



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:11 PM JST

PDB ID : 6KY7 / pdb_00006ky7
Title : Crystal structure of yak lactoperoxidase at 2.27 Å resolution
Authors : Singh, P.K.; Viswanathan, V.; Sharma, P.; Rani, C.; Sharma, S.; Singh, T.P.
Deposited on : 2019-09-16
Resolution : 2.27 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

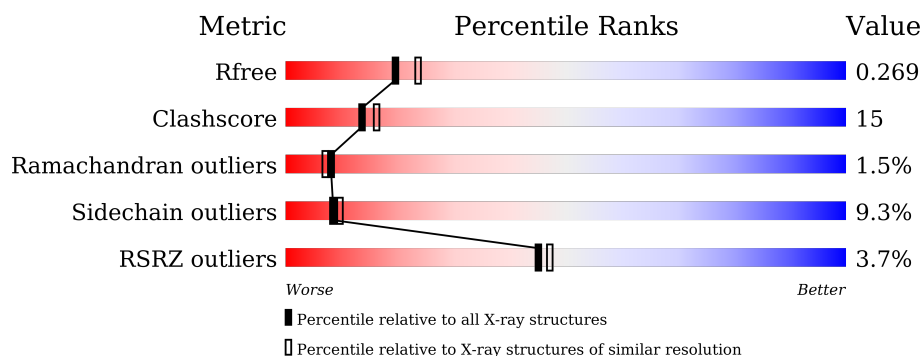
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

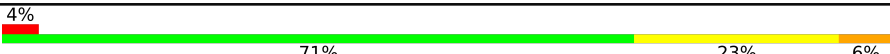
The reported resolution of this entry is 2.27 Å.

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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	

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
6	OSM	A	620	-	-	X	-
6	OSM	A	622	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	PEO	A	628	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5264 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.

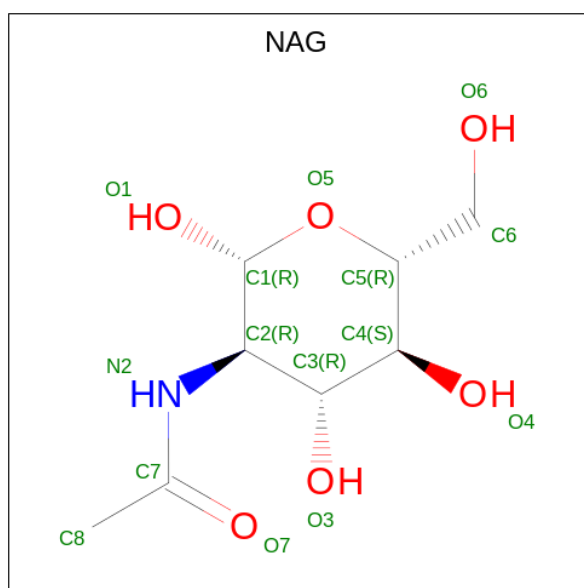
- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	595	4763	3025	847	864	1	26	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	SER	PHE	conflict	UNP L8ICE9
A	254	ALA	PHE	conflict	UNP L8ICE9

- Molecule 2 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
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

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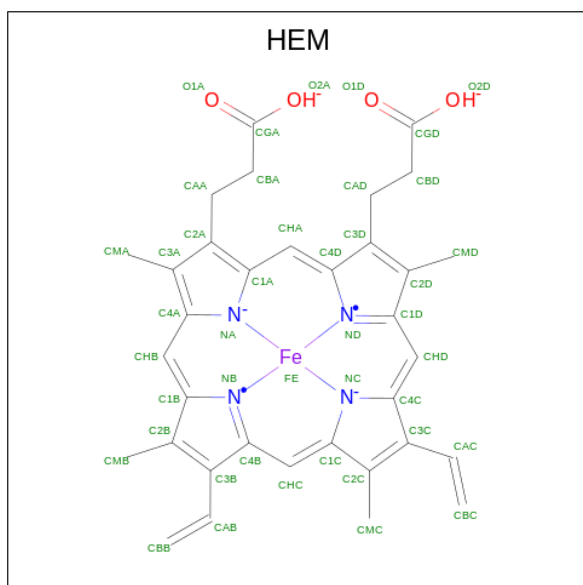
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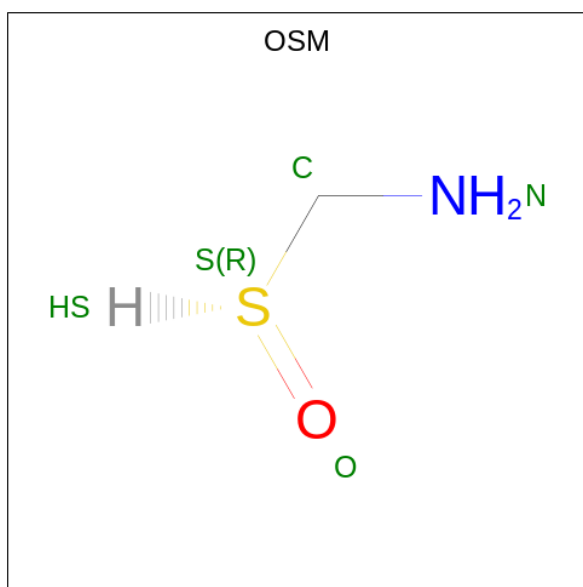
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

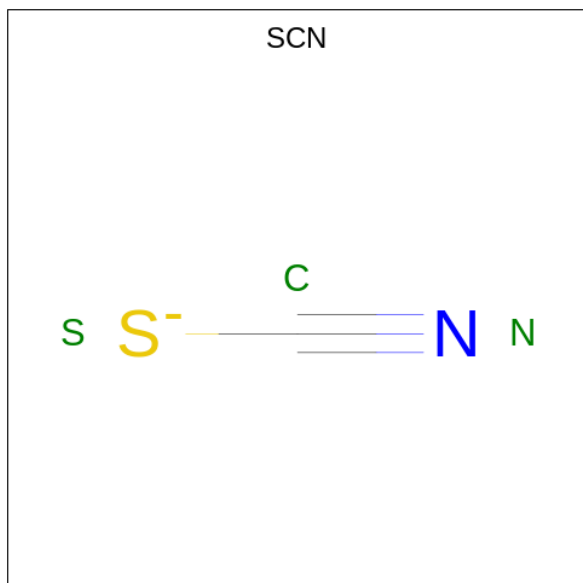
- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).





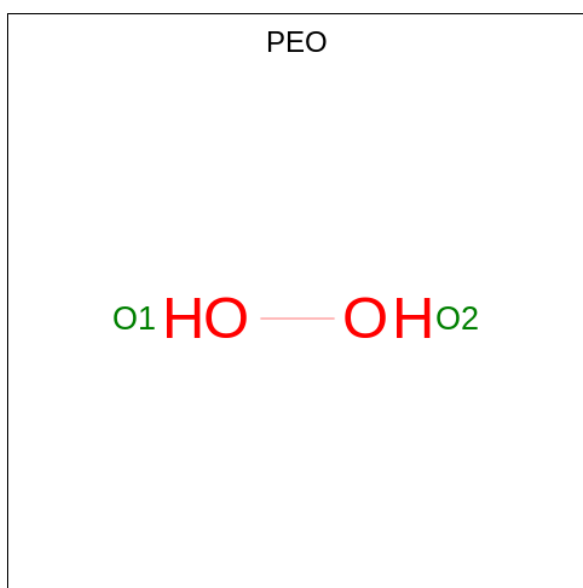
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		

- Molecule 7 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



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

- Molecule 8 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H_2O_2).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	358	Total O 358 358	0	0

3 Residue-property plots

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	54.08Å 80.64Å 76.13Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	52.79 – 2.27 52.79 – 2.27	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.79-2.27) 100.0 (52.79-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.196 , 0.266 0.209 , 0.269	Depositor DCC
R_{free} test set	1020 reflections (3.45%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5264	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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: CA, OSM, NAG, SEP, HEM, SCN, PEO, 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	1.01	0/4878	1.41	6/6617 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	PRO	N-CA-C	8.13	120.62	110.70
1	A	194	GLY	CA-C-O	-7.40	117.13	122.23
1	A	453	ARG	CA-C-N	5.14	125.80	119.99
1	A	453	ARG	C-N-CA	5.14	125.80	119.99
1	A	362	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	341	ASN	N-CA-C	-5.05	105.78	111.28

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	4763	0	4679	136	0
2	A	56	0	52	0	0
3	A	1	0	0	0	0
4	A	43	0	30	4	0
5	A	13	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	16	0	20	5	0
7	A	12	0	0	2	0
8	A	2	0	0	2	0
9	A	358	0	0	22	0
All	All	5264	0	4781	141	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 15.

