Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2023 – 01:11 pm GMT

PDB ID	:	7QOX
Title	:	Factor XI and Plasma Kallikrein apple domain structures reveals different kininogen bound complexes
Authors	:	Li, C.; Awital, B.; Wong, S.; Dreveny, I.; Meijers, J.; Emsley, J.
Deposited on	:	2021-12-29
Resolution	:	2.32 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:

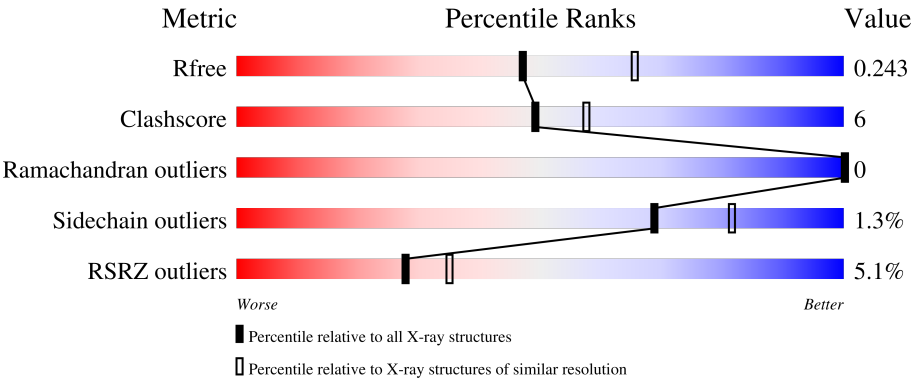
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	367	2% 86% 11%
1	B	367	5% 85% 11%
2	C	29	24% 76%
2	D	29	45% 66% 31%

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
4	PEG	B	406	-	-	-	X
7	NAG	A	408	X	-	-	X
7	NAG	B	410	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6368 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 Plasma kallikrein heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	1	0	0
			2794	1754	485	522	33			
1	B	355	Total	C	N	O	S	10	0	0
			2768	1739	481	515	33			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ARG	-	expression tag	UNP P03952
A	-6	SER	-	expression tag	UNP P03952
A	-5	HIS	-	expression tag	UNP P03952
A	-4	HIS	-	expression tag	UNP P03952
A	-3	HIS	-	expression tag	UNP P03952
A	-2	HIS	-	expression tag	UNP P03952
A	-1	HIS	-	expression tag	UNP P03952
A	0	HIS	-	expression tag	UNP P03952
A	323	ALA	GLU	conflict	UNP P03952
A	325	ALA	LYS	conflict	UNP P03952
B	-7	ARG	-	expression tag	UNP P03952
B	-6	SER	-	expression tag	UNP P03952
B	-5	HIS	-	expression tag	UNP P03952
B	-4	HIS	-	expression tag	UNP P03952
B	-3	HIS	-	expression tag	UNP P03952
B	-2	HIS	-	expression tag	UNP P03952
B	-1	HIS	-	expression tag	UNP P03952
B	0	HIS	-	expression tag	UNP P03952
B	323	ALA	GLU	conflict	UNP P03952
B	325	ALA	LYS	conflict	UNP P03952

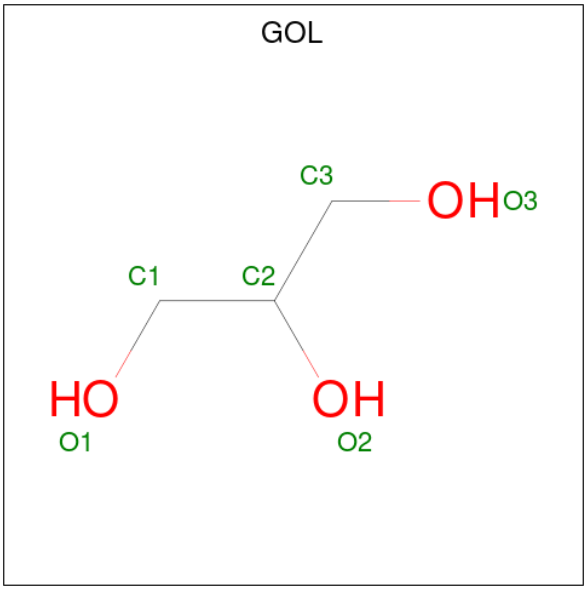
- Molecule 2 is a protein called Kininogen-1 light chain.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	29	Total C N O 230 144 34 52	38	0	0
2	C	7	Total C N O 55 36 7 12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

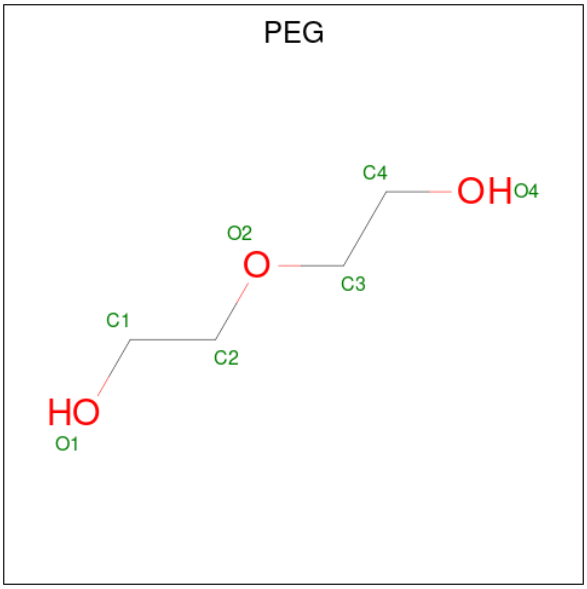
Chain	Residue	Modelled	Actual	Comment	Reference
D	563	THR	-	expression tag	UNP P01042
C	563	THR	-	expression tag	UNP P01042

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



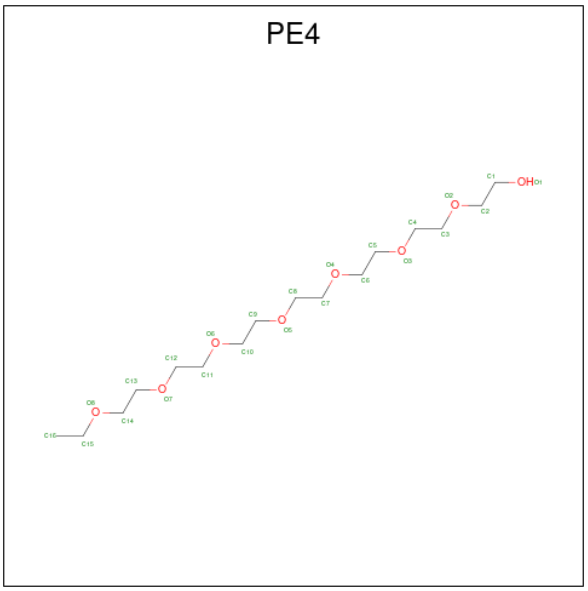
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

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



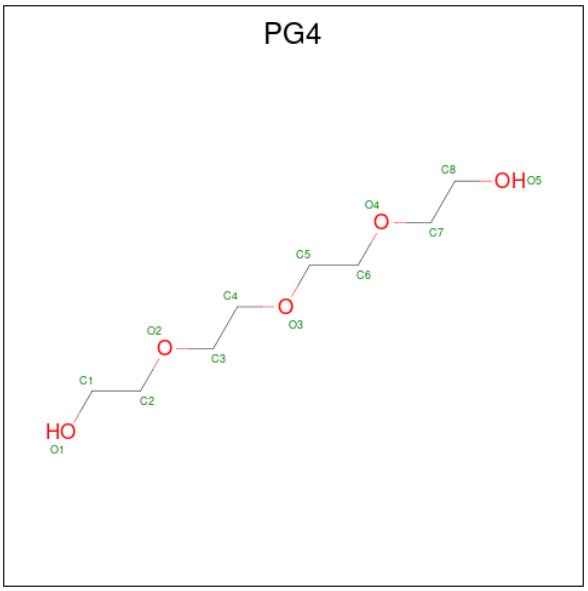
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0

- Molecule 5 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY) -ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 24 16 8	0	0
5	B	1	Total C O 24 16 8	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 8 5	0	0

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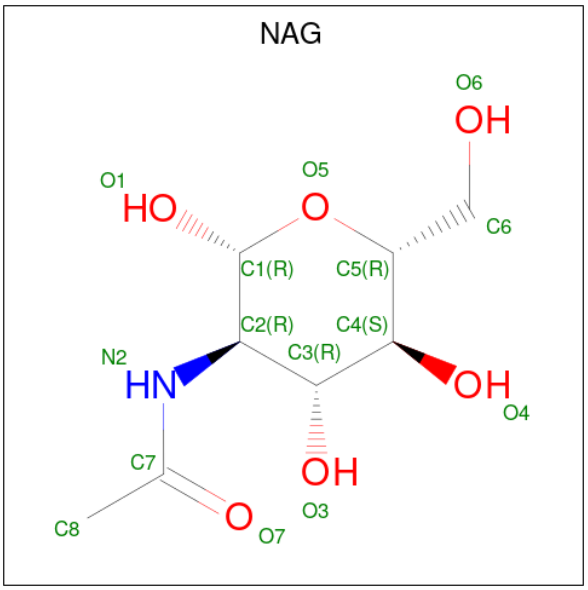
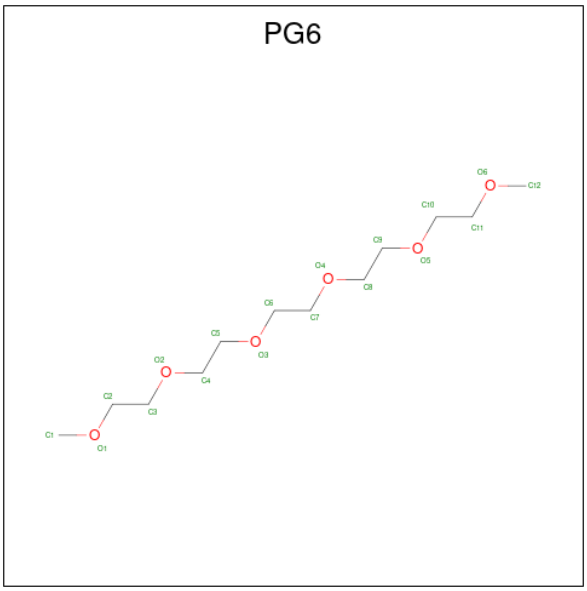
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 8 5	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: $C_{12}H_{26}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 18 12 6	0	0

- Molecule 9 is water.

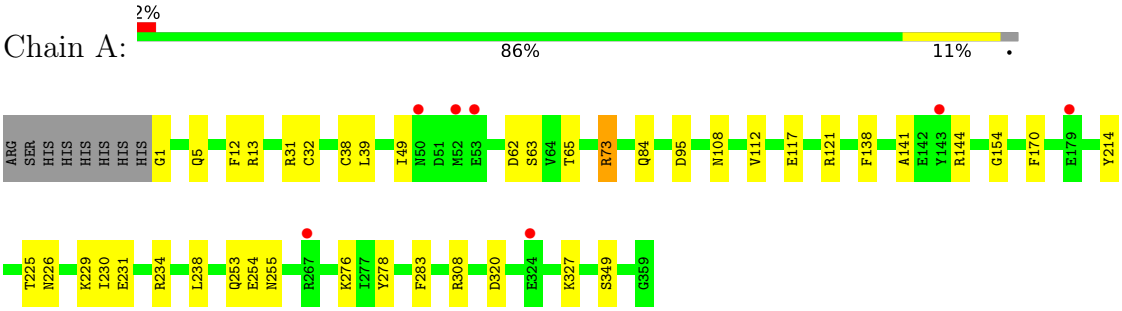
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	187	Total O 187 187	0	0
9	B	132	Total O 132 132	0	0
9	D	9	Total O 9 9	0	0
9	C	2	Total O 2 2	0	0

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.

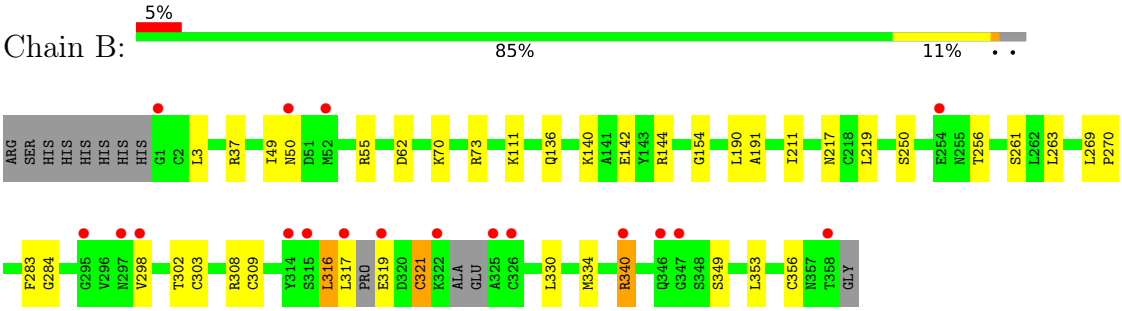
• Molecule 1: Plasma kallikrein heavy chain

Chain A:



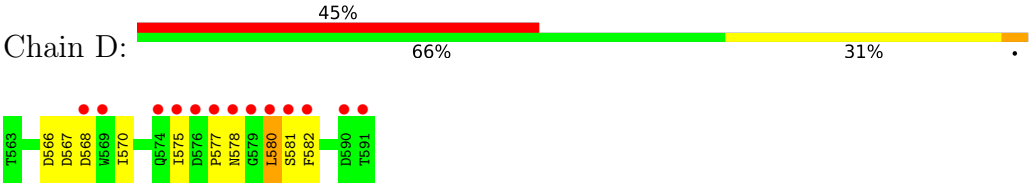
• Molecule 1: Plasma kallikrein heavy chain

Chain B:



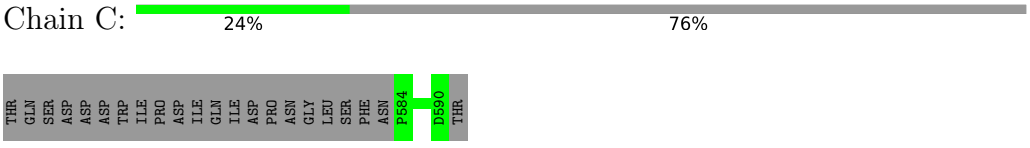
• Molecule 2: Kininogen-1 light chain

Chain D:



• Molecule 2: Kininogen-1 light chain

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.54Å 68.26Å 120.31Å 90.00° 96.55° 90.00°	Depositor
Resolution (Å)	29.64 – 2.32 29.64 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.64-2.32) 99.2 (29.64-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.199 , 0.253 0.203 , 0.243	Depositor DCC
R_{free} test set	1935 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6368	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, PG4, PE4, PEG, PG6

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	0.35	1/2858 (0.0%)	0.67	2/3862 (0.1%)
1	B	0.35	0/2829	0.64	0/3820
2	C	0.40	0/57	0.58	0/77
2	D	0.59	0/237	0.91	0/327
All	All	0.36	1/5981 (0.0%)	0.66	2/8086 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	ARG	C-N	-5.58	1.21	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	13	ARG	O-C-N	6.25	133.82	123.20
1	A	62	ASP	C-N-CA	5.74	136.04	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	73	ARG	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2794	0	2706	30	0
1	B	2768	0	2683	29	0
2	C	55	0	47	0	0
2	D	230	0	198	5	0
3	A	6	0	8	0	0
3	B	30	0	40	3	0
4	A	21	0	30	3	0
4	B	14	0	20	0	0
5	A	24	0	34	4	0
5	B	24	0	34	2	0
6	A	26	0	36	2	0
7	A	14	0	13	3	0
7	B	14	0	13	0	0
8	B	18	0	26	2	0
9	A	187	0	0	1	0
9	B	132	0	0	2	0
9	C	2	0	0	0	0
9	D	9	0	0	0	0
All	All	6368	0	5888	70	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 6.

