Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 02:20 PM JST

PDB ID	:	8IQ9
Title	:	Crystal structure of trimeric K2-2 TSP in complex with tetrasaccharide and octasaccharide
Authors	:	Ye, T.J.; Ko, T.P.; Huang, K.F.; Wu, S.H.
Deposited on	:	2023-03-16
Resolution	:	1.58 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:

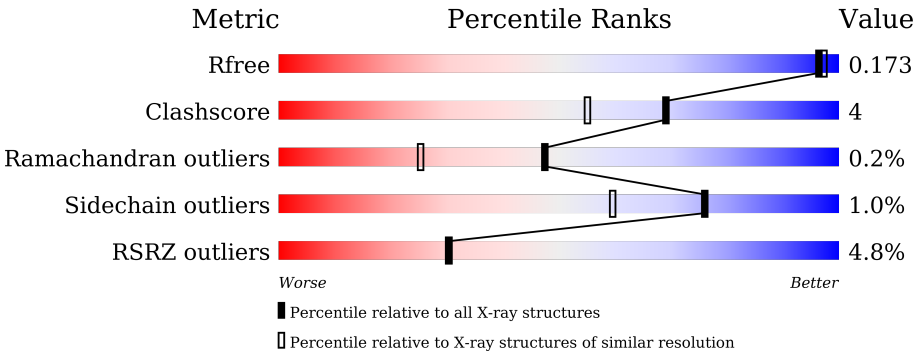
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.58 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	612	86% 6% 8%
1	B	612	11% 83% 8% 8%
1	C	612	85% 7% 8%
2	D	8	62% 38%
2	F	8	38% 62%
3	E	4	50% 50%

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Mol	Chain	Length	Quality of chain
3	G	4	25% 50% 25%
3	H	4	50% 25% 25%

2 Entry composition

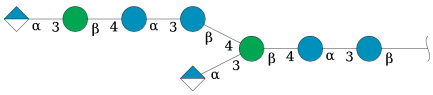
There are 6 unique types of molecules in this entry. The entry contains 15282 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 K2-2 TSP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	10	0
			4212	2648	720	822	22			
1	B	563	Total	C	N	O	S	0	8	0
			4192	2637	717	817	21			
1	C	565	Total	C	N	O	S	0	11	0
			4219	2652	723	823	21			

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranuronic acid-(1-3)-beta-D-mannopyranose-(1-4)-alpha-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[alpha-D-glucopyranuronic acid-(1-3)]beta-D-mannopyranose-(1-4)-alpha-D-glucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	8	Total	C	O	0	0	0
			91	48	43			
2	F	8	Total	C	O	0	1	0
			94	50	44			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranuronic acid-(1-3)-beta-D-mannopyranose-(1-4)-alpha-D-glucopyranose-(1-3)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	4	Total	C	O	0	1	0
			48	25	23			

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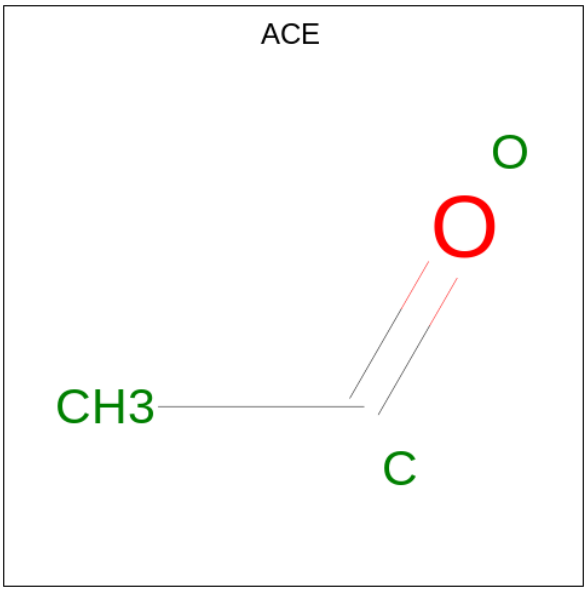
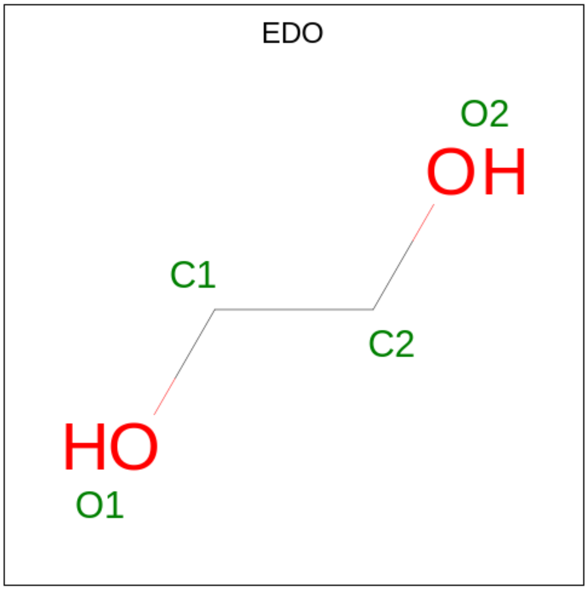
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	G	4	Total C O 46 24 22	0	0	0
3	H	4	Total C O 48 25 23	0	1	0