All (141) 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)
5:A:608:IOD:I	7:A:626:SCN:N	2.56	1.09
1:A:424:PRO:O	5:A:615:IOD:I	2.48	1.00
1:A:167:CYS:CB	1:A:168:PRO:HD2	1.96	0.96
1:A:360:ARG:NH2	1:A:389:ASP:OD2	1.99	0.95
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.48	0.94
1:A:68:ASN:ND2	9:A:701:HOH:O	1.98	0.94
1:A:16:ASP:HB2	9:A:989:HOH:O	1.75	0.85
1:A:196:GLU:HB3	1:A:198:SEP:O2P	1.81	0.81
1:A:10:VAL:HG11	1:A:41:ARG:CZ	2.11	0.80
1:A:420:LYS:NZ	9:A:705:HOH:O	2.16	0.77
1:A:170:PRO:HD2	1:A:171:PRO:HD2	1.65	0.77
1:A:197:PRO:HB3	5:A:618:IOD:I	2.56	0.75
1:A:167:CYS:CB	1:A:168:PRO:CD	2.64	0.75
1:A:8:ALA:HA	9:A:977:HOH:O	1.88	0.72
1:A:468:GLN:NE2	9:A:702:HOH:O	2.09	0.72
1:A:3:GLU:HG3	1:A:175:LEU:HD21	1.72	0.72
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.73	0.70
1:A:89:GLU:HG2	9:A:1007:HOH:O	1.91	0.69
1:A:19:SER:O	9:A:703:HOH:O	2.10	0.69
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.75	0.67
4:A:606:HEM:HMB1	4:A:606:HEM:HBB2	1.75	0.67
1:A:373:GLU:O	7:A:627:SCN:N	2.29	0.66
1:A:555:ASP:OD1	9:A:704:HOH:O	2.14	0.66
1:A:237:CYS:HA	1:A:381:PHE:O	1.96	0.66
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.23	0.65
1:A:407:MET:HB3	1:A:501:MET:CE	2.27	0.64
1:A:281:LYS:HD2	1:A:285:PRO:HA	1.78	0.64
1:A:432:ASP:O	1:A:436:ILE:HG12	1.98	0.64
1:A:16:ASP:OD1	1:A:19:SER:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:606:HEM:HMC1	4:A:606:HEM:HBC2	1.82	0.62
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.83	0.61
1:A:407:MET:CB	1:A:501:MET:CE	2.78	0.60
1:A:467:LEU:HG	1:A:471:LEU:HD22	1.82	0.60
1:A:16:ASP:OD1	1:A:16:ASP:C	2.45	0.60
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.36	0.59
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.37	0.59
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.29	0.58
1:A:378:THR:HG22	6:A:620:OSM:H2	1.85	0.57
1:A:551:ARG:CD	1:A:583:ASP:O	2.53	0.57
1:A:30:ASN:O	1:A:34:PRO:HA	2.05	0.56
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.40	0.56
1:A:168:PRO:CB	1:A:171:PRO:HD2	2.35	0.56
4:A:606:HEM:ND	8:A:628:PEO:O1	2.39	0.56
1:A:407:MET:HB3	1:A:501:MET:HE3	1.88	0.56
1:A:126:LYS:NZ	9:A:720:HOH:O	2.38	0.56
1:A:175:LEU:HA	9:A:980:HOH:O	2.05	0.55
1:A:168:PRO:HB2	1:A:171:PRO:HD2	1.89	0.55
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.04	0.55
1:A:543:SER:OG	1:A:586:ASP:O	2.22	0.54
1:A:284:ASN:HA	1:A:286:HIS:CE1	2.43	0.54
1:A:82:ILE:CD1	1:A:480:LEU:HD13	2.37	0.54
1:A:407:MET:HB2	1:A:501:MET:HE2	1.89	0.54
1:A:159:PRO:HD2	1:A:431:PHE:CE2	2.43	0.54
1:A:592:SER:OG	9:A:706:HOH:O	2.16	0.54
1:A:579:CYS:O	1:A:582:VAL:HG22	2.07	0.53
1:A:588:SER:OG	1:A:589:PRO:HD3	2.08	0.53
1:A:232:LYS:HG3	6:A:621:OSM:H1	1.91	0.53
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.44	0.52
1:A:282:LYS:HD3	9:A:1042:HOH:O	2.10	0.52
1:A:170:PRO:CD	1:A:171:PRO:HD2	2.39	0.51
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.45	0.51
1:A:153:THR:CG2	9:A:742:HOH:O	2.58	0.51
1:A:174:SER:O	1:A:175:LEU:C	2.53	0.51
1:A:197:PRO:HG2	1:A:198:SEP:O1P	2.11	0.51
1:A:246:VAL:CG2	1:A:388:LYS:HE2	2.41	0.51
1:A:21:TYR:OH	1:A:295:GLU:OE1	2.18	0.49
1:A:153:THR:HG22	1:A:154:GLN:HG3	1.94	0.49
1:A:264:THR:HG23	1:A:392:ILE:HB	1.94	0.49
1:A:551:ARG:HD2	1:A:583:ASP:O	2.13	0.49
1:A:559:ILE:O	9:A:707:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.94	0.49
1:A:8:ALA:CB	9:A:977:HOH:O	2.61	0.49
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.48	0.48
1:A:295:GLU:O	1:A:299:ILE:HG12	2.13	0.48
1:A:407:MET:HG2	9:A:793:HOH:O	2.13	0.48
1:A:169:THR:N	1:A:170:PRO:CD	2.76	0.48
1:A:561:LYS:HG3	9:A:914:HOH:O	2.12	0.48
1:A:7:GLY:O	1:A:10:VAL:HG23	2.14	0.48
1:A:16:ASP:CG	1:A:19:SER:HB2	2.39	0.48
1:A:184:THR:OG1	1:A:188:ASP:OD2	2.31	0.47
1:A:268:LEU:HB3	1:A:552:LEU:HD21	1.96	0.47
1:A:407:MET:CB	1:A:501:MET:HE2	2.45	0.47
1:A:407:MET:HB2	1:A:501:MET:CE	2.44	0.47
1:A:138:ASN:O	1:A:161:SER:HA	2.14	0.47
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.49	0.47
1:A:170:PRO:HG2	1:A:171:PRO:HD3	1.97	0.47
1:A:203:LEU:HB3	1:A:213:MET:HE1	1.97	0.46
1:A:580:SER:O	1:A:581:THR:OG1	2.31	0.46
1:A:127:THR:O	1:A:131:GLU:N	2.30	0.46
1:A:322:GLN:OE1	9:A:708:HOH:O	2.21	0.46
1:A:378:THR:HG22	6:A:620:OSM:C	2.46	0.46
1:A:287:TRP:HB3	1:A:292:LEU:HD13	1.98	0.46
1:A:322:GLN:H	1:A:322:GLN:CD	2.24	0.46
1:A:95:ASN:HD22	6:A:622:OSM:C	2.28	0.46
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.51	0.45
1:A:284:ASN:ND2	1:A:287:TRP:CH2	2.85	0.45
1:A:95:ASN:HD22	6:A:622:OSM:H2	1.81	0.45
1:A:478:LYS:HE3	1:A:482:ASP:OD2	2.17	0.45
1:A:464:LEU:O	1:A:468:GLN:HG3	2.16	0.45
1:A:66:THR:HB	1:A:70:PHE:N	2.31	0.45
1:A:106:ILE:HG22	1:A:107:VAL:N	2.32	0.45
1:A:286:HIS:NE2	1:A:592:SER:HB3	2.32	0.45
1:A:541:ARG:O	1:A:545:GLN:HG3	2.17	0.45
1:A:464:LEU:HD22	1:A:468:GLN:HG3	1.99	0.44
1:A:168:PRO:HB3	1:A:171:PRO:HG2	2.00	0.44
1:A:221:ASP:O	1:A:224:LEU:HB2	2.16	0.44
1:A:120:GLY:O	1:A:126:LYS:HE2	2.17	0.44
1:A:150:LYS:HD3	1:A:158:MET:HE2	1.99	0.44
1:A:82:ILE:HD11	1:A:483:LEU:HD12	1.99	0.44
1:A:284:ASN:ND2	1:A:287:TRP:CZ2	2.81	0.44
1:A:551:ARG:HD3	1:A:583:ASP:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HD12	1:A:276:LEU:HA	1.88	0.44
4:A:606:HEM:C4D	8:A:628:PEO:O1	2.71	0.44
1:A:425:THR:HG22	1:A:426:HIS:CE1	2.53	0.44
1:A:193:TYR:CZ	1:A:297:ARG:HA	2.52	0.43
1:A:291:LYS:O	1:A:295:GLU:HB2	2.19	0.43
1:A:393:ASP:OD1	1:A:557:THR:HB	2.18	0.43
1:A:301:GLY:O	1:A:305:GLN:HG3	2.19	0.43
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.65	0.43
1:A:361:LEU:O	1:A:397:ARG:NH1	2.52	0.43
1:A:408:ASN:HB2	9:A:850:HOH:O	2.19	0.43
1:A:168:PRO:HB3	1:A:171:PRO:CG	2.49	0.42
1:A:313:LEU:N	1:A:314:PRO:CD	2.83	0.42
1:A:482:ASP:O	1:A:485:LYS:NZ	2.47	0.42
1:A:170:PRO:HD2	1:A:171:PRO:CD	2.43	0.42
1:A:588:SER:N	1:A:589:PRO:CD	2.82	0.42
1:A:194:GLY:HA2	1:A:252:GLY:O	2.20	0.41
1:A:213:MET:HE3	1:A:213:MET:HB3	1.97	0.41
1:A:309:PHE:CD1	1:A:529:TRP:HH2	2.39	0.41
1:A:168:PRO:CB	1:A:171:PRO:HG2	2.50	0.41
1:A:26:GLY:HA2	9:A:870:HOH:O	2.20	0.41
1:A:57:LEU:HD12	1:A:57:LEU:HA	1.85	0.41
1:A:57:LEU:HG	1:A:61:TRP:CD1	2.56	0.41
1:A:170:PRO:CG	1:A:171:PRO:HD3	2.51	0.41
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.34	0.41
1:A:193:TYR:OH	1:A:297:ARG:HA	2.21	0.40
1:A:584:LYS:HE3	9:A:1015:HOH:O	2.20	0.40
1:A:376:LEU:HG	9:A:874:HOH:O	2.21	0.40
1:A:360:ARG:NH1	1:A:371:GLU:O	2.55	0.40
1:A:551:ARG:HD2	1:A:582:VAL:HG23	2.03	0.40
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	592/595 (100%)	552 (93%)	31 (5%)	9 (2%)	8 7

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	167	CYS
1	A	170	PRO
1	A	581	THR
1	A	583	ASP
1	A	5	GLY
1	A	7	GLY
1	A	173	GLN
1	A	209	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	516/516 (100%)	468 (91%)	48 (9%)	8 10

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	12	LEU
1	A	13	VAL
1	A	16	ASP
1	A	17	GLU
1	A	36	LEU
1	A	57	LEU
1	A	82	ILE
1	A	91	VAL
1	A	98	LEU