All (70) 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:219:LEU:HD23	3:B:402:GOL:H32	1.65	0.77
1:B:284:GLY:HA3	1:B:340:ARG:HG3	1.71	0.72
1:B:37:ARG:HD3	1:B:334:MET:HA	1.72	0.71
1:B:37:ARG:NH1	1:B:334:MET:O	2.23	0.71
1:B:269:LEU:HD12	1:B:270:PRO:HD2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LEU:HD12	9:B:623:HOH:O	1.92	0.69
1:A:5:GLN:NE2	9:A:502:HOH:O	2.25	0.68
1:A:170:PHE:HB3	4:A:404:PEG:H11	1.76	0.68
1:A:63:SER:OG	1:A:65:THR:HG22	1.98	0.63
1:B:317:LEU:C	1:B:319:GLU:HA	2.21	0.60
1:A:112:VAL:HG13	1:A:117:GLU:HB3	1.83	0.60
2:D:575:ILE:HG13	2:D:577:PRO:HD3	1.83	0.59
8:B:409:PG6:H112	9:B:581:HOH:O	2.02	0.59
1:B:140:LYS:HE3	1:B:142:GLU:OE1	2.03	0.59
1:B:263:LEU:HD23	3:B:402:GOL:H2	1.85	0.59
1:A:214:TYR:HB2	6:A:407:PG4:H31	1.86	0.58
1:A:229:LYS:HG3	1:A:230:ILE:HD12	1.88	0.56
1:A:226:ASN:HA	1:A:234:ARG:HG2	1.88	0.56
1:B:261:SER:OG	3:B:402:GOL:H31	2.05	0.56
1:B:70:LYS:NZ	5:B:408:PE4:H72	2.22	0.55
1:A:320:ASP:HB3	1:A:327:LYS:HG2	1.89	0.55
1:A:108:ASN:OD1	7:A:408:NAG:H2	2.06	0.54
1:B:309:CYS:SG	1:B:330:LEU:HG	2.48	0.54
1:B:316:LEU:HA	1:B:321:CYS:SG	2.48	0.53
1:A:12:PHE:CE1	5:A:405:PE4:H163	2.45	0.52
1:B:190:LEU:HD11	1:B:250:SER:HB2	1.91	0.52
1:B:317:LEU:O	1:B:319:GLU:HA	2.09	0.52
1:A:121:ARG:HG2	7:A:408:NAG:H82	1.93	0.49
1:B:136:GLN:O	1:B:144:ARG:HD3	2.12	0.49
1:A:253:GLN:HA	4:A:402:PEG:H41	1.95	0.49
1:B:111:LYS:NZ	1:B:144:ARG:O	2.44	0.48
1:A:141:ALA:HA	1:A:144:ARG:HG3	1.96	0.48
5:A:405:PE4:H51	5:A:405:PE4:H71	1.68	0.47
1:A:276:LYS:HD3	1:A:278:TYR:CE2	2.50	0.47
1:A:112:VAL:HG22	1:A:117:GLU:OE1	2.15	0.47
1:A:231:GLU:HA	1:A:234:ARG:HD2	1.97	0.47
1:B:211:ILE:HD11	8:B:409:PG6:H123	1.96	0.46
2:D:578:ASN:C	2:D:580:LEU:H	2.17	0.46
1:B:49:ILE:CG1	1:B:50:ASN:H	2.28	0.46
1:B:283:PHE:CD2	1:B:349:SER:HB3	2.51	0.46
2:D:580:LEU:O	2:D:581:SER:C	2.55	0.46
7:A:408:NAG:N2	7:A:408:NAG:H5	2.30	0.45
1:A:49:ILE:HG13	1:A:73:ARG:HH21	1.82	0.45
1:A:63:SER:HG	1:A:65:THR:HG22	1.80	0.45
2:D:581:SER:O	2:D:582:PHE:HB2	2.17	0.45
1:A:320:ASP:HB3	1:A:327:LYS:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ASN:HA	1:B:55:ARG:HH21	1.82	0.44
1:A:138:PHE:O	1:A:144:ARG:NH1	2.46	0.44
6:A:407:PG4:H71	6:A:407:PG4:H51	1.69	0.44
1:A:49:ILE:HG13	1:A:73:ARG:NH2	2.32	0.43
1:B:298:VAL:O	1:B:302:THR:HG23	2.18	0.43
5:A:405:PE4:H162	5:A:405:PE4:H141	1.84	0.43
1:A:283:PHE:CD2	1:A:349:SER:HB3	2.53	0.43
1:A:32:CYS:O	1:A:38:CYS:HB3	2.19	0.43
1:B:70:LYS:HZ3	5:B:408:PE4:H72	1.83	0.43
1:B:353:LEU:HB3	1:B:356:CYS:SG	2.59	0.42
1:B:191:ALA:HB2	1:B:256:THR:HG21	2.00	0.42
1:A:225:THR:OG1	1:A:255:ASN:HB3	2.20	0.42
1:A:112:VAL:HG13	1:A:117:GLU:OE1	2.20	0.42
1:A:1:GLY:HA2	1:A:84:GLN:OE1	2.20	0.42
5:A:405:PE4:H82	5:A:405:PE4:H102	1.83	0.42
1:A:31:ARG:NH2	1:A:154:GLY:O	2.46	0.41
2:D:575:ILE:HD11	2:D:577:PRO:HG3	2.03	0.41
1:B:303:CYS:O	1:B:309:CYS:HB3	2.20	0.41
1:B:62:ASP:OD2	1:B:308:ARG:NH1	2.54	0.41
1:A:254:GLU:HB2	4:A:402:PEG:H32	2.03	0.41
1:B:190:LEU:O	1:B:256:THR:HG22	2.21	0.40
1:A:39:LEU:HD11	1:A:308:ARG:HG2	2.02	0.40
1:B:154:GLY:H	1:B:217:ASN:HD21	1.70	0.40
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/367 (97%)	351 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	349/367 (95%)	344 (99%)	5 (1%)	0	100	100
2	C	5/29 (17%)	5 (100%)	0	0	100	100
2	D	27/29 (93%)	23 (85%)	4 (15%)	0	100	100
All	All	738/792 (93%)	723 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/326 (98%)	317 (100%)	1 (0%)	92	96
1	B	316/326 (97%)	313 (99%)	3 (1%)	78	89
2	C	7/28 (25%)	7 (100%)	0	100	100
2	D	28/28 (100%)	23 (82%)	5 (18%)	2	1
All	All	669/708 (94%)	660 (99%)	9 (1%)	69	81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASP
1	B	316	LEU
1	B	321	CYS
1	B	340	ARG
2	D	566	ASP
2	D	567	ASP
2	D	568	ASP
2	D	570	ILE
2	D	580	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	B	402	-	5,5,5	0.10	0	5,5,5	0.32	0
4	PEG	B	407	-	6,6,6	0.11	0	5,5,5	0.08	0
6	PG4	A	406	-	12,12,12	0.13	0	11,11,11	0.14	0
8	PG6	B	409	-	17,17,17	0.11	0	16,16,16	0.20	0
5	PE4	A	405	-	23,23,23	0.12	0	22,22,22	0.13	0
3	GOL	B	404	-	5,5,5	0.10	0	5,5,5	0.31	0
6	PG4	A	407	-	12,12,12	0.12	0	11,11,11	0.17	0
4	PEG	B	406	-	6,6,6	0.12	0	5,5,5	0.10	0
7	NAG	A	408	1	14,14,15	0.47	0	17,19,21	0.80	1 (5%)
4	PEG	A	403	-	6,6,6	0.14	0	5,5,5	0.09	0
3	GOL	B	401	-	5,5,5	0.09	0	5,5,5	0.29	0
7	NAG	B	410	1	14,14,15	0.36	0	17,19,21	0.97	1 (5%)
5	PE4	B	408	-	23,23,23	0.11	0	22,22,22	0.16	0
3	GOL	B	405	-	5,5,5	0.08	0	5,5,5	0.34	0
3	GOL	B	403	-	5,5,5	0.09	0	5,5,5	0.36	0
4	PEG	A	402	-	6,6,6	0.11	0	5,5,5	0.12	0
3	GOL	A	401	-	5,5,5	0.10	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PEG	A	404	-	6,6,6	0.10	0	5,5,5	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	402	-	-	0/4/4/4	-
4	PEG	B	407	-	-	3/4/4/4	-
6	PG4	A	406	-	-	6/10/10/10	-
8	PG6	B	409	-	-	9/15/15/15	-
7	NAG	A	408	1	1/1/5/7	5/6/23/26	0/1/1/1
3	GOL	B	404	-	-	3/4/4/4	-
5	PE4	A	405	-	-	10/21/21/21	-
4	PEG	B	406	-	-	4/4/4/4	-
6	PG4	A	407	-	-	6/10/10/10	-
4	PEG	A	403	-	-	2/4/4/4	-
3	GOL	B	401	-	-	3/4/4/4	-
7	NAG	B	410	1	-	5/6/23/26	0/1/1/1
5	PE4	B	408	-	-	10/21/21/21	-
3	GOL	B	405	-	-	4/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-
4	PEG	A	402	-	-	3/4/4/4	-
3	GOL	A	401	-	-	2/4/4/4	-
4	PEG	A	404	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	410	NAG	C1-O5-C5	-2.39	108.96	112.19
7	A	408	NAG	O5-C5-C6	2.02	110.37	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	408	NAG	C1

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	GOL	O1-C1-C2-C3
3	B	405	GOL	O1-C1-C2-O2
3	B	405	GOL	O1-C1-C2-C3
3	B	405	GOL	C1-C2-C3-O3
7	A	408	NAG	C3-C2-N2-C7
7	A	408	NAG	C8-C7-N2-C2
7	A	408	NAG	O7-C7-N2-C2
7	B	410	NAG	C8-C7-N2-C2
7	B	410	NAG	O7-C7-N2-C2
5	B	408	PE4	O6-C11-C12-O7
6	A	406	PG4	O3-C5-C6-O4
6	A	407	PG4	O3-C5-C6-O4
6	A	406	PG4	O2-C3-C4-O3
7	B	410	NAG	C1-C2-N2-C7
8	B	409	PG6	O4-C8-C9-O5
4	A	402	PEG	C1-C2-O2-C3
5	A	405	PE4	O6-C10-C9-O5
8	B	409	PG6	O2-C4-C5-O3
5	A	405	PE4	O4-C7-C8-O5
3	B	404	GOL	O1-C1-C2-O2
4	B	406	PEG	O1-C1-C2-O2
6	A	407	PG4	O4-C7-C8-O5
5	B	408	PE4	O4-C7-C8-O5
6	A	407	PG4	C5-C6-O4-C7
7	B	410	NAG	O5-C5-C6-O6
4	A	403	PEG	O1-C1-C2-O2
4	A	404	PEG	O2-C3-C4-O4
4	B	407	PEG	O1-C1-C2-O2
5	B	408	PE4	O1-C1-C2-O2
6	A	406	PG4	O4-C7-C8-O5
5	A	405	PE4	C5-C6-O4-C7
3	A	401	GOL	C1-C2-C3-O3
3	B	401	GOL	C1-C2-C3-O3
5	B	408	PE4	O7-C13-C14-O8
3	A	401	GOL	O2-C2-C3-O3
3	B	405	GOL	O2-C2-C3-O3
6	A	407	PG4	C1-C2-O2-C3
8	B	409	PG6	O1-C2-C3-O2
8	B	409	PG6	C9-C8-O4-C7
5	A	405	PE4	O2-C3-C4-O3
7	A	408	NAG	O5-C5-C6-O6
7	B	410	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	405	PE4	C10-C9-O5-C8
3	B	401	GOL	O2-C2-C3-O3
4	A	402	PEG	O2-C3-C4-O4
8	B	409	PG6	O5-C10-C11-O6
6	A	406	PG4	C3-C4-O3-C5
5	A	405	PE4	C14-C13-O7-C12
4	B	406	PEG	C4-C3-O2-C2
6	A	406	PG4	C5-C6-O4-C7
8	B	409	PG6	C5-C4-O2-C3
6	A	406	PG4	C8-C7-O4-C6
5	A	405	PE4	C11-C12-O7-C13
3	B	404	GOL	O2-C2-C3-O3
5	A	405	PE4	C1-C2-O2-C3
5	A	405	PE4	C16-C15-O8-C14
8	B	409	PG6	C4-C5-O3-C6
5	B	408	PE4	C14-C13-O7-C12
4	B	407	PEG	C4-C3-O2-C2
4	A	403	PEG	C4-C3-O2-C2
5	B	408	PE4	C8-C7-O4-C6
5	B	408	PE4	C7-C8-O5-C9
5	B	408	PE4	C12-C11-O6-C10
6	A	407	PG4	C3-C4-O3-C5
4	A	404	PEG	C4-C3-O2-C2
4	B	407	PEG	C1-C2-O2-C3
6	A	407	PG4	O2-C3-C4-O3
4	B	406	PEG	O2-C3-C4-O4
5	A	405	PE4	O6-C11-C12-O7
5	B	408	PE4	C1-C2-O2-C3
5	B	408	PE4	C5-C6-O4-C7
4	A	402	PEG	C4-C3-O2-C2
7	A	408	NAG	C1-C2-N2-C7
8	B	409	PG6	C2-C3-O2-C4
4	B	406	PEG	C1-C2-O2-C3
8	B	409	PG6	C11-C10-O5-C9
3	B	401	GOL	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	GOL	3	0
8	B	409	PG6	2	0

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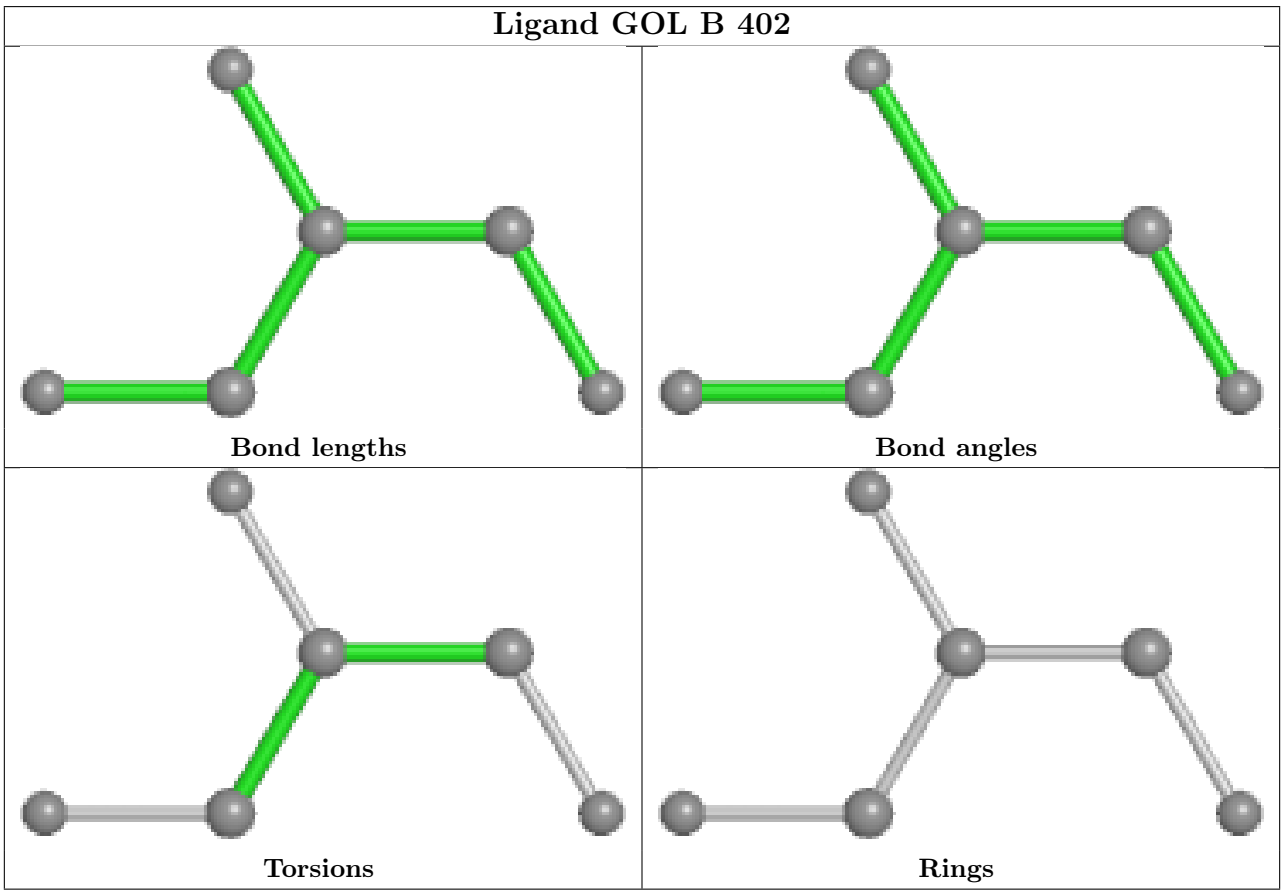
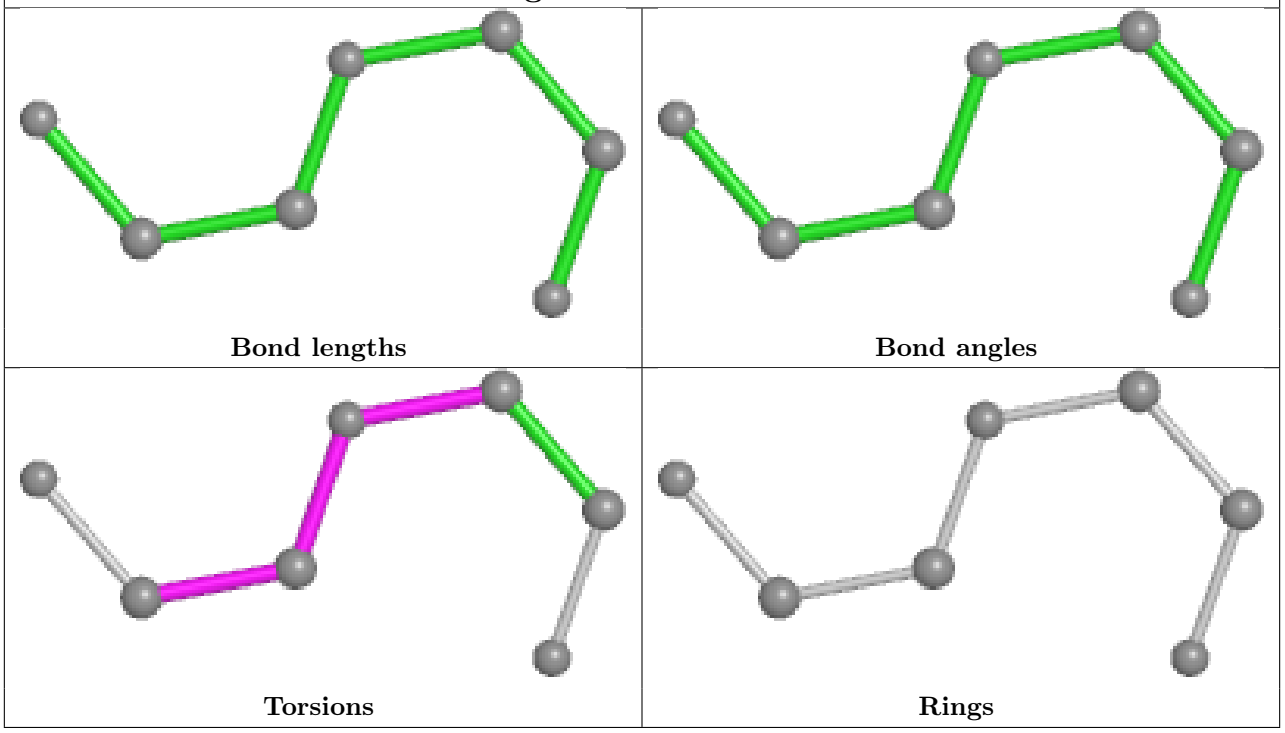
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	PE4	4	0
6	A	407	PG4	2	0
7	A	408	NAG	3	0
5	B	408	PE4	2	0
4	A	402	PEG	2	0
4	A	404	PEG	1	0

