



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:00 PM GMT

PDB ID : 2PUM
Title : Crystal structure of bovine lactoperoxidase complex with catechol and iodide at 2.7 Å resolution
Authors : Singh, A.K.; Singh, N.; Sharma, S.; Kaur, P.; Singh, T.P.
Deposited on : 2007-05-09
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

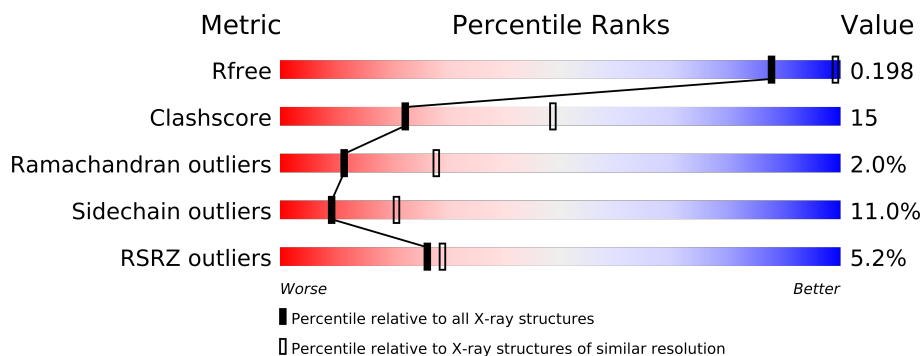
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. 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	CAQ	A	619	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5260 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	1	0
			4780	3041	847	865	1	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	SEP	SER	MODIFIED RESIDUE	UNP P80025

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	SEP	SER	MODIFIED RESIDUE	UNP P80025
A	198	SEP	SER	MODIFIED RESIDUE	UNP P80025

- 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		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

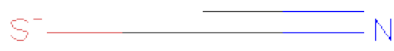
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	SEP	SER	MODIFIED RESIDUE	UNP P80025
A	198	SEP	SER	MODIFIED RESIDUE	UNP P80025

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

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

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

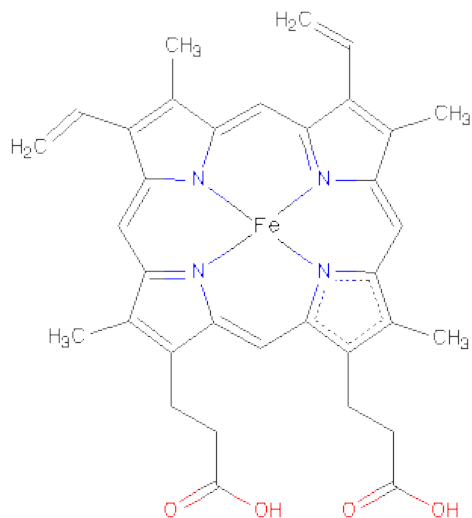


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N S 3 1 1 1	0	0

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

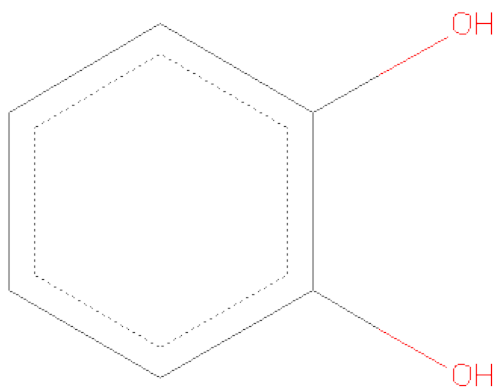
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	10	Total I 10 10	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 8 is CATECHOL (three-letter code: CAQ) (formula: $C_6H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			8	6	2		