- Molecule 4 is ACETYL GROUP (three-letter code: ACE) (formula: C_2H_4O) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	1
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 6 3 3	0	1
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 8 4 4	0	1
5	C	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 6 3 3	0	1
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 8 4 4	0	1

- Molecule 6 is water.

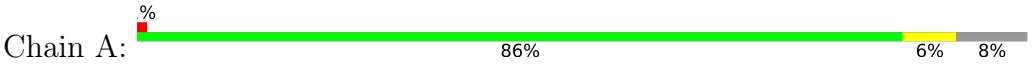
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	818	Total O 818 818	0	0
6	B	656	Total O 656 656	0	0
6	C	766	Total O 766 766	0	0

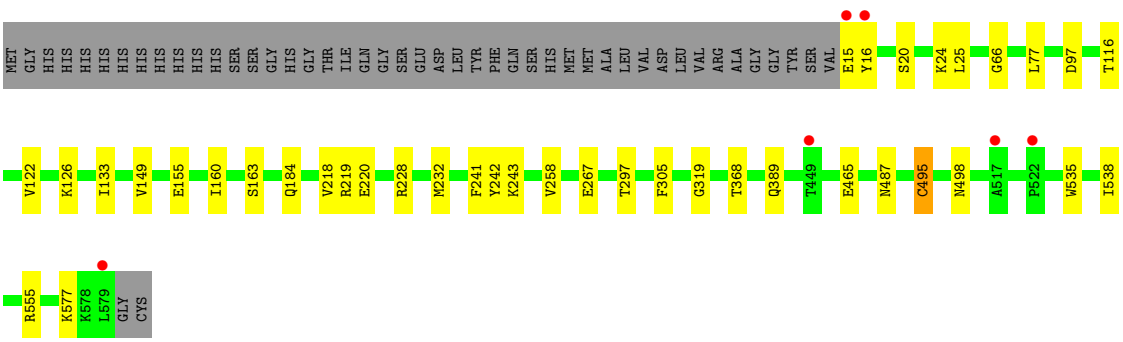
3 Residue-property plots (i)

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: K2-2 TSP

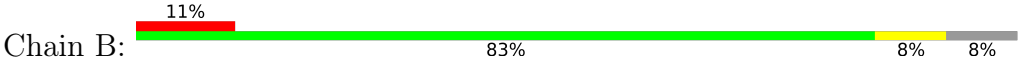
Chain A:

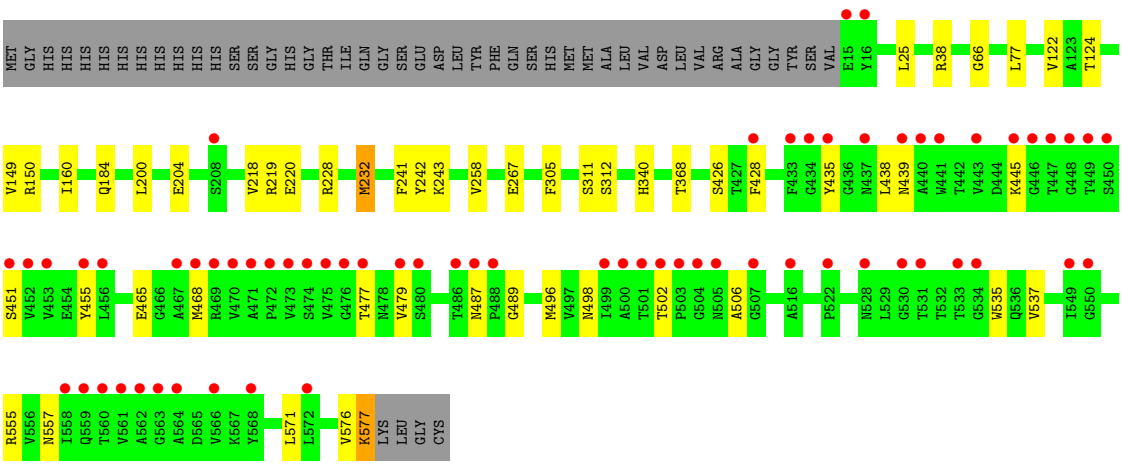




• Molecule 1: K2-2 TSP

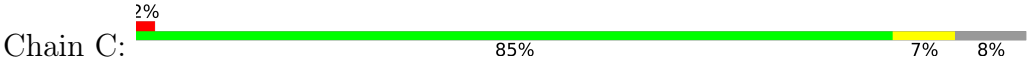
Chain B:

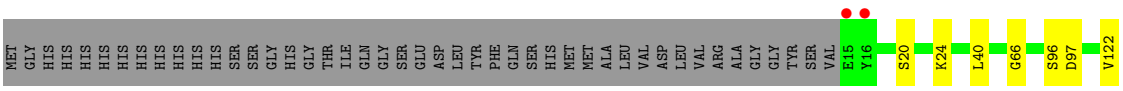


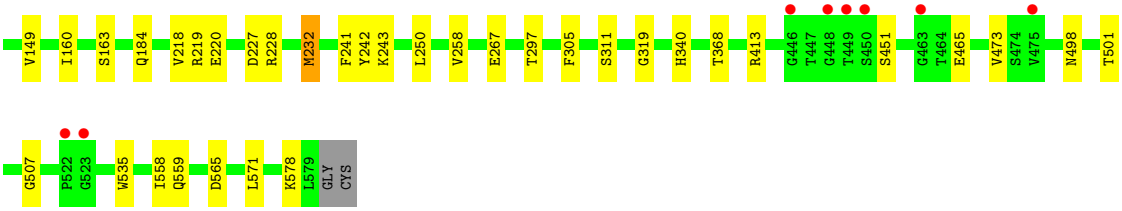


• Molecule 1: K2-2 TSP

Chain C:

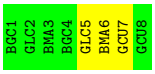






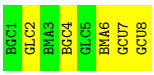
• Molecule 2: alpha-D-glucopyranuronic acid-(1-3)-beta-D-mannopyranose-(1-4)-alpha-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[alpha-D-glucopyranuronic acid-(1-3)]beta-D-mannopyranose-(1-4)-alpha-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain D:



• Molecule 2: alpha-D-glucopyranuronic acid-(1-3)-beta-D-mannopyranose-(1-4)-alpha-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-4)-[alpha-D-glucopyranuronic acid-(1-3)]beta-D-mannopyranose-(1-4)-alpha-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain F:

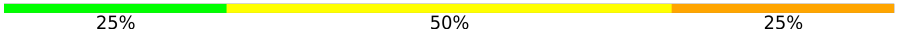


• Molecule 3: alpha-D-glucopyranuronic acid-(1-3)-beta-D-mannopyranose-(1-4)-alpha-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain E:

• Molecule 3: alpha-D-glucopyranuronic acid-(1-3)-beta-D-mannopyranose-(1-4)-alpha-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain G:



• Molecule 3: alpha-D-glucopyranuronic acid-(1-3)-beta-D-mannopyranose-(1-4)-alpha-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	204.41Å 86.36Å 103.42Å 90.00° 110.21° 90.00°	Depositor
Resolution (Å)	26.95 – 1.58 26.95 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.8 (26.95-1.58) 99.9 (26.95-1.58)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 1.58Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.143 , 0.173 0.144 , 0.173	Depositor DCC
R_{free} test set	2000 reflections (0.87%)	wwPDB-VP
Wilson B-factor (Å^2)	16.6	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	15282	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: BMA, GCU, EDO, BGC, ACE, GLC

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	0.49	2/4359 (0.0%)	0.69	0/5933
1	B	0.44	0/4329	0.68	0/5893
1	C	0.45	0/4369	0.68	0/5946
All	All	0.46	2/13057 (0.0%)	0.68	0/17772

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	495[A]	CYS	CB-SG	-6.09	1.72	1.82
1	A	495[B]	CYS	CB-SG	-6.09	1.72	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4212	0	4094	28	1
1	B	4192	0	4070	38	0
1	C	4219	0	4103	26	1
2	D	91	0	68	1	0
2	F	94	0	69	2	0
3	E	48	0	35	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	46	0	36	2	0
3	H	48	0	35	1	0
4	A	3	0	3	0	0
4	C	3	0	3	0	0
5	A	34	0	54	4	0
5	B	26	0	42	1	0
5	C	26	0	42	1	0
6	A	818	0	0	10	5
6	B	656	0	0	9	1
6	C	766	0	0	6	6
All	All	15282	0	12654	95	7

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 4.

