



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:55 PM GMT

PDB ID : 4N7A  
Title : Crystal structure of goat lactoperoxidase with 3-Amino pyrazole at 1.79 Angstrom resolution  
Authors : Tyagi, T.K.; Singh, R.P.; Singh, A.K.; Singh, A.; Bhushan, A.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2013-10-15  
Resolution : 1.79 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

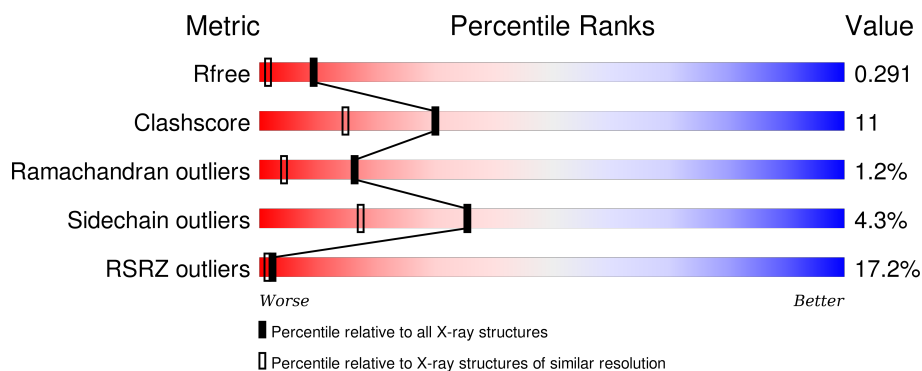
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	IOD	A	610	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SCN	A	613	-	X	-	X
7	EDO	A	616	-	-	-	X
7	EDO	A	618	-	-	X	-
8	GOL	A	619	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5291 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
			Total	C	N	O	P	S			
1	A	595	4758	3021	844	866	1	26	0	0	0

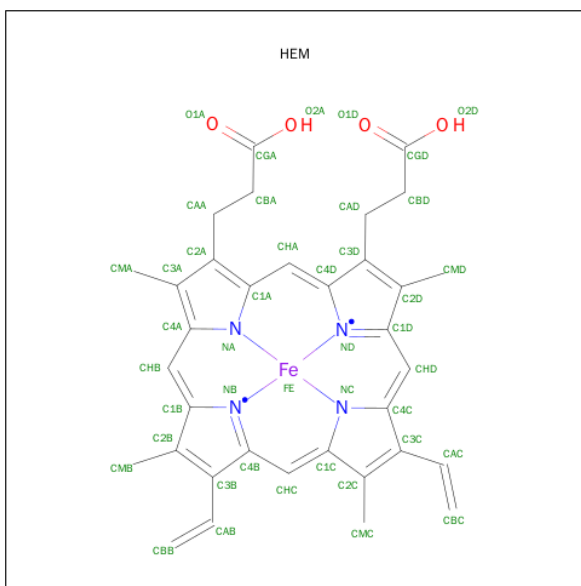
- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula:  $C_{34}H_{32}FeN_4O_4$ ).



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

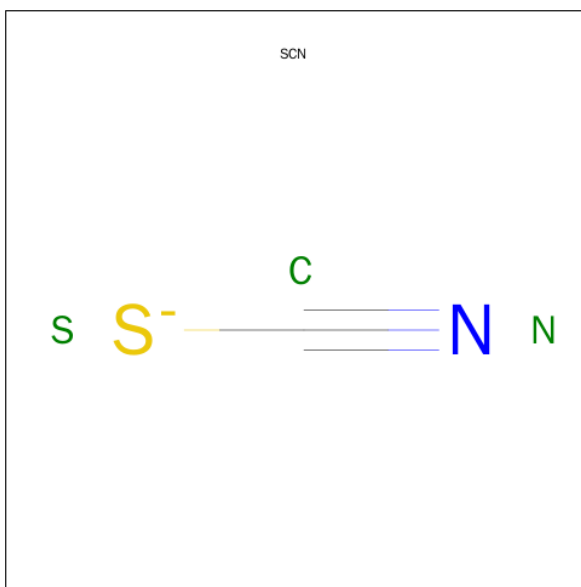
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

