



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:00 AM UTC

PDB ID : 6KMK / pdb_00006kmk
Title : Crystal structure of hydrogen peroxide bound bovine lactoperoxidase at 2.3 Å resolution
Authors : Singh, P.K.; Sirohi, H.V.; Bhusan, A.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2019-07-31
Resolution : 2.30 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

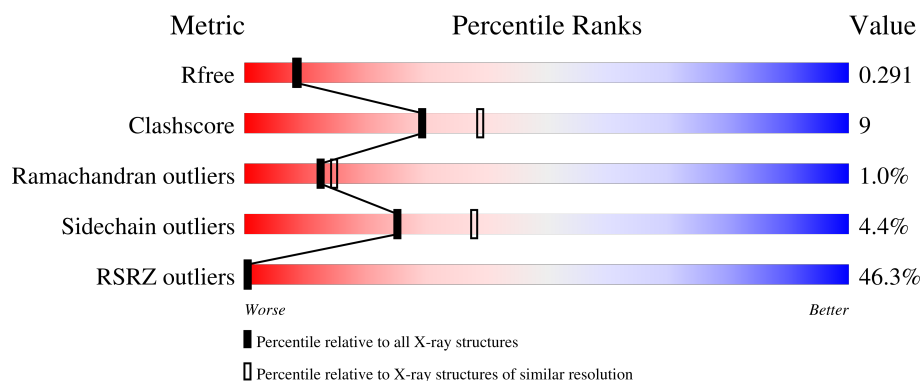
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	46% 80% 18%

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	616	-	-	X	-

Continued on next page...

Continued from previous page...

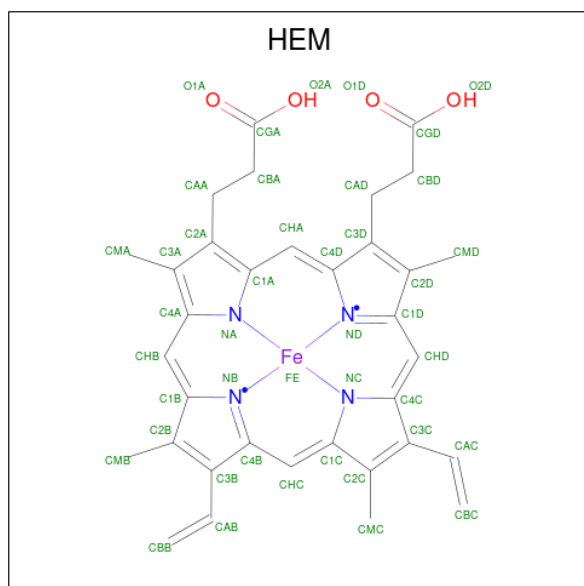
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	IOD	A	621	-	-	X	-

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	P	S	0	0	0
			4774	3037	847	863	1	26			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

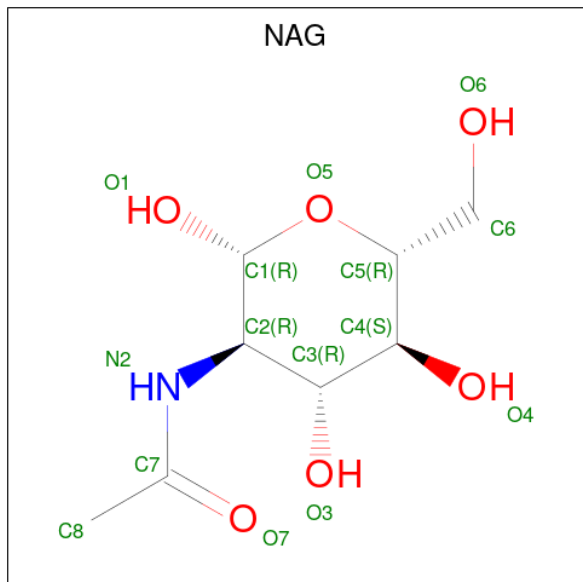


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

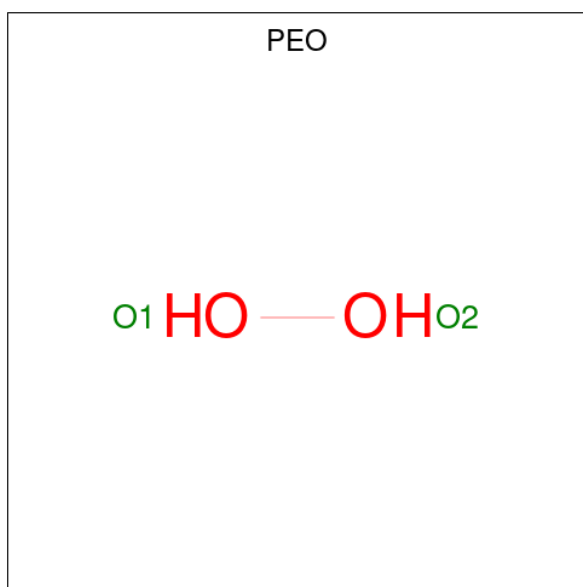


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total	I	0	0
			15	15		

- Molecule 6 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H_2O_2).



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

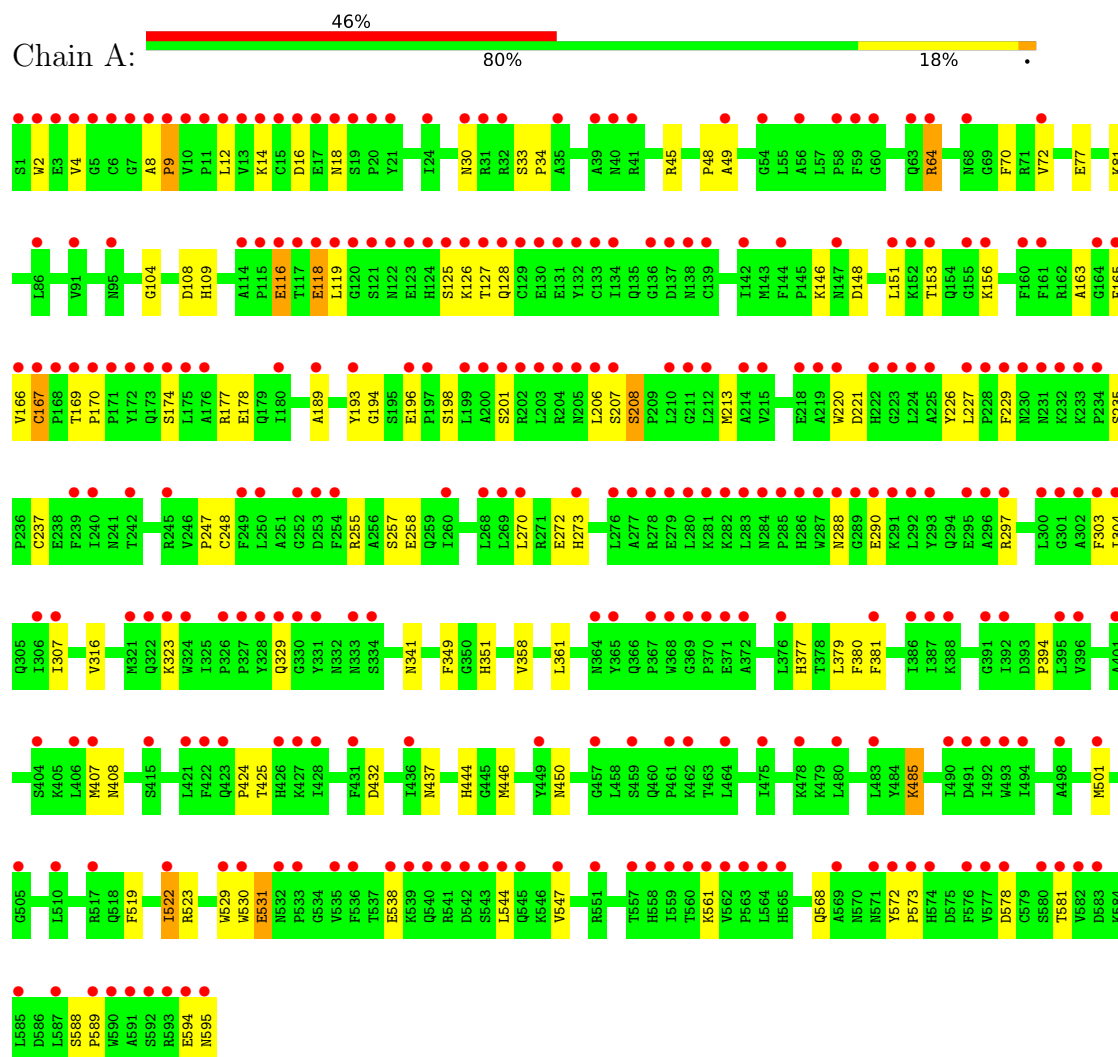
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	251	Total	O	0	0
			251	251		