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Mol	Chain	Res	Type
1	A	106	ILE
1	A	122	ASN
1	A	124	HIS
1	A	127	THR
1	A	153	THR
1	A	173	GLN
1	A	177	ARG
1	A	187	LEU
1	A	201	SER
1	A	203	LEU
1	A	208	SER
1	A	209	PRO
1	A	218	GLU
1	A	232	LYS
1	A	268	LEU
1	A	276	LEU
1	A	279	GLU
1	A	292	LEU
1	A	317	LEU
1	A	322	GLN
1	A	333	ASN
1	A	360	ARG
1	A	363	GLU
1	A	376	LEU
1	A	388	LYS
1	A	407	MET
1	A	425	THR
1	A	464	LEU
1	A	471	LEU
1	A	478	LYS
1	A	480	LEU
1	A	486	THR
1	A	511	LEU
1	A	531	GLU
1	A	543	SER
1	A	545	GLN
1	A	564	LEU
1	A	587	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	122	ASN
1	A	124	HIS
1	A	147	ASN
1	A	154	GLN
1	A	231	ASN
1	A	266	HIS
1	A	322	GLN
1	A	333	ASN
1	A	364	ASN
1	A	429	HIS
1	A	460	GLN
1	A	497	ASN
1	A	520	GLN
1	A	545	GLN
1	A	568	GLN

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	1.13	0	8,12,14	1.24	1 (12%)

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	-	3/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	P-OG-CB	2.28	124.58	118.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 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	NAG	A	601	1	14,14,15	0.71	0	17,19,21	1.17	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SCN	A	627	-	1,2,2	0.68	0	0,1,1	-	-
6	OSM	A	623	-	1,3,3	0.08	0	0,2,2	-	-
6	OSM	A	620	-	1,3,3	0.01	0	0,2,2	-	-
6	OSM	A	622	-	1,3,3	0.05	0	0,2,2	-	-
7	SCN	A	624	-	1,2,2	0.02	0	0,1,1	-	-
7	SCN	A	626	-	1,2,2	1.03	0	0,1,1	-	-
2	NAG	A	604	1	14,14,15	0.44	0	17,19,21	1.11	2 (11%)
4	HEM	A	606	8,1	50,50,50	1.64	11 (22%)	66,82,82	1.70	12 (18%)
2	NAG	A	603	1	14,14,15	1.04	1 (7%)	17,19,21	1.53	1 (5%)
7	SCN	A	625	-	1,2,2	0.73	0	0,1,1	-	-
2	NAG	A	602	1	14,14,15	0.29	0	17,19,21	1.11	1 (5%)
6	OSM	A	621	-	1,3,3	0.09	0	0,2,2	-	-
8	PEO	A	628	4	1,1,1	0.49	0	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
6	OSM	A	623	-	-	0/0/1/1	-
6	OSM	A	620	-	-	0/0/1/1	-
6	OSM	A	622	-	-	0/0/1/1	-
2	NAG	A	604	1	-	2/6/23/26	0/1/1/1
4	HEM	A	606	8,1	-	4/14/54/54	-
2	NAG	A	603	1	-	2/6/23/26	0/1/1/1
2	NAG	A	602	1	-	2/6/23/26	0/1/1/1
6	OSM	A	621	-	-	0/0/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	606	HEM	FE-NB	5.15	2.10	1.94
4	A	606	HEM	FE-NC	3.82	2.08	1.95
4	A	606	HEM	C4D-ND	-3.75	1.33	1.40
2	A	603	NAG	O5-C1	-3.00	1.38	1.43
4	A	606	HEM	C1B-NB	-2.82	1.35	1.40
4	A	606	HEM	C1C-C2C	-2.56	1.40	1.45
4	A	606	HEM	C1D-ND	-2.47	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	606	HEM	C4C-NC	-2.38	1.35	1.39
4	A	606	HEM	FE-NA	2.23	2.02	1.95
4	A	606	HEM	C4B-NB	-2.23	1.34	1.38
4	A	606	HEM	C3B-C4B	2.15	1.49	1.44
4	A	606	HEM	O1A-CGA	2.07	1.29	1.22

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	NAG	C1-O5-C5	-5.14	105.23	112.19
4	A	606	HEM	CHA-C4D-ND	4.67	130.13	124.37
4	A	606	HEM	CHC-C4B-NB	4.33	129.13	124.42
4	A	606	HEM	CMD-C2D-C1D	4.14	131.35	125.04
4	A	606	HEM	C1B-NB-C4B	3.78	108.97	105.07
4	A	606	HEM	CHA-C4D-C3D	-3.49	118.78	125.33
4	A	606	HEM	C4C-NC-C1C	3.40	108.67	105.35
2	A	601	NAG	C1-O5-C5	3.17	116.49	112.19
2	A	604	NAG	C1-C2-N2	-3.02	105.33	110.49
4	A	606	HEM	C4B-C3B-C2B	-2.77	104.92	107.11
2	A	602	NAG	C1-O5-C5	2.54	115.64	112.19
4	A	606	HEM	CBD-CAD-C3D	-2.49	105.69	112.63
4	A	606	HEM	C1A-CHA-C4D	-2.43	120.58	126.34
4	A	606	HEM	CHD-C1D-ND	2.39	127.02	124.42
2	A	604	NAG	C4-C3-C2	2.36	114.47	111.02
2	A	601	NAG	O4-C4-C5	2.20	114.77	109.30
4	A	606	HEM	CMB-C2B-C1B	2.11	128.25	125.04
4	A	606	HEM	CAA-C2A-C1A	2.03	128.88	124.89

There are no chirality outliers.

All (10) torsion outliers are listed below:

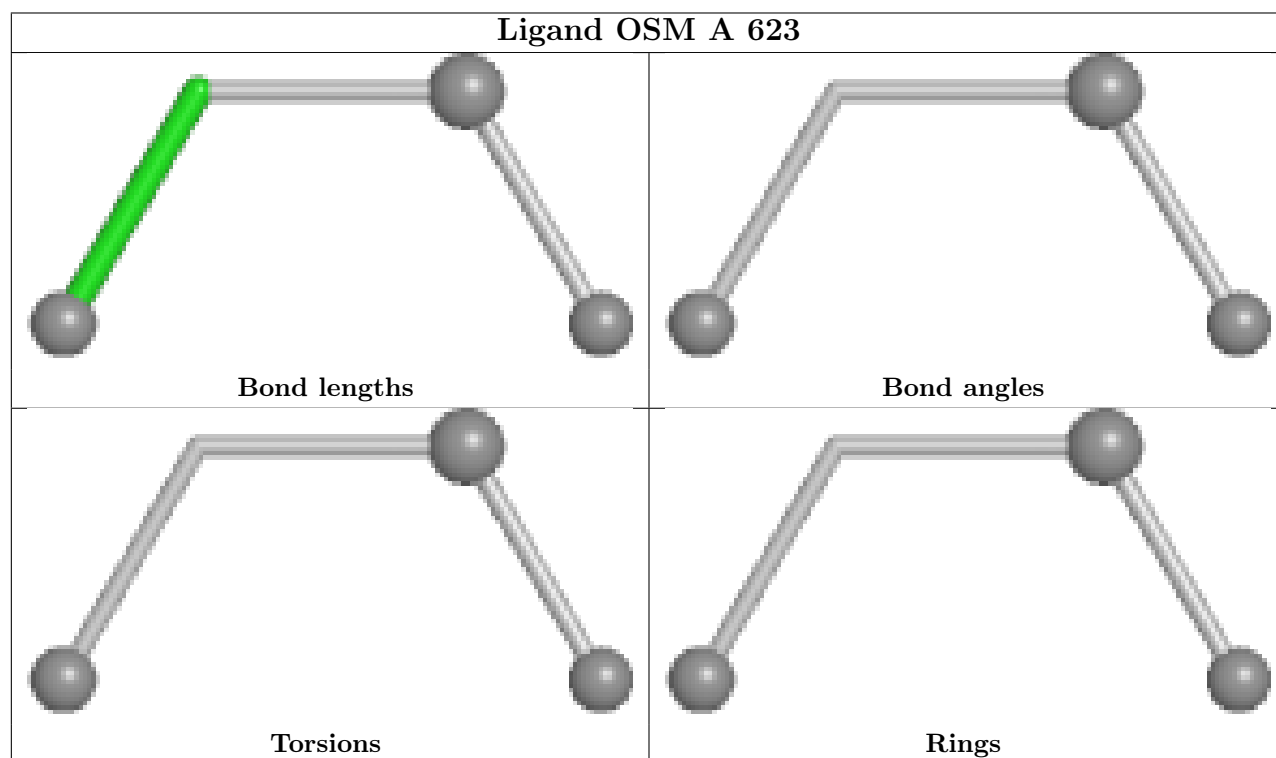
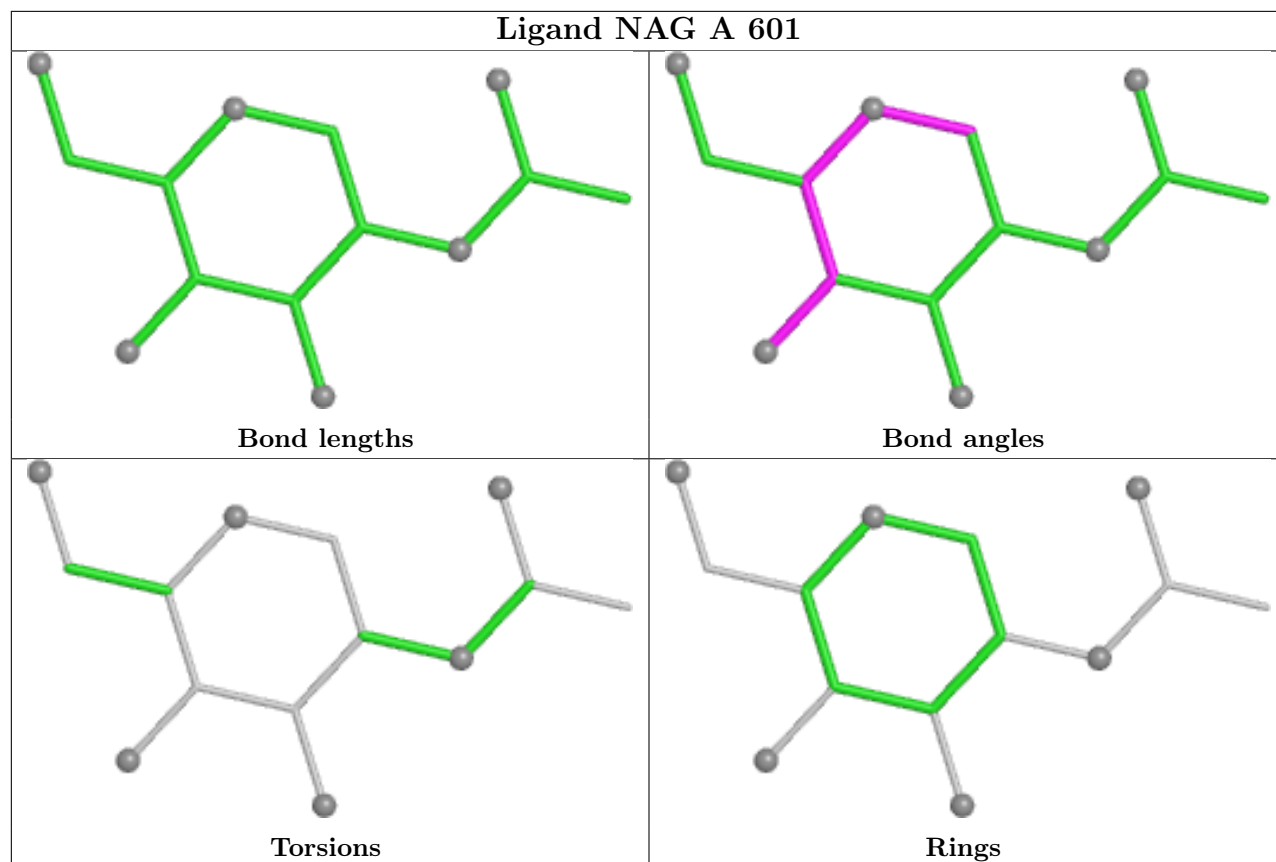
Mol	Chain	Res	Type	Atoms
2	A	604	NAG	O5-C5-C6-O6
2	A	604	NAG	C4-C5-C6-O6
2	A	603	NAG	C4-C5-C6-O6
2	A	603	NAG	O5-C5-C6-O6
2	A	602	NAG	C4-C5-C6-O6
4	A	606	HEM	CAA-CBA-CGA-O1A
4	A	606	HEM	CAA-CBA-CGA-O2A
4	A	606	HEM	CAD-CBD-CGD-O2D
2	A	602	NAG	O5-C5-C6-O6
4	A	606	HEM	CAD-CBD-CGD-O1D