All (95) 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:232[A]:MET:HG2	1:B:258:VAL:HG22	1.62	0.80
1:A:232[B]:MET:HG2	1:A:258:VAL:HG22	1.64	0.79
1:B:571:LEU:O	6:B:701:HOH:O	2.03	0.77
1:B:445:LYS:NZ	1:B:451:SER:O	2.18	0.76
1:C:184[A]:GLN:NE2	6:C:702:HOH:O	2.19	0.76
1:B:555:ARG:NH2	1:B:557:ASN:HD22	1.84	0.74
1:C:220:GLU:HG2	1:C:243:LYS:HE2	1.68	0.73
1:C:232[A]:MET:HG2	1:C:258:VAL:HG22	1.68	0.73
1:A:220:GLU:HG2	1:A:243:LYS:HE2	1.72	0.71
1:A:487:ASN:ND2	6:A:702:HOH:O	2.23	0.71
1:B:220:GLU:HG2	1:B:243:LYS:HE2	1.72	0.71
1:B:428:PHE:O	6:B:702:HOH:O	2.11	0.69
1:A:389[A]:GLN:NE2	6:A:703:HOH:O	2.23	0.69
1:B:160[B]:ILE:HD13	1:B:200:LEU:HB2	1.74	0.69
1:C:97[B]:ASP:OD1	6:C:701:HOH:O	2.12	0.67
1:A:155:GLU:OE2	6:A:701:HOH:O	2.13	0.66
1:A:126:LYS:NZ	6:A:706:HOH:O	2.27	0.66
1:B:576:VAL:O	1:B:577:LYS:HB2	1.95	0.66
1:C:24:LYS:NZ	6:C:708:HOH:O	2.31	0.64
1:A:495[A]:CYS:SG	1:A:538:ILE:HB	2.42	0.60
1:B:487:ASN:ND2	6:B:711:HOH:O	2.37	0.58
1:B:438:LEU:HD11	1:B:455:TYR:HB2	1.86	0.57
5:A:604:EDO:H12	6:A:1021:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:ARG:HH22	1:B:557:ASN:HD22	1.54	0.54
1:B:312:SER:HG	2:F:4[A]:BGC:H6	1.56	0.53
2:D:6:BMA:H62	3:E:1:BGC:O5	2.09	0.53
5:B:605[B]:EDO:H21	6:C:725:HOH:O	2.08	0.52
6:A:702:HOH:O	1:B:426:SER:N	2.42	0.52
1:B:577:LYS:HG2	6:B:1277:HOH:O	2.09	0.51
1:B:577:LYS:HG3	6:B:723:HOH:O	2.11	0.50
6:B:711:HOH:O	1:C:578:LYS:HE2	2.12	0.50
1:B:489:GLY:HA2	1:B:577:LYS:HB2	1.94	0.50
1:C:160:ILE:HD12	1:C:163:SER:HB3	1.94	0.49
1:B:25:LEU:HD11	1:B:77:LEU:HD22	1.94	0.49
1:A:15:GLU:N	6:A:718:HOH:O	2.47	0.48
1:A:184[A]:GLN:NE2	6:A:720:HOH:O	2.47	0.48
1:C:501:THR:HG22	1:C:565:ASP:HB3	1.95	0.48
1:B:368[B]:THR:HG23	6:B:1103:HOH:O	2.13	0.47
1:B:502:THR:HG21	1:B:506:ALA:HB2	1.97	0.47
5:C:606[B]:EDO:H12	6:C:954:HOH:O	2.13	0.47
1:C:20:SER:OG	1:C:24:LYS:HD2	2.15	0.47
1:B:38:ARG:NH1	6:B:705:HOH:O	2.23	0.47
1:C:122:VAL:HA	1:C:149:VAL:HG22	1.97	0.47
1:A:555:ARG:HH11	5:A:608:EDO:H11	1.80	0.46
1:B:267:GLU:OE1	3:G:1:BGC:H1	2.14	0.46
1:C:498:ASN:HB2	1:C:535:TRP:CD2	2.51	0.46
1:A:297:THR:HA	1:A:319:GLY:O	2.16	0.46
1:A:16:TYR:OH	1:C:40:LEU:HB3	2.16	0.45
1:A:267:GLU:OE1	3:E:1:BGC:H1	2.16	0.45
1:B:468:MET:SD	1:B:479:VAL:HG21	2.56	0.45
1:B:160[B]:ILE:HD11	1:B:204:GLU:OE2	2.16	0.45
1:C:297:THR:HA	1:C:319:GLY:O	2.16	0.45
1:B:184[A]:GLN:NE2	6:B:713:HOH:O	2.38	0.45
1:C:507:GLY:HA3	1:C:559:GLN:O	2.16	0.44
1:A:389[B]:GLN:NE2	6:A:726:HOH:O	2.49	0.44
1:B:498:ASN:HB2	1:B:535:TRP:CD2	2.52	0.44
1:C:242:TYR:CE2	1:C:243:LYS:HD3	2.53	0.44
1:A:577:LYS:HB3	1:A:577:LYS:HE2	1.68	0.44
1:C:451:SER:HA	1:C:473[A]:VAL:HG22	2.00	0.44
1:B:122:VAL:HA	1:B:149:VAL:HG22	2.00	0.44
1:A:555:ARG:HB3	5:A:608:EDO:H12	2.00	0.43
1:C:413[B]:ARG:HE	1:C:413[B]:ARG:HB3	1.53	0.43
1:A:25:LEU:HD11	1:A:77:LEU:HD22	2.00	0.43
1:B:489:GLY:HA2	1:B:577:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:ARG:NH2	1:B:557:ASN:ND2	2.62	0.43
1:B:555:ARG:HH22	1:B:557:ASN:ND2	2.17	0.42
1:C:160:ILE:CD1	1:C:163:SER:HB3	2.49	0.42
1:B:124[B]:THR:HG22	1:B:150:ARG:HD3	2.02	0.42
1:B:200:LEU:CD2	1:B:204:GLU:HG2	2.49	0.42
1:A:133:ILE:HG23	5:A:604:EDO:H11	2.02	0.42
1:A:122:VAL:HA	1:A:149:VAL:HG22	2.01	0.42
1:B:311:SER:HA	1:B:340:HIS:O	2.20	0.42
1:C:218:VAL:O	1:C:241:PHE:HA	2.20	0.41
1:A:20:SER:OG	1:A:24:LYS:HD2	2.19	0.41
1:C:227:ASP:HA	1:C:250:LEU:HB3	2.02	0.41
1:A:242:TYR:CE2	1:A:243:LYS:HD3	2.55	0.41
1:C:558:ILE:HD11	1:C:571:LEU:HD13	2.01	0.41
1:B:218:VAL:O	1:B:241:PHE:HA	2.21	0.41
1:A:116:THR:HG23	1:C:122:VAL:HG11	2.02	0.41
1:C:368[A]:THR:HG23	6:C:1097:HOH:O	2.20	0.41
1:A:368[A]:THR:HG23	6:A:1155:HOH:O	2.20	0.41
1:A:160:ILE:HD12	1:A:163:SER:HB3	2.03	0.41
2:F:6:BMA:H62	3:G:1:BGC:O5	2.21	0.41
1:A:498:ASN:HB2	1:A:535:TRP:CD2	2.56	0.40
1:B:496:MET:SD	1:B:537:VAL:HG22	2.61	0.40
1:C:311:SER:HA	1:C:340:HIS:O	2.21	0.40
1:B:124[B]:THR:HG22	1:B:150:ARG:HB3	2.03	0.40
1:C:267:GLU:OE1	3:H:1:BGC:H1	2.21	0.40
1:B:242:TYR:CE2	1:B:243:LYS:HD3	2.57	0.40
1:A:218:VAL:O	1:A:241:PHE:HA	2.21	0.40
1:B:435:TYR:HD2	1:B:439:ASN:HB2	1.87	0.40

