



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:25 AM EDT

PDB ID : 4QJQ / pdb_00004qjq
Title : Crystal structure of goat lactoperoxidase in complex with octopamine at 2.1 Angstrom resolution
Authors : Singh, R.P.; Kushwaha, G.S.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2014-06-04
Resolution : 2.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

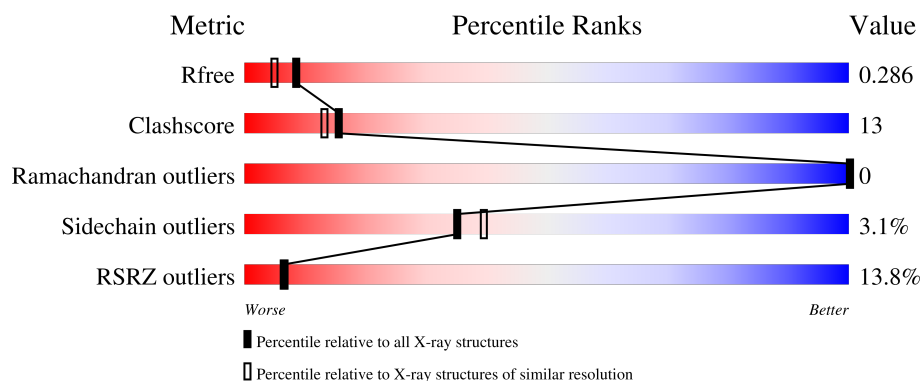
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	14% 79% 19%

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
7	OTR	A	614	-	-	X	-

2 Entry composition [i](#)

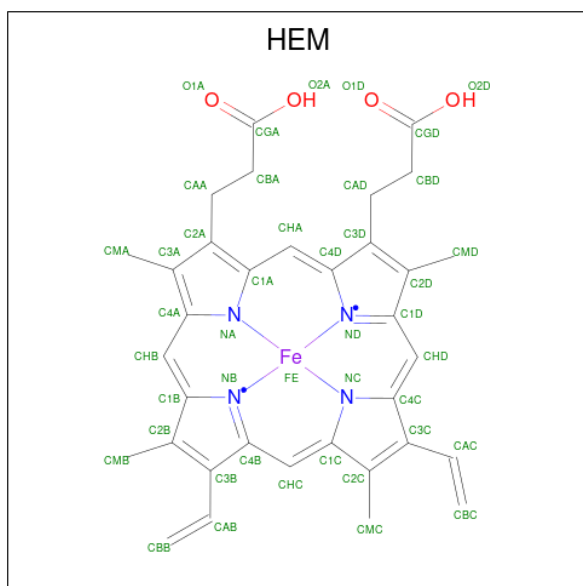
There are 10 unique types of molecules in this entry. The entry contains 5216 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			4758	3021	844	866	1	26			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

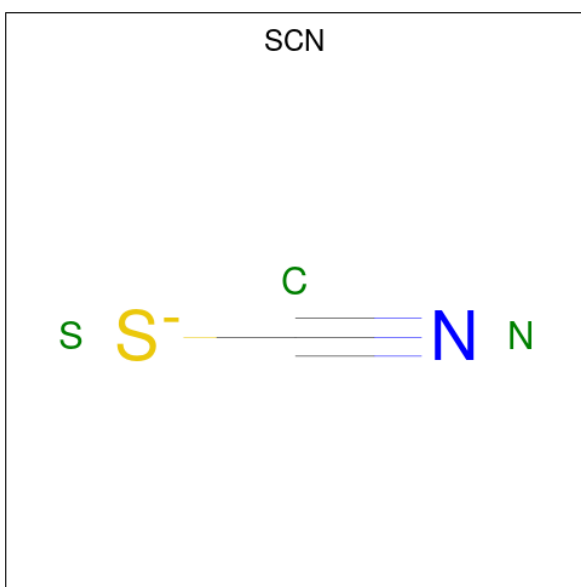
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is IODIDE ION (CCD ID: IOD) (formula: I).

