



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 07:32 PM BST

PDB ID : 6LQW
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

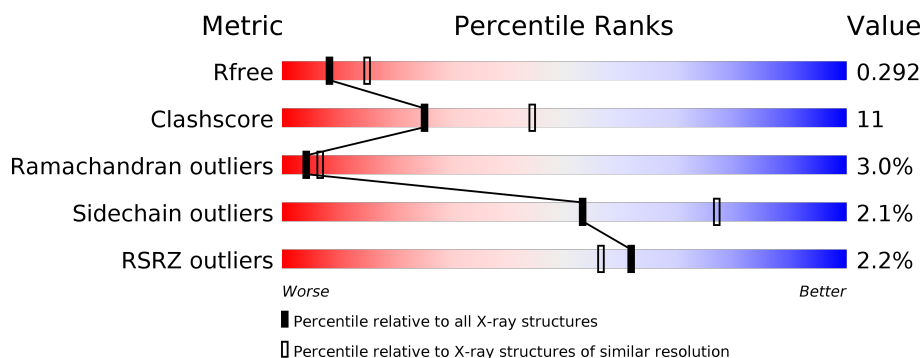
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	595	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>.</div> </div> </div>
1	B	595	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>.</div> </div> </div>

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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by author).



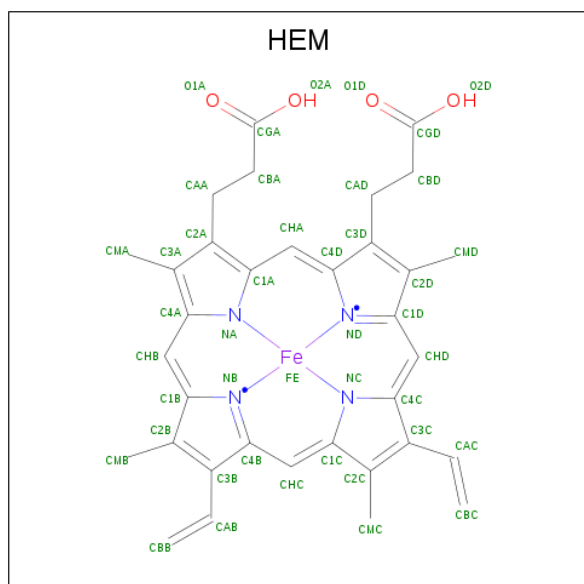
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

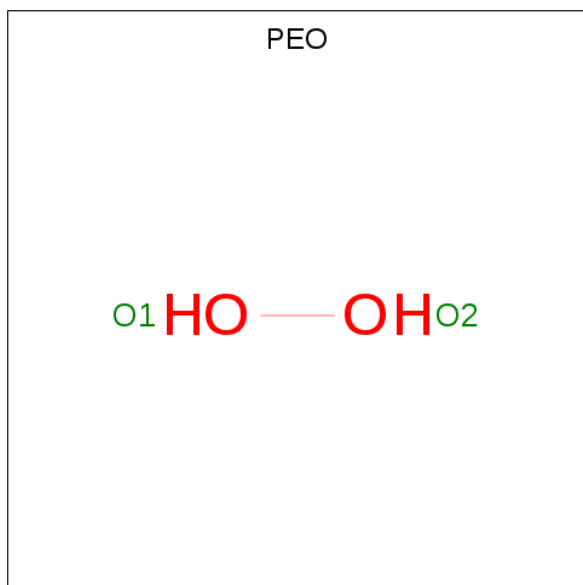
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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





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 (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by author).

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

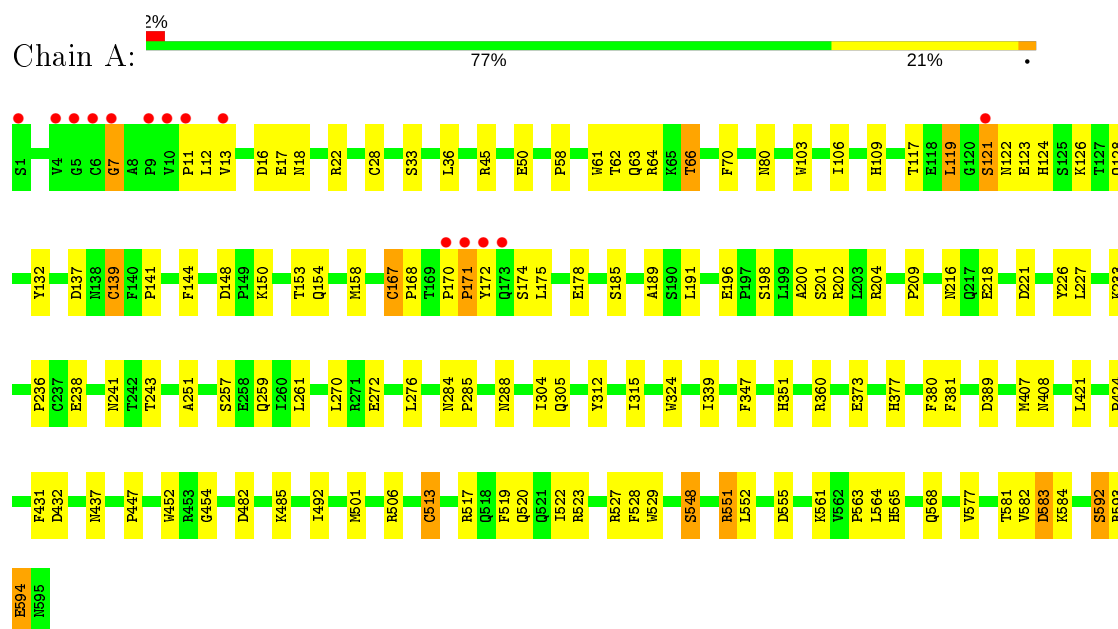
- Molecule 7 is water.

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

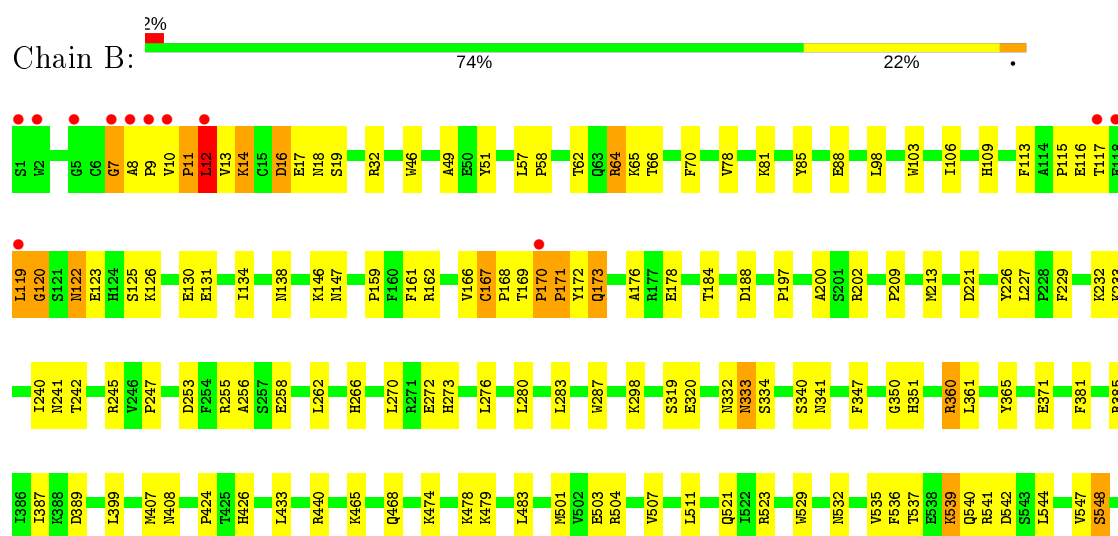
3 Residue-property plots [i](#)

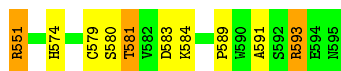
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lactoperoxidase



• Molecule 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 58.24 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.64-2.60) 98.3 (58.24-2.60)	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 (2.65%)	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)	0.33 , 25.9	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	0.92	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, CA, PEO, NAG, CL

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	0.45	0/4898	0.64	0/6645
1	B	0.46	1/4913 (0.0%)	0.61	1/6665 (0.0%)
All	All	0.45	1/9811 (0.0%)	0.62	1/13310 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	579	CYS	CB-SG	5.02	1.90	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	VAL	C-N-CA	5.08	134.39	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	LEU	Peptide

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Mol	Chain	Res	Type	Group
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	101	1
1	B	4779	0	4699	111	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	5	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	206	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 (206) 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
3:B:605:HEM:HMB1	3:B:605:HEM:HBB2	1.65	0.78
1:B:503[B]:GLU:HG2	1:B:504:ARG:HG3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:HBC2	3:B:605:HEM:HMC2	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: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:280:LEU:HD22	1:B:287:TRP:HZ3	1.66	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:A:288:ASN:HB2	1:B:12:LEU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LYS:NZ	1:A:238:GLU:OE1	2.38	0.57
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: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:B:32:ARG:HH21	1:B:333:ASN:CG	2.08	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:128:GLN:HG2	1:A:132:TYR:HE1	1.71	0.56
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:B:226:TYR:CE2	1:B:387:ILE:HG12	2.42	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:B:16:ASP:C	1:B:18:ASN:H	2.10	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:B:280:LEU:HD22	1:B:287:TRP:CZ3	2.44	0.52
1:B:253:ASP:CG	1:B:255:ARG:HH21	2.13	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: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
1:B:474:LYS:HD2	7:B:777:HOH:O	2.11	0.51
2:B:604:NAG:O3	2:B:604:NAG:O7	2.23	0.51
1:A:12:LEU:HD11	1:B:123:GLU:CD	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:PRO:HA	7:B:710:HOH:O	2.10	0.51
1:A:236:PRO:HG3	1:A:424:PRO:HB3	1.93	0.51
1:A:227:LEU:HD23	1:A:251:ALA:HB2	1.92	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:551:ARG:HE	1:A:555:ASP:CG	2.17	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:HMB2	3:A:603:HEM:HBB2	1.94	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
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:B:258:GLU:OE1	3:B:605:HEM:HMB3	2.15	0.47
1:A:12:LEU:HB2	1:B:119:LEU:C	2.35	0.47
1:A:50:GLU:HG3	1:A:447:PRO:HG3	1.97	0.46
1:B:539:LYS:NZ	1:B:542:ASP:OD1	2.33	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: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
1:B:12:LEU:HD23	1:B:14:LYS:N	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:167:CYS:HB3	1:A:168:PRO:CD	2.46	0.46
1:A:28:CYS:O	1:A:527:ARG:NH2	2.37	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:OE2	1:A:594:GLU:N	2.49	0.46
1:B:8:ALA:H	1:B:167:CYS:HA	1.81	0.45
3:B:605:HEM:CMC	3:B:605:HEM:HBC2	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:TYR:OH	1:B:88:GLU:OE1	2.29	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:HA	1:B:270:LEU:HD12	1.87	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: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:CMB	3:A:603:HEM:HBB2	2.50	0.41
1:A:158:MET:HE1	1:A:432:ASP:H	1.86	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:523:ARG:HG3	1:A:529:TRP:CE2	2.55	0.41
1:A:13:VAL:HA	1:B:119:LEU:HG	2.02	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: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:B:407:MET:HB3	1:B:501:MET:CE	2.51	0.41
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.93	0.41
1:A:285:PRO:HD2	1:A:593:ARG:HH11	1.86	0.41
1:A:12:LEU:H	1:B:119:LEU:HD23	1.85	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