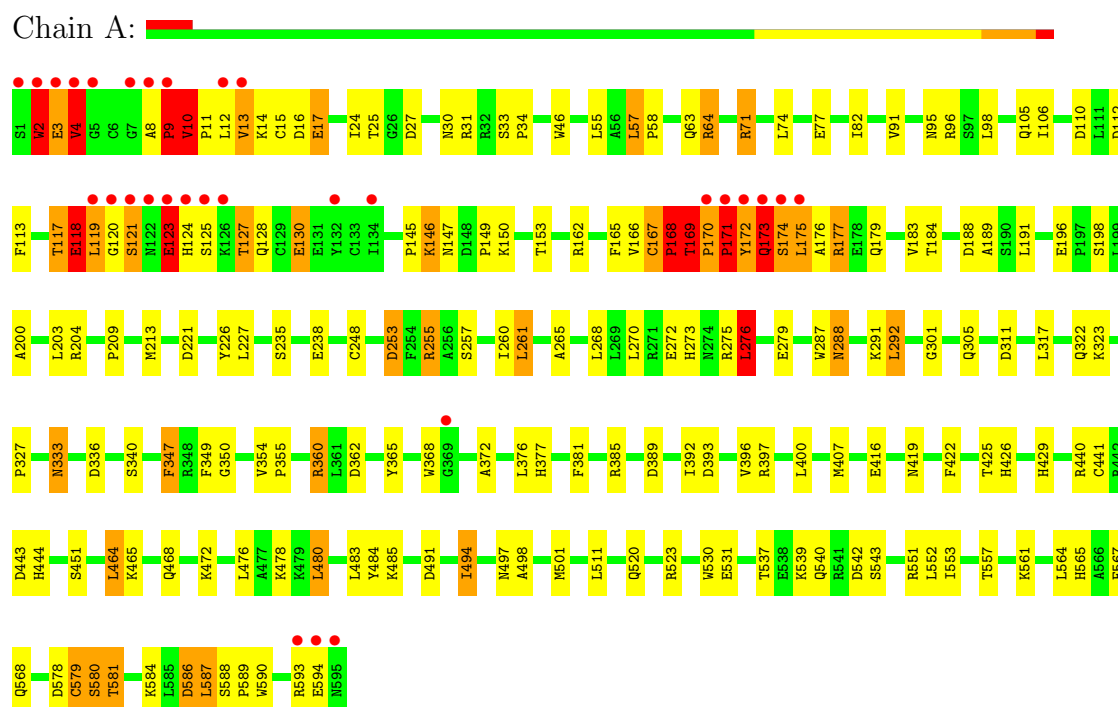
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	281	Total 281	O 281	0	0

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, α , β , γ	54.42Å 80.49Å 77.32Å 90.00° 102.60° 90.00°	Depositor
Resolution (Å)	24.93 – 2.70 24.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.93-2.70) 99.4 (24.93-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.165 , 0.203 0.168 , 0.198	Depositor DCC
R_{free} test set	912 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 17874 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5260	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, CAQ, HEM, IOD, CA, 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	0.77	2/4900 (0.0%)	1.06	31/6646 (0.5%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	VAL	N-CA	-5.62	1.35	1.46
1	A	9	PRO	C-N	-5.38	1.21	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118[A]	GLU	O-C-N	-10.33	106.17	122.70
1	A	118[B]	GLU	O-C-N	-10.33	106.17	122.70
1	A	3	GLU	CA-C-N	-8.72	98.02	117.20
1	A	3	GLU	C-N-CA	8.00	141.69	121.70
1	A	253	ASP	CB-CG-OD2	7.65	125.19	118.30
1	A	3	GLU	N-CA-C	-6.92	92.32	111.00
1	A	3	GLU	N-CA-CB	6.82	122.88	110.60
1	A	27	ASP	CB-CG-OD2	6.71	124.33	118.30
1	A	336	ASP	CB-CG-OD2	6.66	124.30	118.30
1	A	170	PRO	CA-N-CD	-6.58	102.28	111.50
1	A	173	GLN	CA-C-N	6.21	130.86	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	PRO	CA-N-CD	-6.16	102.88	111.50
1	A	2	TRP	C-N-CA	6.08	136.90	121.70
1	A	3	GLU	O-C-N	5.93	132.19	122.70
1	A	172	TYR	CB-CG-CD1	5.81	124.48	121.00
1	A	173	GLN	C-N-CA	-5.78	107.25	121.70
1	A	112	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	311	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	542	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	168	PRO	C-N-CA	5.64	135.81	121.70
1	A	586	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	172	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	A	276	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	9	PRO	CA-C-N	-5.48	105.15	117.20
1	A	174	SER	N-CA-C	5.37	125.50	111.00
1	A	491	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	168	PRO	CA-C-N	-5.09	106.00	117.20
1	A	123	GLU	N-CA-C	5.09	124.75	111.00
1	A	443	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	594	GLU	CB-CA-C	-5.07	100.27	110.40
1	A	288	ASN	N-CA-CB	-5.03	101.55	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118[A]	GLU	Mainchain
1	A	118[B]	GLU	Mainchain

