



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 PM GMT

PDB ID : 3S4F  
Title : Crystal structure of the complex of bovine lactoperoxidase with 1H-pyrazolo[4,3-c] pyridine at 1.99 Å resolution  
Authors : Singh, A.; Singh, A.K.; Singh, R.P.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2011-05-19  
Resolution : 2.00 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

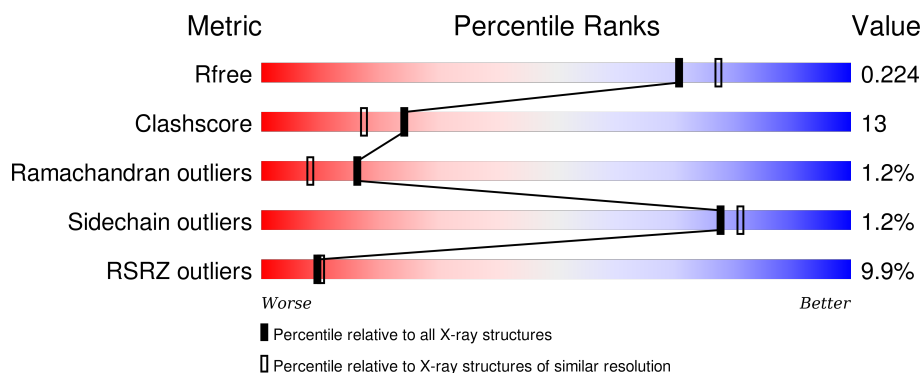
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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	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  $\geq 3$ , 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	<div> <div>10%</div> <div>79%</div> <div>19%</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
10	GOL	A	622	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IOD	A	601	-	-	-	X
5	PZR	A	608	-	-	X	X
9	PEG	A	616	-	-	-	X
9	PEG	A	621	-	-	X	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5410 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		

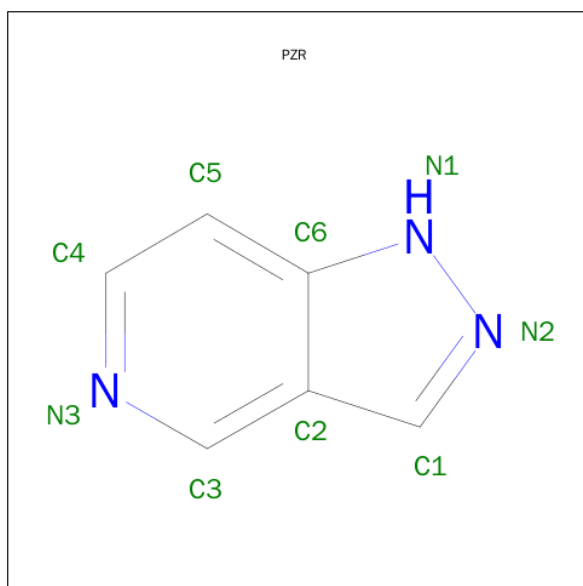
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

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

- Molecule 5 is 1H-PYRAZOLO[4,3-C]PYRIDINE (three-letter code: PZR) (formula: C<sub>6</sub>H<sub>5</sub>N<sub>3</sub>).



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

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

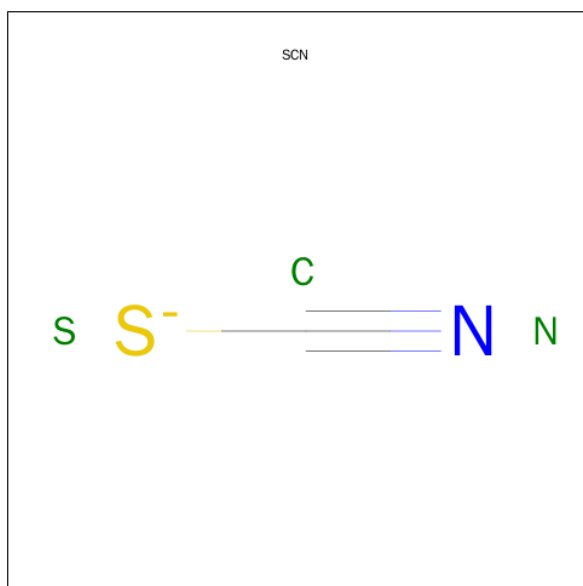
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total C N O 28 16 2 10	0	0
6	A	2	Total C N O 28 16 2 10	0	0

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 8 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 11 is water.