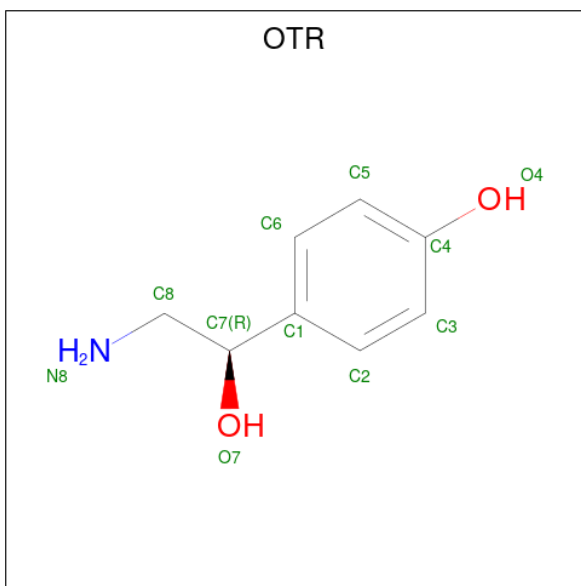
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	I	0	0
			13	13		

- Molecule 6 is THIOCYANATE ION (CCD ID: 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 4-(2R-AMINO-1-HYDROXYETHYL)PHENOL (CCD ID: OTR) (formula: $C_8H_{11}NO_2$).



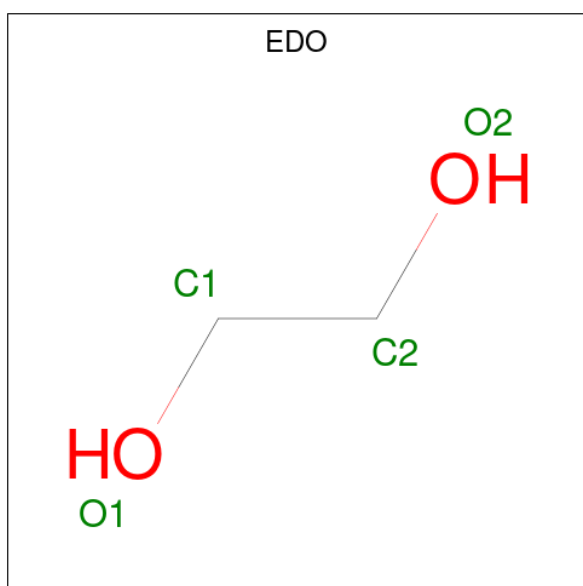
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			11	8	1	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	309	Total 309	O 309	0	0

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.95Å 80.36Å 75.39Å 90.00° 102.81° 90.00°	Depositor
Resolution (Å)	73.51 – 2.10 73.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.7 (73.51-2.10) 99.5 (73.51-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.204 , 0.278 0.220 , 0.286	Depositor DCC
R_{free} test set	1838 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.922	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: SCN, IOD, CA, PEG, EDO, SEP, NAG, HEM, OTR

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	0.88	4/4876 (0.1%)	1.00	9/6621 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	VAL	C-O	-5.40	1.17	1.24
1	A	194	GLY	C-O	-5.34	1.17	1.23
1	A	460	GLN	C-O	-5.11	1.19	1.24
1	A	168	PRO	N-CD	5.10	1.54	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	CYS	N-CA-C	-7.06	103.52	111.07
1	A	369	GLY	CA-C-N	5.92	125.31	118.85
1	A	369	GLY	C-N-CA	5.92	125.31	118.85
1	A	260	ILE	N-CA-C	5.71	118.19	111.05
1	A	12	LEU	N-CA-C	5.70	122.94	110.80
1	A	316	VAL	CB-CA-C	-5.67	104.61	112.04
1	A	395	LEU	N-CA-C	-5.32	105.15	111.69
1	A	152	LYS	N-CA-C	5.25	117.75	111.71
1	A	10	VAL	C-N-CD	-5.03	109.54	120.60