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	53.83Å 80.42Å 75.82Å 90.00° 102.58° 90.00°	Depositor
Resolution (Å)	54.46 – 2.30 54.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (54.46-2.30) 98.7 (54.46-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.245 , 0.295 (Not available) , 0.291	Depositor DCC
R_{free} test set	1405 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	5144	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, NAG, PEO, SEP, CA, 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	1.03	0/4891	1.37	2/6634 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	316	VAL	N-CA-C	-5.71	106.14	111.45
1	A	194	GLY	CA-C-O	-5.45	117.55	122.57

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4687	78	0
2	A	43	0	30	14	0
3	A	1	0	0	0	0
4	A	56	0	52	4	0
5	A	15	0	0	5	1
6	A	4	0	0	1	0
7	A	251	0	0	7	1
All	All	5144	0	4769	83	1

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 9.

All (83) 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:258:GLU:OE2	2:A:601:HEM:CMB	1.77	1.33
1:A:108:ASP:OD2	2:A:601:HEM:CMD	1.82	1.28
1:A:258:GLU:OE2	2:A:601:HEM:HMB1	1.00	1.16
1:A:108:ASP:OD2	2:A:601:HEM:HMD1	0.94	1.10
1:A:64:ARG:NH1	7:A:702:HOH:O	2.10	0.83
1:A:126:LYS:N	1:A:127:THR:HA	1.97	0.78
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.16	0.75
1:A:48:PRO:HD3	5:A:621:IOD:I	2.56	0.75
1:A:108:ASP:CG	2:A:601:HEM:HMD1	2.05	0.73
2:A:601:HEM:HBC2	2:A:601:HEM:HMC1	1.72	0.71
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.37	0.70
1:A:127:THR:N	1:A:128:GLN:HA	2.07	0.69
1:A:407:MET:HB3	1:A:501:MET:CE	2.23	0.69
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.76	0.67
1:A:288:ASN:HD21	1:A:290:GLU:HB3	1.60	0.66
4:A:606:NAG:O6	7:A:701:HOH:O	1.71	0.65
1:A:220:TRP:HB2	7:A:878:HOH:O	1.96	0.65
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.77	0.65
1:A:568:GLN:NE2	4:A:606:NAG:C1	2.61	0.64
1:A:126:LYS:N	1:A:127:THR:CA	2.63	0.62
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.35	0.62
1:A:424:PRO:O	1:A:425:THR:OG1	2.16	0.61
1:A:206:LEU:O	1:A:208:SER:N	2.34	0.61
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.84	0.60
1:A:30:ASN:O	1:A:34:PRO:HA	2.03	0.58
1:A:108:ASP:CG	2:A:601:HEM:CMD	2.70	0.58
1:A:193:TYR:OH	1:A:297:ARG:HA	2.04	0.58
1:A:568:GLN:NE2	4:A:606:NAG:O5	2.37	0.57
1:A:544:LEU:O	1:A:547:VAL:HG22	2.04	0.57
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.35	0.57
1:A:193:TYR:CZ	1:A:297:ARG:HA	2.41	0.56
1:A:148:ASP:O	1:A:151:LEU:HB2	2.06	0.55
1:A:237:CYS:HA	1:A:381:PHE:O	2.07	0.55
1:A:258:GLU:OE2	2:A:601:HEM:HMB2	1.96	0.55
1:A:167:CYS:O	1:A:169:THR:N	2.40	0.55
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.89	0.54
1:A:108:ASP:OD2	2:A:601:HEM:C2D	2.58	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.89	0.54
1:A:125:SER:C	1:A:127:THR:HA	2.34	0.53
1:A:561:LYS:HE2	5:A:611:IOD:I	2.79	0.52
2:A:601:HEM:CMB	2:A:601:HEM:HBB2	2.40	0.51
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.45	0.51
1:A:255:ARG:HD2	5:A:616:IOD:I	2.81	0.51
1:A:116:GLU:HA	1:A:163:ALA:HA	1.93	0.50
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.46	0.50
1:A:70:PHE:CD1	1:A:485:LYS:HG3	2.47	0.50
1:A:568:GLN:HE22	4:A:606:NAG:C1	2.23	0.49
1:A:341:ASN:OD1	1:A:444:HIS:ND1	2.29	0.49
1:A:255:ARG:HB3	5:A:616:IOD:I	2.81	0.49
1:A:519:PHE:CD1	1:A:522:ILE:HD11	2.48	0.49
1:A:109:HIS:NE2	6:A:622:PEO:O1	2.37	0.48
1:A:303:PHE:O	1:A:307:ILE:HG12	2.14	0.48
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.49	0.48
1:A:530:TRP:CZ2	1:A:531:GLU:HG3	2.48	0.48
1:A:594:GLU:HB2	7:A:734:HOH:O	2.14	0.48
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.49	0.47
1:A:237:CYS:HB2	1:A:248:CYS:N	2.30	0.47
1:A:258:GLU:CD	2:A:601:HEM:CMB	2.76	0.47
1:A:45:ARG:CZ	1:A:49:ALA:HB2	2.45	0.47
1:A:127:THR:N	1:A:128:GLN:CA	2.77	0.46
1:A:581:THR:HG22	1:A:581:THR:O	2.16	0.46
1:A:361:LEU:O	1:A:394:PRO:HA	2.15	0.46
1:A:272:GLU:OE1	1:A:272:GLU:HA	2.16	0.45
1:A:45:ARG:HA	5:A:608:IOD:I	2.88	0.44
1:A:116:GLU:O	1:A:119:LEU:CD2	2.66	0.44
1:A:450:ASN:N	7:A:724:HOH:O	2.48	0.44
1:A:407:MET:SD	1:A:408:ASN:N	2.91	0.43
1:A:257:SER:O	1:A:381:PHE:HA	2.19	0.43
1:A:104:GLY:HA3	2:A:601:HEM:CBC	2.47	0.43
1:A:165:PHE:N	1:A:165:PHE:CD1	2.85	0.43
1:A:432:ASP:OD1	1:A:432:ASP:C	2.60	0.43
1:A:358:VAL:HB	1:A:379:LEU:CD1	2.48	0.43
1:A:165:PHE:CD2	1:A:177:ARG:HD2	2.54	0.42
1:A:446:MET:HA	1:A:446:MET:HE2	2.01	0.42
1:A:349:PHE:CD1	1:A:349:PHE:C	2.98	0.42
1:A:178:GLU:HA	1:A:178:GLU:OE2	2.20	0.41
1:A:16:ASP:C	1:A:18:ASN:H	2.28	0.41
1:A:206:LEU:C	1:A:208:SER:H	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:SER:OG	7:A:703:HOH:O	2.21	0.41
1:A:206:LEU:C	1:A:208:SER:N	2.79	0.40
1:A:220:TRP:CB	7:A:878:HOH:O	2.63	0.40
1:A:572:TYR:CD1	1:A:573:PRO:HA	2.55	0.40
1:A:166:VAL:HA	1:A:167:CYS:C	2.45	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:621:IOD:I	7:A:925:HOH:O[2_646]	1.10	1.10