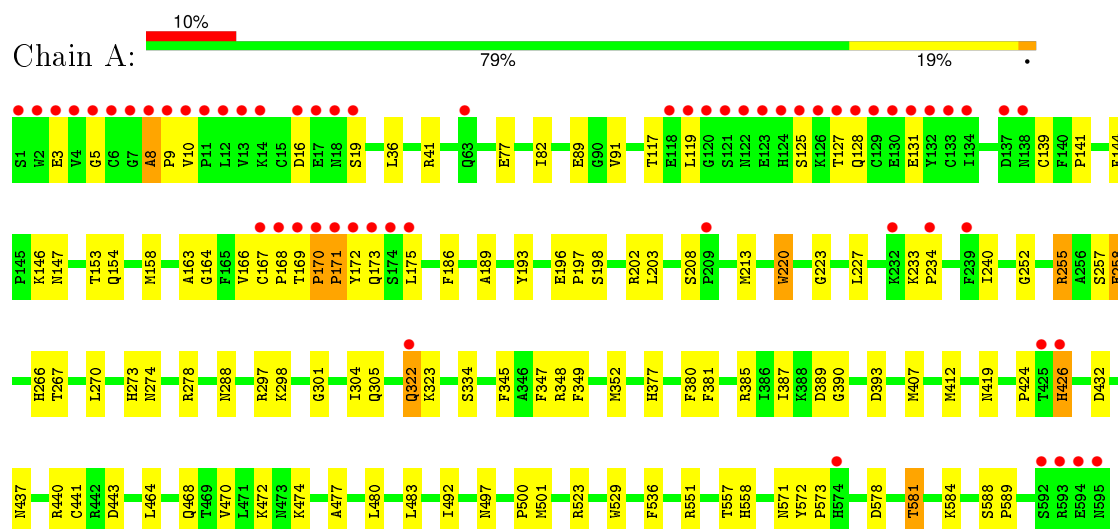
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	431	Total	O	0	0
			431	431		



### 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, $\alpha$ , $\beta$ , $\gamma$	53.35Å 80.33Å 73.39Å 90.00° 103.94° 90.00°	Depositor
Resolution (Å)	43.50 – 2.00 43.52 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.50-2.00) 96.5 (43.52-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.40 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.196 , 0.225 0.193 , 0.224	Depositor DCC
$R_{free}$ test set	1977 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 39356 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5410	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SCN, NAG, SEP, CA, PZR, HEM, PEG, 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	0.68	4/4891 (0.1%)	0.77	5/6634 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	ARG	CD-NE	-8.37	1.32	1.46
1	A	571	ASN	C-N	-5.74	1.20	1.34
1	A	186	PHE	CD1-CE1	-5.62	1.28	1.39
1	A	477	ALA	C-N	-5.38	1.21	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	HIS	CB-CA-C	5.60	121.60	110.40
1	A	258	GLU	CA-CB-CG	-5.50	101.30	113.40
1	A	166	VAL	N-CA-C	5.36	125.48	111.00
1	A	390	GLY	N-CA-C	5.26	126.24	113.10
1	A	255	ARG	CG-CD-NE	5.20	122.72	111.80

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4684	127	0
2	A	43	0	30	8	0
3	A	1	0	0	0	0
4	A	10	0	0	0	0
5	A	9	0	5	8	0
6	A	56	0	50	2	0
7	A	28	0	26	2	0
8	A	3	0	0	0	0
9	A	49	0	70	18	0
10	A	6	0	8	3	0
11	A	431	0	0	12	0
All	All	5410	0	4873	128	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 13.