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	593/595 (100%)	529 (89%)	49 (8%)	15 (2%)	5	9
1	B	595/595 (100%)	529 (89%)	45 (8%)	21 (4%)	3	5
All	All	1188/1190 (100%)	1058 (89%)	94 (8%)	36 (3%)	4	7

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
1	B	171	PRO
1	A	66	THR
1	A	137	ASP
1	A	174	SER
1	A	209	PRO

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Mol	Chain	Res	Type
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%)	508 (98%)	10 (2%)	57	79
1	B	520/518 (100%)	508 (98%)	12 (2%)	50	75
All	All	1038/1036 (100%)	1016 (98%)	22 (2%)	53	77

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	CYS
1	A	202	ARG
1	A	270	LEU
1	A	347	PHE
1	A	360	ARG
1	A	389	ASP
1	A	513	CYS
1	A	548	SER
1	A	551	ARG
1	A	592	SER
1	B	12	LEU
1	B	131	GLU

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Mol	Chain	Res	Type
1	B	173	GLN
1	B	333	ASN
1	B	341	ASN
1	B	347	PHE
1	B	360	ARG
1	B	539	LYS
1	B	548	SER
1	B	551	ARG
1	B	574	HIS
1	B	593	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	B	18	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 monosaccharides 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	$\# Z > 2$
3	HEM	B	605	1	27,50,50	1.81	4 (14%)	17,82,82	1.30	1 (5%)
4	PEO	B	606	-	1,1,1	0.07	0	-		
2	NAG	B	601	1	14,14,15	0.54	0	17,19,21	1.03	1 (5%)
2	NAG	A	608	1	14,14,15	0.99	1 (7%)	17,19,21	1.22	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%)
2	NAG	A	601	1	14,14,15	0.40	0	17,19,21	0.52	0
3	HEM	A	603	1,4	27,50,50	1.87	7 (25%)	17,82,82	1.75	4 (23%)
2	NAG	B	603	1	14,14,15	1.22	1 (7%)	17,19,21	1.33	2 (11%)
2	NAG	A	607	1	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
4	PEO	A	604	3	1,1,1	0.13	0	-		
2	NAG	B	604	1	14,14,15	0.69	1 (7%)	17,19,21	0.92	2 (11%)

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	HEM	C3C-C2C	-4.11	1.34	1.40
3	B	605	HEM	C3B-C2B	-4.09	1.34	1.40
3	B	605	HEM	C3C-C2C	-3.95	1.34	1.40

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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	C3B-C2B	-3.79	1.35	1.40
3	B	605	HEM	C3B-CAB	3.68	1.55	1.47
3	A	603	HEM	C3B-CAB	3.59	1.55	1.47
2	A	608	NAG	O5-C1	3.55	1.49	1.43
3	B	605	HEM	C3C-CAC	3.04	1.54	1.47
3	A	603	HEM	C3C-CAC	2.99	1.53	1.47
3	A	603	HEM	CAD-C3D	2.11	1.55	1.52
3	A	603	HEM	C1C-C2C	2.11	1.47	1.42
3	A	603	HEM	CAA-C2A	2.01	1.55	1.52
2	B	604	NAG	C1-C2	2.00	1.55	1.52

All (14) 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
3	A	603	HEM	CMD-C2D-C1D	-4.18	122.04	128.46
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
3	A	603	HEM	CMB-C2B-C3B	3.28	130.81	124.68
2	A	602	NAG	C1-O5-C5	3.04	116.31	112.19
3	A	603	HEM	CMD-C2D-C3D	2.71	130.05	124.94
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
2	B	602	NAG	C1-O5-C5	2.33	115.34	112.19
3	B	605	HEM	CBA-CAA-C2A	-2.30	108.24	112.49
3	A	603	HEM	CAA-CBA-CGA	-2.29	108.83	112.67
2	B	604	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (12) 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

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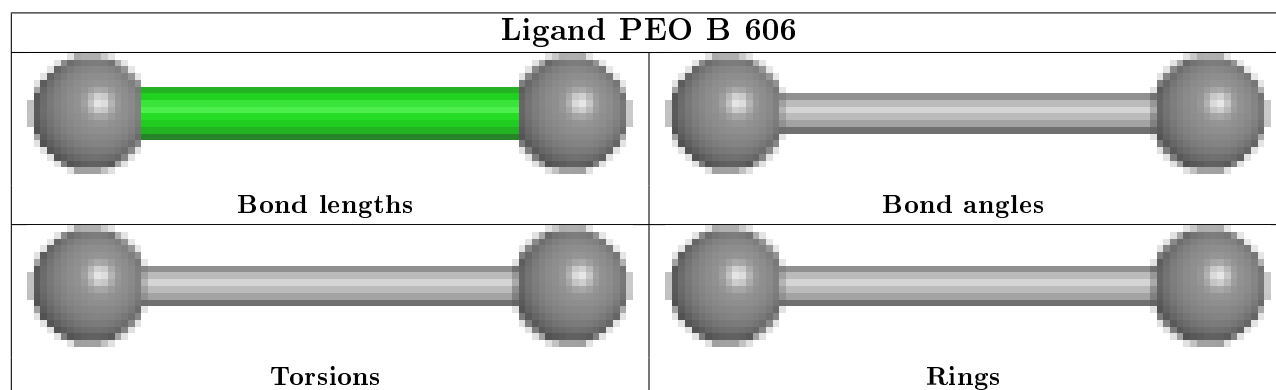
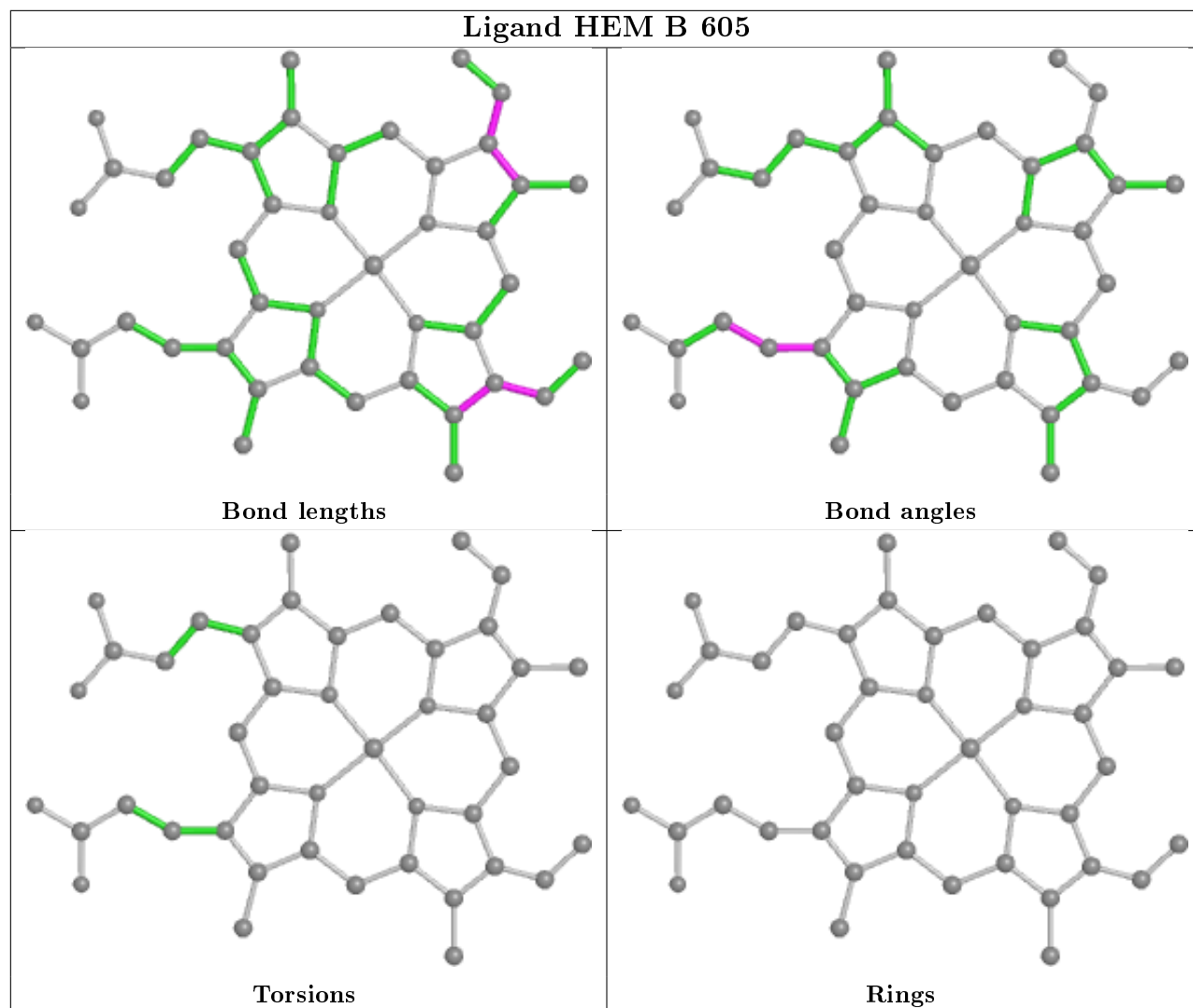
Mol	Chain	Res	Type	Atoms
2	B	604	NAG	C3-C2-N2-C7
2	A	607	NAG	C4-C5-C6-O6
2	B	603	NAG	C1-C2-N2-C7
2	A	607	NAG	O5-C5-C6-O6