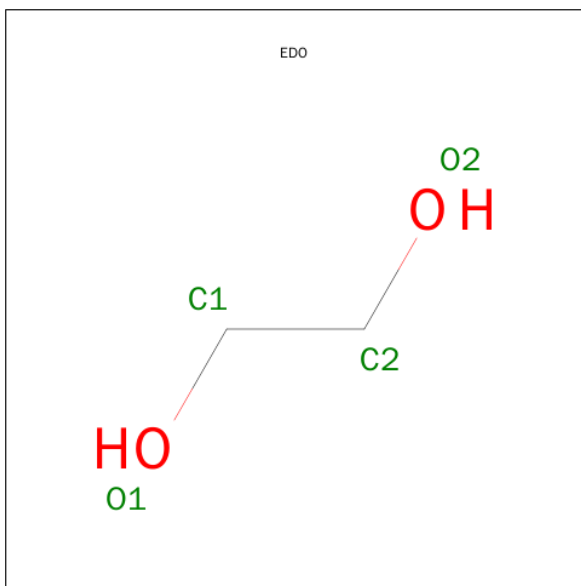
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	I		
			11	11	0	0

- Molecule 6 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

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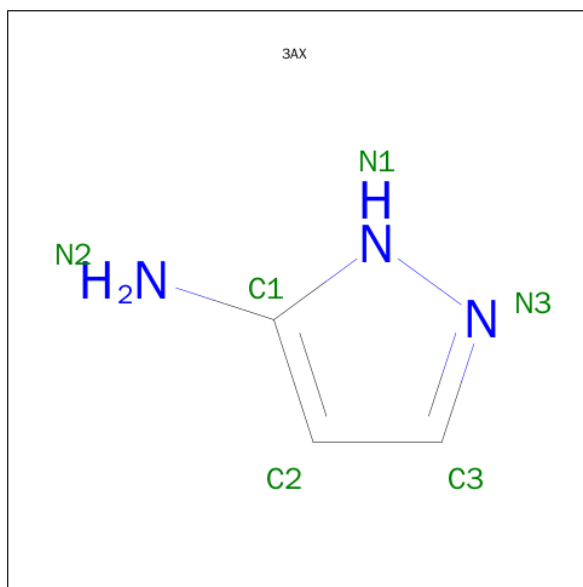
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 1H-PYRAZOL-5-AMINE (three-letter code: 3AX) (formula:  $C_3H_5N_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	N	0	0
			6	3	3		

- Molecule 10 is water.

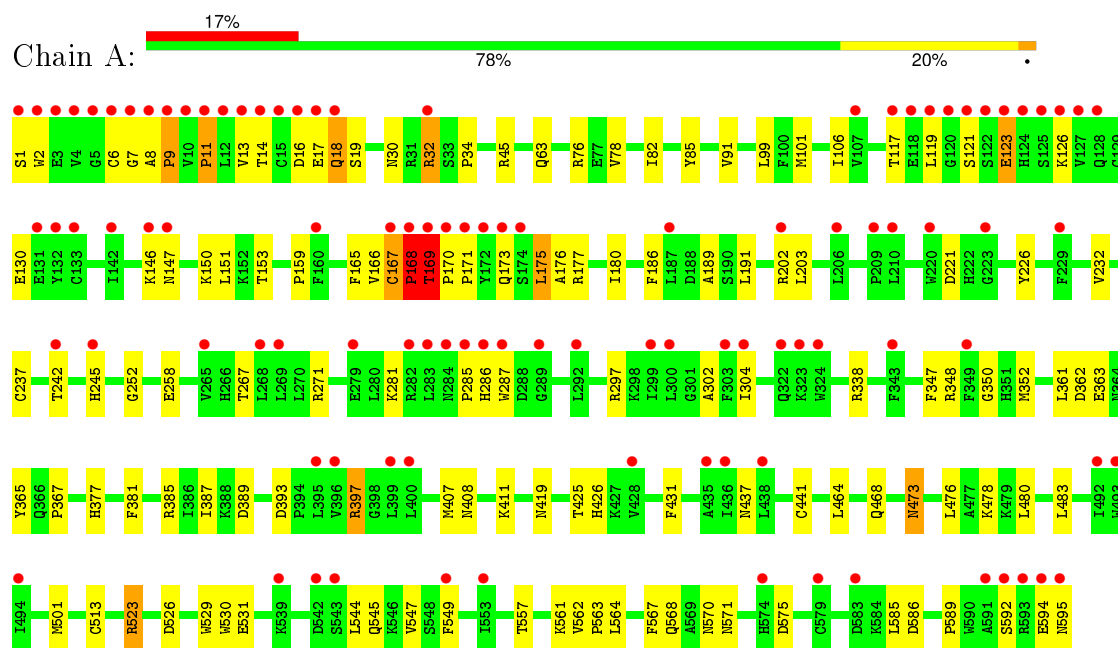
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	387	Total	O	0	0
			387	387		



