



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:26 PM JST

PDB ID : 6LQW / pdb_00006lqw
Title : Crystal structure of a dimeric yak lactoperoxidase at 2.59 Å resolution.
Authors : Viswanathan, V.; Pandey, S.N.; Ahmad, N.; Rani, C.; Sharma, P.; Sharma, S.; Singh, T.P.
Deposited on : 2020-01-14
Resolution : 2.60 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

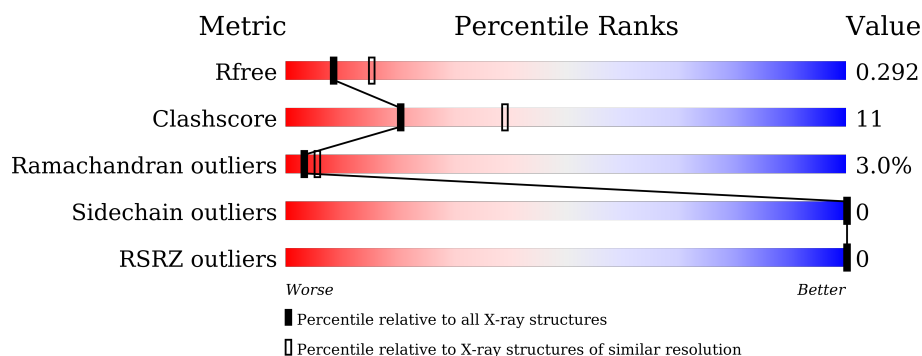
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	 77% 21% .
1	B	595	 75% 23% .

2 Entry composition [i](#)

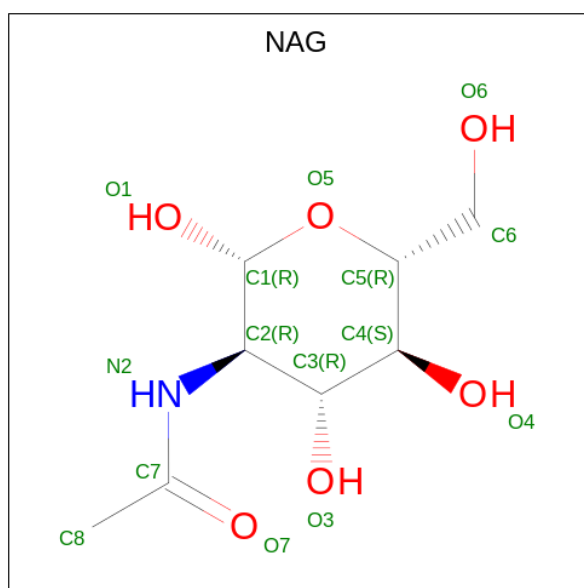
There are 7 unique types of molecules in this entry. The entry contains 10011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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			
1	B	595	Total	C	N	O	S	0	2	0
			4779	3043	847	863	26			

- 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).



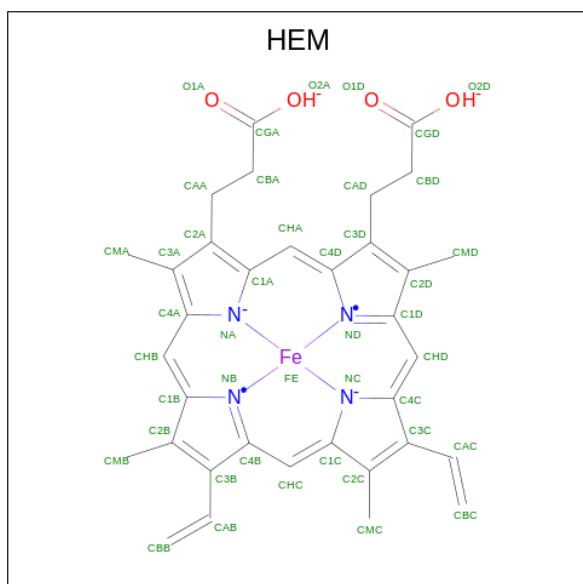
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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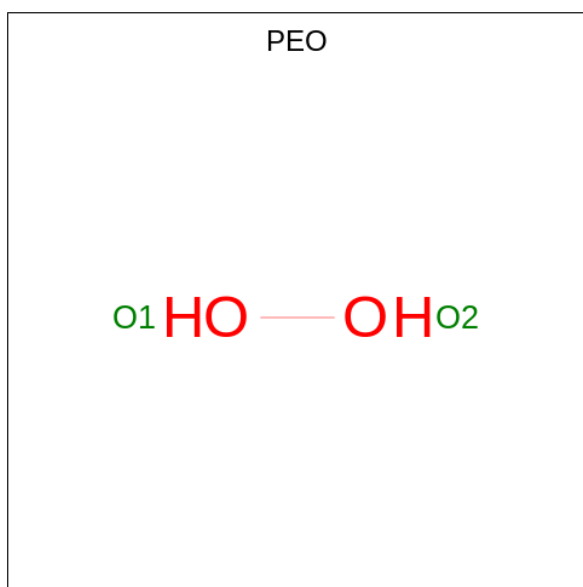
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H_2O_2) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	1	Total Cl 1 1	0	0

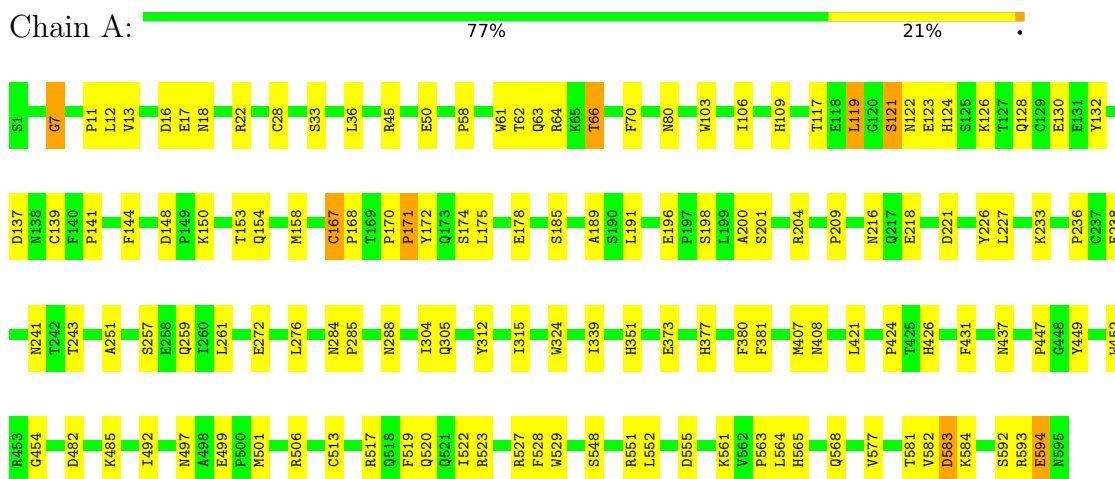
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	141	Total 141	O 141	0	0
7	B	115	Total 115	O 115	0	0

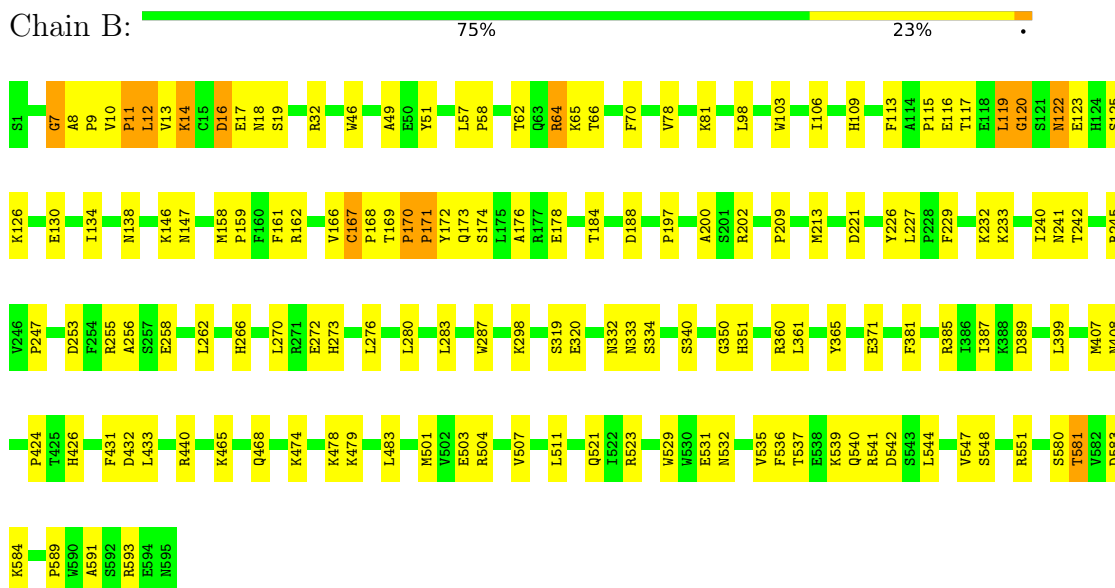
3 Residue-property plots

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



• 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	81.30Å 96.73Å 83.93Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	40.64 – 2.60 40.64 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.64-2.60) 98.4 (40.64-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.212 , 0.292 0.212 , 0.292	Depositor DCC
R_{free} test set	1061 reflections (2.64%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.057 for l,k,-h 0.328 for h,-k,-l 0.056 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10011	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.40	0/4898	0.63	0/6645
1	B	0.39	0/4913	0.61	2/6665 (0.0%)
All	All	0.39	0/9811	0.62	2/13310 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	166	VAL	CA-C-N	5.16	134.39	121.80
1	B	166	VAL	C-N-CA	5.16	134.39	121.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	LEU	Peptide
1	B	122	ASN	Peptide
1	B	581	THR	Peptide