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	4758	0	4644	122	0
2	A	43	0	30	14	0
3	A	56	0	52	0	0
4	A	1	0	0	0	0
5	A	13	0	0	2	0
6	A	3	0	0	0	0
7	A	11	0	10	9	0
8	A	14	0	20	1	0
9	A	8	0	12	2	0
10	A	309	0	0	19	0
All	All	5216	0	4768	130	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 (130) 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:53:ASP:CG	1:A:55:LEU:HB2	1.45	1.42
1:A:258:GLU:OE2	2:A:601:HEM:HMB3	1.45	1.15
1:A:108:ASP:OD2	2:A:601:HEM:HMD1	1.46	1.15
1:A:484:TYR:CE1	1:A:490:ILE:HA	1.91	1.05
1:A:108:ASP:OD2	2:A:601:HEM:CMD	2.06	1.02
2:A:601:HEM:HMB1	2:A:601:HEM:HBB2	1.40	1.02
1:A:53:ASP:CG	1:A:55:LEU:CB	2.31	1.02
1:A:53:ASP:OD1	1:A:55:LEU:HB2	1.63	0.99
1:A:51:TYR:CG	1:A:55:LEU:O	2.22	0.91
1:A:138:GLU:O	1:A:162:ARG:HG3	1.74	0.88
1:A:53:ASP:OD2	1:A:55:LEU:CB	2.22	0.87
1:A:258:GLU:HG3	7:A:614:OTR:C3	2.05	0.85
1:A:53:ASP:OD2	1:A:55:LEU:HB2	1.75	0.83
1:A:258:GLU:OE2	2:A:601:HEM:CMB	2.29	0.80
1:A:10:VAL:HB	1:A:11:PRO:HA	1.64	0.80
1:A:51:TYR:CB	1:A:55:LEU:O	2.30	0.80
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.11	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASP:OD1	1:A:55:LEU:CB	2.29	0.78
5:A:621:IOD:I	10:A:993:HOH:O	2.70	0.77
1:A:258:GLU:HG3	7:A:614:OTR:C2	2.14	0.77
1:A:572:TYR:CG	1:A:573:PRO:HA	2.20	0.76
1:A:258:GLU:HG3	7:A:614:OTR:H3	1.67	0.76
1:A:572:TYR:CD2	1:A:573:PRO:HA	2.20	0.74
1:A:258:GLU:CG	7:A:614:OTR:H3	2.18	0.74
1:A:53:ASP:OD2	1:A:55:LEU:HB3	1.93	0.69
2:A:601:HEM:CHA	10:A:937:HOH:O	2.41	0.69
1:A:350:GLY:HA3	2:A:601:HEM:CAC	2.23	0.68
1:A:51:TYR:CD2	1:A:55:LEU:O	2.46	0.68
1:A:156:LYS:NZ	10:A:981:HOH:O	2.17	0.68
1:A:137:ASP:CB	10:A:925:HOH:O	2.40	0.68
1:A:137:ASP:HB2	10:A:925:HOH:O	1.94	0.68
1:A:278:ARG:NH1	10:A:827:HOH:O	2.26	0.67
1:A:484:TYR:CZ	1:A:490:ILE:HA	2.30	0.67
1:A:132:TYR:HE2	10:A:736:HOH:O	1.78	0.66
1:A:230:ASN:HB2	1:A:250:GLN:HG2	1.78	0.65
1:A:381:PHE:HZ	7:A:614:OTR:H81	1.60	0.64
1:A:481:LEU:O	1:A:485:LYS:HA	1.97	0.64
1:A:484:TYR:CD2	1:A:490:ILE:HG12	2.33	0.64
1:A:106:ILE:HG13	1:A:265:VAL:HG11	1.81	0.63
1:A:230:ASN:HB2	1:A:250:GLN:CG	2.30	0.62
1:A:102:GLN:HG3	1:A:265:VAL:HG21	1.82	0.61
1:A:572:TYR:CZ	1:A:573:PRO:HB3	2.35	0.61
1:A:261:LEU:O	1:A:265:VAL:HG23	2.02	0.60
1:A:407:MET:SD	1:A:408:ASN:N	2.75	0.59
1:A:409:GLN:OE1	1:A:473:ASN:ND2	2.34	0.58
1:A:105:GLN:HG3	2:A:601:HEM:C1C	2.40	0.57
1:A:381:PHE:CZ	7:A:614:OTR:H81	2.40	0.56
1:A:7:GLY:N	1:A:167:CYS:SG	2.77	0.56
1:A:420:LYS:NZ	10:A:912:HOH:O	2.38	0.56
1:A:137:ASP:HB3	10:A:925:HOH:O	2.04	0.56
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.40	0.56
1:A:258:GLU:CB	7:A:614:OTR:H3	2.35	0.56
2:A:601:HEM:HMB1	2:A:601:HEM:CBB	2.26	0.55
1:A:258:GLU:HG3	7:A:614:OTR:H2	1.88	0.55
1:A:424:PRO:O	1:A:425:THR:OG1	2.13	0.55
1:A:53:ASP:OD1	1:A:55:LEU:CA	2.55	0.55
1:A:572:TYR:CG	1:A:573:PRO:CA	2.89	0.55
1:A:173:GLN:NE2	10:A:983:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:HB2	1:A:167:CYS:HB2	1.90	0.54
1:A:169:THR:HB	1:A:170:PRO:HD2	1.89	0.53
1:A:16:ASP:OD1	1:A:16:ASP:C	2.52	0.53
1:A:588:SER:HB2	10:A:940:HOH:O	2.10	0.53