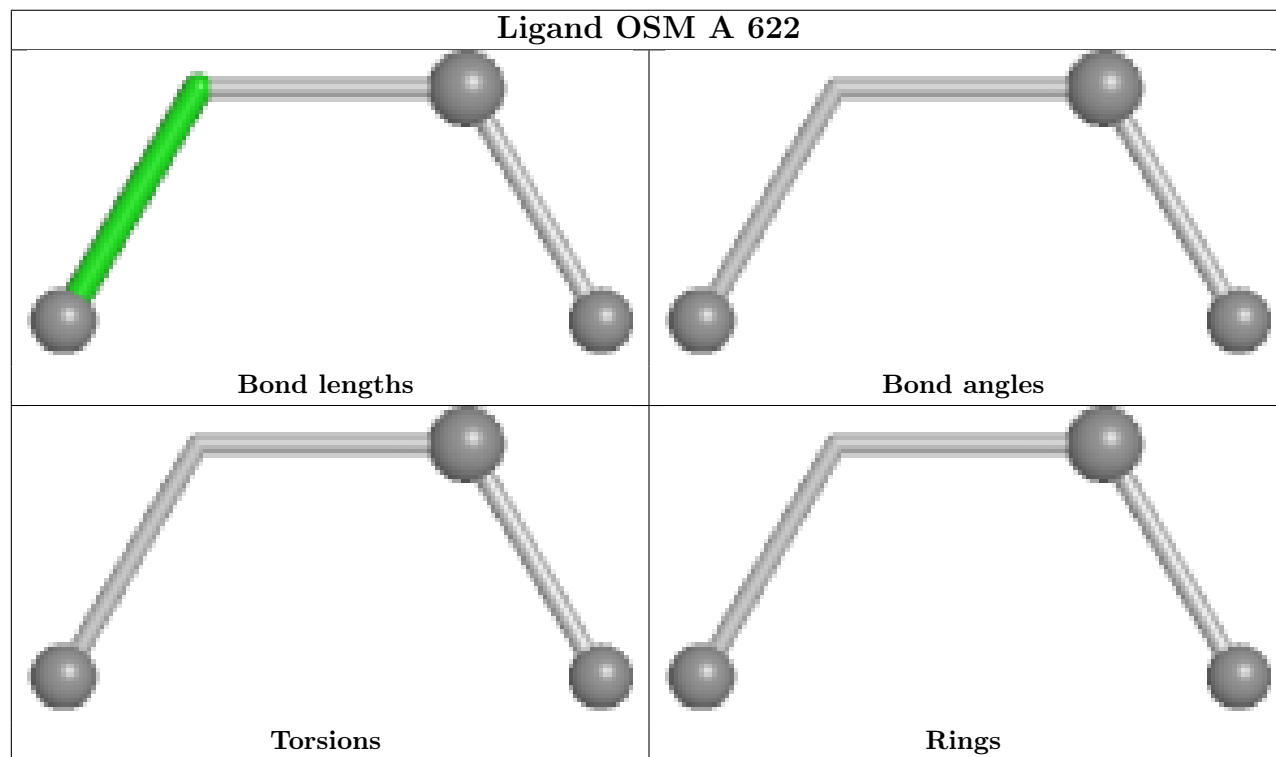
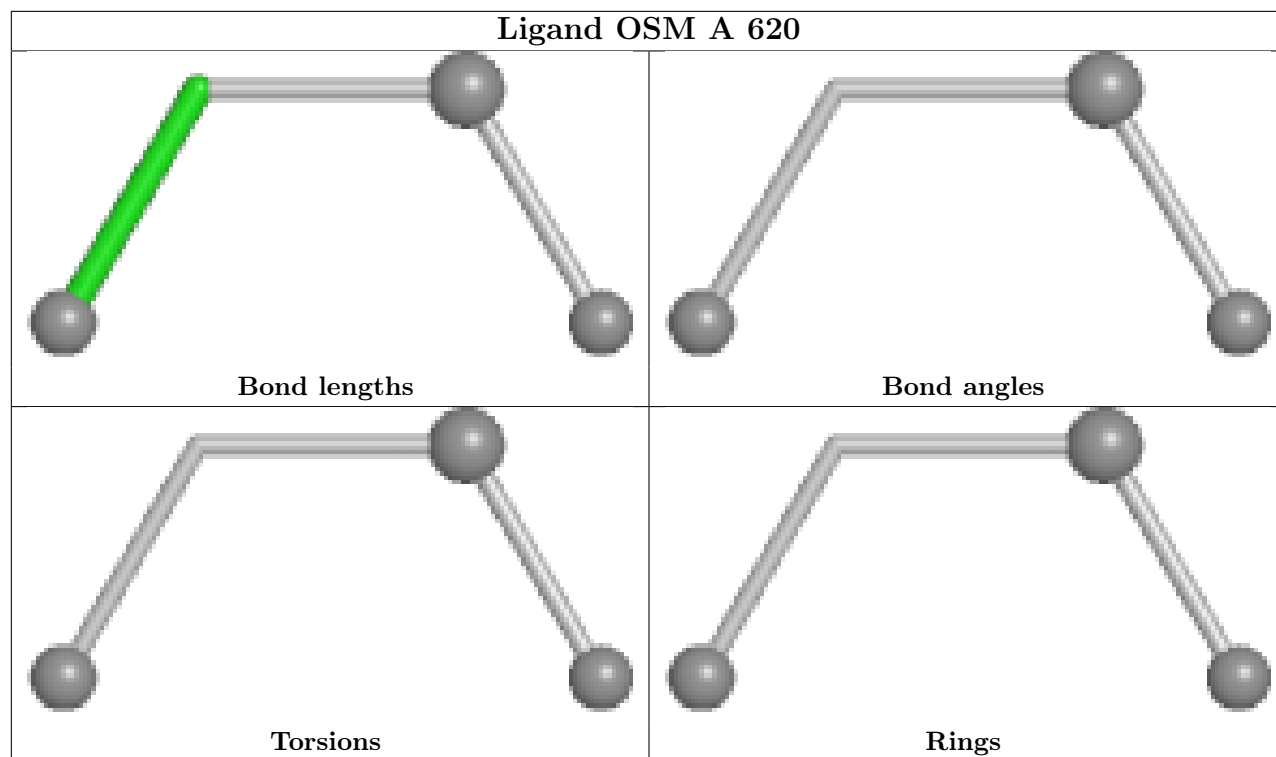
There are no ring outliers.