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	4770	0	4688	104	1
1	B	4779	0	4699	117	1
2	A	56	0	52	0	0
2	B	56	0	52	2	0
3	A	43	0	30	3	0
3	B	43	0	30	6	0
4	A	2	0	0	1	0
4	B	2	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	141	0	0	8	0
7	B	115	0	0	7	0
All	All	10011	0	9551	216	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ARG:NH2	1:B:371:GLU:O	2.05	0.90
1:A:126:LYS:NZ	7:A:701:HOH:O	2.06	0.86
1:A:16:ASP:O	1:A:18:ASN:N	2.15	0.80
1:B:551:ARG:HD3	1:B:584:LYS:HA	1.64	0.79
1:B:167:CYS:HB2	1:B:168:PRO:HD2	1.65	0.78
1:B:503[B]:GLU:HG2	1:B:504:ARG:HG3	1.67	0.77
1:A:12:LEU:HG	1:B:123:GLU:HG2	1.67	0.76
1:B:167:CYS:HB2	1:B:168:PRO:CD	2.16	0.75
1:B:16:ASP:O	1:B:18:ASN:N	2.19	0.75
1:B:258:GLU:OE2	3:B:605:HEM:HMB1	1.86	0.75
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.36	0.73
1:B:12:LEU:HD23	1:B:14:LYS:H	1.53	0.73
1:A:12:LEU:HD11	1:B:123:GLU:OE1	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASN:HD21	1:A:592:SER:H	1.38	0.70
1:B:168:PRO:HB2	1:B:171:PRO:HD2	1.74	0.70
1:A:117:THR:O	7:A:701:HOH:O	2.11	0.69
1:B:130:GLU:OE2	1:B:426:HIS:ND1	2.24	0.68
1:B:287:TRP:O	7:B:701:HOH:O	2.12	0.67
1:B:468:GLN:HE21	1:B:474:LYS:HA	1.58	0.67
1:A:150:LYS:HA	1:A:153:THR:HG22	1.76	0.67
1:B:7:GLY:N	1:B:167:CYS:SG	2.68	0.66
1:B:319:SER:OG	1:B:320:GLU:OE2	2.13	0.66
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.78	0.65
1:A:564:LEU:CD1	1:A:577:VAL:HG21	2.26	0.65
1:A:168:PRO:HB2	1:A:171:PRO:HB3	1.77	0.65
1:A:381:PHE:CZ	1:A:424:PRO:HG3	2.33	0.64
1:A:482:ASP:O	1:A:485:LYS:NZ	2.18	0.64
1:B:78:VAL:HG22	1:B:483:LEU:HD23	1.79	0.63
1:B:32:ARG:HH22	1:B:334:SER:HB3	1.63	0.63
1:B:123:GLU:HG3	1:B:125:SER:H	1.62	0.63
1:A:153:THR:HG23	1:A:154:GLN:HG3	1.80	0.63
1:A:106:ILE:HG13	1:A:191:LEU:HD11	1.82	0.62
3:B:605:HEM:HMC2	3:B:605:HEM:HBC2	1.81	0.62
1:A:117:THR:HG22	1:A:119:LEU:H	1.66	0.61
1:B:381:PHE:CZ	1:B:424:PRO:HG3	2.35	0.61
1:B:32:ARG:HH21	1:B:333:ASN:CG	2.08	0.61
1:B:536:PHE:O	1:B:541:ARG:NH1	2.34	0.61
1:B:16:ASP:O	1:B:19:SER:N	2.34	0.60
1:B:109:HIS:NE2	4:B:606:PEO:O2	2.35	0.60
1:B:548:SER:HB3	1:B:551:ARG:H	1.65	0.60
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.31	0.60
1:B:544:LEU:O	1:B:547:VAL:HG22	2.02	0.59
1:B:202:ARG:NH1	7:B:713:HOH:O	2.36	0.59
1:B:407:MET:HB3	1:B:501:MET:HE3	1.84	0.59
1:B:280:LEU:HD22	1:B:287:TRP:HZ3	1.66	0.59
3:B:605:HEM:HMB2	3:B:605:HEM:HBB2	1.84	0.59
1:A:548:SER:HG	1:A:551:ARG:H	1.52	0.58
1:B:120:GLY:HA3	1:B:126:LYS:HE3	1.85	0.58
1:B:332:ASN:ND2	2:B:603:NAG:O7	2.36	0.58
1:A:121:SER:O	1:A:123:GLU:N	2.37	0.58
1:B:16:ASP:C	1:B:18:ASN:H	2.10	0.57
1:A:288:ASN:HB2	1:B:12:LEU:HB3	1.87	0.57
1:A:233:LYS:NZ	1:A:238:GLU:OE1	2.38	0.57
1:B:529:TRP:CD1	1:B:531:GLU:H	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.39	0.57
1:A:109:HIS:NE2	4:A:604:PEO:O2	2.34	0.57
3:A:603:HEM:HMC2	3:A:603:HEM:HBC2	1.87	0.57
1:A:11:PRO:HB3	1:B:170:PRO:HB3	1.86	0.56
1:B:253:ASP:CG	1:B:255:ARG:HH21	2.13	0.56
1:A:198:SER:HB2	1:B:168:PRO:HB3	1.87	0.56
1:B:123:GLU:OE2	1:B:125:SER:N	2.38	0.56
1:B:319:SER:HA	1:B:504:ARG:HH22	1.70	0.56
1:A:272:GLU:O	1:A:276:LEU:HD22	2.05	0.56
1:A:284:ASN:ND2	1:A:592:SER:H	2.03	0.56
1:A:12:LEU:HD11	1:B:123:GLU:CD	2.30	0.56
1:A:128:GLN:HG2	1:A:132:TYR:HE1	1.71	0.56
1:B:539:LYS:NZ	1:B:542:ASP:OD1	2.33	0.55
1:A:257:SER:O	1:A:381:PHE:HA	2.07	0.55
1:A:58:PRO:HD2	1:A:61:TRP:HB2	1.88	0.54
1:B:227:LEU:HD11	1:B:266:HIS:HB3	1.89	0.54
1:B:116:GLU:HG2	1:B:440:ARG:HH22	1.72	0.54
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.42	0.54
1:B:351:HIS:CE1	1:B:433:LEU:HD21	2.42	0.54
1:A:200:ALA:O	1:A:204:ARG:HG3	2.08	0.54
1:A:454:GLY:HA2	7:A:734:HOH:O	2.07	0.54
1:B:10:VAL:HG12	1:B:11:PRO:O	2.08	0.54
1:A:312:TYR:O	1:A:315:ILE:HG12	2.08	0.54
1:A:407:MET:HB3	1:A:501:MET:HE2	1.89	0.53
1:B:226:TYR:CE2	1:B:387:ILE:HG12	2.42	0.53
1:A:551:ARG:HE	1:A:555:ASP:CG	2.17	0.53
1:B:81:LYS:HD3	1:B:483:LEU:HD11	1.91	0.53
1:A:80:ASN:ND2	1:A:148:ASP:OD2	2.35	0.53
1:A:351:HIS:HD1	1:A:437:ASN:ND2	2.05	0.53
1:A:45:ARG:NE	1:A:178:GLU:OE2	2.40	0.53
1:A:62:THR:O	1:A:64:ARG:N	2.38	0.52
1:B:117:THR:HG21	1:B:138:ASN:ND2	2.24	0.52
1:B:385:ARG:NH1	1:B:389:ASP:OD2	2.35	0.52
1:A:175:LEU:HA	7:A:792:HOH:O	2.10	0.52
1:A:407:MET:HE2	1:A:497:ASN:O	2.08	0.52
1:B:280:LEU:HD22	1:B:287:TRP:CZ3	2.44	0.52
1:B:319:SER:HA	1:B:504:ARG:NH2	2.25	0.52
1:B:170:PRO:CD	1:B:171:PRO:HD3	2.40	0.52
1:A:12:LEU:HB2	1:B:119:LEU:C	2.35	0.51
1:B:221:ASP:HB2	1:B:226:TYR:CZ	2.45	0.51
1:B:273:HIS:HA	1:B:276:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LYS:HD2	7:B:777:HOH:O	2.11	0.51
2:B:604:NAG:O7	2:B:604:NAG:O3	2.23	0.51
1:B:58:PRO:HA	7:B:710:HOH:O	2.10	0.51
1:A:227:LEU:HD23	1:A:251:ALA:HB2	1.92	0.51
1:A:236:PRO:HG3	1:A:424:PRO:HB3	1.93	0.51
1:A:33:SER:HB3	1:A:36:LEU:HD12	1.92	0.50
1:A:12:LEU:O	1:B:119:LEU:HA	2.11	0.50
1:B:532:ASN:HB3	1:B:535:VAL:HG21	1.93	0.50
1:B:540:GLN:HG3	1:B:589:PRO:HB2	1.94	0.49
1:B:184:THR:OG1	1:B:188:ASP:OD2	2.31	0.49
1:B:591:ALA:HB1	1:B:593:ARG:NH2	2.28	0.49
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.94	0.49
1:B:229:PHE:CG	1:B:247:PRO:HG2	2.48	0.49
1:A:324:TRP:CE2	1:A:513:CYS:HA	2.48	0.48
1:B:478:LYS:HE2	7:B:725:HOH:O	2.13	0.48
1:A:128:GLN:HG2	1:A:132:TYR:CE1	2.46	0.48
1:B:465:LYS:HD3	7:B:703:HOH:O	2.12	0.48
1:A:201:SER:HB2	1:B:8:ALA:HB2	1.94	0.48
1:A:123:GLU:HG2	1:A:124:HIS:H	1.78	0.48
3:A:603:HEM:HBB2	3:A:603:HEM:HMB2	1.94	0.48
1:B:158:MET:HE1	1:B:432:ASP:HB2	1.96	0.48
1:A:139:CYS:SG	1:A:141:PRO:HD3	2.54	0.48
1:A:7:GLY:N	1:A:167:CYS:SG	2.87	0.48
1:A:564:LEU:HD11	1:A:577:VAL:HG21	1.96	0.48
1:A:66:THR:HB	1:A:70:PHE:O	2.15	0.47
1:B:103:TRP:O	1:B:106:ILE:HG22	2.14	0.47
1:A:196:GLU:HB3	7:A:732:HOH:O	2.13	0.47
1:B:113:PHE:CE2	1:B:115:PRO:HG3	2.49	0.47
3:B:605:HEM:HBB2	3:B:605:HEM:CMB	2.44	0.47
1:A:168:PRO:O	1:A:171:PRO:HG3	2.14	0.47
1:A:241:ASN:OD1	1:A:243:THR:HB	2.13	0.47
1:A:582:VAL:O	1:A:583:ASP:HB2	2.15	0.47
1:A:158:MET:HE3	1:A:431:PHE:CD2	2.50	0.47
1:A:50:GLU:HG3	1:A:447:PRO:HG3	1.97	0.46
1:B:551:ARG:HD2	1:B:583:ASP:O	2.15	0.46
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.98	0.46
1:B:16:ASP:C	1:B:18:ASN:N	2.72	0.46
1:B:242:THR:HB	1:B:245:ARG:NH1	2.30	0.46
1:B:172:TYR:HB3	1:B:173:GLN:H	1.48	0.46
1:B:232:LYS:HG2	1:B:233:LYS:N	2.30	0.46
1:A:167:CYS:CB	1:A:168:PRO:CD	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LEU:HD23	1:B:14:LYS:N	2.27	0.46
1:B:361:LEU:HB3	1:B:365:TYR:HA	1.97	0.46
1:B:170:PRO:N	1:B:171:PRO:HD3	2.31	0.46
1:A:28:CYS:O	1:A:527:ARG:NH2	2.37	0.46
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.46	0.46
1:A:185:SER:HB3	1:A:339:ILE:HG12	1.97	0.46
1:B:49:ALA:HB1	1:B:51:TYR:CE2	2.50	0.46
1:A:513:CYS:O	1:A:517:ARG:HG3	2.15	0.46
1:A:594:GLU:N	1:A:594:GLU:OE2	2.49	0.46
1:B:8:ALA:H	1:B:167:CYS:HA	1.81	0.45
3:B:605:HEM:HBC2	3:B:605:HEM:CMC	2.46	0.45
1:B:171:PRO:HB2	1:B:172:TYR:H	1.57	0.45
1:B:298:LYS:HG2	1:B:536:PHE:CZ	2.51	0.45
1:B:521:GLN:NE2	7:B:716:HOH:O	2.41	0.45
1:B:46:TRP:CE2	1:B:340:SER:HB3	2.51	0.45
1:A:216:ASN:OD1	1:A:218:GLU:N	2.28	0.45
1:B:537:THR:O	1:B:541:ARG:HG3	2.17	0.45
1:A:150:LYS:O	1:A:154:GLN:N	2.45	0.45
1:A:227:LEU:CD2	1:A:251:ALA:HB2	2.46	0.45
1:A:130:GLU:CD	1:A:426:HIS:HD1	2.25	0.44
1:A:259:GLN:OE1	1:A:261:LEU:N	2.48	0.44
1:A:519:PHE:HA	1:A:522:ILE:HG12	1.99	0.44
1:A:119:LEU:O	7:A:701:HOH:O	2.21	0.44
1:B:242:THR:HB	1:B:245:ARG:CZ	2.48	0.44
1:A:103:TRP:O	1:A:106:ILE:HG22	2.18	0.43
1:B:138:ASN:OD1	1:B:162:ARG:HB2	2.18	0.43
1:B:350:GLY:HA3	3:B:605:HEM:CBC	2.49	0.43
1:B:66:THR:HB	1:B:70:PHE:N	2.32	0.43
1:A:144:PHE:CE1	1:A:158:MET:HG3	2.53	0.43
1:A:272:GLU:HB2	1:A:552:LEU:HD11	2.00	0.43
1:B:479:LYS:O	1:B:483:LEU:HD13	2.18	0.43
1:A:22:ARG:HG2	1:A:528:PHE:CD2	2.54	0.43
1:B:507:VAL:HB	1:B:511:LEU:HB2	2.00	0.43
1:B:523:ARG:HG3	1:B:529:TRP:CE2	2.54	0.43
1:A:106:ILE:HG13	1:A:191:LEU:CD1	2.47	0.43
1:A:305:GLN:HB3	1:A:529:TRP:CH2	2.54	0.43
1:B:11:PRO:HB2	1:B:12:LEU:H	1.68	0.43
1:B:62:THR:O	1:B:64:ARG:N	2.51	0.43
1:B:283:LEU:HD23	1:B:591:ALA:HB2	2.01	0.42
1:A:288:ASN:HD22	1:B:12:LEU:HB3	1.84	0.42
1:B:407:MET:HE3	1:B:501:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:LYS:HA	1:A:577:VAL:O	2.19	0.42
1:A:251:ALA:HA	7:A:723:HOH:O	2.18	0.42
1:A:501:MET:SD	1:A:506:ARG:HA	2.60	0.42
1:A:517:ARG:O	1:A:520:GLN:HB3	2.19	0.42
1:B:176:ALA:HB3	1:B:178:GLU:OE1	2.18	0.42
1:B:270:LEU:HD12	1:B:270:LEU:HA	1.87	0.42
1:A:449:TYR:OH	1:A:499:GLU:OE2	2.30	0.42
1:B:98:LEU:HB3	1:B:399:LEU:HA	2.00	0.42
1:A:407:MET:SD	1:A:408:ASN:N	2.92	0.42
1:B:51:TYR:HB3	1:B:57:LEU:O	2.20	0.42
1:B:256:ALA:O	1:B:262:LEU:HG	2.20	0.42
1:B:158:MET:HE2	1:B:431:PHE:HA	2.02	0.42
1:A:12:LEU:CG	1:B:123:GLU:HG2	2.45	0.41
1:B:407:MET:SD	1:B:408:ASN:N	2.93	0.41
1:A:189:ALA:HB2	1:A:304:ILE:HD12	2.02	0.41
3:A:603:HEM:HBB2	3:A:603:HEM:CMB	2.50	0.41
1:B:130:GLU:HG2	1:B:159:PRO:HG3	2.03	0.41
1:B:272:GLU:O	1:B:276:LEU:HG	2.20	0.41
1:A:13:VAL:HA	1:B:119:LEU:HG	2.02	0.41
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.55	0.41
1:B:134:ILE:HD13	1:B:134:ILE:HA	1.91	0.41
1:B:532:ASN:HB3	1:B:535:VAL:CG2	2.51	0.41
1:A:171:PRO:HB2	1:A:172:TYR:H	1.58	0.41
1:A:380:PHE:CE2	1:A:421:LEU:HA	2.56	0.41
1:B:46:TRP:NE1	1:B:340:SER:HB3	2.36	0.41
1:B:197:PRO:HA	1:B:200:ALA:HB3	2.01	0.41
1:B:117:THR:HG21	1:B:138:ASN:CG	2.45	0.41
1:A:123:GLU:HG2	1:A:124:HIS:ND1	2.36	0.41
1:A:158:MET:HE3	1:A:431:PHE:HD2	1.84	0.41
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.93	0.41
1:B:174:SER:HB2	1:B:176:ALA:C	2.46	0.41
1:A:12:LEU:H	1:B:119:LEU:HD23	1.85	0.41
1:A:285:PRO:HD2	1:A:593:ARG:HH11	1.86	0.41
1:A:565:HIS:O	1:A:568:GLN:HG2	2.21	0.40
1:A:452:TRP:CD1	1:A:492:ILE:HD13	2.56	0.40
1:B:146:LYS:HD3	1:B:147:ASN:N	2.37	0.40
1:A:563:PRO:HB2	7:A:751:HOH:O	2.20	0.40
1:B:213:MET:HG2	1:B:273:HIS:CD2	2.56	0.40
1:B:138:ASN:O	1:B:161:PHE:HA	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLU:OE1	1:B:65:LYS:NZ[2_646]	2.17	0.03

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%)	529 (89%)	49 (8%)	15 (2%)	4	8
1	B	595/595 (100%)	529 (89%)	45 (8%)	21 (4%)	3	4
All	All	1188/1190 (100%)	1058 (89%)	94 (8%)	36 (3%)	3	6

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	122	ASN
1	A	167	CYS
1	A	170	PRO
1	A	171	PRO
1	A	581	THR
1	B	16	ASP
1	B	64	ARG
1	B	122	ASN
1	B	167	CYS
1	B	241	ASN
1	A	121	SER
1	A	583	ASP
1	A	594	GLU
1	B	11	PRO
1	B	12	LEU
1	B	13	VAL
1	B	14	LYS
1	B	17	GLU
1	B	119	LEU