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	4780	0	4692	140	0
2	A	78	0	68	2	0
3	A	56	0	50	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
5	A	3	0	0	0	0
6	A	10	0	0	6	0
7	A	43	0	30	7	0
8	A	8	0	4	0	0
9	A	281	0	0	16	0
All	All	5260	0	4844	146	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 15.

All (146) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:578:ASP:OD1	1:A:580:SER:HB2	1.53	1.05
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.37	1.03
1:A:31:ARG:HD2	6:A:609:IOD:I	2.29	1.02
1:A:33:SER:HB2	9:A:896:HOH:O	1.62	1.00
1:A:118[A]:GLU:HG3	1:A:119:LEU:N	1.75	0.92
1:A:118[A]:GLU:HG3	1:A:119:LEU:H	1.09	0.88
1:A:106:ILE:HD11	1:A:265:ALA:HB1	1.59	0.84
7:A:618:HEM:HMB2	7:A:618:HEM:HBB2	1.60	0.81
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.12	0.80
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.62	0.80
7:A:618:HEM:CMB	7:A:618:HEM:HBB2	2.12	0.78
1:A:8:ALA:N	1:A:9:PRO:HD2	2.02	0.73
1:A:9:PRO:O	1:A:11:PRO:HD3	1.89	0.73
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.52	0.73
1:A:537:THR:OG1	1:A:540:GLN:HG3	1.89	0.72
1:A:167:CYS:CB	1:A:168:PRO:CD	2.67	0.72
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.88	0.72
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.72	0.72
6:A:609:IOD:I	9:A:723:HOH:O	2.78	0.71
1:A:275:ARG:NH1	9:A:800:HOH:O	2.26	0.69
1:A:130:GLU:CD	1:A:426:HIS:HD2	1.95	0.69
1:A:2:TRP:HA	1:A:4:VAL:HG13	1.75	0.69
1:A:327:PRO:HD2	9:A:799:HOH:O	1.93	0.68
7:A:618:HEM:HMB2	7:A:618:HEM:CBB	2.23	0.68
1:A:147:ASN:O	1:A:149:PRO:HD3	1.93	0.67
1:A:578:ASP:C	1:A:580:SER:H	1.98	0.67
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.25	0.67
1:A:8:ALA:N	1:A:9:PRO:CD	2.58	0.67
1:A:464:LEU:O	1:A:468:GLN:HG3	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:360:ARG:NH1	1:A:372:ALA:HA	2.13	0.64
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.33	0.63
1:A:71:ARG:HH11	1:A:71:ARG:CG	2.10	0.63
1:A:150:LYS:NZ	1:A:419:ASN:O	2.30	0.63
1:A:17:GLU:HG3	9:A:894:HOH:O	1.98	0.63
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.81	0.62
1:A:8:ALA:H	1:A:9:PRO:HD2	1.65	0.59
1:A:587:LEU:HD23	1:A:587:LEU:O	2.02	0.59
2:A:598:MAN:H2	9:A:861:HOH:O	2.02	0.59
1:A:121:SER:HB2	9:A:827:HOH:O	2.04	0.58
1:A:82:ILE:HG21	1:A:494:ILE:HD11	1.84	0.58
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.39	0.58
