



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:06 PM GMT

PDB ID : 4NT3
Title : Structure of the complex of bovine lactoperoxidase with 3,3'-dipyridyl ketone at 1.99 Å resolution
Authors : Sirohi, H.V.; Kushwaha, G.S.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2013-11-30
Resolution : 1.99 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

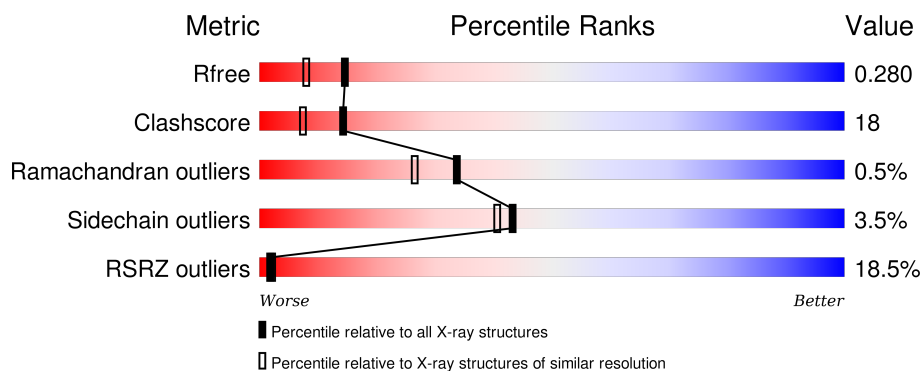
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 $\leq 5\%$. 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>18%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	605	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	607	-	-	-	X
6	IOD	A	613	-	-	-	X
7	ZAW	A	618	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5186 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	C	N	O	P	S	0	0	0
			4774	3037	847	863	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	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

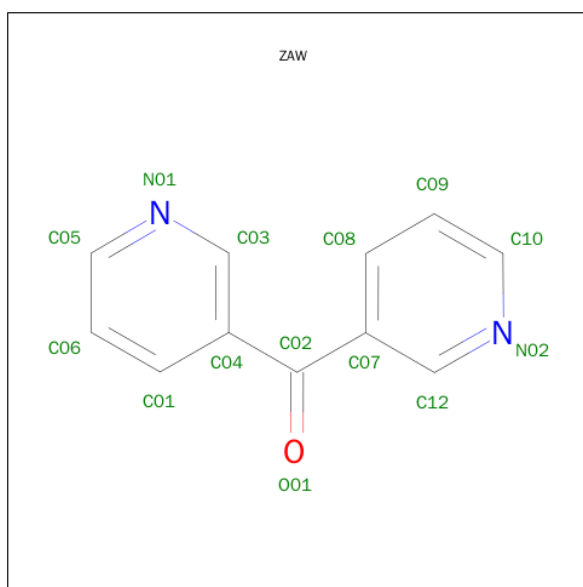


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

- Molecule 7 is DI(PYRIDIN-3-YL)METHANONE (three-letter code: ZAW) (formula: $C_{11}H_8N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	11	2	1		

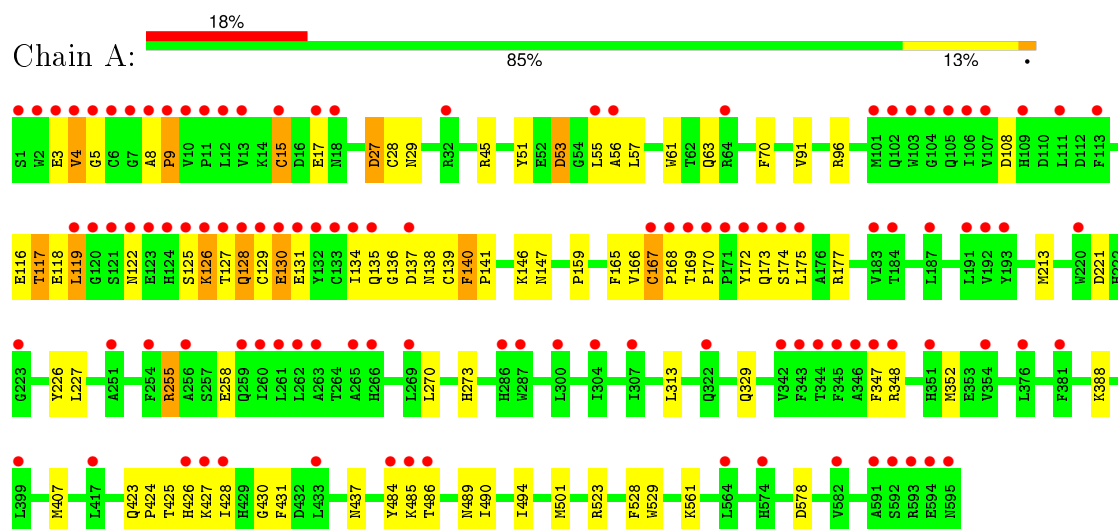
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	274	Total	O	0	0
			274	274		

