



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 06:12 AM EDT

PDB ID : 7P18 / pdb_00007p18
Title : Crystal structure of 3-ketosteroid delta1-dehydrogenase from Sterolibacterium denitrificans in complex with 1,4-androstadiene-3,17-dione
Authors : Wojcik, P.; Mrugala, B.; Kurpiewska, K.; Szaleniec, M.
Deposited on : 2021-07-01
Resolution : 1.84 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 : 2022.3.0, CSD as543be (2022)
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

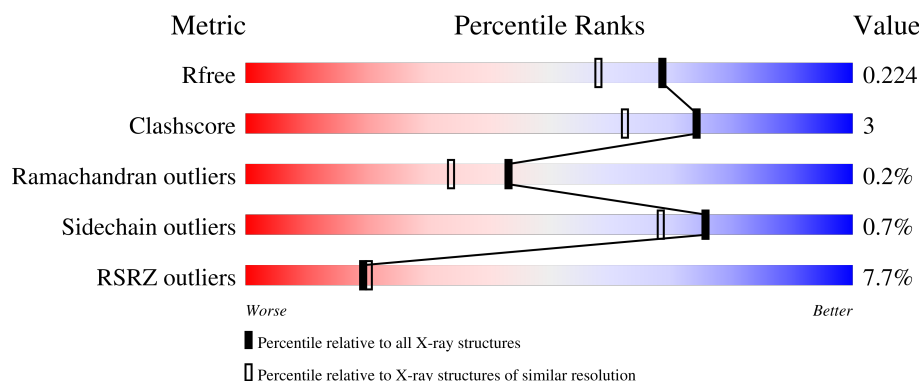
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	561	
1	B	561	

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	GOL	A	606	-	-	X	-

2 Entry composition [i](#)

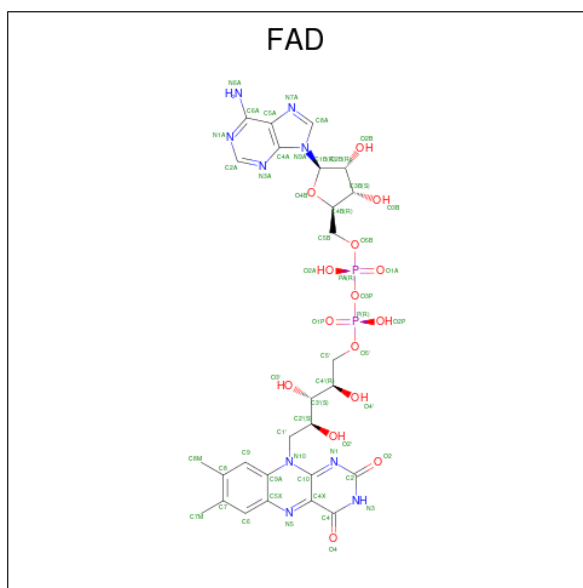
There are 7 unique types of molecules in this entry. The entry contains 9665 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-oxosteroid 1-dehydrogenase.

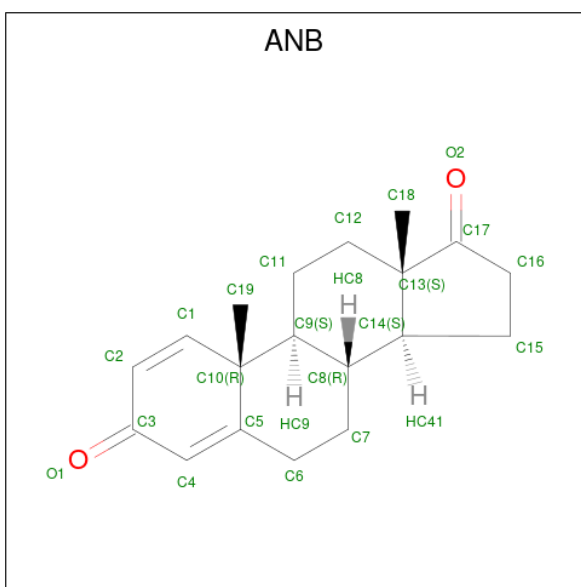
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	4	0
			4322	2734	764	797	27			
1	B	557	Total	C	N	O	S	0	7	0
			4336	2739	770	801	26			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



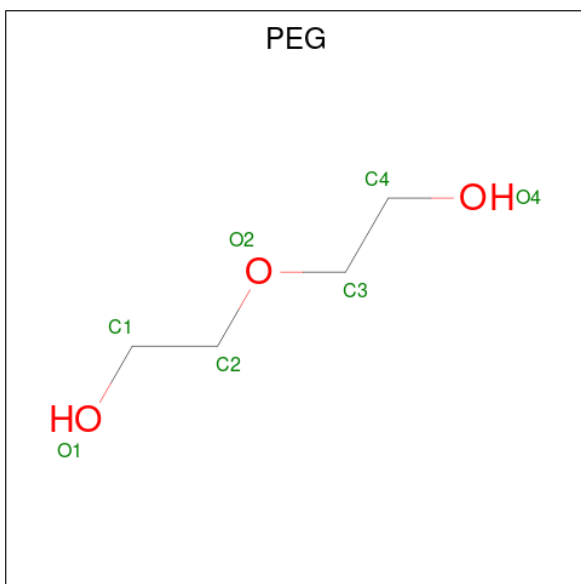
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is ANDROSTA-1,4-DIENE-3,17-DIONE (CCD ID: ANB) (formula: $C_{19}H_{24}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	19	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



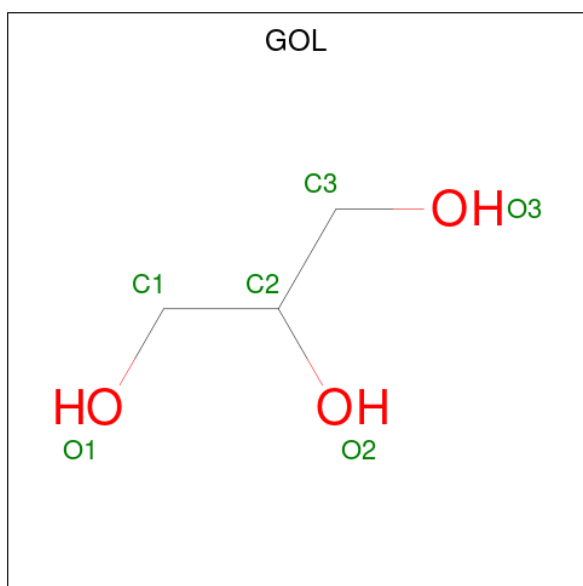
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

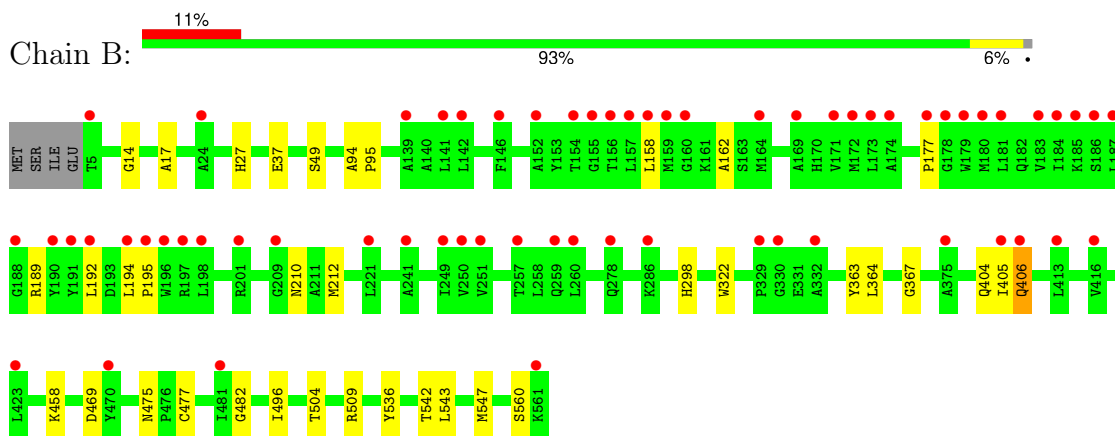
- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	521	Total 521	O 521	0	0
7	B	305	Total 305	O 305	0	0

- Molecule 1: 3-oxosteroid 1-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.37Å 130.37Å 139.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.71 – 1.84 47.71 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.71-1.84) 99.6 (47.71-1.84)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.185 , 0.214 0.195 , 0.224	Depositor DCC
R_{free} test set	2100 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9665	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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: NA, FAD, ANB, GOL, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.07	0/4426	1.24	4/5998 (0.1%)
1	B	1.05	0/4440	1.25	10/6018 (0.2%)
All	All	1.06	0/8866	1.25	14/12016 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	HIS	N-CA-C	7.43	122.34	113.28
1	A	298	HIS	N-CA-C	6.01	120.68	113.23
1	B	475	ASN	CB-CA-C	5.47	116.44	110.15
1	B	177	PRO	CB-CA-C	-5.41	104.48	111.46
1	B	469	ASP	CA-C-N	5.22	128.65	120.82
1	B	469	ASP	C-N-CA	5.22	128.65	120.82
1	B	37	GLU	CA-C-N	5.17	127.20	120.28
1	B	37	GLU	C-N-CA	5.17	127.20	120.28
1	B	14	GLY	CA-C-O	-5.14	117.35	121.77
1	B	189	ARG	CA-C-N	5.10	127.07	120.44
1	B	189	ARG	C-N-CA	5.10	127.07	120.44
1	A	189	ARG	CA-C-N	5.07	127.03	120.44
1	A	189	ARG	C-N-CA	5.07	127.03	120.44
1	A	177	PRO	CB-CA-C	-5.04	104.96	111.46

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	4322	0	4250	33	0
1	B	4336	0	4247	20	0
2	A	53	0	31	2	0
2	B	53	0	31	3	0
3	A	21	0	24	1	0
4	A	21	0	30	5	0
4	B	14	0	20	0	0
5	A	18	0	24	6	0
6	A	1	0	0	0	0
7	A	521	0	0	6	0
7	B	305	0	0	4	0
All	All	9665	0	8657	55	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 3.