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%)	545 (92%)	41 (7%)	6 (1%)	12 15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	GLU
1	A	174	SER
1	A	207	SER
1	A	9	PRO
1	A	170	PRO
1	A	485	LYS

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%)	494 (96%)	23 (4%)	25	38

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	4	VAL
1	A	12	LEU
1	A	14	LYS
1	A	33	SER
1	A	64	ARG
1	A	72	VAL
1	A	116	GLU
1	A	118	GLU
1	A	146	LYS
1	A	153	THR
1	A	156	LYS
1	A	167	CYS
1	A	196	GLU
1	A	201	SER
1	A	208	SER
1	A	323	LYS
1	A	329	GLN
1	A	522	ILE
1	A	531	GLU
1	A	538	GLU
1	A	578	ASP
1	A	595	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	63	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	122	ASN
1	A	288	ASN
1	A	468	GLN
1	A	497	ASN
1	A	568	GLN
1	A	595	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	1.51	1 (12%)	7,12,14	0.66	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	-	6/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-OG	2.87	1.69	1.60

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 16 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	A	601	1,6	50,50,50	1.63	9 (18%)	67,82,82	1.62	14 (20%)
6	PEO	A	622	2	1,1,1	0.31	0	-		
4	NAG	A	604	1	14,14,15	0.62	0	17,19,21	1.86	4 (23%)
6	PEO	A	623	-	1,1,1	0.46	0	-		
4	NAG	A	606	1	14,14,15	0.92	0	17,19,21	2.05	3 (17%)
4	NAG	A	605	1	14,14,15	0.54	0	17,19,21	1.62	3 (17%)
4	NAG	A	603	1	14,14,15	0.65	0	17,19,21	1.54	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	601	1,6	-	4/14/54/54	-
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
4	NAG	A	606	1	-	5/6/23/26	0/1/1/1
4	NAG	A	605	1	-	0/6/23/26	0/1/1/1
4	NAG	A	603	1	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	FE-NB	4.50	2.08	1.94
2	A	601	HEM	C4D-ND	-4.41	1.32	1.40
2	A	601	HEM	FE-NC	3.47	2.06	1.95
2	A	601	HEM	C1B-NB	-3.43	1.34	1.40
2	A	601	HEM	C1C-C2C	-2.95	1.39	1.45
2	A	601	HEM	C4C-NC	-2.11	1.35	1.39
2	A	601	HEM	C3D-C2D	-2.11	1.32	1.36
2	A	601	HEM	C3C-C4C	-2.07	1.42	1.46
2	A	601	HEM	C1D-ND	-2.04	1.34	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	606	NAG	C1-O5-C5	6.46	120.84	112.19
4	A	604	NAG	C1-O5-C5	5.28	119.27	112.19
2	A	601	HEM	CHC-C4B-NB	5.14	129.95	124.42
4	A	605	NAG	C4-C3-C2	4.31	117.34	111.02
2	A	601	HEM	CMD-C2D-C1D	3.91	131.15	125.03
2	A	601	HEM	CHA-C4D-ND	3.57	128.78	124.37
2	A	601	HEM	C1B-NB-C4B	3.34	109.17	105.21
4	A	603	NAG	C3-C4-C5	-3.04	104.71	110.23
2	A	601	HEM	O2D-CGD-O1D	-3.03	115.54	123.33
4	A	603	NAG	O5-C1-C2	-2.92	106.78	111.29
2	A	601	HEM	O2D-CGD-CBD	2.75	122.69	114.00
2	A	601	HEM	O2A-CGA-CBA	2.72	122.58	114.00
4	A	604	NAG	O5-C1-C2	-2.68	107.14	111.29
4	A	604	NAG	O4-C4-C5	2.63	115.81	109.32
2	A	601	HEM	CHA-C4D-C3D	-2.63	120.38	125.23
4	A	605	NAG	C1-O5-C5	2.60	115.66	112.19
2	A	601	HEM	C4B-C3B-C2B	-2.43	105.05	107.28
4	A	606	NAG	C8-C7-N2	2.37	120.05	116.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	NAG	C6-C5-C4	-2.35	107.26	113.02
4	A	605	NAG	O5-C5-C6	2.18	111.90	107.66
2	A	601	HEM	CHD-C1D-ND	2.17	126.76	124.42
4	A	606	NAG	C3-C4-C5	2.11	114.05	110.23
2	A	601	HEM	CHB-C1B-NB	2.10	126.96	124.37
2	A	601	HEM	CBA-CAA-C2A	-2.09	106.75	112.53
2	A	601	HEM	CBD-CAD-C3D	-2.03	106.91	112.53
2	A	601	HEM	C1A-CHA-C4D	-2.02	121.50	126.25
4	A	603	NAG	O4-C4-C3	2.02	115.13	110.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	606	NAG	O5-C5-C6-O6
4	A	606	NAG	C8-C7-N2-C2
4	A	606	NAG	O7-C7-N2-C2
4	A	606	NAG	C4-C5-C6-O6
4	A	603	NAG	O5-C5-C6-O6
2	A	601	HEM	CAA-CBA-CGA-O2A
4	A	606	NAG	C1-C2-N2-C7
2	A	601	HEM	CAA-CBA-CGA-O1A
2	A	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O1D
4	A	603	NAG	C4-C5-C6-O6

