Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 05:17 AM JST

PDB ID	:	6KY7
Title	:	Crystal structure of yak lactoperoxidase at 2.27 A 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 (i) 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 (i)) were used in the production of this report:

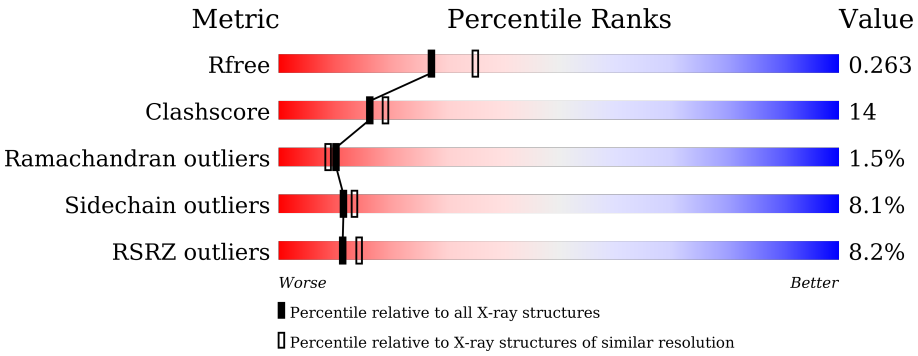
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (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 <=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	8% 72% 23% 5%

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	607	-	-	X	-
6	OSM	A	620	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	OSM	A	622	-	-	X	-
7	SCN	A	626	-	-	X	-
8	PEO	A	628	-	-	X	-

2 Entry composition

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.

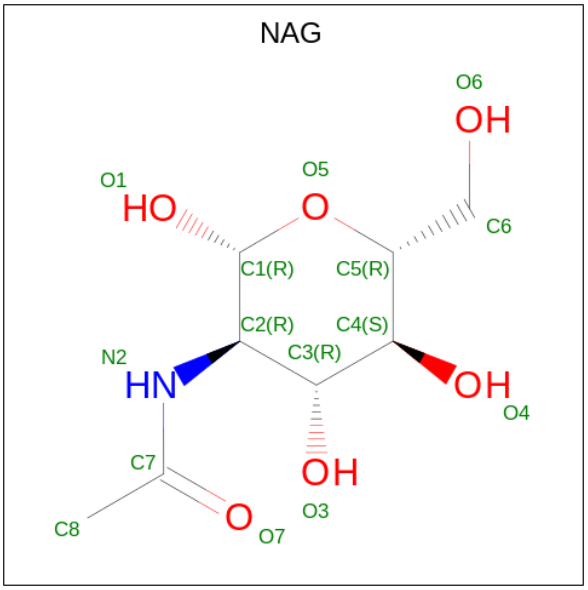
- Molecule 1 is a protein called Lactoperoxidase.

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 (three-letter code: 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
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

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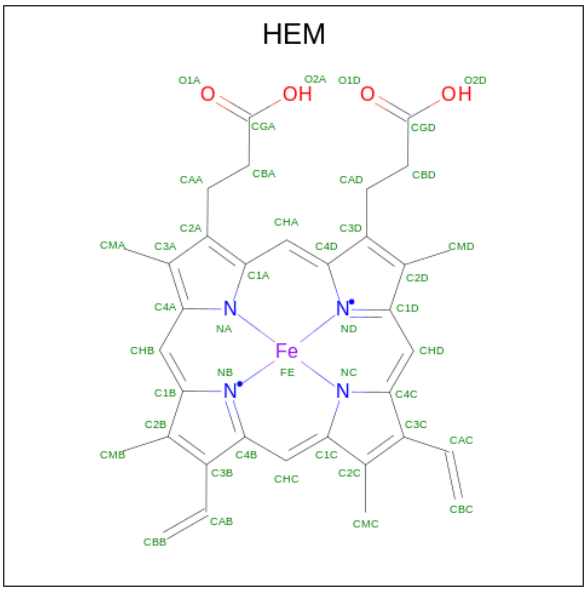
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0

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

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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

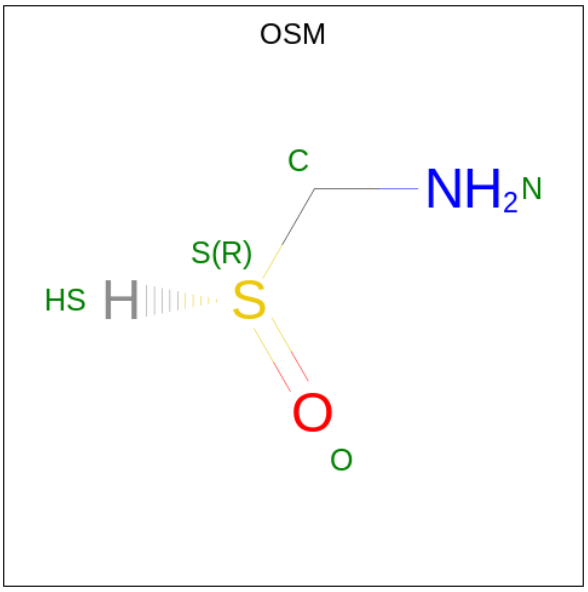


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

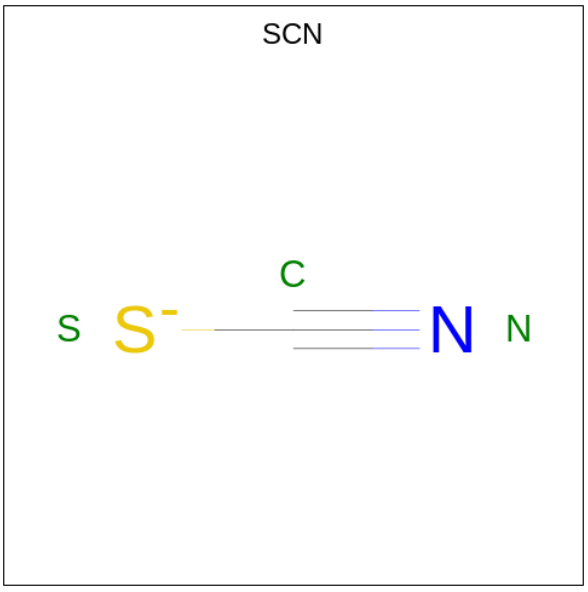
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	13	Total I 13 13	0	0

- Molecule 6 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH_5NOS) (labeled as "Ligand of Interest" by depositor).



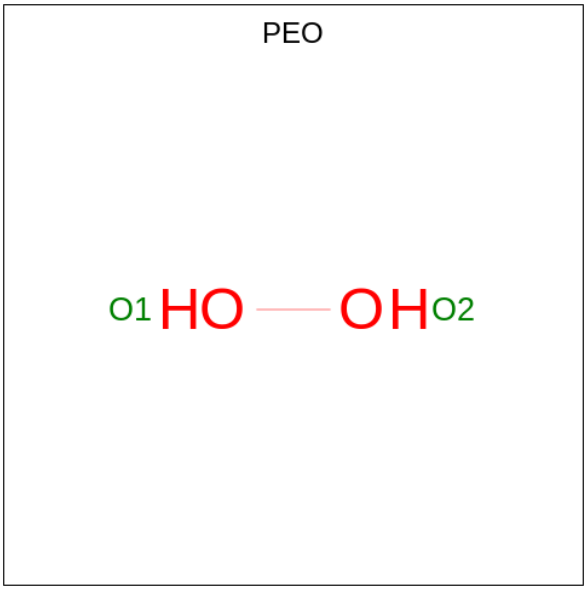
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		

- Molecule 7 is THIOCYANATE ION (three-letter code: 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 (three-letter code: PEO) (formula: H_2O_2).



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

- Molecule 9 is water.