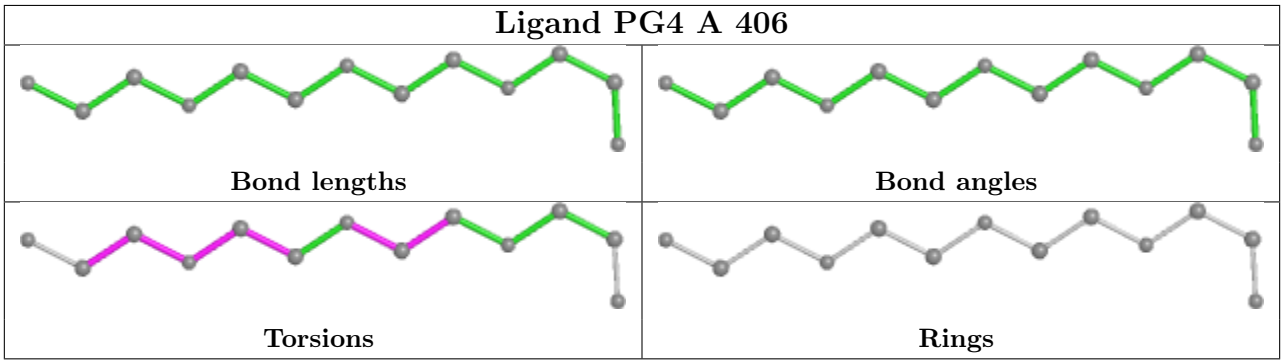
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