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Mol	Chain	Res	Type
1	B	171	PRO
1	A	66	THR
1	A	137	ASP
1	A	174	SER
1	A	209	PRO
1	B	169	THR
1	B	580	SER
1	B	581	THR
1	A	63	GLN
1	B	170	PRO
1	B	209	PRO
1	A	7	GLY
1	B	120	GLY
1	B	240	ILE
1	B	7	GLY
1	B	9	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	518/518 (100%)	518 (100%)	0	100	100
1	B	520/518 (100%)	520 (100%)	0	100	100
All	All	1038/1036 (100%)	1038 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	173	GLN
1	A	468	GLN
1	A	520	GLN
1	A	571	ASN

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Mol	Chain	Res	Type
1	B	18	ASN
1	B	135	GLN
1	B	341	ASN
1	B	468	GLN

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
4	PEO	A	604	3	1,1,1	0.13	0	-		
2	NAG	B	601	1	14,14,15	0.54	0	17,19,21	1.03	1 (5%)
2	NAG	B	602	1	14,14,15	0.57	0	17,19,21	0.74	1 (5%)
2	NAG	A	602	1	14,14,15	0.42	0	17,19,21	0.92	1 (5%)
4	PEO	B	606	-	1,1,1	0.07	0	-		
2	NAG	B	604	1	14,14,15	0.69	1 (7%)	17,19,21	0.92	2 (11%)
2	NAG	A	607	1	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
2	NAG	B	603	1	14,14,15	1.22	1 (7%)	17,19,21	1.33	2 (11%)

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	0.40	0	17,19,21	0.52	0
3	HEM	B	605	1	50,50,50	1.39	7 (14%)	66,82,82	1.15	5 (7%)
2	NAG	A	608	1	14,14,15	0.99	1 (7%)	17,19,21	1.22	1 (5%)
3	HEM	A	603	1,4	50,50,50	1.46	8 (16%)	66,82,82	1.22	4 (6%)

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	B	601	1	-	2/6/23/26	0/1/1/1
2	NAG	B	602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	2/6/23/26	0/1/1/1
2	NAG	B	604	1	-	3/6/23/26	0/1/1/1
2	NAG	A	607	1	-	2/6/23/26	0/1/1/1
2	NAG	B	603	1	-	3/6/23/26	0/1/1/1
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
3	HEM	B	605	1	-	4/14/54/54	-
2	NAG	A	608	1	-	0/6/23/26	0/1/1/1
3	HEM	A	603	1,4	-	4/14/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	603	NAG	O5-C1	-3.93	1.37	1.43
3	A	603	HEM	FE-NA	3.69	2.07	1.95
2	A	608	NAG	O5-C1	3.55	1.49	1.43
3	B	605	HEM	FE-NC	3.53	2.07	1.95
3	B	605	HEM	FE-NB	3.52	2.05	1.94
3	A	603	HEM	FE-NB	3.43	2.05	1.94
3	B	605	HEM	FE-NA	3.00	2.05	1.95
3	B	605	HEM	CAB-C3B	2.93	1.55	1.47
3	A	603	HEM	CAB-C3B	2.87	1.55	1.47
3	A	603	HEM	FE-ND	2.70	2.03	1.94
3	A	603	HEM	CMB-C2B	2.57	1.56	1.50
3	B	605	HEM	FE-ND	2.44	2.02	1.94
3	B	605	HEM	CAC-C3C	2.43	1.54	1.47
3	A	603	HEM	CAC-C3C	2.39	1.53	1.47
3	A	603	HEM	CMA-C3A	2.33	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	HEM	C3C-C4C	-2.11	1.42	1.46
3	B	605	HEM	CMB-C2B	2.07	1.55	1.50
2	B	604	NAG	C1-C2	2.00	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	608	NAG	C1-O5-C5	4.62	118.45	112.19
2	B	603	NAG	C4-C3-C2	3.60	116.29	111.02
2	A	607	NAG	C1-O5-C5	3.49	116.93	112.19
2	B	601	NAG	C1-O5-C5	3.35	116.73	112.19
2	A	602	NAG	C1-O5-C5	3.04	116.31	112.19
3	A	603	HEM	CHD-C4C-NC	2.68	127.33	124.44
3	B	605	HEM	C1B-NB-C4B	2.59	107.75	105.07
3	B	605	HEM	C4D-ND-C1D	2.59	107.75	105.07
2	B	603	NAG	C1-O5-C5	-2.45	108.88	112.19
2	B	604	NAG	C2-N2-C7	2.43	126.36	122.90
3	B	605	HEM	C4A-NA-C1A	2.40	107.70	105.35
3	A	603	HEM	CHD-C1D-ND	2.34	126.96	124.42
2	B	602	NAG	C1-O5-C5	2.33	115.34	112.19
3	B	605	HEM	C4C-NC-C1C	2.33	107.62	105.35
3	B	605	HEM	C3B-C2B-C1B	2.25	108.16	106.49
3	A	603	HEM	CAA-CBA-CGA	-2.22	108.83	113.60
3	A	603	HEM	C4A-NA-C1A	2.11	107.42	105.35
2	B	604	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	603	NAG	C3-C2-N2-C7
2	B	601	NAG	C4-C5-C6-O6
2	B	601	NAG	O5-C5-C6-O6
2	A	602	NAG	O5-C5-C6-O6
2	A	602	NAG	C4-C5-C6-O6
2	B	604	NAG	C1-C2-N2-C7
2	B	604	NAG	O5-C5-C6-O6
2	B	603	NAG	O5-C5-C6-O6
2	B	604	NAG	C3-C2-N2-C7
2	A	607	NAG	C4-C5-C6-O6
2	B	603	NAG	C1-C2-N2-C7
3	A	603	HEM	CAD-CBD-CGD-O2D

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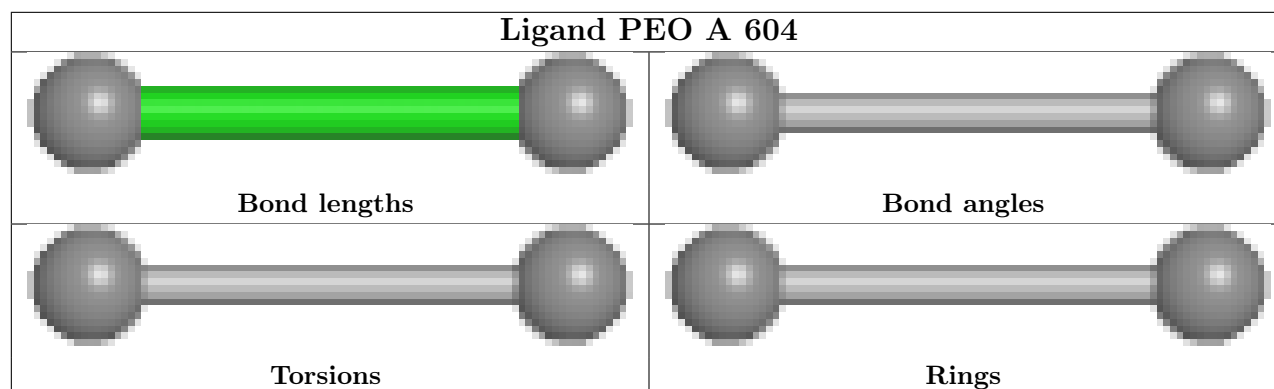
Mol	Chain	Res	Type	Atoms
3	A	603	HEM	CAD-CBD-CGD-O1D
3	B	605	HEM	CAD-CBD-CGD-O1D
3	B	605	HEM	CAD-CBD-CGD-O2D
3	A	603	HEM	CAA-CBA-CGA-O2A
3	B	605	HEM	CAA-CBA-CGA-O2A
3	A	603	HEM	CAA-CBA-CGA-O1A
2	A	607	NAG	O5-C5-C6-O6
3	B	605	HEM	CAA-CBA-CGA-O1A

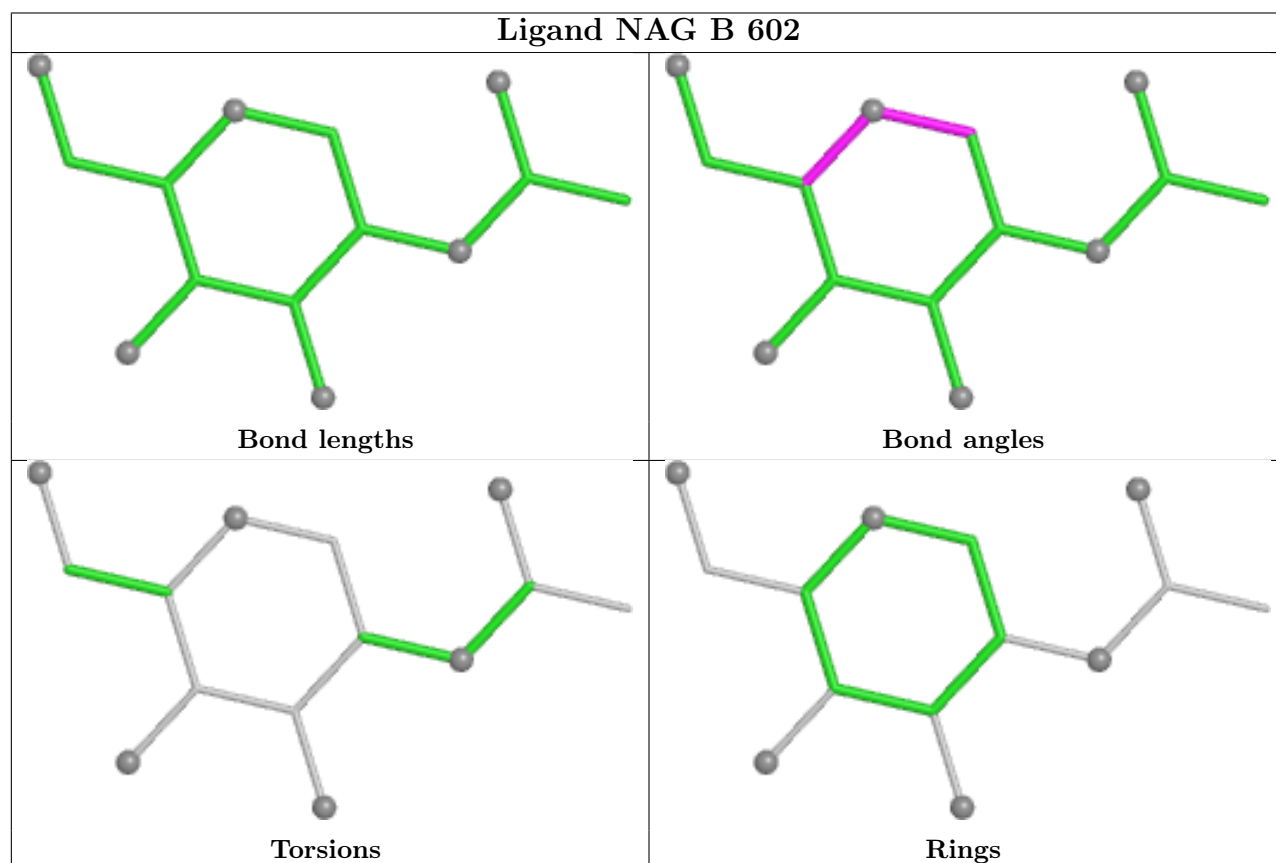
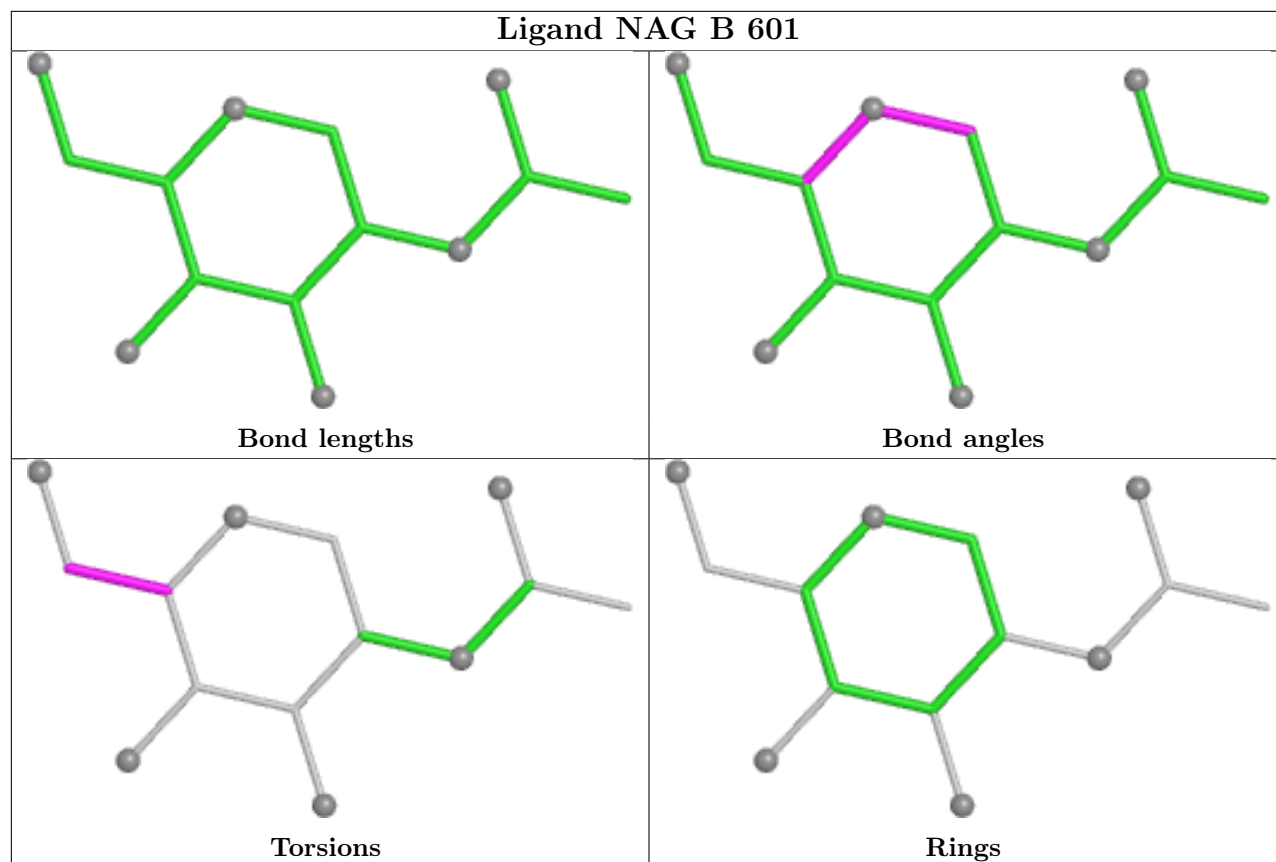
There are no ring outliers.