1:A:10:VAL:CB	1:A:11:PRO:HA	2.36	0.52
1:A:393:ASP:OD1	1:A:557:THR:HB	2.09	0.52
1:A:233:LYS:O	1:A:233:LYS:HG3	2.08	0.51
1:A:259:GLN:HG2	2:A:601:HEM:CBB	2.40	0.51
1:A:116:GLU:HA	1:A:163:ALA:HA	1.92	0.51
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.93	0.51
1:A:298:LYS:HE2	1:A:536:PHE:CE1	2.46	0.51
1:A:361:LEU:O	1:A:397:ARG:NE	2.41	0.51
1:A:481:LEU:O	1:A:485:LYS:N	2.43	0.50
1:A:10:VAL:HB	1:A:11:PRO:CA	2.36	0.50
1:A:108:ASP:OD2	2:A:601:HEM:HMD2	2.06	0.50
1:A:484:TYR:CD1	1:A:490:ILE:HA	2.41	0.50
1:A:117:THR:HG23	1:A:164:GLY:HA2	1.94	0.50
1:A:481:LEU:O	1:A:485:LYS:CA	2.59	0.49
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.46	0.49
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.42	0.49
1:A:237:CYS:HA	1:A:381:PHE:O	2.13	0.48
1:A:560:THR:HA	1:A:579:CYS:SG	2.52	0.48
1:A:57:VAL:HG13	1:A:61:TRP:CG	2.48	0.48
1:A:118:GLU:O	1:A:121:SER:HB2	2.14	0.48
1:A:198:SEP:P	1:A:198:SEP:H	2.36	0.48
1:A:536:PHE:O	1:A:541:ARG:NH1	2.48	0.47
1:A:329:GLN:HG2	10:A:941:HOH:O	2.14	0.47
1:A:588:SER:CB	10:A:940:HOH:O	2.63	0.47
1:A:167:CYS:O	1:A:169:THR:HG23	2.14	0.47
1:A:47:LEU:HA	8:A:616:PEG:H21	1.97	0.46
1:A:167:CYS:O	1:A:168:PRO:C	2.57	0.46
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.50	0.46
1:A:572:TYR:C	1:A:572:TYR:CD1	2.93	0.46
1:A:17:GLU:HG3	1:A:18:GLN:N	2.31	0.45
1:A:51:TYR:HB3	1:A:55:LEU:O	2.14	0.45
1:A:574:HIS:HB2	10:A:903:HOH:O	2.16	0.45
1:A:407:MET:HB3	1:A:501:MET:HE3	1.99	0.45
1:A:530:TRP:CZ2	1:A:531:GLU:HG3	2.51	0.45
1:A:56:ALA:HB1	1:A:177:ARG:HD3	2.00	0.44
1:A:433:LEU:HD13	2:A:601:HEM:HMA1	1.99	0.44
1:A:481:LEU:HD21	1:A:487:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ILE:HD12	1:A:522:ILE:C	2.42	0.44
1:A:53:ASP:OD1	1:A:55:LEU:C	2.61	0.44
9:A:625:EDO:H11	10:A:988:HOH:O	2.17	0.44
1:A:208:SER:C	1:A:210:LEU:H	2.26	0.44
1:A:571:ASN:N	1:A:571:ASN:HD22	2.15	0.44
1:A:424:PRO:HG2	7:A:614:OTR:H82	1.99	0.43
1:A:572:TYR:CE1	1:A:573:PRO:HB3	2.52	0.43
1:A:424:PRO:C	1:A:425:THR:HG23	2.42	0.43
1:A:51:TYR:CD1	1:A:57:VAL:O	2.72	0.43
9:A:625:EDO:C1	10:A:988:HOH:O	2.65	0.43
1:A:171:PRO:HG2	1:A:173:GLN:HB2	2.00	0.43
1:A:484:TYR:O	1:A:485:LYS:HB2	2.18	0.43
1:A:449:TYR:OH	1:A:499:GLU:OE2	2.30	0.43
1:A:51:TYR:HD1	1:A:57:VAL:O	2.02	0.42
1:A:53:ASP:OD1	1:A:55:LEU:N	2.53	0.42
1:A:373:GLU:HB2	5:A:622:IOD:I	2.90	0.42
1:A:291:MET:HE3	1:A:295:GLU:HG3	2.01	0.42
1:A:362:ASP:OD1	1:A:362:ASP:C	2.63	0.42
1:A:9:PRO:CB	1:A:11:PRO:HB3	2.51	0.41
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.55	0.41
1:A:407:MET:HB3	1:A:501:MET:CE	2.50	0.41
1:A:137:ASP:HB3	1:A:138:GLU:H	1.66	0.41
1:A:244:ALA:O	1:A:245:HIS:C	2.64	0.41
1:A:117:THR:CG2	10:A:853:HOH:O	2.68	0.41
1:A:202:ARG:HD3	10:A:933:HOH:O	2.20	0.41
1:A:349:PHE:CD1	1:A:349:PHE:C	2.99	0.41
1:A:432:ASP:OD1	1:A:432:ASP:C	2.63	0.41
1:A:281:LYS:O	1:A:282:ARG:C	2.64	0.41
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.56	0.40
1:A:122:SER:HB2	10:A:797:HOH:O	2.22	0.40
1:A:484:TYR:CE2	1:A:490:ILE:HG12	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%)	564 (95%)	28 (5%)	0	100	100

