



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2020 – 10:10 AM JST

PDB ID : 7DN6
Title : Crystal structure of bovine lactoperoxidase with hydrogen peroxide trapped between heme iron and his109 at 1.69 Å resolution
Authors : Singh, P.K.; Singh, A.K.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2020-12-08
Resolution : 1.70 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.16

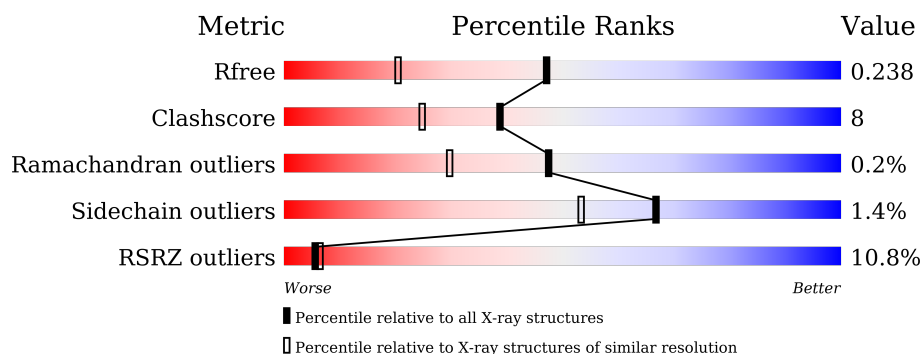
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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>11%</div> <div> <div></div> <div>86%</div> <div>13%</div> </div> </div>
2	C	2	<div> <div>50%</div> <div>50%</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	OSM	A	617	-	-	X	-
10	OSM	A	619	-	-	X	-
11	PEO	A	627	-	-	X	-

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.

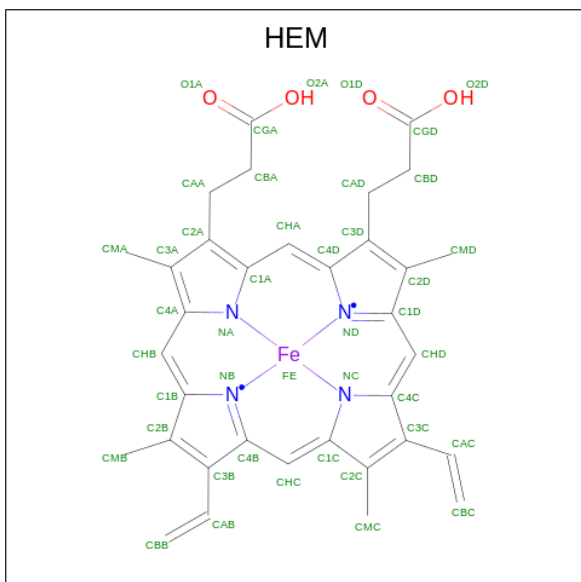
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4770	3037	847	860	26			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

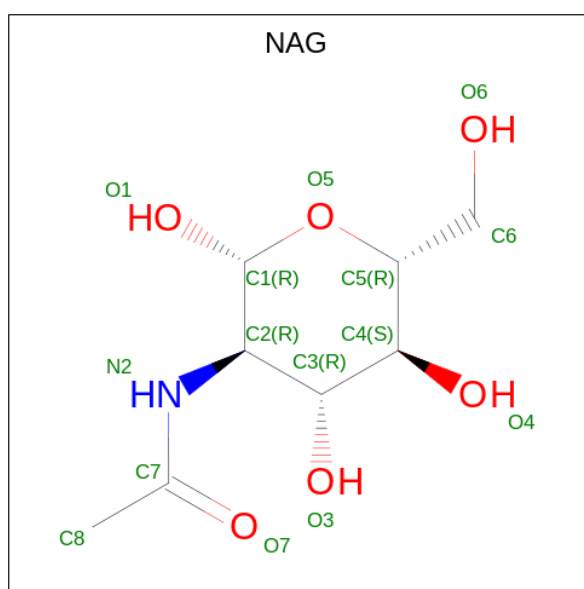


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

- 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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	I		
			19	19	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