1:A:10:VAL:CG2	1:A:10:VAL:O	2.51	0.57
1:A:10:VAL:HG23	1:A:10:VAL:O	2.03	0.57
1:A:95:ASN:O	1:A:96:ARG:HD3	2.05	0.57
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.87	0.56
1:A:365:TYR:CE1	1:A:397:ARG:HB3	2.41	0.56
1:A:191:LEU:H	1:A:191:LEU:HD23	1.71	0.55
1:A:117:THR:OG1	1:A:162:ARG:O	2.23	0.55
1:A:272:GLU:O	1:A:276:LEU:HB2	2.06	0.55
1:A:71:ARG:NH1	1:A:71:ARG:CG	2.68	0.54
1:A:272:GLU:HG3	1:A:276:LEU:HD22	1.89	0.54
1:A:451:SER:HA	9:A:696:HOH:O	2.08	0.53
1:A:14:LYS:HG3	1:A:15:CYS:N	2.23	0.53
1:A:169:THR:OG1	1:A:170:PRO:CD	2.57	0.53
1:A:578:ASP:C	1:A:580:SER:N	2.61	0.53
1:A:484:TYR:O	1:A:485:LYS:HB2	2.08	0.53
1:A:422:PHE:HB2	1:A:429:HIS:CD2	2.44	0.53
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.91	0.52
1:A:288:ASN:O	1:A:292:LEU:HD23	2.10	0.52
1:A:567:PHE:HD2	6:A:617:IOD:I	2.63	0.52
1:A:64:ARG:C	1:A:64:ARG:HD3	2.30	0.52
1:A:127:THR:HA	1:A:130:GLU:HB2	1.91	0.52
1:A:16:ASP:OD1	1:A:16:ASP:C	2.48	0.52
1:A:123:GLU:HG2	1:A:125:SER:HB2	1.92	0.52
1:A:407:MET:HB3	1:A:501:MET:CE	2.40	0.52
1:A:33:SER:CB	9:A:896:HOH:O	2.36	0.51
1:A:16:ASP:HB2	9:A:816:HOH:O	2.09	0.51
1:A:110:ASP:OD2	1:A:189:ALA:N	2.43	0.51
1:A:9:PRO:HG3	9:A:708:HOH:O	2.11	0.51
1:A:360:ARG:HH12	1:A:372:ALA:HA	1.76	0.51
1:A:128:GLN:NE2	9:A:820:HOH:O	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:106:ILE:HD11	1:A:265:ALA:CB	2.36	0.51
1:A:146:LYS:HE3	1:A:147:ASN:HD21	1.76	0.51
1:A:166:VAL:O	1:A:167:CYS:HB2	2.10	0.50
1:A:578:ASP:O	1:A:580:SER:N	2.45	0.50
1:A:333:ASN:HD22	1:A:333:ASN:C	2.15	0.50
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.93	0.50
1:A:9:PRO:O	1:A:11:PRO:CD	2.57	0.50
1:A:362:ASP:OD1	1:A:362:ASP:C	2.51	0.49
1:A:172:TYR:CD1	1:A:173:GLN:N	2.80	0.49
1:A:16:ASP:OD1	1:A:16:ASP:O	2.31	0.49
1:A:385:ARG:O	1:A:389:ASP:HB2	2.13	0.49
1:A:347:PHE:HB3	7:A:618:HEM:CMD	2.43	0.49
1:A:565:HIS:HB3	6:A:617:IOD:I	2.83	0.48
1:A:235:SER:HB3	1:A:238:GLU:HB2	1.94	0.48
1:A:118[A]:GLU:OE2	1:A:120:GLY:N	2.38	0.48
1:A:588:SER:C	1:A:590:TRP:H	2.16	0.48
1:A:268:LEU:CD1	1:A:392:ILE:HD12	2.42	0.48
1:A:580:SER:C	1:A:581:THR:HG1	2.17	0.48
1:A:392:ILE:O	1:A:396:VAL:HG23	2.13	0.48
1:A:165:PHE:CB	1:A:177:ARG:HD2	2.44	0.48
1:A:368:TRP:O	1:A:368:TRP:CE3	2.66	0.48
1:A:82:ILE:CG2	1:A:494:ILE:HD11	2.44	0.48
1:A:169:THR:OG1	1:A:170:PRO:HD3	2.14	0.48
1:A:257:SER:O	1:A:381:PHE:HA	2.14	0.47