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	54.27Å 80.44Å 76.60Å 90.00° 103.20° 90.00°	Depositor
Resolution (Å)	74.50 – 1.99 39.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.6 (74.50-1.99) 92.6 (39.11-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.203 , 0.250 0.239 , 0.280	Depositor DCC
R_{free} test set	2014 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	23 of 40499 reflections (0.057%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5186	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SEP, CA, HEM, ZAW, 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	0.70	0/4891	0.80	4/6634 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	167	CYS	C-N-CD	5.95	140.89	128.40
1	A	96	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	140	PHE	N-CA-CB	-5.12	101.39	110.60
1	A	255	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4687	166	0
2	A	43	0	30	12	0
3	A	1	0	0	0	0
4	A	28	0	25	0	0
5	A	42	0	39	0	0
6	A	10	0	0	2	0
7	A	14	0	8	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	274	0	0	8	0
All	All	5186	0	4789	175	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 18.

All (175) 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:108:ASP:OD2	2:A:601:HEM:CMD	1.70	1.37
1:A:258:GLU:OE2	2:A:601:HEM:CMB	1.78	1.29
1:A:484:TYR:CE1	1:A:490:ILE:HA	1.70	1.26
1:A:258:GLU:OE2	2:A:601:HEM:HMB1	1.07	1.24
7:A:618:ZAW:H1	7:A:618:ZAW:C08	1.59	1.23
1:A:423:GLN:HB2	1:A:426:HIS:CD2	1.80	1.16
1:A:126:LYS:CG	1:A:128:GLN:HG3	1.85	1.05
1:A:126:LYS:CD	1:A:128:GLN:HG3	1.86	1.04
7:A:618:ZAW:H1	7:A:618:ZAW:H5	1.04	1.03
1:A:159:PRO:HG2	1:A:426:HIS:CE1	1.95	1.02
7:A:618:ZAW:C01	7:A:618:ZAW:H5	1.87	1.01
1:A:423:GLN:HB2	1:A:426:HIS:HD2	1.20	1.00
1:A:127:THR:HG23	1:A:129:CYS:N	1.76	0.99
1:A:3:GLU:HG3	1:A:175:LEU:HD22	1.43	0.98
7:A:618:ZAW:C01	7:A:618:ZAW:C08	2.35	0.97
1:A:108:ASP:OD2	2:A:601:HEM:HMD1	0.78	0.95
1:A:127:THR:HG22	1:A:128:GLN:HA	1.48	0.95
1:A:53:ASP:CG	1:A:55:LEU:HB2	1.87	0.94
1:A:159:PRO:HG2	1:A:426:HIS:HE1	1.32	0.93
1:A:56:ALA:HB1	1:A:177:ARG:HD3	1.50	0.92
1:A:426:HIS:NE2	1:A:431:PHE:CE2	2.38	0.92
1:A:3:GLU:CG	1:A:175:LEU:HD22	2.00	0.90
1:A:51:TYR:HB3	1:A:55:LEU:O	1.72	0.90
1:A:51:TYR:CB	1:A:55:LEU:O	2.19	0.89
