



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 03:42 AM BST

PDB ID : 6L9T
Title : Crystal structure of the complex of bovine lactoperoxidase with OSCN at 1.89 Å resolution
Authors : Singh, P.K.; Viswanathan, V.; Pandey, N.; Singh, A.; Sinha, M.; Singh, R.P.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2019-11-11
Resolution : 1.89 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 : 2.14.4.dev1
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) : 2.14.4.dev1

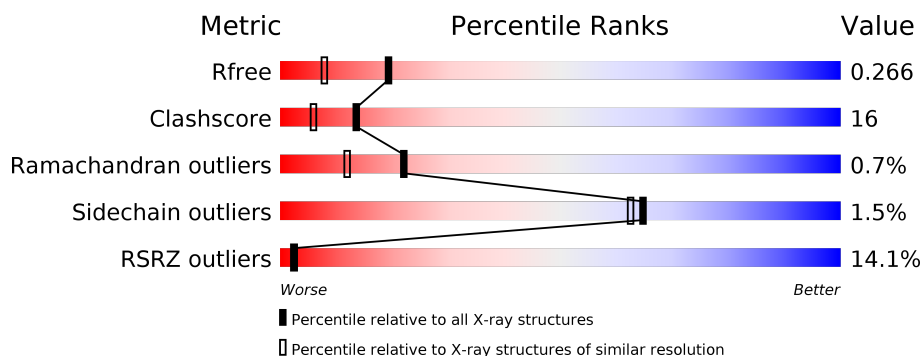
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
2	AeA	2	
2	AhA	2	

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	IOD	A	608	-	-	X	-
7	IOD	A	614	-	-	X	-
7	IOD	A	618	-	-	X	-
7	IOD	A	620	-	-	X	-
7	IOD	A	621	-	-	X	-
7	IOD	A	623	-	-	X	-
7	IOD	A	624	-	-	X	-
8	SCN	A	625	-	-	X	-
8	SCN	A	629	-	-	X	-
9	OSM	A	634	-	-	X	-

2 Entry composition [i](#)

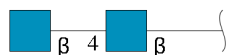
There are 10 unique types of molecules in this entry. The entry contains 5511 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	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	AeA	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	AhA	2	Total	C	N	O	0	0	0
			28	16	2	10			

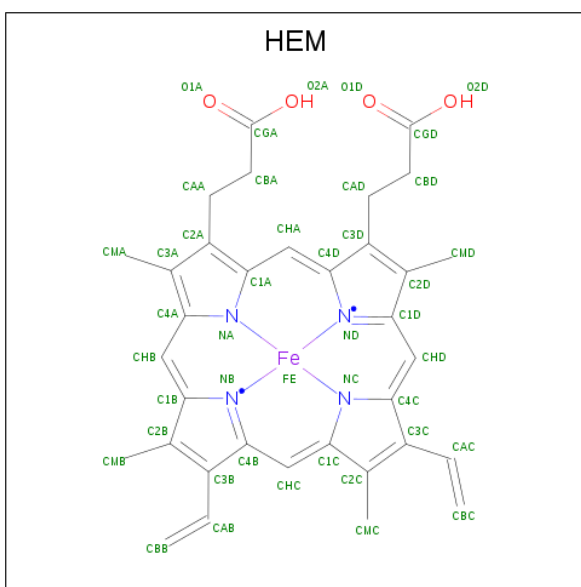
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

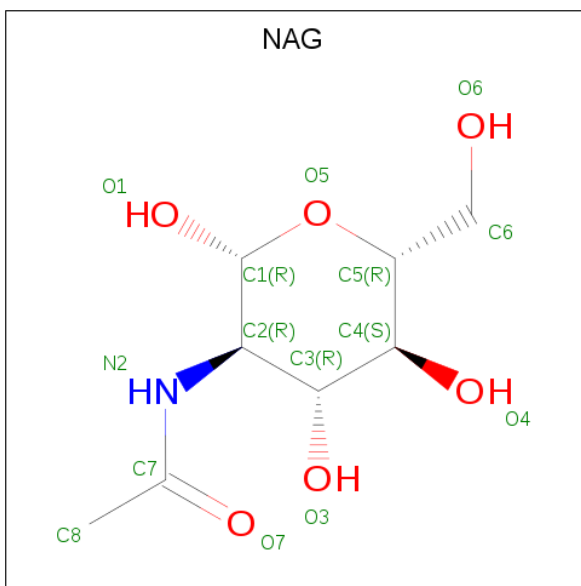
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by author).



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by author).

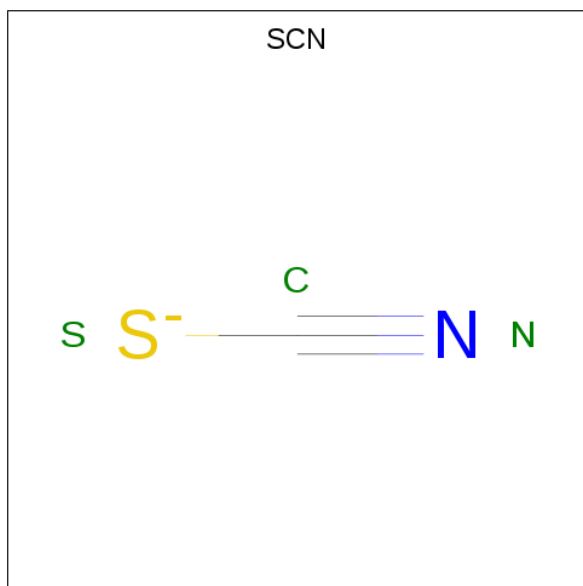


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 14	C 8	N 1	O 5	0	0
6	A	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 7 is IODIDE ION (three-letter code: IOD) (formula: I).

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

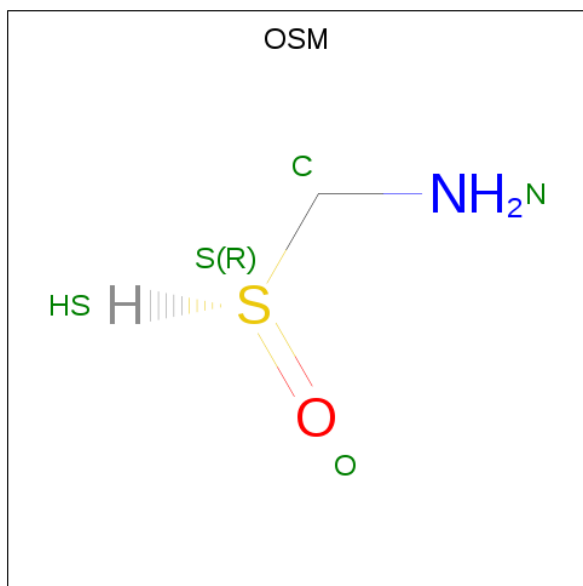
- Molecule 8 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 9 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula:

CH₅NOS) (labeled as "Ligand of Interest" by author).