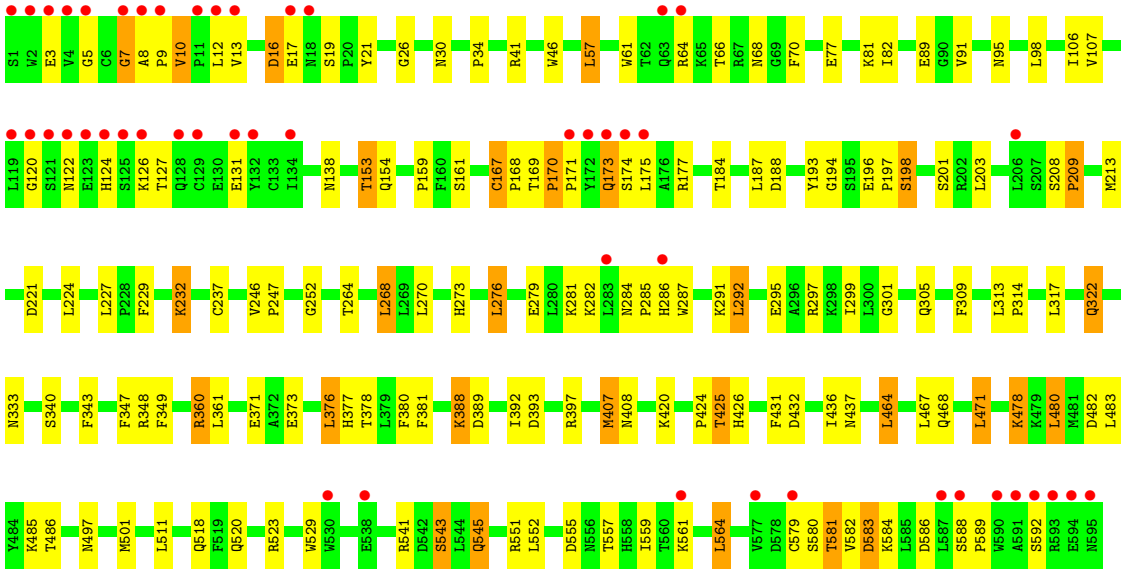
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	358	Total O 358 358	0	0

3 Residue-property plots (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

Chain A:



4 Data and refinement statistics (i)

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 52.74 – 2.27	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.79-2.27) 100.0 (52.74-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.196 , 0.266 0.201 , 0.263	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)	0.29 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, SCN, HEM, PEO, SEP, CA, NAG, OSM

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	0.67	0/4878	0.81	0/6617

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4763	0	4679	132	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	5	0
6	A	16	0	20	5	0
7	A	12	0	0	4	0
8	A	2	0	0	2	0
9	A	358	0	0	22	0
All	All	5264	0	4781	139	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 14.

All (139) 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:607:IOD:I	7:A:626:SCN:C	2.39	1.40
5:A:607:IOD:I	7:A:626:SCN:S	0.96	1.25
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: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:420:LYS:NZ	9:A:705:HOH:O	2.16	0.73
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
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: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:592:SER:OG	9:A:706:HOH:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:175:LEU:HA	9:A:980:HOH:O	2.05	0.55
1:A:16:ASP:OD1	1:A:16:ASP:C	2.45	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:126:LYS:NZ	9:A:720:HOH:O	2.38	0.54
1:A:159:PRO:HD2	1:A:431:PHE:CE2	2.43	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: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
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:184:THR:OG1	1:A:188:ASP:OD2	2.31	0.47
4:A:606:HEM:HMC2	4:A:606:HEM:HBC2	1.96	0.47
1:A:268:LEU:HB3	1:A:552:LEU:HD21	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:407:MET:CB	1:A:501:MET:HE2	2.45	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:174:SER:O	1:A:175:LEU:C	2.53	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: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:82:ILE:HD11	1:A:483:LEU:HD12	1.99	0.44
1:A:407:MET:HB3	1:A:501:MET:HE2	1.97	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
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:16:ASP:CG	1:A:19:SER:HB2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:322:GLN:H	1:A:322:GLN:CD	2.24	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 (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%)	552 (93%)	31 (5%)	9 (2%)	10 9

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

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Mol	Chain	Res	Type
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 (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	516/516 (100%)	474 (92%)	42 (8%)	11 13

All (42) 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	57	LEU
1	A	91	VAL
1	A	98	LEU
1	A	122	ASN
1	A	124	HIS
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	232	LYS
1	A	268	LEU
1	A	276	LEU

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Mol	Chain	Res	Type
1	A	279	GLU
1	A	292	LEU
1	A	317	LEU
1	A	322	GLN
1	A	333	ASN
1	A	347	PHE
1	A	360	ARG
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	520	GLN
1	A	543	SER
1	A	545	GLN
1	A	564	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
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	333	ASN
1	A	437	ASN
1	A	497	ASN
1	A	520	GLN
1	A	545	GLN
1	A	570	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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(^{o})	Ideal(^{o})
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 monosaccharides 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	603	1	14,14,15	1.04	1 (7%)	17,19,21	1.53	1 (5%)
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	-	-
7	SCN	A	627	-	1,2,2	0.68	0	0,1,1	-	-
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%)
4	HEM	A	606	1,8	41,50,50	1.40	8 (19%)	45,82,82	1.95	12 (26%)
6	OSM	A	620	-	1,3,3	0.01	0	0,2,2	-	-
8	PEO	A	628	4	1,1,1	0.49	0	-		
6	OSM	A	622	-	1,3,3	0.05	0	0,2,2	-	-
2	NAG	A	604	1	14,14,15	0.44	0	17,19,21	1.11	2 (11%)
6	OSM	A	621	-	1,3,3	0.09	0	0,2,2	-	-
2	NAG	A	601	1	14,14,15	0.71	0	17,19,21	1.17	2 (11%)
6	OSM	A	623	-	1,3,3	0.08	0	0,2,2	-	-

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	603	1	-	2/6/23/26	0/1/1/1
2	NAG	A	602	1	-	2/6/23/26	0/1/1/1
4	HEM	A	606	1,8	-	4/12/54/54	-
6	OSM	A	620	-	-	0/0/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OSM	A	622	-	-	0/0/1/1	-
2	NAG	A	604	1	-	2/6/23/26	0/1/1/1
6	OSM	A	621	-	-	0/0/1/1	-
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
6	OSM	A	623	-	-	0/0/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	FE-NB	2.82	2.10	1.96
4	A	606	HEM	C1B-NB	-2.82	1.35	1.40
4	A	606	HEM	C1D-ND	-2.47	1.33	1.38
4	A	606	HEM	CHB-C1B	2.38	1.41	1.35
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(^{o})	Ideal(^{o})
2	A	603	NAG	C1-O5-C5	-5.14	105.23	112.19
4	A	606	HEM	CHA-C4D-ND	4.65	130.13	124.38
4	A	606	HEM	CHC-C4B-NB	4.32	129.13	124.43
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
2	A	601	NAG	C1-O5-C5	3.17	116.49	112.19
4	A	606	HEM	CBA-CAA-C2A	-3.02	107.46	112.62
2	A	604	NAG	C1-C2-N2	-3.02	105.33	110.49
4	A	606	HEM	C4A-C3A-C2A	2.78	108.93	107.00
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	CHD-C1D-ND	2.38	127.02	124.43
2	A	604	NAG	C4-C3-C2	2.36	114.47	111.02
4	A	606	HEM	CMC-C2C-C3C	2.21	128.81	124.68
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

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

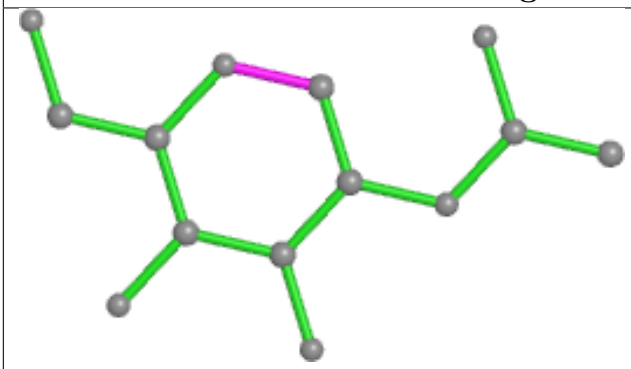
There are no ring outliers.

7 monomers are involved in 13 short contacts:

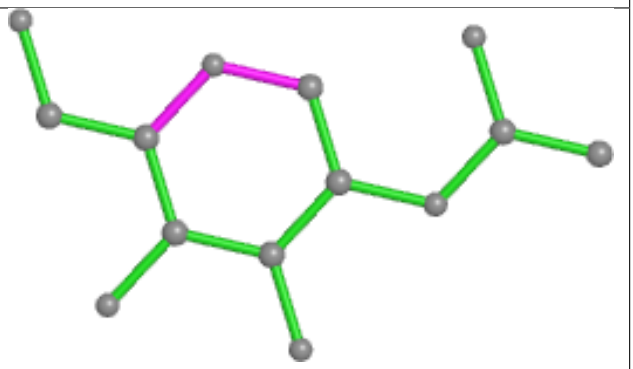
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	626	SCN	3	0
7	A	627	SCN	1	0
4	A	606	HEM	4	0
6	A	620	OSM	2	0
8	A	628	PEO	2	0
6	A	622	OSM	2	0
6	A	621	OSM	1	0

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 then 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.