1:A:188:ASP:O	1:A:189:ALA:HB3	2.14	0.47
1:A:165:PHE:CG	1:A:177:ARG:HD2	2.50	0.47
1:A:301:GLY:O	1:A:305:GLN:HG3	2.15	0.47
1:A:354:VAL:HA	1:A:355:PRO:HD3	1.79	0.47
1:A:287:TRP:CE2	1:A:291:LYS:HD3	2.49	0.47
1:A:255:ARG:HG2	6:A:608:IOD:I	2.85	0.47
1:A:567:PHE:HB2	6:A:617:IOD:I	2.85	0.47
1:A:30:ASN:O	1:A:34:PRO:HA	2.15	0.46
1:A:82:ILE:HD11	1:A:483:LEU:HD12	1.96	0.46
1:A:248:CYS:HB3	1:A:257:SER:OG	2.16	0.46
1:A:288:ASN:O	1:A:292:LEU:CD2	2.64	0.46
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.51	0.46
1:A:105:GLN:NE2	7:A:618:HEM:C4B	2.84	0.45
1:A:58:PRO:HG3	1:A:162:ARG:NH2	2.31	0.45
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.51	0.45
1:A:543:SER:OG	1:A:586:ASP:O	2.25	0.45
1:A:578:ASP:O	1:A:581:THR:HB	2.17	0.45
2:A:602:NAG:H4	2:A:603:MAN:H2	1.61	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:200:ALA:O	1:A:204:ARG:HG3	2.18	0.44
1:A:440:ARG:O	1:A:440:ARG:HG3	2.18	0.44
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.29	0.44
1:A:169:THR:HA	9:A:874:HOH:O	2.18	0.44
1:A:77:GLU:HB2	1:A:145:PRO:HG3	2.00	0.43
1:A:124:HIS:HA	1:A:127:THR:HB	1.99	0.43
1:A:468:GLN:O	1:A:472:LYS:N	2.51	0.43
1:A:63:GLN:HB2	9:A:805:HOH:O	2.18	0.43
1:A:57:LEU:HA	1:A:58:PRO:HD3	1.84	0.43
1:A:82:ILE:CD1	1:A:483:LEU:HD12	2.48	0.42
1:A:253:ASP:OD2	1:A:255:ARG:HD3	2.19	0.42
1:A:480:LEU:HA	1:A:480:LEU:HD12	1.76	0.42
1:A:276:LEU:HD12	1:A:587:LEU:HD11	2.01	0.42
1:A:393:ASP:OD1	1:A:557:THR:HB	2.20	0.42
1:A:292:LEU:HD13	1:A:292:LEU:HA	1.88	0.42
1:A:407:MET:HB3	1:A:501:MET:HE3	2.02	0.42
1:A:113:PHE:HB3	1:A:183:VAL:HG13	2.02	0.42
1:A:478:LYS:HE2	1:A:478:LYS:HB3	1.82	0.41
1:A:15:CYS:HA	9:A:684:HOH:O	2.21	0.41
1:A:63:GLN:O	1:A:71:ARG:NH1	2.53	0.41
1:A:441:CYS:HB3	9:A:672:HOH:O	2.19	0.41
1:A:425:THR:HB	1:A:426:HIS:ND1	2.35	0.41
1:A:25:THR:O	1:A:184:THR:HG22	2.21	0.41
1:A:179:GLN:HG2	1:A:444:HIS:CE1	2.56	0.41
1:A:377:HIS:HB3	1:A:416:GLU:OE2	2.21	0.41
1:A:347:PHE:HB3	7:A:618:HEM:HMD1	2.03	0.41
1:A:350:GLY:HA3	7:A:618:HEM:CBC	2.50	0.41
1:A:260:ILE:HG23	1:A:261:LEU:N	2.36	0.41
1:A:24:ILE:HA	1:A:24:ILE:HD13	1.83	0.41
1:A:261:LEU:HA	1:A:261:LEU:HD12	1.90	0.40
1:A:123:GLU:C	1:A:125:SER:N	2.75	0.40
1:A:287:TRP:CD2	1:A:291:LYS:HD3	2.56	0.40
1:A:12:LEU:O	1:A:13:VAL:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	593/595 (100%)	541 (91%)	40 (7%)	12 (2%)	11	28