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

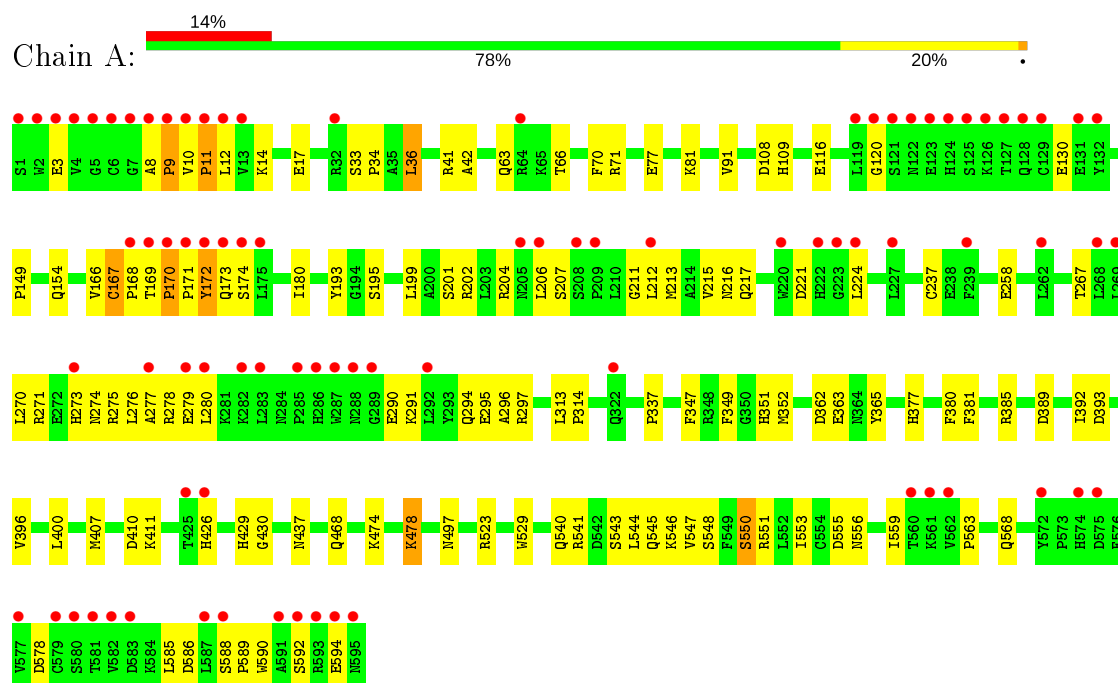
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	562	Total	O	0	0
			562	562		

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



• 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	53.99Å 79.93Å 76.31Å 90.00° 102.18° 90.00°	Depositor
Resolution (Å)	35.33 – 1.89 35.30 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.33-1.89) 100.0 (35.30-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.49 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.205 , 0.264 0.211 , 0.266	Depositor DCC
R_{free} test set	2580 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.788	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.2	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	0.94	EDS
Total number of atoms	5511	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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: ZN, SCN, NAG, CA, 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	0.72	0/4898	0.84	1/6645 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	9	PRO	C-N-CA	5.03	134.27	121.70

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	4770	0	4688	130	0
2	AeA	28	0	25	0	0
2	AhA	28	0	25	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	43	0	30	18	0
6	A	28	0	26	0	0
7	A	19	0	0	23	0
8	A	27	0	0	9	0
9	A	4	0	5	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	562	0	0	31	0
All	All	5511	0	4799	155	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 16.

