WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2017 – 06:05 pm GMT

PDB ID : 3V6Q

Title : Crystal structure of the complex of bovine lactoperoxidase with Carbon monoxide at 2.0 A resolution

Authors : Yamini, S.; Singh, A.K.; Pandey, N.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.

Deposited on : 2011-12-20

Resolution : 2.00 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

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 2.00 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	Percentile Ranks	Value
Rfree		0.272
Clashscore		12
Ramachandran outliers		0.7%
Sidechain outliers		0.8%
RSRZ outliers		9.3%

Worse — Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
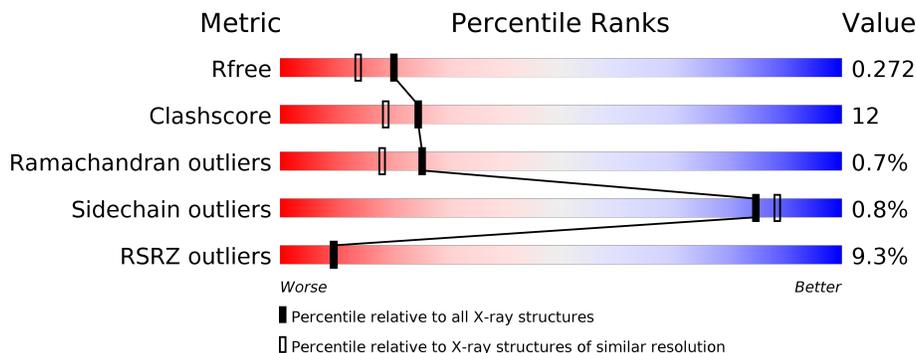
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	9% / 79% / 20% / •

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
11	CMO	A	621	-	-	X	-
6	IOD	A	614	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	IOD	A	615	-	-	X	-
8	MPD	A	617	-	-	-	X
9	EDO	A	619	-	-	-	X

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 5417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total 4774	C 3037	N 847	O 863	P 1	S 26	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
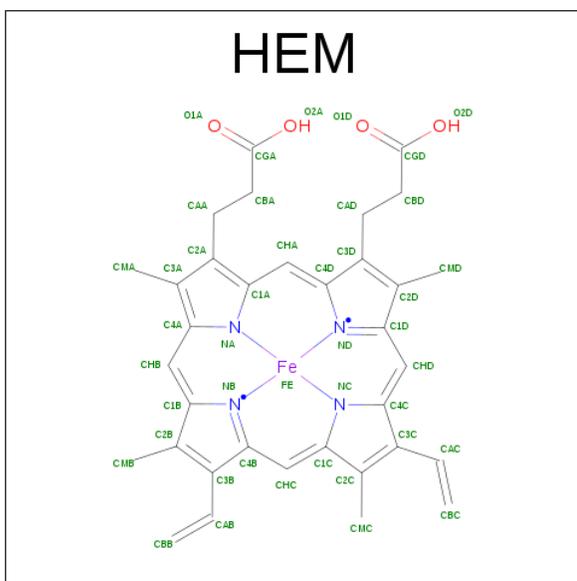
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
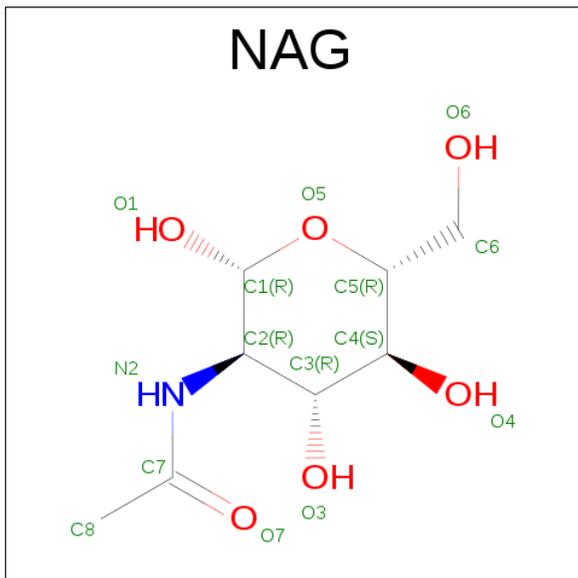
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total 9	I 9	0	0

- Molecule 7 is BROMIDE ION (three-letter code: BR) (formula: Br).