### 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 ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Lactoperoxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.88Å 80.73Å 75.14Å 90.00° 101.53° 90.00°	Depositor
Resolution (Å)	73.62 – 1.79 27.20 – 1.79	Depositor EDS
% Data completeness (in resolution range)	96.4 (73.62-1.79) 96.4 (27.20-1.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.223 , 0.277 0.237 , 0.291	Depositor DCC
$R_{free}$ test set	2915 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 56952 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5291	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, SCN, NAG, SEP, CA, EDO, 3AX, 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	1.10	4/4876 (0.1%)	0.98	11/6621 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	TYR	CE2-CZ	6.30	1.46	1.38
1	A	302	ALA	CA-CB	5.83	1.64	1.52
1	A	186	PHE	C-O	5.29	1.33	1.23
1	A	441	CYS	CB-SG	-5.27	1.73	1.81

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	NE-CZ-NH2	-12.86	113.87	120.30
1	A	167	CYS	C-N-CD	-8.42	102.07	120.60
1	A	177	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	297	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	297	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	A	526	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	338	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	397	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	523	ARG	NE-CZ-NH1	-5.24	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	A	101	MET	CG-SD-CE	5.00	108.21	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	PRO	Peptide
1	A	169	THR	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4758	0	4644	101	0
2	A	56	0	52	1	0
3	A	43	0	30	6	0
4	A	1	0	0	0	0
5	A	11	0	0	4	0
6	A	3	0	0	0	0
7	A	20	0	30	6	0
8	A	6	0	8	3	0
9	A	6	0	5	3	0
10	A	387	0	0	21	0
All	All	5291	0	4769	106	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 11.