1:A:108:ASP:CG	2:A:601:HEM:HMD1	1.91	0.89
1:A:427:LYS:O	1:A:428:ILE:HG23	1.72	0.89
1:A:484:TYR:CZ	1:A:490:ILE:HA	2.06	0.88
1:A:4:VAL:HG12	1:A:5:GLY:HA2	1.54	0.88
1:A:127:THR:CG2	1:A:128:GLN:CA	2.52	0.87
1:A:15:CYS:HA	1:A:28:CYS:SG	2.14	0.87
1:A:127:THR:CG2	1:A:128:GLN:C	2.45	0.84
1:A:426:HIS:CG	1:A:431:PHE:CZ	2.66	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:THR:HG22	1:A:128:GLN:CA	2.07	0.83
1:A:127:THR:CG2	1:A:128:GLN:HA	2.09	0.83
1:A:424:PRO:O	1:A:425:THR:OG1	1.97	0.82
1:A:426:HIS:CD2	1:A:431:PHE:CZ	2.69	0.80
1:A:128:GLN:NE2	1:A:128:GLN:H	1.79	0.80
1:A:51:TYR:CG	1:A:55:LEU:O	2.35	0.80
1:A:137:ASP:O	1:A:138:ASN:HB2	1.81	0.80
1:A:135:GLN:HG2	1:A:139:CYS:O	1.81	0.79
1:A:258:GLU:HG3	7:A:618:ZAW:C08	2.12	0.79
1:A:127:THR:HG23	1:A:128:GLN:C	2.01	0.79
1:A:116:GLU:O	1:A:119:LEU:CD2	2.33	0.77
1:A:70:PHE:CD1	1:A:485:LYS:HG2	2.21	0.76
1:A:127:THR:N	1:A:128:GLN:HA	1.99	0.76
1:A:426:HIS:CE1	1:A:431:PHE:CE2	2.75	0.75
1:A:126:LYS:CG	1:A:128:GLN:CG	2.65	0.74
1:A:426:HIS:HB2	8:A:862:HOH:O	1.88	0.74
1:A:117:THR:O	1:A:118:GLU:HG3	1.87	0.73
1:A:484:TYR:CE1	1:A:490:ILE:CA	2.63	0.73
1:A:126:LYS:HG2	1:A:128:GLN:N	2.04	0.73
1:A:426:HIS:O	1:A:427:LYS:HB2	1.89	0.73
1:A:126:LYS:N	1:A:127:THR:HA	2.04	0.72
1:A:126:LYS:CE	1:A:128:GLN:HG3	2.20	0.72
1:A:128:GLN:OE1	1:A:134:ILE:HB	1.89	0.72
1:A:126:LYS:H	1:A:127:THR:C	1.93	0.72
1:A:27:ASP:O	1:A:28:CYS:HB2	1.90	0.72
1:A:426:HIS:CD2	1:A:431:PHE:CE2	2.78	0.71
1:A:484:TYR:CD1	1:A:490:ILE:HA	2.26	0.71
1:A:127:THR:HG23	1:A:129:CYS:H	1.54	0.70
1:A:423:GLN:CB	1:A:426:HIS:HD2	2.00	0.70
1:A:126:LYS:N	1:A:127:THR:CA	2.54	0.69
1:A:255:ARG:HA	7:A:618:ZAW:H2	1.73	0.69
1:A:484:TYR:CD2	1:A:490:ILE:HG12	2.27	0.69
1:A:127:THR:HG22	1:A:128:GLN:C	2.11	0.69
1:A:126:LYS:HD3	1:A:128:GLN:HG3	1.74	0.69
1:A:172:TYR:HD2	8:A:900:HOH:O	1.75	0.69
1:A:426:HIS:CE1	1:A:431:PHE:CZ	2.82	0.68
1:A:561:LYS:HD2	6:A:613:IOD:I	2.64	0.68
1:A:126:LYS:HG2	1:A:128:GLN:HG3	1.75	0.68
1:A:70:PHE:CE1	1:A:485:LYS:HG2	2.30	0.67
1:A:3:GLU:HG3	1:A:175:LEU:CD2	2.22	0.66
1:A:427:LYS:O	1:A:428:ILE:CG2	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:GLN:O	1:A:426:HIS:HB2	1.96	0.65
1:A:4:VAL:HG12	1:A:5:GLY:CA	2.26	0.65
1:A:426:HIS:CB	8:A:862:HOH:O	2.45	0.64
1:A:61:TRP:CE3	1:A:135:GLN:OE1	2.50	0.64