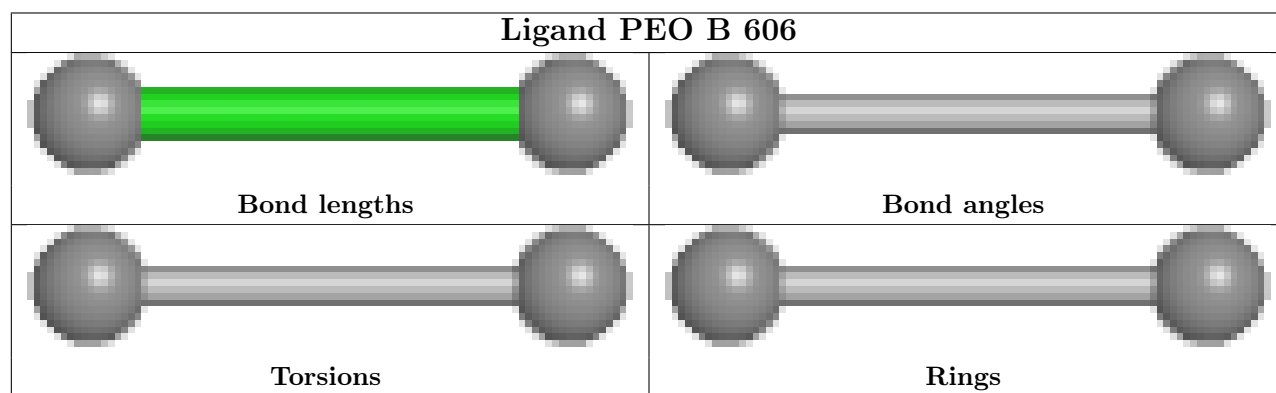
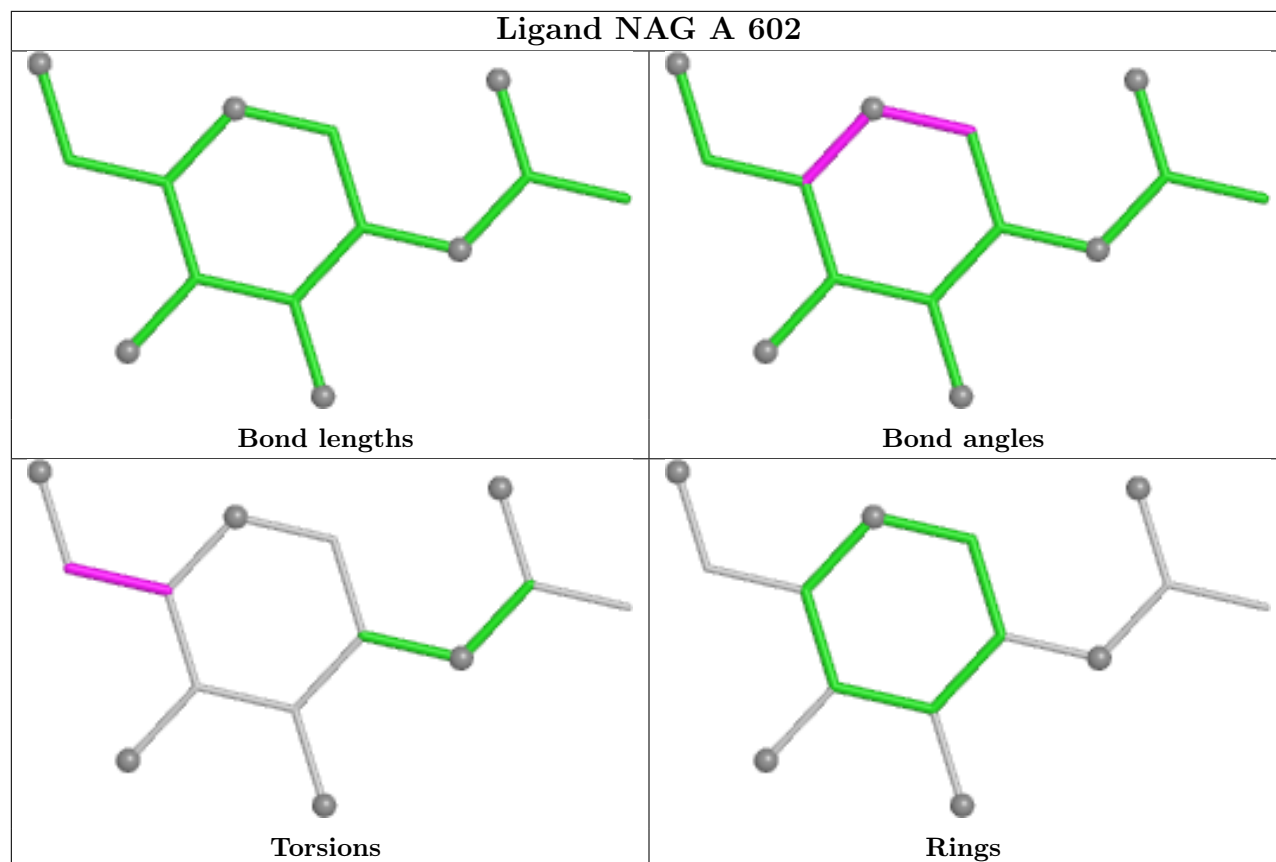
6 monomers are involved in 13 short contacts:

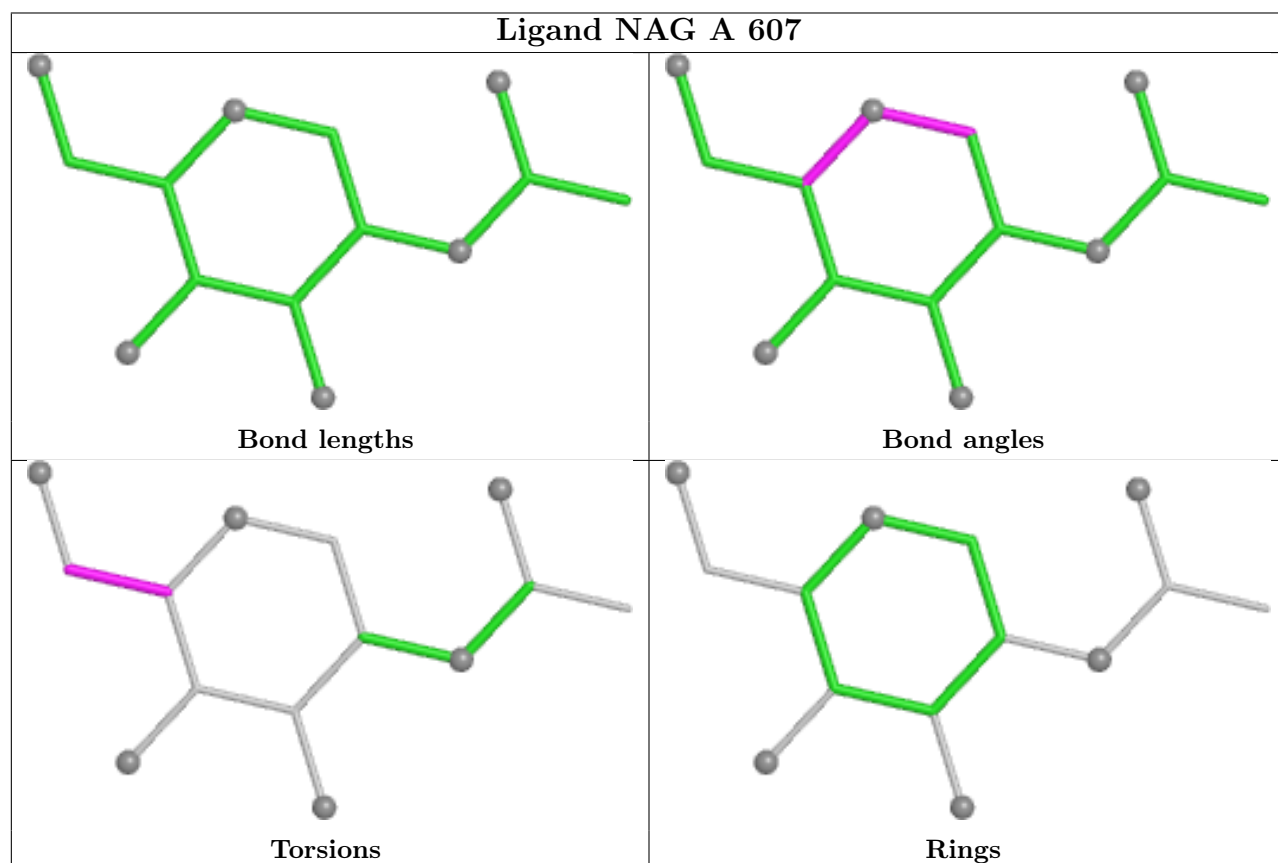
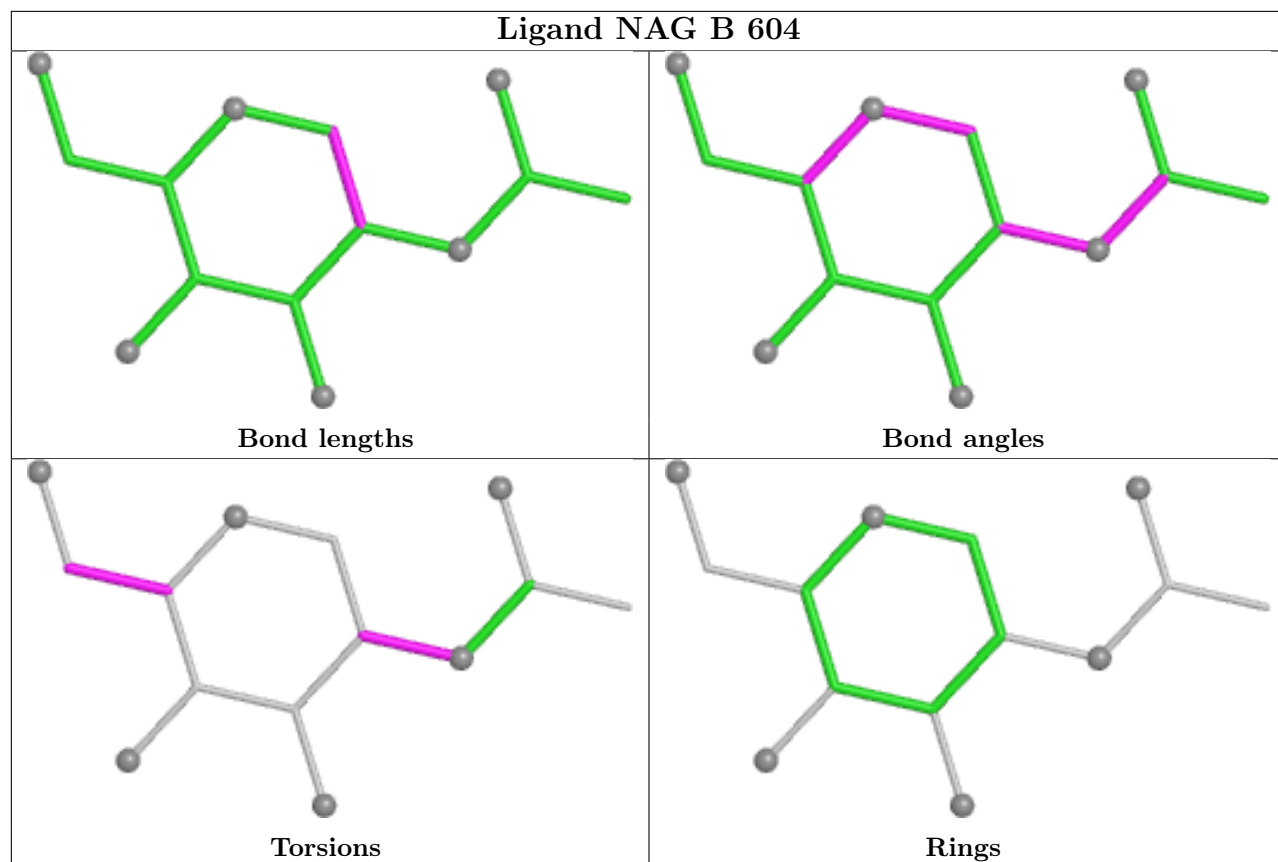
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	PEO	1	0
4	B	606	PEO	1	0
2	B	604	NAG	1	0
2	B	603	NAG	1	0
3	B	605	HEM	6	0
3	A	603	HEM	3	0