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

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:

$C_6H_{14}O_2$).

MPD

(chemical structure diagram showing MPD with atoms O4, OH, C1, C5, C4(S), C3, C2, CM, OH, O2)
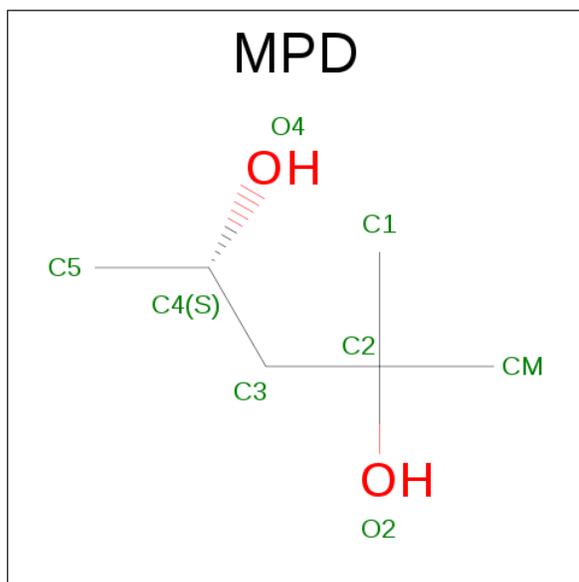
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 8	C 6	O 2	0	0

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

(chemical structure diagram showing EDO with atoms O2, OH, C1, C2, HO, O1)
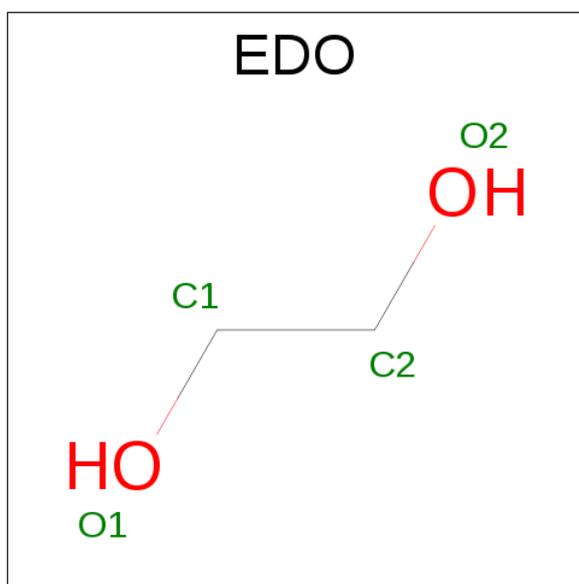
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 4	C 2	O 2	0	0
9	A	1	Total 4	C 2	O 2	0	0

• Molecule 10 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).
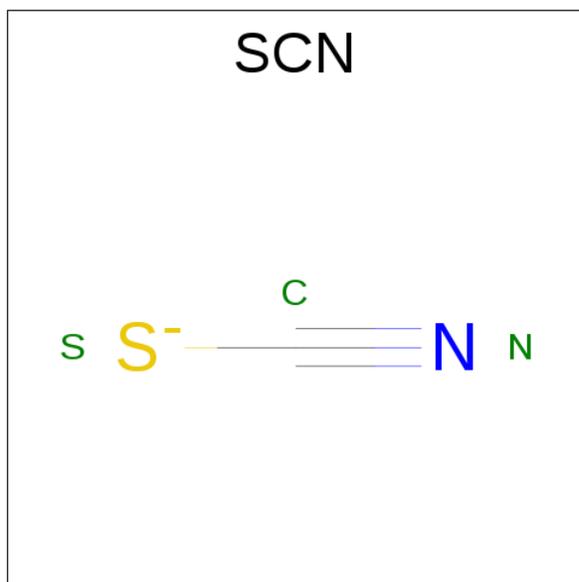
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total 3	C 1	N 1	S 1	0	0