All (55) 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:560[A]:SER:OG	7:B:701:HOH:O	1.90	0.88
1:A:179:TRP:CD1	5:A:606:GOL:HO3	1.96	0.84
1:A:179:TRP:CG	5:A:606:GOL:HO3	1.97	0.82
1:B:406:GLN:O	1:B:406:GLN:HG3	1.92	0.70
1:A:242:GLU:HG3	7:A:1035:HOH:O	1.98	0.64
1:B:496:ILE:HB	2:B:601:FAD:H9	1.81	0.62
1:A:188:GLY:O	1:A:192:LEU:HG	2.00	0.61
1:A:406:GLN:NE2	7:A:703:HOH:O	2.36	0.59
1:A:28:ASP:HB3	5:A:607:GOL:H2	1.86	0.58
1:A:212[B]:MET:CE	1:A:547:MET:HE2	2.36	0.56
1:A:27:HIS:HD2	7:A:1050:HOH:O	1.89	0.55
1:A:158:LEU:HB3	1:A:162:ALA:HB3	1.89	0.54
1:A:496:ILE:HB	2:A:601:FAD:H9	1.89	0.54
1:A:120:GLN:HB3	4:A:603:PEG:H12	1.89	0.54
1:A:560:SER:HB2	7:A:724:HOH:O	2.07	0.54
1:A:179:TRP:CD2	5:A:606:GOL:O2	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:HIS:HB2	4:A:604:PEG:H31	1.91	0.53
1:A:452[B]:LYS:HG2	1:A:454:ARG:NH1	2.24	0.52
1:B:158:LEU:HB3	1:B:162:ALA:HB3	1.91	0.52
1:B:17:ALA:HB1	1:B:212[B]:MET:HE2	1.91	0.52
1:B:192:LEU:HD23	1:B:192:LEU:O	2.10	0.51
1:B:27:HIS:HD2	7:B:905:HOH:O	1.93	0.51
1:A:363:TYR:OH	3:A:602:ANB:C2	2.62	0.47
1:A:94:ALA:HB3	1:A:95:PRO:HD3	1.96	0.46
1:A:245:ARG:HD3	7:B:851:HOH:O	2.16	0.46
1:A:175:LYS:HB3	5:A:606:GOL:H31	1.97	0.45
1:B:212[B]:MET:HE3	1:B:547:MET:HE2	1.98	0.45
1:A:194:LEU:O	1:A:195:PRO:C	2.59	0.44
1:B:49:SER:HA	2:B:601:FAD:C6	2.48	0.44
1:B:94:ALA:HB3	1:B:95:PRO:HD3	2.00	0.44
1:B:536:TYR:HB3	7:B:872:HOH:O	2.17	0.43
1:A:120:GLN:CB	4:A:603:PEG:H12	2.48	0.43
1:B:322:TRP:HB3	1:B:367:GLY:HA3	2.00	0.43
1:A:230:ASN:ND2	7:A:707:HOH:O	2.41	0.43
1:B:194:LEU:O	1:B:195:PRO:C	2.61	0.43
4:A:604:PEG:H32	7:A:860:HOH:O	2.19	0.43
1:B:194:LEU:CB	1:B:195:PRO:CD	2.97	0.43
1:A:39:SER:HB3	1:A:298:HIS:CD2	2.55	0.42
1:A:39:SER:HB2	1:A:298:HIS:NE2	2.34	0.42
2:B:601:FAD:H9	2:B:601:FAD:H1'1	1.83	0.42
1:B:458:LYS:HE2	1:B:477:CYS:HB3	2.01	0.42
1:A:27:HIS:CE1	1:A:223:ARG:HB3	2.55	0.41
1:A:504:THR:HA	1:A:509:ARG:O	2.21	0.41
1:B:212[B]:MET:HE1	1:B:543:LEU:HB3	2.03	0.41
1:A:179:TRP:CE3	5:A:606:GOL:O2	2.73	0.41
1:B:212[B]:MET:CE	1:B:547:MET:HE2	2.50	0.41
1:A:458:LYS:HE2	1:A:477:CYS:HB3	2.03	0.41
1:A:324:PRO:HB2	1:A:491:VAL:HG13	2.03	0.41
1:A:49:SER:HA	2:A:601:FAD:C6	2.51	0.41
1:A:46:SER:HB3	1:A:212[A]:MET:HE3	2.03	0.40
1:B:364:LEU:HD22	1:B:536:TYR:HB2	2.03	0.40
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.91	0.40
1:B:404[B]:GLN:HG3	1:B:405:ILE:HG23	2.03	0.40
1:A:114:ARG:CD	4:A:604:PEG:H22	2.51	0.40
1:B:504:THR:HA	1:B:509:ARG:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	560/561 (100%)	545 (97%)	14 (2%)	1 (0%)	43	34
1	B	562/561 (100%)	545 (97%)	16 (3%)	1 (0%)	43	34
All	All	1122/1122 (100%)	1090 (97%)	30 (3%)	2 (0%)	43	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	482	GLY
1	B	482	GLY

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	436/436 (100%)	434 (100%)	2 (0%)	81	75
1	B	436/436 (100%)	432 (99%)	4 (1%)	70	60
All	All	872/872 (100%)	866 (99%)	6 (1%)	76	68

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	363	TYR
1	B	210	ASN
1	B	363	TYR

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Mol	Chain	Res	Type
1	B	406	GLN
1	B	542	THR

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	27	HIS
1	A	62	GLN
1	A	182	GLN
1	A	218	HIS
1	A	243	ASN
1	A	278	GLN
1	A	394	ASN
1	B	6	ASN
1	B	27	HIS
1	B	182	GLN
1	B	243	ASN
1	B	278	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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	ANB	A	602	-	24,24,24	0.42	0	39,39,39	1.10	4 (10%)
4	PEG	A	603	-	6,6,6	0.31	0	5,5,5	0.24	0
4	PEG	A	605	-	6,6,6	0.43	0	5,5,5	0.28	0
2	FAD	B	601	-	58,58,58	0.85	2 (3%)	85,89,89	0.95	7 (8%)
5	GOL	A	606	-	5,5,5	0.12	0	5,5,5	0.25	0
4	PEG	A	604	-	6,6,6	0.28	0	5,5,5	0.27	0
4	PEG	B	603	-	6,6,6	0.15	0	5,5,5	0.12	0
5	GOL	A	608	-	5,5,5	0.14	0	5,5,5	0.14	0
4	PEG	B	602	-	6,6,6	0.19	0	5,5,5	0.12	0
5	GOL	A	607	-	5,5,5	0.12	0	5,5,5	0.30	0
2	FAD	A	601	-	58,58,58	0.92	3 (5%)	85,89,89	0.80	1 (1%)

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
4	PEG	A	603	-	-	2/4/4/4	-
3	ANB	A	602	-	-	-	0/4/4/4
4	PEG	A	605	-	-	4/4/4/4	-
2	FAD	B	601	-	-	3/34/50/50	0/6/6/6
5	GOL	A	606	-	-	2/4/4/4	-
4	PEG	A	604	-	-	2/4/4/4	-
4	PEG	B	603	-	-	2/4/4/4	-
5	GOL	A	608	-	-	3/4/4/4	-
4	PEG	B	602	-	-	1/4/4/4	-
5	GOL	A	607	-	-	3/4/4/4	-
2	FAD	A	601	-	-	2/34/50/50	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	P-O3P	4.31	1.64	1.59
2	A	601	FAD	PA-O3P	2.48	1.62	1.59
2	B	601	FAD	PA-O3P	2.36	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C2-N3	-2.20	1.34	1.39
2	B	601	FAD	O2-C2	2.11	1.28	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	O2P-P-O1P	3.12	126.97	112.44
3	A	602	ANB	C10-C9-C8	-2.93	109.79	112.07
3	A	602	ANB	C2-C3-C4	-2.75	114.33	117.12
2	B	601	FAD	C1'-C2'-C3'	2.61	116.74	109.66
2	B	601	FAD	O2A-PA-O1A	2.48	123.96	112.44
2	B	601	FAD	O5'-P-O1P	-2.44	99.25	108.94
2	A	601	FAD	O2P-P-O1P	2.15	122.47	112.44
2	B	601	FAD	C4X-C4-N3	2.08	118.56	113.25
3	A	602	ANB	C9-C8-C14	2.05	111.77	109.09
2	B	601	FAD	O3B-C3B-C2B	2.04	118.36	111.82
3	A	602	ANB	C1-C10-C5	-2.03	109.79	111.76
2	B	601	FAD	O2B-C2B-C1B	2.01	117.02	110.10

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	608	GOL	C1-C2-C3-O3
4	A	605	PEG	O1-C1-C2-O2
5	A	607	GOL	O1-C1-C2-C3
5	A	607	GOL	O1-C1-C2-O2
4	A	604	PEG	O1-C1-C2-O2
5	A	608	GOL	O2-C2-C3-O3
4	A	603	PEG	O2-C3-C4-O4
4	B	603	PEG	O1-C1-C2-O2
5	A	606	GOL	O2-C2-C3-O3
2	B	601	FAD	O4B-C4B-C5B-O5B
4	A	603	PEG	C4-C3-O2-C2
4	A	605	PEG	C1-C2-O2-C3
5	A	606	GOL	O1-C1-C2-O2
5	A	608	GOL	O1-C1-C2-C3
4	A	605	PEG	C4-C3-O2-C2
4	A	605	PEG	O2-C3-C4-O4
5	A	607	GOL	O2-C2-C3-O3
4	B	602	PEG	O2-C3-C4-O4
4	B	603	PEG	C4-C3-O2-C2