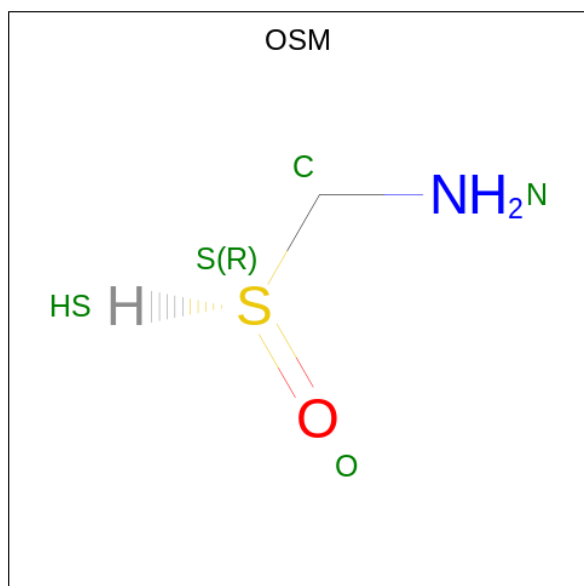


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

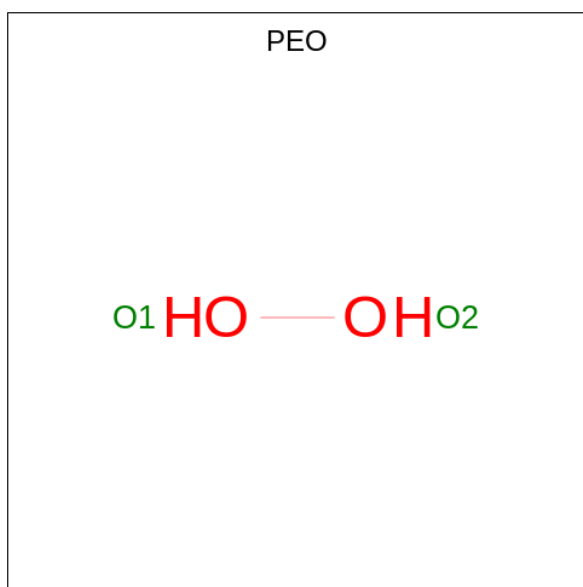
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Zn	0	0
			1	1		

- Molecule 10 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH₅NOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
10	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
10	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		

- Molecule 11 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H₂O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	O	0	0
			2	2		

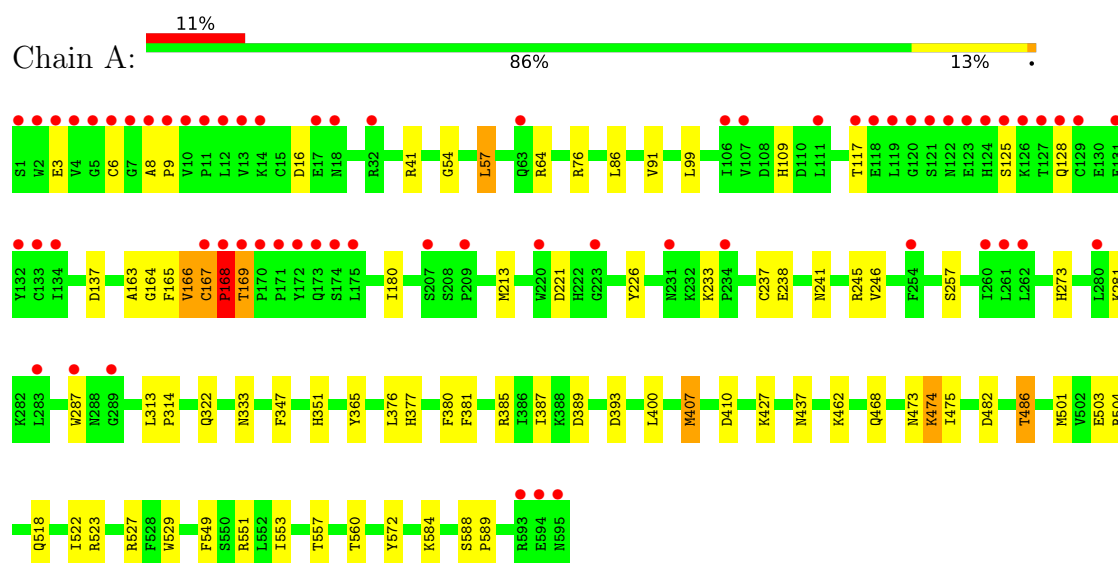
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	654	Total	O	0	0
			654	654		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lactoperoxidase