• Molecule 11 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).
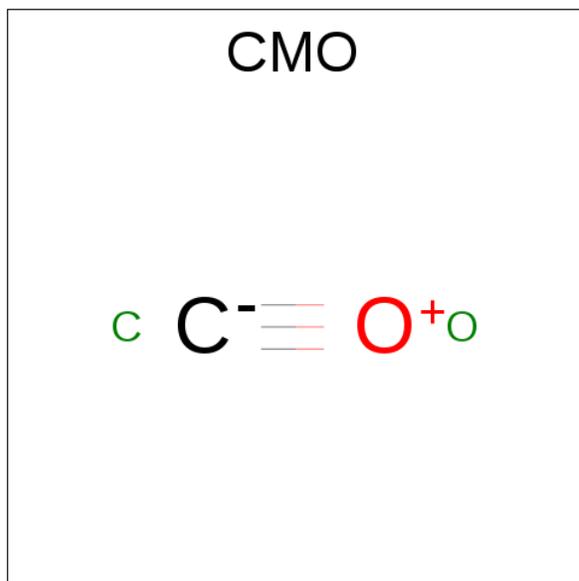
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total 2	C 1	O 1	0	0

• Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	512	Total 512	O 512	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 the various outlier classes 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
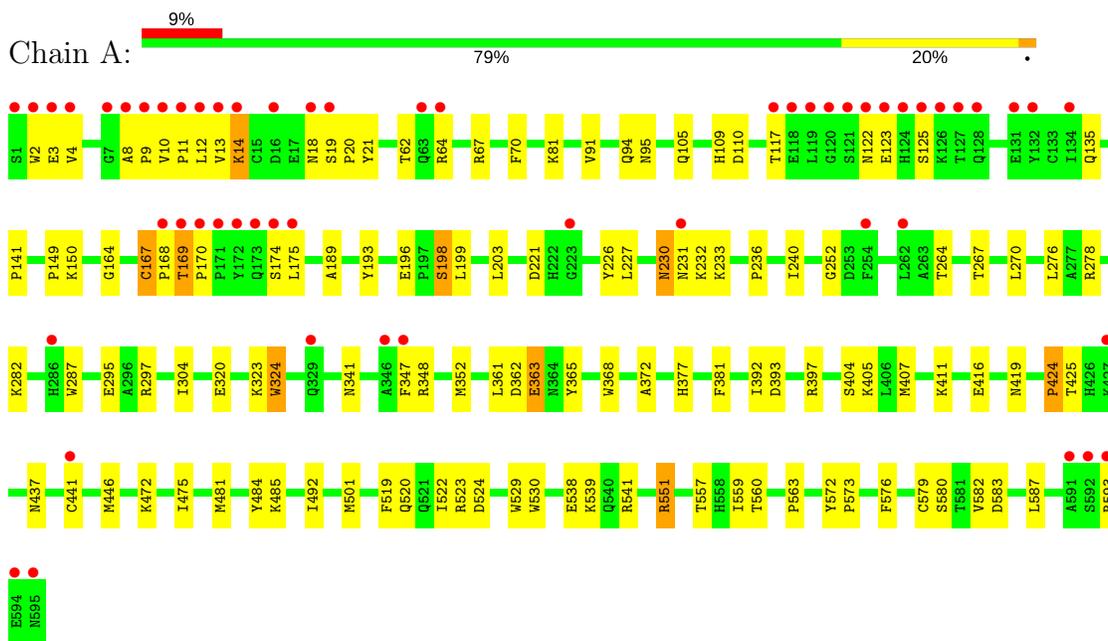
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.30Å 80.00Å 76.55Å 90.00° 103.02° 90.00°	Depositor
Resolution (Å)	44.13 – 2.00 44.13 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.13-2.00) 99.6 (44.13-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.191 , 0.248 0.230 , 0.272	Depositor DCC
R_{free} test set	2159 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5417	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: CMO, MPD, SCN, NAG, SEP, CA, EDO, BR, HEM, IOD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	1.21	3/4891 (0.1%)	0.97	21/6634 (0.3%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	TRP	CB-CG	-5.83	1.39	1.50
1	A	404	SER	CB-OG	5.31	1.49	1.42
1	A	320	GLU	CD-OE1	-5.04	1.20	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	MET	CB-CA-C	-12.85	84.69	110.40
1	A	174	SER	CB-CA-C	-7.74	95.40	110.10
1	A	231	ASN	CB-CA-C	-7.51	95.37	110.40
1	A	593	ARG	N-CA-C	-7.46	90.85	111.00
1	A	240	ILE	CB-CA-C	7.27	126.14	111.60
1	A	230	ASN	CB-CA-C	7.08	124.55	110.40
1	A	10	VAL	C-N-CD	-6.99	105.23	120.60
1	A	231	ASN	N-CA-C	6.93	129.71	111.00
1	A	2	TRP	N-CA-C	6.88	129.59	111.00
1	A	230	ASN	C-N-CA	6.69	138.41	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	LYS	N-CA-C	6.67	129.00	111.00
1	A	110	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	81	LYS	CB-CA-C	6.06	122.52	110.40
1	A	67	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	A	582	VAL	CB-CA-C	5.43	121.71	111.40
1	A	169	THR	CB-CA-C	-5.41	96.99	111.60
1	A	472	LYS	CB-CA-C	5.41	121.21	110.40
1	A	174	SER	N-CA-C	5.33	125.40	111.00
1	A	524	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	551	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	484	TYR	C-N-CA	-5.02	109.16	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	SEP	Mainchain
1	A	230	ASN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4687	115	0
2	A	43	0	30	3	0
3	A	1	0	0	0	0
4	A	28	0	26	0	0
5	A	28	0	25	0	0
6	A	9	0	0	5	0
7	A	1	0	0	0	0
8	A	8	0	13	4	0
9	A	8	0	12	2	0
10	A	3	0	0	0	0
11	A	2	0	0	2	0
12	A	512	0	0	1	0
All	All	5417	0	4793	119	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 12.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:CB	1:A:13:VAL:HA	1.61	1.28
1:A:12:LEU:HB3	1:A:13:VAL:CA	1.71	1.20
1:A:12:LEU:CB	1:A:13:VAL:CA	2.30	1.06
1:A:227:LEU:HD22	1:A:270:LEU:CD2	1.87	1.03
1:A:167:CYS:CB	1:A:168:PRO:HD2	1.89	1.02
