NAG	A	621	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	622	7	-	0/6/23/26	0/1/1/1
7	MAN	A	623	7	-	0/2/19/22	0/1/1/1
8	NAG	A	624	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	625	8	-	0/6/23/26	0/1/1/1
8	BMA	A	626	8	-	0/2/19/22	1/1/1/1
8	MAN	A	627	8	-	0/2/19/22	1/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	622	NAG	O5-C1	-3.90	1.37	1.43
6	A	620	NAG	O5-C1	-3.48	1.37	1.43
7	A	621	NAG	O5-C1	-3.32	1.38	1.43
6	A	619	NAG	O5-C1	-2.65	1.39	1.43
6	A	617	NAG	O5-C1	-2.45	1.39	1.43
7	A	621	NAG	C2-N2	-2.43	1.42	1.46
8	A	625	NAG	C1-C2	2.09	1.55	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	620	NAG	C2-N2-C7	-6.33	114.90	123.04
6	A	620	NAG	C3-C2-N2	-6.09	95.98	110.56
6	A	618	NAG	C2-N2-C7	-5.80	115.59	123.04
6	A	617	NAG	C2-N2-C7	-5.75	115.65	123.04
8	A	624	NAG	C2-N2-C7	-5.43	116.06	123.04
6	A	617	NAG	C1-O5-C5	-4.33	106.76	112.25
8	A	627	MAN	C1-O5-C5	-3.81	107.41	112.25
6	A	617	NAG	O6-C6-C5	-3.30	100.42	111.33
6	A	618	NAG	C6-C5-C4	-3.23	105.05	113.02
6	A	617	NAG	C3-C4-C5	-2.93	105.09	110.20
8	A	624	NAG	O6-C6-C5	-2.86	101.88	111.33
7	A	621	NAG	C1-O5-C5	-2.71	108.81	112.25
6	A	620	NAG	O4-C4-C3	-2.60	104.49	110.34
6	A	619	NAG	C3-C2-N2	-2.58	104.37	110.56
8	A	624	NAG	C6-C5-C4	-2.50	106.85	113.02
7	A	621	NAG	O6-C6-C5	-2.45	103.23	111.33
6	A	618	NAG	O7-C7-C8	-2.35	117.74	122.06
8	A	624	NAG	O3-C3-C4	-2.31	105.13	110.34
8	A	625	NAG	C6-C5-C4	-2.20	107.58	113.02
7	A	621	NAG	C3-C2-N2	-2.05	105.65	110.56
6	A	618	NAG	O3-C3-C2	-2.03	105.09	109.11
6	A	618	NAG	C3-C4-C5	2.05	113.77	110.20
8	A	624	NAG	O5-C5-C6	2.12	111.94	107.35
6	A	620	NAG	C4-C3-C2	2.21	114.67	111.23
6	A	618	NAG	O5-C5-C6	2.33	112.39	107.35
8	A	625	NAG	C1-O5-C5	2.33	115.20	112.25
6	A	619	NAG	O3-C3-C4	2.36	115.64	110.34
8	A	626	BMA	O5-C5-C6	2.48	112.71	107.35
6	A	620	NAG	O7-C7-C8	2.70	127.01	122.06
6	A	618	NAG	C8-C7-N2	2.82	121.51	116.11
7	A	623	MAN	C2-C3-C4	3.10	116.31	111.04
6	A	620	NAG	O4-C4-C5	3.23	117.79	109.24
8	A	625	NAG	C3-C4-C5	3.36	116.05	110.20
8	A	625	NAG	C4-C3-C2	3.61	116.84	111.23
6	A	618	NAG	C4-C3-C2	3.78	117.10	111.23
7	A	623	MAN	O5-C5-C6	3.98	115.97	107.35
8	A	624	NAG	C4-C3-C2	4.51	118.24	111.23
8	A	626	BMA	C1-O5-C5	4.94	118.52	112.25
7	A	623	MAN	C1-C2-C3	8.31	119.37	109.54
7	A	622	NAG	C1-O5-C5	8.42	122.94	112.25

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	627	MAN	C1-C2-C3-C4-C5-O5
8	A	626	BMA	C1-C2-C3-C4-C5-O5

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	618	NAG	2	0
6	A	620	NAG	2	0
7	A	622	NAG	2	0
7	A	623	MAN	2	0
8	A	624	NAG	1	0
8	A	625	NAG	5	0
8	A	626	BMA	4	0
8	A	627	MAN	2	0