All (128) 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:19:SER:HB2	11:A:885:HOH:O	1.36	1.20
1:A:322:GLN:HE21	1:A:322:GLN:CA	1.54	1.18
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.14	1.12
1:A:258:GLU:OE2	2:A:605:HEM:HMB3	1.57	1.04
1:A:322:GLN:HA	1:A:322:GLN:NE2	1.48	1.04
1:A:170:PRO:CB	1:A:171:PRO:HD3	1.96	0.94
1:A:472:LYS:NZ	9:A:621:PEG:H32	1.89	0.87
1:A:202:ARG:HH11	10:A:622:GOL:H11	1.37	0.87
1:A:348:ARG:CG	2:A:605:HEM:HMD3	2.05	0.86
1:A:322:GLN:HE21	1:A:322:GLN:HA	0.72	0.85
1:A:170:PRO:HB2	1:A:171:PRO:CD	2.04	0.84
1:A:163:ALA:HB2	1:A:440:ARG:NH1	1.93	0.82
1:A:258:GLU:OE2	2:A:605:HEM:CMB	2.33	0.77
1:A:470:VAL:HG22	9:A:620:PEG:H11	1.68	0.76
1:A:227:LEU:HD21	1:A:267:THR:HA	1.68	0.76
1:A:348:ARG:HG3	2:A:605:HEM:HMD3	1.67	0.75
1:A:202:ARG:NH1	10:A:622:GOL:H11	2.02	0.74
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.68	0.74
1:A:348:ARG:HG2	2:A:605:HEM:HMD3	1.68	0.73
1:A:407:MET:HB3	1:A:501:MET:CE	2.19	0.72
1:A:163:ALA:HB2	1:A:440:ARG:HH11	1.52	0.71
1:A:258:GLU:HG3	5:A:608:PZR:H3	1.72	0.70
1:A:220:TRP:HB3	9:A:618:PEG:H31	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:HE2	1:A:175:LEU:H	1.43	0.66
1:A:258:GLU:HG3	5:A:608:PZR:C3	2.26	0.66
1:A:197:PRO:HB3	9:A:619:PEG:H41	1.77	0.66
1:A:197:PRO:CB	9:A:619:PEG:H41	2.27	0.65
1:A:407:MET:HB3	1:A:501:MET:HE1	1.81	0.63
2:A:605:HEM:HBD2	11:A:1019:HOH:O	1.99	0.62
1:A:227:LEU:HD13	1:A:270:LEU:HD22	1.82	0.62
1:A:393:ASP:OD2	1:A:558:HIS:HB2	2.00	0.61
1:A:258:GLU:HG3	5:A:608:PZR:C1	2.31	0.60
1:A:170:PRO:CB	1:A:171:PRO:CD	2.70	0.60
1:A:258:GLU:CG	5:A:608:PZR:H3	2.31	0.60
1:A:117:THR:HG22	1:A:164:GLY:HA2	1.84	0.59
1:A:500:PRO:HB2	9:A:621:PEG:H22	1.85	0.59
1:A:10:VAL:HB	1:A:41:ARG:NH2	2.18	0.58
1:A:352:MET:SD	1:A:407:MET:SD	3.01	0.58
1:A:472:LYS:HZ2	9:A:621:PEG:H32	1.68	0.58
1:A:8:ALA:H	1:A:9:PRO:CD	2.16	0.58
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.41	0.56
1:A:202:ARG:HD2	10:A:622:GOL:H32	1.87	0.55
1:A:258:GLU:CD	2:A:605:HEM:HMB3	2.25	0.55
1:A:258:GLU:HG3	5:A:608:PZR:C2	2.37	0.55
1:A:572:TYR:CD1	1:A:573:PRO:HA	2.42	0.54
1:A:501:MET:O	9:A:621:PEG:H21	2.07	0.54
1:A:472:LYS:HZ1	9:A:621:PEG:H32	1.67	0.54
1:A:227:LEU:HD23	11:A:728:HOH:O	2.07	0.54
1:A:470:VAL:CG2	9:A:620:PEG:H11	2.37	0.54
1:A:348:ARG:HG2	2:A:605:HEM:CMD	2.36	0.54
1:A:240:ILE:HD12	11:A:757:HOH:O	2.08	0.54
1:A:578:ASP:O	1:A:581:THR:HB	2.08	0.54
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.43	0.53
1:A:258:GLU:HG3	5:A:608:PZR:H1	1.90	0.53
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.07	0.53
1:A:158:MET:HE1	1:A:432:ASP:H	1.73	0.53
1:A:197:PRO:HB3	9:A:619:PEG:C4	2.39	0.53
1:A:208:SER:HB3	6:A:611:NAG:H62	1.91	0.53
1:A:119:LEU:HD13	1:A:170:PRO:HG3	1.90	0.53
1:A:472:LYS:CE	9:A:621:PEG:H32	2.38	0.53
1:A:8:ALA:N	1:A:9:PRO:CD	2.72	0.52
1:A:153:THR:HG22	1:A:154:GLN:HG3	1.92	0.52
1:A:257:SER:O	1:A:381:PHE:HA	2.09	0.52
1:A:8:ALA:H	1:A:9:PRO:HD3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:MET:HB3	1:A:501:MET:HE3	1.91	0.51
1:A:16:ASP:OD1	1:A:19:SER:HB3	2.10	0.51
1:A:441:CYS:SG	1:A:492:ILE:HG22	2.51	0.50