There are no Ramachandran outliers to report.

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%)	500 (97%)	16 (3%)	35	39

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	32	ARG
1	A	117	THR
1	A	118	GLU
1	A	128	GLN
1	A	138	GLU
1	A	146	LYS
1	A	233	LYS
1	A	250	GLN
1	A	410	ASN
1	A	423	GLN
1	A	474	LYS
1	A	481	LEU
1	A	503	GLU
1	A	538	GLU
1	A	545	GLN

Sometimes 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	94	GLN
1	A	147	ASN
1	A	250	GLN
1	A	329	GLN
1	A	429	HIS
1	A	521	GLN
1	A	545	GLN
1	A	556	ASN
1	A	565	HIS
1	A	571	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	0.76	0	7,12,14	1.17	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
1	SEP	A	198	1	-	5/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	N-CA-CB-OG
1	A	198	SEP	CA-CB-OG-P
1	A	198	SEP	CB-OG-P-O1P
1	A	198	SEP	CB-OG-P-O2P
1	A	198	SEP	CB-OG-P-O3P

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 14 are monoatomic - leaving 11 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$
9	EDO	A	624	-	3,3,3	0.47	0	2,2,2	0.19	0
3	NAG	A	605	1	14,14,15	0.57	0	17,19,21	1.45	2 (11%)
8	PEG	A	616	-	6,6,6	0.52	0	5,5,5	0.80	0
7	OTR	A	614	-	11,11,11	2.40	5 (45%)	14,14,14	1.80	2 (14%)
3	NAG	A	603	1	14,14,15	0.65	0	17,19,21	1.51	3 (17%)
3	NAG	A	604	1	14,14,15	0.61	0	17,19,21	1.53	3 (17%)
2	HEM	A	601	10	50,50,50	1.55	8 (16%)	67,82,82	1.60	12 (17%)
3	NAG	A	602	1	14,14,15	0.83	1 (7%)	17,19,21	1.25	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SCN	A	613	-	1,2,2	1.23	0	0,1,1	-	-
9	EDO	A	625	-	3,3,3	0.46	0	2,2,2	1.16	0
8	PEG	A	615	-	6,6,6	0.50	0	5,5,5	0.34	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
9	EDO	A	624	-	-	1/1/1/1	-
3	NAG	A	605	1	-	0/6/23/26	0/1/1/1
8	PEG	A	616	-	-	3/4/4/4	-
7	OTR	A	614	-	-	4/6/6/6	0/1/1/1
3	NAG	A	603	1	-	0/6/23/26	0/1/1/1
3	NAG	A	604	1	-	1/6/23/26	0/1/1/1
2	HEM	A	601	10	-	4/14/54/54	-
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
9	EDO	A	625	-	-	1/1/1/1	-
8	PEG	A	615	-	-	1/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	FE-NB	5.13	2.10	1.94
7	A	614	OTR	C1-C7	-4.41	1.44	1.51
2	A	601	HEM	FE-NC	4.09	2.08	1.95
7	A	614	OTR	C3-C4	-3.60	1.32	1.39
2	A	601	HEM	C4D-ND	-3.27	1.34	1.40
2	A	601	HEM	C1B-NB	-3.27	1.34	1.40
7	A	614	OTR	C2-C1	-2.92	1.34	1.39
7	A	614	OTR	O4-C4	-2.79	1.30	1.37
7	A	614	OTR	C5-C4	-2.78	1.33	1.39
2	A	601	HEM	FE-ND	-2.58	1.87	1.94
3	A	602	NAG	O5-C1	-2.34	1.39	1.43
2	A	601	HEM	C1C-C2C	-2.29	1.40	1.45
2	A	601	HEM	C1D-ND	-2.12	1.34	1.38
2	A	601	HEM	C4B-NB	-2.05	1.34	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	CHC-C4B-NB	4.35	129.10	124.42
7	A	614	OTR	O7-C7-C1	-4.12	101.14	111.05
3	A	605	NAG	O5-C1-C2	-4.06	105.00	111.29
2	A	601	HEM	C1B-NB-C4B	3.93	109.86	105.21
2	A	601	HEM	CHD-C1D-ND	3.88	128.60	124.42
3	A	603	NAG	C1-O5-C5	3.76	117.22	112.19
2	A	601	HEM	C3B-C4B-NB	-3.17	107.19	109.47
2	A	601	HEM	CHA-C4D-ND	2.96	128.03	124.37
2	A	601	HEM	CHB-C1B-NB	2.96	128.03	124.37
7	A	614	OTR	C3-C2-C1	-2.89	118.30	121.18
2	A	601	HEM	C1A-CHA-C4D	-2.72	119.84	126.25
3	A	604	NAG	O7-C7-C8	-2.60	117.43	122.05
3	A	603	NAG	O6-C6-C5	-2.56	102.61	111.33
2	A	601	HEM	C4D-ND-C1D	2.56	108.24	105.21
2	A	601	HEM	C1C-CHC-C4B	-2.37	120.99	126.02
3	A	603	NAG	O5-C1-C2	-2.34	107.68	111.29
3	A	605	NAG	C1-O5-C5	2.27	115.22	112.19
3	A	602	NAG	C1-O5-C5	2.21	115.14	112.19
2	A	601	HEM	CHD-C4C-NC	2.20	126.84	124.45
3	A	604	NAG	C4-C3-C2	2.12	114.12	111.02
2	A	601	HEM	C4C-CHD-C1D	-2.09	121.57	126.02
2	A	601	HEM	C4C-NC-C1C	2.01	109.10	105.82
3	A	604	NAG	O5-C5-C6	2.00	111.56	107.66