1:A:168:PRO:HB2	1:A:170:PRO:HD2	1.39	1.01
1:A:227:LEU:CD2	1:A:270:LEU:HD22	1.90	1.01
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.42	0.98
1:A:227:LEU:HD22	1:A:270:LEU:HD22	0.99	0.97
1:A:167:CYS:CB	1:A:168:PRO:CD	2.42	0.96
1:A:12:LEU:HB2	1:A:13:VAL:HB	1.53	0.90
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.01	0.89
1:A:9:PRO:HD3	1:A:167:CYS:O	1.74	0.87
1:A:3:GLU:HB2	1:A:175:LEU:HD22	1.57	0.84
1:A:3:GLU:CD	1:A:4:VAL:H	1.81	0.83
1:A:551:ARG:HD3	1:A:583:ASP:O	1.80	0.82
1:A:12:LEU:HB2	1:A:13:VAL:CB	2.09	0.80
1:A:91:VAL:HG12	1:A:405:LYS:HG3	1.66	0.77
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.65	0.77
1:A:12:LEU:HB3	1:A:13:VAL:HA	0.79	0.75
1:A:522:ILE:HD12	1:A:522:ILE:C	2.09	0.73
1:A:3:GLU:HB2	1:A:175:LEU:CD2	2.20	0.71
1:A:19:SER:O	1:A:21:TYR:N	2.22	0.70
1:A:236:PRO:HG3	1:A:424:PRO:HB3	1.74	0.70
1:A:227:LEU:N	1:A:227:LEU:HD23	2.07	0.69
1:A:117:THR:HG22	1:A:164:GLY:HA2	1.75	0.68
1:A:123:GLU:C	1:A:125:SER:H	1.95	0.68
1:A:94:GLN:C	1:A:95:ASN:HD22	1.98	0.67
1:A:12:LEU:HB2	1:A:13:VAL:CA	2.24	0.66
2:A:601:HEM:HBC2	2:A:601:HEM:HMC1	1.76	0.65
1:A:362:ASP:OD1	1:A:362:ASP:C	2.35	0.65
1:A:522:ILE:HD12	1:A:523:ARG:N	2.13	0.64
1:A:381:PHE:CZ	1:A:424:PRO:HG3	2.33	0.64
1:A:199:LEU:HA	8:A:617:MPD:HM2	1.81	0.63
1:A:227:LEU:CD2	1:A:270:LEU:CD2	2.64	0.63
1:A:169:THR:N	1:A:170:PRO:CD	2.62	0.62
1:A:278:ARG:O	1:A:282:LYS:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:OG1	1:A:170:PRO:HD3	2.00	0.62
1:A:12:LEU:CB	1:A:13:VAL:CB	2.72	0.61
1:A:580:SER:CB	6:A:615:IOD:I	3.19	0.61
1:A:3:GLU:CG	1:A:4:VAL:N	2.64	0.60
1:A:323:LYS:HE3	1:A:324:TRP:CZ2	2.38	0.59
1:A:368:TRP:O	1:A:372:ALA:HB2	2.03	0.58
1:A:122:ASN:CG	1:A:122:ASN:O	2.42	0.57
1:A:123:GLU:C	1:A:125:SER:N	2.57	0.57
1:A:3:GLU:OE1	1:A:3:GLU:HA	2.05	0.57
1:A:377:HIS:CD2	9:A:618:EDO:H21	2.41	0.56
1:A:530:TRP:CZ3	1:A:541:ARG:HG2	2.41	0.55
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.42	0.55
1:A:377:HIS:ND1	1:A:416:GLU:OE2	2.35	0.54
1:A:425:THR:O	1:A:425:THR:HG22	2.08	0.54
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.71	0.53
1:A:149:PRO:HB2	6:A:614:IOD:I	2.79	0.53
1:A:12:LEU:CD1	1:A:13:VAL:HG23	2.38	0.53
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.44	0.52
1:A:3:GLU:CD	1:A:4:VAL:N	2.56	0.52
1:A:377:HIS:HD2	9:A:618:EDO:H21	1.73	0.51
1:A:323:LYS:HE3	1:A:324:TRP:CE2	2.46	0.51
1:A:91:VAL:CG2	1:A:411:LYS:HD3	2.41	0.51
1:A:18:ASN:O	1:A:19:SER:C	2.49	0.50
1:A:199:LEU:CA	8:A:617:MPD:HM2	2.42	0.50
1:A:199:LEU:HB2	8:A:617:MPD:HM2	1.93	0.50
1:A:352:MET:CB	1:A:407:MET:HG2	2.42	0.50
1:A:393:ASP:OD1	1:A:557:THR:HB	2.11	0.50
1:A:193:TYR:OH	1:A:297:ARG:HA	2.11	0.50
1:A:441:CYS:SG	1:A:492:ILE:HG22	2.52	0.50
1:A:580:SER:HB3	6:A:615:IOD:I	2.82	0.50
1:A:122:ASN:ND2	1:A:122:ASN:O	2.44	0.49
1:A:407:MET:HB3	1:A:501:MET:CE	2.43	0.49
1:A:362:ASP:OD1	1:A:363:GLU:N	2.46	0.48
1:A:580:SER:HB2	6:A:615:IOD:I	2.83	0.48