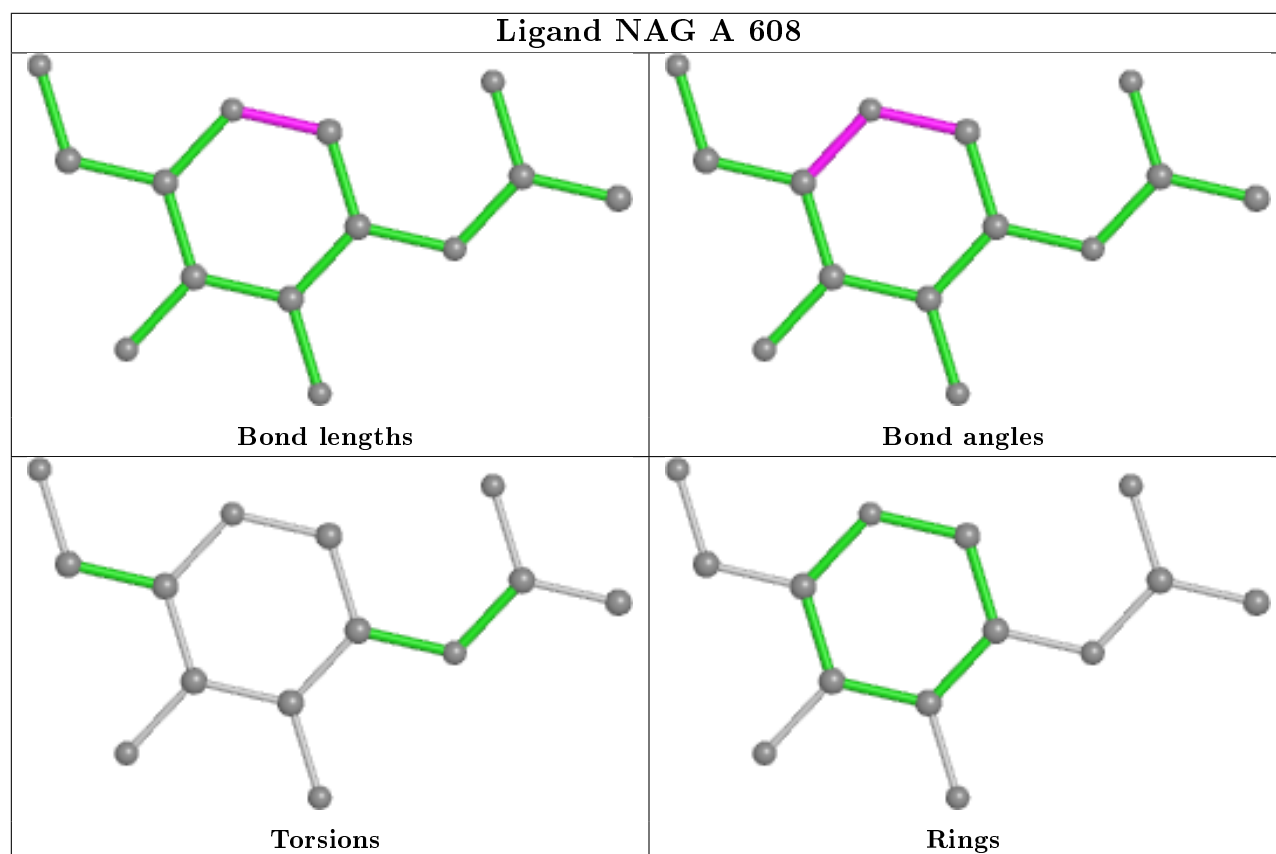
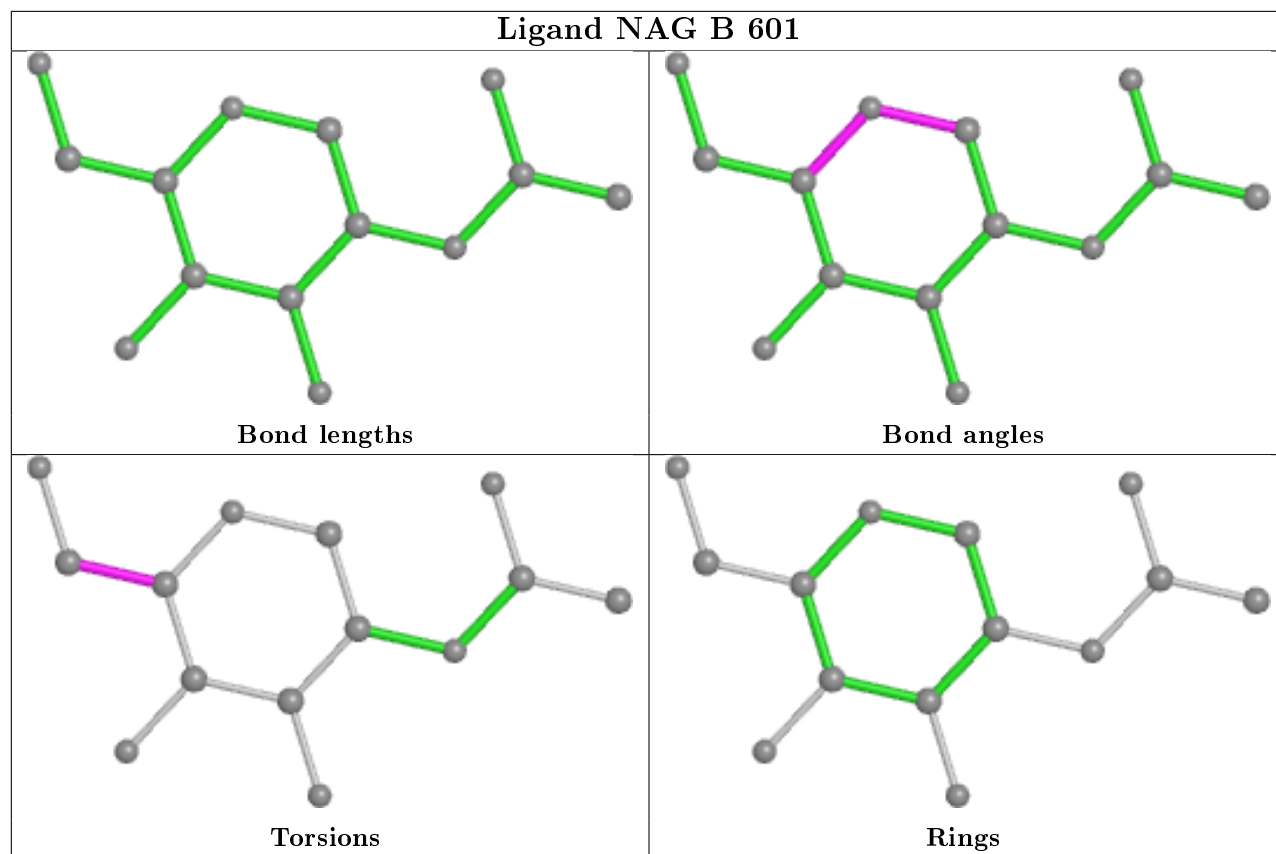
There are no ring outliers.

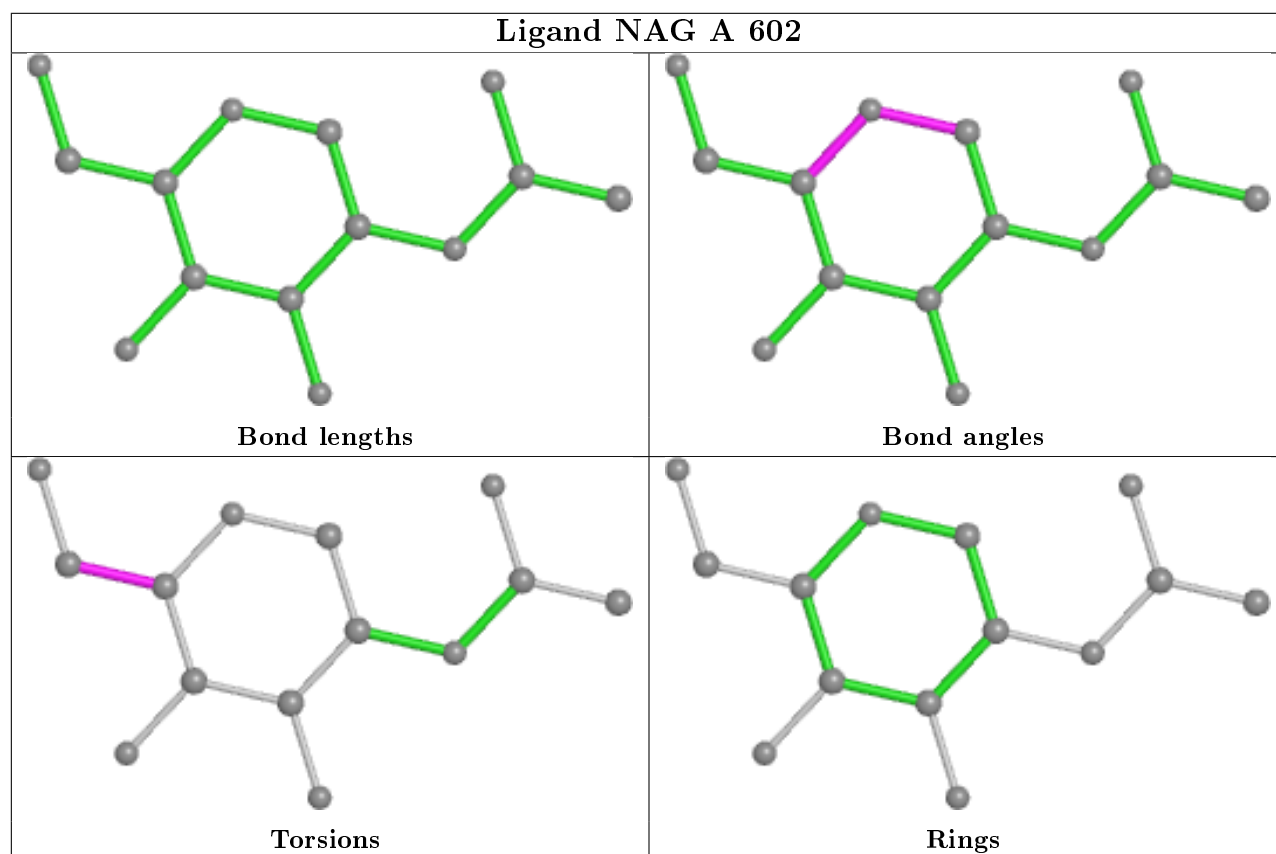
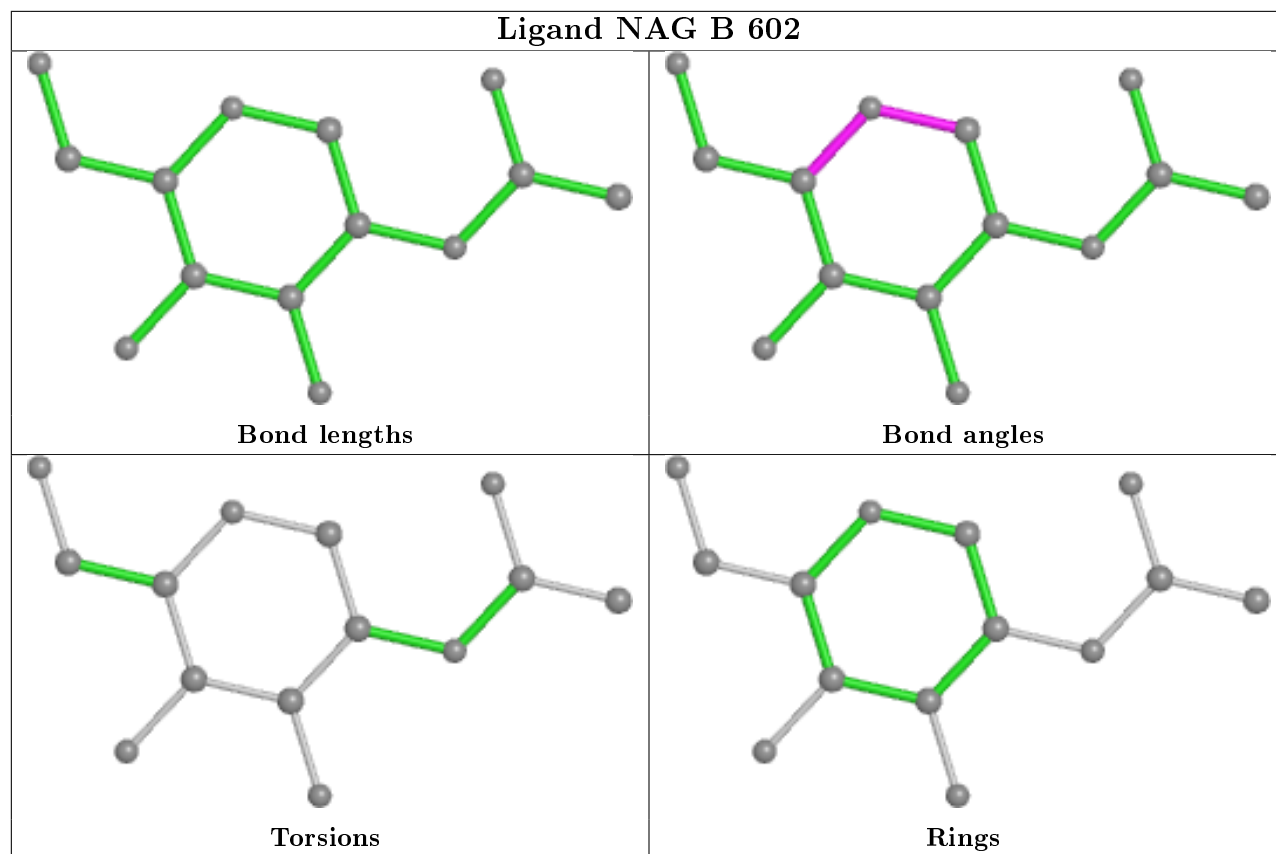
6 monomers are involved in 12 short contacts:

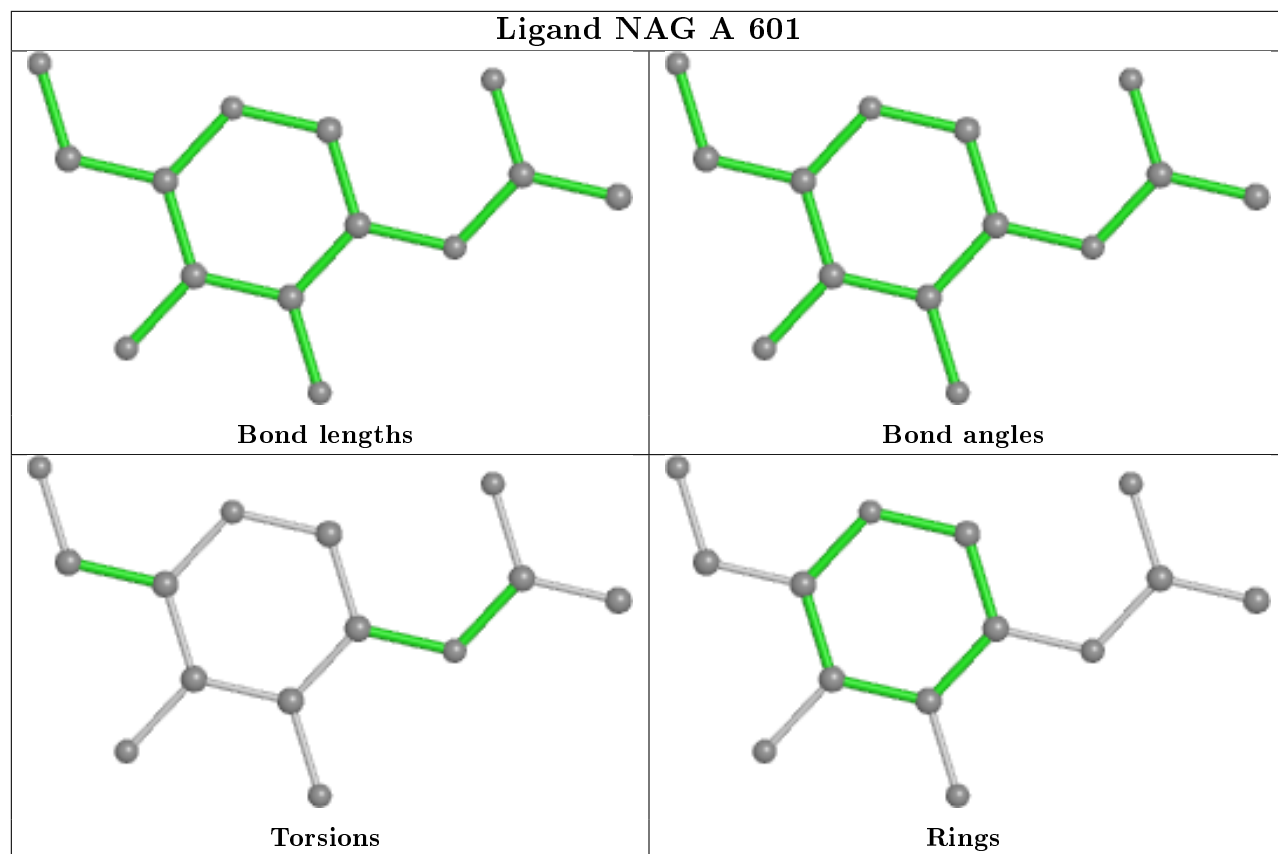
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	605	HEM	5	0
4	B	606	PEO	1	0
3	A	603	HEM	3	0
2	B	603	NAG	1	0
4	A	604	PEO	1	0
2	B	604	NAG	1	0

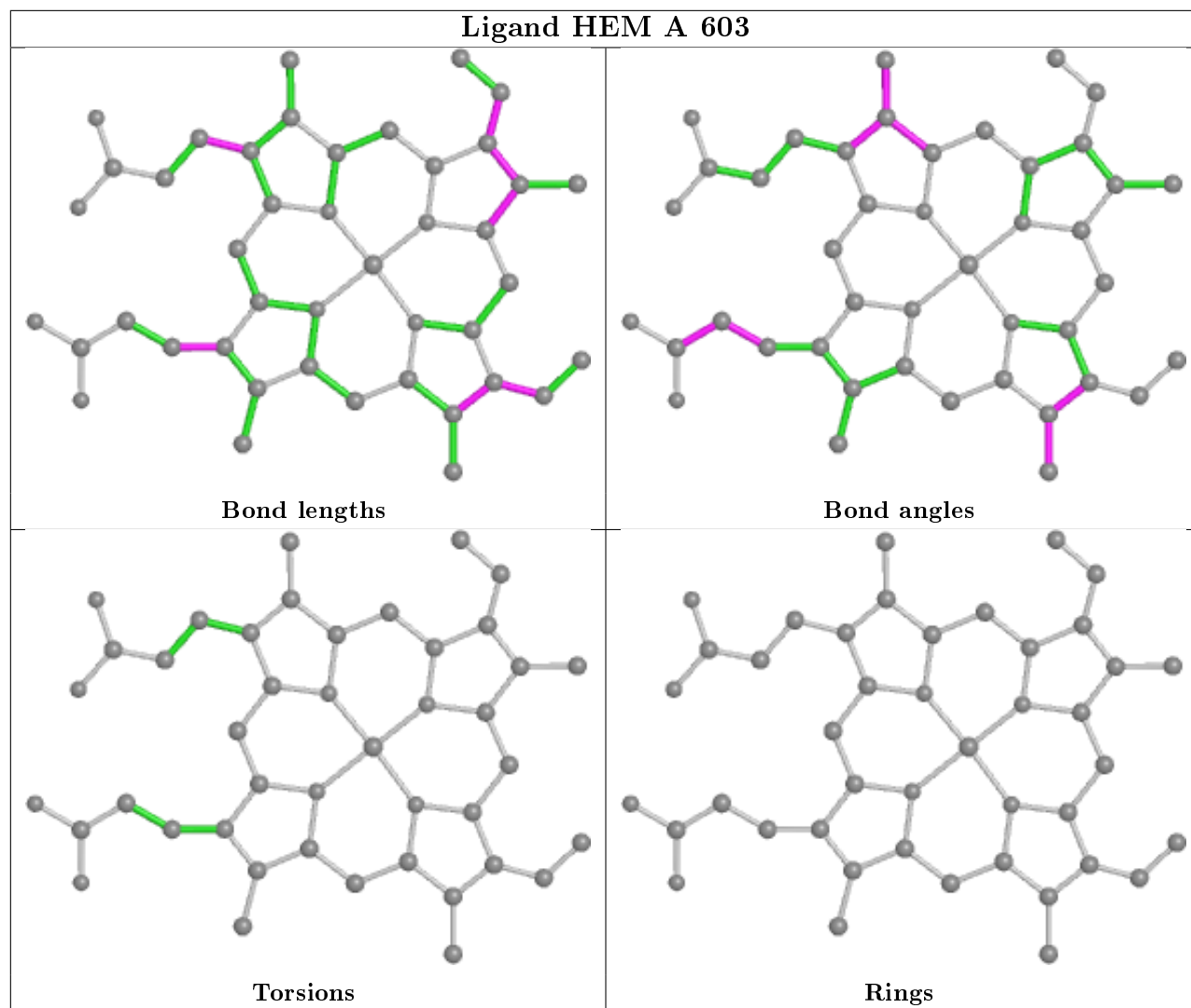
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

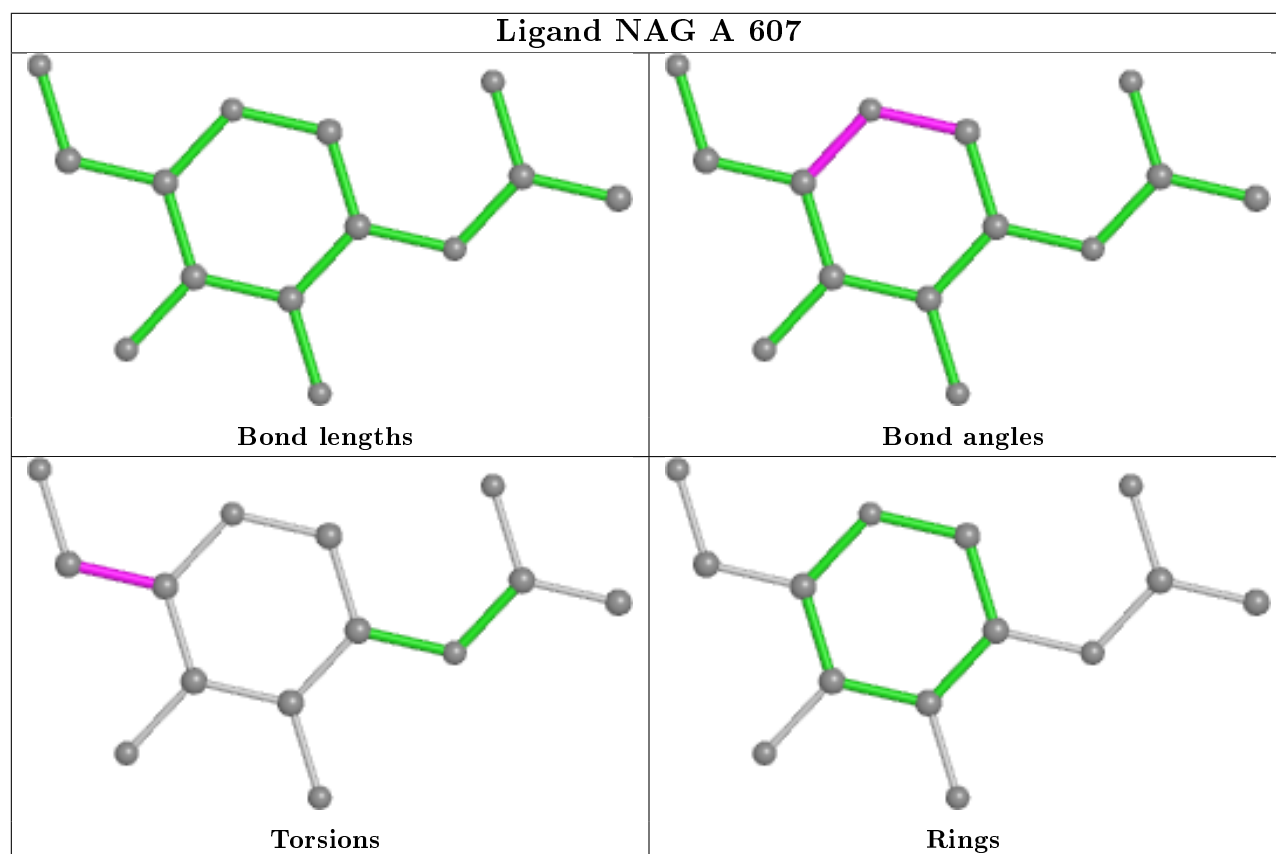
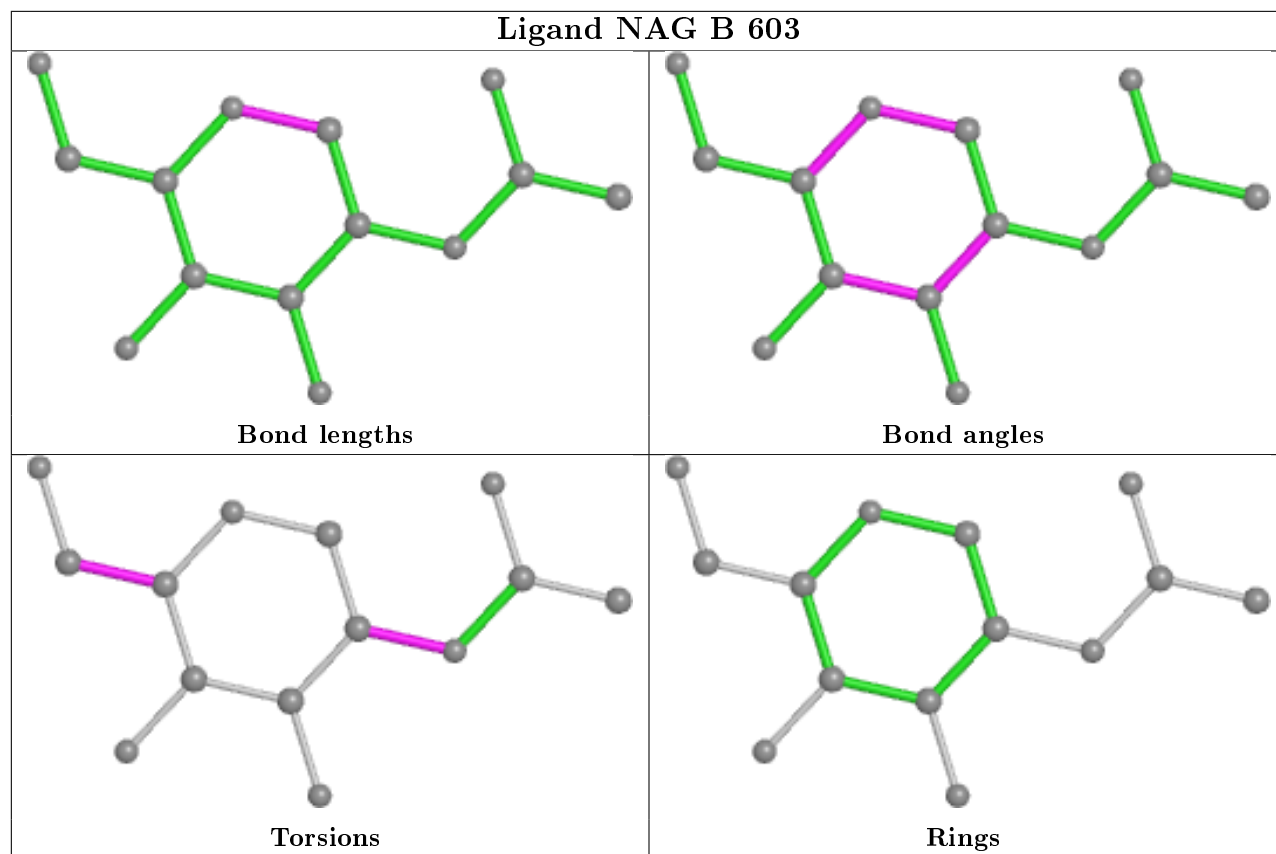