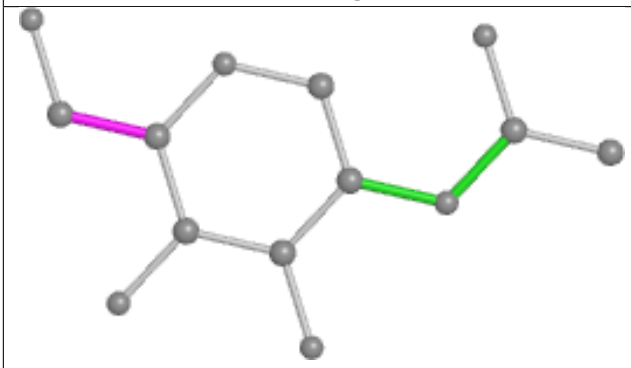
Ligand NAG A 603



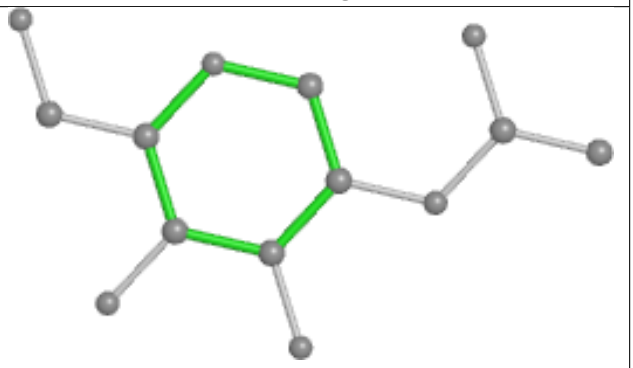
Bond lengths



Bond angles

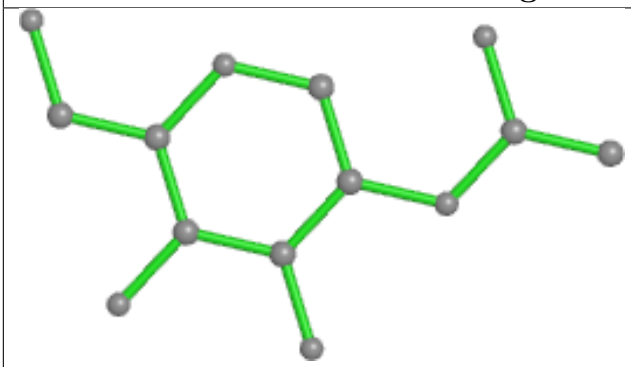


Torsions



Rings

Ligand NAG A 602



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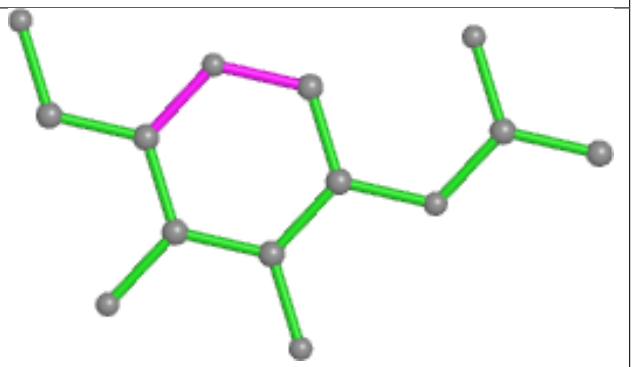
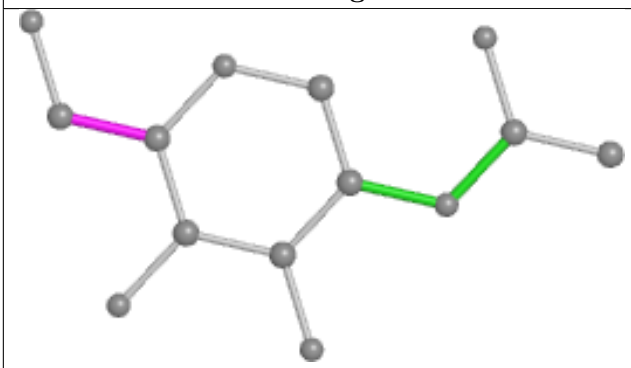


Bond angles



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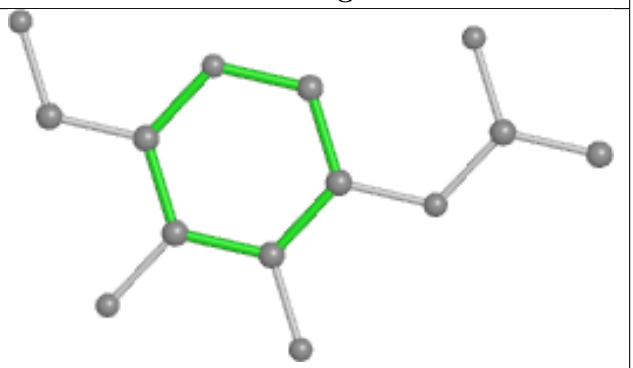
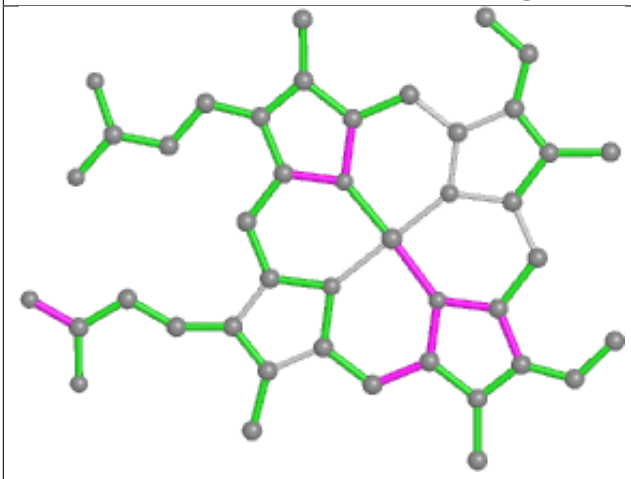
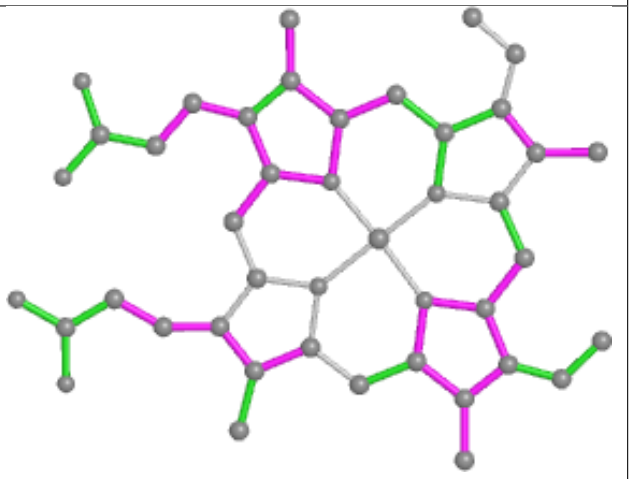