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.91Å 79.69Å 76.97Å 90.00° 102.23° 90.00°	Depositor
Resolution (Å)	39.41 – 1.70 39.41 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.41-1.70) 97.6 (39.41-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.197 , 0.235 0.204 , 0.238	Depositor DCC
R_{free} test set	3464 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5568	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, NAG, CA, EDO, PEO, OSM, 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	0.73	3/4898 (0.1%)	0.87	5/6645 (0.1%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	CYS	C-N	8.97	1.51	1.34
1	A	486	THR	C-N	7.18	1.47	1.34
1	A	57	LEU	C-N	7.11	1.47	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	PRO	N-CA-CB	-6.49	95.46	102.60
1	A	76	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	473	ASN	CB-CA-C	5.29	120.99	110.40
1	A	137	ASP	CB-CA-C	5.22	120.84	110.40
1	A	166	VAL	C-N-CA	5.05	134.32	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	CYS	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	4770	0	4689	66	0
2	C	28	0	25	1	0
3	A	43	0	30	0	0
4	A	1	0	0	0	0
5	A	28	0	26	0	0
6	A	19	0	0	4	0
7	A	6	0	8	0	0
8	A	4	0	6	0	0
9	A	1	0	0	0	0
10	A	12	0	14	5	0
11	A	2	0	0	2	0
12	A	654	0	0	28	0
All	All	5568	0	4798	73	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 8.