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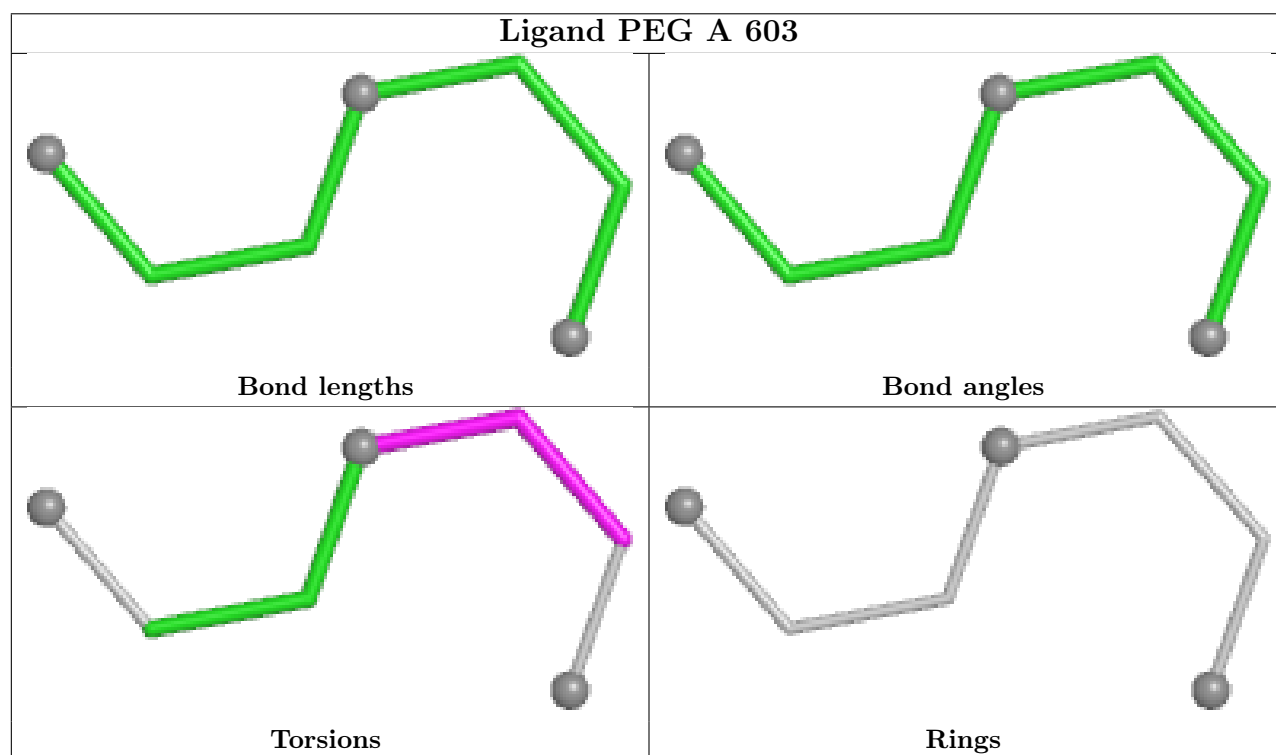
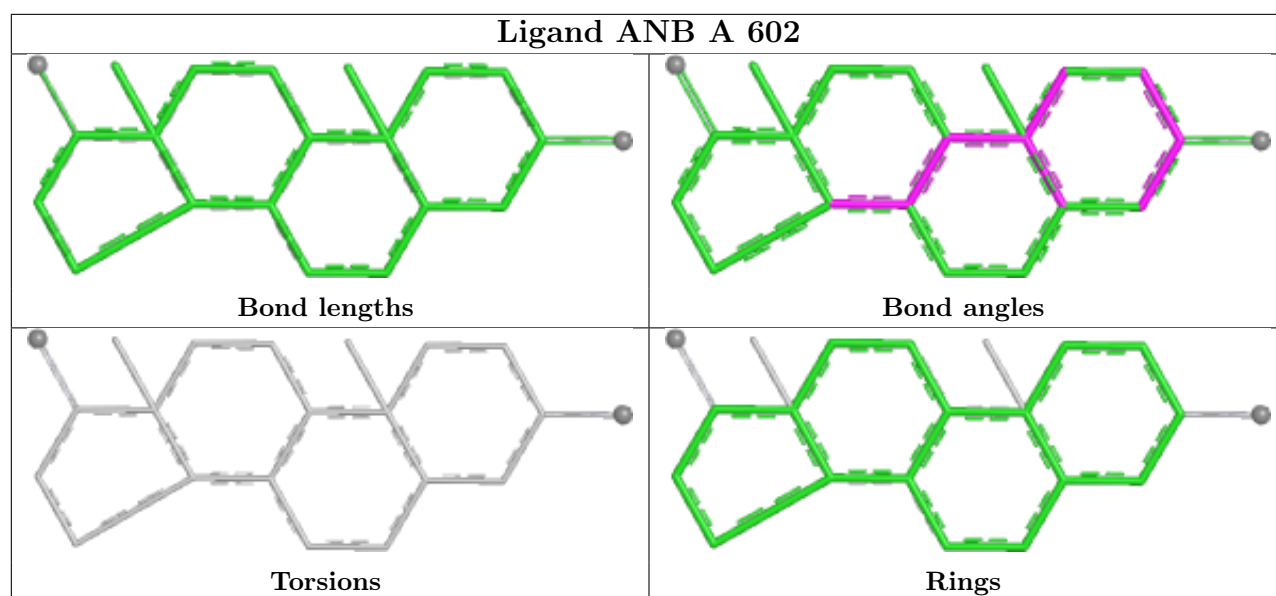
Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C2B-C1B-N9A-C8A
2	A	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	C2B-C1B-N9A-C8A
4	A	604	PEG	C1-C2-O2-C3
2	B	601	FAD	C3B-C4B-C5B-O5B

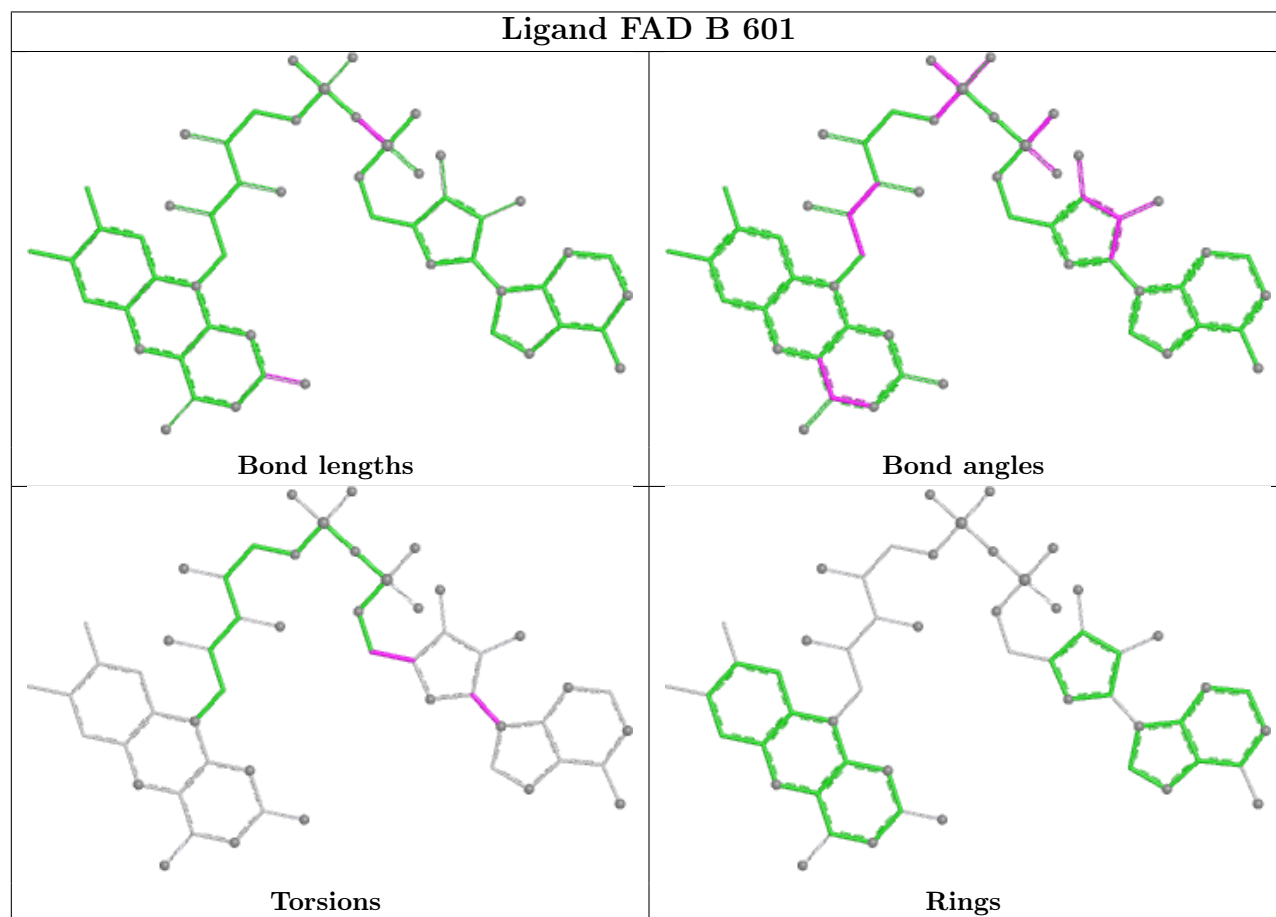
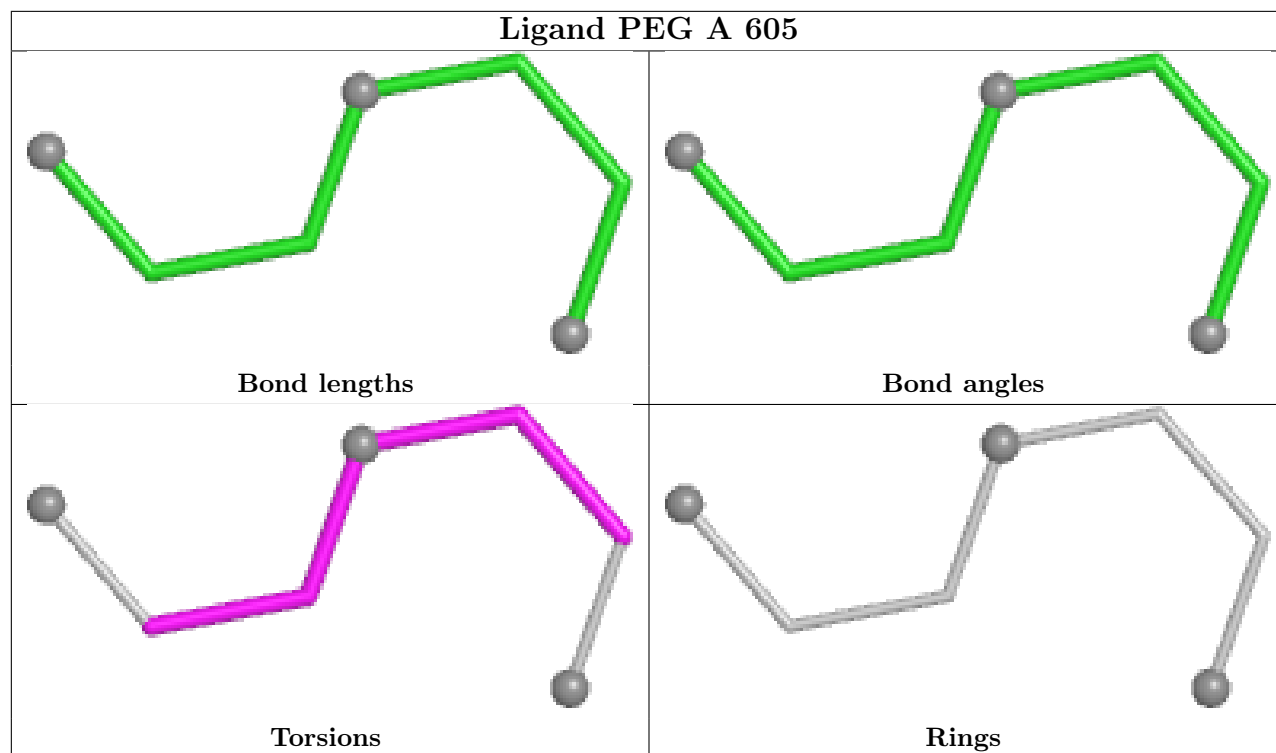
There are no ring outliers.