All (106) 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)
5:A:609:IOD:I	10:A:1071:HOH:O	2.40	1.08
1:A:258:GLU:OE2	3:A:604:HEM:HMB1	0.84	1.01
1:A:367:PRO:HG3	7:A:618:EDO:H22	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:HB	10:A:1046:HOH:O	1.66	0.93
1:A:258:GLU:HG3	9:A:622:3AX:H3	1.41	0.85
1:A:377:HIS:NE2	7:A:614:EDO:H11	1.92	0.85
1:A:63:GLN:HG2	10:A:852:HOH:O	1.77	0.83
5:A:620:IOD:I	10:A:1038:HOH:O	2.66	0.81
1:A:258:GLU:CD	3:A:604:HEM:HMB1	2.00	0.80
1:A:18:GLN:HE21	1:A:18:GLN:HA	1.48	0.79
1:A:8:ALA:H	1:A:9:PRO:HD3	1.51	0.75
2:A:625:NAG:H3	10:A:871:HOH:O	1.86	0.75
7:A:618:EDO:H11	10:A:708:HOH:O	1.85	0.74
1:A:567:PHE:HD1	5:A:610:IOD:I	2.42	0.72
1:A:8:ALA:N	1:A:9:PRO:HD3	2.06	0.70
1:A:78:VAL:HG13	1:A:82:ILE:HD12	1.73	0.70
1:A:159:PRO:HD2	1:A:431:PHE:CE2	2.27	0.69
1:A:130:GLU:OE1	1:A:426:HIS:ND1	2.22	0.68
1:A:258:GLU:HG3	9:A:622:3AX:N1	2.11	0.66
1:A:258:GLU:CD	3:A:604:HEM:CMB	2.59	0.66
1:A:258:GLU:CG	9:A:622:3AX:H3	2.09	0.65
1:A:348:ARG:HH11	1:A:437:ASN:ND2	1.96	0.63
1:A:407:MET:HB3	1:A:501:MET:CE	2.29	0.63
1:A:153:THR:HG22	1:A:153:THR:O	2.00	0.61
1:A:363:GLU:H	1:A:363:GLU:CD	2.04	0.61
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.48	0.60
1:A:281:LYS:HE3	1:A:285:PRO:HA	1.84	0.59
1:A:408:ASN:HB2	10:A:918:HOH:O	2.01	0.58
1:A:14:THR:N	10:A:997:HOH:O	2.36	0.58
1:A:82:ILE:HD13	1:A:480:LEU:HD23	1.86	0.58
1:A:407:MET:HB3	1:A:501:MET:HE3	1.86	0.57
1:A:99:LEU:HD21	1:A:549:PHE:CD1	2.39	0.57
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.87	0.57
1:A:6:CYS:HB2	10:A:1034:HOH:O	2.04	0.56
1:A:407:MET:HE3	1:A:407:MET:C	2.27	0.55
1:A:258:GLU:OE2	3:A:604:HEM:HMB2	1.92	0.55
1:A:464:LEU:O	1:A:468:GLN:HG3	2.07	0.54
1:A:352:MET:HB3	1:A:407:MET:HG2	1.88	0.54
1:A:159:PRO:HD2	1:A:431:PHE:CZ	2.44	0.53
1:A:352:MET:CB	1:A:407:MET:HG2	2.38	0.53
1:A:377:HIS:CD2	7:A:614:EDO:H11	2.44	0.53
1:A:530:TRP:CZ2	1:A:531:GLU:HG3	2.44	0.53
1:A:544:LEU:O	1:A:547:VAL:HG22	2.09	0.52
1:A:119:LEU:HD13	1:A:169:THR:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLU:HG3	10:A:1003:HOH:O	2.10	0.52
1:A:130:GLU:HG3	1:A:159:PRO:HG3	1.93	0.51
1:A:393:ASP:OD1	1:A:557:THR:HB	2.10	0.51
1:A:13:VAL:HB	10:A:1015:HOH:O	2.11	0.51
1:A:150:LYS:HG3	8:A:619:GOL:H12	1.93	0.51
1:A:8:ALA:N	1:A:9:PRO:CD	2.74	0.50
1:A:419:ASN:CG	8:A:619:GOL:H11	2.31	0.50
1:A:82:ILE:HD13	1:A:480:LEU:CD2	2.42	0.50
1:A:286:HIS:NE2	1:A:594:GLU:OE2	2.41	0.49