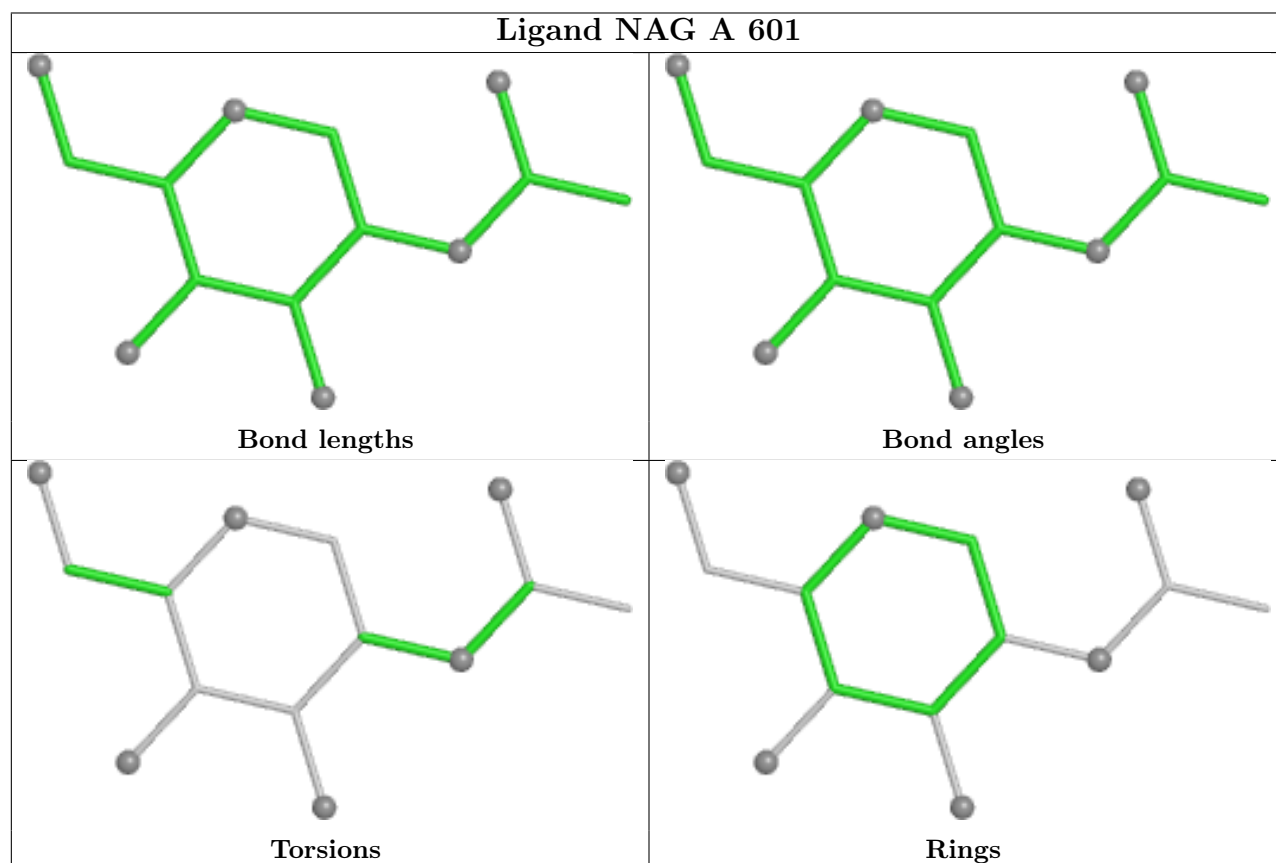
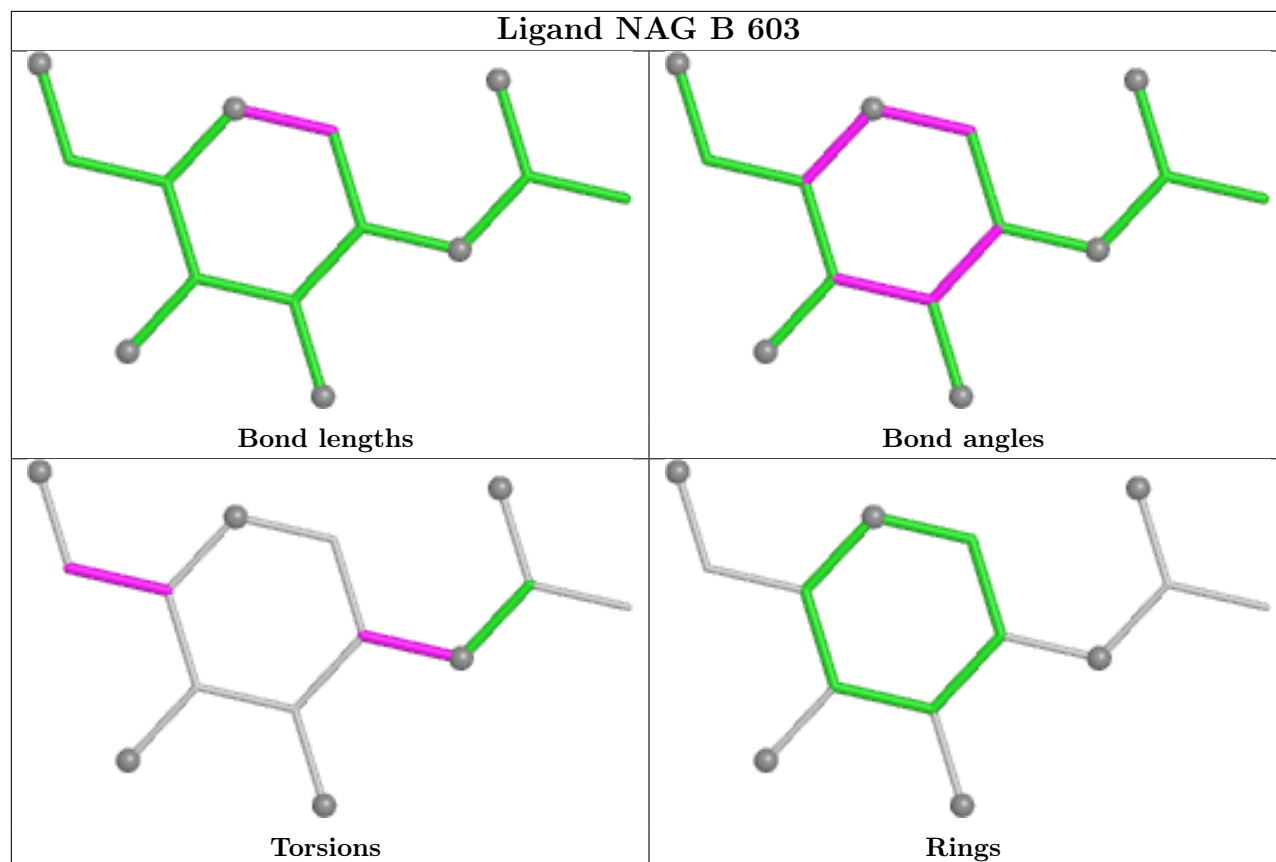
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