1:A:55:LEU:HD13	8:A:788:HOH:O	1.95	0.64
1:A:116:GLU:O	1:A:119:LEU:HD21	1.98	0.64
1:A:168:PRO:O	1:A:169:THR:HG23	1.98	0.64
1:A:56:ALA:CB	1:A:177:ARG:HD3	2.24	0.64
1:A:4:VAL:CG1	1:A:5:GLY:HA2	2.28	0.63
1:A:127:THR:HG23	1:A:128:GLN:CA	2.25	0.63
1:A:53:ASP:OD1	1:A:53:ASP:N	2.33	0.62
1:A:146:LYS:O	1:A:147:ASN:HB2	1.99	0.61
1:A:127:THR:CG2	1:A:129:CYS:N	2.56	0.61
1:A:53:ASP:CG	1:A:55:LEU:CB	2.65	0.61
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.36	0.60
7:A:618:ZAW:H7	8:A:887:HOH:O	2.02	0.60
1:A:159:PRO:CG	1:A:426:HIS:CE1	2.80	0.60
1:A:61:TRP:CD2	1:A:135:GLN:OE1	2.54	0.60
1:A:126:LYS:N	1:A:127:THR:C	2.55	0.59
1:A:126:LYS:HG3	1:A:128:GLN:HB3	1.83	0.59
1:A:135:GLN:HB2	1:A:141:PRO:HD2	1.85	0.59
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.85	0.59
1:A:428:ILE:HA	8:A:890:HOH:O	2.02	0.58
1:A:127:THR:HG21	1:A:130:GLU:H	1.68	0.58
1:A:53:ASP:CB	1:A:55:LEU:HB2	2.33	0.57
1:A:117:THR:O	1:A:118:GLU:CG	2.52	0.57
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.87	0.57
1:A:423:GLN:CB	1:A:426:HIS:CD2	2.72	0.57
1:A:125:SER:HA	1:A:127:THR:O	2.05	0.57
1:A:258:GLU:OE2	2:A:601:HEM:HMB2	1.93	0.56
1:A:426:HIS:ND1	1:A:431:PHE:CZ	2.73	0.56
1:A:258:GLU:HG3	7:A:618:ZAW:C09	2.35	0.56
1:A:128:GLN:H	1:A:128:GLN:HE21	1.51	0.56
1:A:255:ARG:HA	7:A:618:ZAW:C06	2.36	0.56
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.88	0.55
1:A:108:ASP:CG	2:A:601:HEM:CMD	2.63	0.55
1:A:117:THR:C	1:A:118:GLU:CG	2.74	0.55
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.05	0.54
1:A:258:GLU:CB	7:A:618:ZAW:H6	2.37	0.54
1:A:427:LYS:HB2	1:A:427:LYS:NZ	2.22	0.54
1:A:126:LYS:CG	1:A:128:GLN:CB	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLN:CG	1:A:140:PHE:HA	2.37	0.54
1:A:29:ASN:ND2	1:A:528:PHE:HD2	2.06	0.54
1:A:126:LYS:HG2	1:A:128:GLN:CB	2.38	0.53
1:A:135:GLN:HG2	1:A:140:PHE:HA	1.91	0.52
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.44	0.52
1:A:258:GLU:HB2	7:A:618:ZAW:H5	1.92	0.52
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.57	0.52
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.45	0.52
1:A:127:THR:N	1:A:128:GLN:CA	2.72	0.52
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.91	0.51
1:A:130:GLU:HG3	1:A:131:GLU:N	2.26	0.51