All (155) 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)
7:A:608:IOD:I	8:A:625:SCN:S	1.71	1.41
1:A:108:ASP:OD2	5:A:603:HEM:CMD	1.68	1.37
7:A:614:IOD:I	8:A:629:SCN:S	1.66	1.35
1:A:258:GLU:OE2	5:A:603:HEM:CMB	1.73	1.34
7:A:608:IOD:I	8:A:625:SCN:C	0.76	1.16
5:A:603:HEM:HBD2	9:A:634:OSM:HN2	1.12	1.10
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.32	1.09
1:A:170:PRO:HG2	1:A:171:PRO:HD2	1.31	1.09
1:A:216:ASN:HA	8:A:625:SCN:S	1.93	1.08
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.23	1.07
9:A:634:OSM:H1	10:A:884:HOH:O	1.55	1.06
1:A:170:PRO:HB2	1:A:171:PRO:CD	1.87	1.04
1:A:167:CYS:CB	1:A:168:PRO:HD3	1.85	1.02
7:A:619:IOD:I	10:A:748:HOH:O	2.46	1.02
1:A:429:HIS:O	7:A:621:IOD:I	2.48	1.02
1:A:258:GLU:OE2	5:A:603:HEM:HMB1	0.84	1.01
1:A:130:GLU:OE1	1:A:426:HIS:ND1	1.94	1.01
7:A:608:IOD:I	8:A:625:SCN:N	1.35	0.99
1:A:410:ASP:OD1	10:A:701:HOH:O	1.81	0.98
7:A:623:IOD:I	9:A:634:OSM:S	2.92	0.97
1:A:109:HIS:NE2	9:A:634:OSM:S	2.03	0.96
1:A:108:ASP:CG	5:A:603:HEM:HMD1	1.87	0.95
1:A:108:ASP:OD2	5:A:603:HEM:HMD1	0.77	0.94
1:A:173:GLN:NE2	10:A:703:HOH:O	1.99	0.94
1:A:109:HIS:CE1	9:A:634:OSM:HS	1.85	0.93
1:A:36:LEU:HD12	1:A:337:PRO:HD2	1.49	0.93
1:A:170:PRO:CG	1:A:171:PRO:HD2	2.01	0.89
1:A:170:PRO:CB	1:A:171:PRO:CD	2.50	0.87
1:A:258:GLU:CD	5:A:603:HEM:HMB1	1.94	0.87
1:A:195:SER:O	10:A:702:HOH:O	1.92	0.86
9:A:634:OSM:C	10:A:884:HOH:O	2.16	0.86
5:A:603:HEM:CBD	9:A:634:OSM:HN2	1.86	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:603:HEM:HBD2	9:A:634:OSM:N	1.91	0.85
1:A:207:SER:HA	10:A:992:HOH:O	1.78	0.83
1:A:63:GLN:O	1:A:71:ARG:NH1	2.09	0.83
5:A:603:HEM:CHA	9:A:634:OSM:H2	2.08	0.83
1:A:224:LEU:HD13	1:A:271:ARG:NH1	1.94	0.82
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.25	0.82
1:A:559:ILE:HA	8:A:627:SCN:S	2.20	0.80
7:A:620:IOD:I	10:A:1117:HOH:O	2.69	0.79
1:A:550:SER:OG	1:A:563:PRO:O	2.00	0.79
1:A:8:ALA:H	1:A:9:PRO:HD3	1.46	0.79
1:A:10:VAL:HG23	1:A:41:ARG:NH2	1.99	0.78
1:A:168:PRO:HG2	1:A:172:TYR:HB2	1.64	0.78
8:A:633:SCN:S	9:A:634:OSM:S	2.83	0.77
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.12	0.76
1:A:12:LEU:HB2	1:A:14:LYS:HE2	1.69	0.74
1:A:221:ASP:HB3	1:A:224:LEU:HB2	1.70	0.73
1:A:167:CYS:CB	1:A:168:PRO:CD	2.68	0.71
1:A:377:HIS:NE2	7:A:618:IOD:I	2.93	0.71
5:A:603:HEM:C1A	9:A:634:OSM:H2	2.27	0.70
1:A:204:ARG:O	10:A:706:HOH:O	2.10	0.70
7:A:614:IOD:I	8:A:629:SCN:N	1.24	0.69
1:A:199:LEU:HA	7:A:624:IOD:I	2.63	0.69
1:A:290:GLU:OE2	10:A:705:HOH:O	2.10	0.69
1:A:578:ASP:OD1	10:A:708:HOH:O	2.12	0.68
1:A:294:GLN:OE1	10:A:707:HOH:O	2.12	0.66
1:A:116:GLU:O	10:A:709:HOH:O	2.13	0.66
7:A:615:IOD:I	10:A:1167:HOH:O	2.84	0.66
1:A:8:ALA:N	1:A:9:PRO:CD	2.58	0.66
1:A:291:LYS:CD	10:A:886:HOH:O	2.43	0.65
1:A:586:ASP:N	10:A:716:HOH:O	2.26	0.65
1:A:108:ASP:CG	5:A:603:HEM:CMD	2.57	0.65
1:A:362:ASP:O	1:A:365:TYR:N	2.28	0.64
1:A:237:CYS:O	10:A:710:HOH:O	2.14	0.64
1:A:541:ARG:O	1:A:545:GLN:HB2	1.97	0.64
7:A:617:IOD:I	10:A:862:HOH:O	2.85	0.64
1:A:540:GLN:O	1:A:544:LEU:N	2.28	0.64
1:A:8:ALA:H	1:A:9:PRO:CD	2.10	0.63
1:A:224:LEU:HD13	1:A:271:ARG:HH11	1.64	0.63
7:A:623:IOD:I	9:A:634:OSM:C	3.18	0.62
7:A:614:IOD:I	8:A:629:SCN:C	0.22	0.62
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:O	10:A:711:HOH:O	2.16	0.61
1:A:548:SER:OG	1:A:551:ARG:CB	2.49	0.61
1:A:548:SER:OG	1:A:551:ARG:N	2.30	0.61
1:A:36:LEU:CD1	1:A:337:PRO:HD2	2.26	0.61
1:A:17:GLU:OE2	10:A:712:HOH:O	2.17	0.60
1:A:224:LEU:CD1	1:A:271:ARG:NH1	2.65	0.60
1:A:36:LEU:HD12	1:A:337:PRO:CD	2.28	0.60
1:A:291:LYS:HD2	10:A:886:HOH:O	2.01	0.59
1:A:258:GLU:CD	5:A:603:HEM:CMB	2.60	0.59
1:A:548:SER:HG	1:A:551:ARG:H	1.50	0.58
1:A:363:GLU:HA	7:A:611:IOD:I	2.73	0.58
1:A:169:THR:OG1	1:A:170:PRO:HD3	2.04	0.58
1:A:237:CYS:HA	1:A:381:PHE:O	2.03	0.58
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.40	0.56
1:A:551:ARG:NH2	1:A:555:ASP:OD1	2.41	0.54
1:A:377:HIS:CD2	7:A:618:IOD:I	3.32	0.53
5:A:603:HEM:HMC2	5:A:603:HEM:HBC2	1.91	0.53
1:A:170:PRO:CG	1:A:171:PRO:CD	2.77	0.53
1:A:212:LEU:HD13	10:A:1210:HOH:O	2.07	0.53
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.90	0.53
1:A:478:LYS:NZ	10:A:727:HOH:O	2.38	0.53
5:A:603:HEM:C4D	9:A:634:OSM:H2	2.44	0.53
1:A:149:PRO:HB2	7:A:620:IOD:I	2.80	0.51
1:A:166:VAL:HG13	1:A:180:ILE:HG12	1.92	0.51
1:A:215:VAL:HG23	1:A:217:GLN:HE21	1.75	0.50
1:A:540:GLN:NE2	10:A:715:HOH:O	2.43	0.50
1:A:548:SER:OG	1:A:551:ARG:HB2	2.12	0.50
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.48	0.49
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.93	0.49
1:A:267:THR:CG2	1:A:392:ILE:HD13	2.43	0.49
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.41	0.49
1:A:172:TYR:CE2	1:A:174:SER:HB2	2.48	0.48
1:A:202:ARG:HD3	7:A:624:IOD:I	2.84	0.48
1:A:207:SER:N	10:A:739:HOH:O	2.45	0.48
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.48	0.48
1:A:392:ILE:O	1:A:396:VAL:HG23	2.14	0.47
1:A:66:THR:HB	1:A:70:PHE:N	2.29	0.47
1:A:215:VAL:HG23	1:A:217:GLN:NE2	2.28	0.47
7:A:623:IOD:I	9:A:634:OSM:H1	2.84	0.47
1:A:393:ASP:HB2	10:A:844:HOH:O	2.15	0.47
1:A:91:VAL:HG12	1:A:411:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ALA:O	1:A:280:LEU:HB2	2.15	0.46
1:A:273:HIS:HE1	1:A:296:ALA:HB3	1.80	0.46
1:A:588:SER:N	1:A:589:PRO:CD	2.79	0.46
1:A:291:LYS:HD3	10:A:886:HOH:O	2.13	0.45
1:A:8:ALA:N	1:A:9:PRO:HD3	2.13	0.45
1:A:592:SER:OG	1:A:594:GLU:OE1	2.35	0.45
1:A:385:ARG:O	1:A:389:ASP:HB3	2.16	0.45
1:A:274:ASN:HB3	1:A:278:ARG:NH1	2.31	0.45
1:A:273:HIS:CE1	1:A:296:ALA:HB3	2.52	0.45
1:A:548:SER:HG	1:A:551:ARG:HB2	1.82	0.44
1:A:544:LEU:O	1:A:547:VAL:HG22	2.17	0.44
5:A:603:HEM:CBD	9:A:634:OSM:N	2.65	0.44
1:A:109:HIS:CD2	9:A:634:OSM:S	3.03	0.44
1:A:430:GLY:HA2	7:A:621:IOD:I	2.88	0.44
1:A:42:ALA:HB2	1:A:166:VAL:HG21	1.98	0.44
1:A:291:LYS:O	1:A:295:GLU:HB2	2.18	0.44
1:A:154:GLN:OE1	10:A:713:HOH:O	2.21	0.44
1:A:276:LEU:HD21	1:A:585:LEU:HD23	2.00	0.44
1:A:556:ASN:HA	10:A:724:HOH:O	2.17	0.44
1:A:544:LEU:HG	1:A:590:TRP:HH2	1.82	0.43
1:A:211:GLY:HA2	10:A:780:HOH:O	2.17	0.43
1:A:221:ASP:HB2	1:A:271:ARG:NH2	2.33	0.43
1:A:34:PRO:HD2	7:A:610:IOD:I	2.89	0.43
1:A:270:LEU:HD13	10:A:1010:HOH:O	2.18	0.43
1:A:10:VAL:HG23	1:A:41:ARG:HH22	1.76	0.42
1:A:275:ARG:O	1:A:279:GLU:HG2	2.18	0.42
1:A:172:TYR:CD1	1:A:172:TYR:O	2.73	0.42
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.84	0.42
1:A:221:ASP:CB	1:A:271:ARG:NH2	2.83	0.42
1:A:193:TYR:CZ	1:A:297:ARG:HA	2.55	0.42
1:A:313:LEU:N	1:A:314:PRO:CD	2.83	0.42
1:A:10:VAL:HA	1:A:11:PRO:HD3	1.91	0.41
1:A:543:SER:HA	1:A:546:LYS:HG3	2.02	0.41
1:A:169:THR:N	1:A:170:PRO:CD	2.83	0.41
1:A:544:LEU:HG	1:A:590:TRP:CH2	2.56	0.41
1:A:258:GLU:OE2	5:A:603:HEM:C2B	2.64	0.40
5:A:603:HEM:C4D	9:A:634:OSM:C	3.04	0.40
1:A:294:GLN:OE1	1:A:294:GLN:HA	2.21	0.40
1:A:352:MET:CB	1:A:407:MET:HG2	2.52	0.40
1:A:33:SER:O	1:A:36:LEU:HB2	2.21	0.40
1:A:199:LEU:HD13	7:A:624:IOD:I	2.91	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	593/595 (100%)	553 (93%)	36 (6%)	4 (1%)	22 12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	167	CYS
1	A	170	PRO
1	A	120	GLY