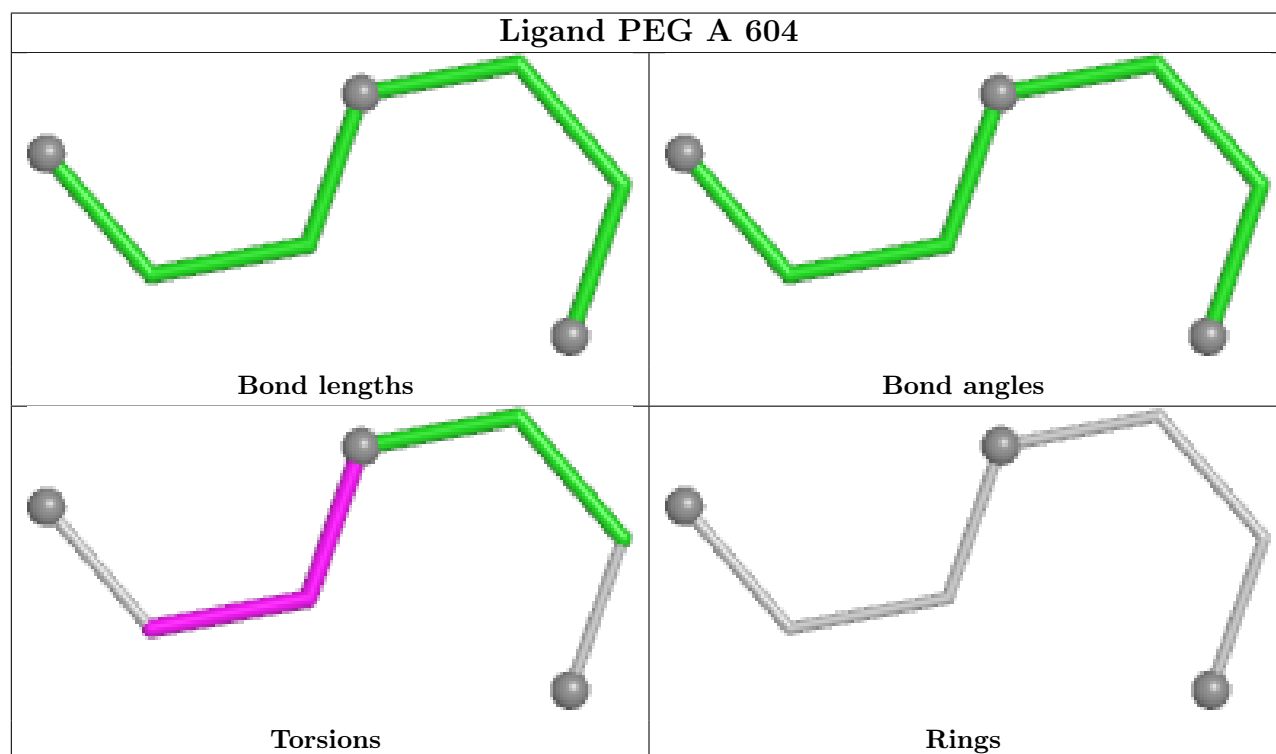
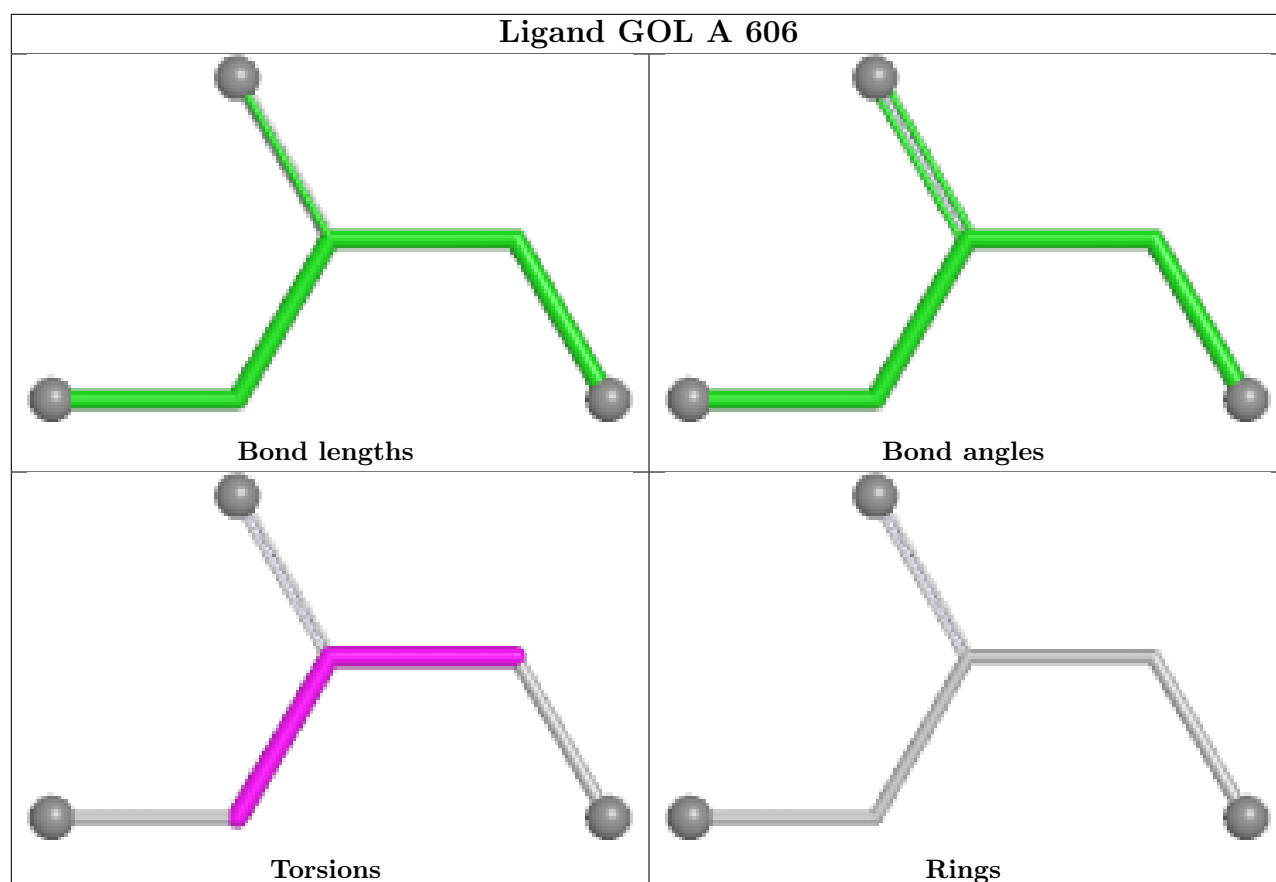
7 monomers are involved in 17 short contacts:

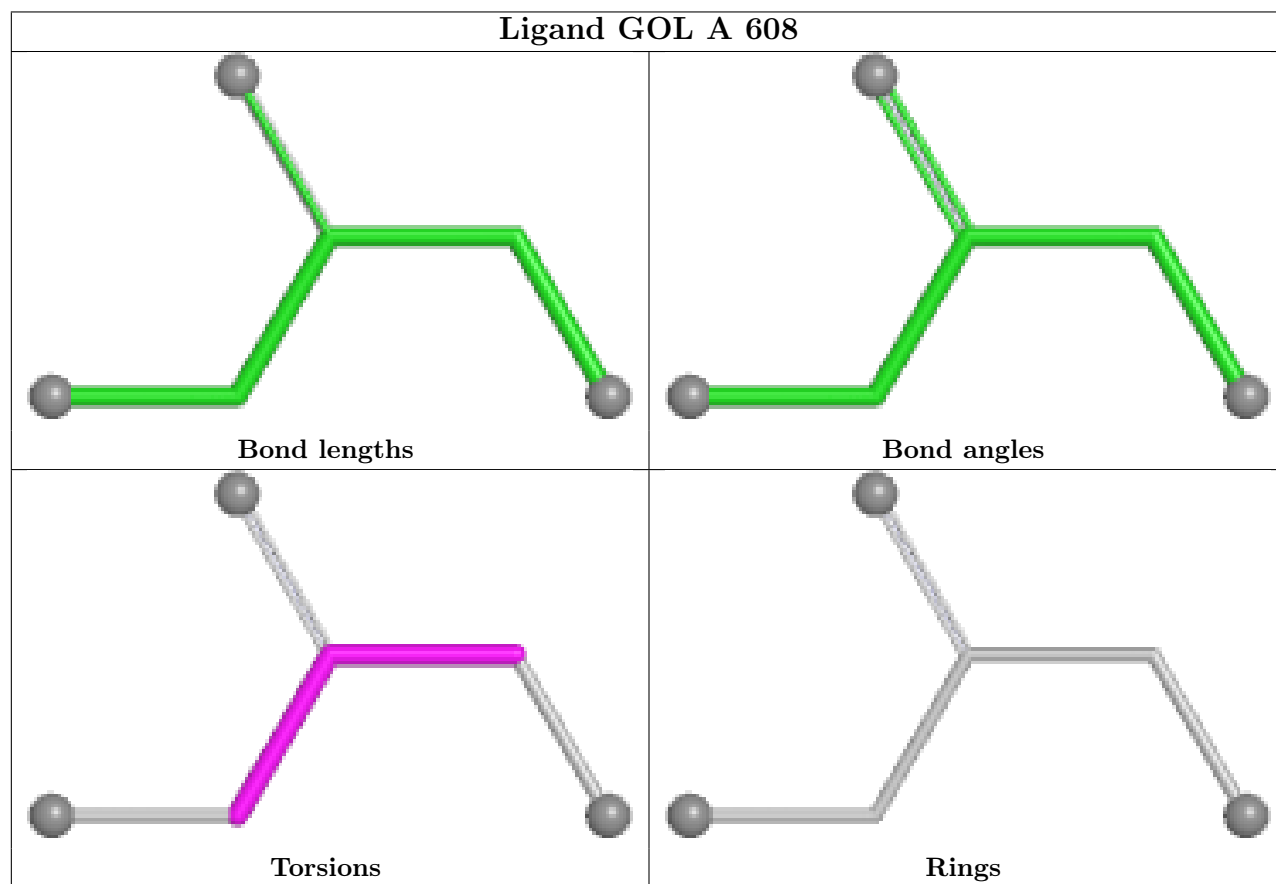
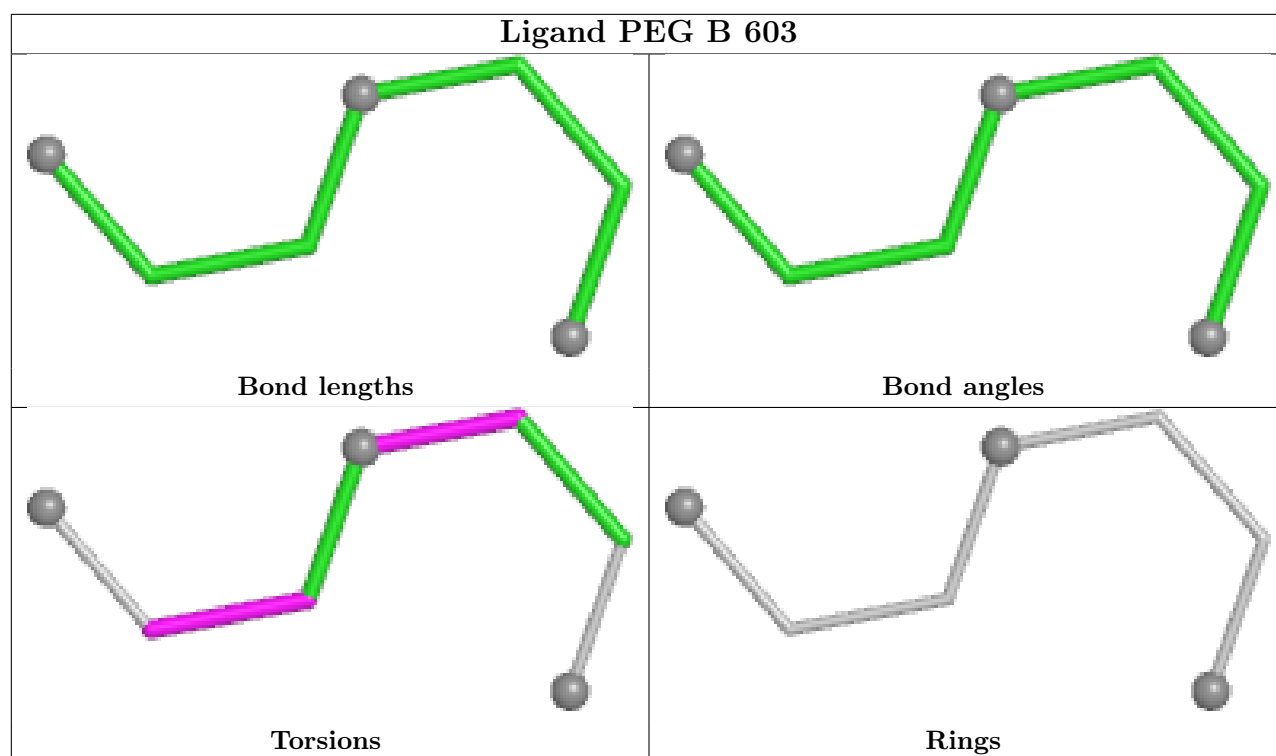
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	ANB	1	0
4	A	603	PEG	2	0
2	B	601	FAD	3	0
5	A	606	GOL	5	0
4	A	604	PEG	3	0
5	A	607	GOL	1	0
2	A	601	FAD	2	0