1:A:232:VAL:O	1:A:232:VAL:HG23	2.12	0.49
1:A:586:ASP:O	1:A:589:PRO:HD2	2.13	0.49
1:A:126:LYS:HE2	1:A:425:THR:HG21	1.93	0.49
1:A:13:VAL:HA	10:A:997:HOH:O	2.11	0.49
1:A:242:THR:HG22	1:A:242:THR:O	2.13	0.48
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.48	0.48
1:A:175:LEU:HG	1:A:176:ALA:H	1.78	0.48
1:A:126:LYS:NZ	1:A:425:THR:HG21	2.28	0.48
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.49	0.48
1:A:153:THR:O	1:A:153:THR:CG2	2.61	0.47
1:A:169:THR:HG22	10:A:1045:HOH:O	2.13	0.47
1:A:570:ASN:HD22	1:A:575:ASP:HB3	1.79	0.47
1:A:267:THR:O	1:A:271:ARG:HG3	2.16	0.46
1:A:1:SER:CB	1:A:175:LEU:HD13	2.46	0.46
1:A:419:ASN:ND2	8:A:619:GOL:H11	2.31	0.45
1:A:568:GLN:NE2	10:A:1064:HOH:O	2.48	0.45
1:A:361:LEU:CD2	7:A:618:EDO:H21	2.46	0.45
1:A:82:ILE:CD1	1:A:480:LEU:HD23	2.47	0.45
1:A:287:TRP:HA	10:A:950:HOH:O	2.16	0.45
1:A:385:ARG:O	1:A:389:ASP:HB3	2.16	0.45
1:A:7:GLY:HA3	10:A:1084:HOH:O	2.17	0.45
1:A:166:VAL:HG12	1:A:180:ILE:HG12	1.99	0.45
1:A:165:PHE:CE2	1:A:171:PRO:HB3	2.53	0.44
1:A:567:PHE:CD1	5:A:610:IOD:I	3.32	0.44
1:A:106:ILE:HG23	1:A:191:LEU:HD11	2.00	0.44
1:A:562:VAL:HB	1:A:563:PRO:HD2	2.00	0.43
1:A:473:ASN:HD22	1:A:473:ASN:C	2.22	0.43
1:A:32:ARG:HG3	1:A:32:ARG:H	1.48	0.43
1:A:126:LYS:CE	1:A:425:THR:HG21	2.49	0.43
1:A:350:GLY:HA3	3:A:604:HEM:CBC	2.49	0.43
3:A:604:HEM:HBC2	3:A:604:HEM:HMC2	2.01	0.43
1:A:367:PRO:CG	7:A:618:EDO:H22	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ASN:ND2	1:A:476:LEU:H	2.17	0.43
1:A:570:ASN:ND2	10:A:1064:HOH:O	2.52	0.43
1:A:1:SER:HB2	1:A:175:LEU:HD13	2.02	0.42
1:A:365:TYR:CE2	1:A:397:ARG:HB3	2.54	0.42
1:A:16:ASP:O	1:A:16:ASP:OD1	2.37	0.42
1:A:203:LEU:HD11	1:A:252:GLY:HA2	2.02	0.42
1:A:76:ARG:HH12	1:A:419:ASN:ND2	2.17	0.42
1:A:237:CYS:HA	1:A:381:PHE:O	2.20	0.42
1:A:362:ASP:HB2	1:A:363:GLU:OE2	2.19	0.42
1:A:91:VAL:HG12	1:A:411:LYS:CD	2.50	0.42
1:A:146:LYS:O	1:A:147:ASN:HB2	2.20	0.41
1:A:19:SER:HA	10:A:937:HOH:O	2.21	0.41
1:A:91:VAL:HG12	1:A:411:LYS:HD3	2.02	0.41
1:A:76:ARG:HH22	1:A:419:ASN:ND2	2.19	0.41
1:A:11:PRO:HA	10:A:929:HOH:O	2.20	0.41
1:A:571:ASN:HB3	10:A:1076:HOH:O	2.21	0.41
1:A:168:PRO:HG2	1:A:169:THR:H	1.85	0.40
1:A:30:ASN:O	1:A:34:PRO:HA	2.21	0.40
1:A:407:MET:CB	1:A:501:MET:CE	2.97	0.40
1:A:6:CYS:CB	10:A:1034:HOH:O	2.68	0.40
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.57	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%)	559 (94%)	26 (4%)	7 (1%)	16	4