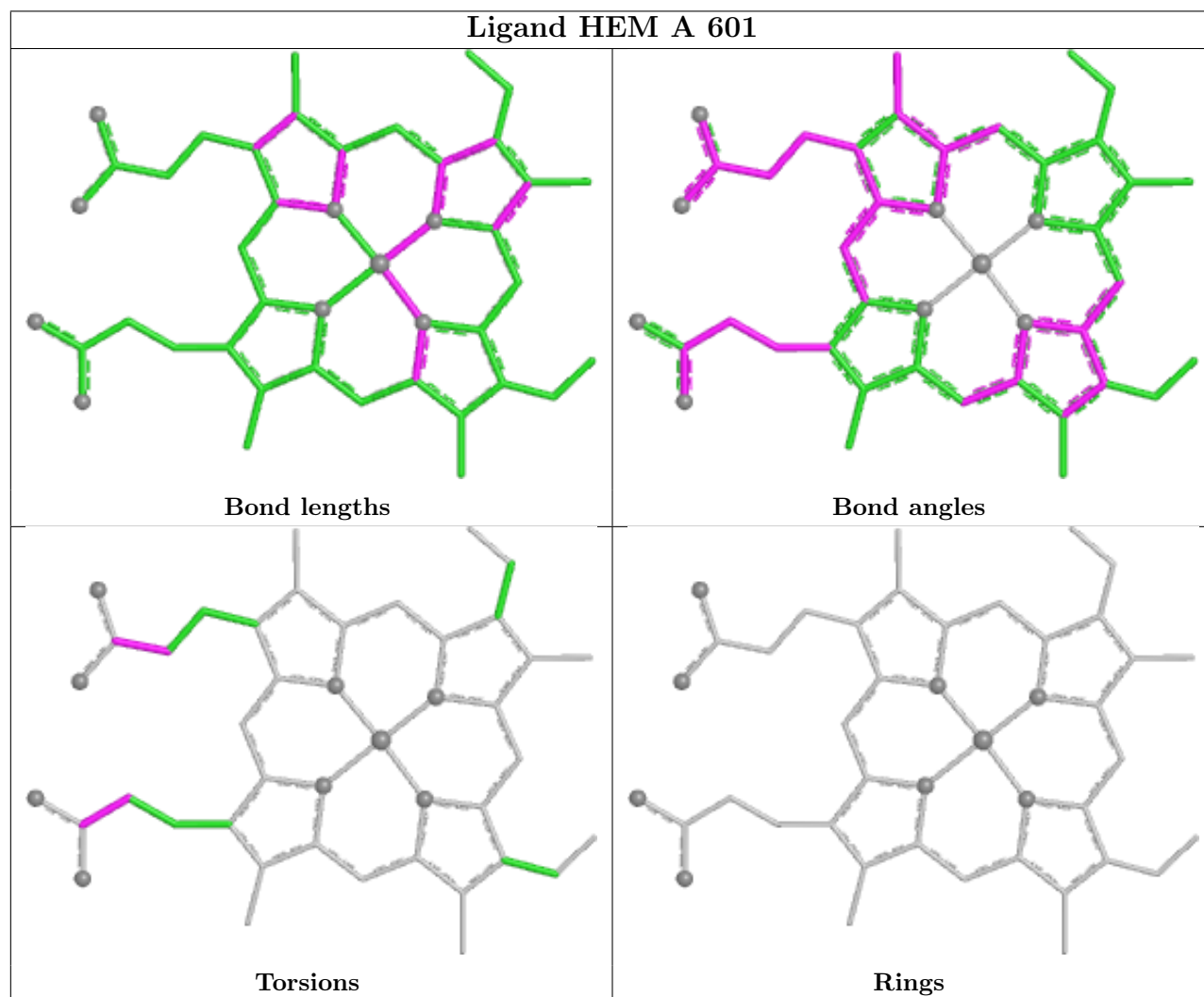
There are no ring outliers.

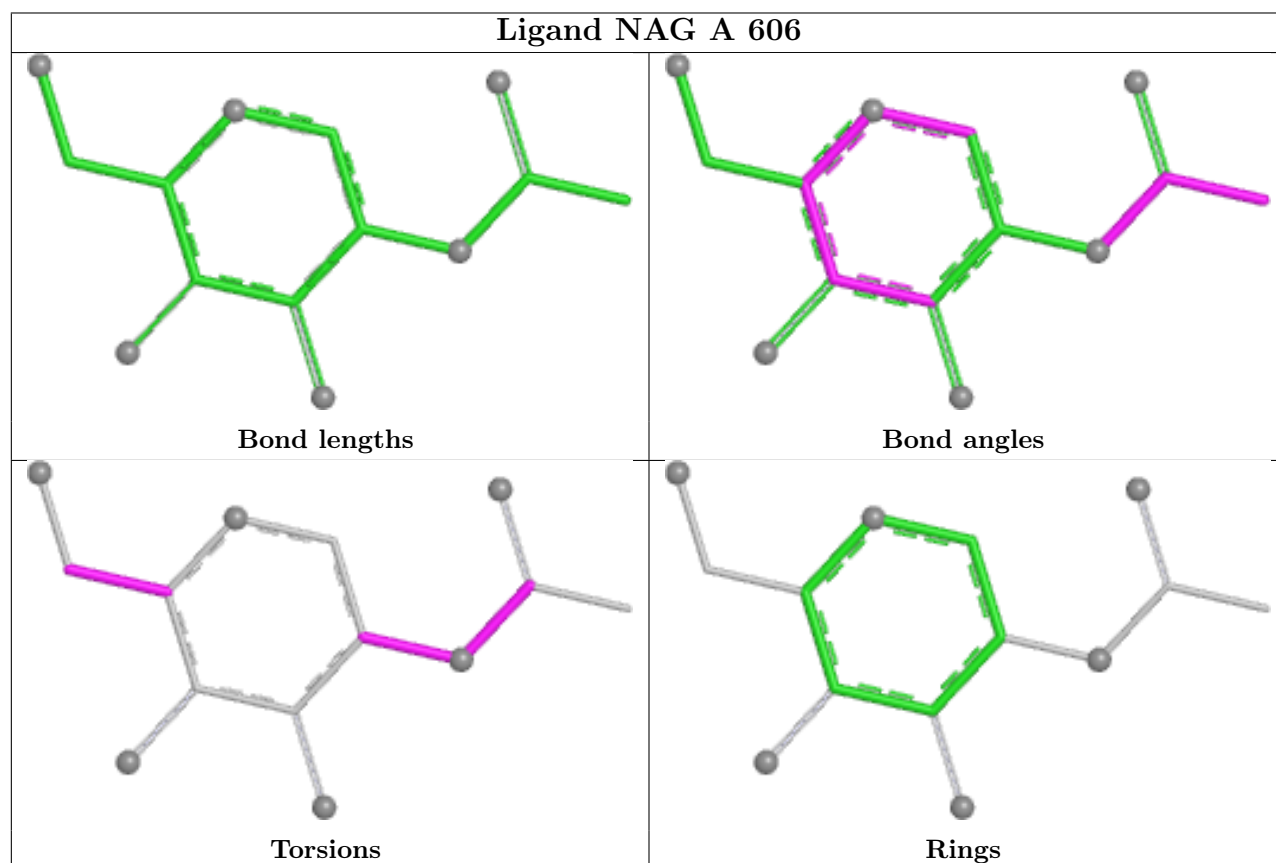
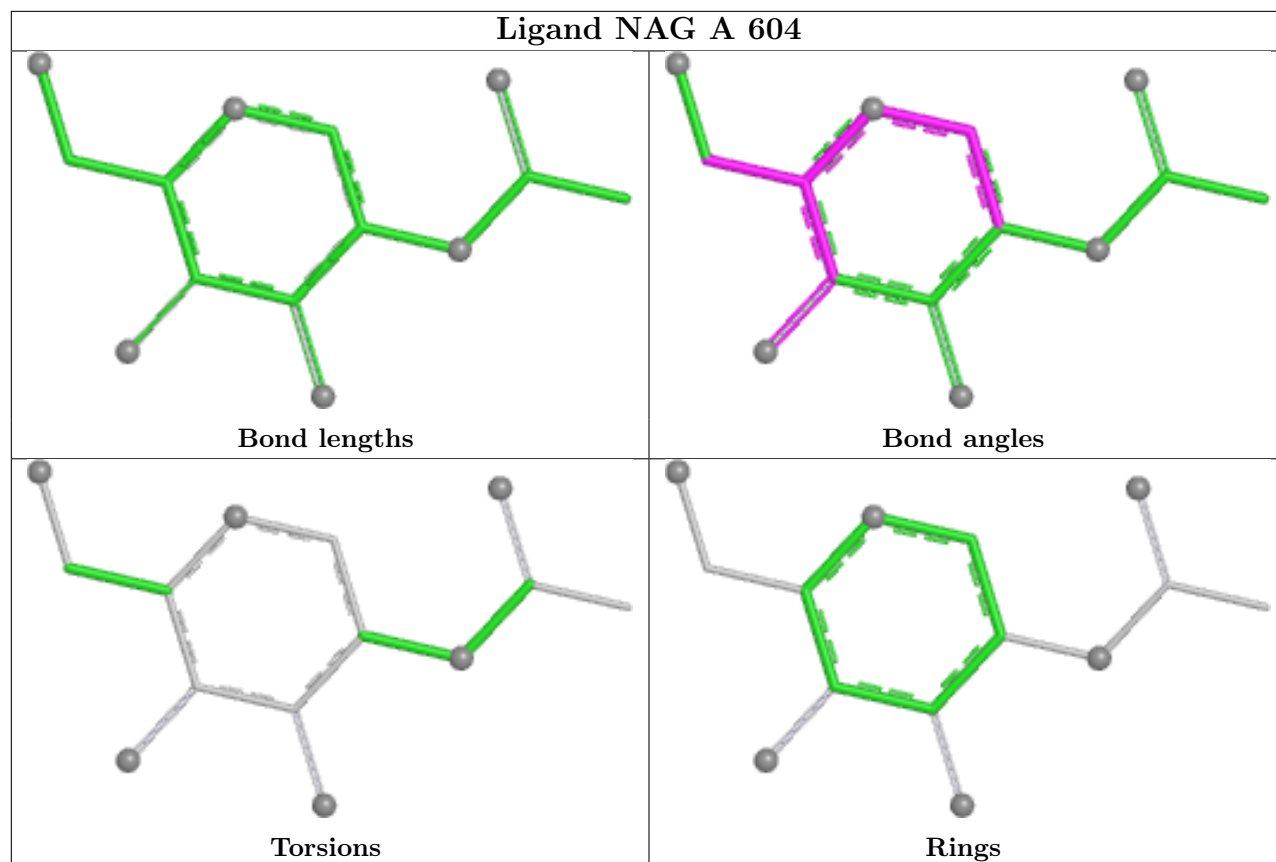
3 monomers are involved in 19 short contacts:

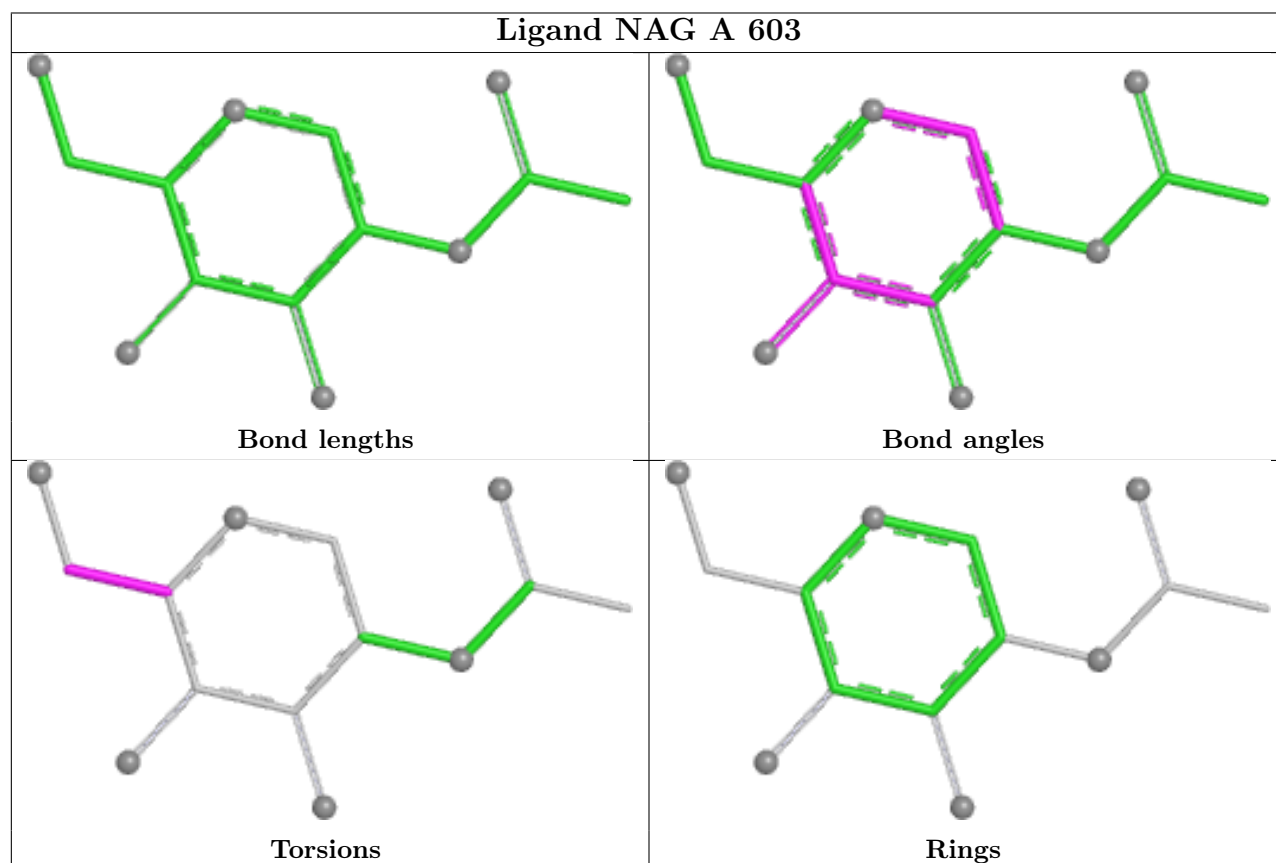
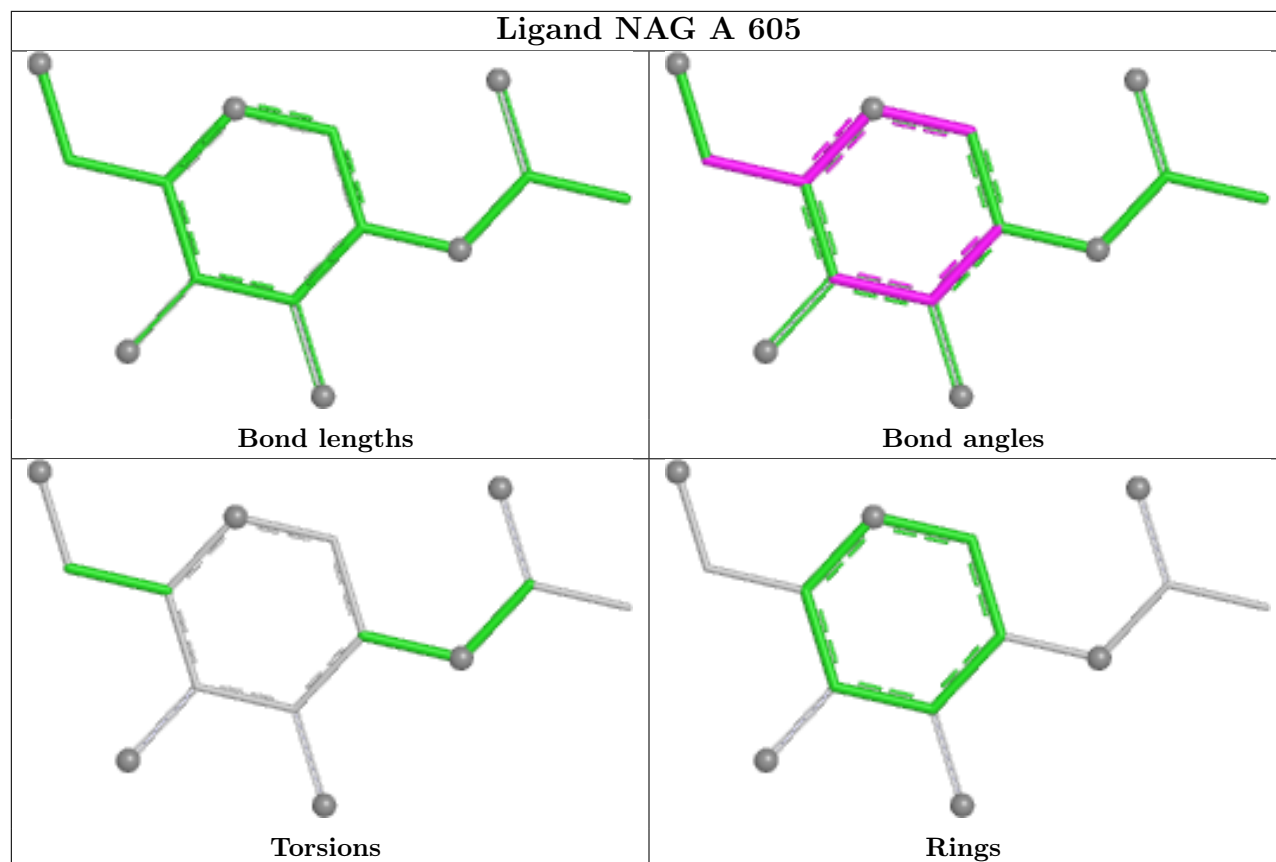
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	14	0
6	A	622	PEO	1	0
4	A	606	NAG	4	0