1:A:352:MET:HB2	1:A:407:MET:HG2	1.95	0.47
1:A:91:VAL:HG22	1:A:411:LYS:CD	2.44	0.47
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.12	0.47
1:A:3:GLU:HG3	1:A:4:VAL:N	2.29	0.47
1:A:3:GLU:CG	1:A:4:VAL:H	2.23	0.47
2:A:601:HEM:CMB	2:A:601:HEM:HBB2	2.44	0.47
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:VAL:HG22	1:A:411:LYS:HD3	1.97	0.46
1:A:62:THR:HG22	1:A:64:ARG:HG2	1.97	0.46
1:A:559:ILE:HG23	6:A:611:IOD:I	2.85	0.46
1:A:8:ALA:HB3	1:A:167:CYS:HA	1.98	0.46
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.51	0.46
1:A:407:MET:HE3	1:A:407:MET:C	2.37	0.45
1:A:168:PRO:CB	1:A:170:PRO:HD2	2.28	0.45
1:A:538:GLU:HG3	1:A:539:LYS:N	2.32	0.44
1:A:196:GLU:HB3	1:A:198:SEP:O3P	2.18	0.44
1:A:362:ASP:O	1:A:365:TYR:N	2.44	0.44
1:A:3:GLU:CB	1:A:175:LEU:CD2	2.93	0.44
1:A:227:LEU:N	1:A:227:LEU:CD2	2.79	0.44
1:A:276:LEU:HD23	1:A:587:LEU:HD11	2.00	0.44
1:A:150:LYS:NZ	1:A:419:ASN:O	2.45	0.43
1:A:227:LEU:HD21	1:A:267:THR:HA	2.00	0.43
1:A:70:PHE:CG	1:A:485:LYS:HB2	2.54	0.43
1:A:109:HIS:NE2	11:A:621:CMO:O	2.49	0.43
1:A:560:THR:HA	1:A:579:CYS:SG	2.59	0.43
1:A:13:VAL:HG22	1:A:14:LYS:N	2.33	0.43
1:A:9:PRO:CD	1:A:167:CYS:O	2.57	0.43
1:A:441:CYS:SG	1:A:446:MET:HG3	2.58	0.42
1:A:105:GLN:HE21	11:A:621:CMO:C	2.33	0.42
1:A:12:LEU:HD12	1:A:13:VAL:HG23	2.01	0.42
1:A:95:ASN:N	1:A:95:ASN:HD22	2.16	0.42
1:A:135:GLN:HB2	1:A:141:PRO:HD2	2.02	0.41
1:A:232:LYS:HG3	1:A:233:LYS:N	2.35	0.41
1:A:361:LEU:O	1:A:397:ARG:HD2	2.20	0.41
1:A:522:ILE:CD1	1:A:522:ILE:C	2.84	0.41
1:A:19:SER:C	1:A:21:TYR:H	2.16	0.41
1:A:287:TRP:CZ3	1:A:295:GLU:HG2	2.55	0.41
1:A:519:PHE:HA	1:A:522:ILE:HG13	2.02	0.41
1:A:563:PRO:HD3	1:A:576:PHE:CD2	2.55	0.41
1:A:9:PRO:HG3	12:A:704:HOH:O	2.20	0.41
1:A:264:THR:HG23	1:A:392:ILE:HB	2.02	0.41
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.46	0.41
1:A:341:ASN:HB3	1:A:446:MET:CE	2.51	0.41
1:A:175:LEU:HD12	1:A:175:LEU:HA	1.75	0.40
1:A:203:LEU:HD11	1:A:252:GLY:HA2	2.04	0.40
1:A:572:TYR:CG	1:A:573:PRO:HA	2.57	0.40
1:A:3:GLU:OE1	1:A:3:GLU:CA	2.65	0.40
8:A:617:MPD:H4	8:A:617:MPD:HM1	1.90	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%)	568 (96%)	20 (3%)	4 (1%)	25	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	PRO
1	A	167	CYS
1	A	11	PRO
1	A	424	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/517 (100%)	513 (99%)	4 (1%)	85	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	347	PHE
1	A	363	GLU
1	A	475	ILE
1	A	520	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	128	GLN
1	A	138	ASN
1	A	364	ASN
1	A	426	HIS
1	A	468	GLN
1	A	497	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	SEP	A	198	1	9,9,10	0.67	0	9,12,14	1.31	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	198	1	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	SEP	O-C-CA	-2.36	118.51	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates ⓘ