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.94	0.50
1:A:208:SER:CB	6:A:611:NAG:H62	2.42	0.50
1:A:193:TYR:CE1	1:A:297:ARG:HG3	2.46	0.50
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.75	0.50
1:A:419:ASN:HD21	9:A:615:PEG:H32	1.77	0.50
1:A:127:THR:O	1:A:131:GLU:N	2.36	0.50
1:A:322:GLN:CA	1:A:322:GLN:NE2	2.28	0.50
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.94	0.49
1:A:322:GLN:HG2	11:A:963:HOH:O	2.12	0.49
1:A:464:LEU:O	1:A:468:GLN:HG3	2.12	0.49
1:A:440:ARG:NH1	1:A:443:ASP:OD2	2.46	0.49
1:A:227:LEU:HD12	11:A:738:HOH:O	2.11	0.49
1:A:158:MET:CE	1:A:432:ASP:H	2.25	0.49
1:A:266:HIS:HE1	11:A:670:HOH:O	1.96	0.49
1:A:220:TRP:CE3	9:A:618:PEG:H32	2.48	0.48
1:A:220:TRP:HE3	9:A:618:PEG:H32	1.78	0.48
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.48	0.48
1:A:393:ASP:OD1	1:A:557:THR:HB	2.14	0.48
1:A:227:LEU:HD21	1:A:267:THR:CA	2.42	0.48
1:A:172:TYR:OH	1:A:175:LEU:HB2	2.14	0.48
1:A:223:GLY:HA3	11:A:1034:HOH:O	2.14	0.48
1:A:298:LYS:HG2	1:A:536:PHE:CZ	2.49	0.47
1:A:117:THR:CG2	1:A:164:GLY:HA2	2.44	0.47
1:A:255:ARG:HD2	5:A:608:PZR:C4	2.45	0.47
1:A:146:LYS:O	1:A:147:ASN:HB2	2.15	0.47
1:A:255:ARG:HD2	5:A:608:PZR:C5	2.46	0.46
1:A:440:ARG:HD2	11:A:666:HOH:O	2.16	0.46
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.28	0.46
1:A:227:LEU:CD2	1:A:267:THR:HA	2.42	0.45
1:A:36:LEU:CD2	9:A:616:PEG:H42	2.46	0.45
1:A:91:VAL:O	1:A:91:VAL:HG22	2.17	0.45
1:A:220:TRP:CD1	1:A:220:TRP:C	2.89	0.45
1:A:82:ILE:HD13	1:A:480:LEU:CD2	2.47	0.45
1:A:77:GLU:HG2	1:A:483:LEU:HD21	1.99	0.44
1:A:278:ARG:HD2	11:A:905:HOH:O	2.17	0.44
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.43	0.44
1:A:345:PHE:CE2	1:A:440:ARG:HG3	2.52	0.44
1:A:203:LEU:HD11	1:A:252:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LYS:HD2	11:A:977:HOH:O	2.17	0.43
1:A:144:PHE:CE2	1:A:158:MET:HG3	2.53	0.43
1:A:163:ALA:N	1:A:440:ARG:HH12	2.16	0.43
1:A:584:LYS:NZ	1:A:584:LYS:HB3	2.33	0.43
1:A:301:GLY:O	1:A:305:GLN:HG3	2.18	0.43
1:A:36:LEU:HD21	9:A:616:PEG:H42	2.01	0.43
1:A:468:GLN:CD	1:A:474:LYS:HG2	2.39	0.42
1:A:233:LYS:HA	1:A:234:PRO:C	2.39	0.42
1:A:385:ARG:O	1:A:389:ASP:HB3	2.19	0.42
1:A:3:GLU:O	1:A:3:GLU:HG2	2.18	0.42
1:A:426:HIS:HA	11:A:922:HOH:O	2.20	0.42
1:A:334:SER:HB2	7:A:613:NAG:H5	2.01	0.41
1:A:387:ILE:CG2	9:A:617:PEG:H21	2.50	0.41
1:A:189:ALA:HB2	1:A:304:ILE:HD12	2.02	0.41
1:A:125:SER:HA	1:A:128:GLN:HB3	2.01	0.41
1:A:274:ASN:O	1:A:278:ARG:HG3	2.21	0.41
1:A:139:CYS:SG	1:A:141:PRO:HG3	2.60	0.41
1:A:196:GLU:HB3	1:A:198:SEP:OG	2.21	0.41
1:A:82:ILE:HD11	1:A:483:LEU:HD12	2.03	0.40
1:A:322:GLN:HE21	1:A:322:GLN:N	2.09	0.40
1:A:407:MET:HE3	1:A:412:MET:HG2	2.03	0.40
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.67	0.40
1:A:334:SER:CB	7:A:613:NAG:H5	2.51	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%)	560 (95%)	25 (4%)	7 (1%)	16 8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	PRO
1	A	173	GLN
1	A	424	PRO
1	A	169	THR
1	A	5	GLY
1	A	8	ALA
1	A	171	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	517/517 (100%)	511 (99%)	6 (1%)	78 81