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%)	2.23	275 (46%) 0 0	18, 37, 104, 148	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	ALA	10.9
1	A	11	PRO	9.7
1	A	7	GLY	9.5
1	A	4	VAL	8.9
1	A	120	GLY	8.6
1	A	12	LEU	8.3
1	A	172	TYR	8.3
1	A	2	TRP	8.0
1	A	119	LEU	7.3
1	A	9	PRO	7.2
1	A	10	VAL	7.2
1	A	6	CYS	7.1
1	A	117	THR	7.0
1	A	170	PRO	6.9
1	A	254	PHE	6.8
1	A	13	VAL	6.8
1	A	127	THR	6.5
1	A	5	GLY	6.5
1	A	169	THR	6.3
1	A	124	HIS	6.1
1	A	174	SER	6.0
1	A	211	GLY	6.0
1	A	595	ASN	5.8
1	A	15	CYS	5.8
1	A	168	PRO	5.8
1	A	1	SER	5.8
1	A	166	VAL	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	3	GLU	5.6
1	A	132	TYR	5.4
1	A	283	LEU	5.4
1	A	220	TRP	5.4
1	A	40	ASN	5.3
1	A	173	GLN	5.3
1	A	161	PHE	5.2
1	A	21	TYR	5.2
1	A	17	GLU	5.2
1	A	125	SER	5.2
1	A	530	TRP	5.1
1	A	126	LYS	5.0
1	A	544	LEU	5.0
1	A	171	PRO	5.0
1	A	64	ARG	4.9
1	A	280	LEU	4.8
1	A	581	THR	4.8
1	A	138	ASN	4.7
1	A	14	LYS	4.7
1	A	121	SER	4.7
1	A	19	SER	4.6
1	A	587	LEU	4.6
1	A	233	LYS	4.6
1	A	564	LEU	4.6
1	A	122	ASN	4.5
1	A	167	CYS	4.5
1	A	130	GLU	4.5
1	A	231	ASN	4.5
1	A	16	ASP	4.4
1	A	590	TRP	4.4
1	A	219	ALA	4.4
1	A	535	VAL	4.4
1	A	572	TYR	4.4
1	A	123	GLU	4.2
1	A	368	TRP	4.2
1	A	387	ILE	4.2
1	A	223	GLY	4.2
1	A	279	GLU	4.2
1	A	287	TRP	4.2
1	A	593	ARG	4.1
1	A	129	CYS	4.1
1	A	269	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	210	LEU	4.0
1	A	592	SER	4.0
1	A	574	HIS	4.0
1	A	539	LYS	4.0
1	A	128	GLN	4.0
1	A	224	LEU	3.9
1	A	175	LEU	3.9
1	A	290	GLU	3.8
1	A	131	GLU	3.8
1	A	20	PRO	3.7
1	A	591	ALA	3.6
1	A	156	LYS	3.6
1	A	331	TYR	3.6
1	A	116	GLU	3.6
1	A	293	TYR	3.6
1	A	328	TYR	3.6
1	A	155	GLY	3.6
1	A	270	LEU	3.6
1	A	232	LYS	3.6
1	A	560	THR	3.6
1	A	225	ALA	3.5
1	A	296	ALA	3.5
1	A	86	LEU	3.5
1	A	203	LEU	3.5
1	A	292	LEU	3.5
1	A	427	LYS	3.5
1	A	288	ASN	3.5
1	A	245	ARG	3.4
1	A	276	LEU	3.4
1	A	302	ALA	3.4
1	A	228	PRO	3.4
1	A	222	HIS	3.4
1	A	153	THR	3.3
1	A	204	ARG	3.3
1	A	229	PHE	3.3
1	A	322	GLN	3.3
1	A	529	TRP	3.3
1	A	543	SER	3.3
1	A	582	VAL	3.2
1	A	56	ALA	3.2
1	A	152	LYS	3.2
1	A	242	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	505	GLY	3.1
1	A	227	LEU	3.1
1	A	533	PRO	3.1
1	A	536	PHE	3.1
1	A	589	PRO	3.1
1	A	562	VAL	3.1
1	A	212	LEU	3.1
1	A	326	PRO	3.1
1	A	164	GLY	3.1
1	A	189	ALA	3.1
1	A	461	PRO	3.1
1	A	580	SER	3.0
1	A	144	PHE	3.0
1	A	333	ASN	3.0
1	A	431	PHE	3.0
1	A	371	GLU	3.0
1	A	240	ILE	3.0
1	A	136	GLY	3.0
1	A	583	ASP	3.0
1	A	18	ASN	3.0
1	A	60	GLY	3.0
1	A	137	ASP	3.0
1	A	230	ASN	3.0
1	A	324	TRP	3.0
1	A	391	GLY	3.0
1	A	422	PHE	3.0
1	A	576	PHE	3.0
1	A	278	ARG	3.0
1	A	165	PHE	2.9
1	A	303	PHE	2.9
1	A	569	ALA	2.9
1	A	196	GLU	2.9
1	A	365	TYR	2.9
1	A	364	ASN	2.9
1	A	206	LEU	2.9
1	A	547	VAL	2.9
1	A	301	GLY	2.9
1	A	72	VAL	2.9
1	A	594	GLU	2.9
1	A	202	ARG	2.8
1	A	483	LEU	2.8
1	A	585	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	215	VAL	2.8
1	A	538	GLU	2.8
1	A	134	ILE	2.8
1	A	369	GLY	2.8
1	A	197	PRO	2.8
1	A	41	ARG	2.8
1	A	139	CYS	2.8
1	A	252	GLY	2.8
1	A	239	PHE	2.8
1	A	284	ASN	2.8
1	A	541	ARG	2.8
1	A	396	VAL	2.8
1	A	95	ASN	2.7
1	A	323	LYS	2.7
1	A	388	LYS	2.7
1	A	253	ASP	2.7
1	A	457	GLY	2.7
1	A	407	MET	2.7
1	A	498	ALA	2.7
1	A	260	ILE	2.7
1	A	367	PRO	2.7
1	A	91	VAL	2.7
1	A	462	LYS	2.7
1	A	578	ASP	2.7
1	A	559	ILE	2.7
1	A	285	PRO	2.7
1	A	459	SER	2.7
1	A	151	LEU	2.7
1	A	286	HIS	2.6
1	A	401	ALA	2.6
1	A	205	ASN	2.6
1	A	565	HIS	2.6
1	A	329	GLN	2.6
1	A	214	ALA	2.6
1	A	327	PRO	2.6
1	A	268	LEU	2.6
1	A	115	PRO	2.6
1	A	392	ILE	2.6
1	A	372	ALA	2.6
1	A	289	GLY	2.6
1	A	573	PRO	2.6
1	A	522	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	32	ARG	2.5
1	A	35	ALA	2.5
1	A	49	ALA	2.5
1	A	201	SER	2.5
1	A	273	HIS	2.5
1	A	118	GLU	2.5
1	A	494	ILE	2.5
1	A	281	LYS	2.5
1	A	532	ASN	2.5
1	A	133	CYS	2.5
1	A	24	ILE	2.5
1	A	31	ARG	2.5
1	A	577	VAL	2.5
1	A	63	GLN	2.5
1	A	291	LYS	2.4
1	A	297	ARG	2.4
1	A	542	ASP	2.4
1	A	295	GLU	2.4
1	A	234	PRO	2.4
1	A	180	ILE	2.4
1	A	501	MET	2.4
1	A	493	TRP	2.4
1	A	423	GLN	2.4
1	A	68	ASN	2.4
1	A	39	ALA	2.4
1	A	54	GLY	2.4
1	A	199	LEU	2.4
1	A	250	LEU	2.4
1	A	376	LEU	2.4
1	A	30	ASN	2.3
1	A	147	ASN	2.3
1	A	334	SER	2.3
1	A	540	GLN	2.3
1	A	277	ALA	2.3
1	A	406	LEU	2.3
1	A	464	LEU	2.3
1	A	428	ILE	2.3
1	A	415	SER	2.3
1	A	561	LYS	2.3
1	A	381	PHE	2.2
1	A	551	ARG	2.2
1	A	176	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	218	GLU	2.2
1	A	404	SER	2.2
1	A	142	ILE	2.2
1	A	421	LEU	2.2
1	A	160	PHE	2.2
1	A	249	PHE	2.2
1	A	330	GLY	2.2
1	A	426	HIS	2.2
1	A	200	ALA	2.2
1	A	306	ILE	2.2
1	A	436	ILE	2.2
1	A	449	TYR	2.1
1	A	307	ILE	2.1
1	A	395	LEU	2.1
1	A	480	LEU	2.1
1	A	492	ILE	2.1
1	A	510	LEU	2.1
1	A	491	ASP	2.1
1	A	58	PRO	2.1
1	A	370	PRO	2.1
1	A	563	PRO	2.1
1	A	59	PHE	2.1
1	A	207	SER	2.1
1	A	557	THR	2.1
1	A	282	LYS	2.1
1	A	545	GLN	2.1
1	A	478	LYS	2.0
1	A	321	MET	2.0
1	A	304	ILE	2.0
1	A	193	TYR	2.0
1	A	114	ALA	2.0
1	A	558	HIS	2.0
1	A	300	LEU	2.0
1	A	571	ASN	2.0
1	A	386	ILE	2.0
1	A	475	ILE	2.0
1	A	490	ILE	2.0
1	A	517	ARG	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	0.88	0.16	26,41,45,45	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
4	NAG	A	605	14/15	0.44	0.26	68,83,87,89	0
4	NAG	A	606	14/15	0.58	0.21	53,59,66,67	0
4	NAG	A	604	14/15	0.72	0.21	52,57,59,61	0
6	PEO	A	623	2/2	0.74	0.20	42,42,42,49	0
4	NAG	A	603	14/15	0.79	0.17	39,42,45,48	0
5	IOD	A	619	1/1	0.89	0.11	79,79,79,79	1
5	IOD	A	615	1/1	0.89	0.09	45,45,45,45	1
5	IOD	A	617	1/1	0.90	0.13	68,68,68,68	1
5	IOD	A	620	1/1	0.91	0.08	62,62,62,62	1
3	CA	A	602	1/1	0.92	0.07	29,29,29,29	0
6	PEO	A	622	2/2	0.93	0.15	36,36,36,41	0
5	IOD	A	612	1/1	0.93	0.07	43,43,43,43	1
2	HEM	A	601	43/43	0.94	0.10	16,21,28,30	0
5	IOD	A	621	1/1	0.96	0.09	81,81,81,81	1
5	IOD	A	609	1/1	0.96	0.05	44,44,44,44	0
5	IOD	A	613	1/1	0.96	0.06	61,61,61,61	0
5	IOD	A	618	1/1	0.97	0.06	48,48,48,48	1
5	IOD	A	607	1/1	0.97	0.07	55,55,55,55	0
5	IOD	A	614	1/1	0.98	0.04	57,57,57,57	0
5	IOD	A	611	1/1	0.98	0.04	42,42,42,42	1
5	IOD	A	616	1/1	0.98	0.08	55,55,55,55	1