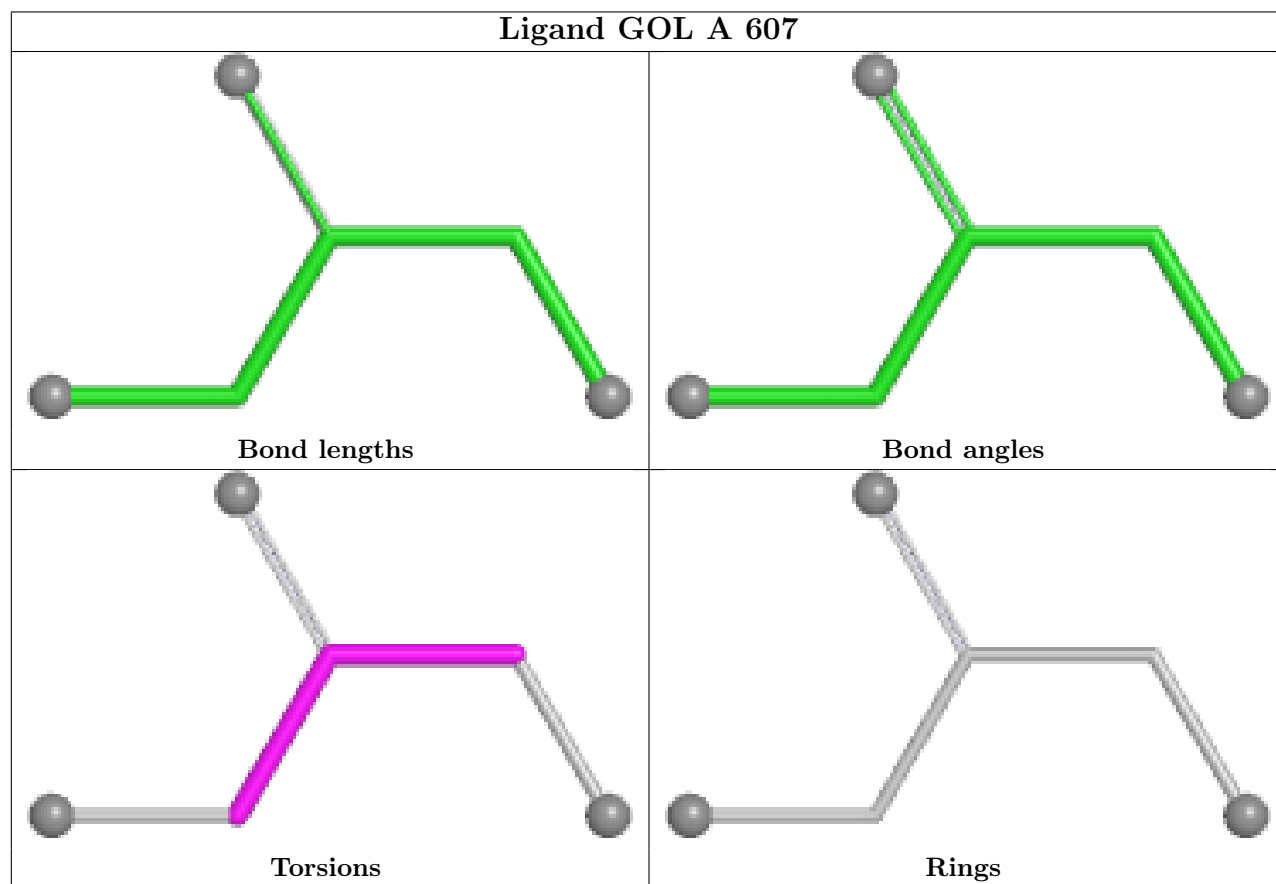
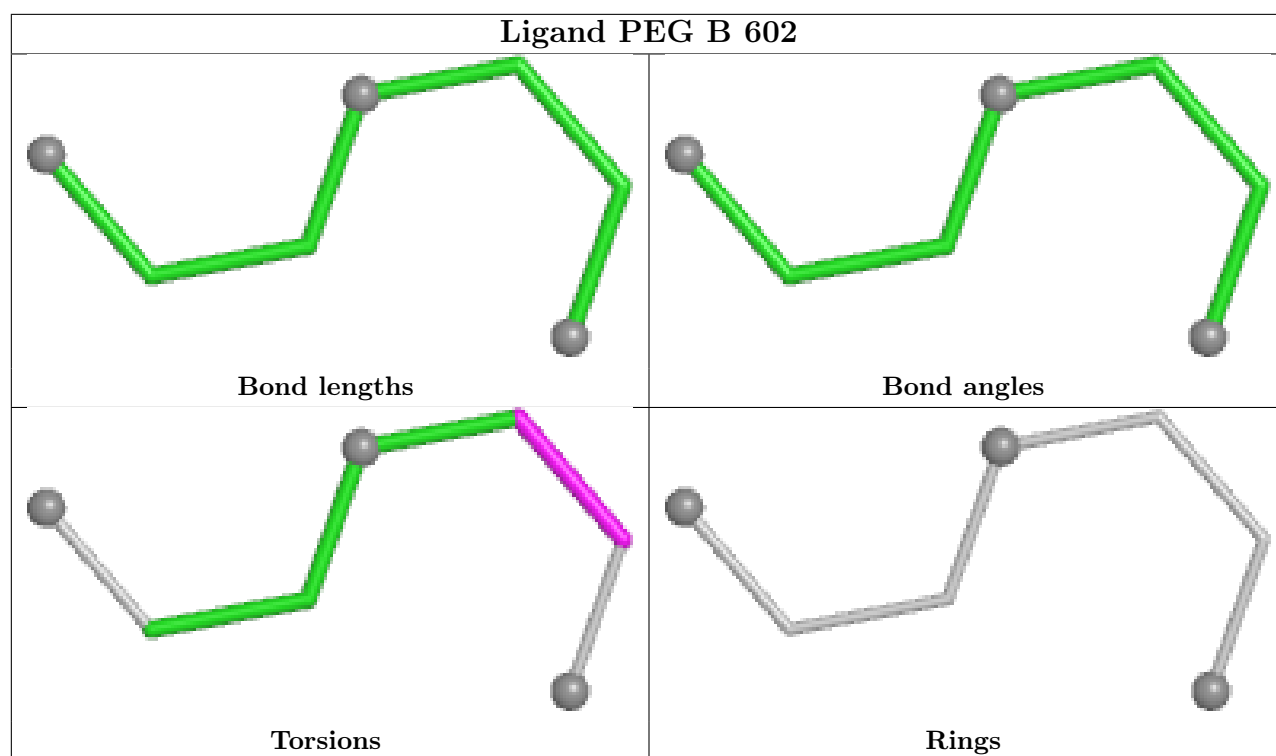
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