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%)	510 (98%)	8 (2%)	65 62

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	36	LEU
1	A	172	TYR
1	A	201	SER

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Mol	Chain	Res	Type
1	A	347	PHE
1	A	478	LYS
1	A	550	SER
1	A	568	GLN

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

Mol	Chain	Res	Type
1	A	128	GLN
1	A	273	HIS
1	A	468	GLN
1	A	497	ASN
1	A	558	HIS
1	A	570	ASN

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 [i](#)

4 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	AeA	1	1,2	14,14,15	0.78	0	17,19,21	1.62	6 (35%)
2	NAG	AeA	2	2	14,14,15	0.56	0	17,19,21	2.27	3 (17%)
2	NAG	AhA	1	1,2	14,14,15	0.42	0	17,19,21	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	AhA	2	2	14,14,15	0.74	0	17,19,21	2.08	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	AeA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	AeA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	AhA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	AhA	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AeA	2	NAG	C1-O5-C5	6.99	121.66	112.19
2	AhA	2	NAG	C4-C3-C2	4.56	117.71	111.02
2	AeA	2	NAG	C4-C3-C2	-4.30	104.71	111.02
2	AhA	2	NAG	O5-C5-C4	-3.59	102.08	110.83
2	AhA	2	NAG	O5-C5-C6	3.15	112.14	107.20
2	AhA	2	NAG	C2-N2-C7	3.06	127.26	122.90
2	AhA	1	NAG	O5-C5-C6	2.91	111.76	107.20
2	AhA	2	NAG	O5-C1-C2	2.55	115.32	111.29
2	AeA	2	NAG	O3-C3-C2	2.48	114.60	109.47
2	AeA	1	NAG	C6-C5-C4	2.37	118.55	113.00
2	AeA	1	NAG	O5-C1-C2	2.34	114.98	111.29
2	AeA	1	NAG	C1-O5-C5	2.34	115.36	112.19
2	AeA	1	NAG	O7-C7-N2	2.18	125.95	121.95
2	AeA	1	NAG	O7-C7-C8	-2.08	118.20	122.06
2	AeA	1	NAG	O4-C4-C5	2.04	114.37	109.30

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AhA	2	NAG	C1-C2-N2-C7
2	AhA	2	NAG	O5-C5-C6-O6
2	AhA	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	AhA	1	NAG	O5-C5-C6-O6
2	AhA	1	NAG	C4-C5-C6-O6
2	AhA	2	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 34 ligands modelled in this entry, 21 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEM	A	603	1,9	27,50,50	1.02	1 (3%)	17,82,82	1.46	5 (29%)
8	SCN	A	629	-	1,2,2	0.76	0	0,1,1	0.00	-
8	SCN	A	631	-	1,2,2	0.08	0	0,1,1	0.00	-
6	NAG	A	605	1	14,14,15	0.57	0	17,19,21	1.03	1 (5%)
8	SCN	A	625	-	1,2,2	1.61	0	0,1,1	0.00	-
6	NAG	A	604	1	14,14,15	0.61	0	17,19,21	0.99	0
8	SCN	A	632	-	1,2,2	0.26	0	0,1,1	0.00	-
8	SCN	A	628	-	1,2,2	1.35	0	0,1,1	0.00	-
9	OSM	A	634	5	1,3,3	0.02	0	0,2,2	0.00	-
8	SCN	A	627	-	1,2,2	1.19	0	0,1,1	0.00	-
8	SCN	A	633	-	1,2,2	0.10	0	0,1,1	0.00	-
8	SCN	A	630	-	1,2,2	0.36	0	0,1,1	0.00	-
8	SCN	A	626	-	1,2,2	1.06	0	0,1,1	0.00	-

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
5	HEM	A	603	1,9	-	0/6/54/54	-
6	NAG	A	604	1	-	1/6/23/26	0/1/1/1
9	OSM	A	634	5	-	0/0/1/1	-
6	NAG	A	605	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	603	HEM	C3B-C2B	-3.46	1.35	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	605	NAG	O5-C1-C2	-2.65	107.10	111.29
5	A	603	HEM	CMC-C2C-C3C	2.60	129.54	124.68
5	A	603	HEM	CBD-CAD-C3D	-2.21	108.40	112.48
5	A	603	HEM	CMA-C3A-C4A	-2.13	125.19	128.46
5	A	603	HEM	CMD-C2D-C1D	2.10	131.70	128.46
5	A	603	HEM	CMD-C2D-C3D	-2.09	120.99	124.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	604	NAG	C4-C5-C6-O6