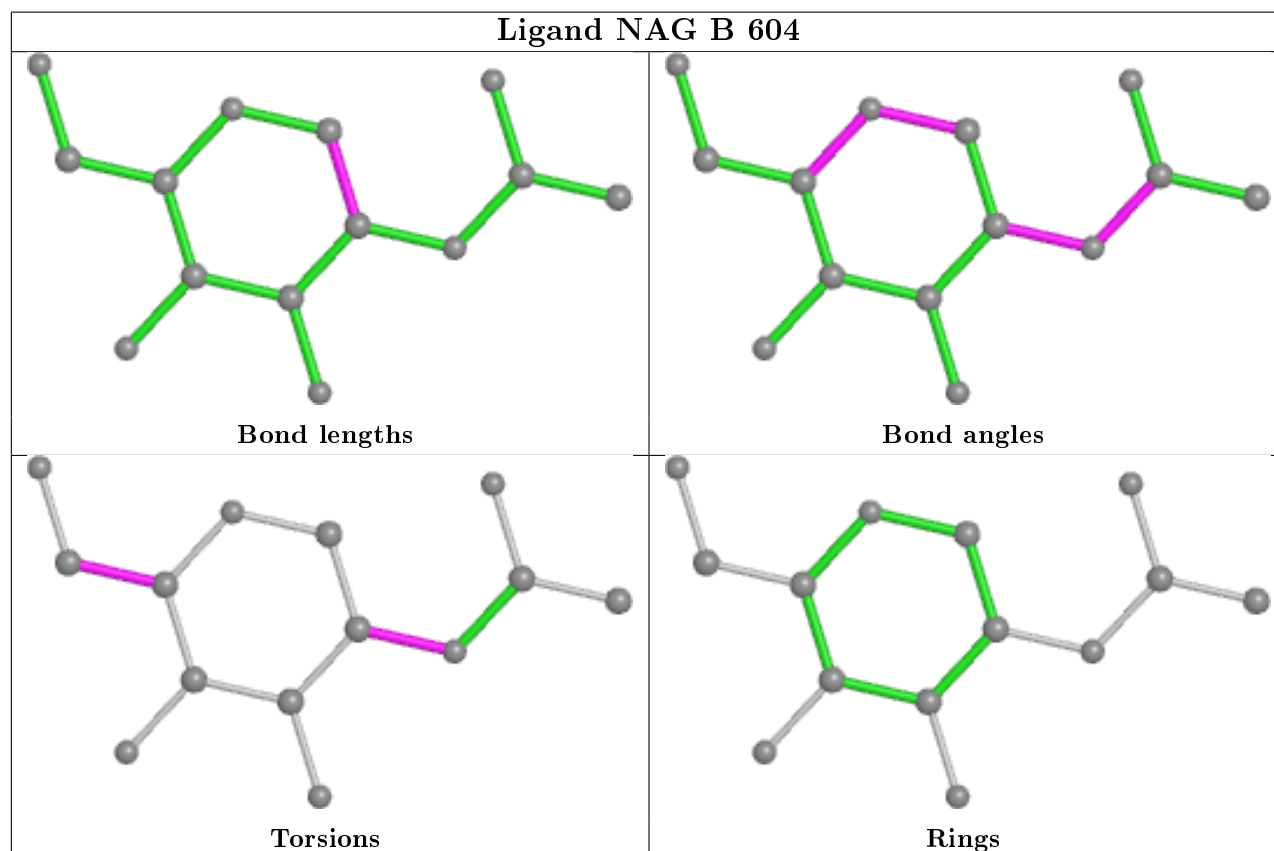
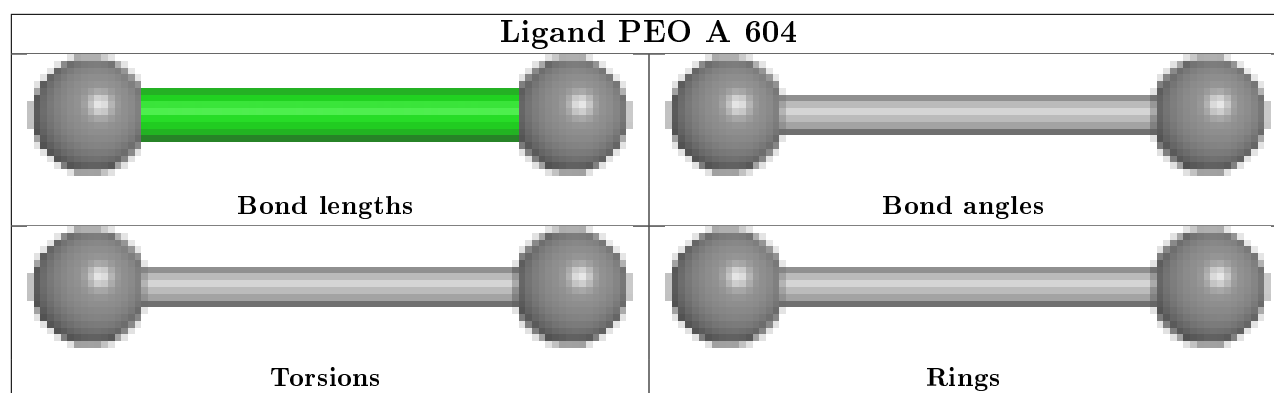












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	595/595 (100%)	-0.59	14 (2%) 59 53	13, 25, 74, 135	0
1	B	595/595 (100%)	-0.55	12 (2%) 65 60	15, 30, 65, 136	0
All	All	1190/1190 (100%)	-0.57	26 (2%) 62 56	13, 27, 69, 136	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	SER	8.9
1	A	6	CYS	7.2
1	B	2	TRP	6.7
1	A	7	GLY	6.5
1	A	172	TYR	5.5
1	A	10	VAL	4.9
1	A	11	PRO	4.9
1	B	119	LEU	4.8
1	B	8	ALA	4.7
1	A	171	PRO	4.6
1	A	5	GLY	4.5
1	B	5	GLY	4.5
1	B	10	VAL	4.5
1	B	9	PRO	4.3
1	A	4	VAL	4.2
1	A	13	VAL	4.1
1	B	7	GLY	4.1
1	A	173	GLN	3.9
1	B	12	LEU	3.9
1	A	121	SER	3.7
1	A	170	PRO	3.5
1	B	118	GLU	3.1
1	A	9	PRO	3.0
1	B	117	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1	SER	2.3
1	B	170	PRO	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

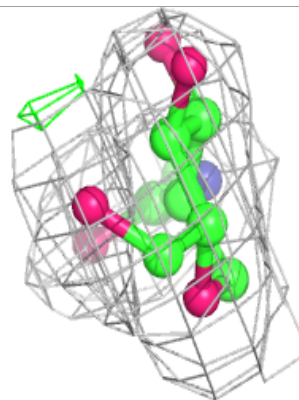
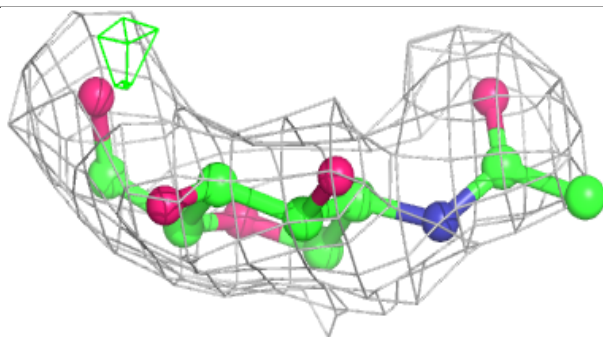
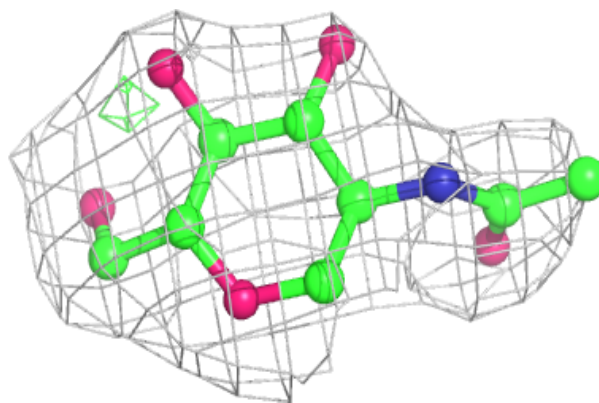
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	B	601	14/15	0.90	0.14	40,44,49,51	0
2	NAG	A	602	14/15	0.90	0.15	32,41,49,52	0
2	NAG	B	604	14/15	0.92	0.26	40,52,61,66	0
2	NAG	A	608	14/15	0.93	0.12	27,33,38,40	0
2	NAG	B	603	14/15	0.93	0.16	34,43,55,58	0
2	NAG	A	601	14/15	0.94	0.11	31,38,48,52	0
2	NAG	B	602	14/15	0.95	0.15	29,34,43,49	0
2	NAG	A	607	14/15	0.96	0.10	25,30,36,40	0
3	HEM	B	605	43/43	0.97	0.12	11,16,21,31	0
4	PEO	B	606	2/2	0.97	0.09	20,20,20,31	0
5	CA	A	605	1/1	0.98	0.08	18,18,18,18	0
6	CL	B	608	1/1	0.98	0.15	46,46,46,46	0
4	PEO	A	604	2/2	0.98	0.11	16,16,16,20	0
3	HEM	A	603	43/43	0.98	0.11	12,16,22,24	0
5	CA	B	607	1/1	0.99	0.05	32,32,32,32	0
6	CL	A	606	1/1	0.99	0.13	34,34,34,34	0