All (7) 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:97[B]:ASP:OD2	1:C:96:SER:OG[4_555]	1.95	0.25
6:A:1231:HOH:O	6:C:713:HOH:O[3_455]	2.11	0.09
6:A:1331:HOH:O	6:C:1222:HOH:O[3_455]	2.11	0.09
6:A:1231:HOH:O	6:C:1312:HOH:O[3_455]	2.12	0.08
6:A:1331:HOH:O	6:C:1286:HOH:O[3_455]	2.12	0.08
6:B:1128:HOH:O	6:C:990:HOH:O[4_556]	2.13	0.07
6:A:1358:HOH:O	6:C:865:HOH:O[3_455]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	573/612 (94%)	553 (96%)	19 (3%)	1 (0%)	47	25
1	B	569/612 (93%)	545 (96%)	23 (4%)	1 (0%)	47	25
1	C	574/612 (94%)	555 (97%)	18 (3%)	1 (0%)	47	25
All	All	1716/1836 (94%)	1653 (96%)	60 (4%)	3 (0%)	47	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	GLY
1	B	66	GLY
1	C	66	GLY

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	461/489 (94%)	458 (99%)	3 (1%)	84	72
1	B	457/489 (94%)	450 (98%)	7 (2%)	65	42
1	C	462/489 (94%)	457 (99%)	5 (1%)	73	55
All	All	1380/1467 (94%)	1365 (99%)	15 (1%)	76	55

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	ARG
1	A	305	PHE
1	A	465	GLU
1	B	228	ARG
1	B	232[A]	MET
1	B	232[B]	MET
1	B	305	PHE
1	B	465	GLU
1	B	477	THR
1	B	577	LYS
1	C	228	ARG
1	C	232[A]	MET
1	C	232[B]	MET
1	C	305	PHE
1	C	465	GLU

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

Mol	Chain	Res	Type
1	B	18	GLN
1	B	528	ASN
1	B	557	ASN

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)