Continued on next page...

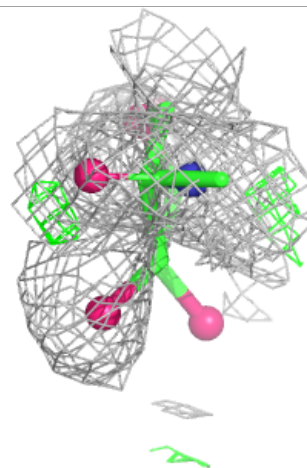
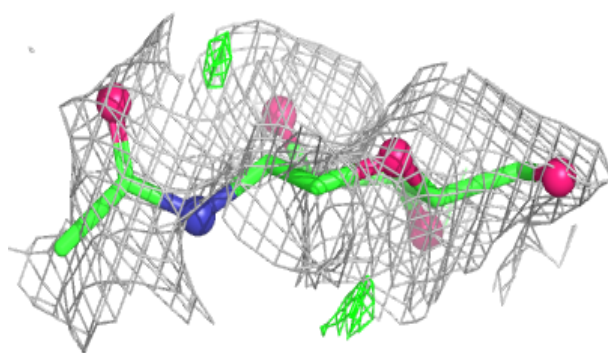
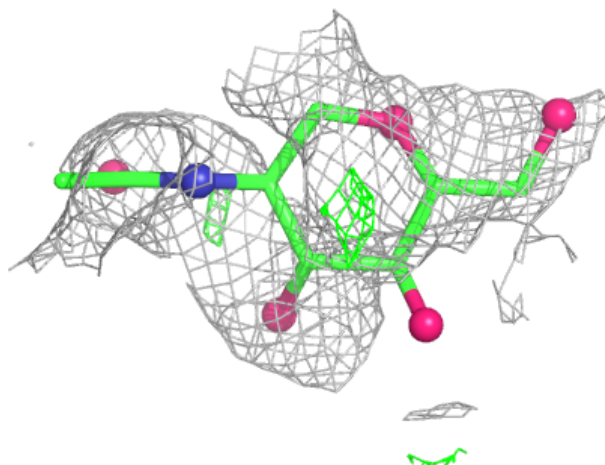
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	IOD	A	608	1/1	0.98	0.07	36,36,36,36	1
5	IOD	A	610	1/1	0.98	0.05	51,51,51,51	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.