Rings

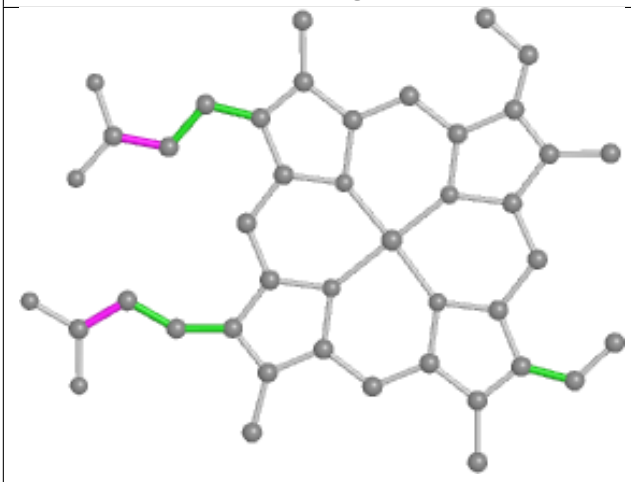
Ligand HEM A 606



Bond lengths



Bond angles



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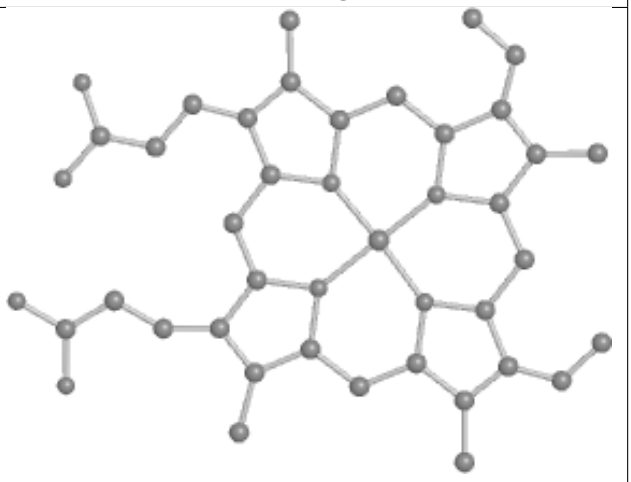
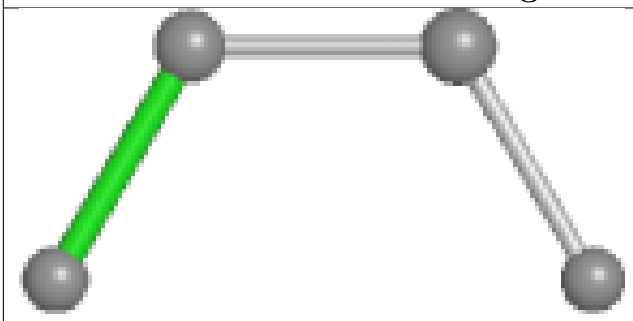
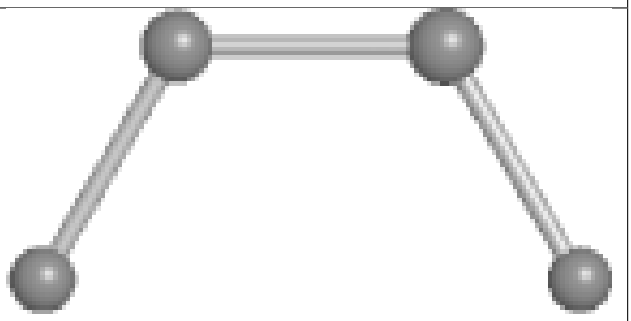


Rings

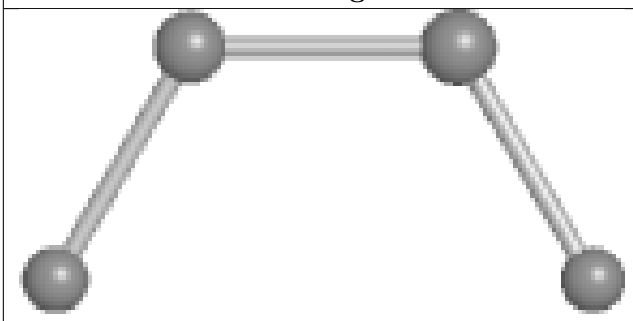
Ligand OSM A 620



Bond lengths



Bond angles



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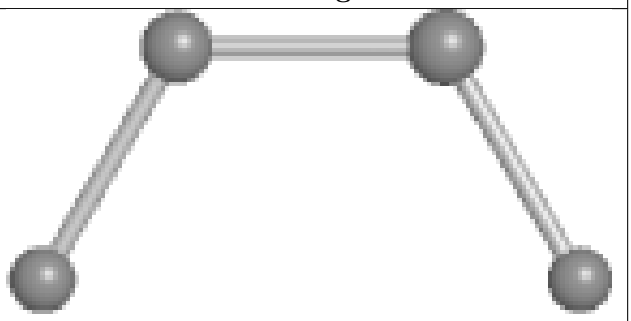
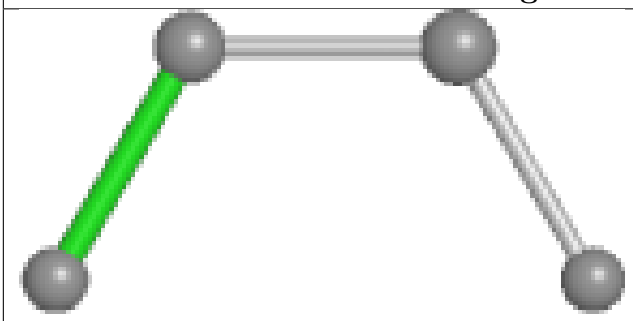
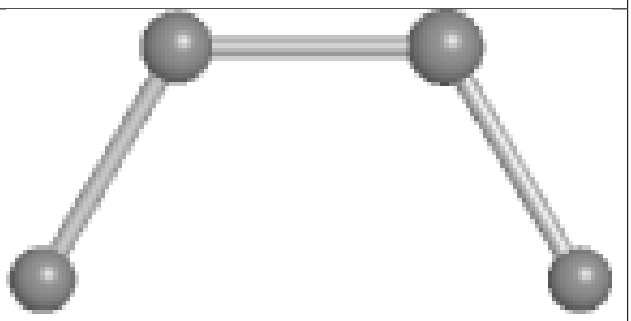


Rings

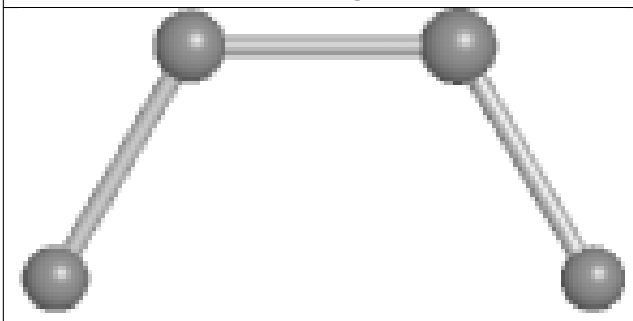
Ligand OSM A 622



Bond lengths



Bond angles



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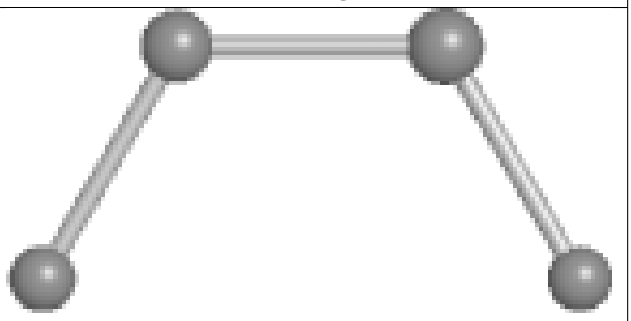
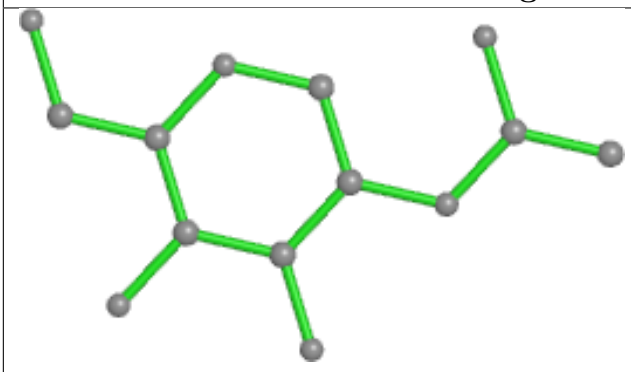
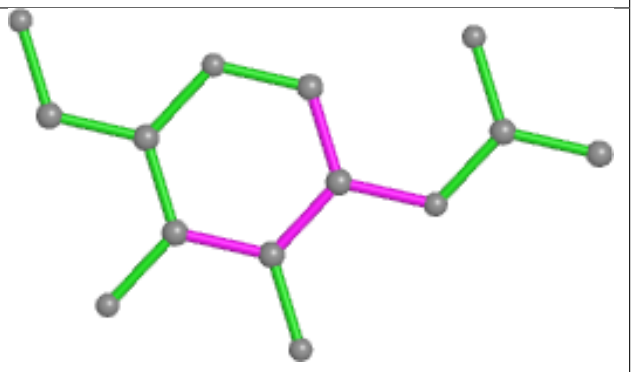