There are no chirality outliers.

All (15) torsion outliers are listed below:

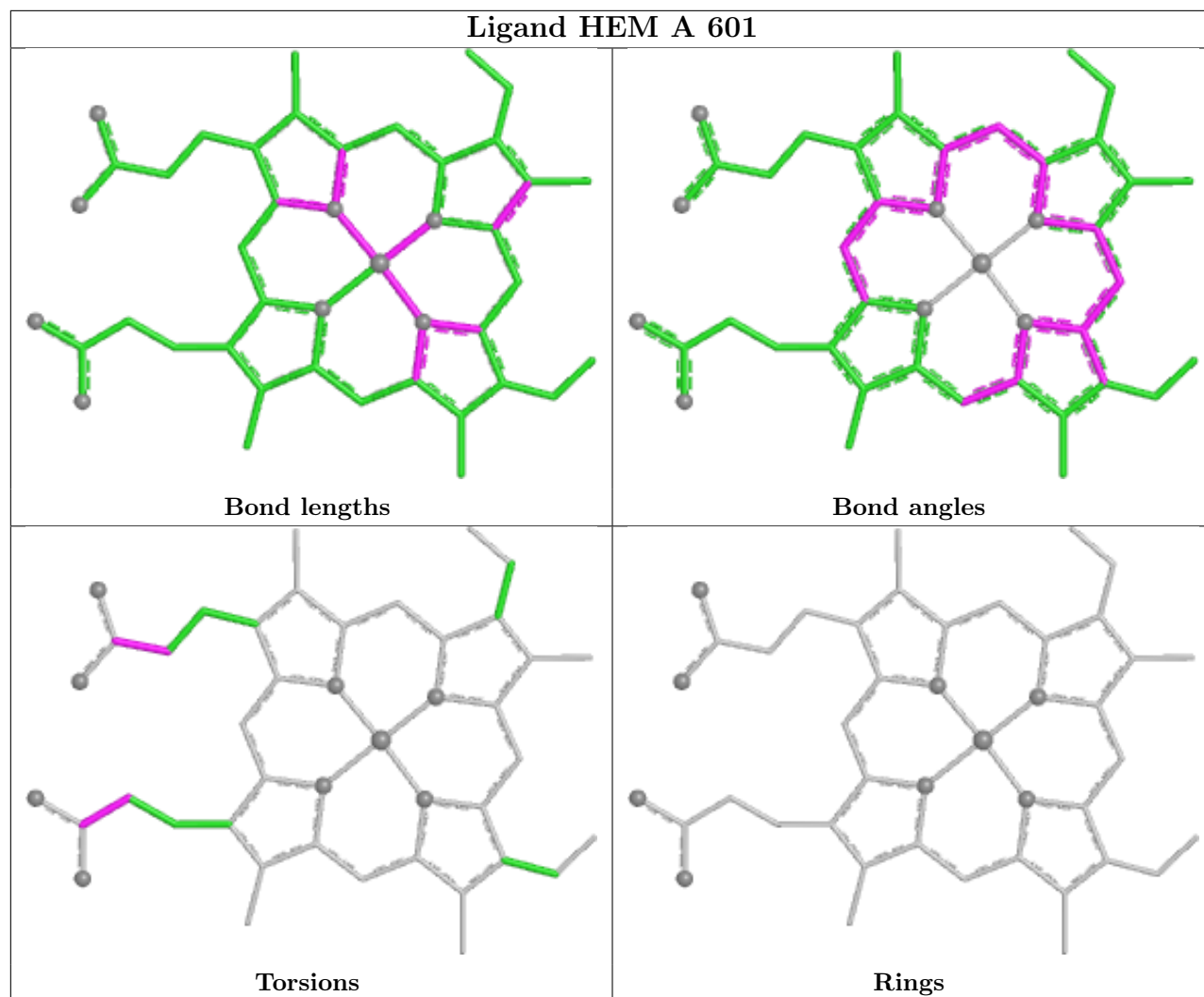
Mol	Chain	Res	Type	Atoms
7	A	614	OTR	O7-C7-C8-N8
8	A	616	PEG	O1-C1-C2-O2
3	A	604	NAG	O5-C5-C6-O6
8	A	615	PEG	O1-C1-C2-O2
7	A	614	OTR	C1-C7-C8-N8
8	A	616	PEG	C1-C2-O2-C3
9	A	624	EDO	O1-C1-C2-O2
9	A	625	EDO	O1-C1-C2-O2
7	A	614	OTR	C2-C1-C7-C8
7	A	614	OTR	C6-C1-C7-C8
2	A	601	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAA-CBA-CGA-O1A
2	A	601	HEM	CAD-CBD-CGD-O2D
8	A	616	PEG	O2-C3-C4-O4
2	A	601	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	616	PEG	1	0
7	A	614	OTR	9	0
2	A	601	HEM	14	0
9	A	625	EDO	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	594/595 (99%)	1.05	82 (13%) 6 6	37, 58, 118, 207	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	LEU	9.3
1	A	168	PRO	5.5
1	A	484	TYR	5.2
1	A	119	LEU	4.5
1	A	6	CYS	4.2
1	A	172	TYR	4.1
1	A	171	PRO	4.0
1	A	169	THR	3.8
1	A	166	VAL	3.8
1	A	572	TYR	3.7
1	A	57	VAL	3.6
1	A	10	VAL	3.6
1	A	4	VAL	3.5
1	A	425	THR	3.5
1	A	127	VAL	3.4
1	A	283	LEU	3.4
1	A	231	ASN	3.3
1	A	486	THR	3.2
1	A	206	LEU	3.2
1	A	20	PRO	3.2
1	A	129	CYS	3.2
1	A	167	CYS	3.2
1	A	582	VAL	3.2
1	A	54	GLY	3.1
1	A	211	GLY	3.1
1	A	13	VAL	3.1
1	A	579	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	227	PRO	2.9
1	A	562	VAL	2.9