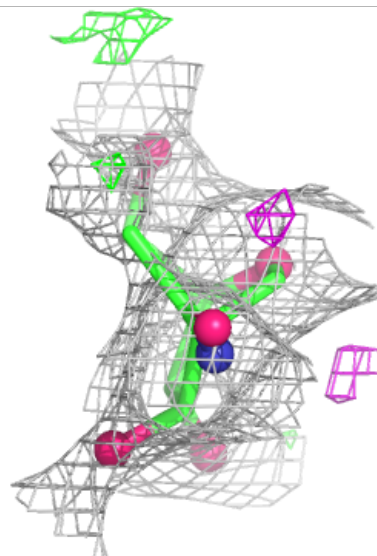
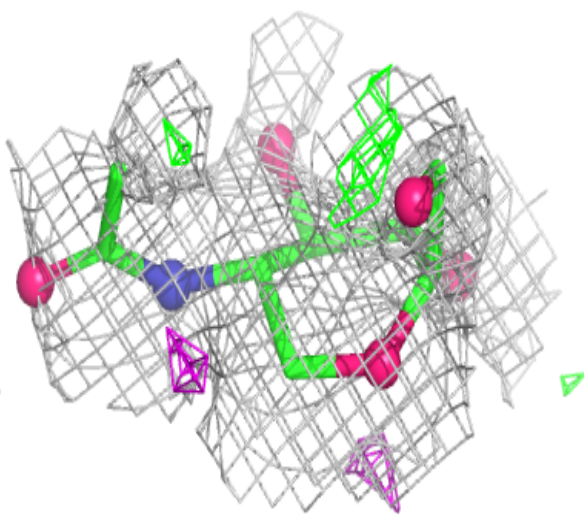
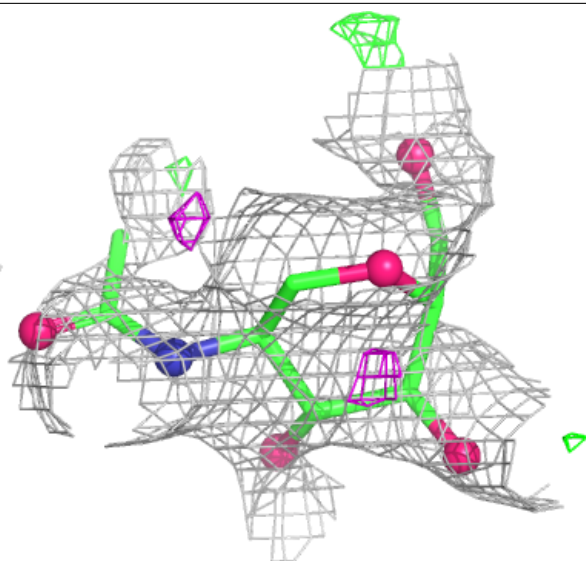
Electron density around NAG A 605:

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



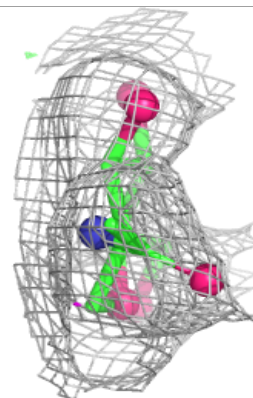
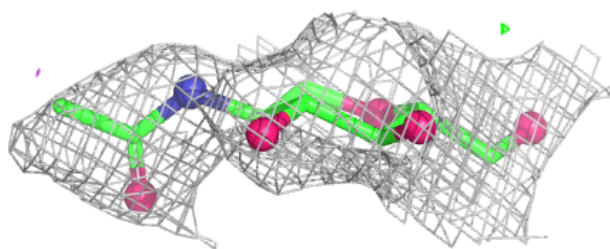
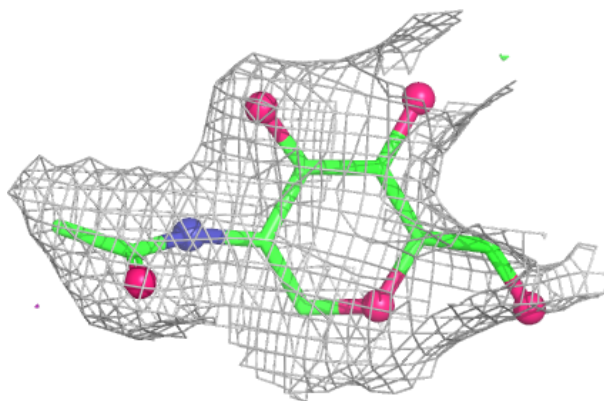
Electron density around NAG A 606:

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

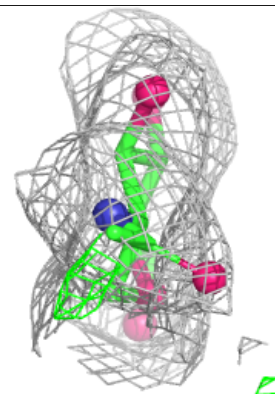
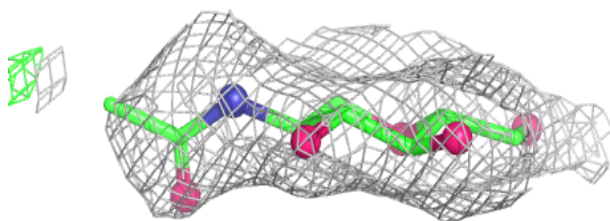
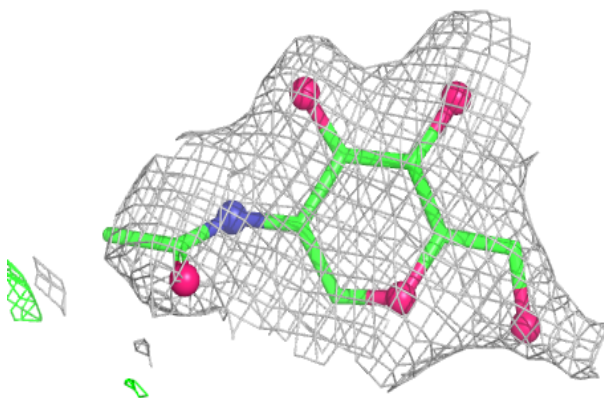


Electron density around NAG A 604:

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

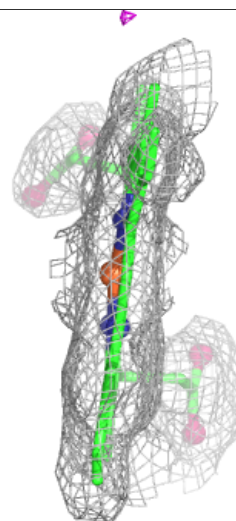
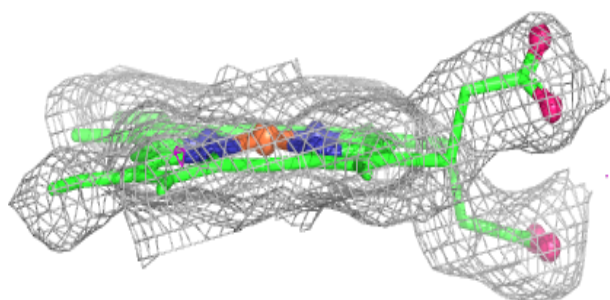
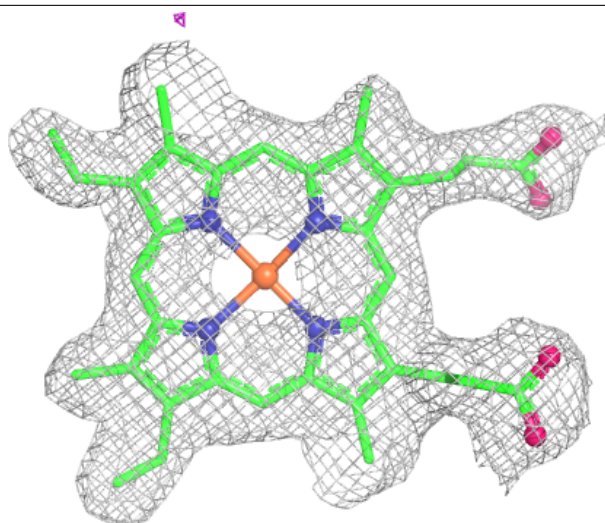
**Electron density around NAG A 603:**

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



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.