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	220	TRP
1	A	288	ASN
1	A	322	GLN
1	A	347	PHE
1	A	581	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	266	HIS
1	A	288	ASN
1	A	322	GLN
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	0.91	0	8,12,14	2.29	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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O3P-P-O1P	-3.35	99.80	110.58
1	A	198	SEP	OG-CB-CA	2.86	110.71	108.27
1	A	198	SEP	O2P-P-OG	2.91	114.95	106.56
1	A	198	SEP	O3P-P-OG	2.96	115.08	106.56

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 [i](#)

4 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	NAG	A	609	1,6	14,14,15	0.25	0	15,19,21	0.83	1 (6%)
6	NAG	A	610	6	14,14,15	0.55	0	15,19,21	0.58	0
6	NAG	A	611	1,6	14,14,15	1.18	2 (14%)	15,19,21	1.14	1 (6%)
6	NAG	A	612	6	14,14,15	0.71	0	15,19,21	2.40	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
6	NAG	A	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	610	6	-	0/6/23/26	0/1/1/1
6	NAG	A	611	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	612	6	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	611	NAG	O5-C1	-2.42	1.39	1.43
6	A	611	NAG	O7-C7	-2.32	1.17	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	612	NAG	C2-N2-C7	-7.86	112.95	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	612	NAG	O6-C6-C5	-3.41	100.06	111.33
6	A	609	NAG	C3-C2-N2	-2.31	105.04	110.56
6	A	612	NAG	C3-C4-C5	2.14	113.93	110.20
6	A	611	NAG	C1-O5-C5	2.59	115.53	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	611	NAG	2	0