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	167	CYS
1	A	168	PRO
1	A	176	ALA
1	A	169	THR
1	A	175	LEU
1	A	581	THR
1	A	3	GLU
1	A	589	PRO
1	A	579	CYS
1	A	209	PRO
1	A	171	PRO

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	518/517 (100%)	460 (89%)	58 (11%)	9	20

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	4	VAL
1	A	9	PRO
1	A	10	VAL
1	A	13	VAL
1	A	17	GLU
1	A	55	LEU
1	A	57	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	64	ARG
1	A	71	ARG
1	A	74	LEU
1	A	91	VAL
1	A	98	LEU
1	A	117	THR
1	A	118[A]	GLU
1	A	118[B]	GLU
1	A	119	LEU
1	A	121	SER
1	A	123	GLU
1	A	127	THR
1	A	130	GLU
1	A	146	LYS
1	A	153	THR
1	A	169	THR
1	A	171	PRO
1	A	173	GLN
1	A	174	SER
1	A	175	LEU
1	A	177	ARG
1	A	203	LEU
1	A	255	ARG
1	A	261	LEU
1	A	276	LEU
1	A	279	GLU
1	A	292	LEU
1	A	317	LEU
1	A	322	GLN
1	A	323	LYS
1	A	333	ASN
1	A	347	PHE
1	A	360	ARG
1	A	376	LEU
1	A	464	LEU
1	A	465	LYS
1	A	480	LEU
1	A	494	ILE
1	A	511	LEU
1	A	520	GLN
1	A	523	ARG
1	A	539	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	552	LEU
1	A	561	LYS
1	A	564	LEU
1	A	568	GLN
1	A	579	CYS
1	A	580	SER
1	A	587	LEU
1	A	593	ARG

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	40	ASN
1	A	322	GLN
1	A	329	GLN
1	A	333	ASN
1	A	341	ASN
1	A	364	ASN
1	A	423	GLN
1	A	426	HIS
1	A	497	ASN
1	A	545	GLN
1	A	574	HIS

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	6.55	2 (22%)	10,12,14	2.02	3 (30%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	O-C	18.93	1.24	1.11
1	A	198	SEP	CA-C	4.59	1.57	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	P-OG-CB	3.17	127.37	118.19
1	A	198	SEP	C-CA-N	-3.08	110.75	113.83
1	A	198	SEP	O2P-P-O1P	-2.26	103.04	110.44

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
2	NAG	A	596	1,2	12,14,15	0.61	0	15,19,21	1.93	3 (20%)
2	NAG	A	597	2	12,14,15	0.55	0	15,19,21	0.99	0
2	MAN	A	598	2	10,11,12	0.60	0	11,15,17	1.24	1 (9%)
3	NAG	A	599	1,3	12,14,15	0.76	1 (8%)	15,19,21	1.04	1 (6%)
3	NAG	A	600	3	12,14,15	0.74	1 (8%)	15,19,21	1.59	3 (20%)
2	NAG	A	601	1,2	12,14,15	0.81	1 (8%)	15,19,21	1.70	4 (26%)
2	NAG	A	602	2	12,14,15	0.55	0	15,19,21	1.34	2 (13%)
2	MAN	A	603	2	10,11,12	0.64	0	11,15,17	1.60	3 (27%)
3	NAG	A	604	1,3	12,14,15	0.92	1 (8%)	15,19,21	1.68	4 (26%)
3	NAG	A	605	3	12,14,15	0.76	1 (8%)	15,19,21	1.24	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
2	NAG	A	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	597	2	-	0/6/23/26	0/1/1/1
2	MAN	A	598	2	-	0/2/19/22	0/1/1/1
3	NAG	A	599	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	600	3	-	0/6/23/26	0/1/1/1
2	NAG	A	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	2	-	0/6/23/26	0/1/1/1
2	MAN	A	603	2	-	0/2/19/22	0/1/1/1
3	NAG	A	604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	605	3	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	NAG	O5-C5	-2.63	1.40	1.45
3	A	605	NAG	O5-C5	-2.25	1.41	1.45
2	A	601	NAG	O5-C5	-2.18	1.41	1.45
3	A	599	NAG	O5-C5	-2.04	1.41	1.45
3	A	600	NAG	O5-C5	-2.01	1.41	1.45