All (73) 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:407:MET:CG	1:A:501:MET:HE3	1.81	1.09
1:A:407:MET:HG3	1:A:501:MET:CE	1.83	1.08
1:A:407:MET:HG3	1:A:501:MET:HE3	1.09	1.05
1:A:407:MET:CG	1:A:501:MET:CE	2.37	1.01
1:A:117:THR:HG22	1:A:164:GLY:HA2	1.40	1.00
1:A:3:GLU:OE1	12:A:701:HOH:O	1.88	0.92
6:A:623:IOD:I	12:A:1166:HOH:O	2.58	0.91
1:A:109:HIS:NE2	11:A:627:PEO:O1	2.09	0.84
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.22	0.83
6:A:620:IOD:I	11:A:627:PEO:O1	2.67	0.83
1:A:462:LYS:HD2	12:A:816:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ASP:OD1	12:A:702:HOH:O	2.05	0.74
1:A:365:TYR:O	12:A:703:HOH:O	2.07	0.71
6:A:622:IOD:I	12:A:1343:HOH:O	2.79	0.70
1:A:165:PHE:CZ	1:A:169:THR:O	2.45	0.70
1:A:86:LEU:O	12:A:704:HOH:O	2.12	0.68
1:A:407:MET:HG2	1:A:501:MET:CE	2.23	0.65
10:A:617:OSM:N	12:A:716:HOH:O	2.30	0.63
10:A:617:OSM:H2	12:A:883:HOH:O	1.98	0.63
1:A:385:ARG:O	1:A:389:ASP:HB3	2.01	0.61
1:A:407:MET:CG	1:A:501:MET:HE2	2.26	0.60
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.38	0.58
1:A:287:TRP:O	12:A:706:HOH:O	2.18	0.57
1:A:246:VAL:HG11	1:A:387:ILE:HG13	1.87	0.57
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.41	0.56
1:A:125:SER:HA	1:A:128:GLN:HB3	1.88	0.56
1:A:117:THR:CG2	1:A:164:GLY:HA2	2.26	0.56
1:A:407:MET:HG2	1:A:501:MET:HE2	1.84	0.56
1:A:54:GLY:HA2	12:A:973:HOH:O	2.06	0.56
1:A:6:CYS:N	12:A:727:HOH:O	2.39	0.55
1:A:238:GLU:O	1:A:241:ASN:O	2.25	0.54
1:A:3:GLU:HA	1:A:3:GLU:OE2	2.08	0.54
1:A:64:ARG:NH2	12:A:725:HOH:O	2.38	0.54
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.43	0.54
1:A:560:THR:OG1	12:A:708:HOH:O	2.19	0.54
1:A:333:ASN:HD22	10:A:619:OSM:HS	1.56	0.54
1:A:237:CYS:HA	1:A:381:PHE:O	2.09	0.52
1:A:527:ARG:HD2	10:A:619:OSM:HN2	1.74	0.52
1:A:41:ARG:NH1	12:A:733:HOH:O	2.43	0.51
1:A:588:SER:OG	1:A:589:PRO:HD3	2.11	0.51
1:A:117:THR:HG22	1:A:164:GLY:CA	2.29	0.50
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.46	0.50
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.93	0.50
1:A:16:ASP:OD1	1:A:16:ASP:C	2.51	0.49
1:A:233:LYS:CE	12:A:1010:HOH:O	2.60	0.49
1:A:365:TYR:HB2	1:A:572:TYR:CD2	2.48	0.49
1:A:333:ASN:ND2	10:A:619:OSM:HS	2.12	0.48
1:A:281:LYS:NZ	12:A:706:HOH:O	2.47	0.47
1:A:588:SER:N	1:A:589:PRO:CD	2.78	0.47
1:A:518:GLN:O	1:A:522:ILE:HG23	2.15	0.47
1:A:313:LEU:N	1:A:314:PRO:CD	2.78	0.46
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ILE:HG23	12:A:1042:HOH:O	2.16	0.46
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.97	0.45
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.98	0.45
1:A:99:LEU:HD21	1:A:549:PHE:CD1	2.52	0.45
1:A:322:GLN:OE1	12:A:709:HOH:O	2.20	0.45
1:A:503:GLU:HG2	1:A:504:ARG:HG3	1.99	0.45
12:A:1146:HOH:O	2:C:2:NAG:H82	2.17	0.44
1:A:221:ASP:HB2	1:A:226:TYR:CE1	2.52	0.43
1:A:376:LEU:HD13	12:A:1060:HOH:O	2.19	0.43
1:A:169:THR:HG21	12:A:1230:HOH:O	2.18	0.43
1:A:245:ARG:NH2	12:A:754:HOH:O	2.50	0.43
1:A:117:THR:HG23	1:A:163:ALA:C	2.39	0.43
1:A:64:ARG:O	12:A:711:HOH:O	2.22	0.43
1:A:233:LYS:HE3	12:A:1010:HOH:O	2.20	0.42
1:A:393:ASP:OD1	1:A:557:THR:HB	2.19	0.42
1:A:427:LYS:HG2	12:A:1176:HOH:O	2.19	0.41
1:A:257:SER:O	1:A:381:PHE:HA	2.20	0.41
1:A:482:ASP:OD2	12:A:710:HOH:O	2.21	0.41
6:A:611:IOD:I	12:A:959:HOH:O	2.93	0.41
1:A:166:VAL:HG12	1:A:180:ILE:HG12	2.03	0.41
1:A:57:LEU:HD23	1:A:57:LEU:HA	1.87	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	593/595 (100%)	563 (95%)	29 (5%)	1 (0%)	47 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	518/518 (100%)	511 (99%)	7 (1%)	67 53

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	VAL
1	A	168	PRO
1	A	169	THR
1	A	347	PHE
1	A	407	MET
1	A	474	LYS
1	A	486	THR

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

Mol	Chain	Res	Type
1	A	135	GLN
1	A	147	ASN
1	A	173	GLN
1	A	333	ASN
1	A	521	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	0.84	0	17,19,21	1.18	2 (11%)
2	NAG	C	2	2	14,14,15	0.64	0	17,19,21	2.33	5 (29%)