1:A:126:LYS:CG	1:A:128:GLN:HB3	2.40	0.51
1:A:146:LYS:O	1:A:147:ASN:CB	2.59	0.51
1:A:56:ALA:HB1	1:A:177:ARG:CD	2.31	0.51
1:A:407:MET:HB3	1:A:501:MET:CE	2.42	0.50
1:A:4:VAL:N	1:A:5:GLY:CA	2.75	0.50
1:A:126:LYS:HG2	1:A:128:GLN:CG	2.37	0.49
1:A:4:VAL:CG1	1:A:5:GLY:CA	2.89	0.49
1:A:126:LYS:HG3	1:A:128:GLN:HG3	1.86	0.49
1:A:4:VAL:N	1:A:5:GLY:HA2	2.27	0.48
1:A:61:TRP:CE3	1:A:135:GLN:CD	2.82	0.48
1:A:159:PRO:CG	1:A:426:HIS:HE1	2.16	0.48
1:A:117:THR:HB	1:A:118:GLU:HG2	1.95	0.48
2:A:601:HEM:CMB	2:A:601:HEM:HBB2	2.44	0.47
1:A:15:CYS:CA	1:A:28:CYS:SG	2.97	0.47
1:A:484:TYR:O	1:A:485:LYS:CB	2.62	0.47
1:A:117:THR:C	1:A:118:GLU:HG2	2.36	0.47
1:A:172:TYR:CB	8:A:785:HOH:O	2.63	0.47
1:A:135:GLN:CB	1:A:141:PRO:HD2	2.44	0.46
1:A:484:TYR:CE1	1:A:489:ASN:O	2.68	0.46
1:A:127:THR:H	1:A:128:GLN:HA	1.80	0.46
1:A:126:LYS:CE	1:A:128:GLN:CG	2.92	0.45
1:A:258:GLU:CG	7:A:618:ZAW:C09	2.95	0.45
1:A:424:PRO:O	1:A:425:THR:CB	2.63	0.45
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.45	0.45
1:A:125:SER:C	1:A:127:THR:HA	2.37	0.45
1:A:352:MET:SD	1:A:407:MET:SD	3.14	0.44
1:A:258:GLU:HG3	7:A:618:ZAW:H5	1.97	0.44
1:A:126:LYS:HG3	1:A:128:GLN:CG	2.45	0.44
1:A:126:LYS:HE2	1:A:128:GLN:HG3	1.98	0.44
1:A:3:GLU:CG	1:A:175:LEU:CD2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASP:OD2	1:A:57:LEU:HD12	2.18	0.44
1:A:51:TYR:HB2	1:A:55:LEU:H	1.83	0.43
1:A:135:GLN:HG3	1:A:140:PHE:HA	2.00	0.42
1:A:126:LYS:HE2	1:A:128:GLN:CG	2.49	0.42
1:A:165:PHE:CD1	1:A:177:ARG:CZ	3.02	0.42
1:A:258:GLU:OE2	2:A:601:HEM:C2B	2.63	0.42
1:A:15:CYS:HB3	1:A:17:GLU:HG3	2.01	0.42
1:A:426:HIS:CE1	1:A:431:PHE:HE2	2.35	0.42
1:A:166:VAL:O	1:A:172:TYR:CE1	2.73	0.42
1:A:426:HIS:ND1	1:A:431:PHE:HZ	2.17	0.41
1:A:126:LYS:N	1:A:127:THR:O	2.47	0.41
1:A:313:LEU:HA	1:A:313:LEU:HD23	1.83	0.41
1:A:126:LYS:HG3	1:A:128:GLN:CB	2.47	0.41
1:A:136:GLY:O	1:A:139:CYS:HB3	2.21	0.41
1:A:484:TYR:HB3	1:A:486:THR:O	2.21	0.41
1:A:388:LYS:NZ	8:A:972:HOH:O	2.53	0.41
1:A:494:ILE:HD12	1:A:494:ILE:HA	1.92	0.41
1:A:51:TYR:CD1	1:A:56:ALA:O	2.74	0.40
1:A:45:ARG:HA	6:A:609:IOD:I	2.92	0.40
1:A:484:TYR:O	1:A:485:LYS:HB3	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	592/595 (100%)	566 (96%)	23 (4%)	3 (0%)	34 26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	PRO