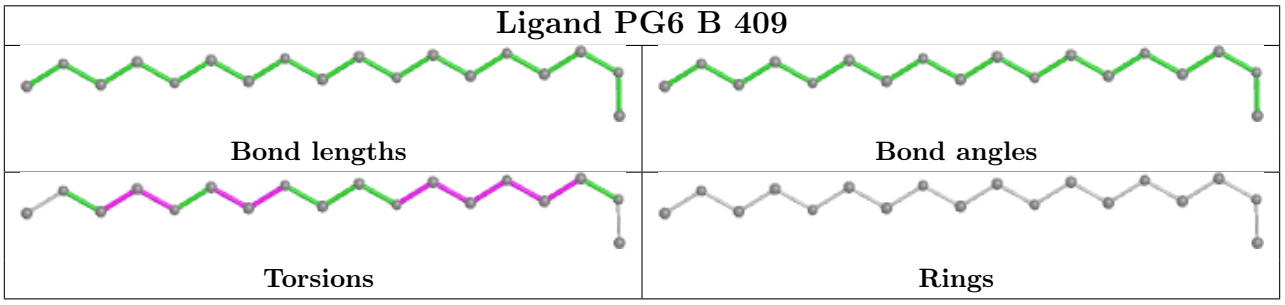
Ligand PEG B 407



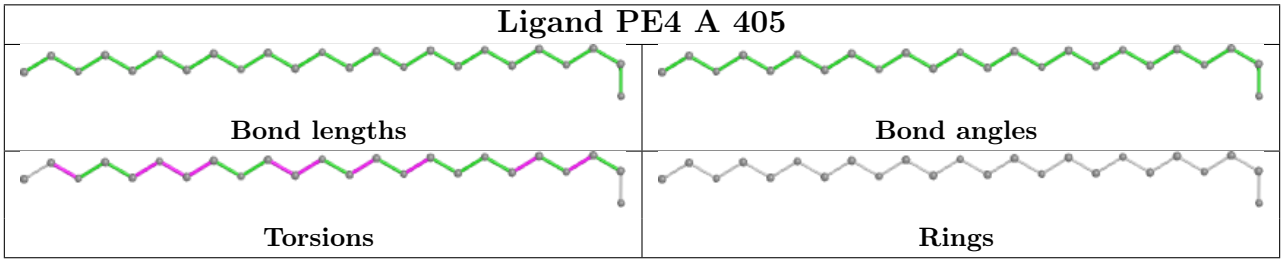
Ligand PG4 A 406



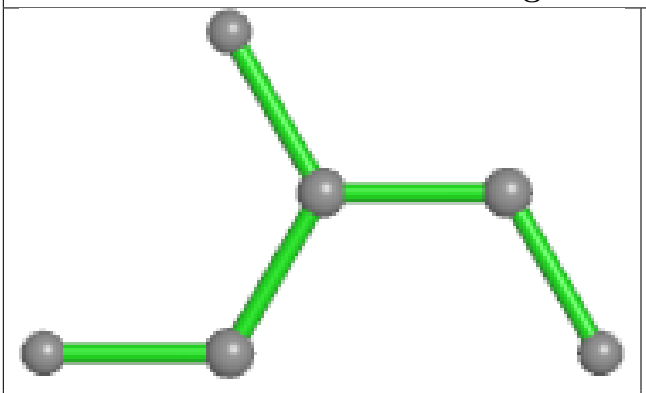
Ligand PG6 B 409



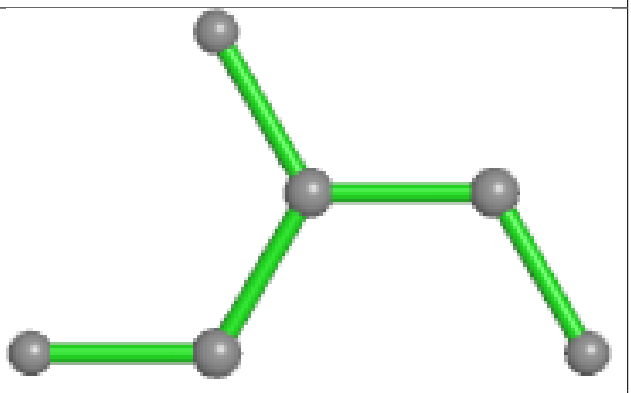
Ligand PE4 A 405



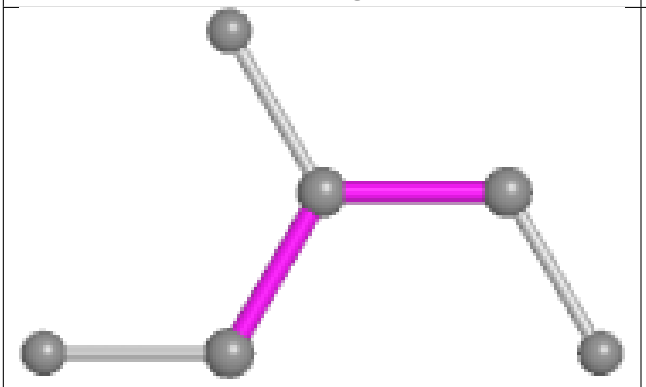
Ligand GOL B 404



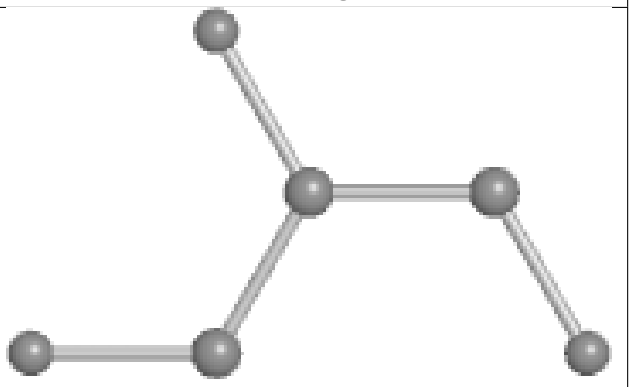
Bond lengths



Bond angles

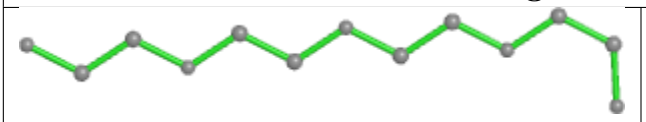


Torsions

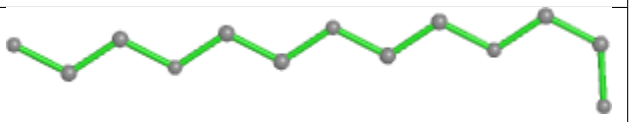


Rings

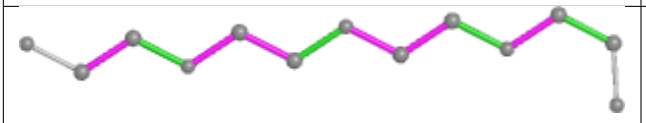
Ligand PG4 A 407



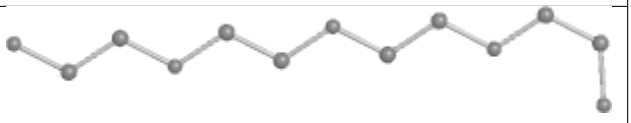
Bond lengths



Bond angles

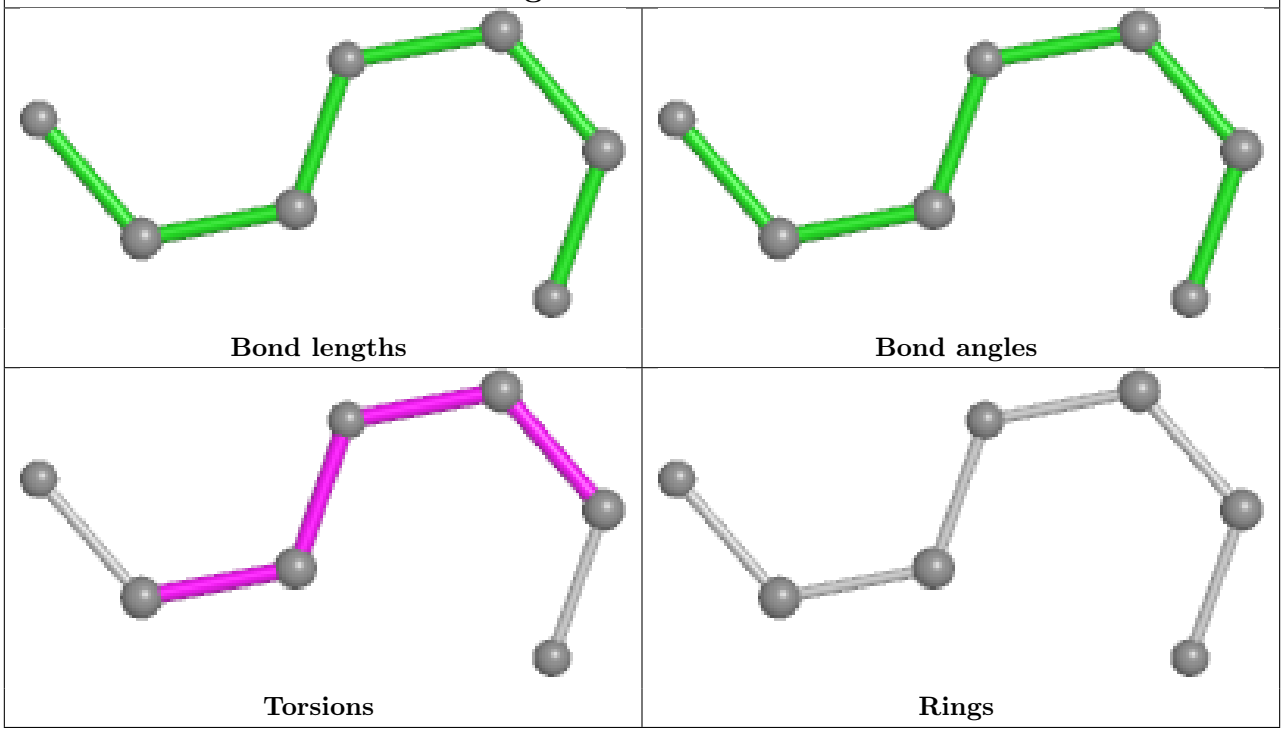


Torsions

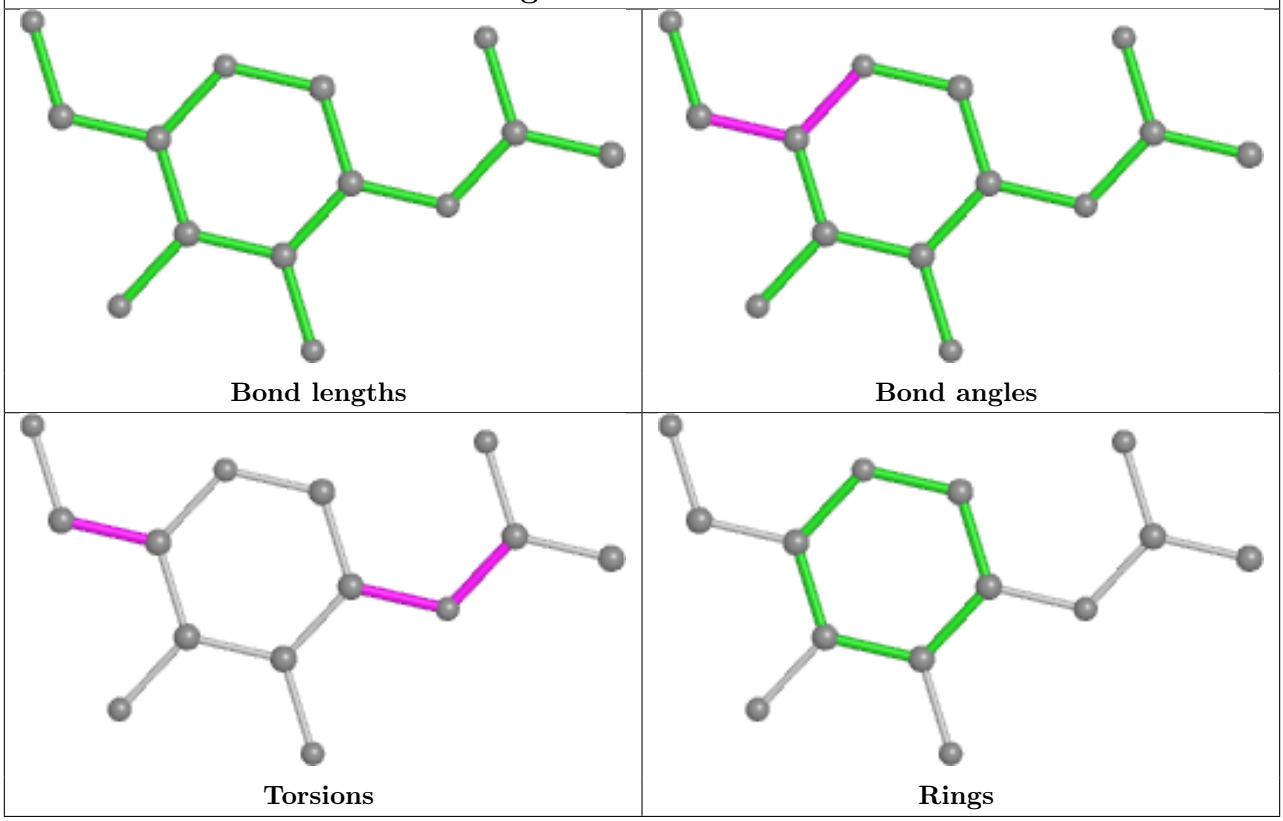


Rings

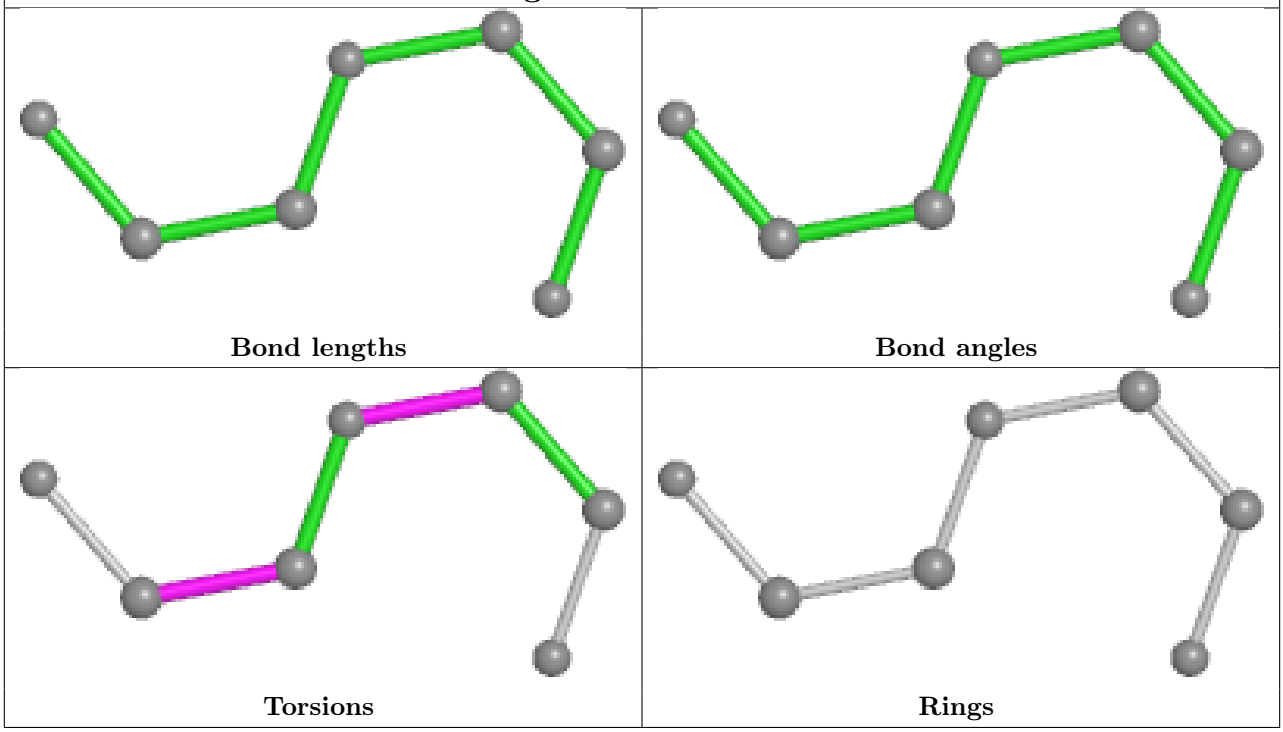
Ligand PEG B 406



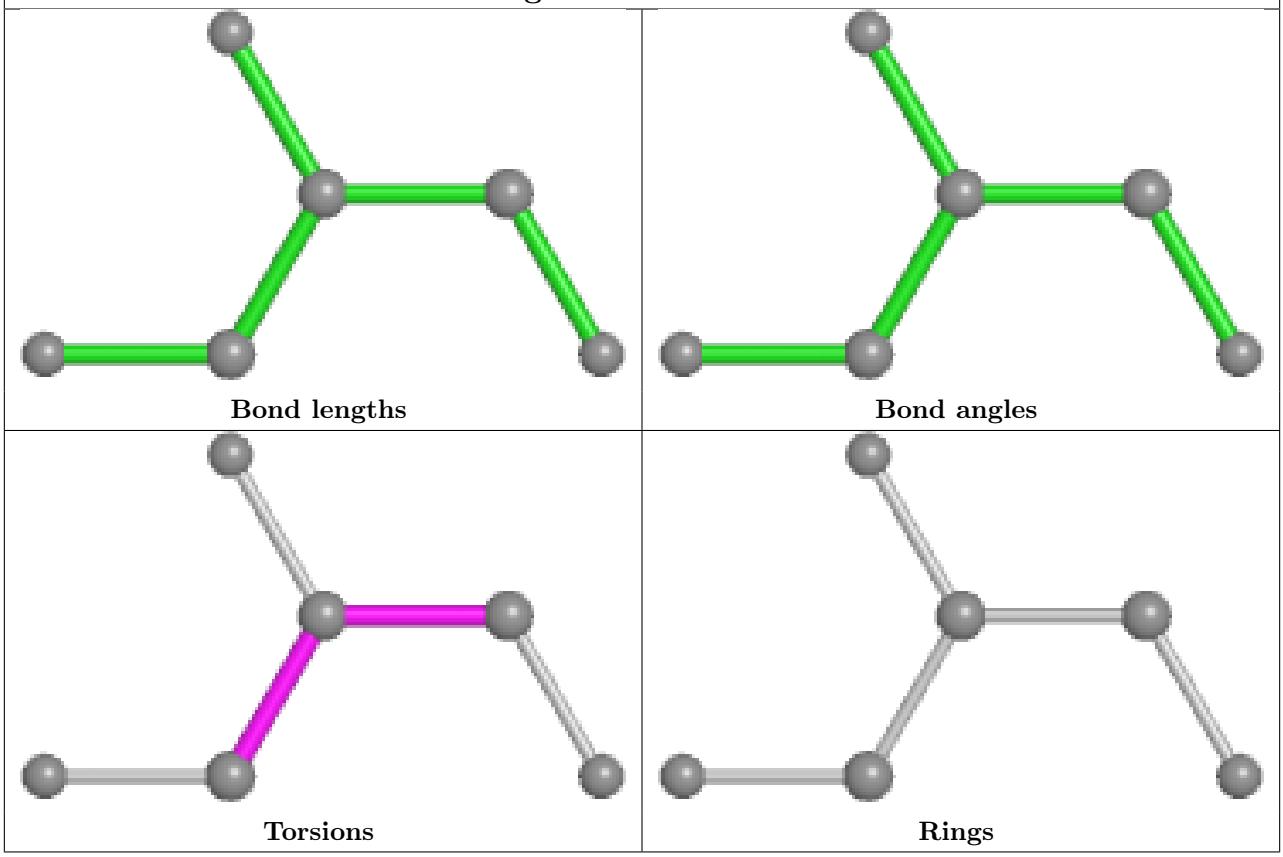
Ligand NAG A 408



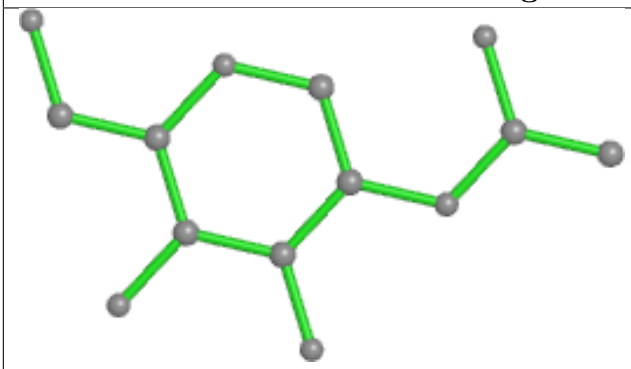
Ligand PEG A 403



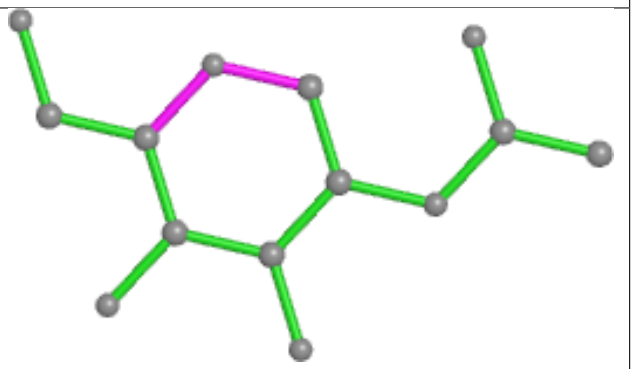
Ligand GOL B 401



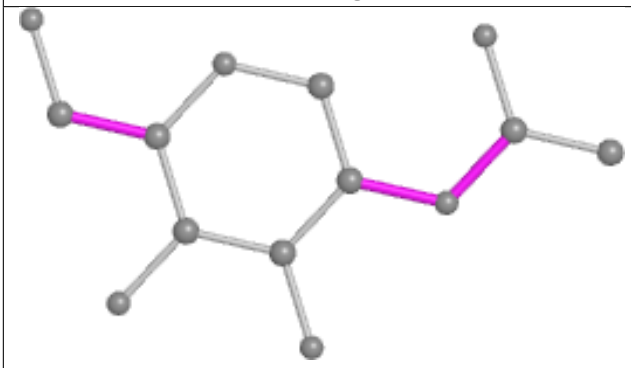
Ligand NAG B 410



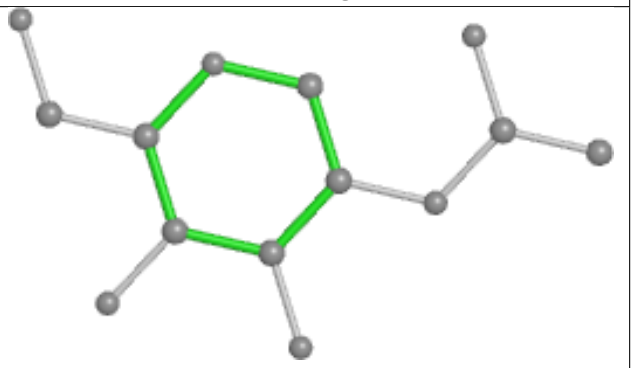
Bond lengths



Bond angles

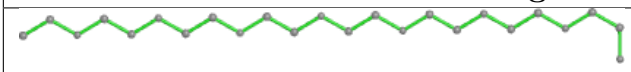


Torsions

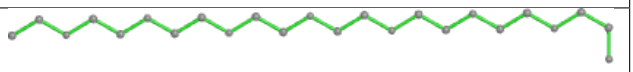


Rings

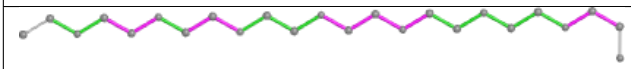
Ligand PE4 B 408



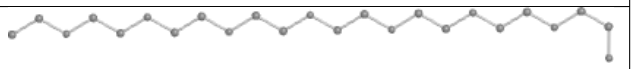
Bond lengths



Bond angles

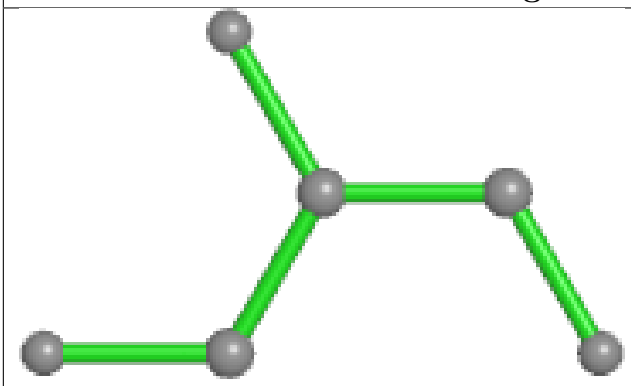


Torsions

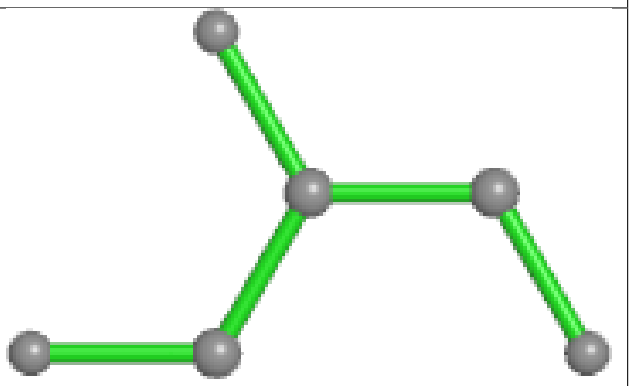


Rings

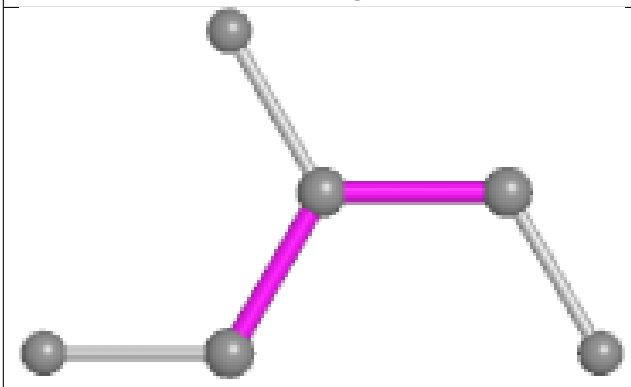
Ligand GOL B 405



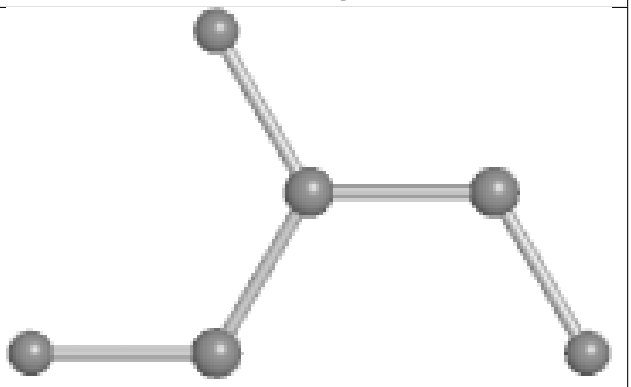
Bond lengths



Bond angles

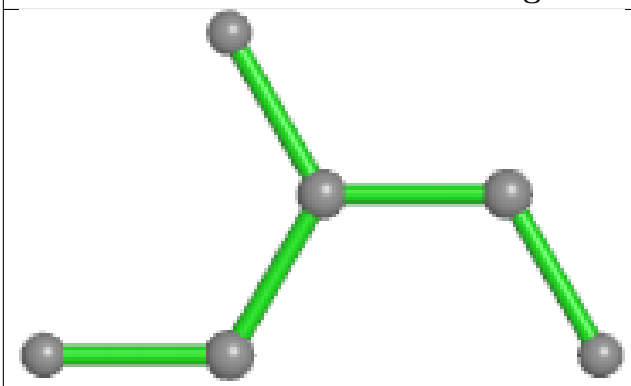


Torsions

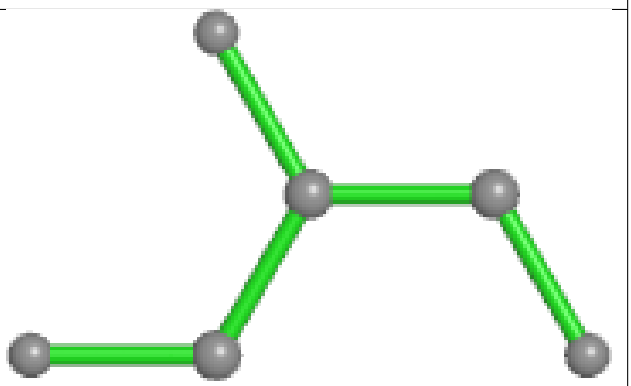


Rings

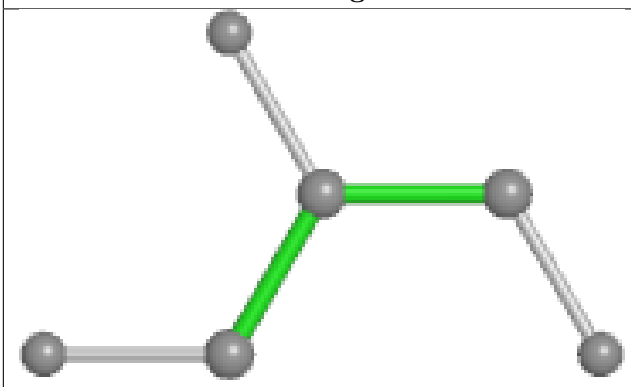
Ligand GOL B 403



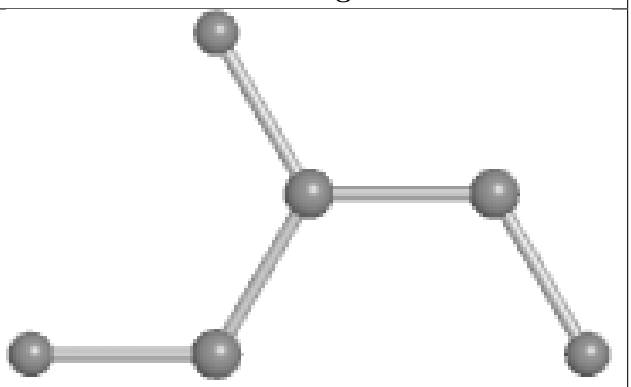
Bond lengths



Bond angles

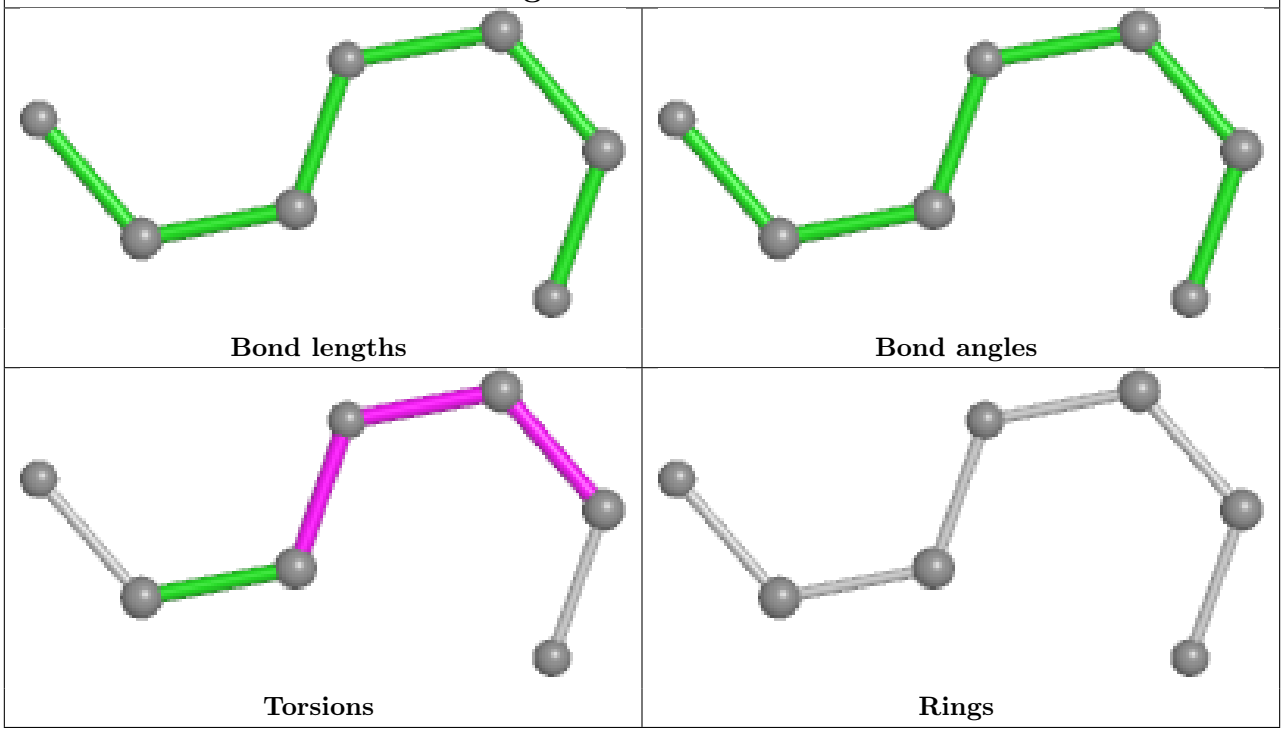


Torsions

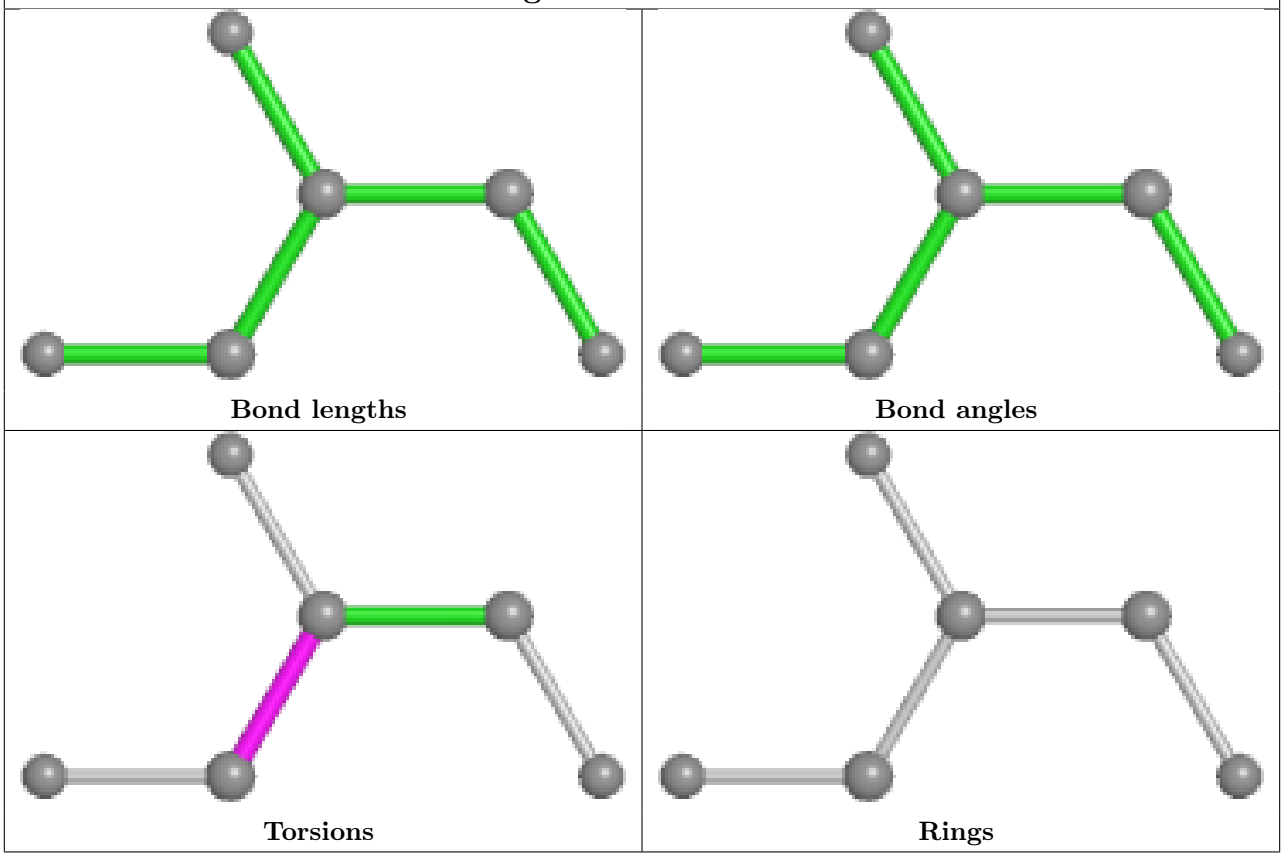


Rings

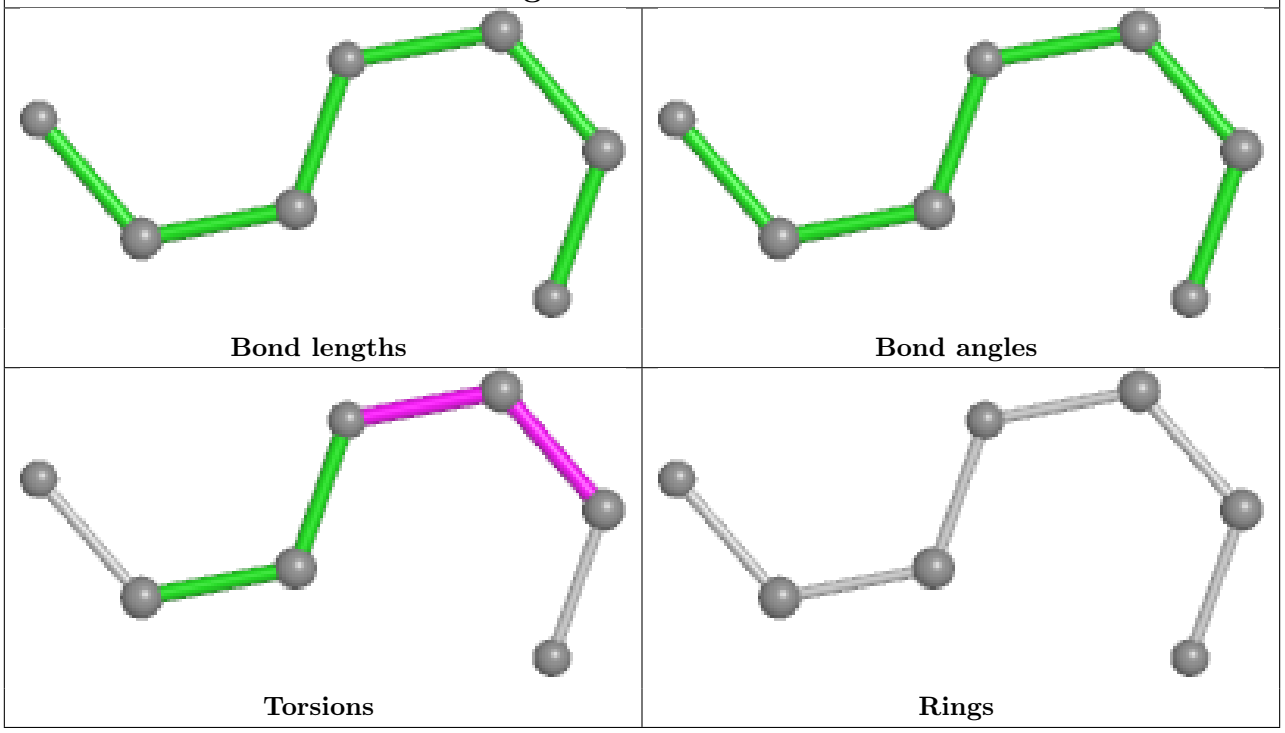
Ligand PEG A 402



Ligand GOL A 401



Ligand PEG A 404