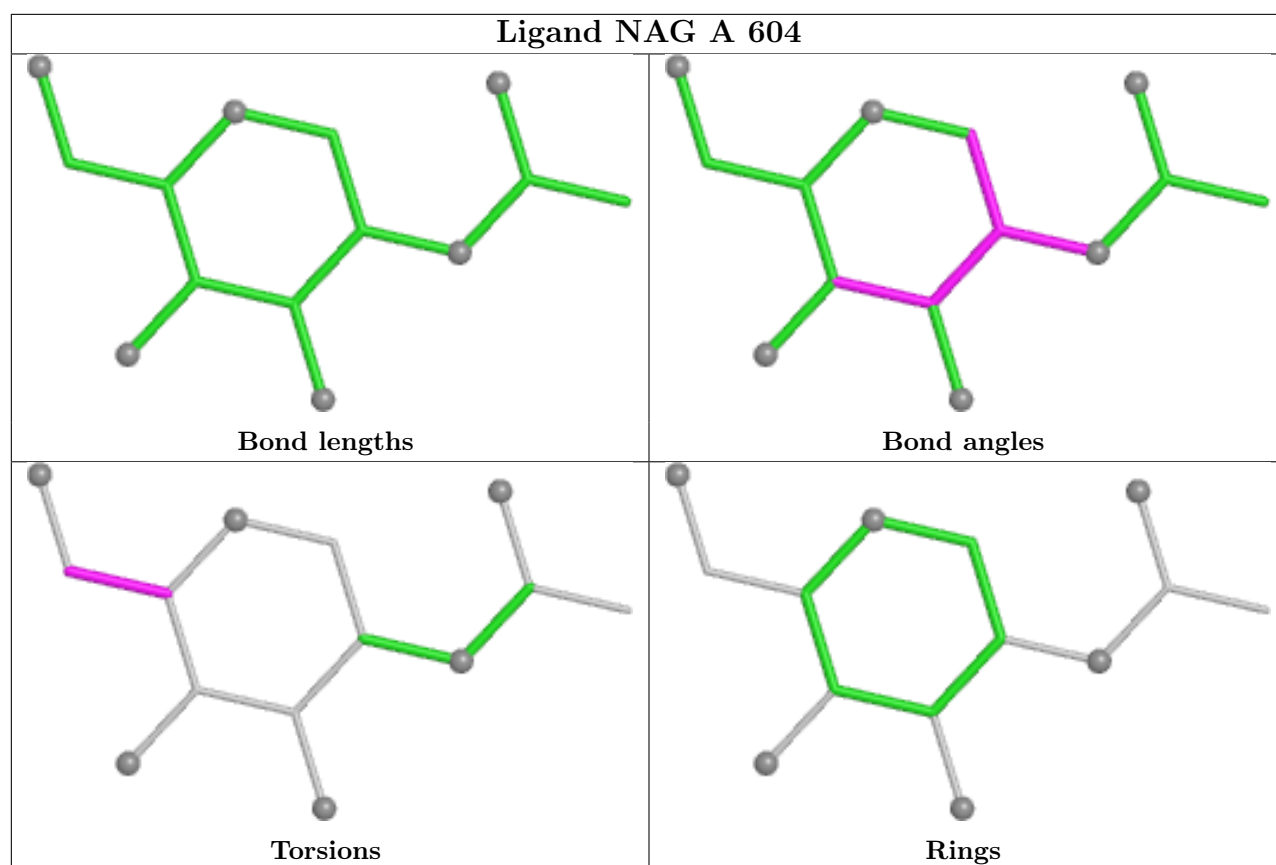
7 monomers are involved in 11 short contacts:

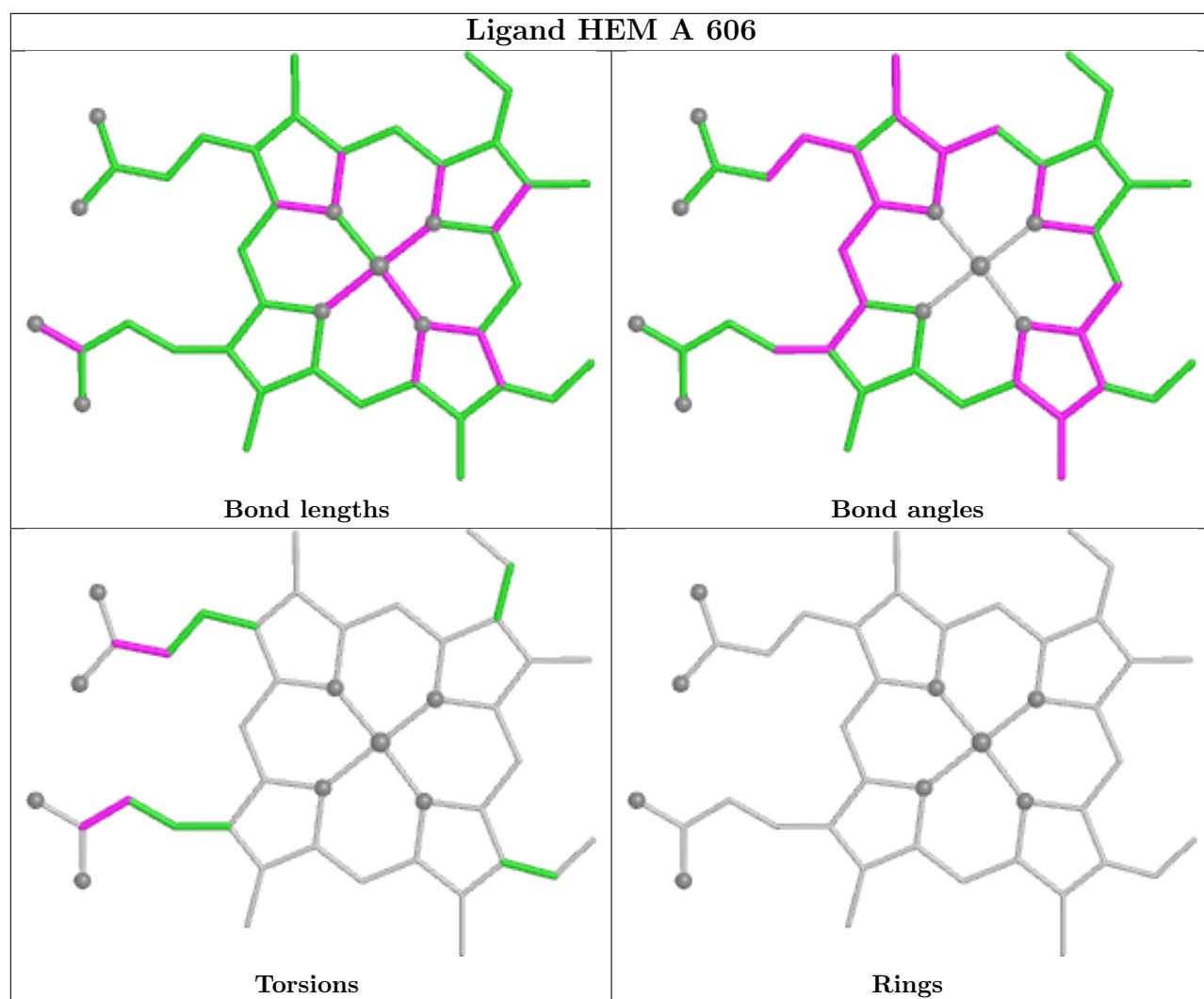
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	627	SCN	1	0
6	A	620	OSM	2	0
6	A	622	OSM	2	0
7	A	626	SCN	1	0
4	A	606	HEM	4	0
6	A	621	OSM	1	0
8	A	628	PEO	2	0