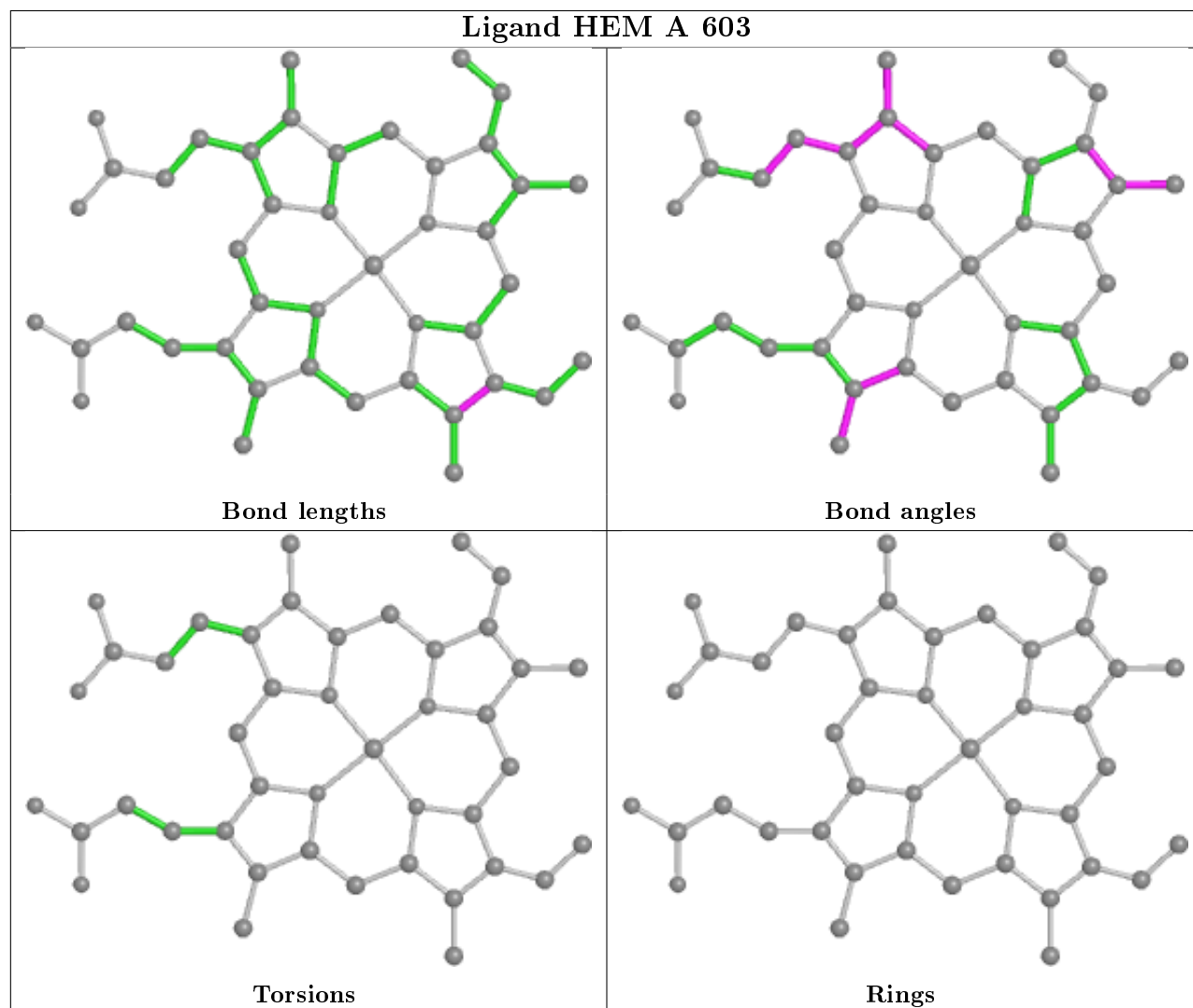
There are no ring outliers.

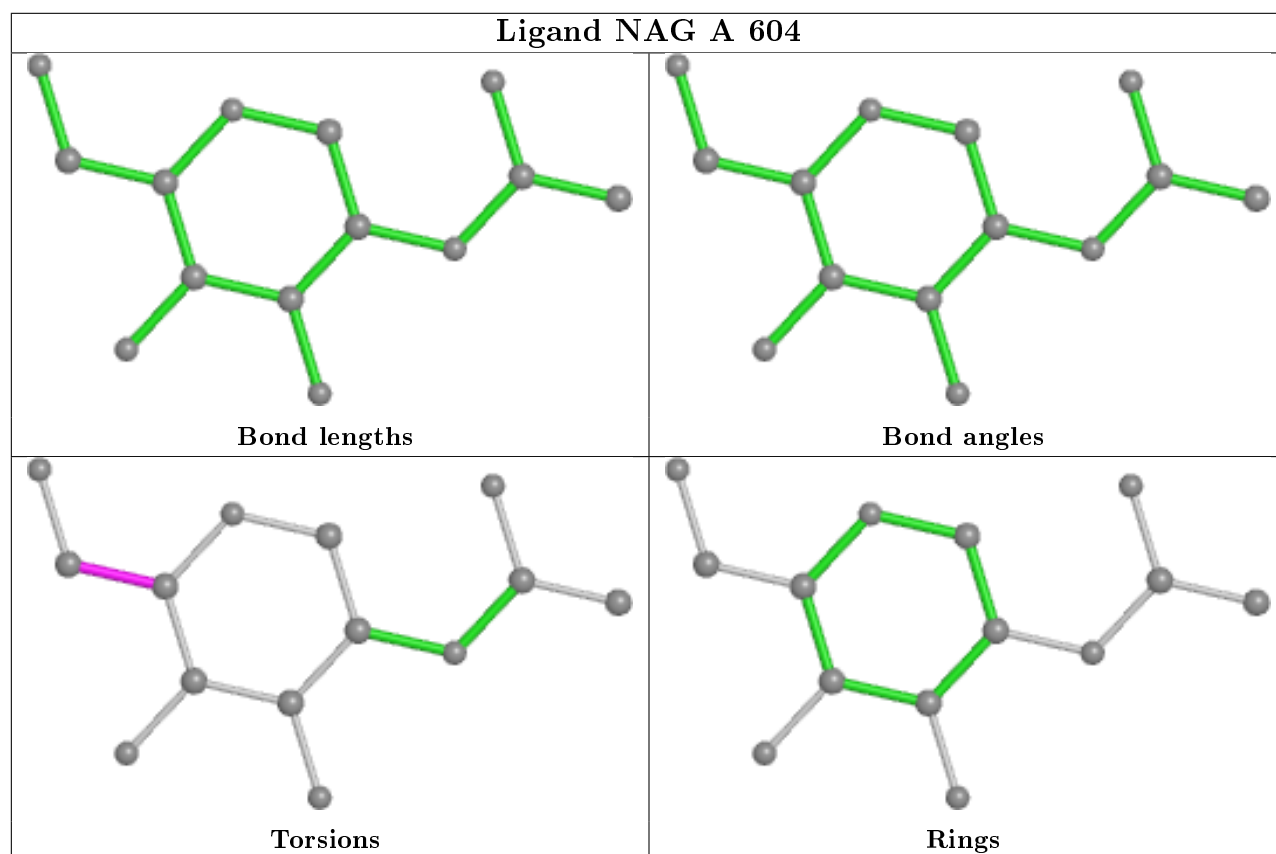
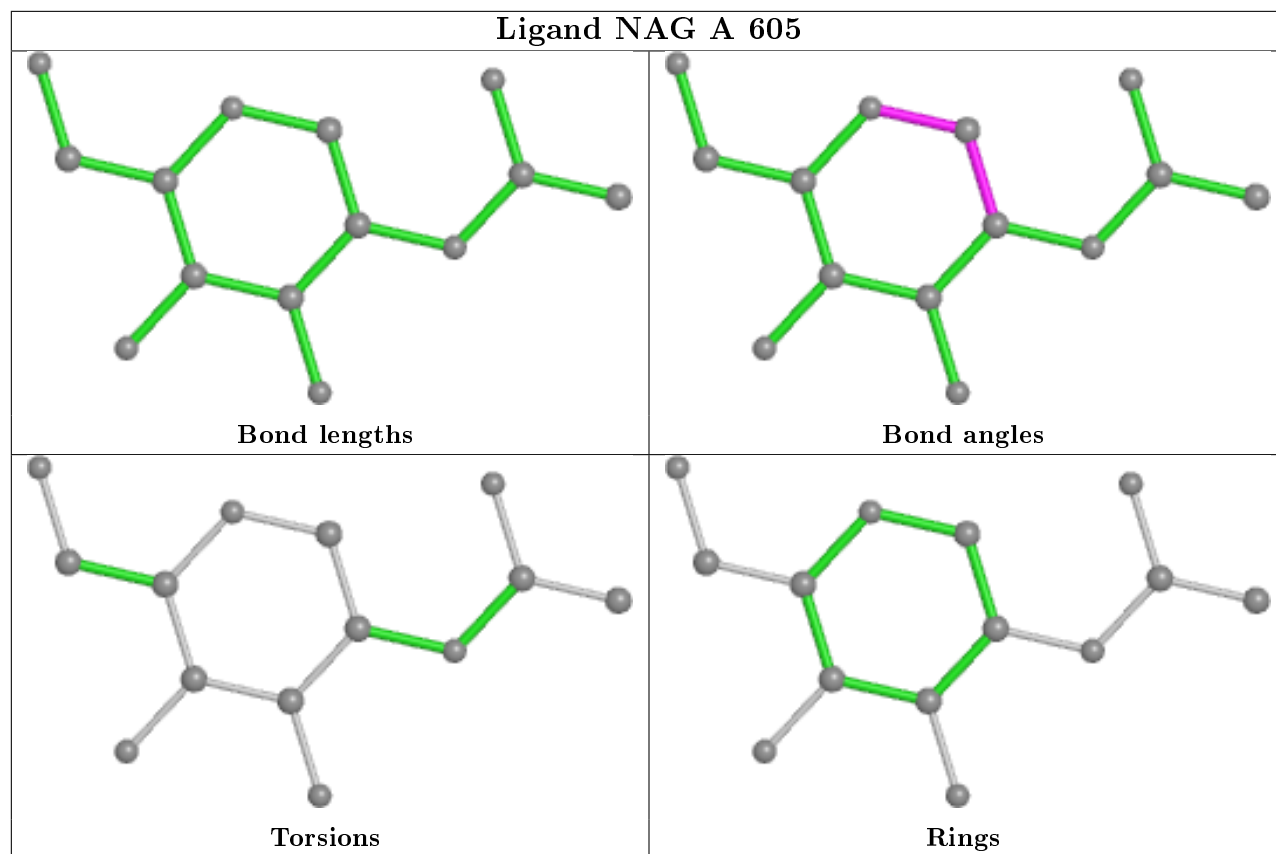
6 monomers are involved in 35 short contacts:

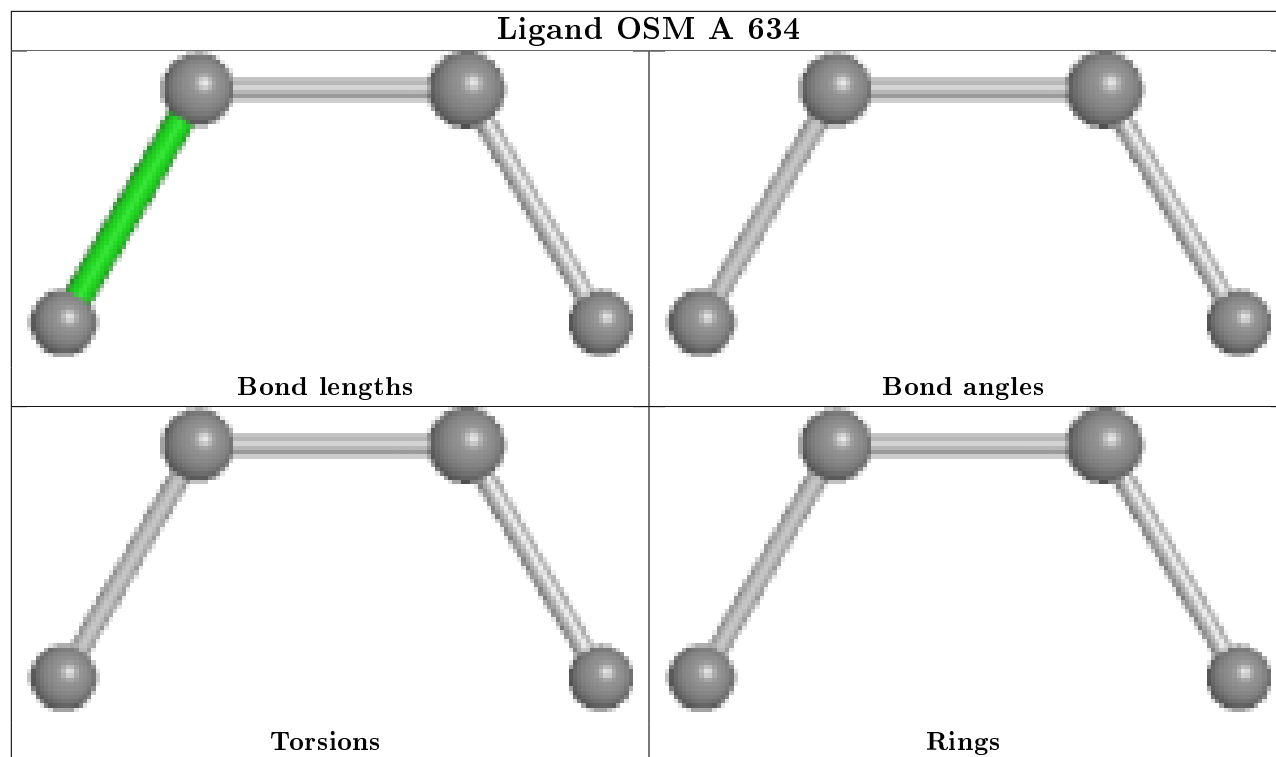
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	603	HEM	18	0
8	A	629	SCN	3	0
8	A	625	SCN	4	0
9	A	634	OSM	17	0
8	A	627	SCN	1	0
8	A	633	SCN	1	0