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	359/367 (97%)	-0.04	7 (1%) 66 73	18, 27, 44, 70	1 (0%)
1	B	355/367 (96%)	0.22	18 (5%) 28 35	19, 31, 60, 80	5 (1%)
2	C	7/29 (24%)	1.21	0 100 100	35, 41, 57, 61	0
2	D	24/29 (82%)	4.28	13 (54%) 0 0	29, 57, 72, 74	0
All	All	745/792 (94%)	0.24	38 (5%) 28 35	18, 30, 60, 80	6 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	577	PRO	18.1
2	D	580	LEU	12.1
2	D	581	SER	11.4
2	D	579	GLY	10.9
2	D	578	ASN	8.0
2	D	575	ILE	7.9
2	D	569	TRP	7.1
2	D	576	ASP	6.0
1	B	358	THR	5.7
1	B	346	GLN	5.5
2	D	568	ASP	4.8
1	B	317	LEU	4.8
1	B	52	MET	4.1
2	D	574	GLN	3.8
1	B	298	VAL	3.8
2	D	591	THR	3.7
1	A	267	ARG	3.7
1	B	347	GLY	3.7
1	B	314	TYR	3.5
1	A	52	MET	3.3
2	D	582	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	322	LYS	3.1
1	B	297	ASN	3.0
1	B	319	GLU	3.0
1	B	1	GLY	2.9
1	A	50	ASN	2.9
1	A	53	GLU	2.8
1	A	324	GLU	2.5
1	B	50	ASN	2.5
1	A	179	GLU	2.4
1	B	254	GLU	2.3
1	B	315	SER	2.3
1	B	295	GLY	2.2
1	B	325	ALA	2.2
2	D	590	ASP	2.2
1	B	340	ARG	2.1
1	B	326	CYS	2.0
1	A	143	TYR	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	405	6/6	0.62	0.26	60,62,66,72	0
7	NAG	B	410	14/15	0.64	0.50	74,80,97,99	0
7	NAG	A	408	14/15	0.72	0.45	20,20,20,20	0
4	PEG	B	406	7/7	0.72	0.43	47,49,54,55	0
4	PEG	A	404	7/7	0.73	0.36	32,40,44,45	0
4	PEG	A	402	7/7	0.79	0.25	37,42,50,50	0

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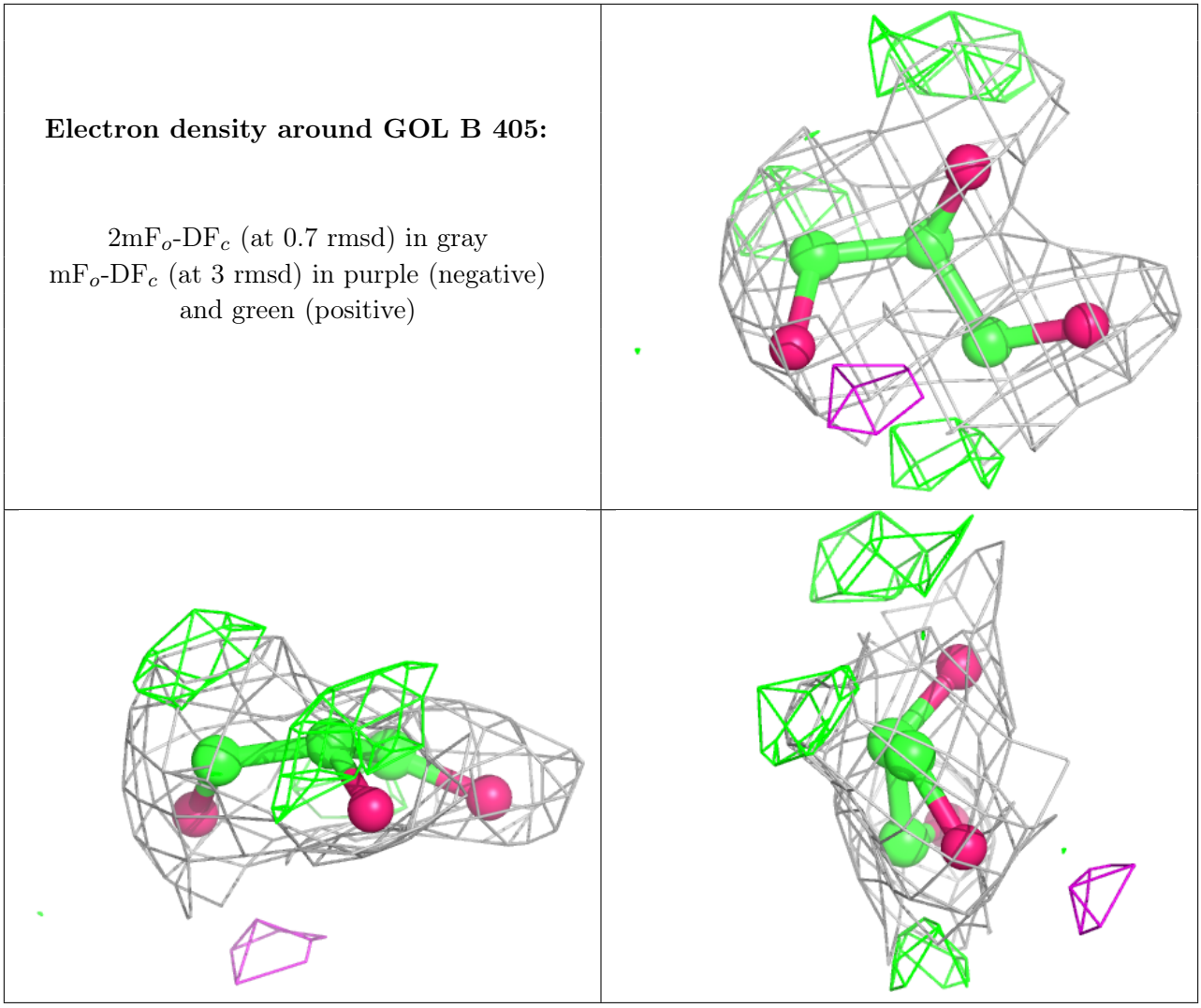
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	401	6/6	0.84	0.34	41,42,44,46	0
4	PEG	B	407	7/7	0.84	0.20	45,50,53,54	0
6	PG4	A	406	13/13	0.87	0.28	52,56,61,65	0
4	PEG	A	403	7/7	0.88	0.26	33,40,48,49	0
6	PG4	A	407	13/13	0.88	0.23	37,43,49,53	0
3	GOL	A	401	6/6	0.91	0.26	32,34,35,41	0
3	GOL	B	403	6/6	0.91	0.18	29,34,35,35	0
5	PE4	A	405	24/24	0.91	0.14	22,28,39,44	0
5	PE4	B	408	24/24	0.91	0.14	26,36,46,50	0
3	GOL	B	402	6/6	0.92	0.23	17,25,27,50	0
8	PG6	B	409	18/18	0.93	0.18	36,43,50,50	0
3	GOL	B	404	6/6	0.94	0.23	43,44,47,53	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.