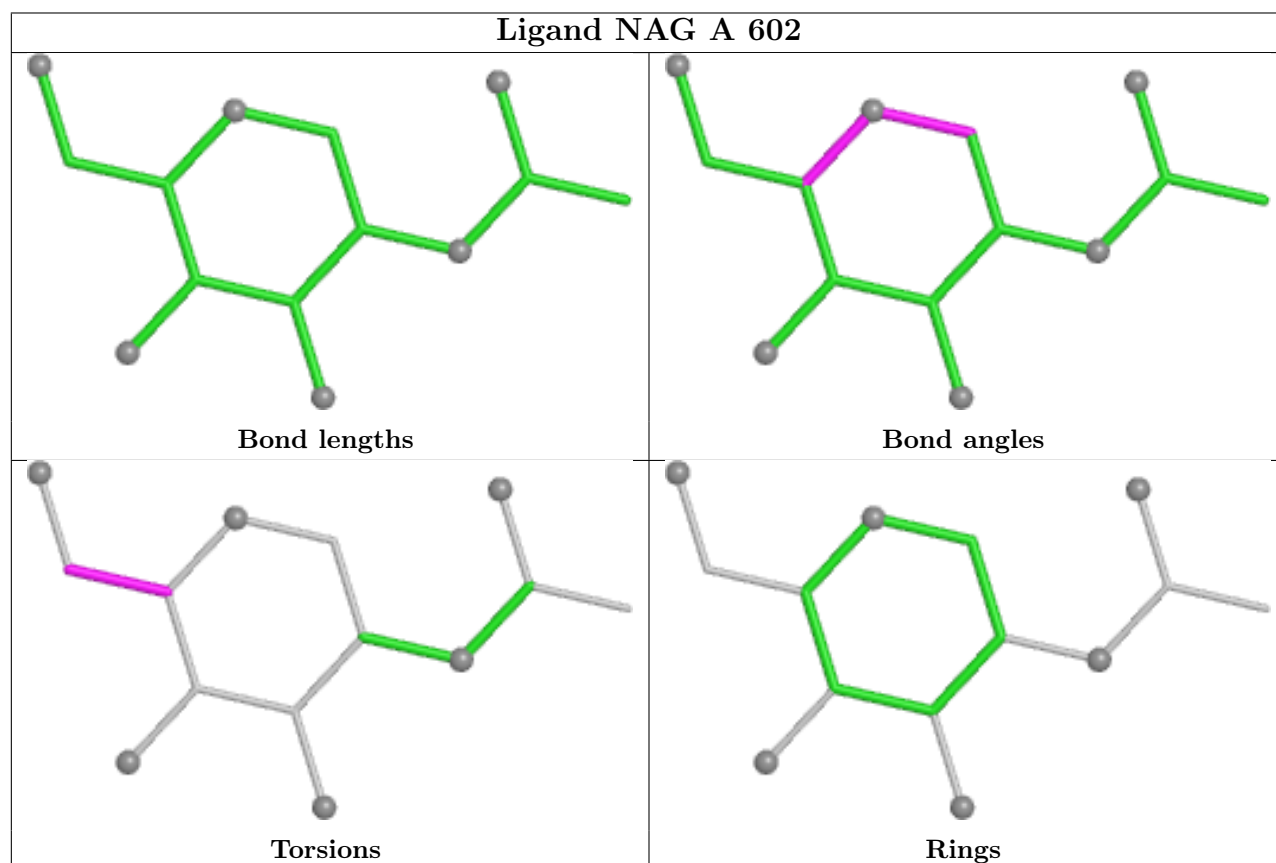
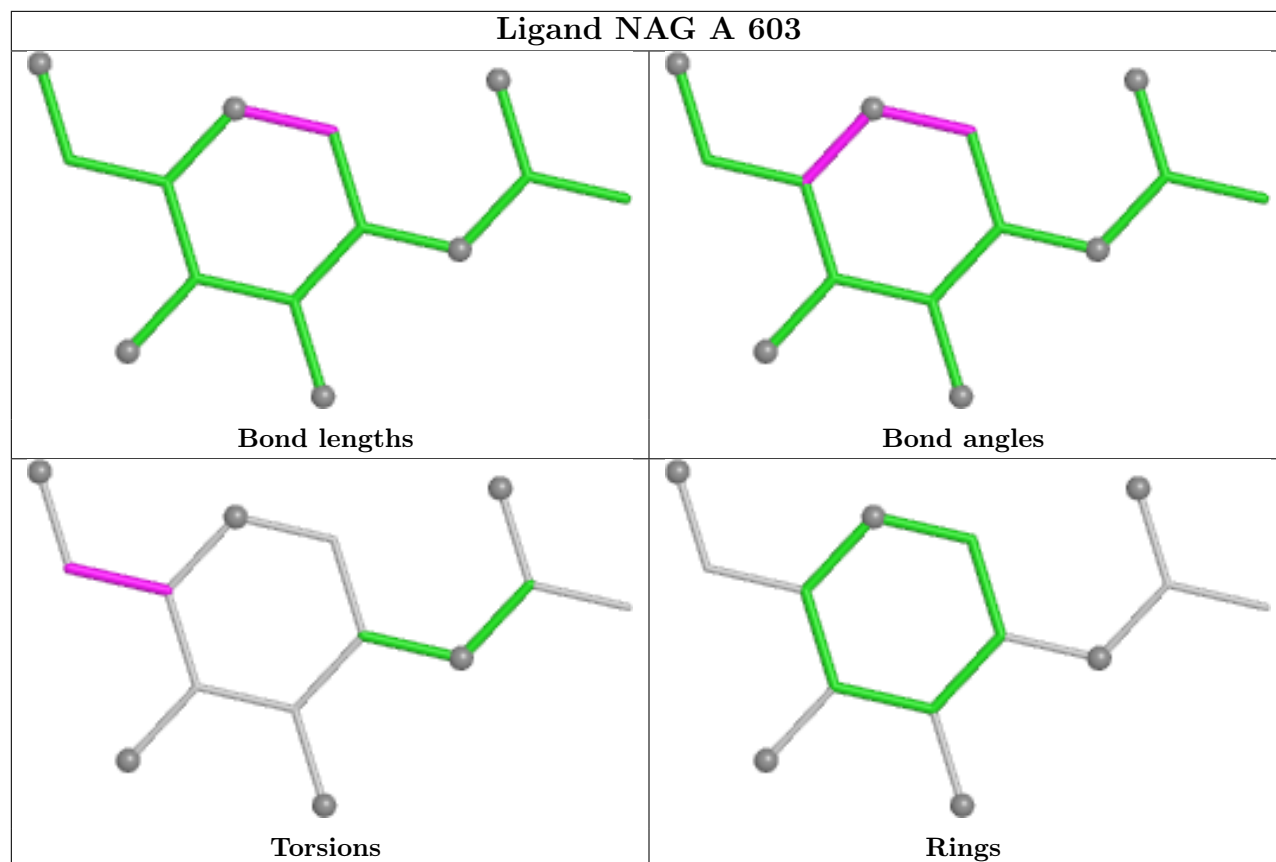
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

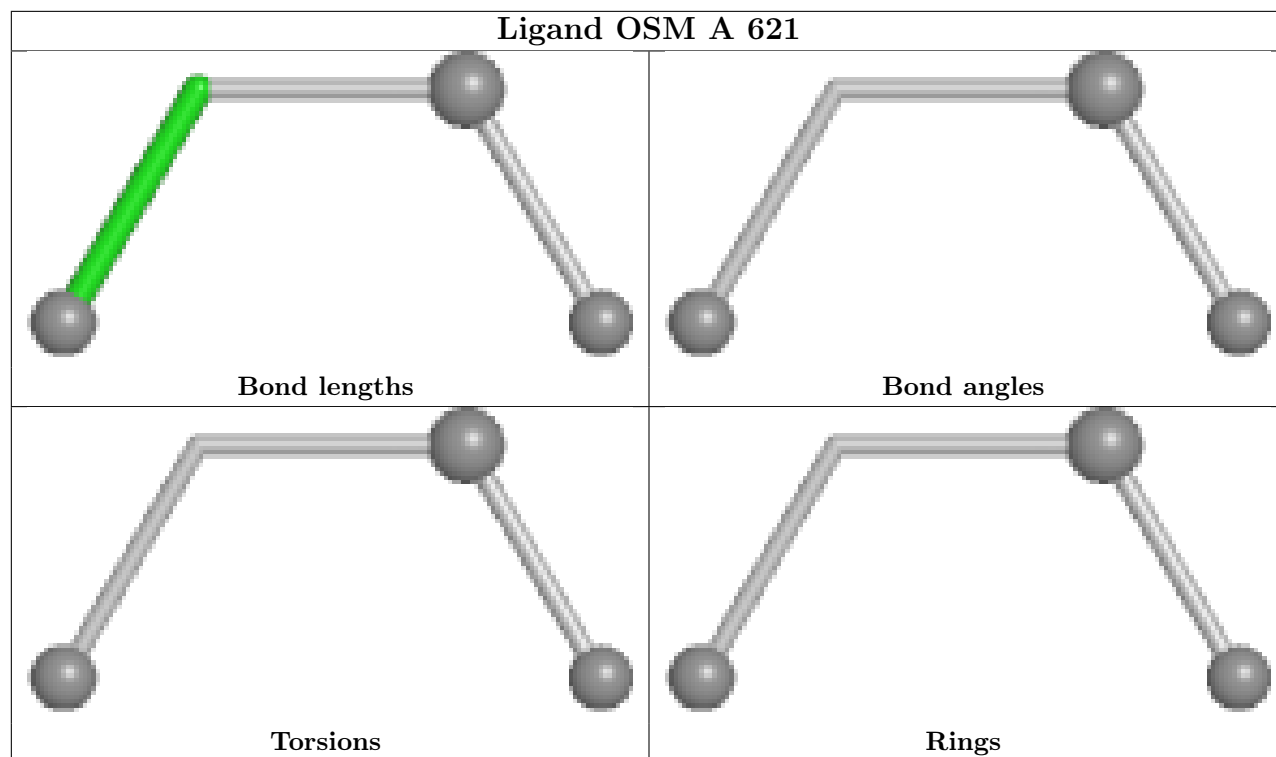












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	594/595 (99%)	0.29	22 (3%)	45 47	31, 52, 112, 177	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	SER	4.2
1	A	175	LEU	3.8
1	A	2	TRP	3.6
1	A	171	PRO	3.6
1	A	169	THR	3.4
1	A	530	TRP	3.3
1	A	172	TYR	3.1
1	A	4	VAL	3.1
1	A	170	PRO	3.1
1	A	9	PRO	3.0
1	A	11	PRO	2.6
1	A	5	GLY	2.6
1	A	120	GLY	2.5
1	A	12	LEU	2.4
1	A	7	GLY	2.3
1	A	8	ALA	2.3
1	A	302	ALA	2.3
1	A	121	SER	2.2
1	A	119	LEU	2.2
1	A	587	LEU	2.1
1	A	1	SER	2.1
1	A	595	ASN	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	0.92	0.12	37,52,62,66	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.