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	167	CYS
1	A	168	PRO
1	A	170	PRO
1	A	9	PRO
1	A	123	GLU
1	A	17	GLU

### 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	516/516 (100%)	494 (96%)	22 (4%)	35 17

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	18	GLN
1	A	32	ARG
1	A	121	SER
1	A	151	LEU
1	A	169	THR
1	A	173	GLN
1	A	175	LEU
1	A	202	ARG
1	A	245	HIS
1	A	347	PHE
1	A	387	ILE
1	A	473	ASN
1	A	478	LYS
1	A	483	LEU
1	A	513	CYS
1	A	545	GLN
1	A	561	LYS
1	A	564	LEU
1	A	585	LEU

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Mol	Chain	Res	Type
1	A	592	SER
1	A	595	ASN

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	18	GLN
1	A	128	GLN
1	A	147	ASN
1	A	329	GLN
1	A	419	ASN
1	A	437	ASN
1	A	468	GLN
1	A	473	ASN
1	A	497	ASN
1	A	568	GLN
1	A	570	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	2.59	3 (37%)	8,12,14	3.43	2 (25%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	2.33	1.58	1.51
1	A	198	SEP	P-OG	2.99	1.70	1.60
1	A	198	SEP	P-O3P	5.51	1.74	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O3P-P-OG	6.05	123.98	106.56
1	A	198	SEP	OG-CB-CA	7.28	114.49	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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 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	NAG	A	601	1	14,14,15	0.46	0	15,19,21	1.38	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	602	1	14,14,15	0.56	0	15,19,21	1.27	2 (13%)
2	NAG	A	603	1	14,14,15	0.97	1 (7%)	15,19,21	1.58	4 (26%)
3	HEM	A	604	1	30,50,50	2.51	10 (33%)	24,82,82	2.83	12 (50%)
6	SCN	A	613	-	2,2,2	2.48	1 (50%)	1,1,1	2.69	1 (100%)
7	EDO	A	614	-	3,3,3	0.37	0	2,2,2	1.25	0
7	EDO	A	615	-	3,3,3	0.65	0	2,2,2	0.68	0
7	EDO	A	616	-	3,3,3	0.52	0	2,2,2	0.23	0
7	EDO	A	617	-	3,3,3	0.43	0	2,2,2	0.18	0
7	EDO	A	618	-	3,3,3	0.51	0	2,2,2	1.21	0
8	GOL	A	619	-	5,5,5	0.77	0	5,5,5	1.60	1 (20%)
9	3AX	A	622	-	4,6,6	3.89	3 (75%)	3,7,7	1.48	0
2	NAG	A	625	1	14,14,15	0.44	0	15,19,21	2.35	3 (20%)

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	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	603	1	-	0/6/23/26	0/1/1/1
3	HEM	A	604	1	-	0/10/54/54	0/0/8/8
6	SCN	A	613	-	-	0/0/0/0	0/0/0/0
7	EDO	A	614	-	-	0/1/1/1	0/0/0/0
7	EDO	A	615	-	-	0/1/1/1	0/0/0/0
7	EDO	A	616	-	-	0/1/1/1	0/0/0/0
7	EDO	A	617	-	-	0/1/1/1	0/0/0/0
7	EDO	A	618	-	-	0/1/1/1	0/0/0/0
8	GOL	A	619	-	-	0/4/4/4	0/0/0/0
9	3AX	A	622	-	-	0/0/0/0	0/1/1/1
2	NAG	A	625	1	-	0/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	HEM	C3B-C4B	-8.44	1.44	1.51
3	A	604	HEM	C2C-C1C	-5.64	1.41	1.52
9	A	622	3AX	C1-N1	-5.23	1.27	1.34
9	A	622	3AX	N3-N1	-4.58	1.27	1.37
9	A	622	3AX	C3-N3	-3.51	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	HEM	C2D-C3D	-3.14	1.45	1.54
3	A	604	HEM	C4C-NC	-3.13	1.32	1.36
3	A	604	HEM	C3D-C4D	-2.43	1.48	1.51
3	A	604	HEM	C2B-C1B	-2.35	1.44	1.51
3	A	604	HEM	FE-ND	2.17	2.09	1.97
3	A	604	HEM	CMC-C2C	2.82	1.59	1.53
2	A	603	NAG	C1-C2	2.84	1.56	1.52
6	A	613	SCN	C-S	2.93	1.82	1.63
3	A	604	HEM	C3B-CAB	2.95	1.56	1.51
3	A	604	HEM	FE-NC	3.56	2.09	1.95