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Mol	Chain	Res	Type
1	A	9	PRO
1	A	430	GLY

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%)	499 (96%)	18 (4%)	43 40

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	15	CYS
1	A	27	ASP
1	A	53	ASP
1	A	63	GLN
1	A	91	VAL
1	A	117	THR
1	A	119	LEU
1	A	122	ASN
1	A	126	LYS
1	A	128	GLN
1	A	130	GLU
1	A	167	CYS
1	A	173	GLN
1	A	174	SER
1	A	329	GLN
1	A	347	PHE
1	A	578	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN

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Mol	Chain	Res	Type
1	A	128	GLN
1	A	426	HIS
1	A	437	ASN
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	8,9,10	3.00	6 (75%)	8,12,14	3.74	4 (50%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	-4.91	1.35	1.51
1	A	198	SEP	P-O2P	-4.04	1.40	1.54
1	A	198	SEP	P-O3P	-2.88	1.44	1.54
1	A	198	SEP	CB-CA	2.42	1.59	1.52
1	A	198	SEP	P-OG	2.66	1.69	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	OG-CB	2.74	1.56	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-P-O1P	-2.05	101.93	107.14
1	A	198	SEP	O2P-P-OG	2.54	113.86	106.56
1	A	198	SEP	O3P-P-O1P	3.55	122.01	110.58
1	A	198	SEP	OG-CB-CA	9.14	116.07	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

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	$\# Z > 2$
4	NAG	A	603	1,4	14,14,15	0.75	0	15,19,21	1.22	1 (6%)
4	NAG	A	604	4	14,14,15	0.70	0	15,19,21	2.16	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
4	NAG	A	603	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	604	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	NAG	O7-C7-C8	-2.68	117.14	122.06
4	A	604	NAG	O3-C3-C4	-2.39	104.97	110.34
4	A	604	NAG	C4-C3-C2	2.23	114.69	111.23
4	A	604	NAG	O5-C5-C6	2.40	112.54	107.35
4	A	604	NAG	C1-O5-C5	6.57	120.58	112.25

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 16 ligands modelled in this entry, 11 are monoatomic - leaving 5 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	1,8	30,50,50	2.50	7 (23%)	24,82,82	2.33	8 (33%)
5	NAG	A	605	1	14,14,15	0.74	0	15,19,21	2.10	7 (46%)
5	NAG	A	606	1	14,14,15	0.50	0	15,19,21	1.78	2 (13%)
5	NAG	A	607	1	14,14,15	1.05	0	15,19,21	2.65	5 (33%)
7	ZAW	A	618	-	15,15,15	3.86	7 (46%)	17,19,19	3.01	7 (41%)

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	1,8	-	0/10/54/54	0/0/8/8
5	NAG	A	605	1	-	0/6/23/26	0/1/1/1
5	NAG	A	606	1	-	0/6/23/26	0/1/1/1
5	NAG	A	607	1	-	0/6/23/26	0/1/1/1
7	ZAW	A	618	-	-	0/8/8/8	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C2D-C3D	-7.50	1.32	1.54
2	A	601	HEM	C2C-C1C	-6.07	1.41	1.52
7	A	618	ZAW	C04-C02	-5.79	1.39	1.49
7	A	618	ZAW	C07-C02	-5.69	1.39	1.49
2	A	601	HEM	C3B-C4B	-4.79	1.47	1.51
2	A	601	HEM	C3D-C4D	-4.24	1.46	1.51
2	A	601	HEM	C3C-CAC	-3.90	1.44	1.51
2	A	601	HEM	C2D-C1D	-3.15	1.41	1.51
2	A	601	HEM	C2B-C1B	-2.46	1.43	1.51
7	A	618	ZAW	C05-N01	2.19	1.40	1.33
7	A	618	ZAW	C10-N02	2.21	1.40	1.33
7	A	618	ZAW	C03-N01	2.79	1.40	1.34
7	A	618	ZAW	C12-N02	2.79	1.40	1.34
7	A	618	ZAW	O01-C02	11.48	1.43	1.22