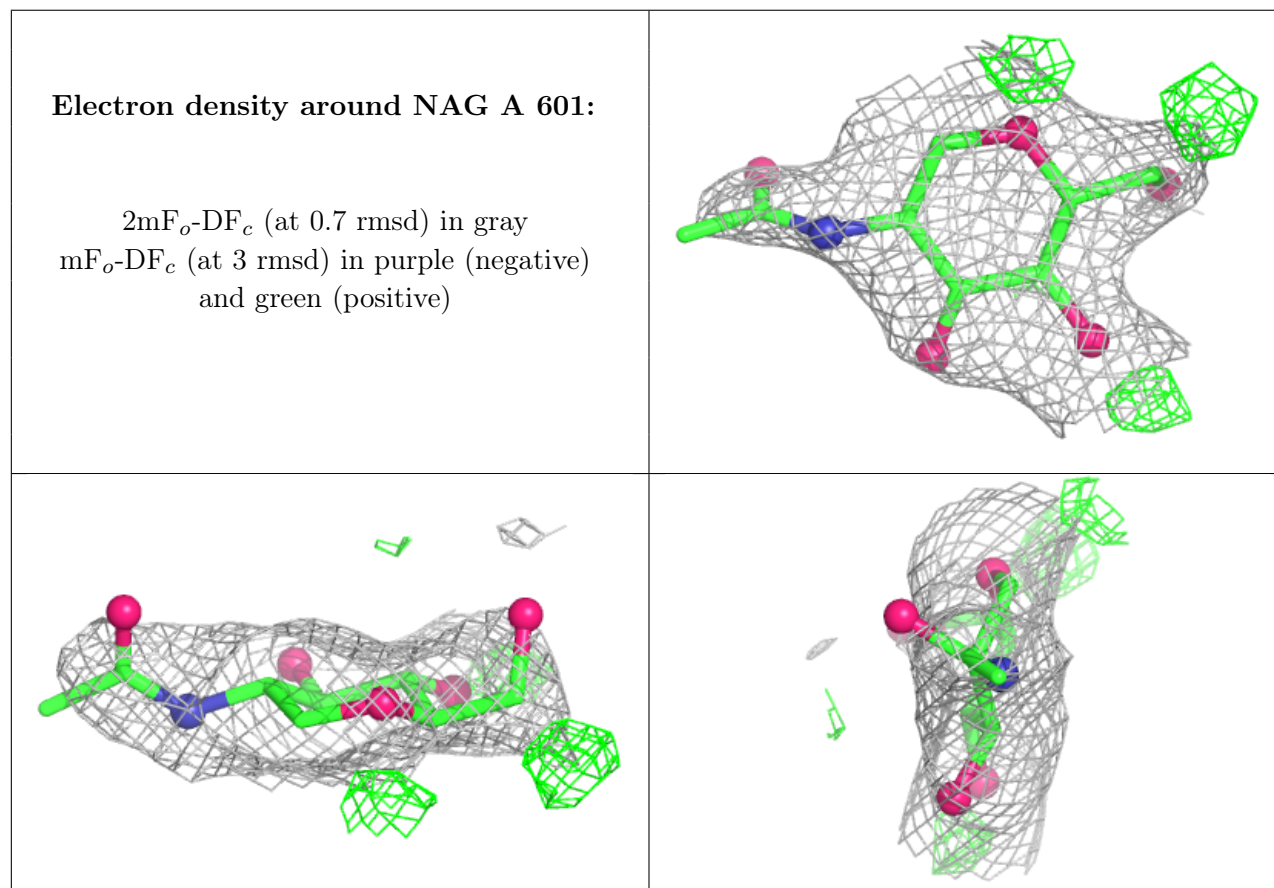
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	601	14/15	0.69	0.14	75,86,98,101	0
2	NAG	A	603	14/15	0.81	0.12	52,62,67,80	0
2	NAG	A	604	14/15	0.82	0.10	77,89,96,96	0
2	NAG	A	602	14/15	0.85	0.13	72,78,94,99	0
6	OSM	A	621	4/4	0.87	0.12	54,56,60,60	0
8	PEO	A	628	2/2	0.95	0.10	42,42,42,60	0
5	IOD	A	618	1/1	0.96	0.09	76,76,76,76	1
6	OSM	A	620	4/4	0.96	0.11	30,31,33,36	0
5	IOD	A	614	1/1	0.96	0.07	81,81,81,81	0
6	OSM	A	622	4/4	0.96	0.06	49,50,50,51	0
7	SCN	A	625	3/3	0.96	0.08	56,56,58,62	0
5	IOD	A	616	1/1	0.96	0.09	74,74,74,74	1
5	IOD	A	617	1/1	0.97	0.06	74,74,74,74	1
4	HEM	A	606	43/43	0.97	0.07	28,37,42,48	0
6	OSM	A	623	4/4	0.97	0.12	26,28,34,34	0
7	SCN	A	624	3/3	0.97	0.07	44,44,52,58	0
5	IOD	A	619	1/1	0.97	0.12	81,81,81,81	1
7	SCN	A	627	3/3	0.97	0.08	44,44,50,60	0
5	IOD	A	611	1/1	0.97	0.05	65,65,65,65	1
5	IOD	A	608	1/1	0.98	0.12	67,67,67,67	1
5	IOD	A	609	1/1	0.98	0.04	60,60,60,60	0

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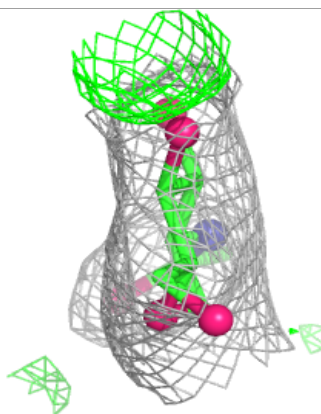
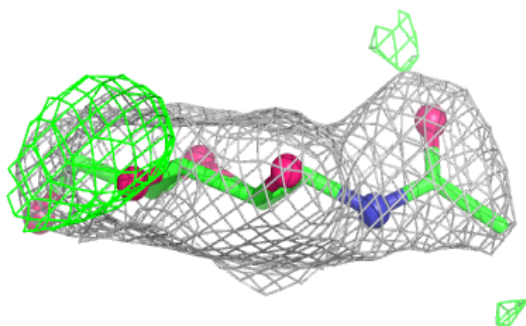
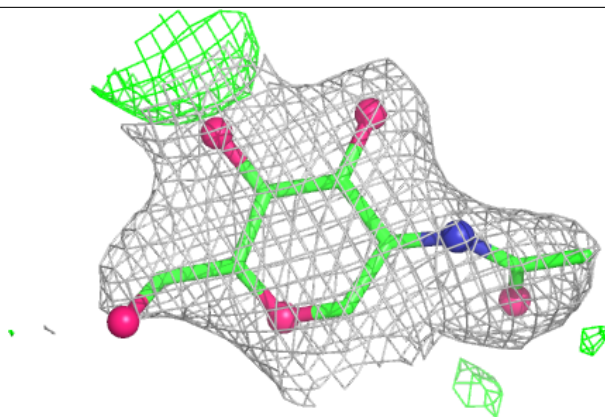
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	IOD	A	610	1/1	0.98	0.05	59,59,59,59	1
3	CA	A	605	1/1	0.98	0.03	46,46,46,46	0
7	SCN	A	626	3/3	0.98	0.07	30,30,34,35	3
5	IOD	A	607	1/1	0.98	0.04	51,51,51,51	1
5	IOD	A	615	1/1	0.98	0.05	56,56,56,56	0
5	IOD	A	613	1/1	0.99	0.04	44,44,44,44	0
5	IOD	A	612	1/1	0.99	0.03	69,69,69,69	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.

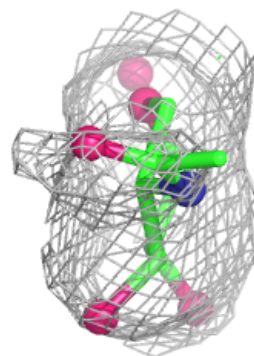
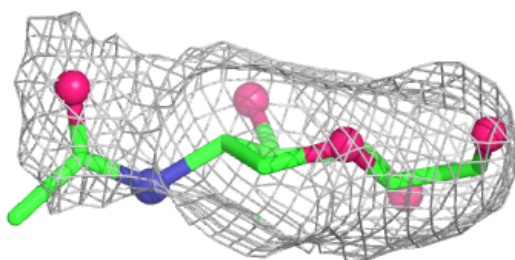
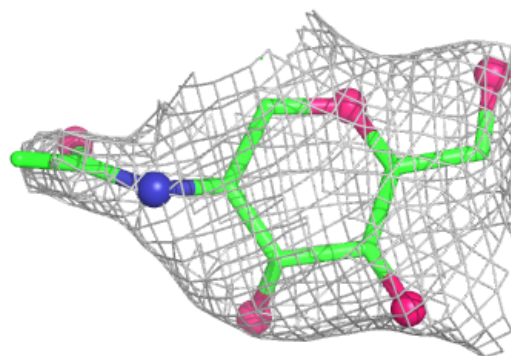


Electron density around NAG A 603:

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

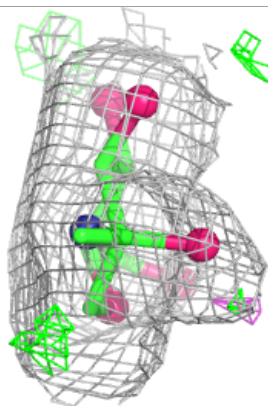
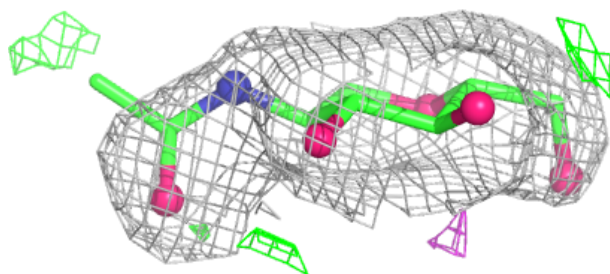
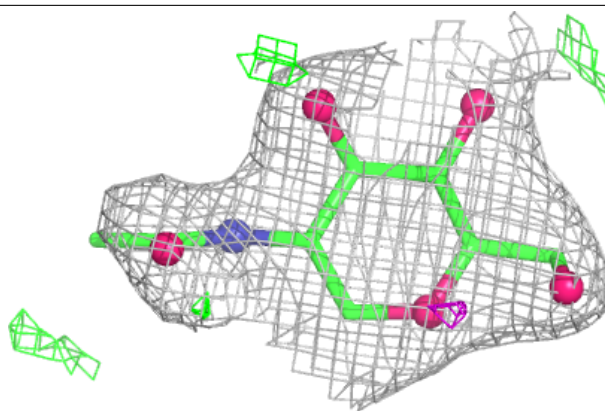
**Electron density around NAG A 604:**

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

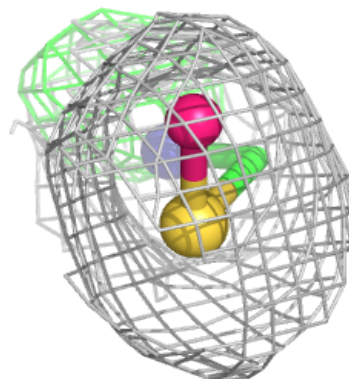
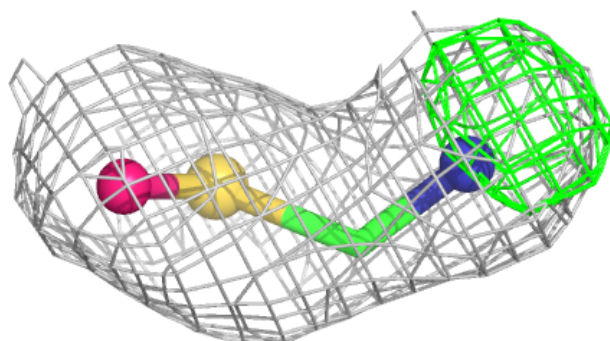
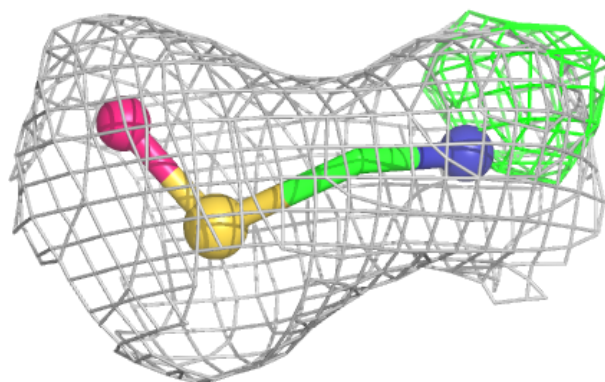