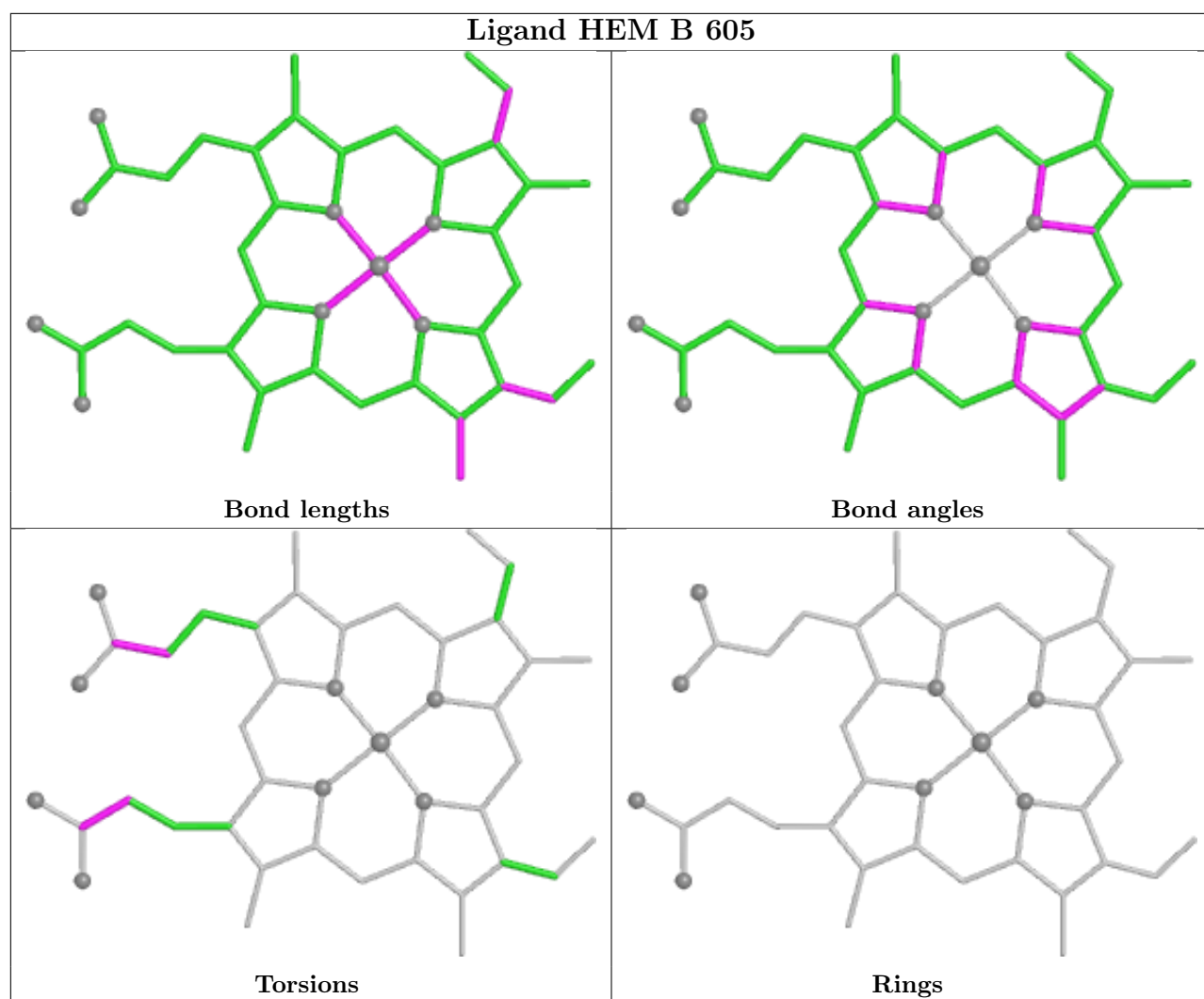


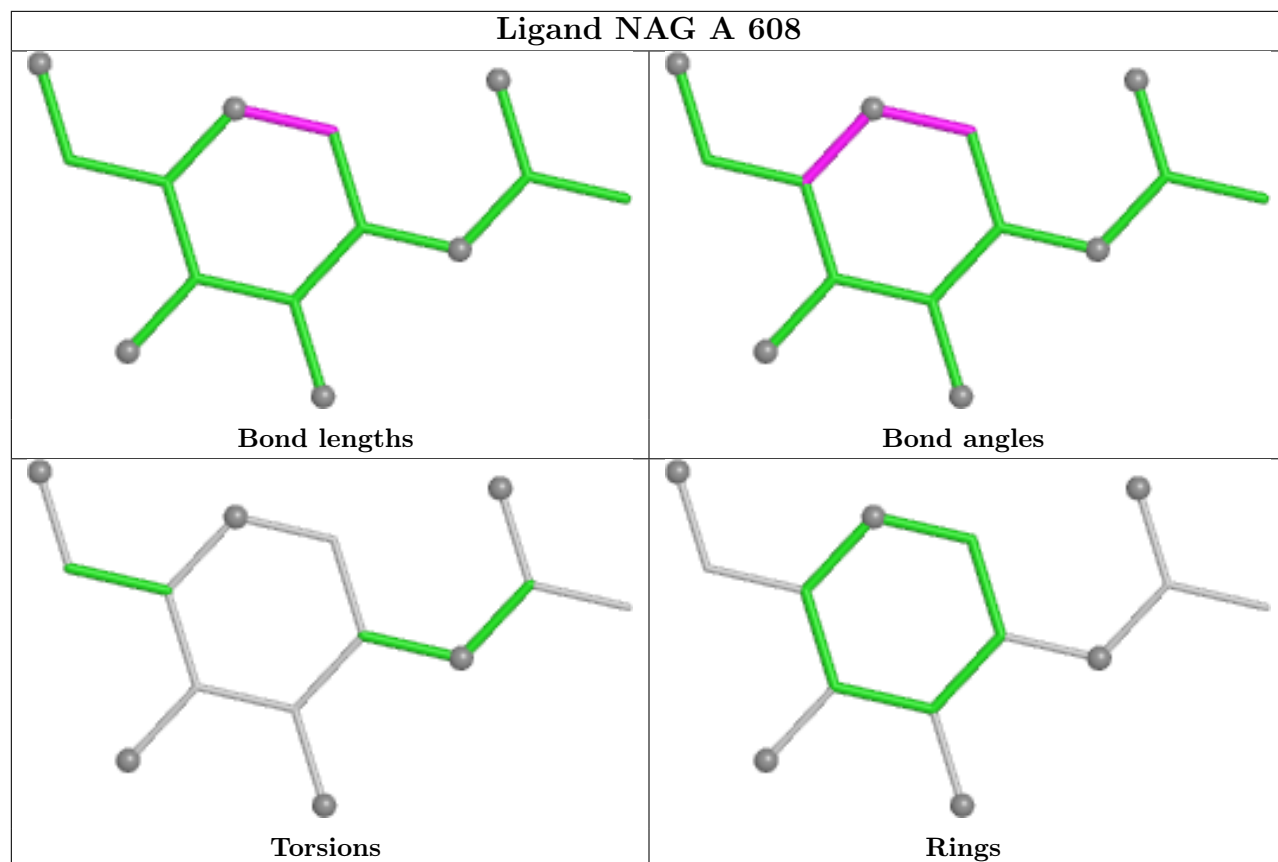


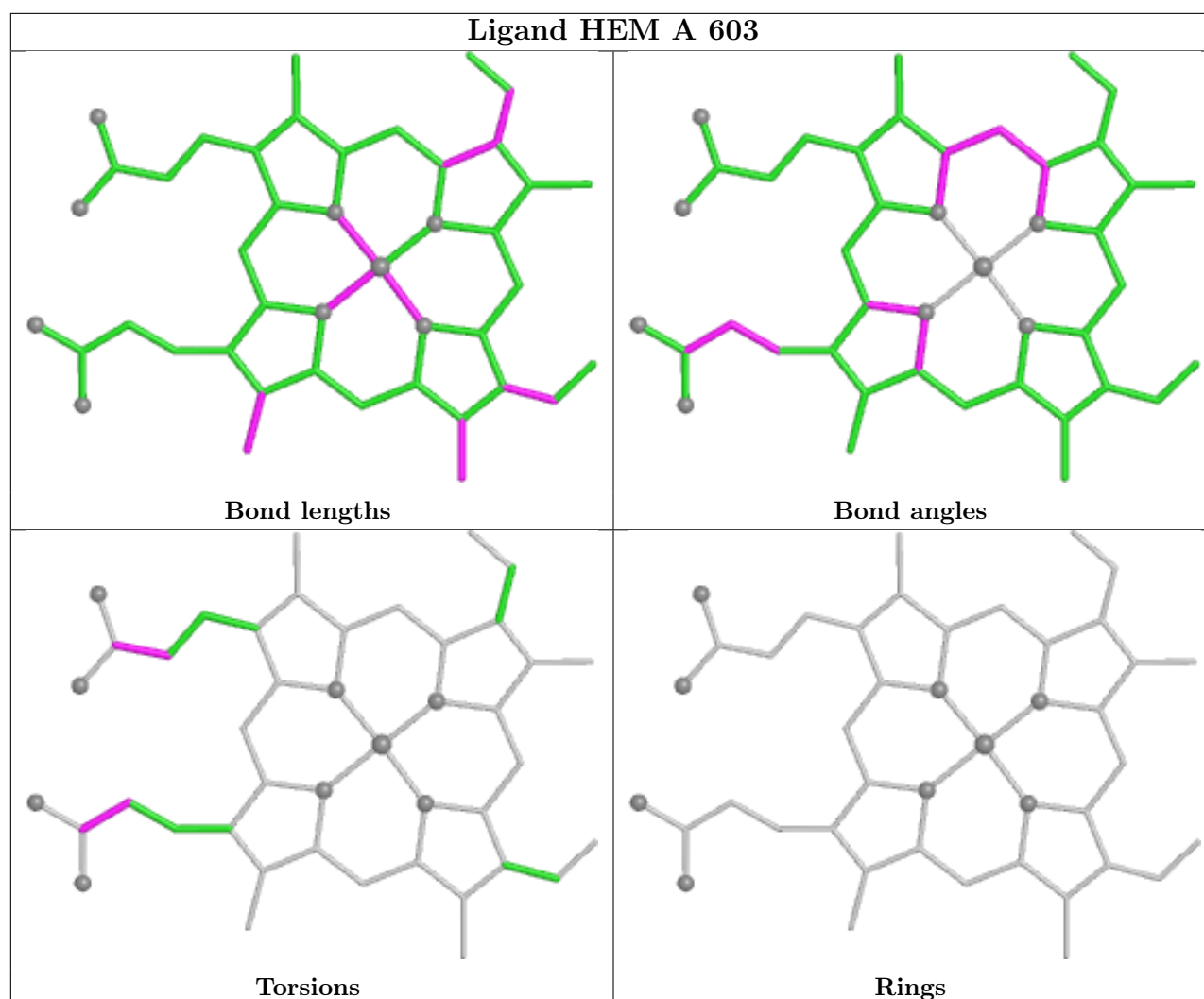












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-1.48	0 100 100	13, 25, 74, 135	0
1	B	595/595 (100%)	-1.49	0 100 100	15, 30, 65, 136	2 (0%)
All	All	1190/1190 (100%)	-1.49	0 100 100	13, 27, 69, 136	2 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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.

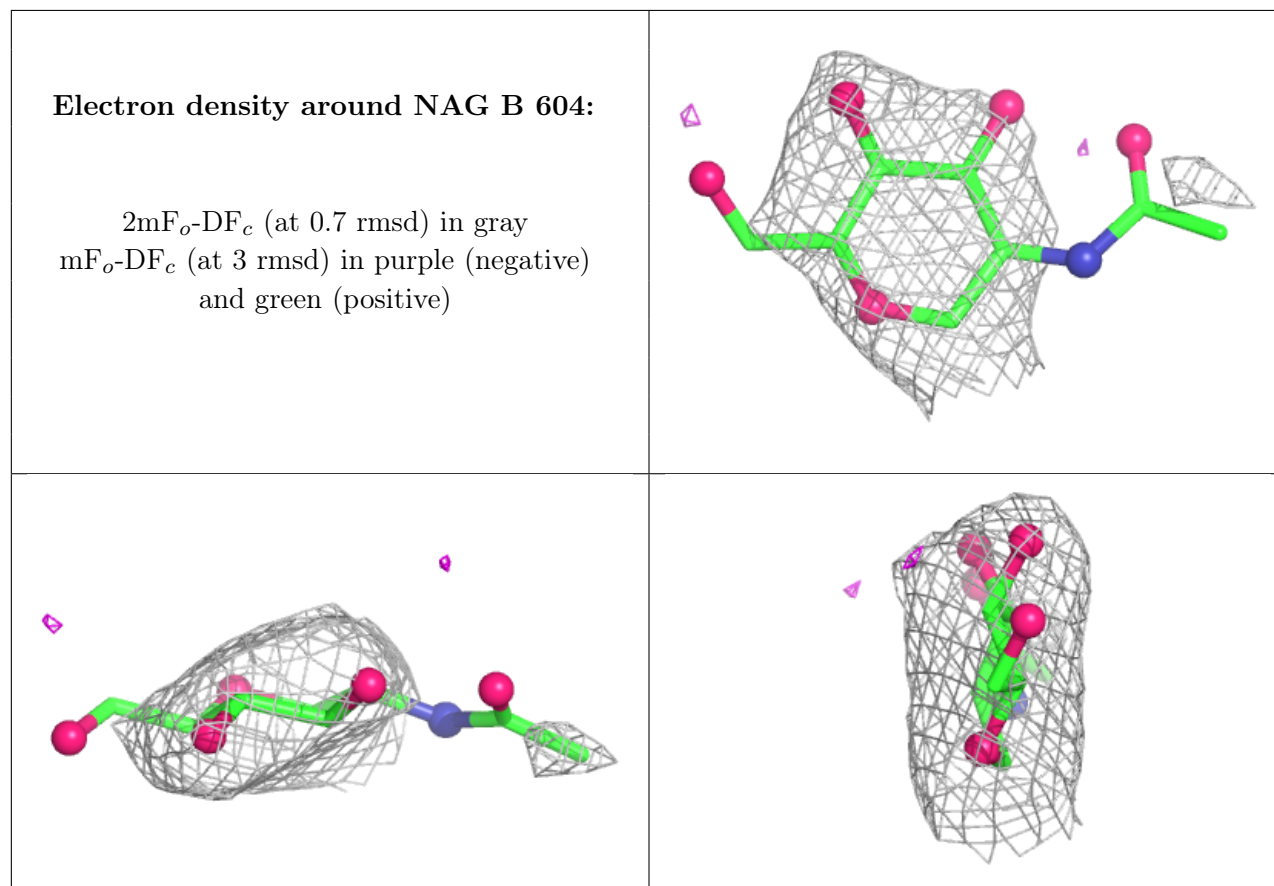
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	604	14/15	0.98	0.06	40,52,61,66	0
2	NAG	A	602	14/15	0.99	0.04	32,41,49,52	0
2	NAG	A	607	14/15	0.99	0.04	25,30,36,40	0
2	NAG	A	608	14/15	0.99	0.03	27,33,38,40	0
2	NAG	B	601	14/15	0.99	0.04	40,44,49,51	0
2	NAG	B	602	14/15	0.99	0.03	29,34,43,49	0
2	NAG	B	603	14/15	0.99	0.04	34,43,55,58	0

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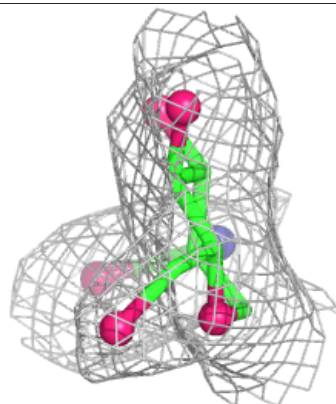
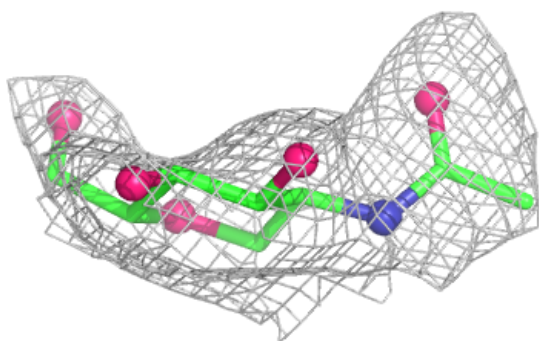
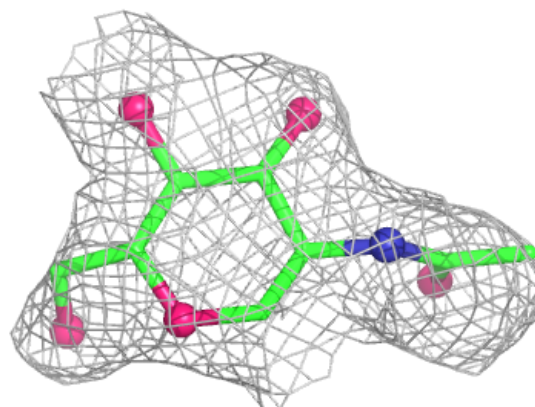
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	601	14/15	0.99	0.03	31,38,48,52	0
4	PEO	A	604	2/2	0.99	0.02	16,16,16,20	0
4	PEO	B	606	2/2	0.99	0.03	20,20,20,31	0
6	CL	B	608	1/1	0.99	0.06	46,46,46,46	0
3	HEM	B	605	43/43	1.00	0.03	11,16,21,31	0
5	CA	A	605	1/1	1.00	0.00	18,18,18,18	0
5	CA	B	607	1/1	1.00	0.01	32,32,32,32	0
6	CL	A	606	1/1	1.00	0.02	34,34,34,34	0
3	HEM	A	603	43/43	1.00	0.02	12,16,22,24	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.

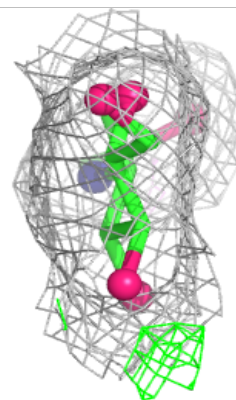
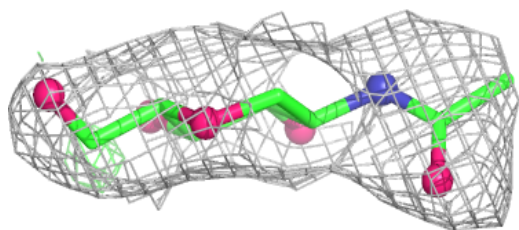
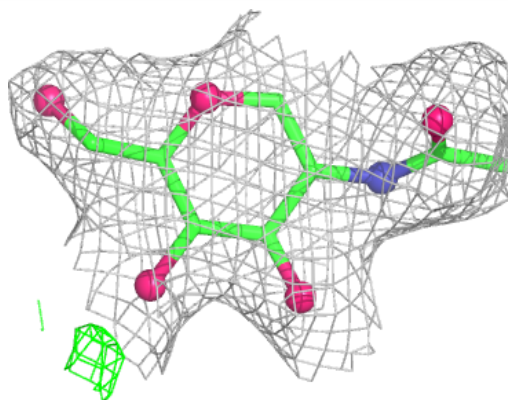


Electron density around NAG A 602:

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

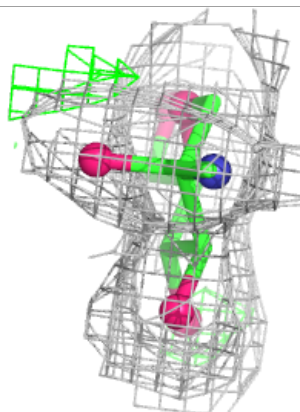
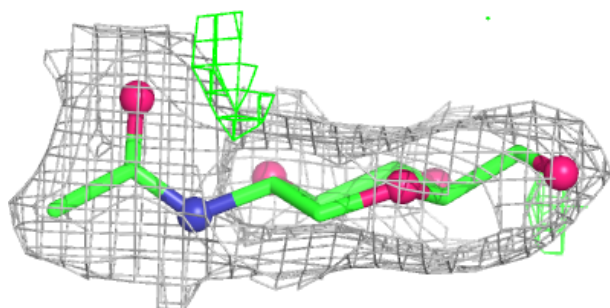
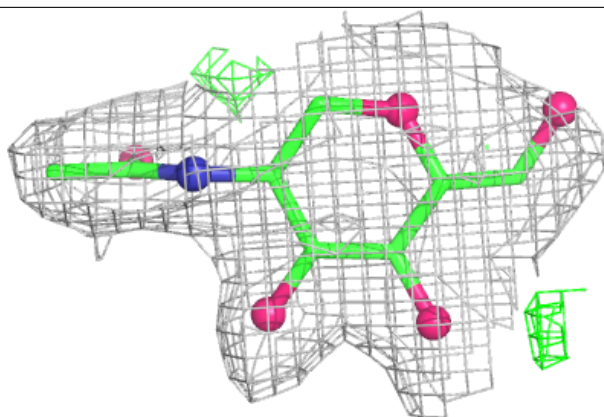
**Electron density around NAG A 607:**

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

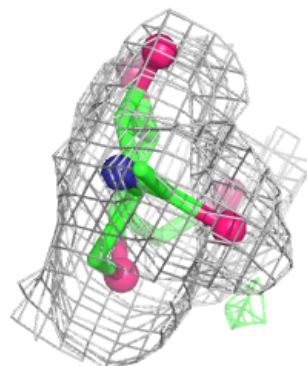
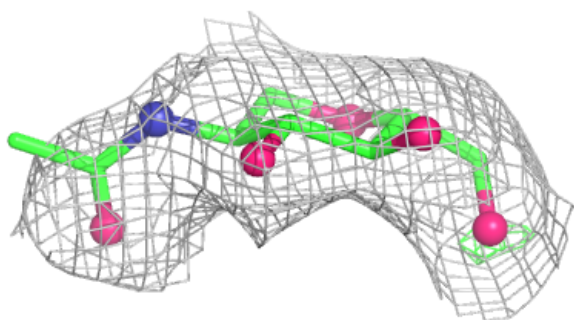
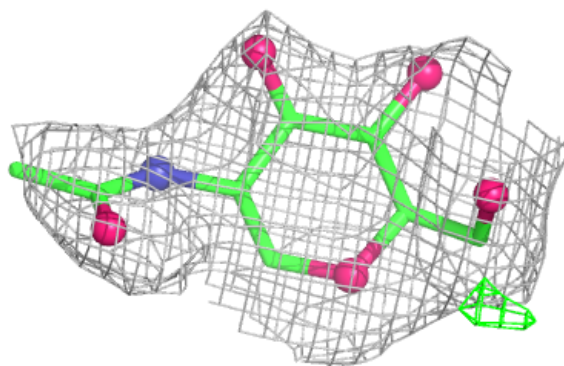