31 monosaccharides 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	$\#\|Z\| > 2$
2	BGC	D	1	2	12,12,12	0.17	0	17,17,17	0.25	0
2	GLC	D	2	2	11,11,12	0.52	0	15,15,17	0.99	0
2	BMA	D	3	2,4	11,11,12	0.90	0	15,15,17	0.87	0
2	BGC	D	4	2	11,11,12	0.30	0	15,15,17	0.49	0
2	GLC	D	5	2	11,11,12	0.65	0	15,15,17	0.91	1 (6%)
2	BMA	D	6	2	11,11,12	0.73	0	15,15,17	0.89	0
2	GCU	D	7	2	12,12,13	0.80	0	14,17,19	0.82	1 (7%)
2	GCU	D	8	2	12,12,13	0.75	0	14,17,19	0.95	0
3	BGC	E	1	3	12,12,12	0.45	0	17,17,17	0.82	0
3	GLC	E	2	3	11,11,12	0.44	0	15,15,17	0.86	1 (6%)
3	BMA	E	3[A]	-	11,11,12	0.70	0	15,15,17	0.74	0
3	BMA	E	3[B]	-	11,11,12	0.69	0	15,15,17	0.70	0
3	GCU	E	4	3	12,12,13	0.74	0	14,17,19	0.67	0
2	BGC	F	1	2	12,12,12	0.16	0	17,17,17	0.34	0
2	GLC	F	2	2	11,11,12	0.53	0	15,15,17	1.37	2 (13%)
2	BMA	F	3	2,4	11,11,12	0.65	0	15,15,17	0.76	0
2	BGC	F	4[A]	-	11,11,12	0.35	0	15,15,17	0.58	0
2	BGC	F	4[B]	-	11,11,12	0.36	0	15,15,17	0.60	0
2	GLC	F	5	2	11,11,12	0.74	0	15,15,17	1.05	0
2	BMA	F	6	2	11,11,12	0.79	0	15,15,17	0.74	0
2	GCU	F	7	2	12,12,13	0.77	0	14,17,19	0.97	1 (7%)
2	GCU	F	8	2	12,12,13	0.87	0	14,17,19	0.95	1 (7%)
3	BGC	G	1	3	12,12,12	0.40	0	17,17,17	0.90	1 (5%)
3	GLC	G	2	3	11,11,12	0.45	0	15,15,17	0.90	1 (6%)
3	BMA	G	3	3	11,11,12	0.53	0	15,15,17	0.70	0
3	GCU	G	4	3	12,12,13	0.71	0	14,17,19	0.93	1 (7%)
3	BGC	H	1	3	12,12,12	0.50	0	17,17,17	0.89	1 (5%)
3	GLC	H	2	3	11,11,12	0.55	0	15,15,17	0.97	1 (6%)
3	BMA	H	3[A]	-	11,11,12	0.64	0	15,15,17	0.84	0
3	BMA	H	3[B]	-	11,11,12	0.62	0	15,15,17	0.77	0
3	GCU	H	4	3	12,12,13	0.64	0	14,17,19	0.80	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
2	BGC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	BMA	D	3	2,4	-	0/2/19/22	0/1/1/1
2	BGC	D	4	2	-	0/2/19/22	0/1/1/1
2	GLC	D	5	2	-	0/2/19/22	0/1/1/1
2	BMA	D	6	2	-	0/2/19/22	0/1/1/1
2	GCU	D	7	2	-	0/4/21/24	0/1/1/1
2	GCU	D	8	2	-	0/4/21/24	0/1/1/1
3	BGC	E	1	3	-	0/2/22/22	0/1/1/1
3	GLC	E	2	3	-	0/2/19/22	0/1/1/1
3	BMA	E	3[A]	-	-	0/2/19/22	0/1/1/1
3	BMA	E	3[B]	-	-	0/2/19/22	0/1/1/1
3	GCU	E	4	3	-	0/4/21/24	0/1/1/1
2	BGC	F	1	2	-	1/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	BMA	F	3	2,4	-	0/2/19/22	0/1/1/1
2	BGC	F	4[A]	-	-	2/2/19/22	0/1/1/1
2	BGC	F	4[B]	-	-	0/2/19/22	0/1/1/1
2	GLC	F	5	2	-	0/2/19/22	0/1/1/1
2	BMA	F	6	2	-	0/2/19/22	0/1/1/1
2	GCU	F	7	2	-	2/4/21/24	0/1/1/1
2	GCU	F	8	2	-	0/4/21/24	0/1/1/1
3	BGC	G	1	3	-	0/2/22/22	0/1/1/1
3	GLC	G	2	3	-	0/2/19/22	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	GCU	G	4	3	-	0/4/21/24	0/1/1/1
3	BGC	H	1	3	-	0/2/22/22	0/1/1/1
3	GLC	H	2	3	-	0/2/19/22	0/1/1/1
3	BMA	H	3[A]	-	-	1/2/19/22	0/1/1/1
3	BMA	H	3[B]	-	-	0/2/19/22	0/1/1/1
3	GCU	H	4	3	-	0/4/21/24	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	GLC	C1-O5-C5	3.03	116.29	112.19
2	D	5	GLC	C1-O5-C5	2.66	115.80	112.19
2	F	7	GCU	O5-C1-C2	-2.65	106.68	110.77
3	G	4	GCU	O5-C1-C2	-2.32	107.19	110.77
3	G	2	GLC	C1-O5-C5	2.30	115.31	112.19
3	G	1	BGC	C1-C2-C3	2.24	114.96	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	2	GLC	C1-O5-C5	2.24	115.22	112.19
3	E	2	GLC	O5-C1-C2	-2.22	107.35	110.77
3	H	1	BGC	C1-C2-C3	2.20	114.88	110.31
2	F	2	GLC	O5-C1-C2	-2.09	107.55	110.77
2	D	7	GCU	O5-C1-C2	-2.09	107.55	110.77
2	F	8	GCU	C1-C2-C3	2.03	112.16	109.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	7	GCU	C4-C5-C6-O6A
2	F	7	GCU	C4-C5-C6-O6B
2	D	1	BGC	O5-C5-C6-O6
2	F	4[A]	BGC	C4-C5-C6-O6
2	D	1	BGC	C4-C5-C6-O6
2	F	4[A]	BGC	O5-C5-C6-O6
3	H	3[A]	BMA	O5-C5-C6-O6
2	F	1	BGC	C4-C5-C6-O6