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	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	6.63	121.17	112.19
2	C	2	NAG	C4-C3-C2	-3.80	105.44	111.02
2	C	2	NAG	O3-C3-C2	2.76	115.18	109.47
2	C	2	NAG	O5-C1-C2	-2.47	107.38	111.29
2	C	1	NAG	O4-C4-C5	2.37	115.17	109.30
2	C	1	NAG	O5-C1-C2	-2.26	107.72	111.29
2	C	2	NAG	C1-C2-N2	2.06	114.02	110.49

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 21 are monoatomic - leaving 9 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	$\# Z > 2$
10	OSM	A	617	-	1,3,3	0.03	0	0,2,2	0.00	-
3	HEM	A	601	1,11	27,50,50	1.18	3 (11%)	17,82,82	2.01	6 (35%)
7	GOL	A	614	-	5,5,5	0.23	0	5,5,5	0.36	0
10	OSM	A	618	-	1,3,3	0.02	0	0,2,2	0.00	-
5	NAG	A	603	1	14,14,15	0.51	0	17,19,21	1.68	3 (17%)
8	EDO	A	615	-	3,3,3	0.71	0	2,2,2	0.11	0
10	OSM	A	619	-	1,3,3	0.02	0	0,2,2	0.00	-
5	NAG	A	630	1	14,14,15	0.60	0	17,19,21	1.33	2 (11%)
11	PEO	A	627	3	1,1,1	0.55	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
10	OSM	A	617	-	-	0/0/1/1	-
3	HEM	A	601	1,11	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	614	-	-	4/4/4/4	-
10	OSM	A	618	-	-	0/0/1/1	-
5	NAG	A	603	1	-	0/6/23/26	0/1/1/1
8	EDO	A	615	-	-	1/1/1/1	-
10	OSM	A	619	-	-	0/0/1/1	-
5	NAG	A	630	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	HEM	C3C-C2C	-3.28	1.35	1.40
3	A	601	HEM	C3B-C2B	-2.51	1.36	1.40
3	A	601	HEM	C4D-C3D	2.00	1.47	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	HEM	C1D-C2D-C3D	-4.27	104.03	107.00
5	A	603	NAG	O5-C1-C2	-4.20	104.66	111.29
3	A	601	HEM	CMC-C2C-C3C	3.16	130.59	124.68
3	A	601	HEM	CMB-C2B-C3B	2.71	129.75	124.68
3	A	601	HEM	C4A-C3A-C2A	-2.68	105.13	107.00
5	A	630	NAG	C2-N2-C7	-2.60	119.20	122.90
5	A	630	NAG	O5-C5-C4	-2.60	104.51	110.83
5	A	603	NAG	O5-C5-C6	2.55	111.20	107.20
3	A	601	HEM	C4C-C3C-C2C	-2.41	105.21	106.90
3	A	601	HEM	C3B-C4B-NB	-2.36	106.16	109.21
5	A	603	NAG	C1-C2-N2	-2.08	106.94	110.49

There are no chirality outliers.

All (7) torsion outliers are listed below:

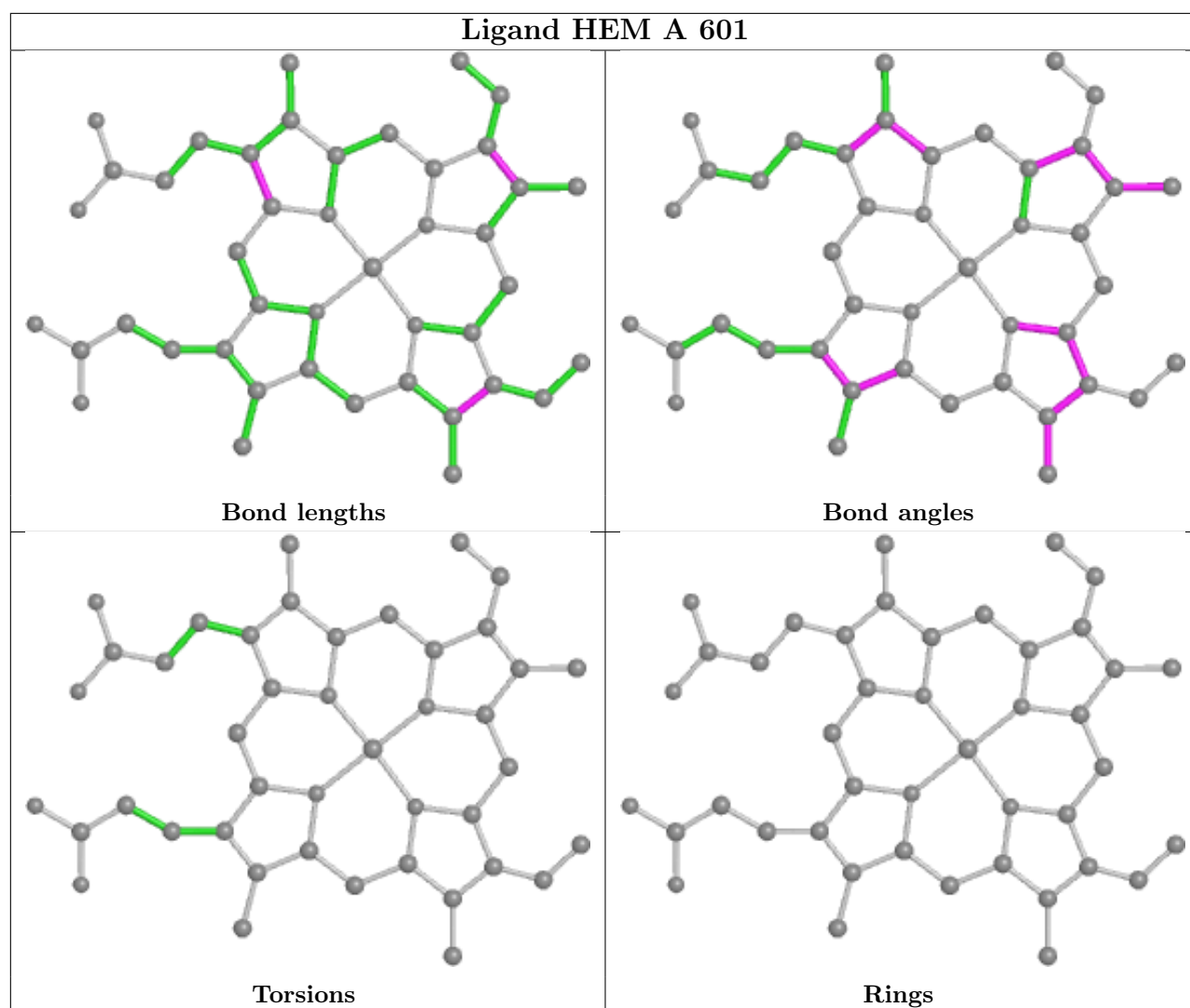
Mol	Chain	Res	Type	Atoms
7	A	614	GOL	O1-C1-C2-C3
7	A	614	GOL	C1-C2-C3-O3
5	A	630	NAG	C4-C5-C6-O6
7	A	614	GOL	O2-C2-C3-O3
7	A	614	GOL	O1-C1-C2-O2
5	A	630	NAG	O5-C5-C6-O6
8	A	615	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	617	OSM	2	0
10	A	619	OSM	3	0
11	A	627	PEO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	595/595 (100%)	0.89	64 (10%) 5 6	16, 31, 100, 173	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	SER	35.0
1	A	120	GLY	27.9
1	A	7	GLY	21.9
1	A	172	TYR	21.0
1	A	119	LEU	18.8
1	A	1	SER	16.8
1	A	171	PRO	13.6
1	A	121	SER	13.0
1	A	2	TRP	13.0
1	A	4	VAL	12.4
1	A	124	HIS	12.1
1	A	8	ALA	11.9
1	A	173	GLN	11.1
1	A	122	ASN	10.1
1	A	13	VAL	10.0
1	A	10	VAL	9.5
1	A	125	SER	9.4
1	A	170	PRO	8.8
1	A	595	ASN	8.1
1	A	6	CYS	8.0