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	HEM	CAA-C2A-C1A	-4.27	122.37	127.01
3	A	604	HEM	CAA-CBA-CGA	-3.76	105.86	112.75
3	A	604	HEM	CBA-CAA-C2A	-3.68	105.93	112.53
2	A	601	NAG	C2-N2-C7	-3.31	118.79	123.04
2	A	603	NAG	C1-O5-C5	-3.26	108.11	112.25
3	A	604	HEM	CBD-CAD-C3D	-3.23	104.14	113.55
6	A	613	SCN	S-C-N	-2.69	157.76	175.94
3	A	604	HEM	C3B-CAB-CBB	-2.48	120.65	124.46
2	A	603	NAG	C3-C4-C5	-2.39	106.03	110.20
2	A	601	NAG	O6-C6-C5	-2.32	103.66	111.33
2	A	603	NAG	O6-C6-C5	-2.12	104.34	111.33
3	A	604	HEM	C2C-C1C-NC	-2.11	106.66	110.21
2	A	625	NAG	O3-C3-C2	2.06	113.19	109.11
2	A	602	NAG	C2-N2-C7	2.10	125.73	123.04
3	A	604	HEM	C2C-C1C-CHC	2.15	126.95	123.68
2	A	603	NAG	C6-C5-C4	2.16	118.35	113.02
2	A	601	NAG	C1-O5-C5	2.21	115.05	112.25
8	A	619	GOL	C3-C2-C1	2.49	120.89	111.12
3	A	604	HEM	CMD-C2D-C3D	2.52	125.49	114.35
2	A	602	NAG	C1-O5-C5	2.80	115.80	112.25
2	A	625	NAG	O5-C5-C6	3.03	113.91	107.35
3	A	604	HEM	CAD-C3D-C4D	4.15	127.11	112.47
3	A	604	HEM	CMB-C2B-C3B	4.39	127.48	116.53
3	A	604	HEM	CMC-C2C-C3C	5.09	129.24	116.53
3	A	604	HEM	CAD-C3D-C2D	5.58	129.27	113.22
2	A	625	NAG	C2-N2-C7	7.22	132.32	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	HEM	6	0
7	A	614	EDO	2	0
7	A	618	EDO	4	0
8	A	619	GOL	3	0
9	A	622	3AX	3	0
2	A	625	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	594/595 (99%)	1.12	102 (17%) 2 1	14, 33, 80, 110	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	TYR	14.2
1	A	119	LEU	14.1
1	A	2	TRP	13.9
1	A	12	LEU	13.2
1	A	122	SER	13.1
1	A	13	VAL	11.2
1	A	120	GLY	10.2
1	A	121	SER	9.3
1	A	124	HIS	8.1
1	A	127	VAL	6.7
1	A	170	PRO	6.6
1	A	125	SER	6.5
1	A	283	LEU	6.5
1	A	171	PRO	6.3
1	A	4	VAL	6.3
1	A	15	CYS	6.0
1	A	174	SER	5.8
1	A	167	CYS	5.6
1	A	173	GLN	5.4
1	A	117	THR	5.3
1	A	168	PRO	5.2
1	A	595	ASN	5.2
1	A	324	TRP	5.2
1	A	594	GLU	5.0
1	A	10	VAL	5.0
1	A	1	SER	5.0
1	A	539	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	7	GLY	4.9
1	A	593	ARG	4.9
1	A	8	ALA	4.9
1	A	118	GLU	4.8
1	A	126	LYS	4.7
1	A	591	ALA	4.4
1	A	292	LEU	4.2
1	A	187	LEU	4.2
1	A	14	THR	4.1
1	A	210	LEU	4.0
1	A	11	PRO	4.0
1	A	169	THR	4.0
1	A	287	TRP	3.8
1	A	9	PRO	3.7
1	A	549	PHE	3.6
1	A	282	ARG	3.5
1	A	132	TYR	3.5
1	A	574	HIS	3.5
1	A	131	GLU	3.4
1	A	494	ILE	3.4
1	A	128	GLN	3.4
1	A	279	GLU	3.3
1	A	32	ARG	3.2
1	A	123	GLU	3.2
1	A	304	ILE	3.2
1	A	220	TRP	3.1
1	A	6	CYS	3.1
1	A	284	ASN	3.0
1	A	428	VAL	3.0
1	A	285	PRO	2.9
1	A	436	ILE	2.9
1	A	5	GLY	2.9
1	A	209	PRO	2.9
1	A	146	LYS	2.8
1	A	242	THR	2.8
1	A	492	ILE	2.8
1	A	229	PHE	2.8
1	A	322	GLN	2.8
1	A	142	ILE	2.8
1	A	592	SER	2.8
1	A	493	TRP	2.8
1	A	543	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	245	HIS	2.7
1	A	269	LEU	2.6
1	A	17	GLU	2.6
1	A	579	CYS	2.6
1	A	396	VAL	2.6
1	A	16	ASP	2.6
1	A	268	LEU	2.6
1	A	133	CYS	2.5
1	A	286	HIS	2.5
1	A	299	ILE	2.5
1	A	300	LEU	2.5
1	A	223	GLY	2.5
1	A	265	VAL	2.4
1	A	147	ASN	2.4
1	A	206	LEU	2.4
1	A	160	PHE	2.4
1	A	343	PHE	2.4
1	A	202	ARG	2.3
1	A	18	GLN	2.3
1	A	583	ASP	2.3
1	A	323	LYS	2.3
1	A	303	PHE	2.3
1	A	553	ILE	2.2
1	A	107	VAL	2.2
1	A	438	LEU	2.2
1	A	542	ASP	2.2
1	A	349	PHE	2.1
1	A	3	GLU	2.1
1	A	435	ALA	2.1
1	A	400	LEU	2.1
1	A	395	LEU	2.1
1	A	289	GLY	2.0
1	A	399	LEU	2.0