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%)	0.95	84 (14%) 2 2	12, 30, 80, 158	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	SER	31.6
1	A	173	GLN	22.8
1	A	172	TYR	20.6
1	A	2	TRP	15.5
1	A	13	VAL	13.6
1	A	120	GLY	12.8
1	A	119	LEU	11.9
1	A	169	THR	11.4
1	A	1	SER	10.8
1	A	595	ASN	10.6
1	A	121	SER	10.1
1	A	7	GLY	9.4
1	A	8	ALA	9.3
1	A	124	HIS	9.1
1	A	10	VAL	9.0
1	A	280	LEU	8.0
1	A	122	ASN	8.0
1	A	4	VAL	7.5
1	A	168	PRO	7.2
1	A	171	PRO	6.7
1	A	283	LEU	6.5
1	A	170	PRO	6.5
1	A	11	PRO	6.2
1	A	593	ARG	6.0
1	A	224	LEU	5.9
1	A	5	GLY	5.7
1	A	220	TRP	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	12	LEU	5.5
1	A	125	SER	5.4
1	A	175	LEU	5.3
1	A	123	GLU	4.8
1	A	9	PRO	4.7
1	A	425	THR	4.5
1	A	287	TRP	4.5
1	A	574	HIS	4.4
1	A	209	PRO	4.3
1	A	127	THR	4.1
1	A	582	VAL	4.0
1	A	223	GLY	3.9
1	A	222	HIS	3.9
1	A	208	SER	3.7
1	A	594	GLU	3.6
1	A	592	SER	3.6
1	A	212	LEU	3.6
1	A	591	ALA	3.6
1	A	577	VAL	3.2
1	A	3	GLU	3.1
1	A	268	LEU	3.0
1	A	285	PRO	2.9
1	A	206	LEU	2.9
1	A	561	LYS	2.9
1	A	227	LEU	2.9
1	A	580	SER	2.9
1	A	587	LEU	2.9
1	A	132	TYR	2.8
1	A	426	HIS	2.7
1	A	6	CYS	2.7
1	A	322	GLN	2.7
1	A	286	HIS	2.7
1	A	572	TYR	2.7
1	A	126	LYS	2.6
1	A	128	GLN	2.6
1	A	269	LEU	2.6
1	A	282	LYS	2.6
1	A	579	CYS	2.6
1	A	588	SER	2.6
1	A	131	GLU	2.5
1	A	277	ALA	2.4
1	A	581	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	288	ASN	2.4
1	A	562	VAL	2.4
1	A	279	GLU	2.3
1	A	129	CYS	2.3
1	A	292	LEU	2.2
1	A	64	ARG	2.2
1	A	289	GLY	2.2
1	A	575	ASP	2.1
1	A	239	PHE	2.1
1	A	583	ASP	2.1
1	A	32	ARG	2.1
1	A	262	LEU	2.1
1	A	560	THR	2.0
1	A	273	HIS	2.0
1	A	205	ASN	2.0

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 ⓘ

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	AhA	2	14/15	0.67	0.37	66,74,84,86	0
2	NAG	AeA	2	14/15	0.69	0.26	56,69,71,71	0
2	NAG	AeA	1	14/15	0.72	0.21	36,57,61,65	0
2	NAG	AhA	1	14/15	0.84	0.18	45,54,59,69	0

6.4 Ligands ⓘ

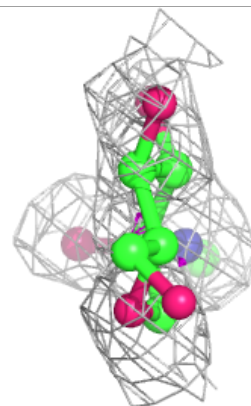
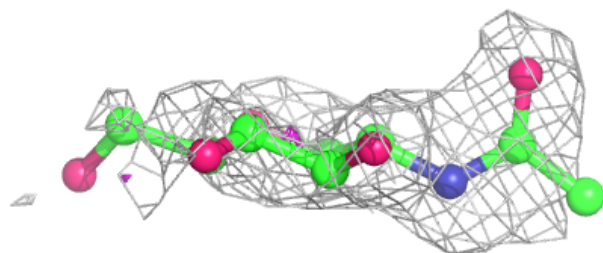
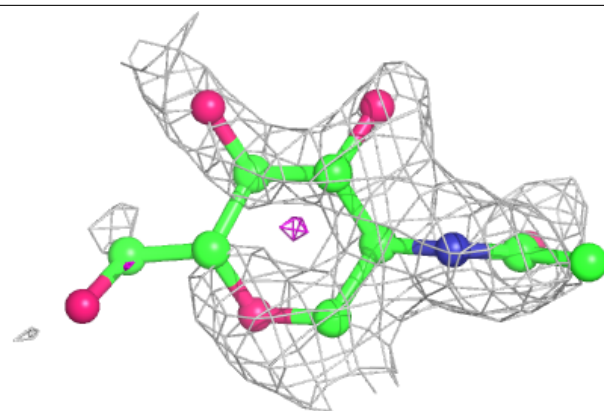
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	A	604	14/15	0.73	0.28	50,58,67,71	0
7	IOD	A	617	1/1	0.85	0.07	64,64,64,64	1
4	ZN	A	602	1/1	0.88	0.08	54,54,54,54	0
6	NAG	A	605	14/15	0.89	0.10	33,38,41,42	0
7	IOD	A	622	1/1	0.94	0.06	91,91,91,91	0
8	SCN	A	627	3/3	0.95	0.15	3,3,4,4	3
9	OSM	A	634	4/4	0.95	0.16	24,30,33,35	0
7	IOD	A	609	1/1	0.96	0.06	37,37,37,37	0
8	SCN	A	629	3/3	0.97	0.07	9,9,9,11	3
8	SCN	A	632	3/3	0.97	0.12	14,14,16,16	3
5	HEM	A	603	43/43	0.97	0.13	12,14,19,24	0
7	IOD	A	611	1/1	0.97	0.05	32,32,32,32	1
7	IOD	A	615	1/1	0.97	0.03	55,55,55,55	1
7	IOD	A	614	1/1	0.97	0.08	75,75,75,75	1
7	IOD	A	610	1/1	0.97	0.10	68,68,68,68	1
7	IOD	A	620	1/1	0.98	0.04	39,39,39,39	1
8	SCN	A	625	3/3	0.98	0.09	6,6,6,6	3
8	SCN	A	630	3/3	0.98	0.05	12,12,12,14	3
7	IOD	A	616	1/1	0.98	0.03	42,42,42,42	1
7	IOD	A	607	1/1	0.98	0.02	29,29,29,29	1
8	SCN	A	631	3/3	0.98	0.08	21,21,21,23	3
7	IOD	A	608	1/1	0.98	0.05	25,25,25,25	1
7	IOD	A	613	1/1	0.99	0.04	36,36,36,36	1
3	CA	A	601	1/1	0.99	0.08	17,17,17,17	0
7	IOD	A	621	1/1	0.99	0.02	31,31,31,31	1
8	SCN	A	628	3/3	0.99	0.06	0,0,0,0	3
8	SCN	A	626	3/3	0.99	0.06	17,17,18,19	3
7	IOD	A	624	1/1	0.99	0.07	29,29,29,29	1
7	IOD	A	612	1/1	0.99	0.03	33,33,33,33	0
7	IOD	A	618	1/1	0.99	0.05	61,61,61,61	1
7	IOD	A	619	1/1	1.00	0.03	30,30,30,30	1
7	IOD	A	623	1/1	1.00	0.07	18,18,18,18	1
8	SCN	A	633	3/3	1.00	0.09	13,13,13,13	3
7	IOD	A	606	1/1	1.00	0.04	18,18,18,18	0