Rings

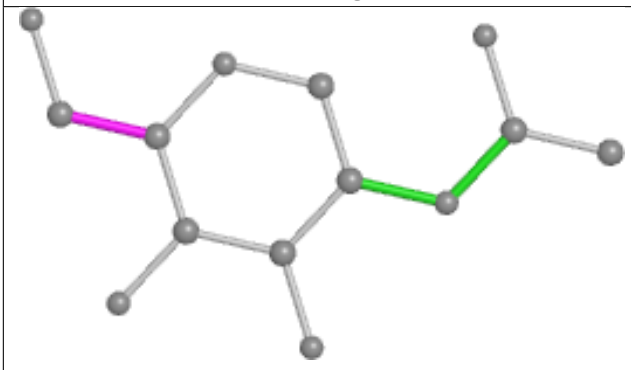
Ligand NAG A 604



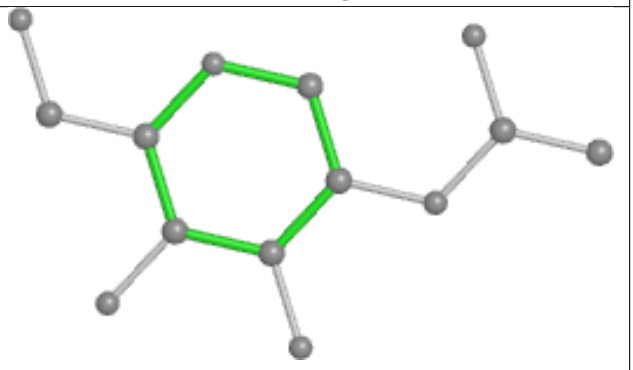
Bond lengths



Bond angles

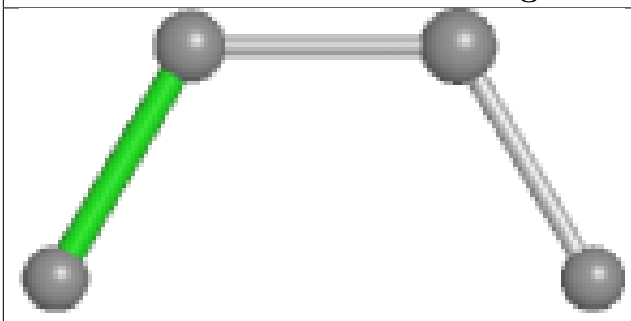


Torsions

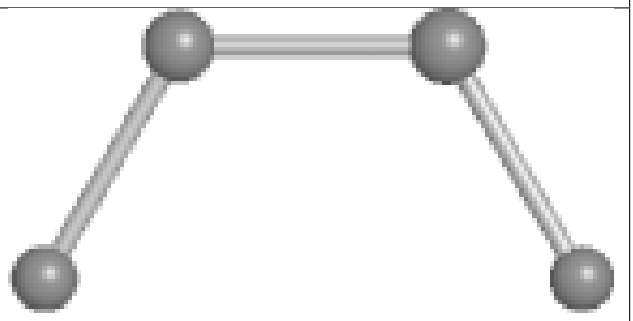


Rings

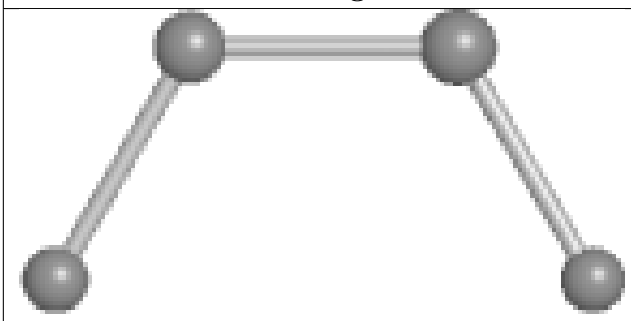
Ligand OSM A 621



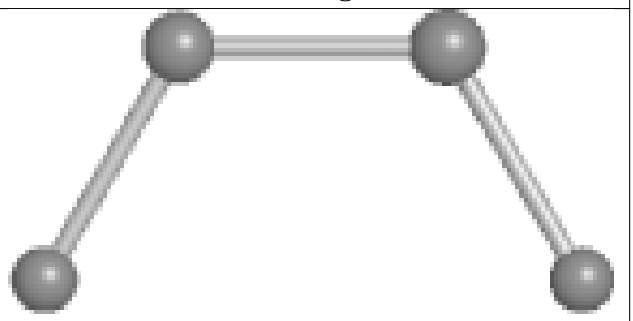
Bond lengths



Bond angles

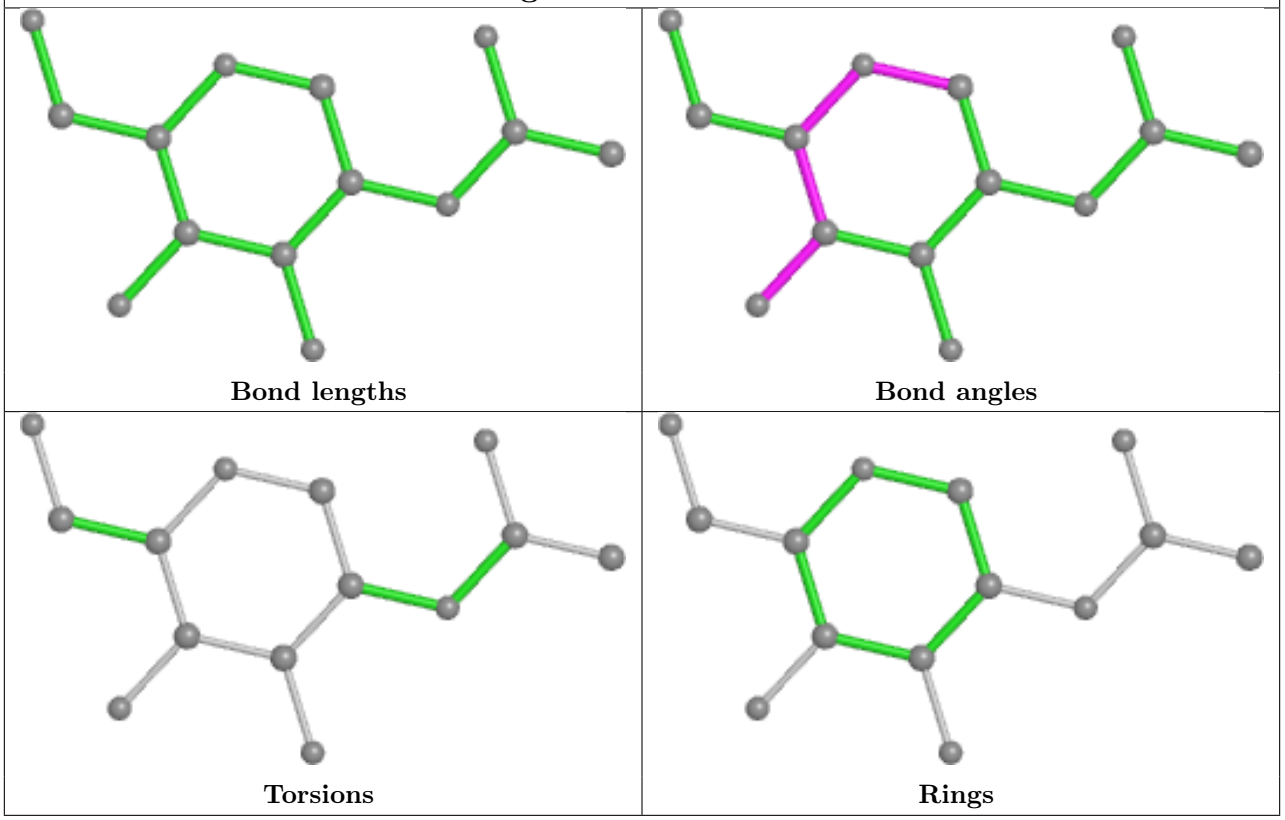


Torsions

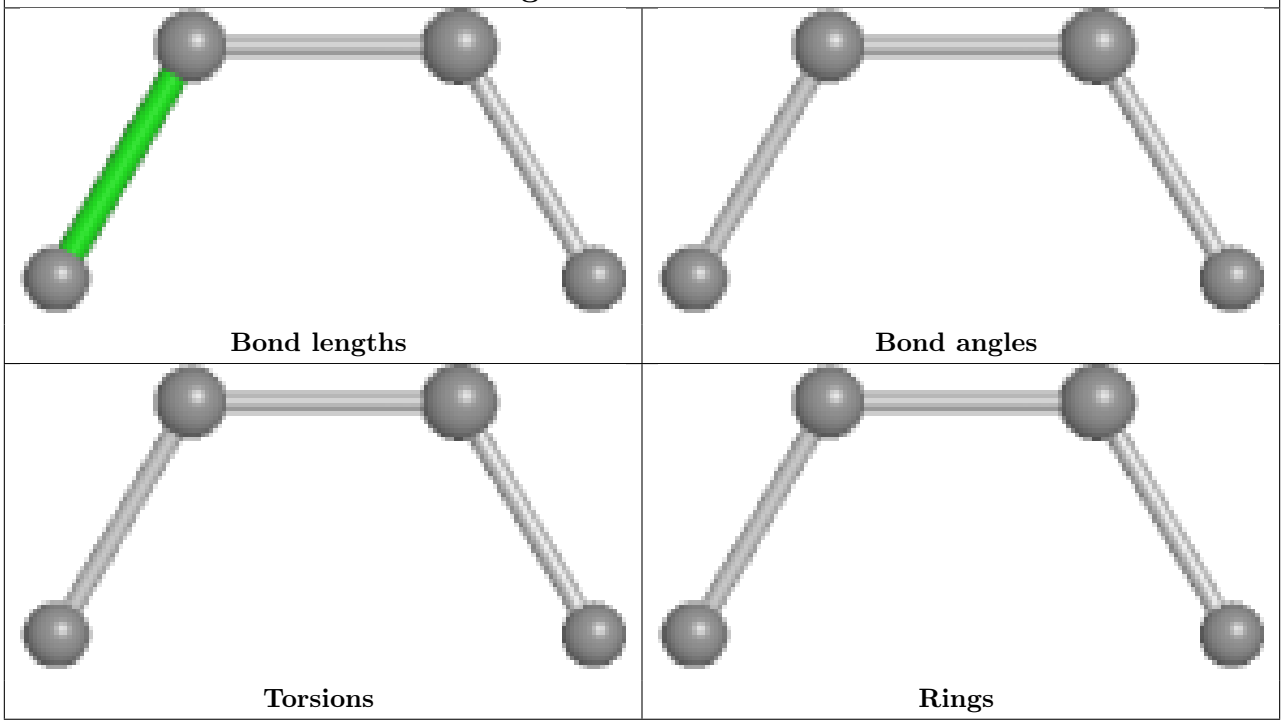


Rings

Ligand NAG A 601



Ligand OSM A 623



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, 95^{th} 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%)	0.55	49 (8%)	11	14	31, 52, 112, 177	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	20.7
1	A	121	SER	18.1
1	A	7	GLY	15.4
1	A	1	SER	14.2
1	A	173	GLN	14.1
1	A	172	TYR	13.7
1	A	174	SER	12.7
1	A	122	ASN	8.8
1	A	595	ASN	7.7
1	A	592	SER	7.6
1	A	124	HIS	6.3
1	A	120	GLY	6.3
1	A	593	ARG	5.7
1	A	594	GLU	5.5
1	A	591	ALA	4.9
1	A	4	VAL	4.9
1	A	8	ALA	4.6
1	A	283	LEU	3.7
1	A	206	LEU	3.3
1	A	587	LEU	3.3
1	A	171	PRO	3.3
1	A	175	LEU	3.2
1	A	13	VAL	3.1
1	A	63	GLN	3.1
1	A	128	GLN	3.1
1	A	9	PRO	3.1
1	A	119	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	64	ARG	3.0
1	A	11	PRO	3.0
1	A	132	TYR	2.8
1	A	530	TRP	2.7
1	A	129	CYS	2.7
1	A	126	LYS	2.7
1	A	123	GLU	2.5
1	A	17	GLU	2.5
1	A	588	SER	2.5
1	A	590	TRP	2.5
1	A	5	GLY	2.5
1	A	286	HIS	2.3
1	A	3	GLU	2.3
1	A	561	LYS	2.3
1	A	125	SER	2.3
1	A	134	ILE	2.3
1	A	577	VAL	2.2
1	A	12	LEU	2.1
1	A	538	GLU	2.1
1	A	18	ASN	2.1
1	A	131	GLU	2.0
1	A	579	CYS	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, 95^{th} 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	0.96	0.19	37,52,62,66	0

6.3 Carbohydrates (i)