Electron density around NAG A 602:

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

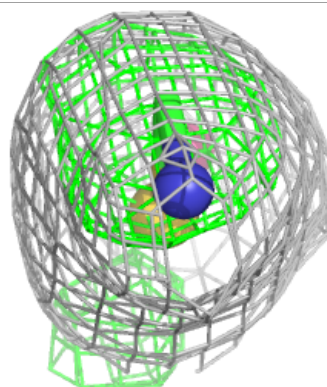
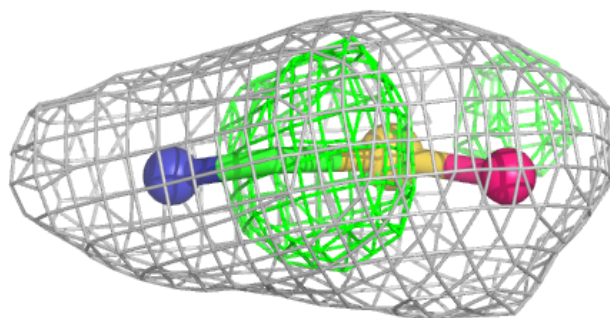
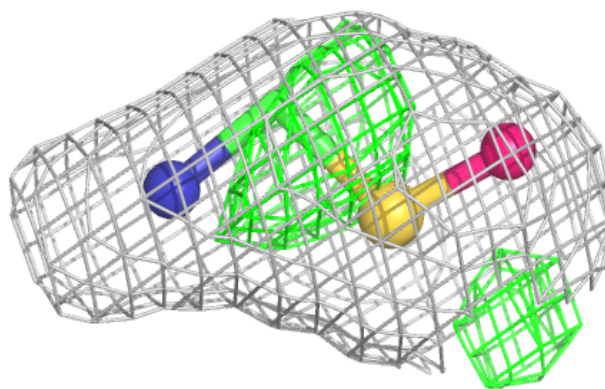
**Electron density around OSM A 621:**

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

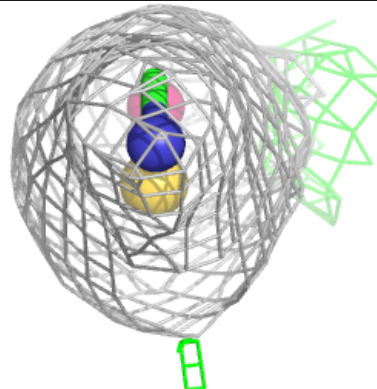
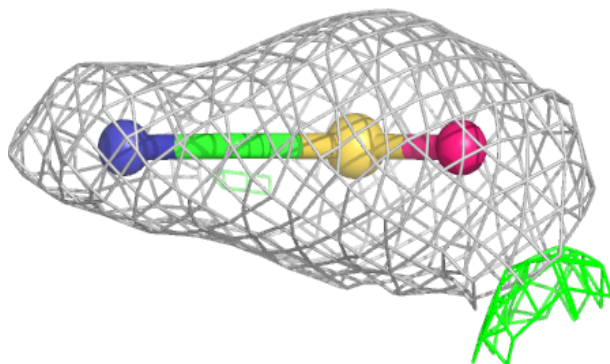
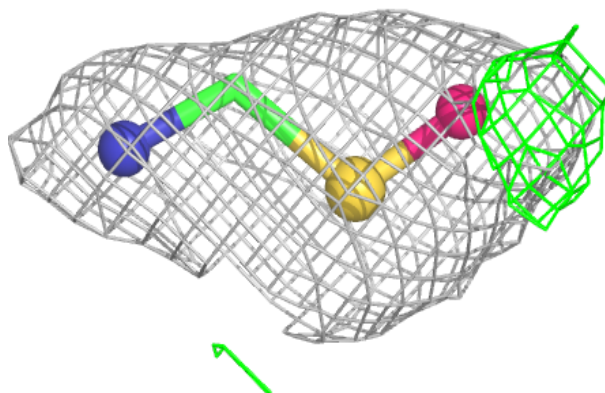


Electron density around OSM A 620:

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

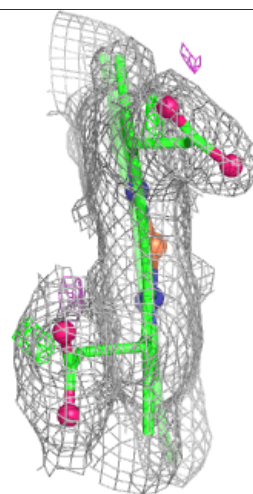
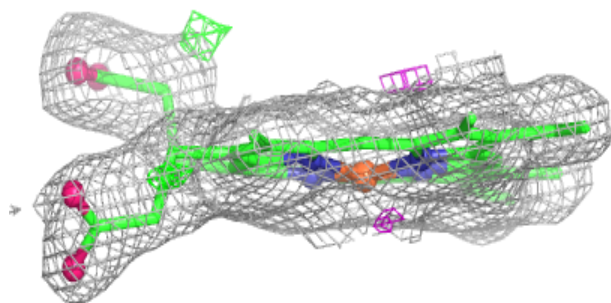
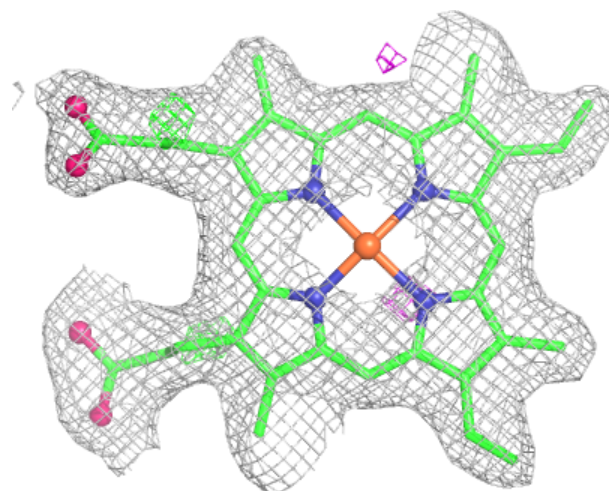
**Electron density around OSM A 622:**

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



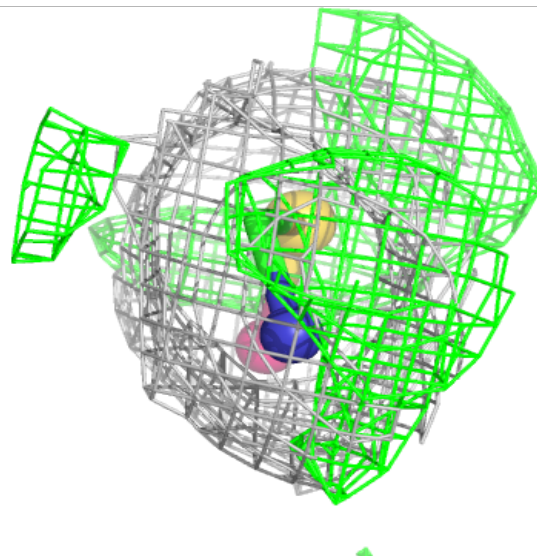
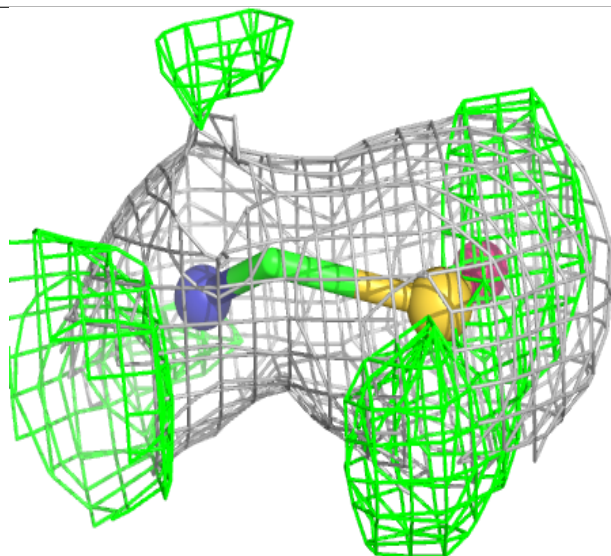
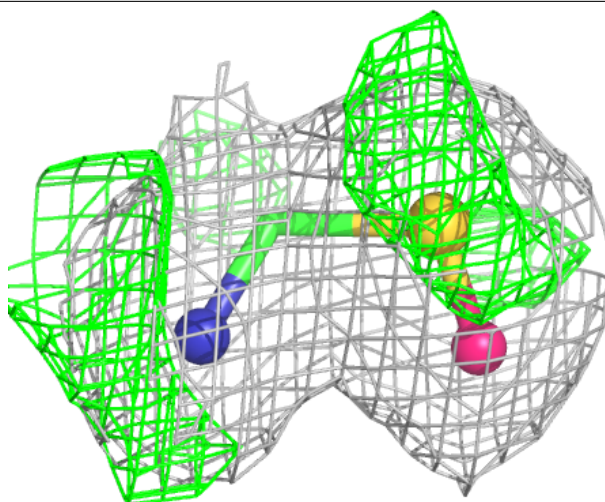
Electron density around HEM A 606:

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



Electron density around OSM A 623:

$2mF_o-DF_c$ (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.