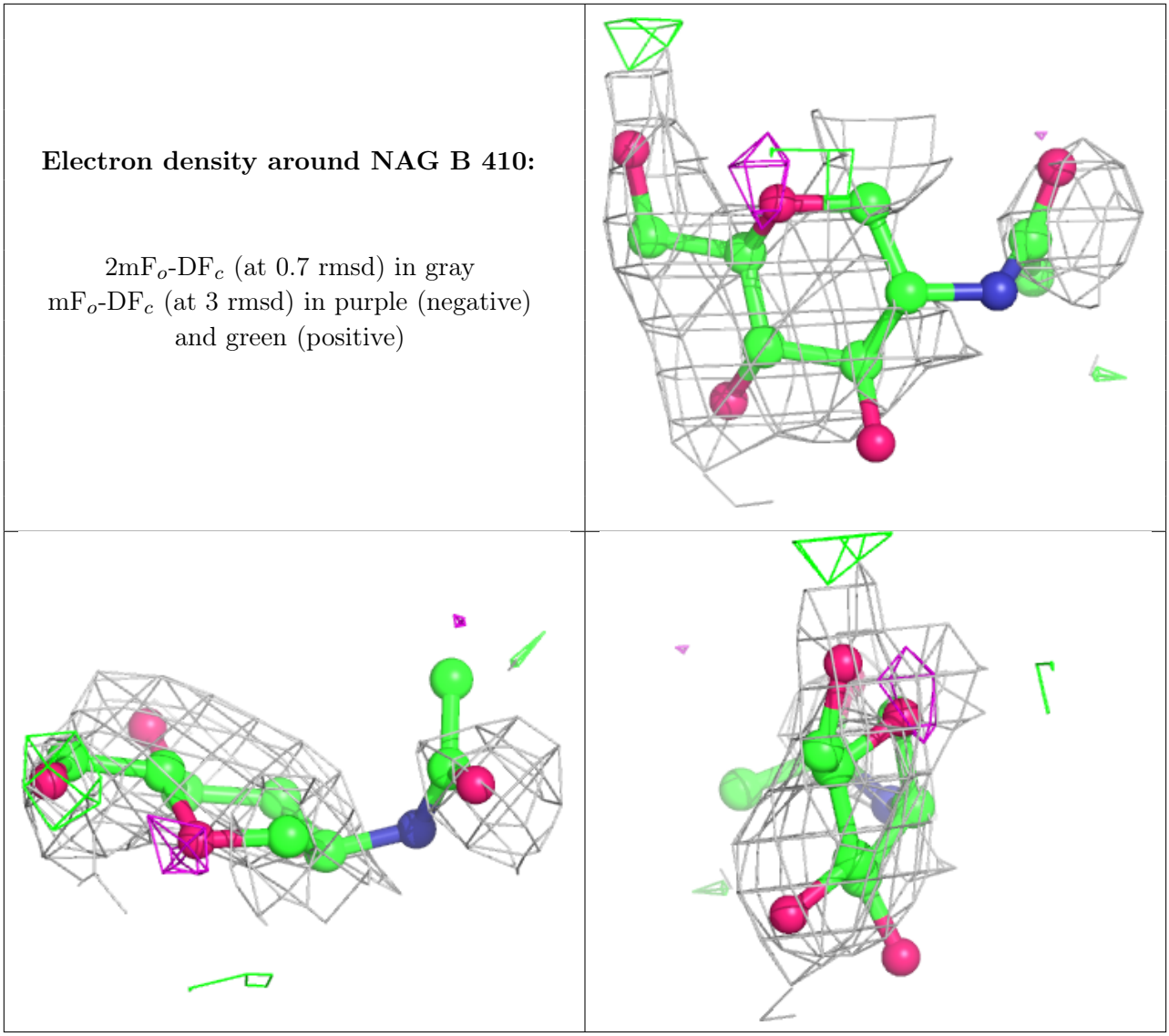
Electron density around GOL B 405:

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



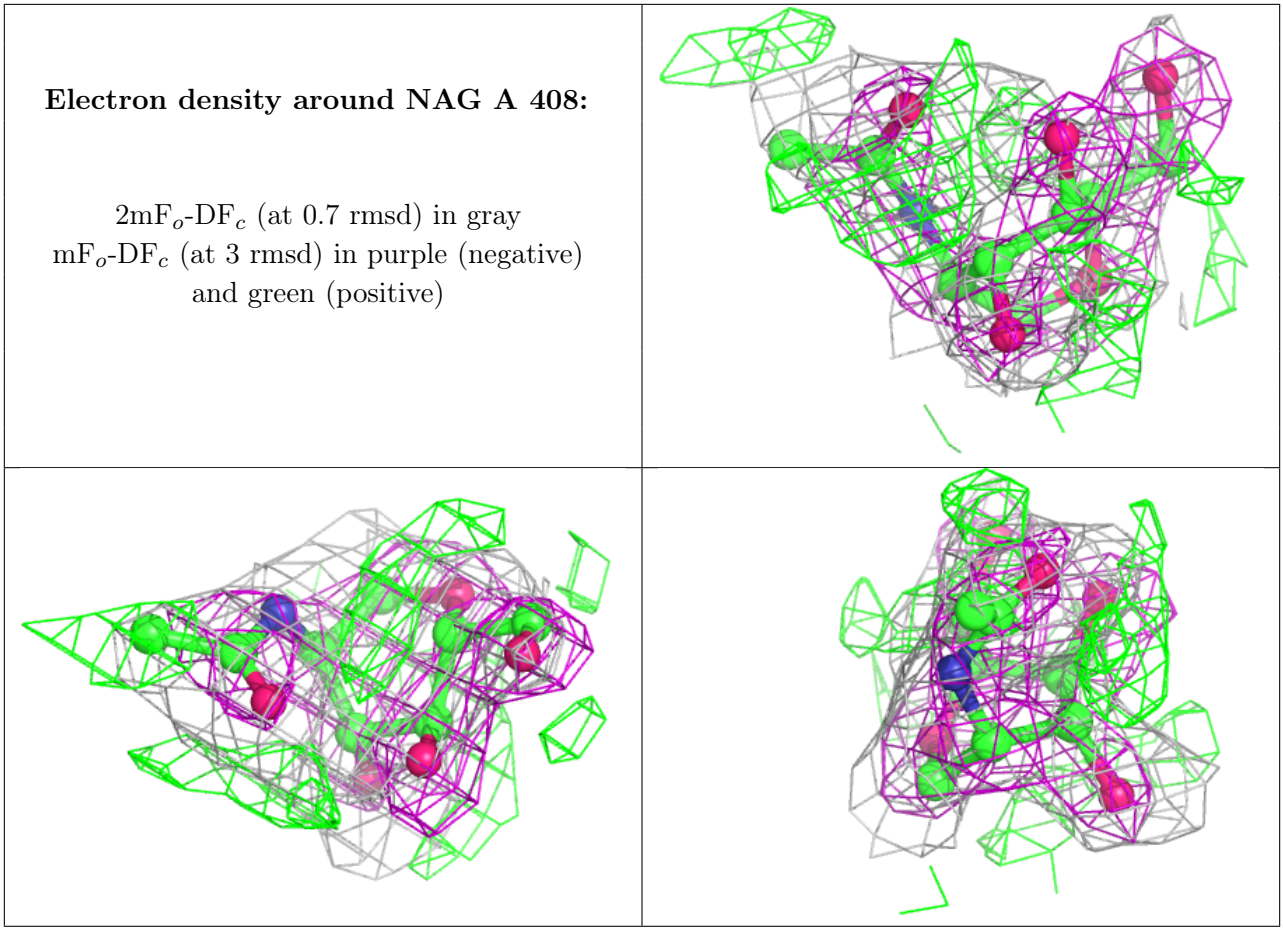
Electron density around NAG B 410:

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



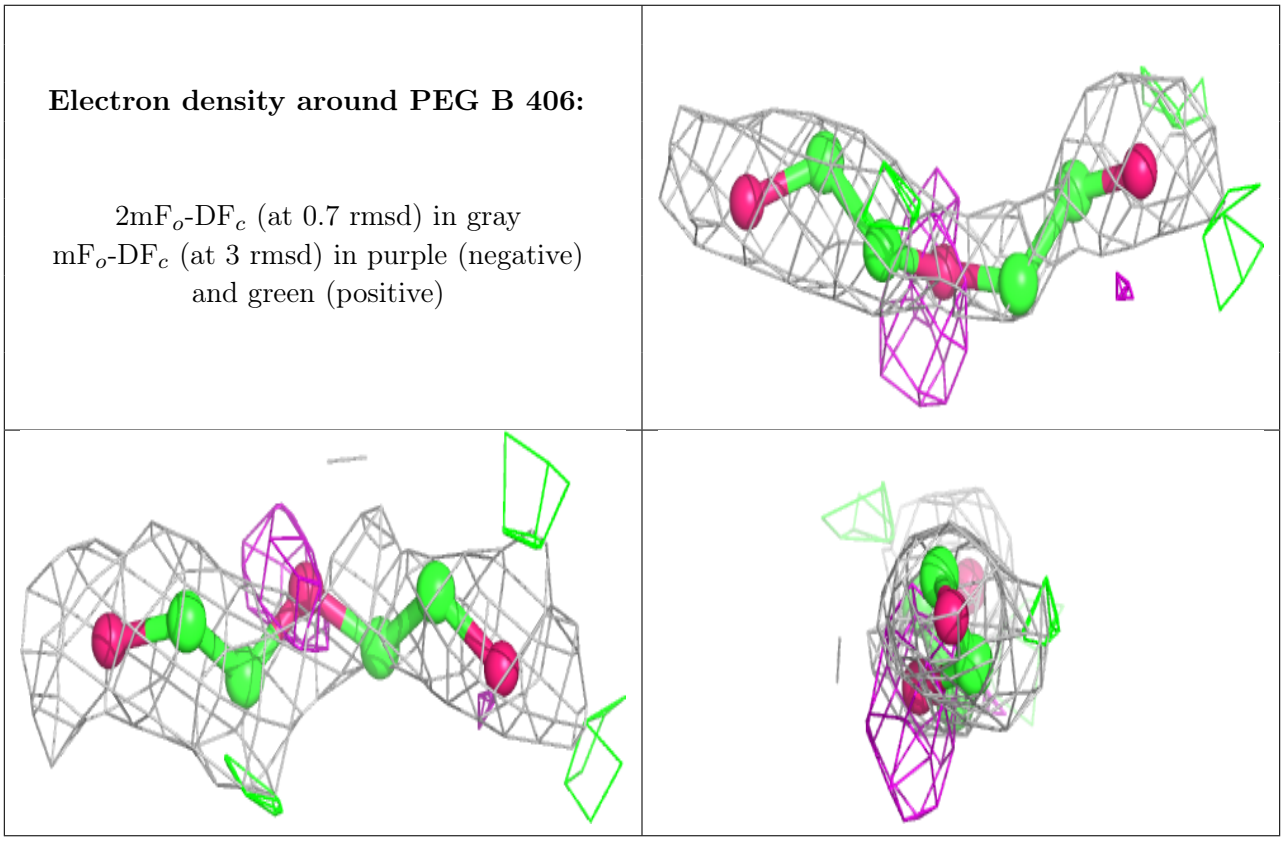
Electron density around NAG A 408:

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



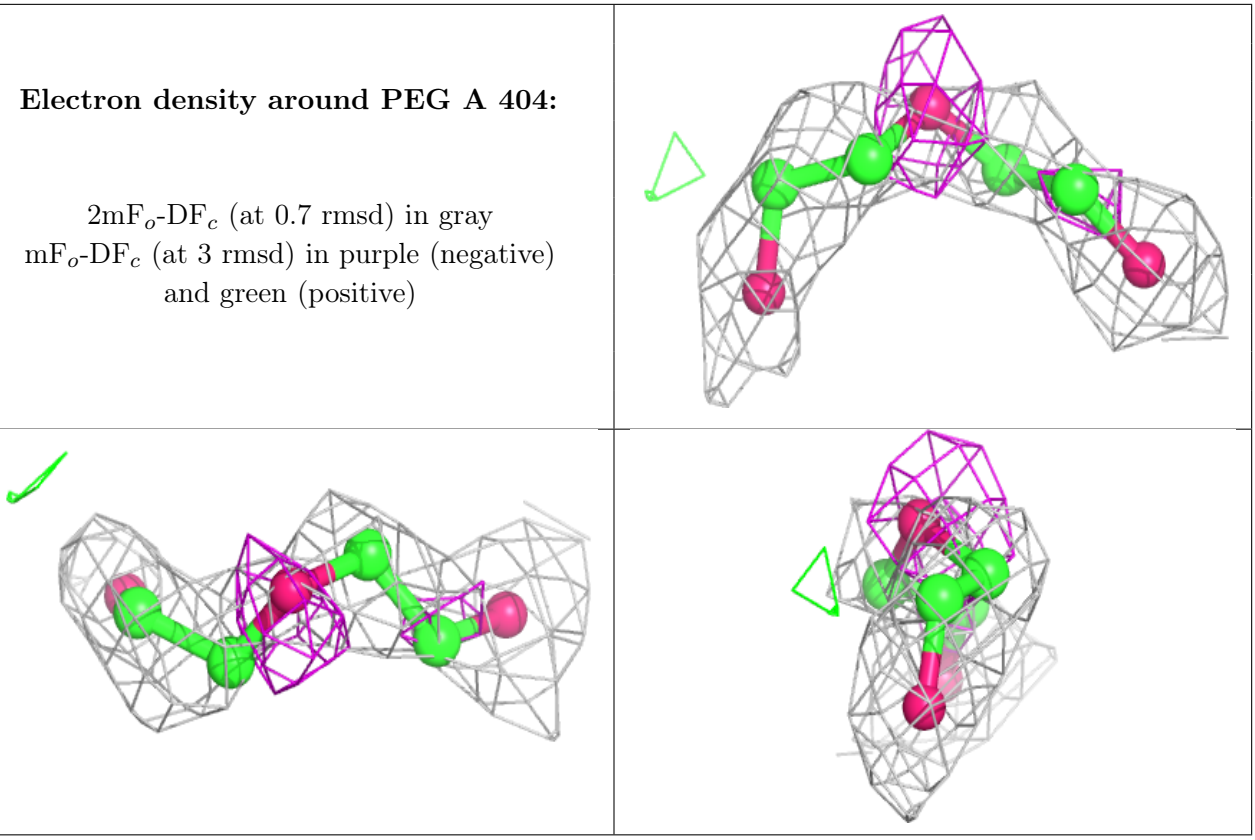
Electron density around PEG B 406:

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



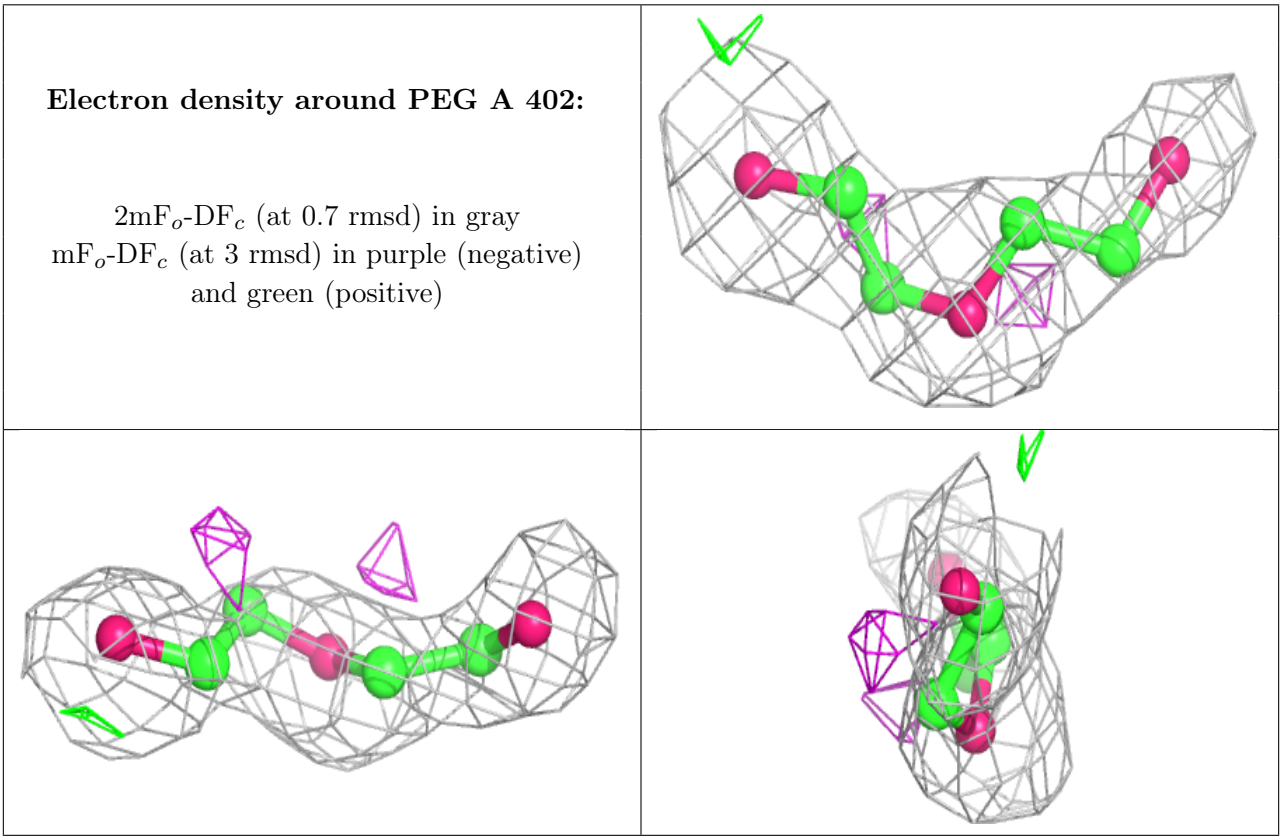
Electron density around PEG A 404:

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



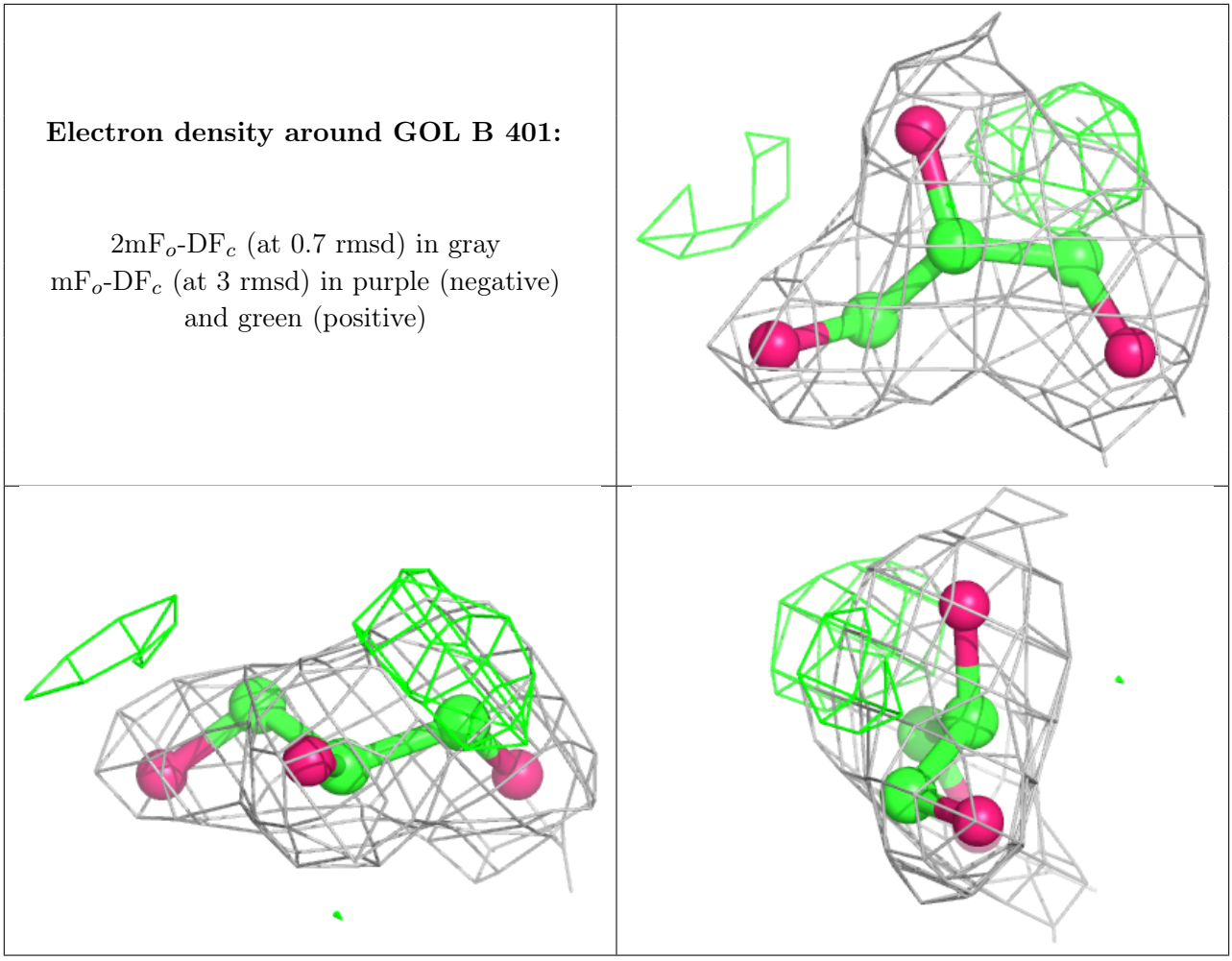
Electron density around PEG A 402:

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



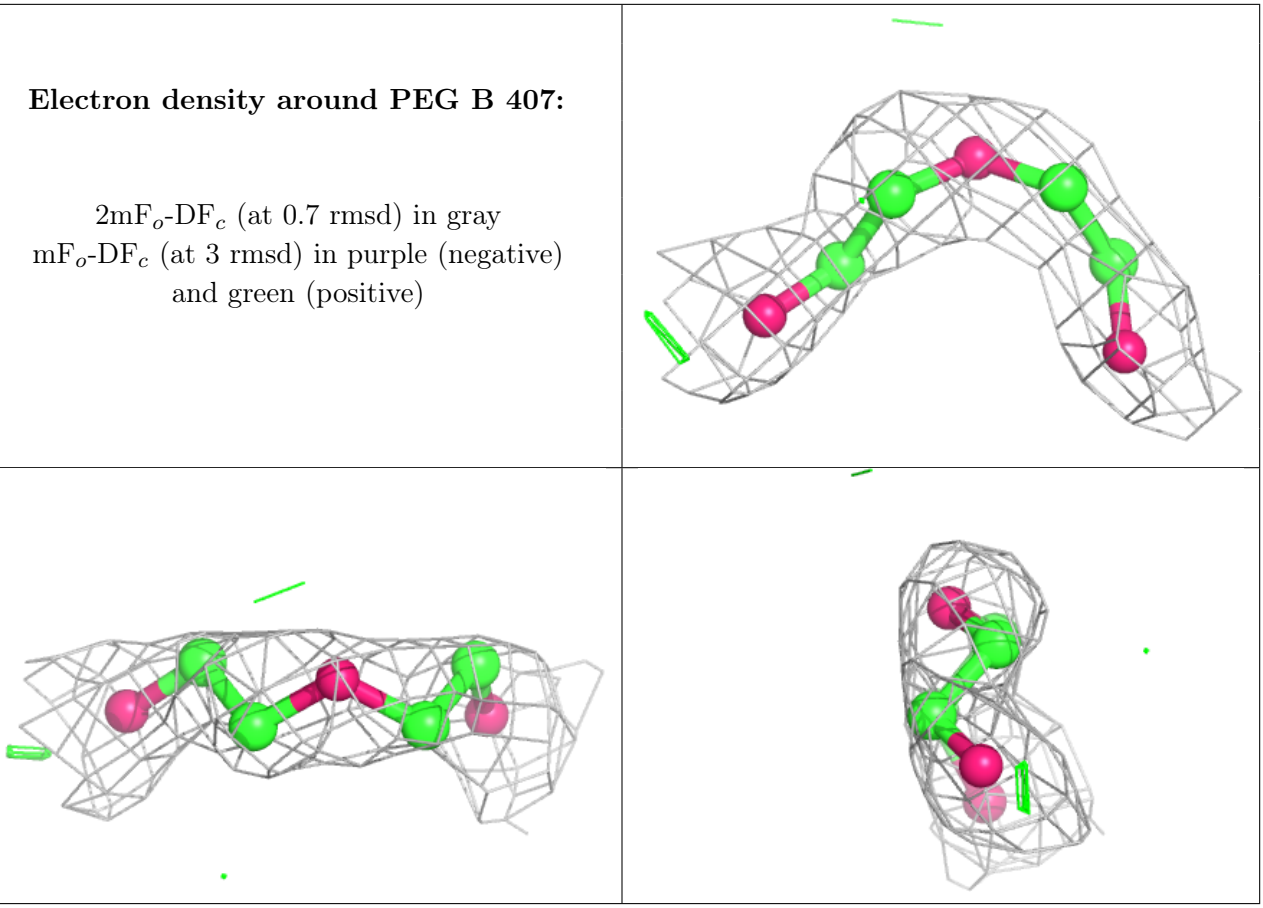
Electron density around GOL B 401:

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



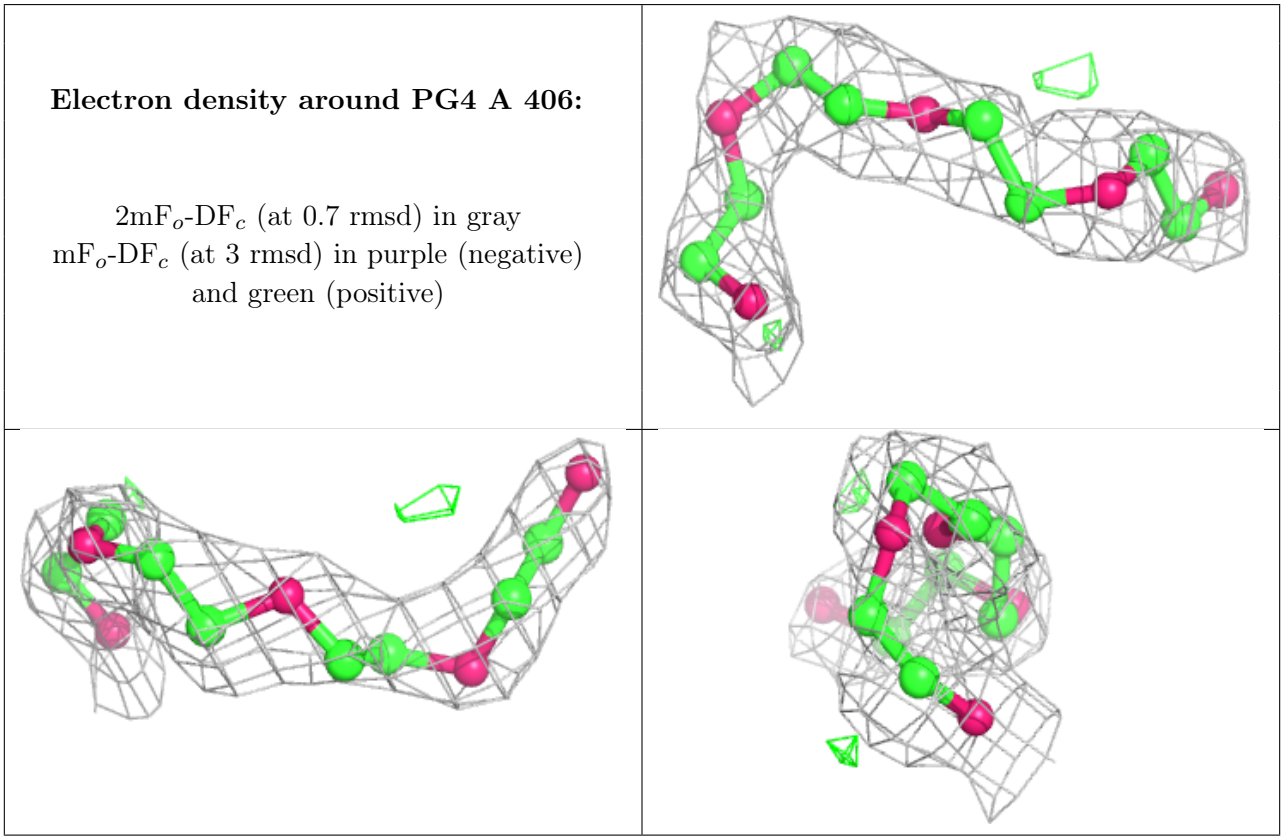
Electron density around PEG B 407:

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



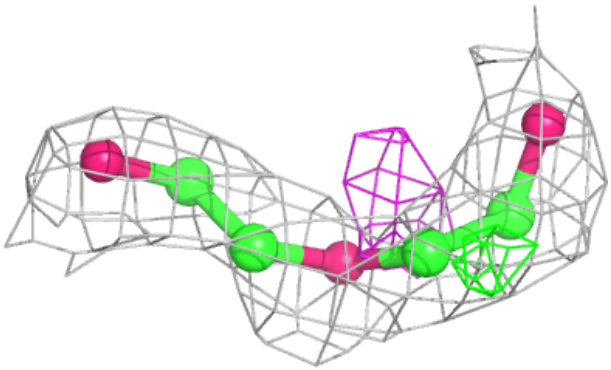
Electron density around PG4 A 406:

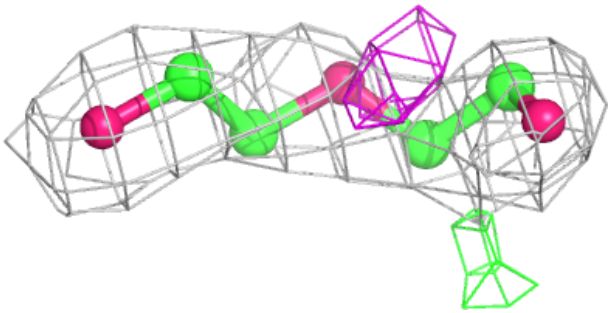
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

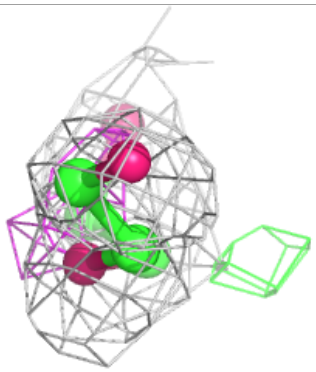


Electron density around PEG A 403:

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

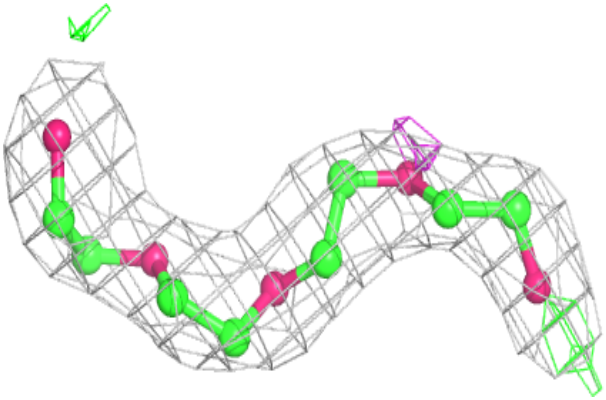


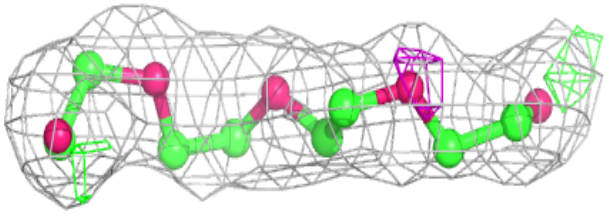


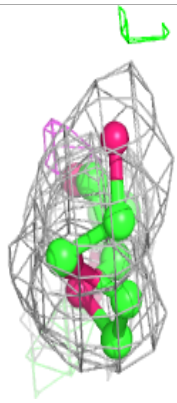


Electron density around PG4 A 407:

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

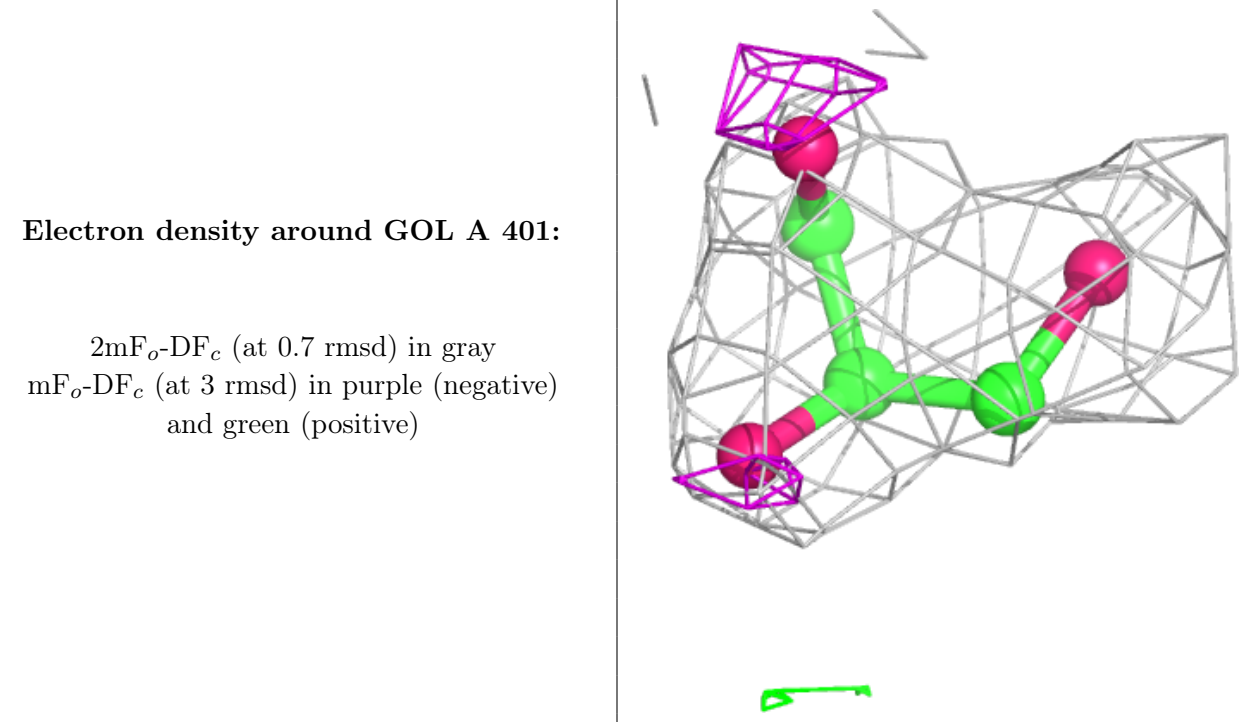


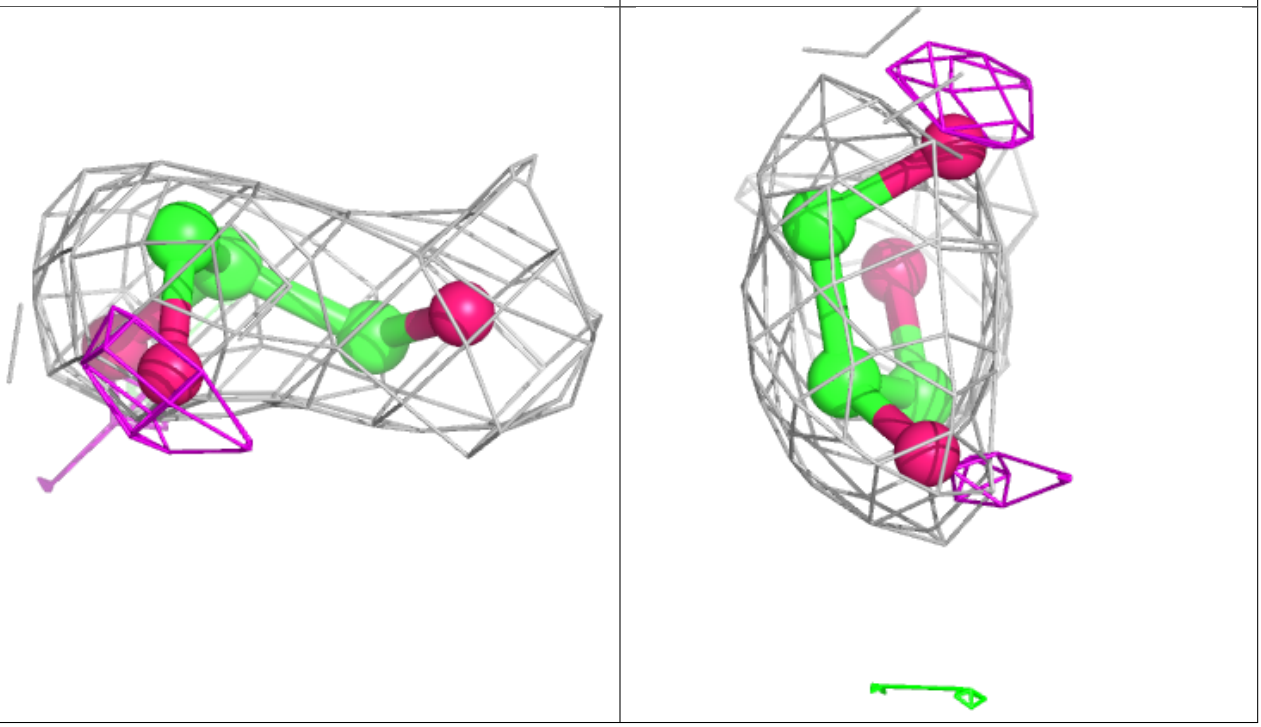




Electron density around GOL A 401:

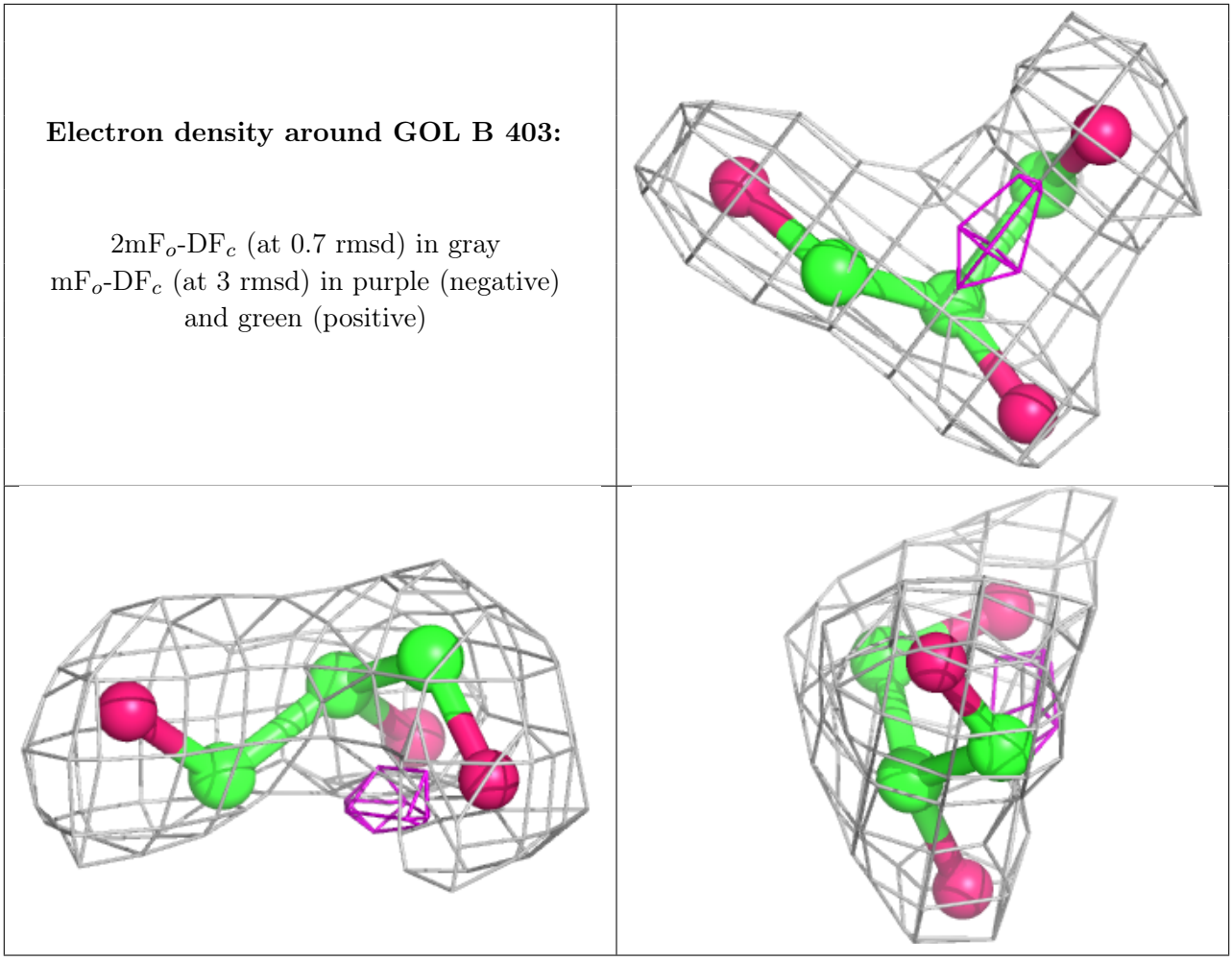
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





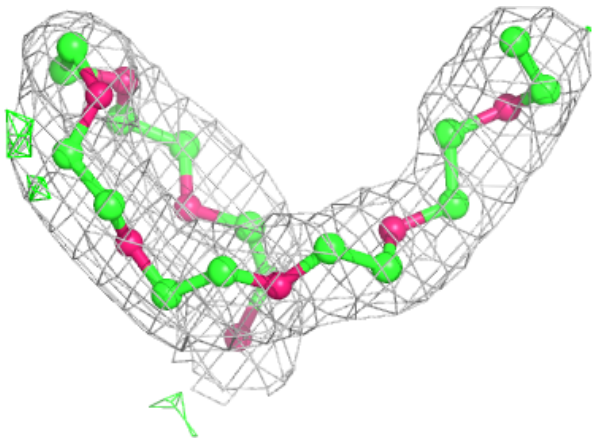
Electron density around GOL B 403:

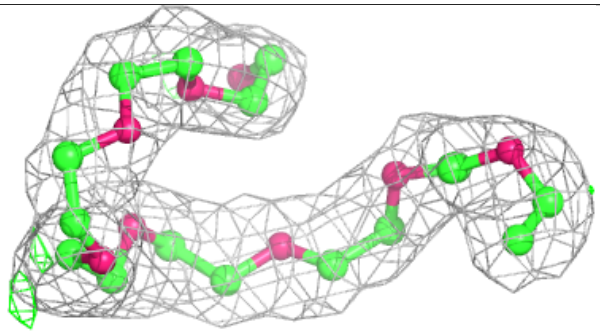
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

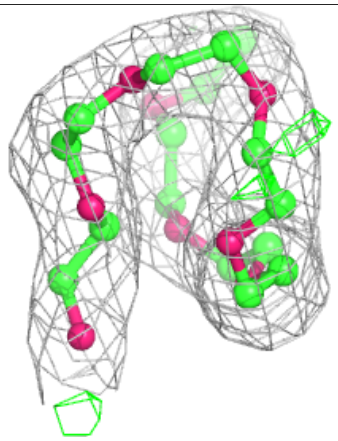


Electron density around PE4 A 405:

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

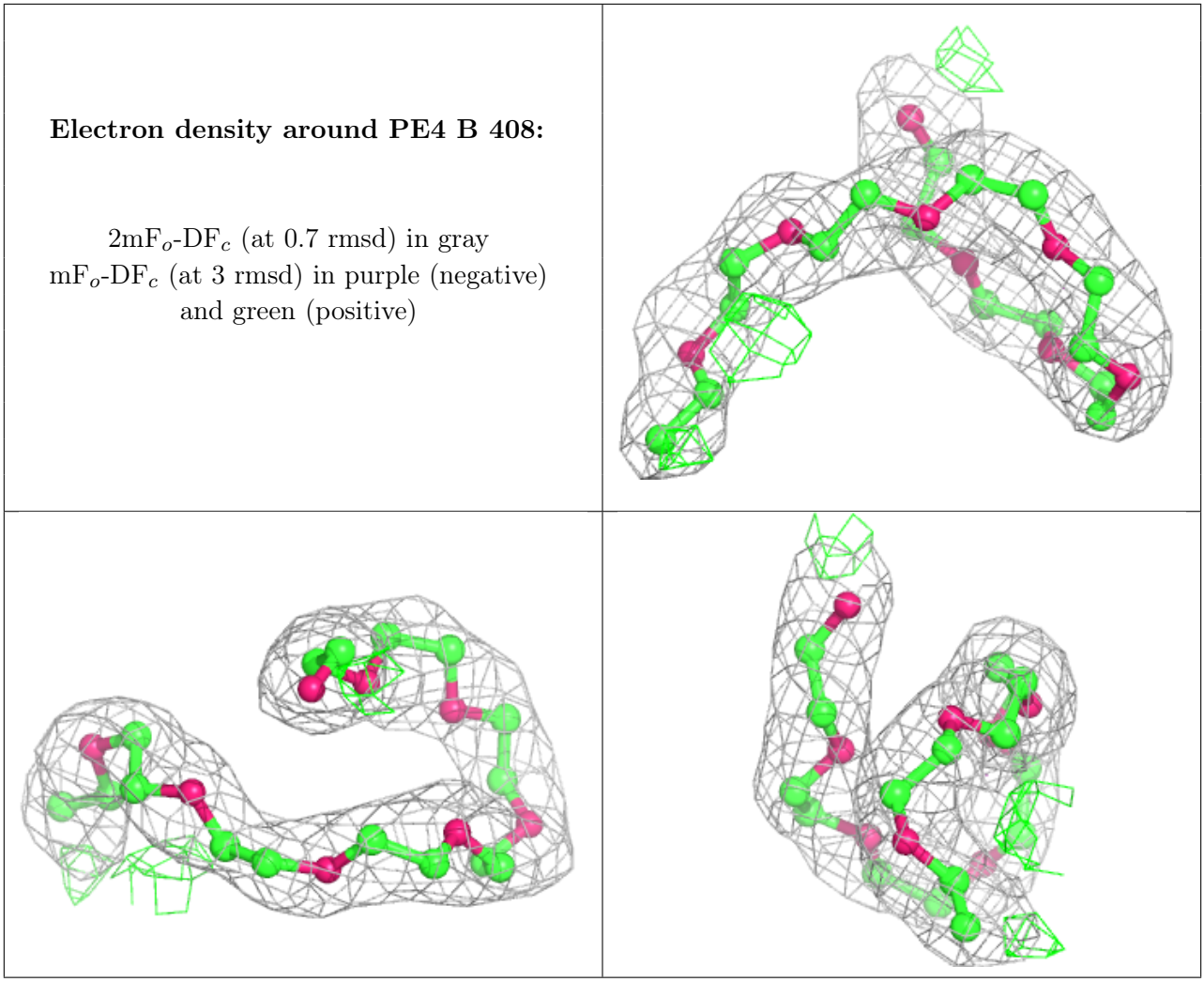






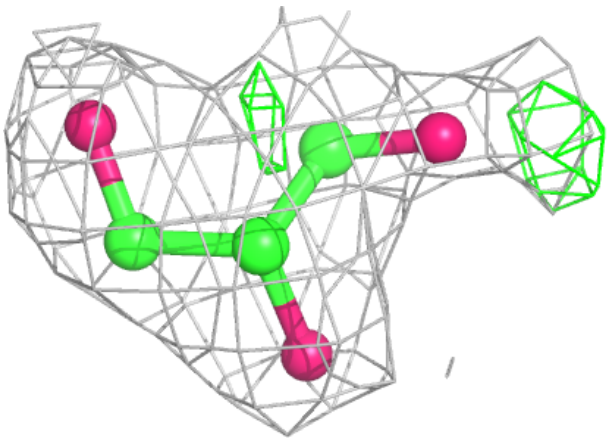
Electron density around PE4 B 408:

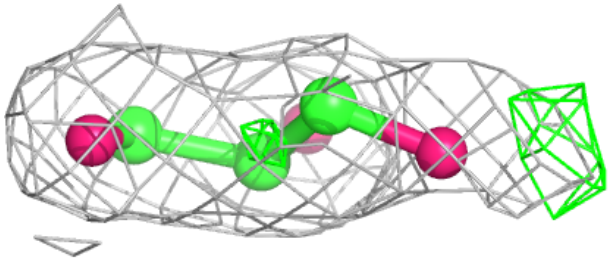
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

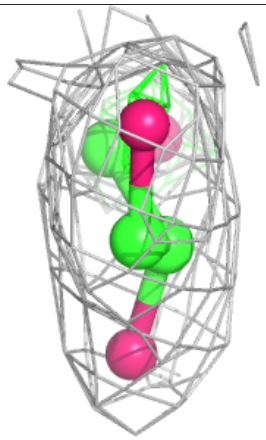


Electron density around GOL B 402:

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

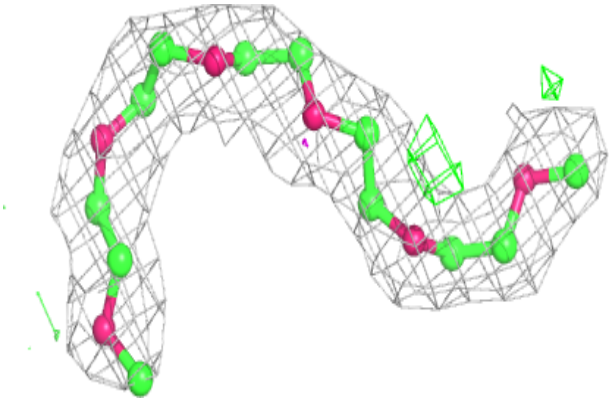


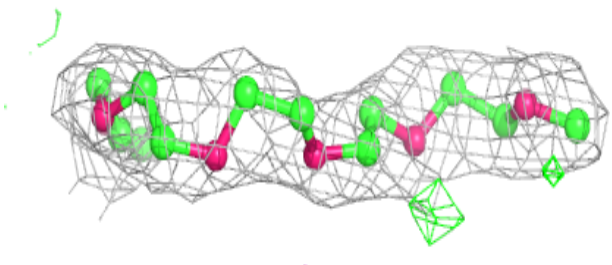


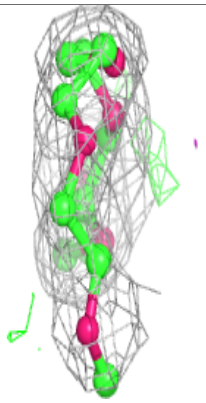


Electron density around PG6 B 409:

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

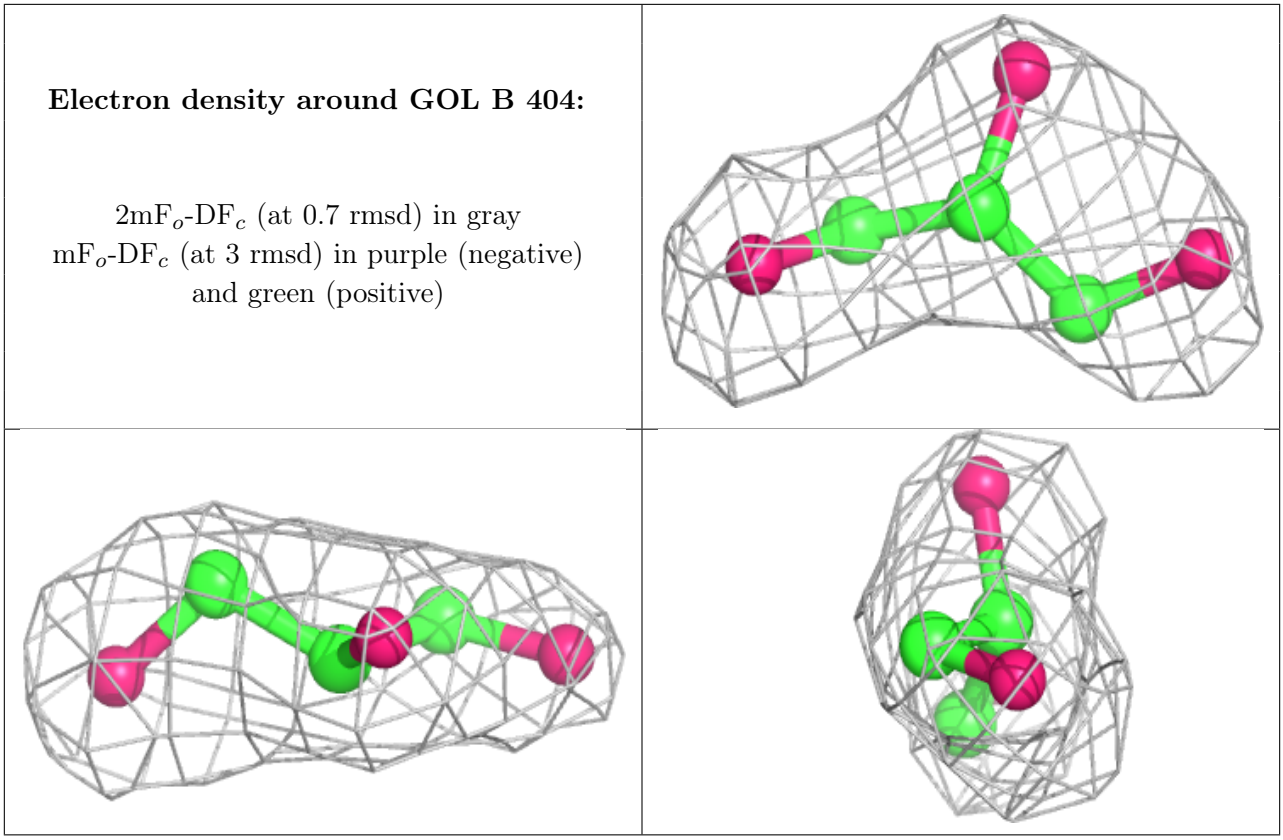






Electron density around GOL B 404:

$2mF_o$-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.