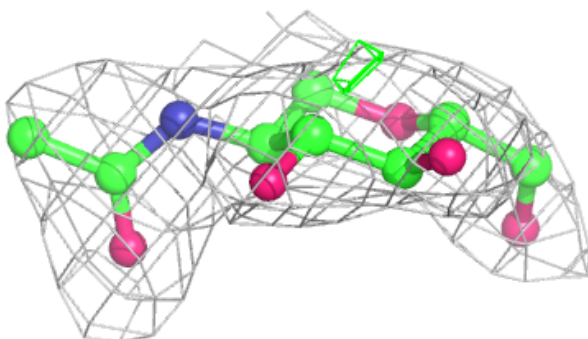
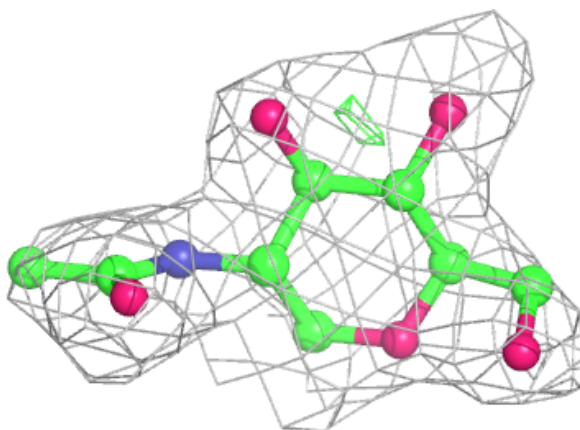
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG B 601:

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

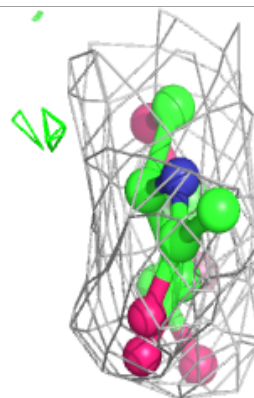
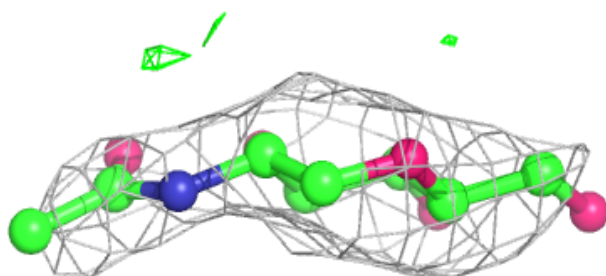
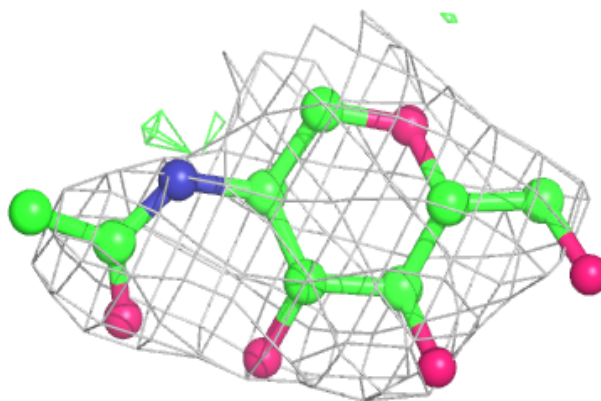
**Electron density around NAG A 602:**

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

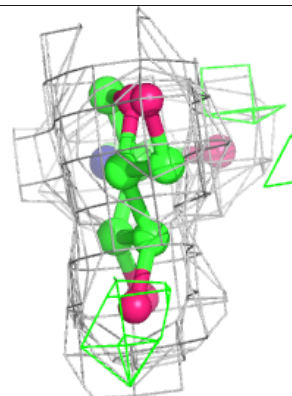
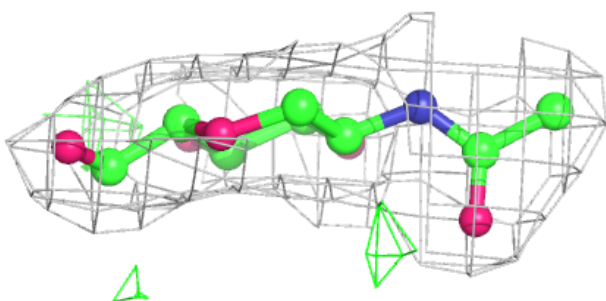
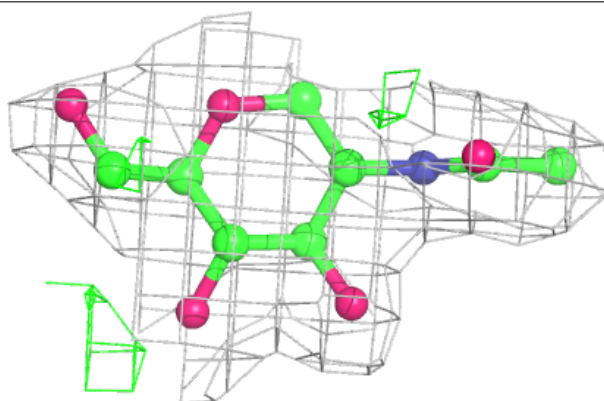


Electron density around NAG B 604:

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

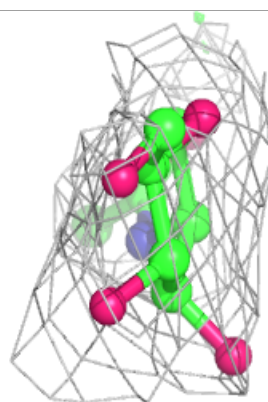
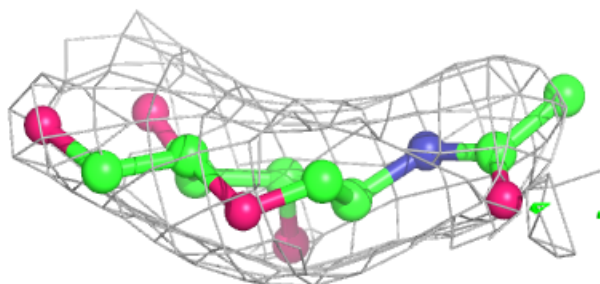
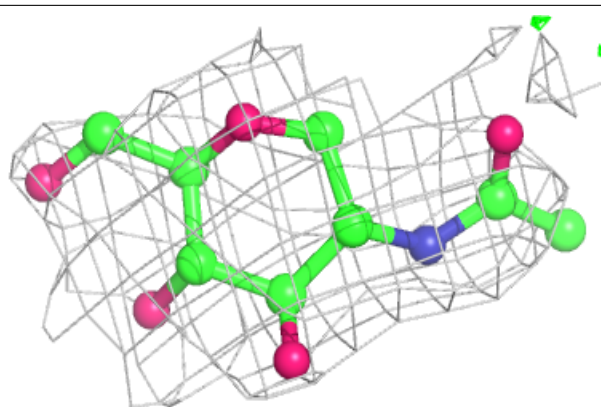
**Electron density around NAG A 608:**

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

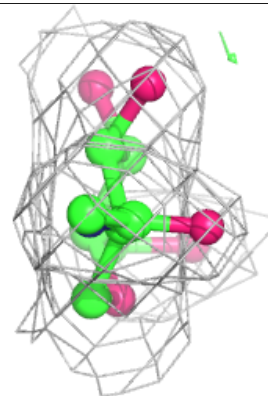
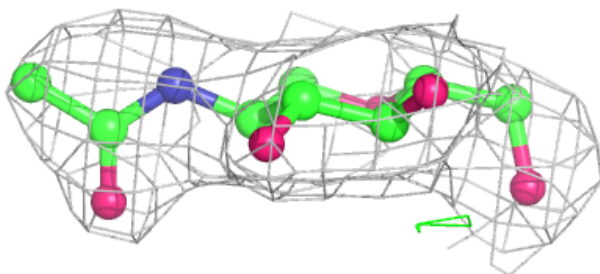
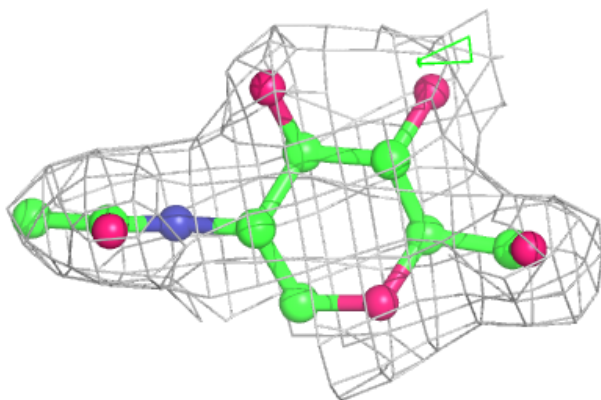


Electron density around NAG B 603:

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

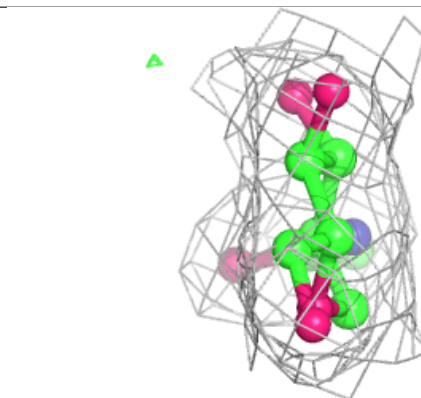
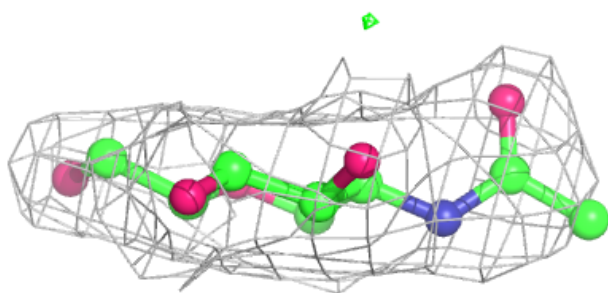
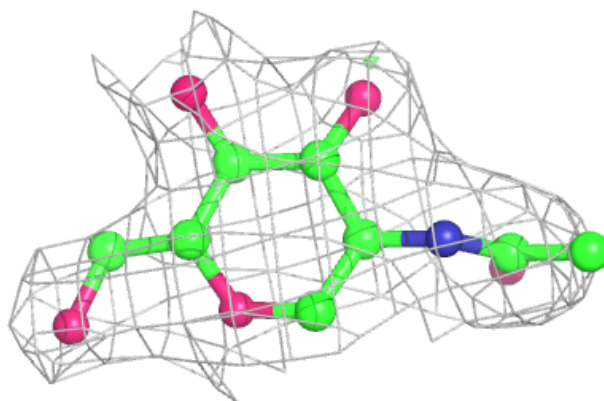
**Electron density around NAG A 601:**