1	A	174	SER	2.9
1	A	230	ASN	2.9
1	A	9	PRO	2.8
1	A	581	ALA	2.8
1	A	569	ALA	2.7
1	A	292	LEU	2.7
1	A	122	SER	2.7
1	A	56	ALA	2.7
1	A	220	TRP	2.7
1	A	138	GLU	2.6
1	A	8	ALA	2.6
1	A	11	PRO	2.6
1	A	12	LEU	2.6
1	A	5	GLY	2.6
1	A	554	CYS	2.6
1	A	120	GLY	2.5
1	A	170	PRO	2.5
1	A	265	VAL	2.5
1	A	238	GLU	2.5
1	A	291	MET	2.5
1	A	403	ASN	2.5
1	A	125	SER	2.5
1	A	124	HIS	2.5
1	A	118	GLU	2.4
1	A	2	TRP	2.4
1	A	15	CYS	2.4
1	A	280	LEU	2.3
1	A	481	LEU	2.3
1	A	592	SER	2.3
1	A	1	SER	2.3
1	A	232	VAL	2.3
1	A	117	THR	2.3
1	A	287	TRP	2.3
1	A	210	LEU	2.3
1	A	564	LEU	2.3
1	A	368	TRP	2.3
1	A	3	GLU	2.2
1	A	121	SER	2.2
1	A	219	ALA	2.2
1	A	591	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	139	CYS	2.2
1	A	545	GLN	2.2
1	A	208	SER	2.2
1	A	427	LYS	2.2
1	A	315	ILE	2.2
1	A	324	TRP	2.2
1	A	40	ASN	2.1
1	A	137	ASP	2.1
1	A	400	LEU	2.1
1	A	279	GLU	2.1
1	A	549	PHE	2.1
1	A	175	LEU	2.0
1	A	539	LYS	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. 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
1	SEP	A	198	10/11	0.72	0.23	51,57,69,79	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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
3	NAG	A	604	14/15	0.65	0.13	71,86,93,98	0
3	NAG	A	603	14/15	0.66	0.12	76,85,92,93	0
8	PEG	A	616	7/7	0.69	0.18	67,71,77,79	0
6	SCN	A	613	3/3	0.75	0.18	62,62,83,93	0