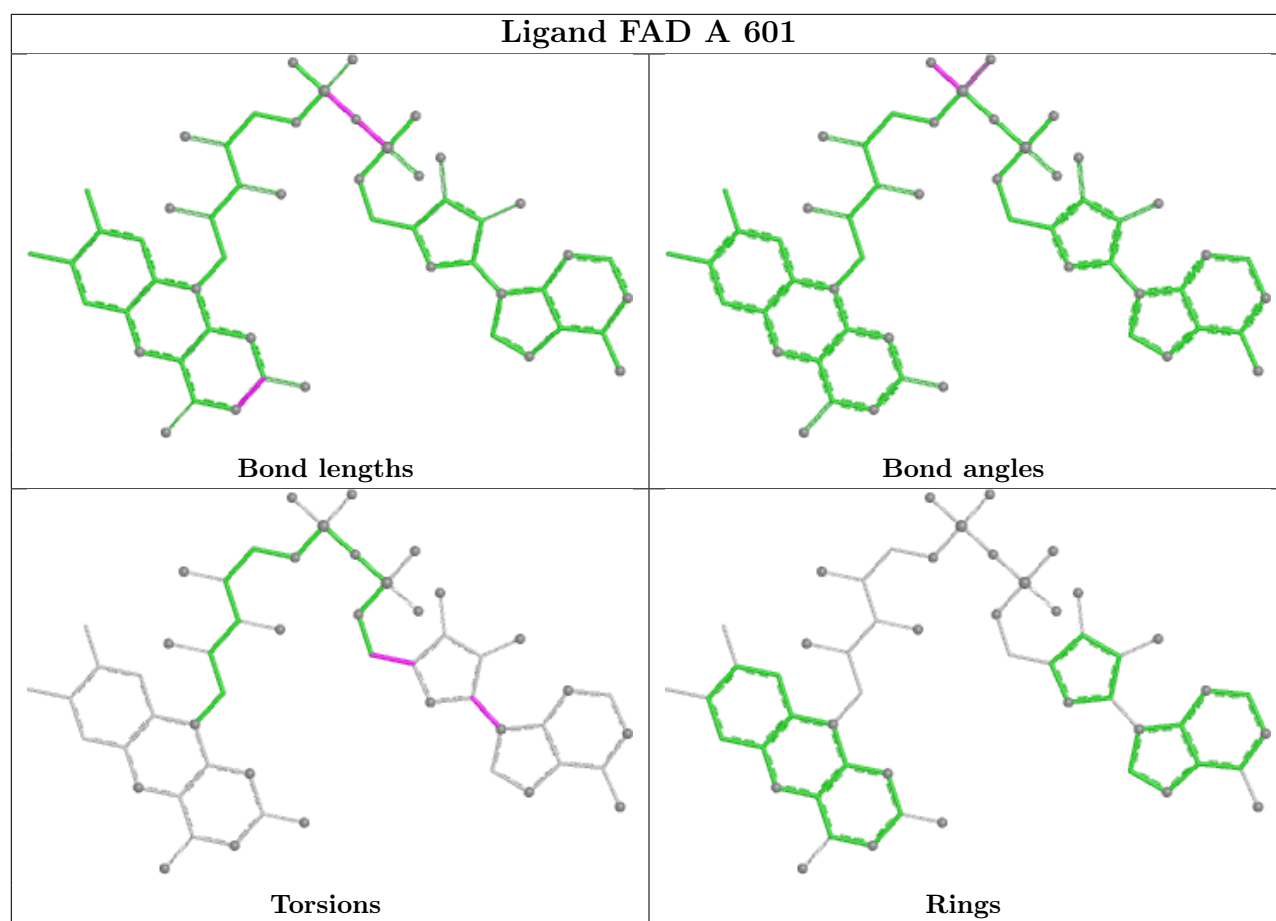












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	558/561 (99%)	0.02	23 (4%)	41	44	12, 27, 56, 109	4 (0%)
1	B	557/561 (99%)	0.79	63 (11%)	10	10	14, 40, 74, 104	7 (1%)
All	All	1115/1122 (99%)	0.40	86 (7%)	19	20	12, 34, 68, 109	11 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	TRP	5.7
1	B	190	TYR	5.4
1	B	198	LEU	4.8
1	B	241	ALA	4.7
1	B	194	LEU	4.7
1	A	194	LEU	4.6
1	A	179	TRP	4.6
1	B	180	MET	4.6
1	B	174	ALA	4.6
1	B	183	VAL	4.4
1	B	195	PRO	4.2
1	A	180	MET	4.1
1	B	184	ILE	4.0
1	A	174	ALA	4.0
1	B	187	LEU	3.9
1	B	154	THR	3.9
1	B	171	VAL	3.8
1	B	169	ALA	3.6
1	B	164	MET	3.5
1	A	470	TYR	3.5
1	B	196	TRP	3.4
1	A	171	VAL	3.4
1	A	5	THR	3.4
1	B	181	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	158	LEU	3.3
1	B	191	TYR	3.2
1	B	192	LEU	3.1
1	B	172[A]	MET	3.1
1	B	141	LEU	3.0
1	A	164	MET	3.0
1	B	157	LEU	3.0
1	A	173	LEU	3.0
1	A	195	PRO	3.0
1	A	198	LEU	2.9
1	A	298	HIS	2.9
1	B	173	LEU	2.9
1	A	159	MET	2.9
1	B	146	PHE	2.9
1	B	159	MET	2.9
1	B	186	SER	2.9
1	B	160	GLY	2.9
1	B	330	GLY	2.8
1	B	332	ALA	2.8
1	B	250	VAL	2.8
1	B	152	ALA	2.7
1	A	183	VAL	2.7
1	A	181	LEU	2.7
1	B	260	LEU	2.7
1	A	169	ALA	2.6
1	A	241	ALA	2.6
1	B	405	ILE	2.6
1	B	178	GLY	2.6
1	A	187	LEU	2.6
1	B	188	GLY	2.6
1	B	561	LYS	2.6
1	B	470	TYR	2.5
1	B	185	LYS	2.5
1	B	142	LEU	2.5
1	A	184	ILE	2.5
1	B	139	ALA	2.5
1	B	413	LEU	2.4
1	B	423	LEU	2.3
1	B	155	GLY	2.3
1	A	405	ILE	2.3
1	B	197	ARG	2.2
1	B	257	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	375	ALA	2.2
1	A	185	LYS	2.2
1	B	5	THR	2.2
1	B	221	LEU	2.2
1	B	406	GLN	2.2
1	B	259	GLN	2.2
1	B	249	ILE	2.1
1	B	416	VAL	2.1
1	B	177	PRO	2.1
1	B	24	ALA	2.1
1	B	156	THR	2.1
1	B	286	LYS	2.1
1	A	190	TYR	2.1
1	B	209	GLY	2.1
1	B	278	GLN	2.1
1	A	4	GLU	2.0
1	B	481	ILE	2.0
1	B	201	ARG	2.0
1	B	329	PRO	2.0
1	B	251	VAL	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 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.

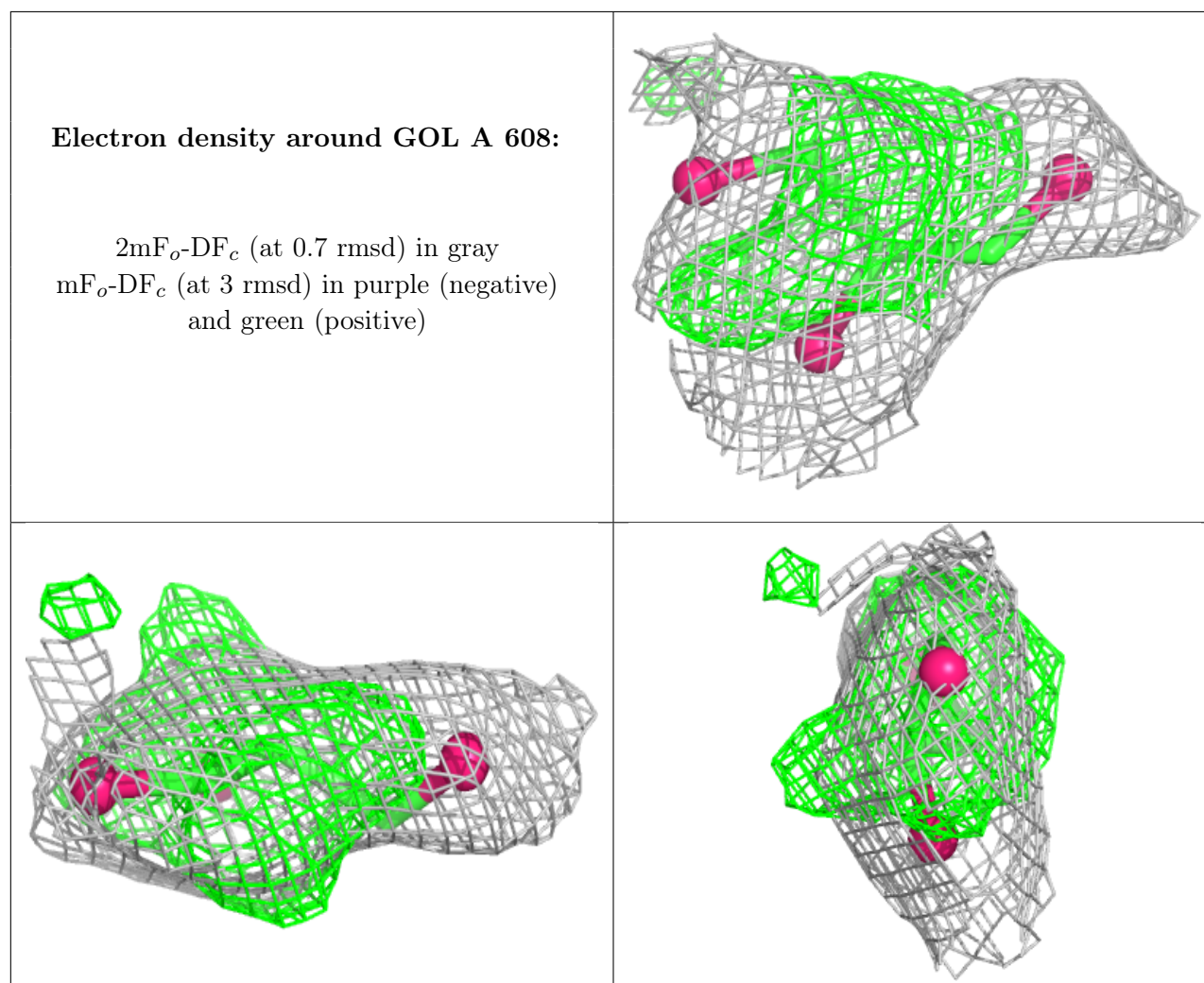
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	608	6/6	0.70	0.28	45,46,47,49	6
4	PEG	B	603	7/7	0.76	0.23	47,49,52,53	7
5	GOL	A	607	6/6	0.79	0.37	41,42,44,49	6

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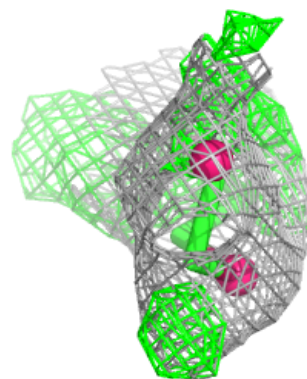
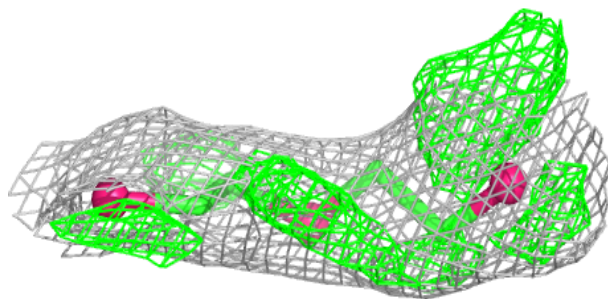
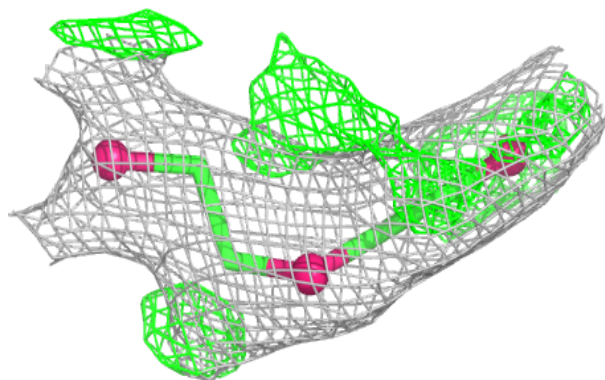
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	606	6/6	0.84	0.24	59,60,62,62	6
4	PEG	A	604	7/7	0.84	0.17	41,43,47,50	5
3	ANB	A	602	21/21	0.84	0.25	29,60,71,73	21
4	PEG	A	605	7/7	0.86	0.23	38,46,50,53	7
4	PEG	A	603	7/7	0.88	0.15	28,41,49,50	3
4	PEG	B	602	7/7	0.92	0.12	41,43,53,57	7
2	FAD	B	601	53/53	0.94	0.08	27,32,40,41	0
2	FAD	A	601	53/53	0.98	0.05	19,22,24,27	0
6	NA	A	609	1/1	0.98	0.11	28,28,28,28	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.