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	596	NAG	O5-C5-C6	5.17	112.40	106.98
2	A	601	NAG	O5-C5-C6	3.87	111.04	106.98
2	A	603	MAN	O5-C5-C6	3.55	110.71	106.98
2	A	598	MAN	O5-C5-C6	3.54	110.69	106.98
2	A	602	NAG	O5-C5-C6	3.51	110.67	106.98
3	A	605	NAG	O5-C5-C6	3.43	110.58	106.98
2	A	596	NAG	C3-C4-C5	-3.37	104.19	110.20
3	A	604	NAG	O5-C5-C4	-3.11	106.71	110.65
2	A	602	NAG	O5-C5-C4	3.07	114.54	110.65
3	A	604	NAG	C4-C3-C2	3.02	118.72	111.32
2	A	601	NAG	O4-C4-C3	-2.98	103.68	110.35
3	A	600	NAG	C3-C2-N2	-2.96	107.25	111.76
3	A	600	NAG	C2-N2-C7	-2.89	118.24	123.09
2	A	596	NAG	O4-C4-C5	2.64	116.23	109.28
2	A	601	NAG	C3-C2-N2	-2.40	108.10	111.76
2	A	603	MAN	C4-C3-C2	-2.36	107.34	110.50
2	A	603	MAN	C3-C4-C5	-2.33	106.05	110.20
3	A	599	NAG	C3-C2-N2	-2.30	108.25	111.76
3	A	600	NAG	O5-C5-C6	2.30	109.40	106.98
3	A	604	NAG	C3-C2-N2	-2.19	108.42	111.76
2	A	601	NAG	C2-N2-C7	-2.12	119.53	123.09
3	A	604	NAG	O4-C4-C3	2.05	114.95	110.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 11 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	$\# Z > 2$
5	SCN	A	607	-	2,2,2	1.72	1 (50%)	1,1,1	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	HEM	A	618	1,9	49,50,50	2.69	14 (28%)	46,82,82	1.65	8 (17%)
8	CAQ	A	619	-	8,8,8	1.98	1 (12%)	10,10,10	2.00	3 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SCN	A	607	-	-	0/0/0/0	0/0/0/0
7	HEM	A	618	1,9	-	0/14/114/114	0/0/8/8
8	CAQ	A	619	-	-	0/0/0/0	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	618	HEM	C3D-C4D	11.35	1.47	1.44
7	A	618	HEM	C3B-C2B	-6.71	1.32	1.43
8	A	619	CAQ	C4-C3	5.37	1.50	1.40
7	A	618	HEM	C3D-C2D	4.96	1.52	1.43
7	A	618	HEM	C3C-CAC	4.80	1.55	1.40
7	A	618	HEM	C3C-C2C	-4.53	1.35	1.43
7	A	618	HEM	C3B-CAB	4.38	1.54	1.40
7	A	618	HEM	FE-NC	3.48	2.10	1.97
7	A	618	HEM	C4A-C3A	3.40	1.44	1.40
7	A	618	HEM	C2B-C1B	3.21	1.45	1.44
7	A	618	HEM	CMC-C2C	2.60	1.55	1.47
7	A	618	HEM	CAA-C2A	2.59	1.56	1.52
5	A	607	SCN	C-S	2.43	1.79	1.63
7	A	618	HEM	FE-NB	2.36	2.06	1.97
7	A	618	HEM	CMB-C2B	2.25	1.54	1.47
7	A	618	HEM	CMD-C2D	2.10	1.53	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	618	HEM	C3B-C4B-NB	-6.52	109.34	114.00
7	A	618	HEM	C4D-ND-C1D	4.07	109.32	105.16
8	A	619	CAQ	C5-C4-C3	-3.73	114.87	119.74
7	A	618	HEM	CAD-C3D-C4D	2.80	129.56	124.53
8	A	619	CAQ	C1-C6-C5	2.78	124.81	120.17
7	A	618	HEM	C4A-C3A-C2A	2.70	108.88	107.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	618	HEM	CBD-CAD-C3D	-2.50	108.92	114.37
8	A	619	CAQ	O3-C3-C4	2.34	124.00	118.30
7	A	618	HEM	O1A-CGA-CBA	-2.19	115.50	123.03
7	A	618	HEM	CMA-C3A-C4A	-2.18	125.28	128.62
7	A	618	HEM	O2A-CGA-CBA	2.14	121.78	114.22