2 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	NAG	A	604	1,5	14,14,15	0.71	0	15,19,21	1.70	4 (26%)
5	NAG	A	605	5	14,14,15	0.93	0	15,19,21	2.67	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	604	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	605	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	605	NAG	O5-C1-C2	-3.94	105.99	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	604	NAG	O4-C4-C3	-3.38	103.01	110.36
5	A	605	NAG	C4-C3-C2	-3.00	106.62	111.02
5	A	604	NAG	O6-C6-C5	-2.31	103.56	111.34
5	A	604	NAG	O3-C3-C2	-2.26	104.54	109.39
5	A	605	NAG	O3-C3-C4	-2.18	105.62	110.36
5	A	604	NAG	C2-N2-C7	3.12	127.50	122.94
5	A	605	NAG	C1-O5-C5	8.01	123.21	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 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	601	1,11	28,50,50	1.75	6 (21%)	17,82,82	2.25	8 (47%)
4	NAG	A	603	1	14,14,15	0.99	1 (7%)	15,19,21	1.52	5 (33%)
4	NAG	A	606	1	14,14,15	0.69	0	15,19,21	1.22	1 (6%)
8	MPD	A	617	-	7,7,7	4.39	3 (42%)	9,10,10	1.23	1 (11%)
9	EDO	A	618	-	3,3,3	1.08	0	2,2,2	1.30	0
9	EDO	A	619	-	3,3,3	0.62	0	2,2,2	1.20	0
10	SCN	A	620	-	1,2,2	1.06	0	0,1,1	0.00	-
11	CMO	A	621	2	0,1,1	0.00	-	0,0,0	0.00	-