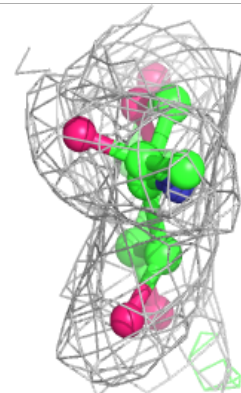
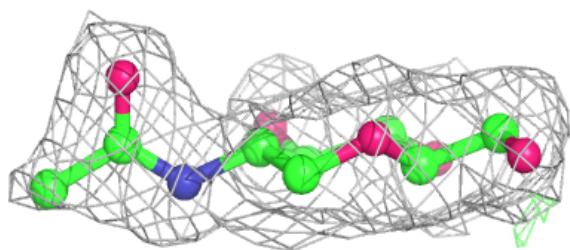
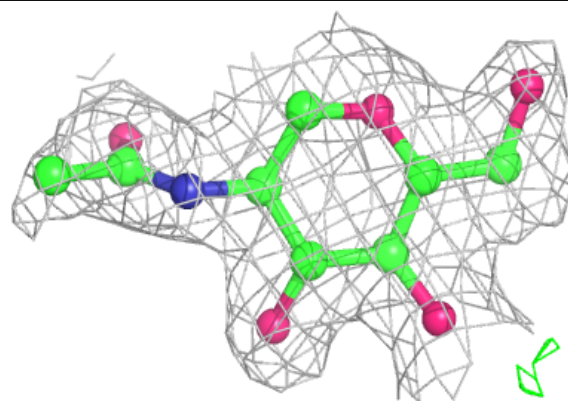
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 604:

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

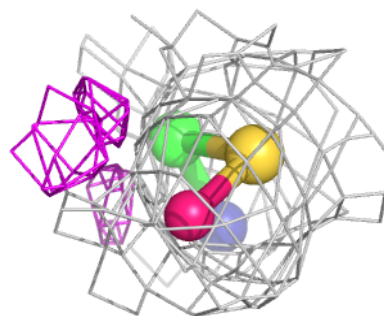
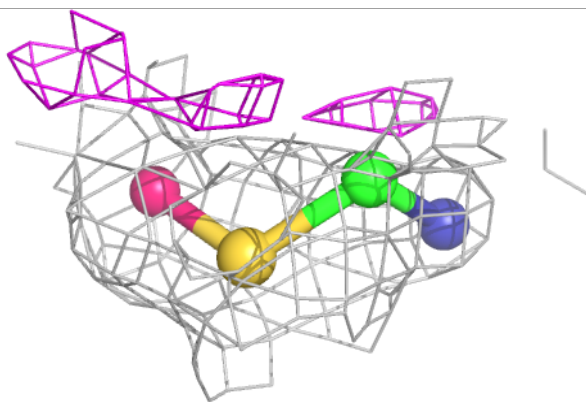
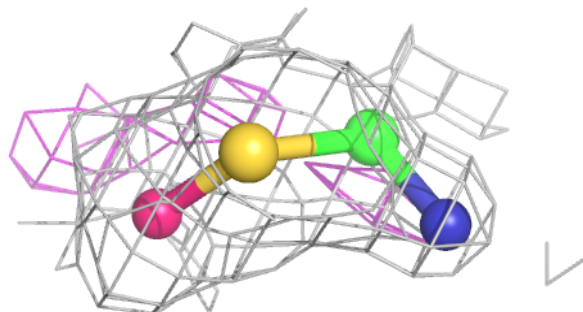
**Electron density around NAG A 605:**

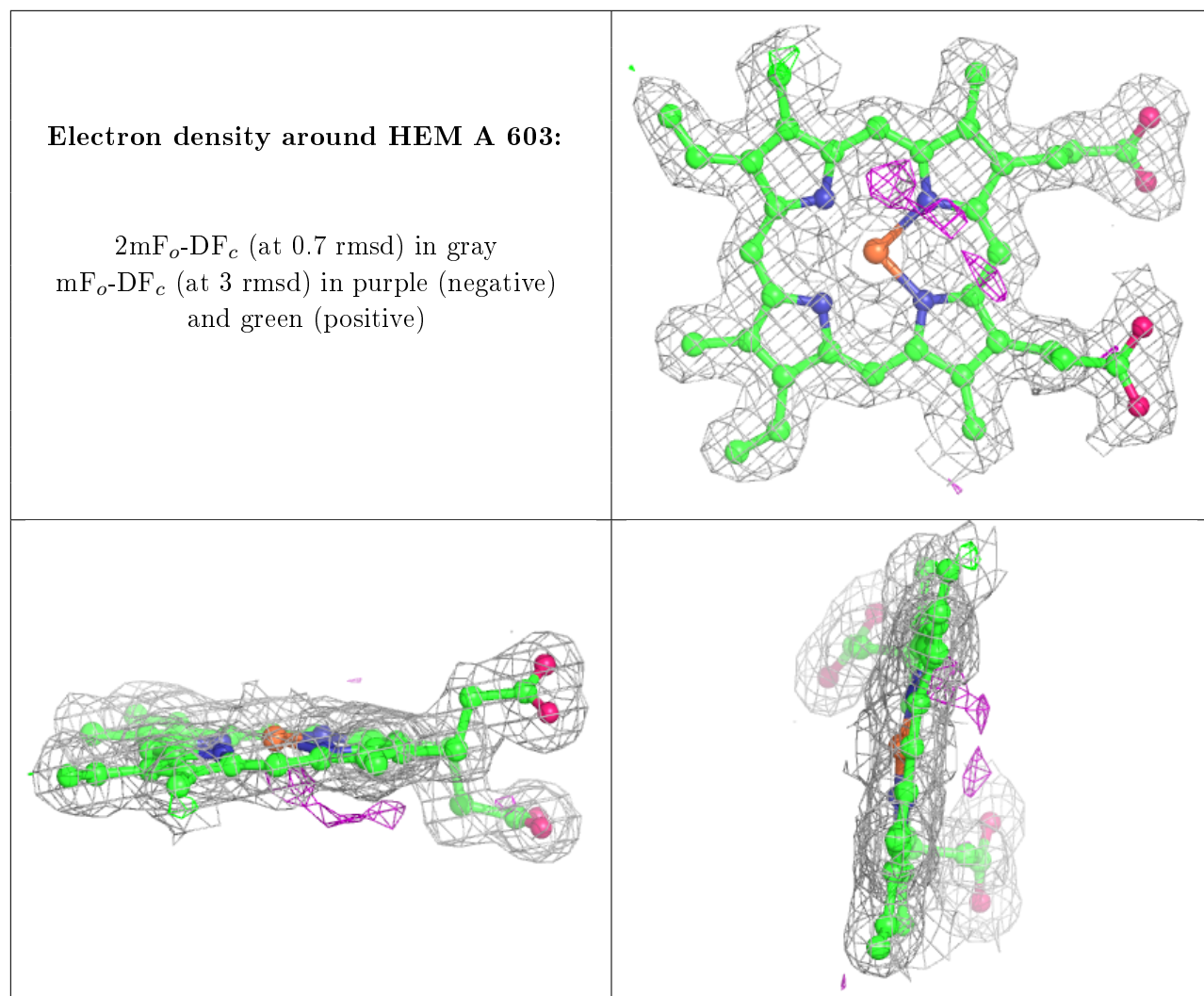
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OSM A 634:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.