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	618	ZAW	O01-C02-C07	-6.68	109.44	120.12
7	A	618	ZAW	O01-C02-C04	-6.65	109.49	120.12
7	A	618	ZAW	C04-C02-C07	-5.94	109.49	120.26
5	A	605	NAG	C3-C4-C5	-4.14	102.98	110.20
5	A	606	NAG	C3-C4-C5	-3.54	104.03	110.20
2	A	601	HEM	CBA-CAA-C2A	-3.28	106.65	112.53
7	A	618	ZAW	C07-C12-N02	-2.54	119.85	123.52
7	A	618	ZAW	C04-C03-N01	-2.53	119.87	123.52
5	A	605	NAG	C4-C3-C2	-2.47	107.39	111.23
5	A	607	NAG	O7-C7-C8	-2.35	117.75	122.06
2	A	601	HEM	C3B-C4B-NB	-2.31	107.21	111.63
5	A	605	NAG	O6-C6-C5	-2.21	104.02	111.33
7	A	618	ZAW	C01-C04-C03	2.01	120.03	117.67
2	A	601	HEM	CAA-C2A-C1A	2.05	129.23	127.01
7	A	618	ZAW	C08-C07-C12	2.05	120.07	117.67
5	A	605	NAG	C2-N2-C7	2.19	125.85	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	C2D-C3D-C4D	2.38	105.53	101.50
5	A	607	NAG	O6-C6-C5	2.48	119.53	111.33
5	A	605	NAG	O7-C7-N2	2.78	127.53	121.86
5	A	605	NAG	C1-O5-C5	2.88	115.90	112.25
5	A	607	NAG	C8-C7-N2	3.07	121.98	116.11
5	A	605	NAG	O4-C4-C5	3.16	117.62	109.24
2	A	601	HEM	CMB-C2B-C3B	3.62	125.57	116.53
2	A	601	HEM	CAD-C3D-C2D	4.21	125.33	113.22
2	A	601	HEM	CAD-C3D-C4D	4.70	129.05	112.47
5	A	607	NAG	O5-C5-C6	5.31	118.84	107.35
5	A	606	NAG	C1-O5-C5	5.31	118.99	112.25
2	A	601	HEM	CMC-C2C-C3C	5.35	129.88	116.53
5	A	607	NAG	C1-O5-C5	6.40	120.37	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	12	0
7	A	618	ZAW	13	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.39	110 (18%) 2 2	29, 46, 110, 178	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	30.4
1	A	122	ASN	23.5
1	A	172	TYR	21.6
1	A	120	GLY	21.4
1	A	12	LEU	21.1
1	A	174	SER	19.8
1	A	11	PRO	19.2
1	A	173	GLN	18.4
1	A	1	SER	15.5
1	A	121	SER	15.4
1	A	119	LEU	15.3
1	A	8	ALA	13.3
1	A	55	LEU	13.3
1	A	7	GLY	12.3
1	A	169	THR	10.8
1	A	3	GLU	10.7
1	A	10	VAL	10.3
1	A	123	GLU	10.3
1	A	595	ASN	10.0
1	A	128	GLN	9.9
1	A	171	PRO	9.4
1	A	126	LYS	9.3
1	A	593	ARG	9.2
1	A	4	VAL	8.9
1	A	170	PRO	8.8
1	A	13	VAL	8.6
1	A	6	CYS	8.5