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 8 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	1,9	30,50,50	2.95	9 (30%)	24,82,82	2.43	8 (33%)
3	SCN	A	607	-	2,2,2	1.50	1 (50%)	1,1,1	0.45	0
3	SCN	A	608	-	2,2,2	1.74	1 (50%)	1,1,1	0.52	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
2	HEM	A	605	1,9	-	0/10/54/54	0/0/8/8
3	SCN	A	607	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SCN	A	608	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C3B-C4B	-12.58	1.40	1.51
2	A	605	HEM	C2C-C1C	-3.58	1.45	1.52
3	A	607	SCN	C-S	2.11	1.77	1.63
3	A	608	SCN	C-S	2.46	1.79	1.63
2	A	605	HEM	C3C-CAC	2.47	1.56	1.51
2	A	605	HEM	FE-NC	2.51	2.05	1.95
2	A	605	HEM	CMA-C3A	2.81	1.57	1.51
2	A	605	HEM	CAA-C2A	2.83	1.56	1.52
2	A	605	HEM	C1C-NC	2.95	1.39	1.36
2	A	605	HEM	C3B-CAB	2.96	1.56	1.51
2	A	605	HEM	C4C-NC	4.59	1.41	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEM	C3B-CAB-CBB	-4.54	117.49	124.46
2	A	605	HEM	CBA-CAA-C2A	-2.62	107.84	112.53
2	A	605	HEM	C4B-CHC-C1C	-2.25	122.06	125.82
2	A	605	HEM	CMD-C2D-C3D	2.63	125.97	114.35
2	A	605	HEM	CMB-C2B-C3B	4.13	126.84	116.53
2	A	605	HEM	CMC-C2C-C3C	4.30	127.26	116.53
2	A	605	HEM	CAD-C3D-C4D	4.64	128.85	112.47
2	A	605	HEM	CAD-C3D-C2D	4.69	126.71	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	605	HEM	5	0
3	A	608	SCN	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, 95th 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 ²)	Q<0.9
1	A	594/595 (99%)	-0.06	35 (5%) 26 26	19, 34, 76, 100	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	10.5
1	A	119	LEU	8.7
1	A	172	TYR	8.3
1	A	7	GLY	7.8
1	A	593	ARG	7.1
1	A	122	ASN	7.0
1	A	594	GLU	6.6
1	A	2	TRP	6.1
1	A	121	SER	5.7
1	A	174	SER	5.4
1	A	120	GLY	5.4
1	A	595	ASN	5.3
1	A	171	PRO	4.8
1	A	169	THR	4.6
1	A	168	PRO	4.5
1	A	124	HIS	4.4
1	A	173	GLN	4.4
1	A	170	PRO	4.3
1	A	175	LEU	4.1
1	A	4	VAL	3.8
1	A	123	GLU	3.3
1	A	12	LEU	3.1
1	A	9	PRO	3.1
1	A	6	CYS	2.8
1	A	167	CYS	2.7
1	A	125	SER	2.7
1	A	8	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	231	ASN	2.4
1	A	581	THR	2.4
1	A	11	PRO	2.3
1	A	254	PHE	2.3
1	A	5	GLY	2.2
1	A	368	TRP	2.2
1	A	132	TYR	2.1
1	A	234	PRO	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, 95th 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 ²)	Q<0.9
1	SEP	A	198	10/11	0.94	0.15	-	21,32,37,39	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, 95th 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 ²)	Q<0.9
6	NAG	A	617	14/15	0.89	0.22	0.41	52,59,71,72	0
7	NAG	A	621	14/15	0.95	0.10	-1.08	35,44,48,55	0
6	NAG	A	619	14/15	0.96	0.11	-1.33	38,42,55,57	0
8	NAG	A	624	14/15	0.79	0.31	-	58,66,74,84	0
8	BMA	A	626	11/12	0.71	0.42	-	109,111,112,113	0
6	NAG	A	618	14/15	0.74	0.54	-	77,84,90,91	0
6	NAG	A	620	14/15	0.81	0.34	-	64,71,73,73	0
7	MAN	A	623	11/12	0.70	0.36	-	87,89,91,92	0
7	NAG	A	622	14/15	0.84	0.28	-	61,73,76,81	0
8	MAN	A	627	11/12	0.65	0.45	-	111,113,114,114	0
8	NAG	A	625	14/15	0.79	0.42	-	92,97,101,105	0

6.4 Ligands [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, 95th 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 ²)	Q<0.9
3	SCN	A	608	3/3	0.94	0.16	1.56	21,21,26,34	0
4	CA	A	609	1/1	0.99	0.14	0.18	25,25,25,25	0
3	SCN	A	607	3/3	0.96	0.13	-0.82	20,20,20,26	0
5	IOD	A	616	1/1	1.00	0.07	-0.93	54,54,54,54	0
5	IOD	A	615	1/1	1.00	0.09	-1.62	28,28,28,28	0
2	HEM	A	605	43/43	0.97	0.09	-1.66	7,20,26,27	0
5	IOD	A	612	1/1	1.00	0.05	-2.38	75,75,75,75	0
5	IOD	A	613	1/1	0.88	0.06	-3.19	88,88,88,88	0
5	IOD	A	614	1/1	0.98	0.05	-4.02	69,69,69,69	0
5	IOD	A	611	1/1	0.86	0.11	-	100,100,100,100	0
5	IOD	A	610	1/1	0.97	0.07	-	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.