There are no monosaccharides 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,

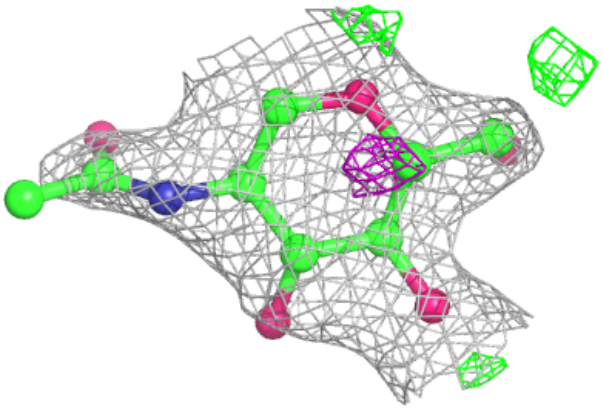
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

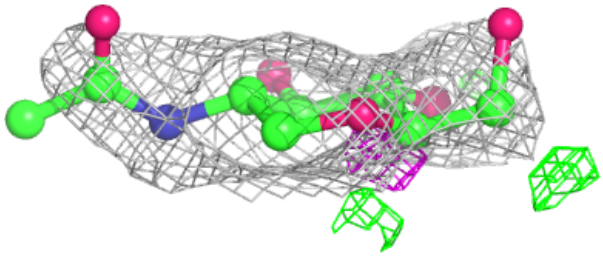
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	601	14/15	0.76	0.24	75,86,98,101	0
2	NAG	A	604	14/15	0.84	0.23	77,89,96,96	0
2	NAG	A	602	14/15	0.91	0.14	72,78,94,99	0
6	OSM	A	621	4/4	0.92	0.25	54,56,60,60	0
2	NAG	A	603	14/15	0.93	0.11	52,62,67,80	0
7	SCN	A	625	3/3	0.94	0.19	56,56,58,62	0
5	IOD	A	619	1/1	0.95	0.13	81,81,81,81	1
5	IOD	A	617	1/1	0.96	0.07	74,74,74,74	1
4	HEM	A	606	43/43	0.96	0.15	28,37,42,48	0
3	CA	A	605	1/1	0.97	0.07	46,46,46,46	0
5	IOD	A	618	1/1	0.97	0.11	76,76,76,76	1
5	IOD	A	611	1/1	0.97	0.10	65,65,65,65	1
6	OSM	A	620	4/4	0.97	0.20	30,31,33,36	0
5	IOD	A	614	1/1	0.97	0.05	81,81,81,81	0
6	OSM	A	622	4/4	0.97	0.14	49,50,50,51	0
5	IOD	A	616	1/1	0.97	0.04	74,74,74,74	1
5	IOD	A	608	1/1	0.98	0.07	67,67,67,67	1
6	OSM	A	623	4/4	0.98	0.27	26,28,34,34	0
5	IOD	A	609	1/1	0.98	0.10	60,60,60,60	0
7	SCN	A	627	3/3	0.98	0.17	44,44,50,60	0
5	IOD	A	610	1/1	0.99	0.06	59,59,59,59	1
5	IOD	A	615	1/1	0.99	0.08	56,56,56,56	0
7	SCN	A	624	3/3	0.99	0.12	44,44,52,58	0
5	IOD	A	607	1/1	0.99	0.13	51,51,51,51	1
7	SCN	A	626	3/3	0.99	0.15	30,30,34,35	3
5	IOD	A	612	1/1	0.99	0.07	69,69,69,69	0
8	PEO	A	628	2/2	0.99	0.14	42,42,42,60	0
5	IOD	A	613	1/1	1.00	0.10	44,44,44,44	0

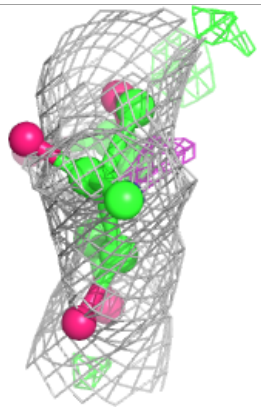
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 601:

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

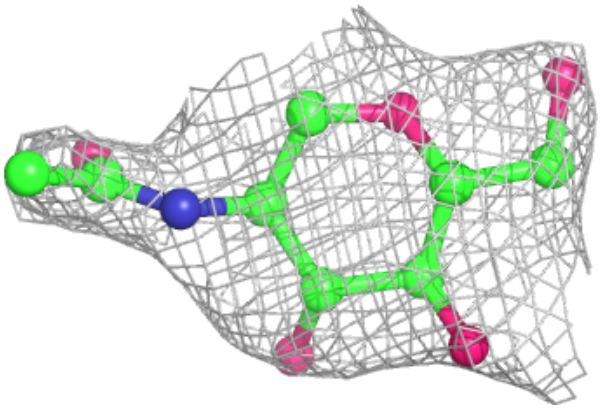


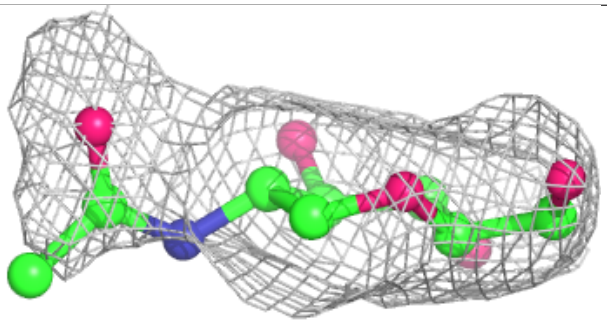


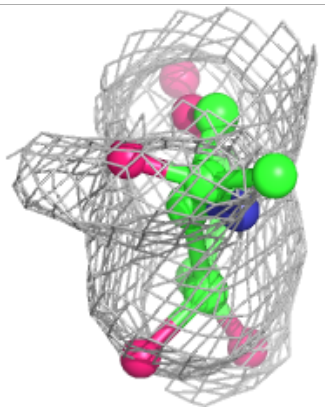


Electron density around NAG A 604:

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

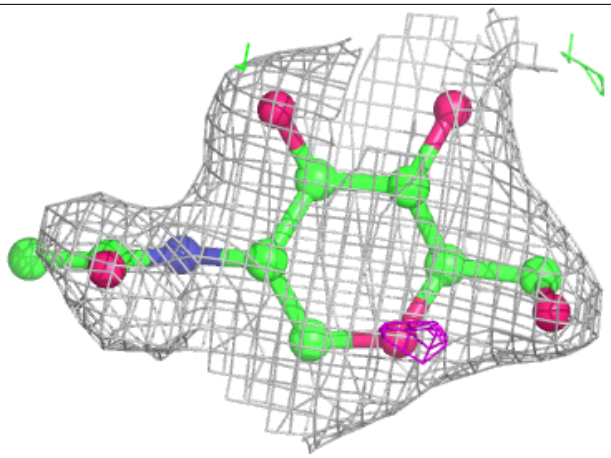


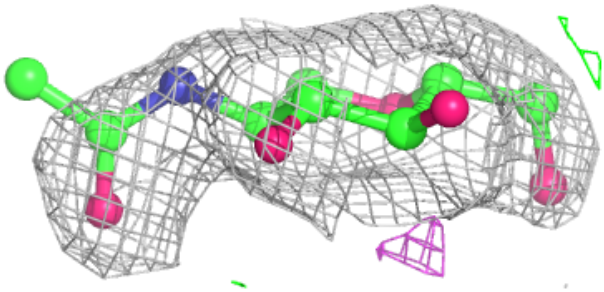


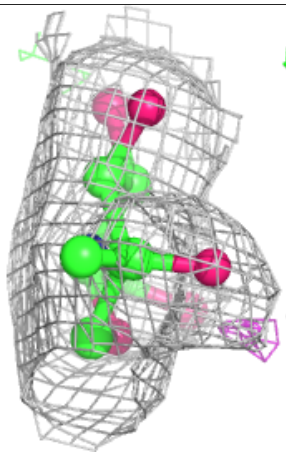


Electron density around NAG A 602:

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

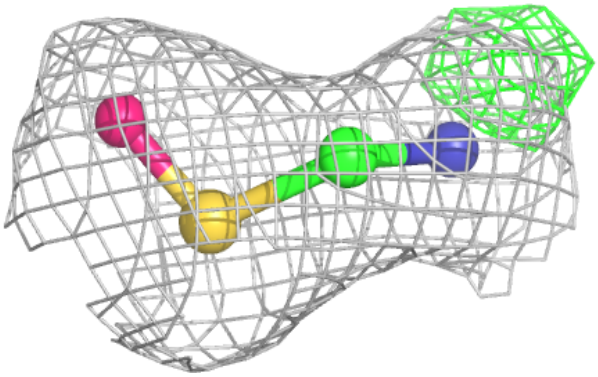


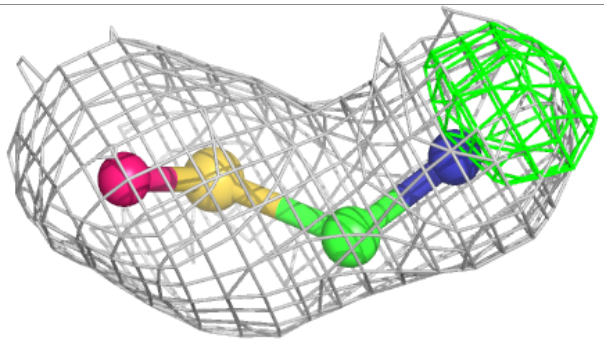


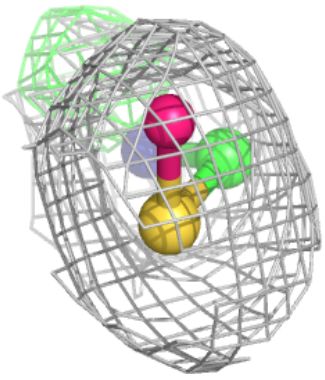


Electron density around OSM A 621:

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

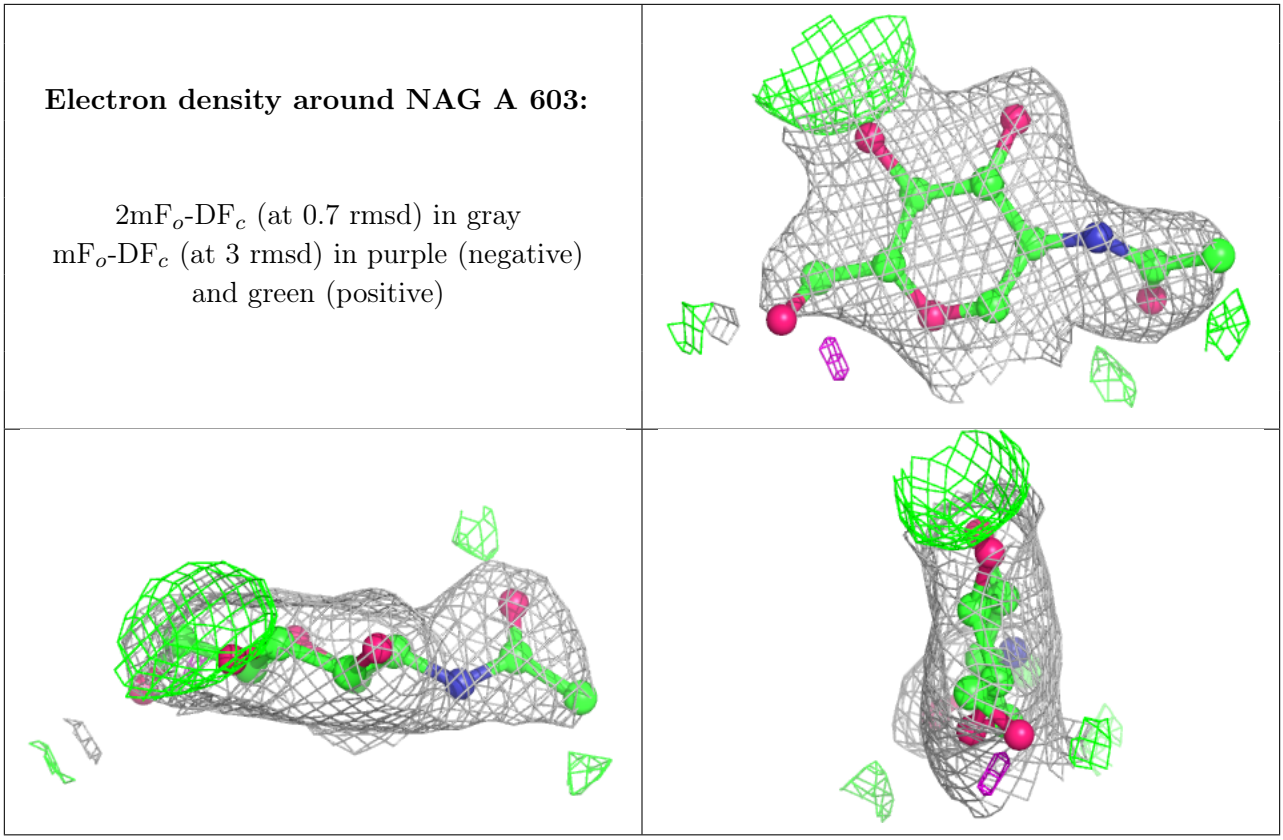






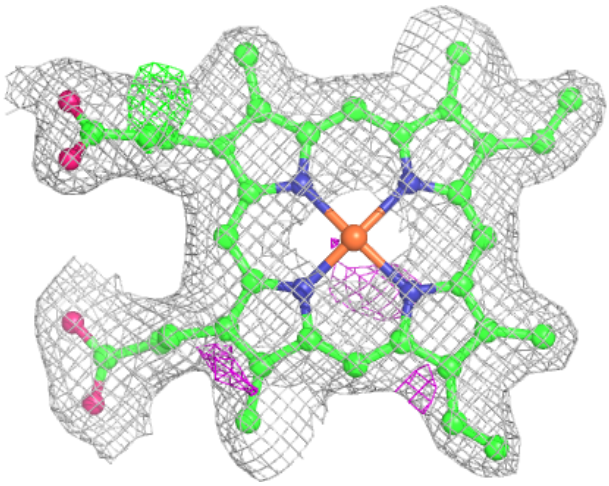
Electron density around NAG A 603:

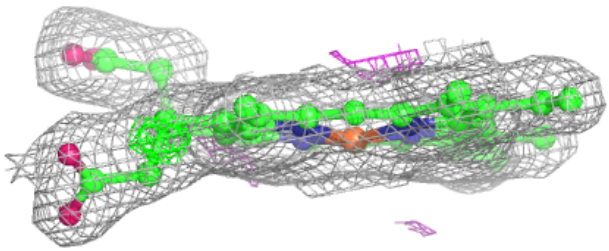
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

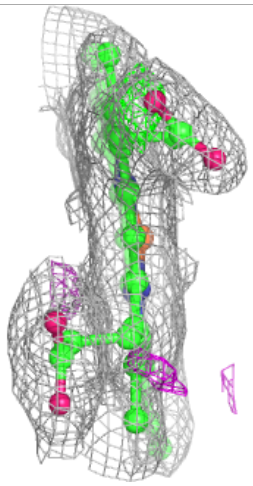


Electron density around HEM A 606:

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

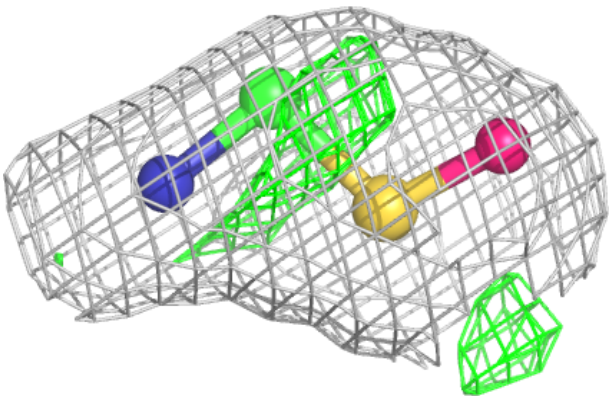


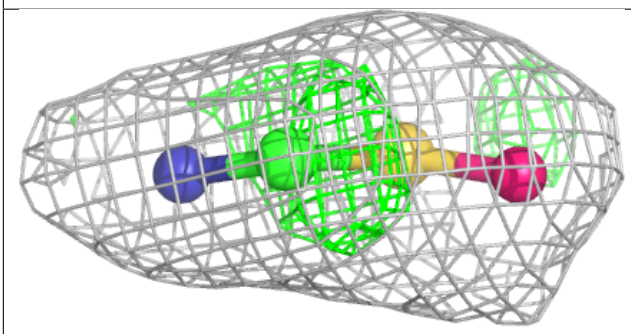


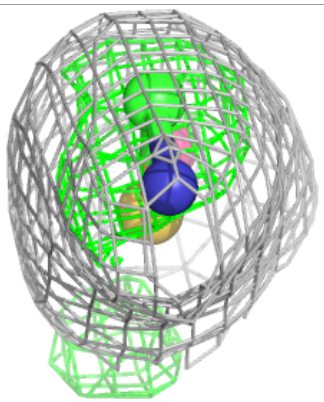


Electron density around OSM A 620:

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

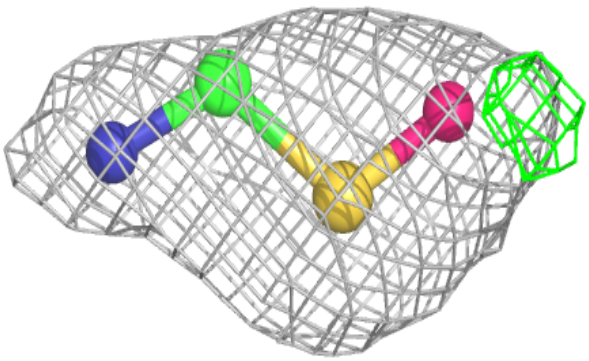


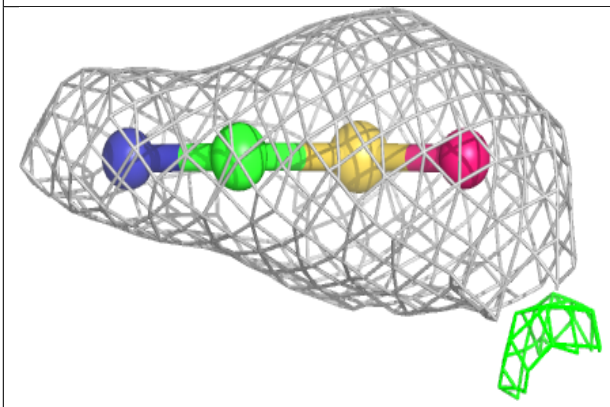


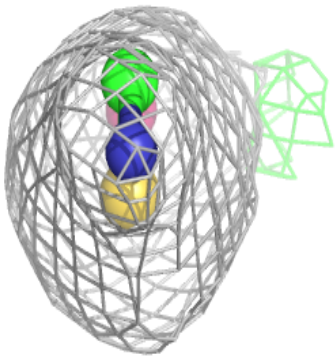


Electron density around OSM A 622:

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

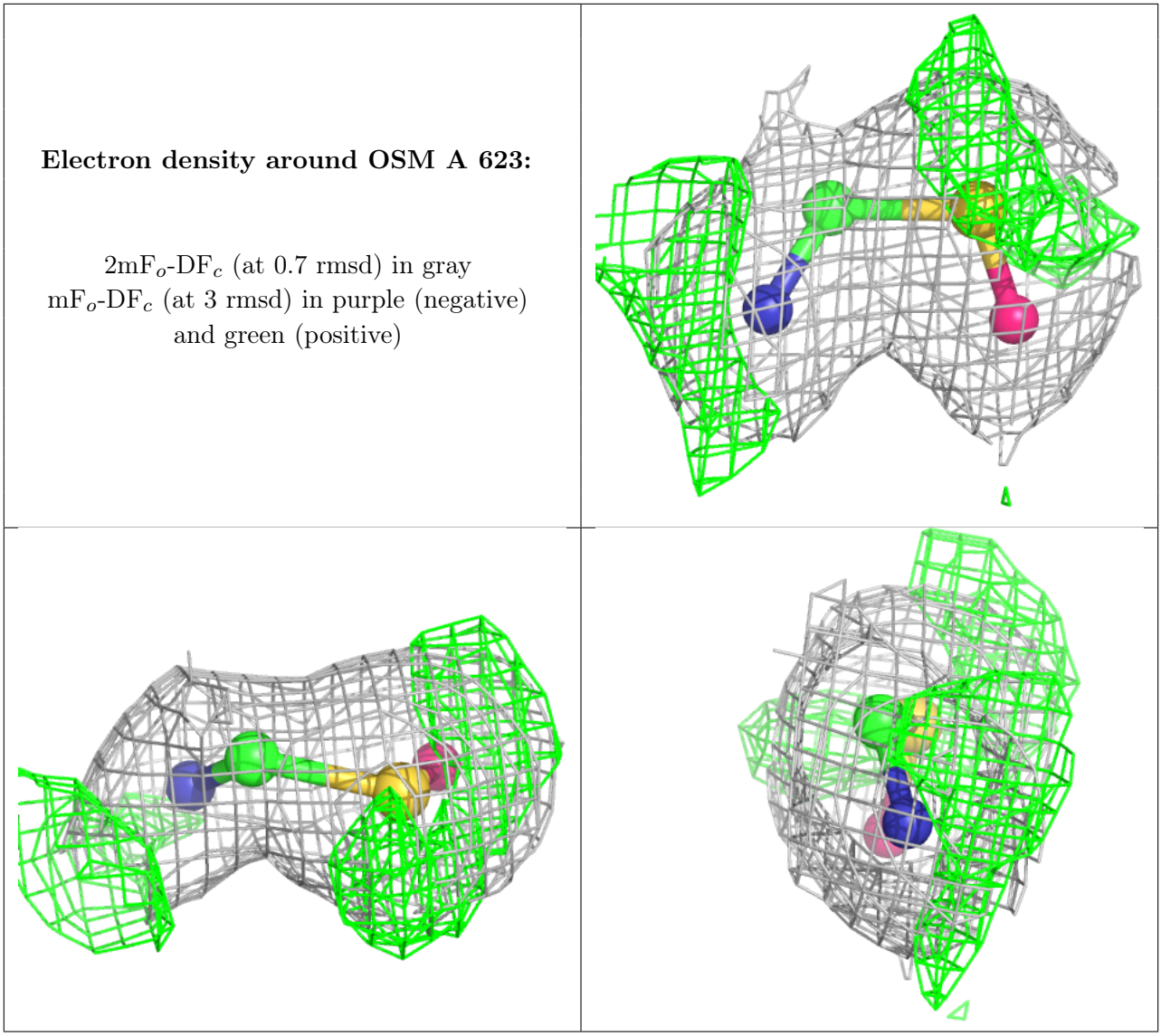






Electron density around OSM A 623:

$2mF_o$-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.