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Mol	Chain	Res	Type	RSRZ
1	A	125	SER	7.3
1	A	426	HIS	7.1
1	A	15	CYS	6.7
1	A	137	ASP	6.2
1	A	129	CYS	6.2
1	A	484	TYR	6.0
1	A	106	ILE	5.6
1	A	124	HIS	5.5
1	A	107	VAL	5.3
1	A	594	GLU	5.2
1	A	262	LEU	4.8
1	A	261	LEU	4.6
1	A	5	GLY	4.6
1	A	56	ALA	4.6
1	A	582	VAL	4.3
1	A	9	PRO	4.2
1	A	127	THR	4.2
1	A	111	LEU	4.2
1	A	64	ARG	4.0
1	A	167	CYS	4.0
1	A	134	ILE	3.7
1	A	346	ALA	3.7
1	A	132	TYR	3.7
1	A	135	GLN	3.6
1	A	183	VAL	3.6
1	A	342	VAL	3.5
1	A	376	LEU	3.5
1	A	17	GLU	3.5
1	A	354	VAL	3.5
1	A	564	LEU	3.4
1	A	428	ILE	3.4
1	A	105	GLN	3.4
1	A	220	TRP	3.2
1	A	187	LEU	3.1
1	A	344	THR	3.0
1	A	168	PRO	3.0
1	A	109	HIS	2.9
1	A	103	TRP	2.9
1	A	102	GLN	2.9
1	A	191	LEU	2.9
1	A	131	GLU	2.9
1	A	433	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	192	VAL	2.8
1	A	113	PHE	2.8
1	A	307	ILE	2.8
1	A	265	ALA	2.8
1	A	348	ARG	2.7
1	A	254	PHE	2.7
1	A	223	GLY	2.6
1	A	269	LEU	2.6
1	A	266	HIS	2.6
1	A	104	GLY	2.5
1	A	343	PHE	2.5
1	A	18	ASN	2.5
1	A	381	PHE	2.5
1	A	399	LEU	2.5
1	A	101	MET	2.4
1	A	345	PHE	2.4
1	A	347	PHE	2.4
1	A	175	LEU	2.4
1	A	32	ARG	2.4
1	A	322	GLN	2.4
1	A	574	HIS	2.4
1	A	486	THR	2.3
1	A	591	ALA	2.2
1	A	287	TRP	2.2
1	A	286	HIS	2.2
1	A	193	TYR	2.1
1	A	417	LEU	2.1
1	A	251	ALA	2.1
1	A	263	ALA	2.1
1	A	592	SER	2.1
1	A	256	ALA	2.1
1	A	130	GLU	2.1
1	A	260	ILE	2.1
1	A	351	HIS	2.1
1	A	427	LYS	2.0
1	A	304	ILE	2.0
1	A	300	LEU	2.0
1	A	133	CYS	2.0
1	A	485	LYS	2.0
1	A	184	THR	2.0
1	A	259	GLN	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	0.97	0.17	-	30,44,54,54	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
4	NAG	A	603	14/15	0.93	0.18	0.25	26,30,33,41	0
4	NAG	A	604	14/15	0.80	0.29	-	38,46,52,53	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
5	NAG	A	607	14/15	0.71	0.33	6.14	44,66,71,79	0
6	IOD	A	613	1/1	0.82	0.22	4.31	52,52,52,52	1
5	NAG	A	605	14/15	0.77	0.24	3.28	30,34,38,40	0
7	ZAW	A	618	14/14	0.65	0.36	1.86	23,42,47,47	0
6	IOD	A	614	1/1	0.99	0.09	-0.48	41,41,41,41	1
6	IOD	A	611	1/1	0.99	0.03	-0.79	63,63,63,63	0
2	HEM	A	601	43/43	0.97	0.17	-0.80	20,23,27,30	0
6	IOD	A	609	1/1	0.99	0.09	-0.98	36,36,36,36	0
6	IOD	A	608	1/1	0.96	0.07	-1.70	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	IOD	A	616	1/1	0.96	0.07	-1.92	57,57,57,57	1
6	IOD	A	610	1/1	0.99	0.08	-2.14	52,52,52,52	0
3	CA	A	602	1/1	0.99	0.02	-4.60	23,23,23,23	0
6	IOD	A	617	1/1	0.96	0.09	-	61,61,61,61	1
5	NAG	A	606	14/15	0.84	0.24	-	56,66,70,71	0
6	IOD	A	615	1/1	0.95	0.10	-	52,52,52,52	1
6	IOD	A	612	1/1	0.99	0.04	-	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.