1	A	594	GLU	7.8
1	A	12	LEU	7.1
1	A	11	PRO	6.9
1	A	168	PRO	6.7
1	A	169	THR	6.4
1	A	126	LYS	5.9
1	A	129	CYS	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	593	ARG	5.7
1	A	123	GLU	5.2
1	A	283	LEU	5.1
1	A	132	TYR	5.0
1	A	127	THR	4.7
1	A	128	GLN	4.6
1	A	175	LEU	4.4
1	A	118	GLU	4.1
1	A	5	GLY	4.1
1	A	3	GLU	3.4
1	A	287	TRP	3.4
1	A	209	PRO	3.3
1	A	167	CYS	3.3
1	A	280	LEU	3.1
1	A	14	LYS	3.1
1	A	223	GLY	3.1
1	A	17	GLU	3.1
1	A	9	PRO	3.0
1	A	18	ASN	2.9
1	A	106	ILE	2.7
1	A	107	VAL	2.7
1	A	220	TRP	2.6
1	A	117	THR	2.6
1	A	111	LEU	2.5
1	A	63	GLN	2.5
1	A	289	GLY	2.5
1	A	254	PHE	2.3
1	A	260	ILE	2.3
1	A	133	CYS	2.3
1	A	134	ILE	2.2
1	A	32	ARG	2.2
1	A	261	LEU	2.2
1	A	262	LEU	2.2
1	A	207	SER	2.1
1	A	231	ASN	2.1
1	A	234	PRO	2.1
1	A	131	GLU	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