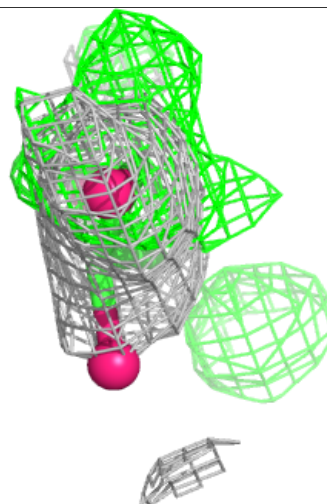
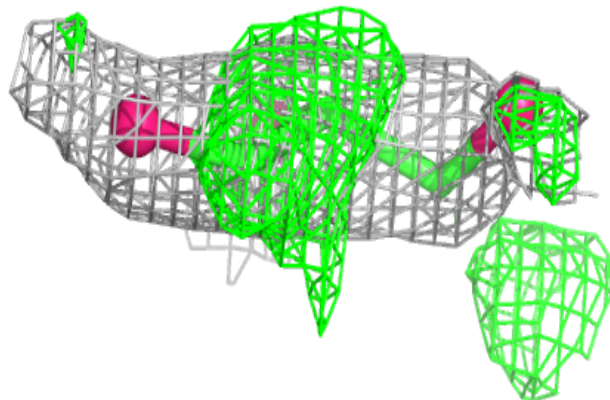
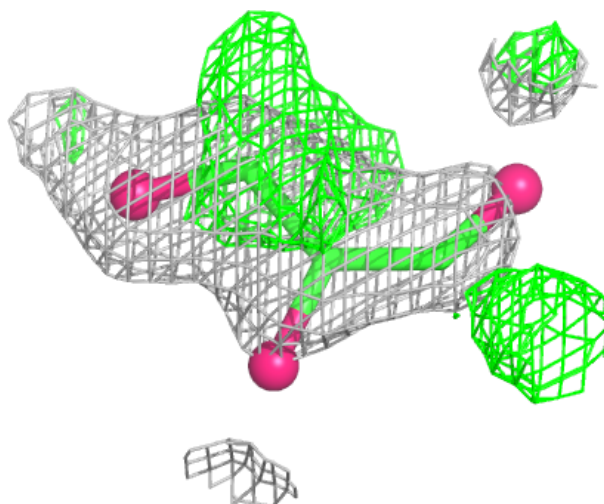
Electron density around PEG B 603:

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



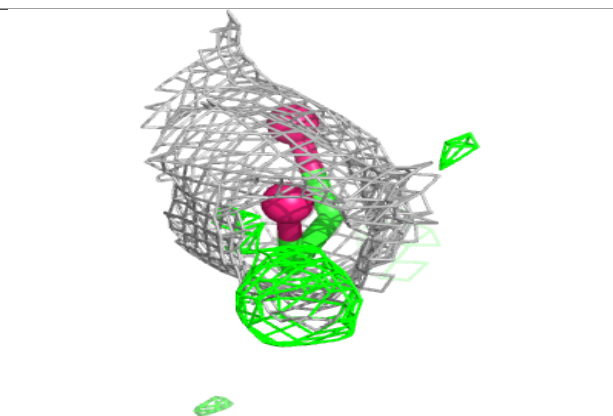
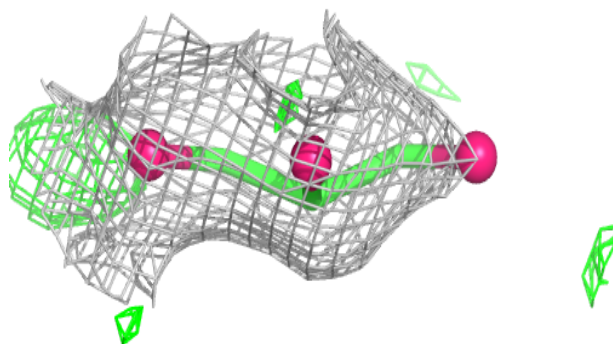
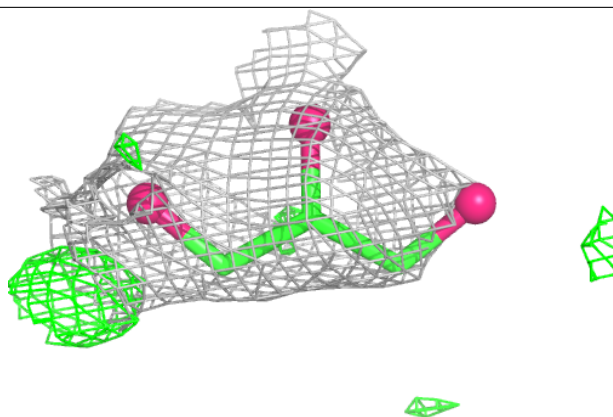
Electron density around GOL A 607:

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

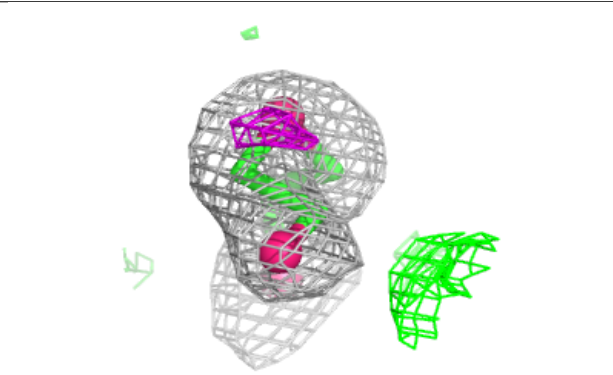
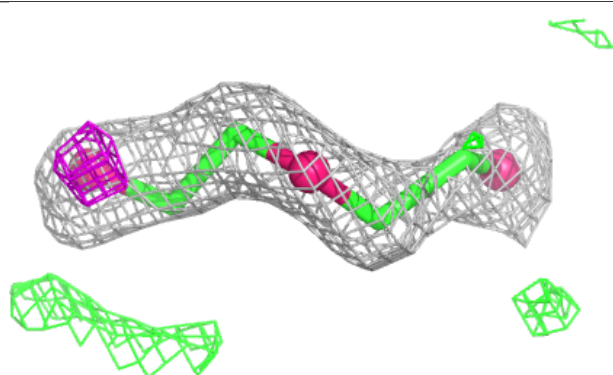
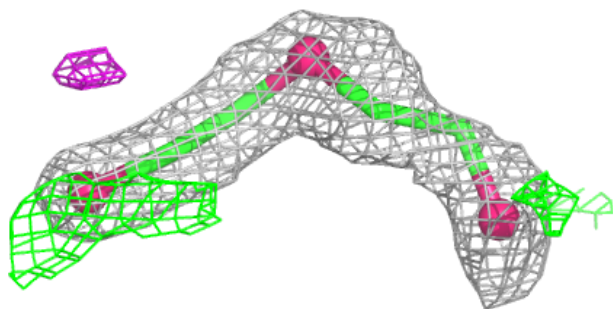


Electron density around GOL A 606:

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

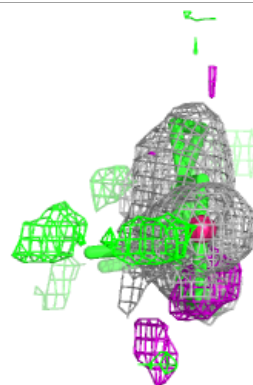
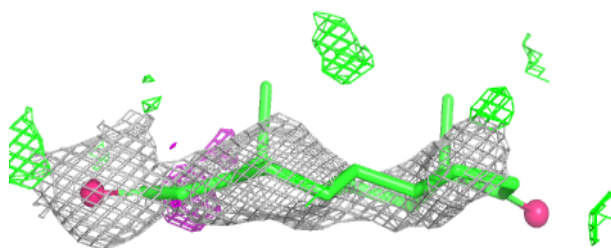
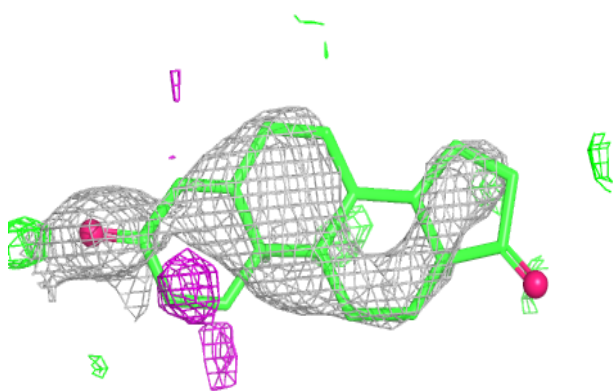
**Electron density around PEG A 604:**

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

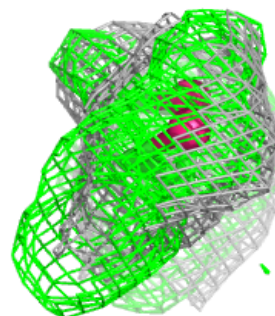
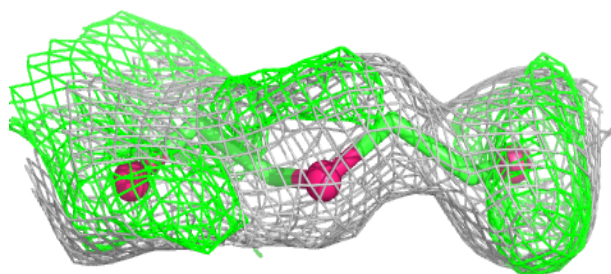
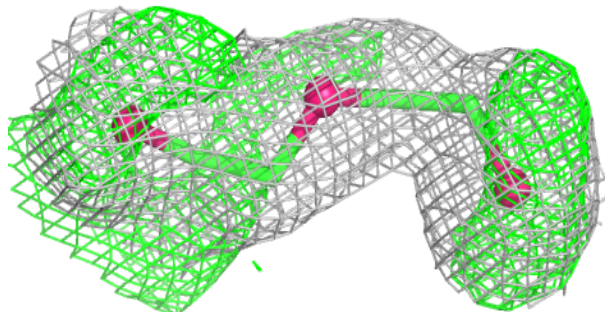