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	601	1,11	-	0/6/54/54	0/0/8/8
4	NAG	A	603	1	-	0/6/23/26	0/1/1/1
4	NAG	A	606	1	-	0/6/23/26	0/1/1/1
8	MPD	A	617	-	-	0/5/5/5	0/0/0/0
9	EDO	A	618	-	-	0/1/1/1	0/0/0/0
9	EDO	A	619	-	-	0/1/1/1	0/0/0/0
10	SCN	A	620	-	-	0/0/0/0	0/0/0/0
11	CMO	A	621	2	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	617	MPD	C1-C2	-7.33	1.28	1.52
8	A	617	MPD	O2-C2	-6.46	1.27	1.44
8	A	617	MPD	CM-C2	-5.91	1.32	1.52
2	A	601	HEM	C3B-C2B	-3.16	1.36	1.40
2	A	601	HEM	C3C-C2C	-3.15	1.36	1.40
4	A	603	NAG	O7-C7	2.08	1.28	1.23
2	A	601	HEM	CMC-C2C	2.66	1.57	1.51
2	A	601	HEM	C3B-CAB	3.19	1.54	1.47
2	A	601	HEM	C3D-C2D	3.72	1.48	1.37
2	A	601	HEM	C3C-CAC	4.31	1.56	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	CBA-CAA-C2A	-4.42	104.03	112.48
2	A	601	HEM	CAD-CBD-CGD	-3.92	105.97	112.66
2	A	601	HEM	CBD-CAD-C3D	-3.45	105.89	112.47
2	A	601	HEM	C3B-C4B-NB	-3.35	104.88	109.21
4	A	606	NAG	C3-C4-C5	-3.22	104.54	110.22
4	A	603	NAG	C8-C7-N2	-2.63	111.36	116.11
4	A	603	NAG	O3-C3-C4	-2.60	104.69	110.36
2	A	601	HEM	CMA-C3A-C4A	-2.54	124.56	128.46
4	A	603	NAG	C3-C4-C5	-2.41	105.97	110.22
8	A	617	MPD	O2-C2-C1	-2.13	100.63	108.00
4	A	603	NAG	C6-C5-C4	-2.11	108.07	113.00
4	A	603	NAG	O7-C7-N2	2.05	125.87	121.92
2	A	601	HEM	C4A-C3A-C2A	2.09	108.45	107.00
2	A	601	HEM	CMC-C2C-C3C	2.17	128.91	124.89
2	A	601	HEM	C4C-C3C-C2C	2.39	108.57	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	3	0
8	A	617	MPD	4	0
9	A	618	EDO	2	0
11	A	621	CMO	2	0