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. 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	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.73	0.28	64,77,89,91	0
2	NAG	C	1	14/15	0.94	0.10	29,40,48,55	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. 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.

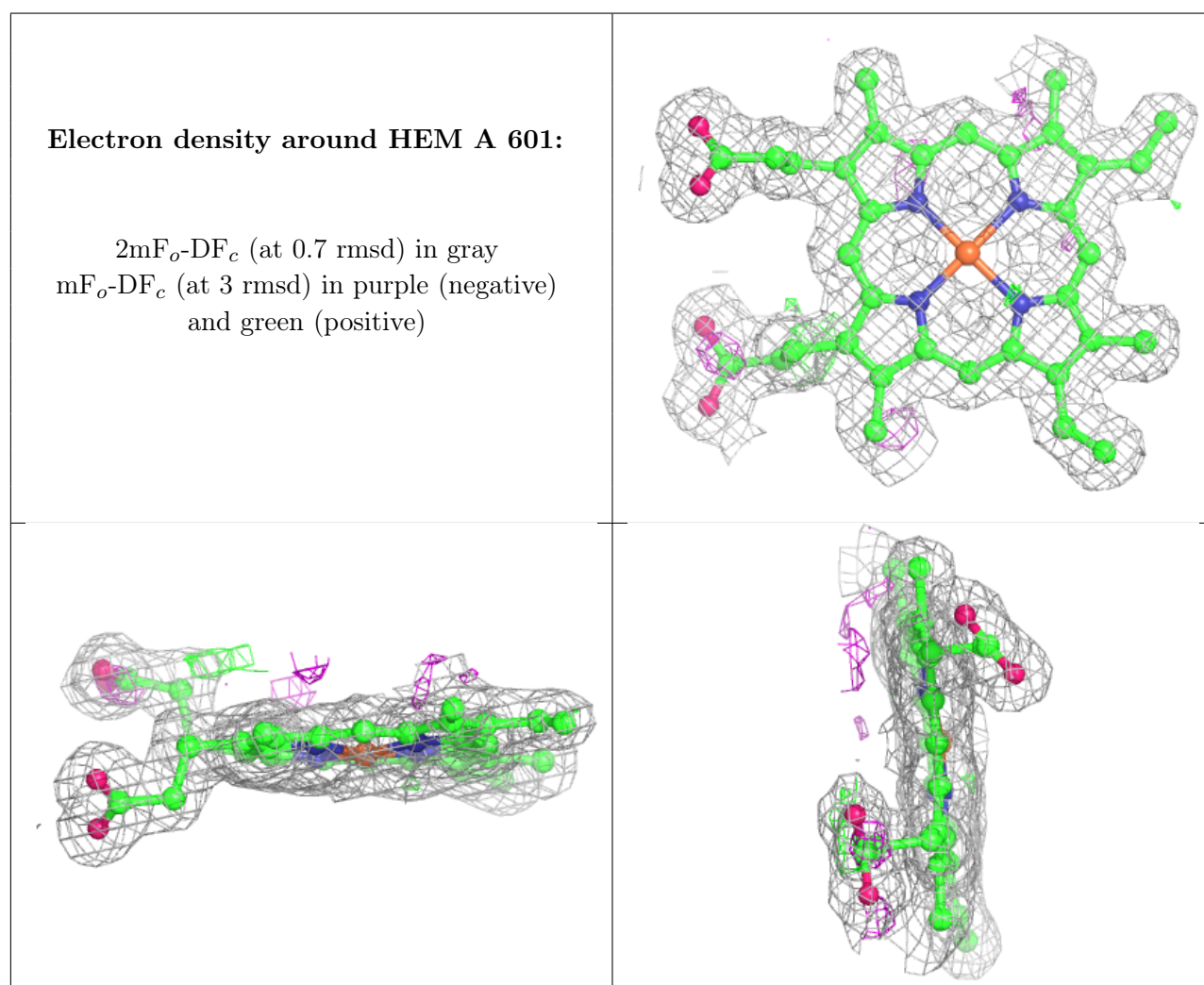
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	630	14/15	0.81	0.13	37,44,50,59	0
5	NAG	A	603	14/15	0.83	0.20	43,51,56,56	0
6	IOD	A	610	1/1	0.85	0.10	60,60,60,60	1
7	GOL	A	614	6/6	0.88	0.17	35,42,52,53	0
8	EDO	A	615	4/4	0.92	0.11	29,31,31,31	0
10	OSM	A	617	4/4	0.93	0.11	40,42,43,53	0
10	OSM	A	619	4/4	0.93	0.23	30,32,36,37	4
6	IOD	A	626	1/1	0.93	0.05	45,45,45,45	0
6	IOD	A	611	1/1	0.94	0.04	48,48,48,48	1
6	IOD	A	612	1/1	0.94	0.04	46,46,46,46	1
11	PEO	A	627	2/2	0.96	0.20	16,16,16,29	0
6	IOD	A	621	1/1	0.96	0.04	45,45,45,45	1
6	IOD	A	625	1/1	0.96	0.05	40,40,40,40	1
10	OSM	A	618	4/4	0.96	0.13	35,35,36,38	0
6	IOD	A	622	1/1	0.96	0.05	41,41,41,41	1
6	IOD	A	606	1/1	0.96	0.06	47,47,47,47	1
6	IOD	A	628	1/1	0.96	0.09	54,54,54,54	1
6	IOD	A	607	1/1	0.97	0.03	44,44,44,44	1
6	IOD	A	623	1/1	0.97	0.10	51,51,51,51	1
9	ZN	A	616	1/1	0.97	0.04	39,39,39,39	0
6	IOD	A	609	1/1	0.98	0.05	40,40,40,40	1
6	IOD	A	605	1/1	0.98	0.04	32,32,32,32	1
3	HEM	A	601	43/43	0.98	0.17	16,18,23,25	0
6	IOD	A	629	1/1	0.98	0.07	58,58,58,58	1
6	IOD	A	613	1/1	0.98	0.14	42,42,42,42	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	IOD	A	620	1/1	0.99	0.07	28,28,28,28	1
6	IOD	A	624	1/1	0.99	0.03	39,39,39,39	1
6	IOD	A	608	1/1	0.99	0.03	32,32,32,32	0
4	CA	A	602	1/1	1.00	0.06	20,20,20,20	0
6	IOD	A	604	1/1	1.00	0.06	19,19,19,19	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.