Electron density around ANB A 602:

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

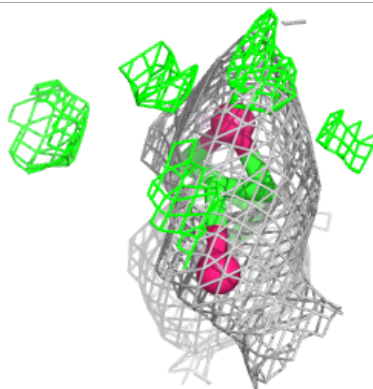
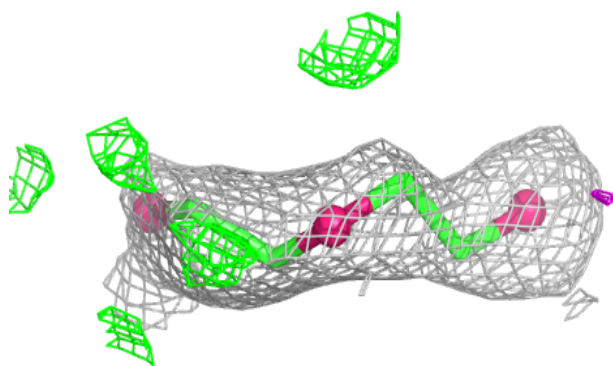
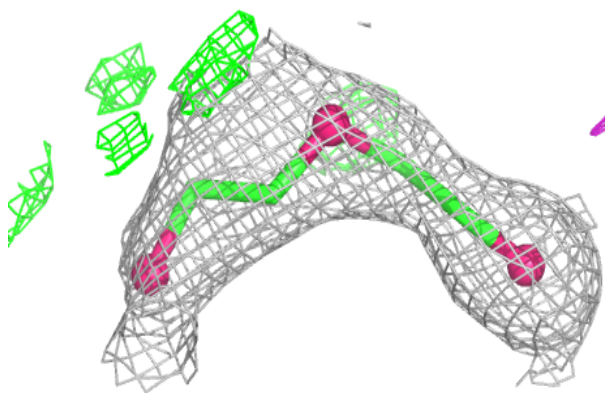
**Electron density around PEG A 605:**

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

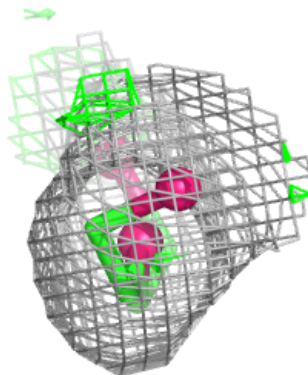
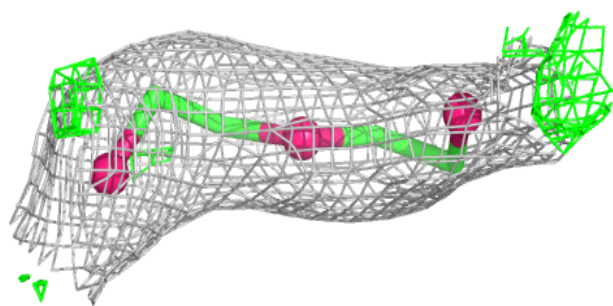
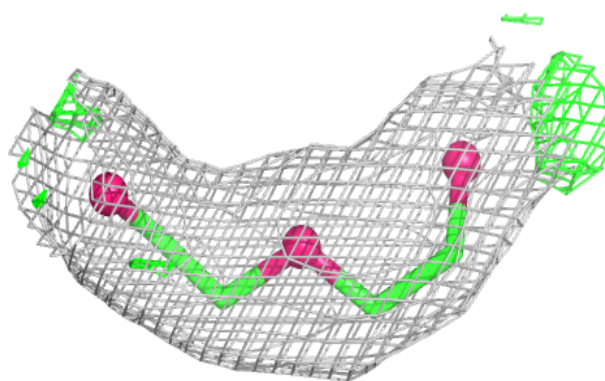


Electron density around PEG A 603:

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

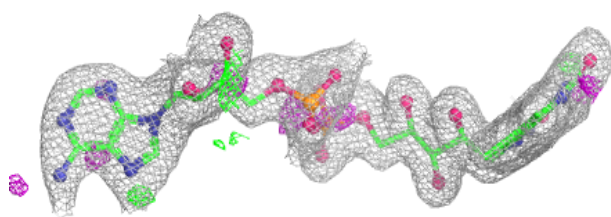
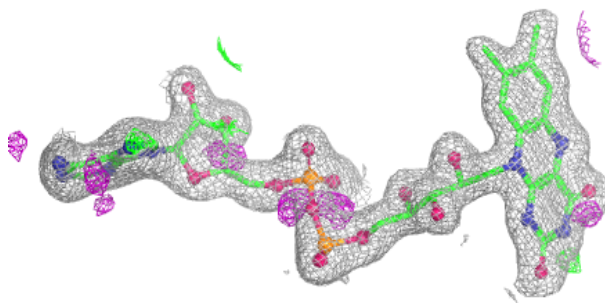
**Electron density around PEG B 602:**

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

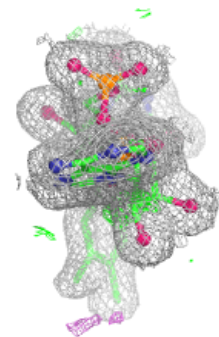
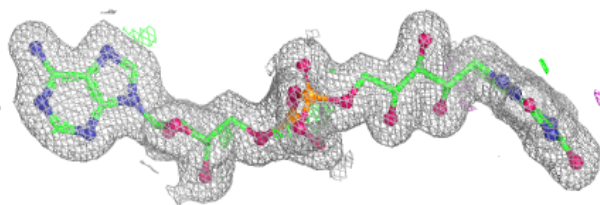
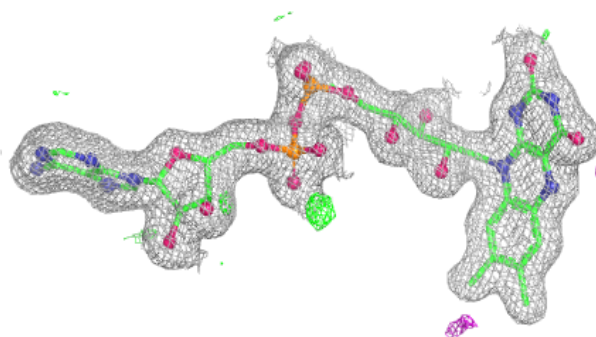


Electron density around FAD B 601:

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

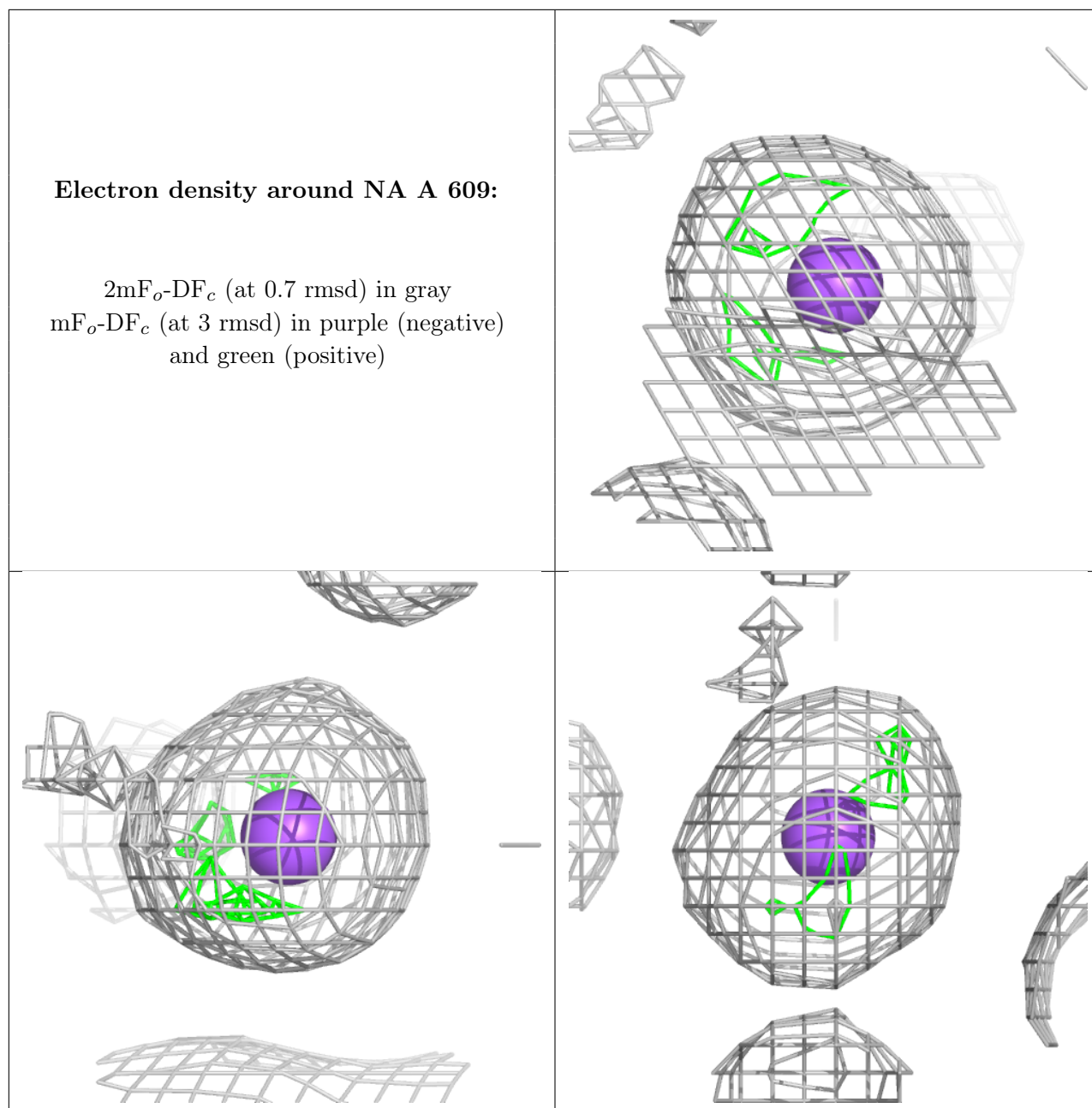
**Electron density around FAD A 601:**

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



Electron density around NA A 609:

$2mF_o-DF_c$ (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.