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	594/595 (99%)	0.56	55 (9%)	9	9	20, 32, 66, 99	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	12.8
1	A	8	ALA	12.7
1	A	121	SER	12.5
1	A	172	TYR	12.3
1	A	174	SER	11.6
1	A	1	SER	11.5
1	A	595	ASN	10.4
1	A	12	LEU	10.2
1	A	124	HIS	10.0
1	A	13	VAL	9.7
1	A	173	GLN	9.7
1	A	4	VAL	9.7
1	A	119	LEU	9.0
1	A	170	PRO	8.6
1	A	120	GLY	8.1
1	A	122	ASN	8.0
1	A	10	VAL	7.6
1	A	7	GLY	7.0
1	A	171	PRO	7.0
1	A	168	PRO	6.9
1	A	118	GLU	6.3
1	A	126	LYS	6.1
1	A	132	TYR	5.8
1	A	594	GLU	5.4
1	A	593	ARG	5.3
1	A	125	SER	4.4
1	A	11	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	18	ASN	4.3
1	A	127	THR	4.1
1	A	123	GLU	4.0
1	A	9	PRO	4.0
1	A	254	PHE	3.9
1	A	16	ASP	3.8
1	A	64	ARG	3.7
1	A	169	THR	3.6
1	A	286	HIS	3.4
1	A	262	LEU	3.4
1	A	128	GLN	3.4
1	A	3	GLU	3.4
1	A	131	GLU	3.3
1	A	231	ASN	3.1
1	A	175	LEU	3.1
1	A	134	ILE	3.0
1	A	117	THR	2.9
1	A	592	SER	2.9
1	A	427	LYS	2.7
1	A	14	LYS	2.7
1	A	441	CYS	2.6
1	A	346	ALA	2.5
1	A	591	ALA	2.4
1	A	329	GLN	2.4
1	A	63	GLN	2.2
1	A	19	SER	2.2
1	A	223	GLY	2.1
1	A	347	PHE	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, 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	0.75	0.45	-	51,52,53,54	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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	A	604	14/15	0.91	0.12	-0.43	29,31,34,38	0
5	NAG	A	605	14/15	0.66	0.35	-	34,37,40,46	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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	IOD	A	614	1/1	0.98	0.31	39.43	39,39,39,39	0
9	EDO	A	619	4/4	0.80	0.29	3.64	26,28,33,34	0
8	MPD	A	617	8/8	0.81	0.37	2.96	18,26,33,37	0
4	NAG	A	603	14/15	0.89	0.15	1.32	25,32,34,37	0
2	HEM	A	601	43/43	0.98	0.19	0.77	16,22,26,27	0
6	IOD	A	609	1/1	0.99	0.16	0.72	36,36,36,36	0
6	IOD	A	611	1/1	0.93	0.13	0.03	37,37,37,37	0
10	SCN	A	620	3/3	0.92	0.14	-0.26	34,34,34,34	0
6	IOD	A	608	1/1	0.99	0.09	-0.53	34,34,34,34	0
6	IOD	A	607	1/1	0.99	0.08	-1.43	23,23,23,23	0
3	CA	A	602	1/1	0.99	0.08	-2.72	24,24,24,24	0
6	IOD	A	610	1/1	0.99	0.02	-10.63	31,31,31,31	0
9	EDO	A	618	4/4	0.75	0.38	-	26,26,27,28	0
4	NAG	A	606	14/15	0.83	0.25	-	31,34,38,41	0
7	BR	A	616	1/1	0.98	0.07	-	29,29,29,29	0
6	IOD	A	613	1/1	1.00	0.01	-	29,29,29,29	0
6	IOD	A	612	1/1	0.98	0.09	-	35,35,35,35	0
11	CMO	A	621	2/2	0.98	0.21	-	33,33,33,36	0
6	IOD	A	615	1/1	0.91	0.28	-	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.