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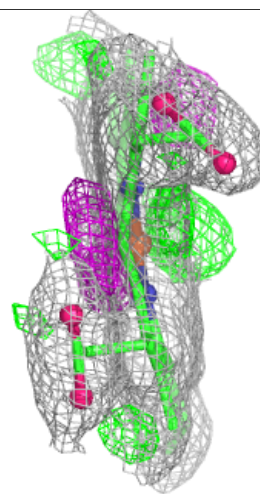
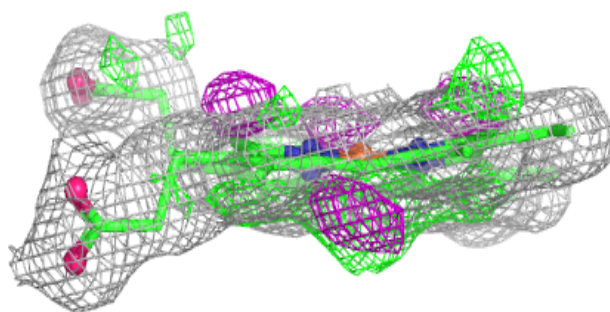
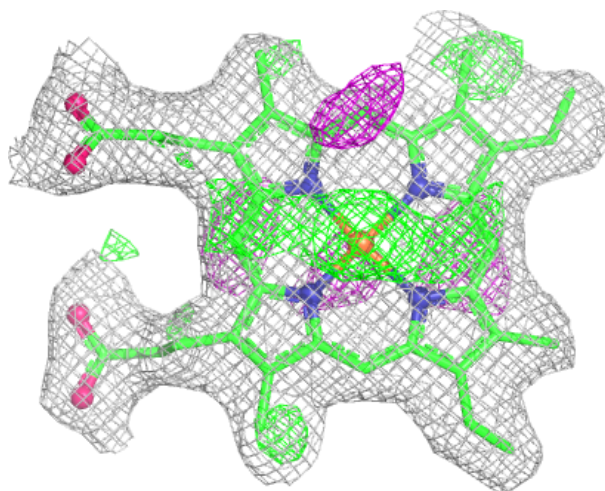
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	PEG	A	615	7/7	0.79	0.16	63,69,73,76	0
9	EDO	A	624	4/4	0.82	0.13	54,55,57,58	0
3	NAG	A	602	14/15	0.84	0.12	50,59,72,77	0
5	IOD	A	618	1/1	0.85	0.20	149,149,149,149	0
7	OTR	A	614	11/11	0.86	0.14	28,52,63,68	0
3	NAG	A	605	14/15	0.86	0.09	56,62,72,74	0
5	IOD	A	621	1/1	0.88	0.15	134,134,134,134	0
5	IOD	A	619	1/1	0.88	0.18	148,148,148,148	0
2	HEM	A	601	43/43	0.89	0.14	31,37,47,52	0
5	IOD	A	617	1/1	0.89	0.18	105,105,105,105	0
5	IOD	A	623	1/1	0.90	0.14	119,119,119,119	0
5	IOD	A	622	1/1	0.90	0.23	123,123,123,123	0
9	EDO	A	625	4/4	0.92	0.12	40,40,43,52	0
5	IOD	A	609	1/1	0.93	0.08	79,79,79,79	0
5	IOD	A	612	1/1	0.93	0.13	113,113,113,113	0
5	IOD	A	620	1/1	0.96	0.07	83,83,83,83	0
5	IOD	A	611	1/1	0.97	0.07	88,88,88,88	0
5	IOD	A	608	1/1	0.97	0.06	71,71,71,71	0
5	IOD	A	610	1/1	0.97	0.08	82,82,82,82	0
5	IOD	A	607	1/1	0.98	0.04	49,49,49,49	0
4	CA	A	606	1/1	0.99	0.03	45,45,45,45	0

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.

Electron density around HEM A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.