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 11 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	HEM	A	605	11,1	30,50,50	3.51	16 (53%)	24,82,82	3.14	11 (45%)
5	PZR	A	608	-	8,10,10	1.50	2 (25%)	8,13,13	1.64	2 (25%)
7	NAG	A	613	1	14,14,15	0.70	1 (7%)	15,19,21	1.12	1 (6%)
7	NAG	A	614	1	14,14,15	0.74	0	15,19,21	1.56	3 (20%)
9	PEG	A	615	-	6,6,6	0.83	0	5,5,5	2.16	1 (20%)
9	PEG	A	616	-	6,6,6	1.15	0	5,5,5	2.30	2 (40%)
9	PEG	A	617	-	6,6,6	0.77	0	5,5,5	2.11	1 (20%)
9	PEG	A	618	-	6,6,6	1.10	0	5,5,5	2.39	2 (40%)
9	PEG	A	619	-	6,6,6	0.98	0	5,5,5	2.55	2 (40%)
9	PEG	A	620	-	6,6,6	0.94	0	5,5,5	1.24	1 (20%)
9	PEG	A	621	-	6,6,6	0.86	0	5,5,5	2.32	2 (40%)
10	GOL	A	622	-	5,5,5	0.33	0	5,5,5	2.41	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SCN	A	6788	-	2,2,2	1.37	0	1,1,1	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	605	11,1	-	0/10/54/54	0/0/8/8
5	PZR	A	608	-	-	0/0/0/0	0/2/2/2
7	NAG	A	613	1	-	0/6/23/26	0/1/1/1
7	NAG	A	614	1	-	0/6/23/26	0/1/1/1
9	PEG	A	615	-	-	0/4/4/4	0/0/0/0
9	PEG	A	616	-	-	0/4/4/4	0/0/0/0
9	PEG	A	617	-	-	0/4/4/4	0/0/0/0
9	PEG	A	618	-	-	0/4/4/4	0/0/0/0
9	PEG	A	619	-	-	0/4/4/4	0/0/0/0
9	PEG	A	620	-	-	0/4/4/4	0/0/0/0
9	PEG	A	621	-	-	0/4/4/4	0/0/0/0
10	GOL	A	622	-	-	0/4/4/4	0/0/0/0
8	SCN	A	6788	-	-	0/0/0/0	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C3B-C4B	-9.43	1.43	1.51
2	A	605	HEM	C1C-NC	-5.45	1.29	1.36
2	A	605	HEM	C2C-C1C	-4.95	1.43	1.52
2	A	605	HEM	C4C-NC	-4.41	1.30	1.36
2	A	605	HEM	C2B-C1B	-3.02	1.42	1.51
5	A	608	PZR	C5-C6	-2.38	1.37	1.41
7	A	613	NAG	C1-C2	-2.09	1.49	1.52
2	A	605	HEM	CAD-C3D	-2.03	1.50	1.54
2	A	605	HEM	C4A-CHB	2.05	1.45	1.39
2	A	605	HEM	C3B-CAB	2.08	1.55	1.51
2	A	605	HEM	FE-NB	2.46	2.10	1.97
5	A	608	PZR	C1-C2	2.74	1.46	1.40
2	A	605	HEM	C2A-C3A	3.20	1.47	1.37
2	A	605	HEM	FE-ND	3.54	2.16	1.97
2	A	605	HEM	C1A-CHA	3.61	1.49	1.39
2	A	605	HEM	FE-NC	4.46	2.13	1.95
2	A	605	HEM	CHC-C1C	5.51	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	CHD-C1D	5.76	1.54	1.38
2	A	605	HEM	CHD-C4C	6.90	1.52	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEM	CBA-CAA-C2A	-6.30	101.23	112.53
10	A	622	GOL	O2-C2-C3	-5.35	84.14	108.65
9	A	619	PEG	O2-C3-C4	-4.54	89.53	110.43
9	A	618	PEG	O2-C3-C4	-4.31	90.60	110.43
9	A	616	PEG	O2-C3-C4	-4.28	90.74	110.43
9	A	615	PEG	O2-C3-C4	-4.25	90.88	110.43
9	A	617	PEG	O2-C3-C4	-4.07	91.68	110.43