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

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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SEP	A	198	10/11	0.92	0.14	-	28,37,42,45	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SCN	A	613	3/3	0.30	0.54	18.26	103,103,104,106	0
7	EDO	A	616	4/4	0.82	0.18	5.69	39,44,50,55	0
8	GOL	A	619	6/6	0.89	0.15	4.61	24,38,41,44	0
7	EDO	A	618	4/4	0.96	0.15	1.95	19,36,38,40	0
7	EDO	A	615	4/4	0.88	0.15	0.76	27,43,46,49	0
2	NAG	A	603	14/15	0.86	0.13	-0.04	34,42,49,53	0
5	IOD	A	620	1/1	0.91	0.11	-0.18	65,65,65,65	1
2	NAG	A	602	14/15	0.88	0.14	-0.21	47,52,57,59	0
7	EDO	A	617	4/4	0.96	0.13	-0.71	34,38,40,51	0
3	HEM	A	604	43/43	0.98	0.09	-0.94	11,16,23,26	0
5	IOD	A	621	1/1	0.96	0.07	-0.98	60,60,60,60	1
5	IOD	A	606	1/1	1.00	0.08	-1.21	20,20,20,20	0
4	CA	A	605	1/1	0.99	0.06	-1.43	22,22,22,22	0
5	IOD	A	608	1/1	0.98	0.03	-1.67	42,42,42,42	0
5	IOD	A	623	1/1	0.94	0.05	-2.58	43,43,43,43	0
5	IOD	A	607	1/1	0.94	0.06	-2.79	56,56,56,56	1
5	IOD	A	611	1/1	0.99	0.06	-2.90	40,40,40,40	1
5	IOD	A	624	1/1	0.96	0.05	-3.77	39,39,39,39	0
5	IOD	A	609	1/1	0.97	0.04	-	63,63,63,63	1
2	NAG	A	601	14/15	0.82	0.23	-	46,51,54,55	0
9	3AX	A	622	6/6	0.87	0.20	-	10,19,32,33	0
5	IOD	A	610	1/1	0.96	0.06	-	56,56,56,56	1
7	EDO	A	614	4/4	0.88	0.25	-	25,33,38,47	0
5	IOD	A	612	1/1	0.95	0.08	-	65,65,65,65	1
2	NAG	A	625	14/15	0.52	0.22	-	41,45,47,51	14

## 6.5 Other polymers [i](#)

There are no such residues in this entry.