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

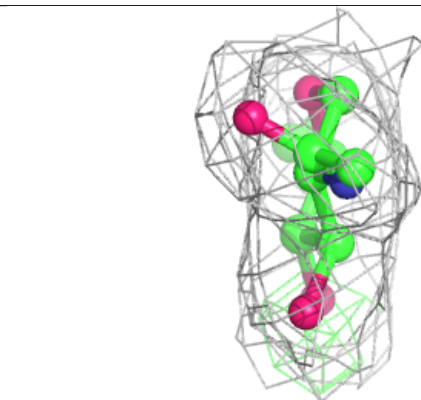
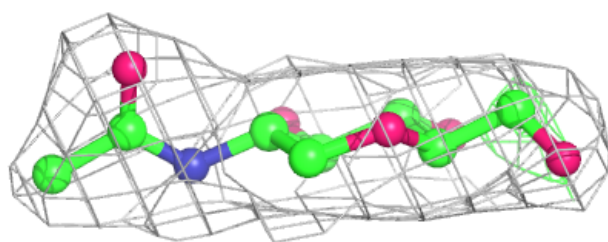
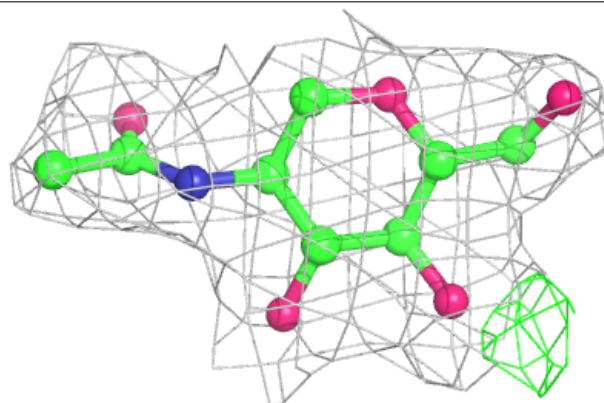


Electron density around NAG B 602:

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

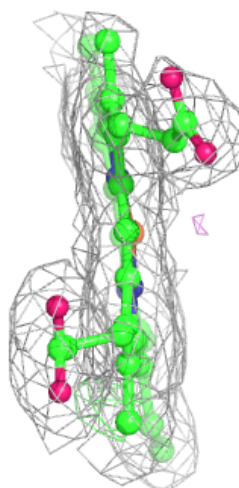
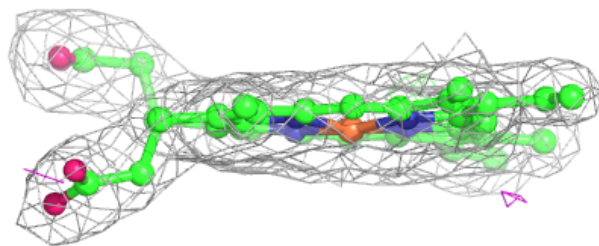
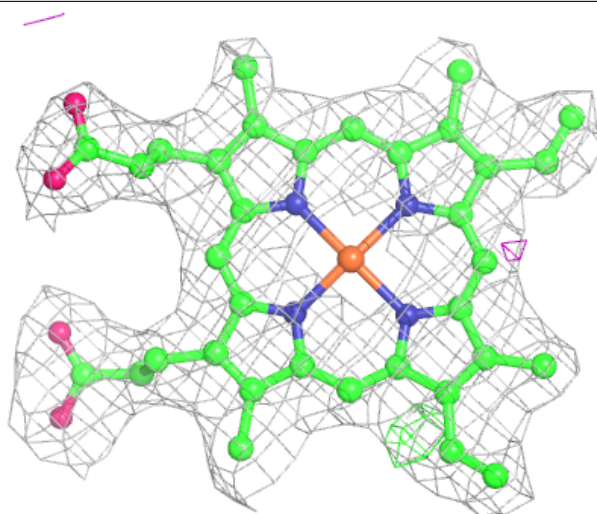
**Electron density around NAG A 607:**

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



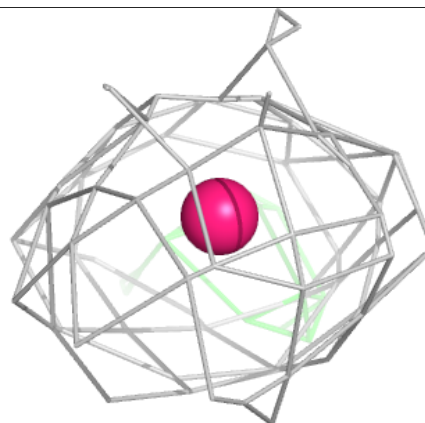
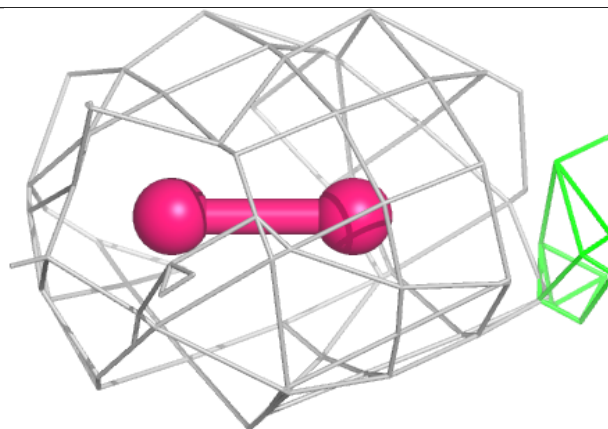
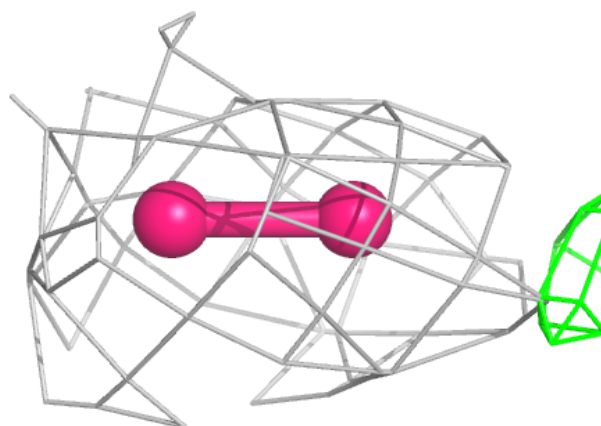
Electron density around HEM B 605:

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



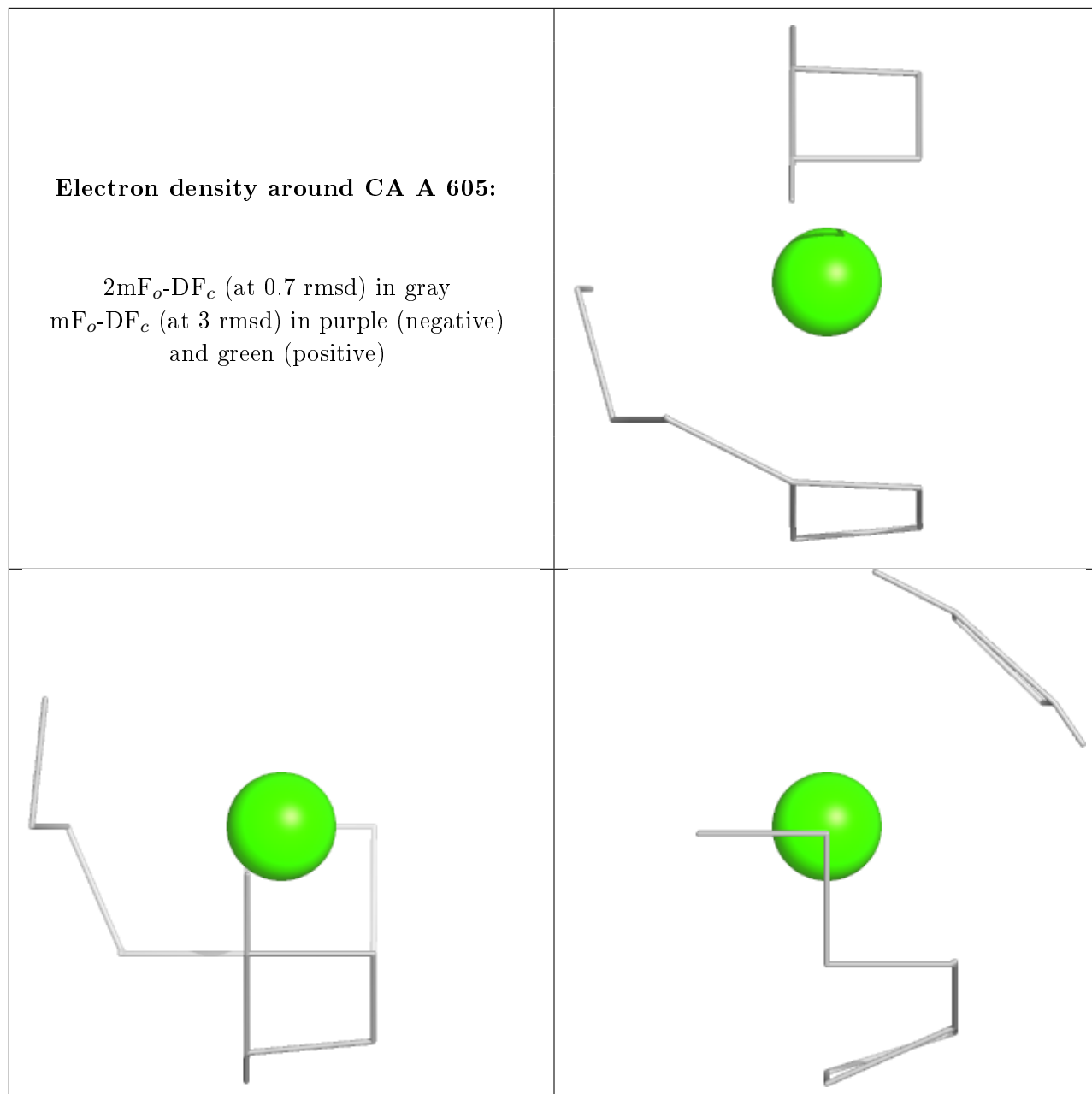
Electron density around PEO B 606:

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



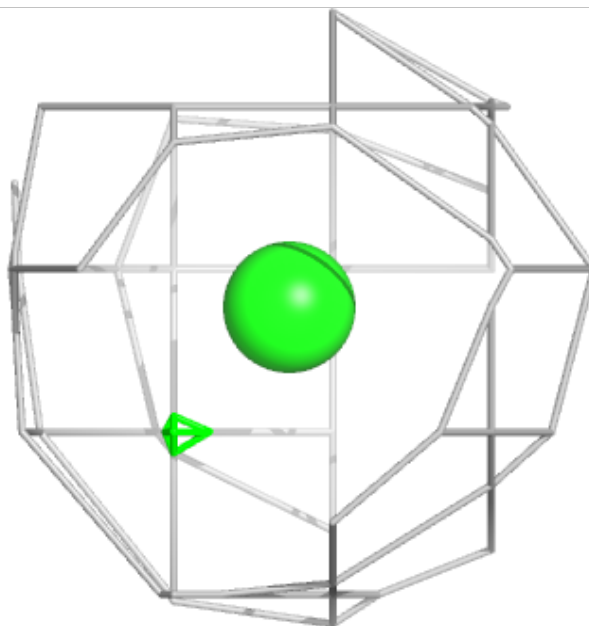
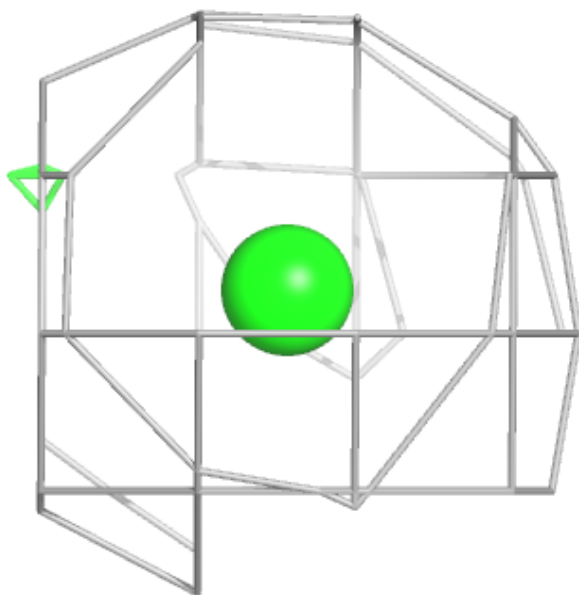
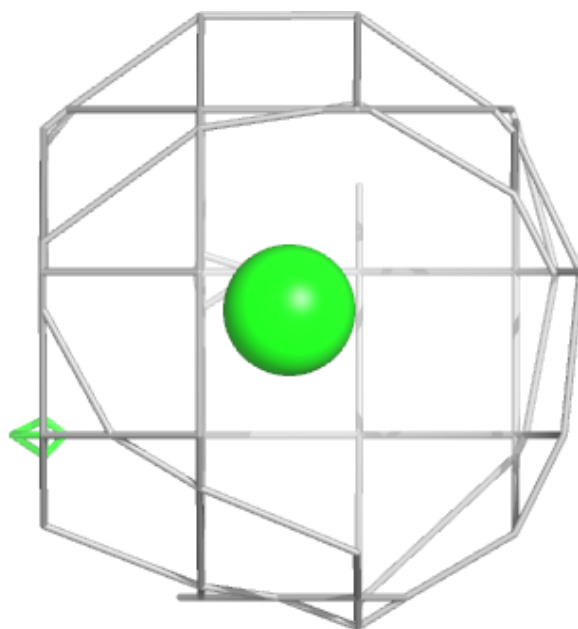
Electron density around CA A 605:

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



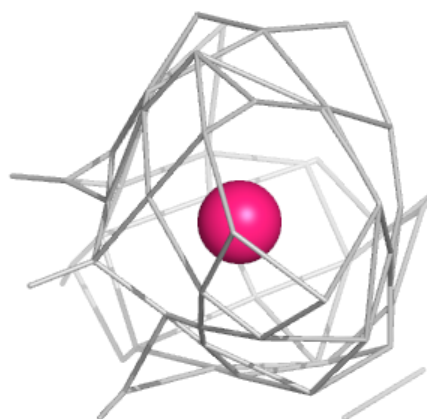
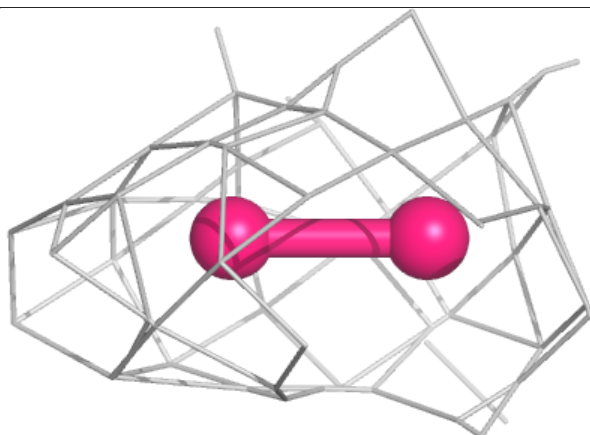
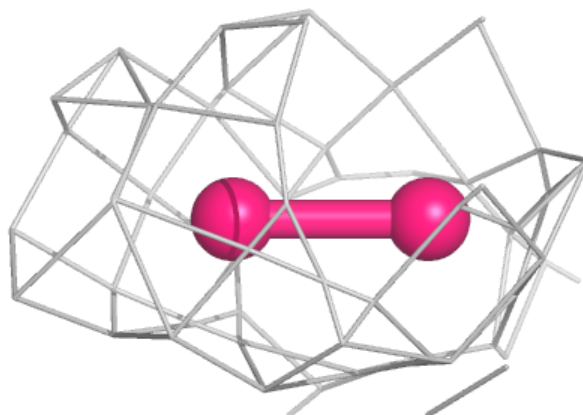
Electron density around CL B 608:

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



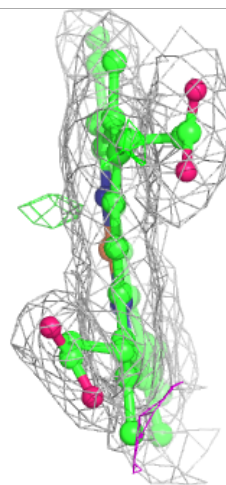
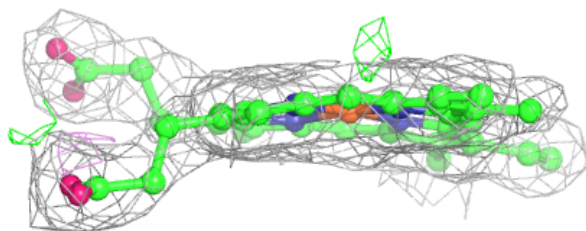
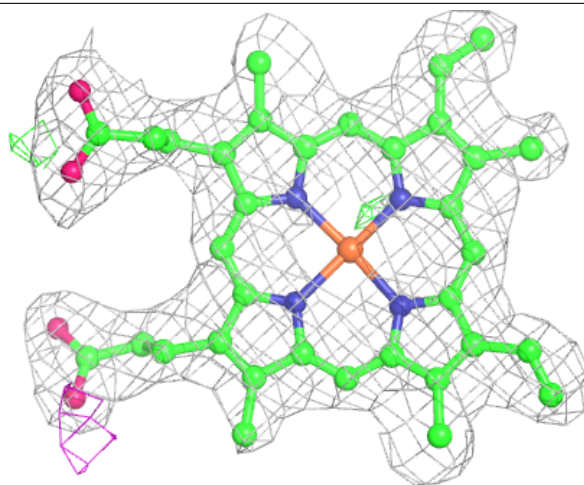
Electron density around PEO A 604:

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



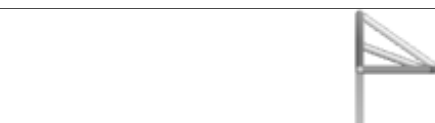
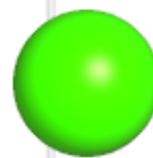
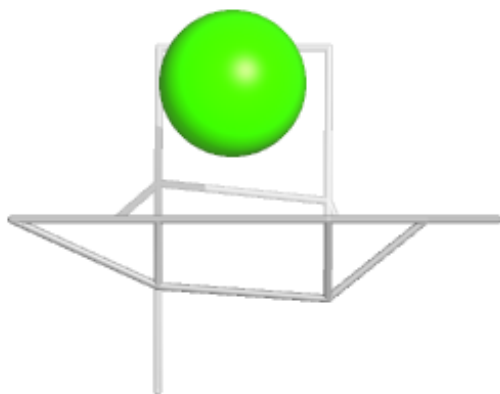
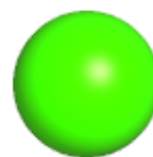
Electron density around HEM A 603:

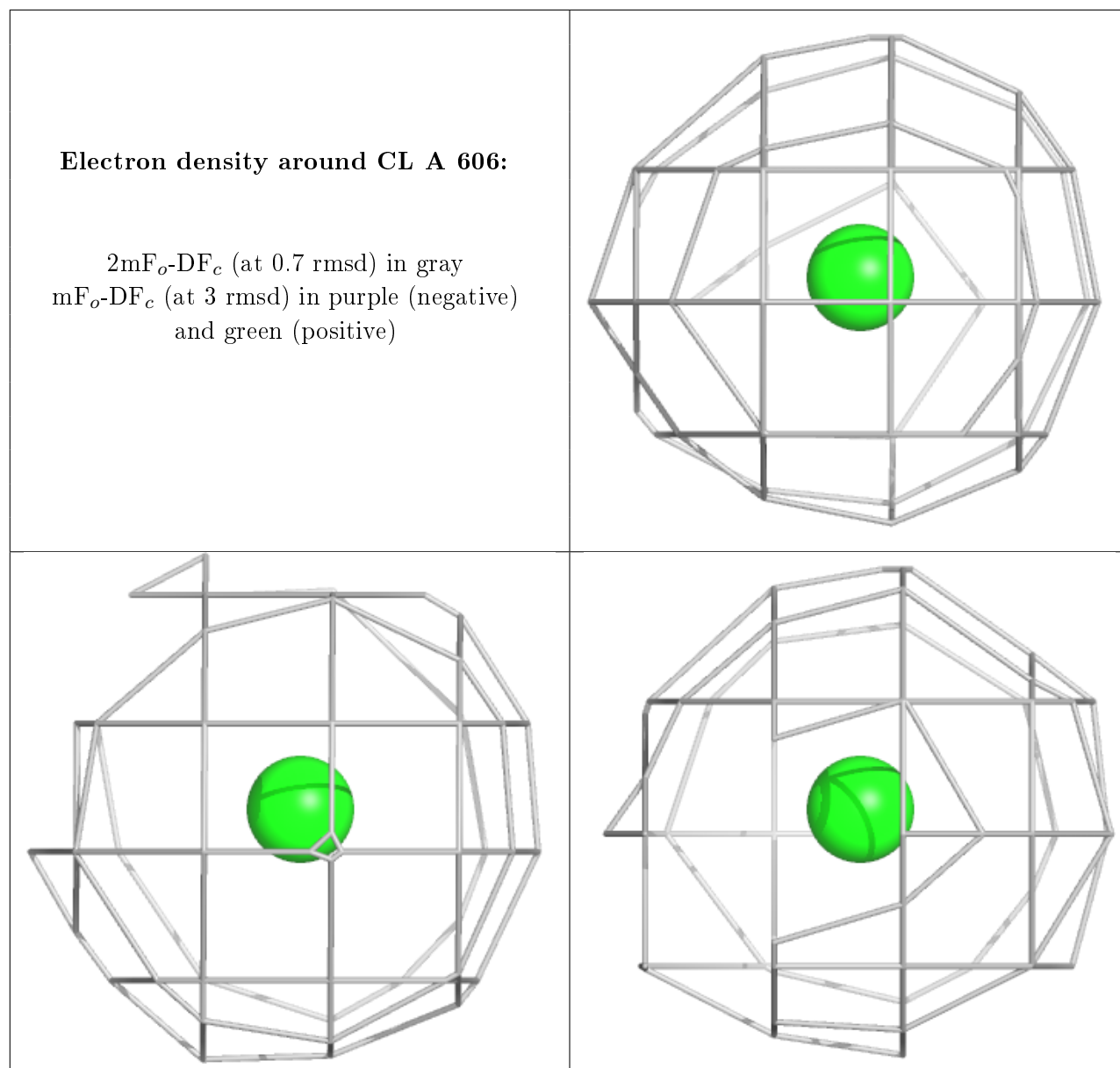
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 607:

$2mF_o-DF_c$ (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.