2	A	605	HEM	CAD-CBD-CGD	-3.79	97.55	113.02
9	A	621	PEG	O2-C3-C4	-3.55	94.08	110.43
2	A	605	HEM	C2C-C1C-CHC	-3.43	118.45	123.68
7	A	614	NAG	C1-O5-C5	-3.20	108.19	112.25
7	A	614	NAG	C2-N2-C7	-2.87	119.35	123.04
7	A	614	NAG	O6-C6-C5	-2.71	102.38	111.33
7	A	613	NAG	O4-C4-C3	-2.49	104.74	110.34
9	A	620	PEG	O2-C3-C4	-2.34	99.67	110.43
5	A	608	PZR	C5-C4-N3	-2.08	122.00	123.91
2	A	605	HEM	C3C-CAC-CBC	2.05	127.59	124.46
9	A	616	PEG	C3-O2-C2	2.30	123.21	113.31
9	A	618	PEG	C3-O2-C2	2.47	123.93	113.31
2	A	605	HEM	C3B-C4B-CHC	2.62	126.85	123.16
2	A	605	HEM	C2C-C1C-NC	2.71	114.78	110.21
9	A	619	PEG	C3-O2-C2	2.92	125.87	113.31
5	A	608	PZR	C5-C6-N1	3.39	135.94	130.22
9	A	621	PEG	C3-O2-C2	3.65	129.00	113.31
2	A	605	HEM	CAD-C3D-C4D	3.77	125.78	112.47
2	A	605	HEM	C3B-CAB-CBB	3.98	130.56	124.46
2	A	605	HEM	CBD-CAD-C3D	4.02	125.25	113.55
2	A	605	HEM	CMB-C2B-C3B	4.49	127.73	116.53
2	A	605	HEM	CMC-C2C-C3C	7.93	136.33	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	605	HEM	8	0
5	A	608	PZR	8	0
7	A	613	NAG	2	0
9	A	615	PEG	1	0
9	A	616	PEG	2	0
9	A	617	PEG	1	0
9	A	618	PEG	3	0
9	A	619	PEG	3	0
9	A	620	PEG	2	0
9	A	621	PEG	6	0
10	A	622	GOL	3	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%)	0.62	59 (9%) 9 10	12, 23, 76, 115	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	20.9
1	A	121	SER	19.1
1	A	13	VAL	16.3
1	A	172	TYR	16.0
1	A	173	GLN	13.8
1	A	119	LEU	13.1
1	A	5	GLY	12.4
1	A	6	CYS	12.2
1	A	122	ASN	11.7
1	A	7	GLY	11.6
1	A	120	GLY	11.4
1	A	124	HIS	10.9
1	A	3	GLU	9.5
1	A	595	ASN	8.9
1	A	8	ALA	8.7
1	A	132	TYR	7.6
1	A	10	VAL	7.5
1	A	11	PRO	7.3
1	A	128	GLN	7.1
1	A	118	GLU	7.0
1	A	12	LEU	6.7
1	A	171	PRO	6.5
1	A	127	THR	6.5
1	A	1	SER	6.5
1	A	125	SER	6.4
1	A	129	CYS	6.3
1	A	169	THR	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	4	VAL	6.2
1	A	123	GLU	6.2
1	A	234	PRO	6.1
1	A	170	PRO	5.3
1	A	594	GLU	5.1
1	A	19	SER	4.7
1	A	126	LYS	4.5
1	A	168	PRO	4.4
1	A	134	ILE	4.4
1	A	18	ASN	3.9
1	A	167	CYS	3.9
1	A	593	ARG	3.9
1	A	174	SER	3.7
1	A	14	LYS	3.5
1	A	131	GLU	3.4
1	A	175	LEU	3.4
1	A	16	ASP	3.3
1	A	9	PRO	3.2
1	A	138	ASN	3.2
1	A	17	GLU	3.0
1	A	426	HIS	2.8
1	A	63	GLN	2.8
1	A	137	ASP	2.7
1	A	130	GLU	2.5
1	A	574	HIS	2.4
1	A	133	CYS	2.3
1	A	209	PRO	2.3
1	A	232	LYS	2.2
1	A	239	PHE	2.2
1	A	592	SER	2.2
1	A	322	GLN	2.1
1	A	425	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	0.72	0.25	-	34,38,44,45	0