Electron density around NAG A 608:

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

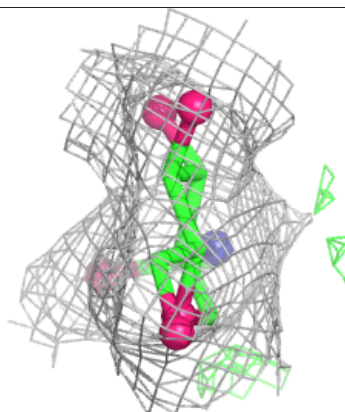
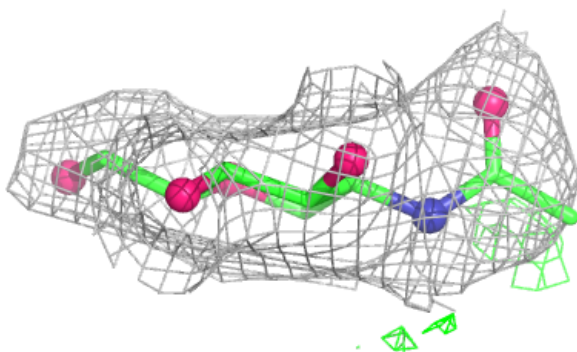
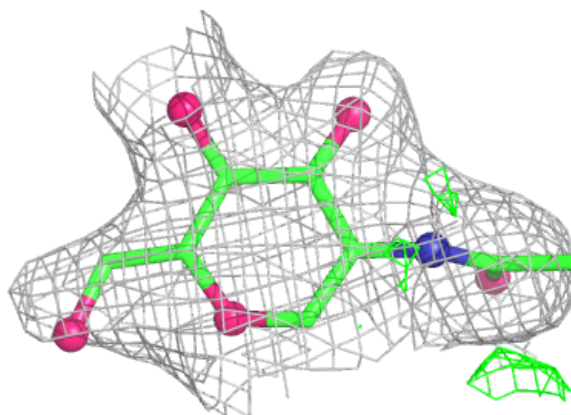
**Electron density around NAG B 601:**

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

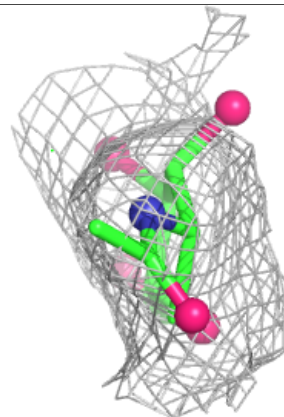
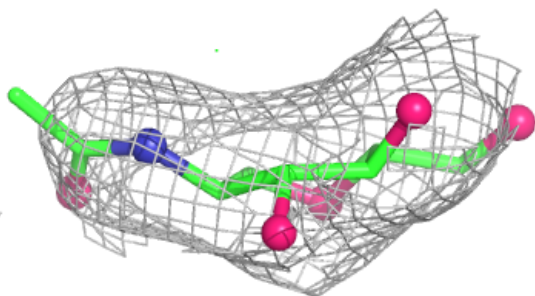
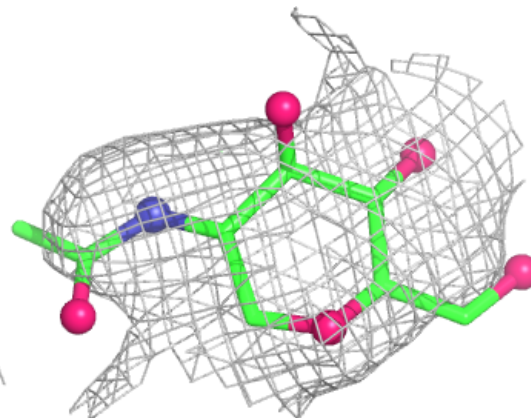


Electron density around NAG B 602:

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

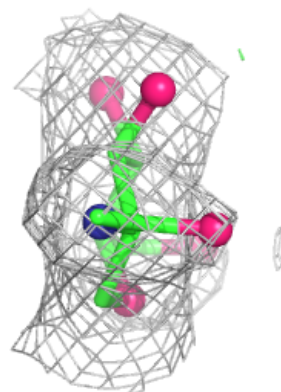
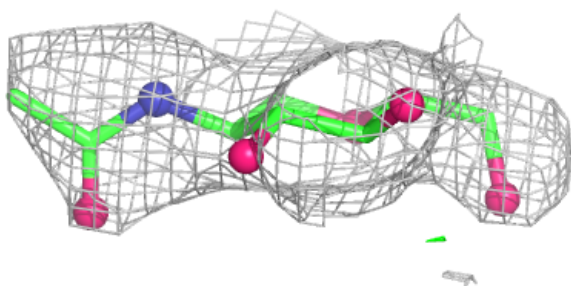
**Electron density around NAG B 603:**

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



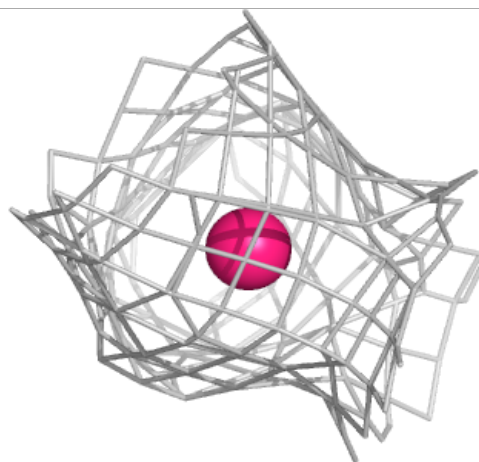
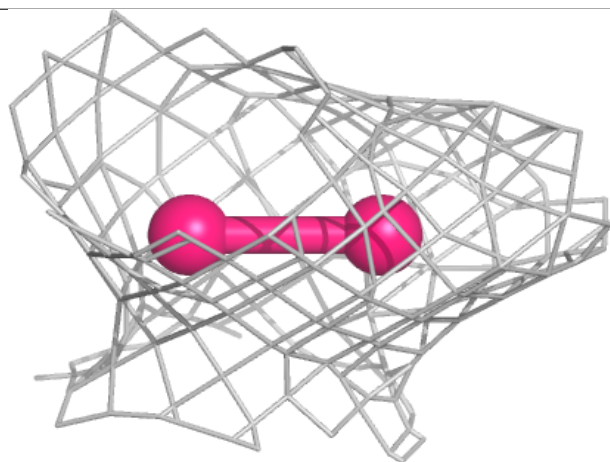
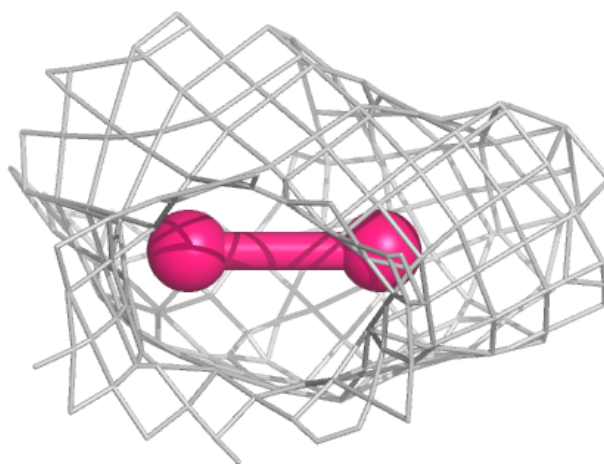
Electron density around NAG A 601:

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



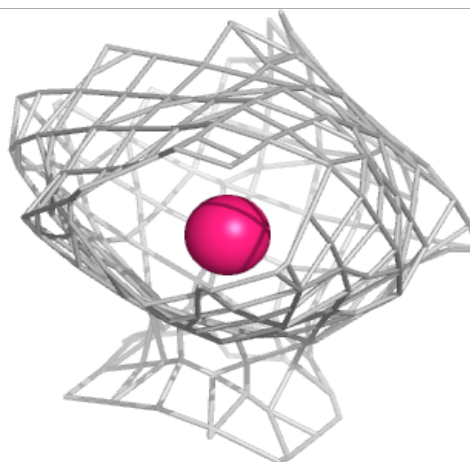
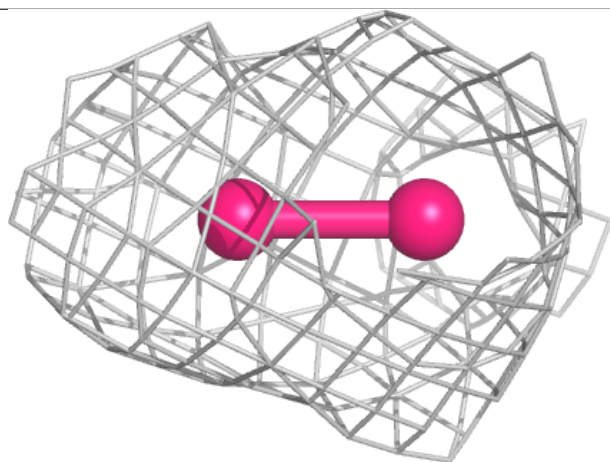
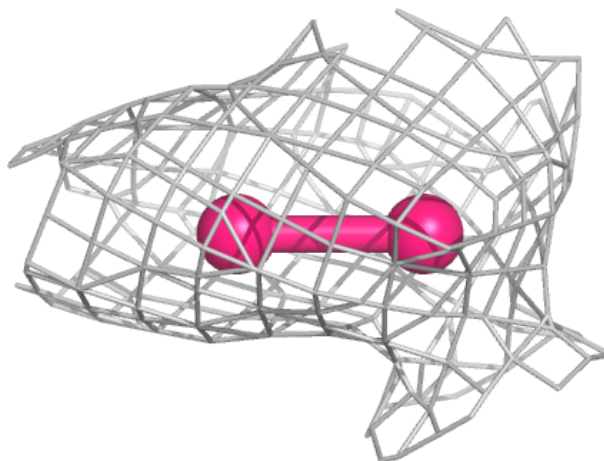
Electron density around PEO A 604:

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



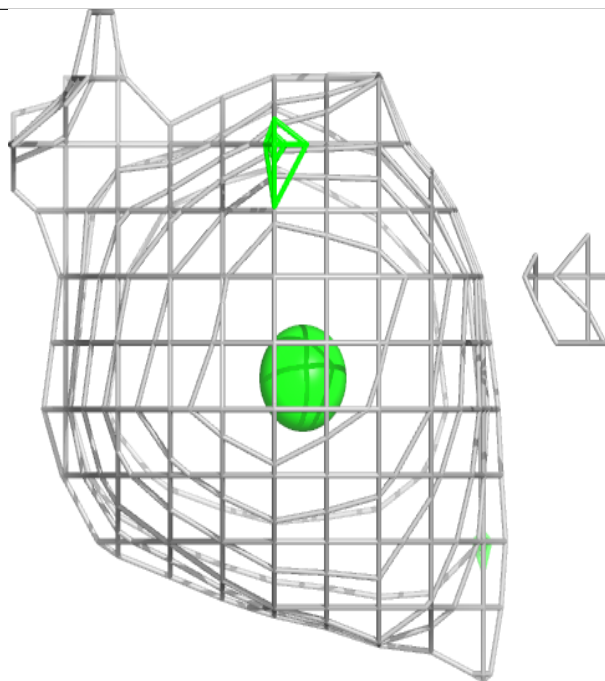
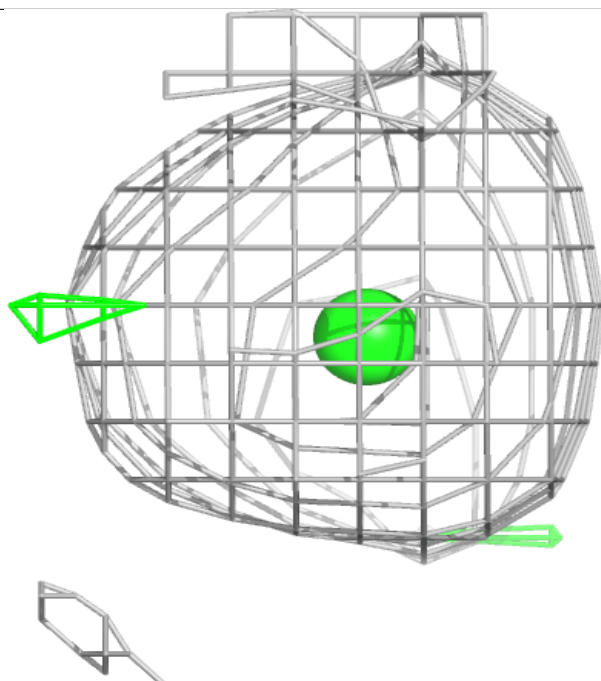
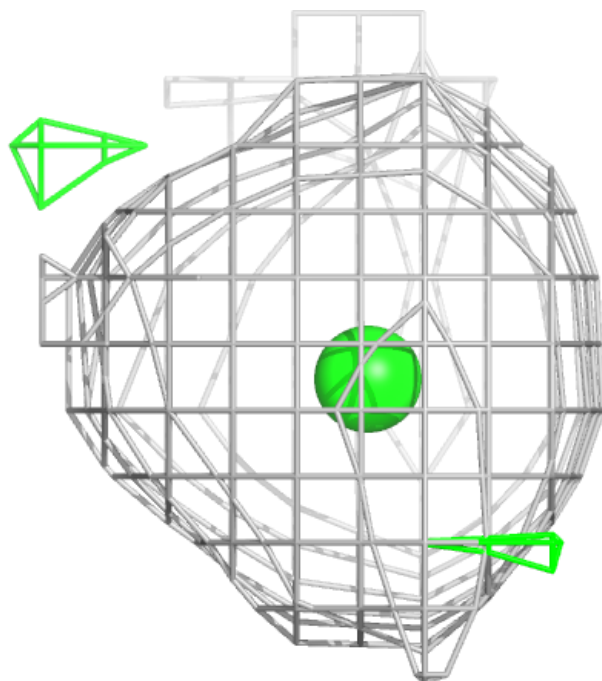
Electron density around PEO B 606:

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



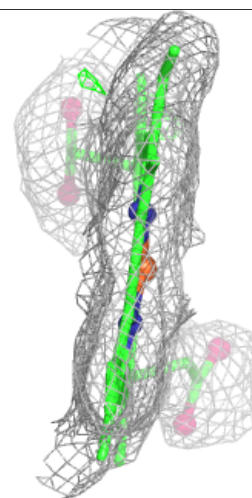
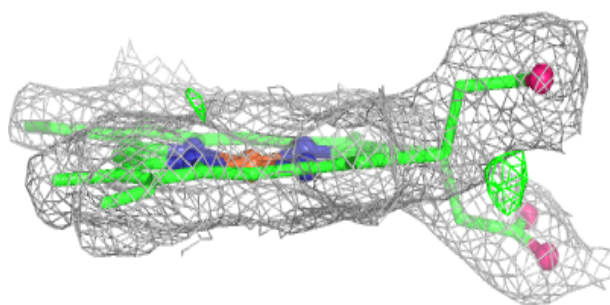
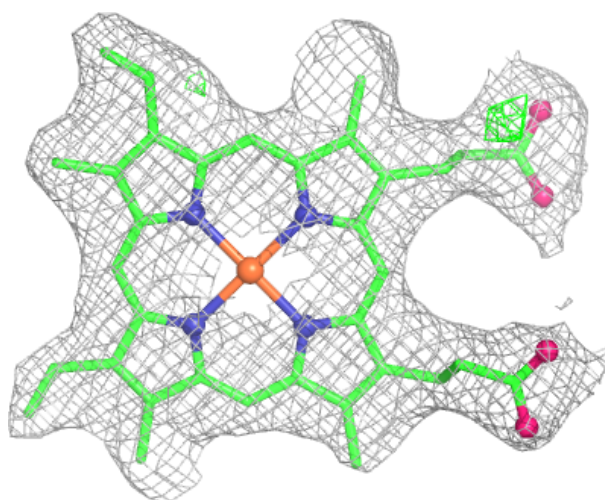
Electron density around CL B 608:

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



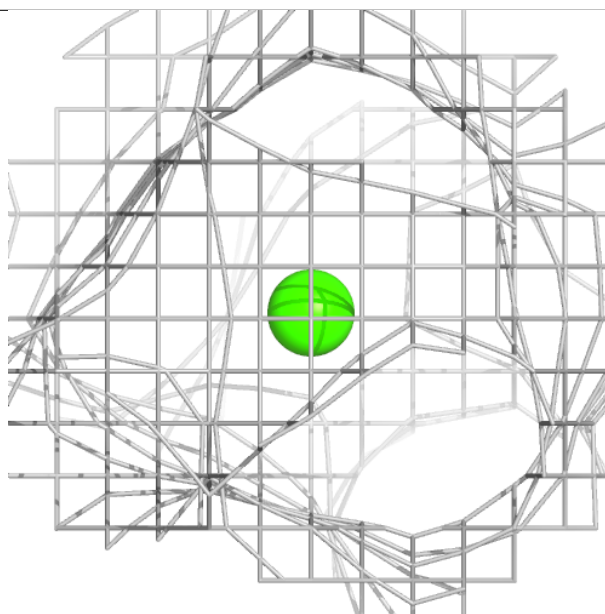
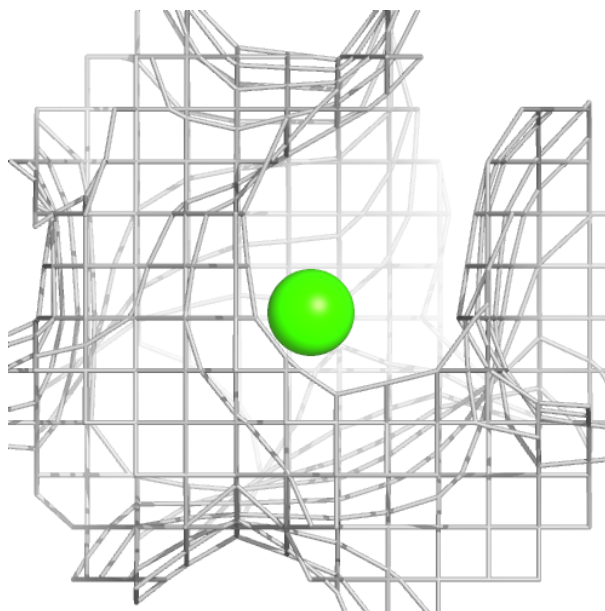
Electron density around HEM B 605:

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



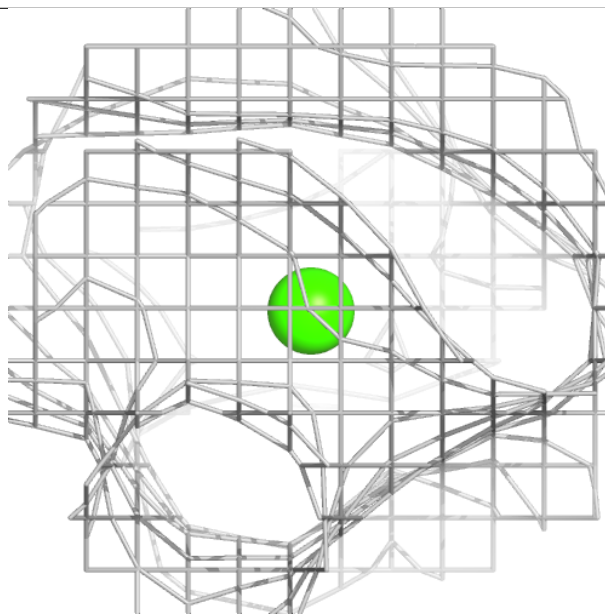
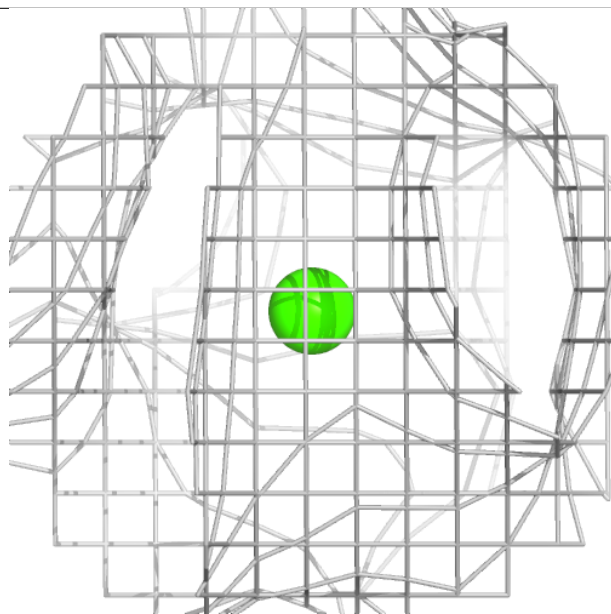
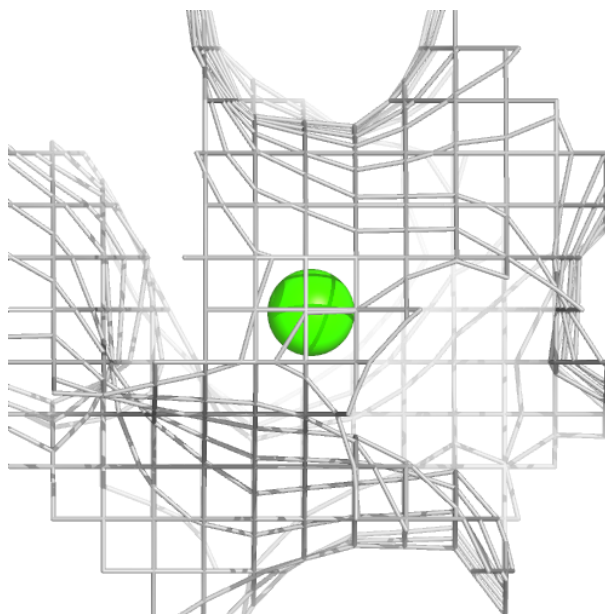
Electron density around CA A 605:

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



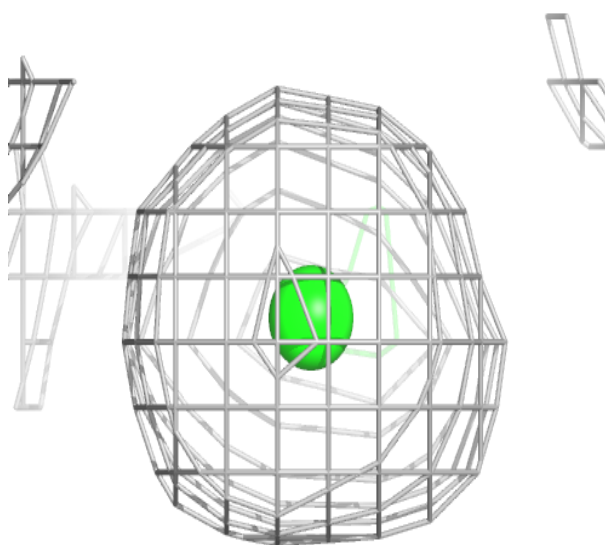
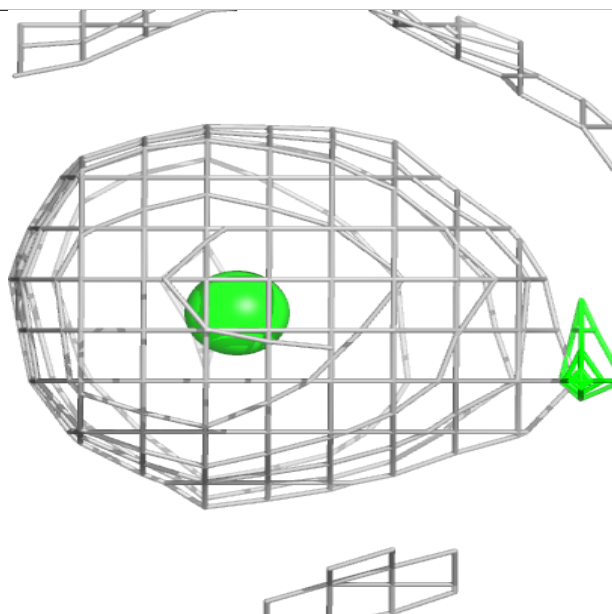
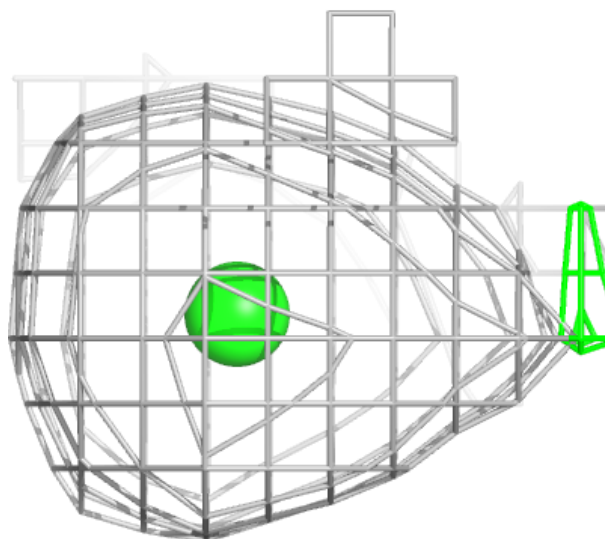
Electron density around CA B 607:

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



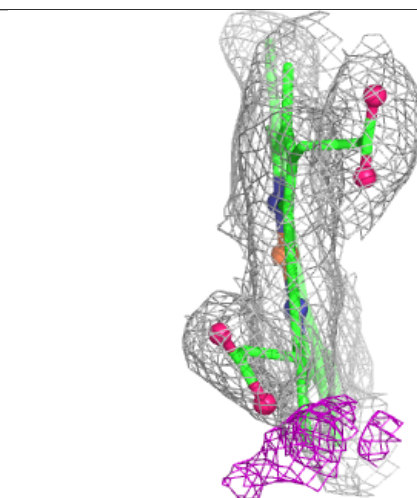
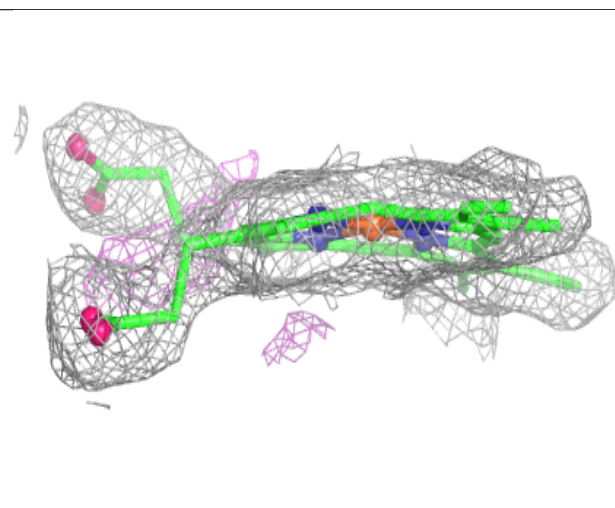
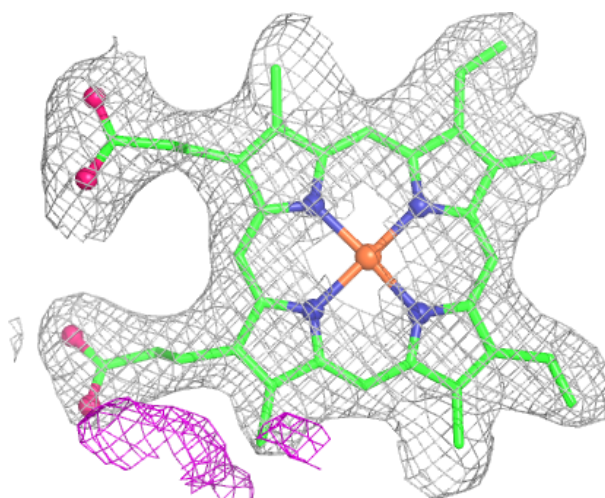
Electron density around CL A 606:

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.