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, 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	595/595 (100%)	-0.32	30 (5%)	28 30	12, 27, 69, 106	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	9.9
1	A	174	SER	8.4
1	A	1	SER	6.9
1	A	121	SER	6.2
1	A	120	GLY	5.7
1	A	171	PRO	5.2
1	A	8	ALA	5.1
1	A	595	ASN	5.0
1	A	170	PRO	4.9
1	A	4	VAL	4.5
1	A	124	HIS	4.3
1	A	172	TYR	4.2
1	A	7	GLY	4.0
1	A	173	GLN	3.9
1	A	126	LYS	3.8
1	A	594	GLU	3.8
1	A	9	PRO	3.8
1	A	125	SER	3.7
1	A	593	ARG	3.7
1	A	122	ASN	3.7
1	A	13	VAL	3.6
1	A	123	GLU	3.4
1	A	3	GLU	3.1
1	A	175	LEU	3.1
1	A	12	LEU	3.0
1	A	119	LEU	2.9
1	A	134	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	132	TYR	2.3
1	A	369	GLY	2.3
1	A	5	GLY	2.2

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	A	198	10/11	0.16	0.38	20,27,28,30	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	597	14/15	0.56	17.68	76,82,84,87	0
3	NAG	A	604	14/15	0.22	3.85	51,60,63,67	0
2	NAG	A	596	14/15	0.28	3.44	47,53,61,68	0
2	NAG	A	602	14/15	0.29	2.54	67,73,76,82	0
3	NAG	A	599	14/15	0.17	0.99	42,44,47,49	0
2	NAG	A	601	14/15	0.15	0.13	44,47,54,59	0
3	NAG	A	600	14/15	0.28	-	53,58,61,61	0
3	NAG	A	605	14/15	0.48	-	70,73,75,77	0
2	MAN	A	598	11/12	0.45	-	91,92,93,94	0
2	MAN	A	603	11/12	0.42	-	86,89,91,92	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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	CAQ	A	619	8/8	0.47	139.30	36,37,39,41	0
6	IOD	A	617	1/1	0.16	1.47	99,99,99,99	0
5	SCN	A	607	3/3	0.16	1.14	18,18,18,20	0
6	IOD	A	609	1/1	0.16	0.01	98,98,98,98	0
7	HEM	A	618	43/43	0.11	-0.39	8,16,18,25	0
4	CA	A	606	1/1	0.09	-1.09	17,17,17,17	0
6	IOD	A	611	1/1	0.05	-1.39	86,86,86,86	0
6	IOD	A	612	1/1	0.05	-1.72	99,99,99,99	0
6	IOD	A	610	1/1	0.06	-2.14	21,21,21,21	0
6	IOD	A	616	1/1	0.05	-2.45	54,54,54,54	0
6	IOD	A	608	1/1	0.07	-3.03	65,65,65,65	0
6	IOD	A	613	1/1	0.03	-3.10	59,59,59,59	0
6	IOD	A	614	1/1	0.04	-4.16	77,77,77,77	0
6	IOD	A	615	1/1	0.02	-4.67	58,58,58,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.