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	NAG	A	609	14/15	0.82	0.17	1.65	34,40,42,42	0
6	NAG	A	611	14/15	0.89	0.12	-0.15	28,39,42,43	0
6	NAG	A	610	14/15	0.59	0.36	-	40,43,46,48	0
6	NAG	A	612	14/15	0.79	0.30	-	42,45,46,48	0

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
5	PZR	A	608	9/9	0.81	0.39	6.94	28,30,32,32	0
9	PEG	A	621	7/7	0.77	0.24	5.65	50,51,51,51	0
10	GOL	A	622	6/6	0.67	0.28	5.50	20,21,22,23	0
4	IOD	A	601	1/1	1.00	0.17	4.38	8,8,8,8	1
9	PEG	A	616	7/7	0.75	0.20	2.74	46,48,50,51	0
9	PEG	A	619	7/7	0.87	0.16	1.72	37,40,44,45	0
9	PEG	A	618	7/7	0.74	0.20	1.58	52,52,52,53	0
4	IOD	A	600	1/1	1.00	0.14	1.51	14,14,14,14	1
9	PEG	A	620	7/7	0.70	0.25	0.98	49,50,51,51	0
9	PEG	A	617	7/7	0.80	0.15	0.92	53,53,53,53	0
4	IOD	A	598	1/1	0.99	0.15	0.81	17,17,17,17	1
2	HEM	A	605	43/43	0.95	0.17	0.74	12,13,17,18	0
3	CA	A	606	1/1	0.98	0.13	0.33	18,18,18,18	0
8	SCN	A	6788	3/3	0.81	0.15	0.01	24,24,25,30	0
9	PEG	A	615	7/7	0.89	0.19	0.00	26,26,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	IOD	A	604	1/1	0.99	0.05	-0.73	44,44,44,44	0
4	IOD	A	599	1/1	0.98	0.09	-0.91	14,14,14,14	1
4	IOD	A	597	1/1	0.97	0.07	-1.48	61,61,61,61	1
4	IOD	A	603	1/1	0.96	0.07	-	85,85,85,85	0
4	IOD	A	596	1/1	0.99	0.09	-	24,24,24,24	1
7	NAG	A	613	14/15	0.84	0.26	-	36,40,44,47	0
4	IOD	A	602	1/1	0.94	0.08	-	54,54,54,54	1
4	IOD	A	607	1/1	0.99	0.23	-	50,50,50,50	0
7	NAG	A	614	14/15	0.84	0.29	-	30,35,39,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.