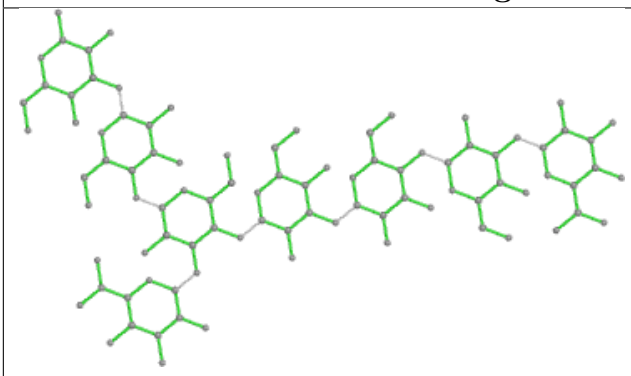
There are no ring outliers.

6 monomers are involved in 6 short contacts:

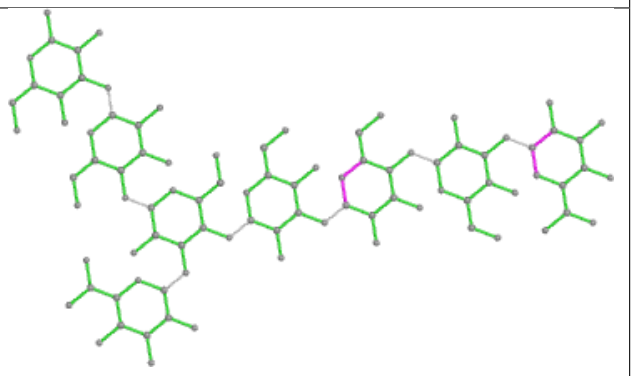
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	6	BMA	1	0
2	F	4[A]	BGC	1	0
2	F	6	BMA	1	0
3	H	1	BGC	1	0
3	G	1	BGC	2	0
3	E	1	BGC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

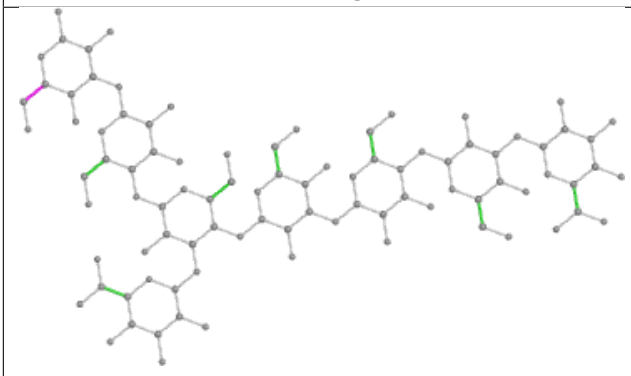
Oligosaccharide Chain D



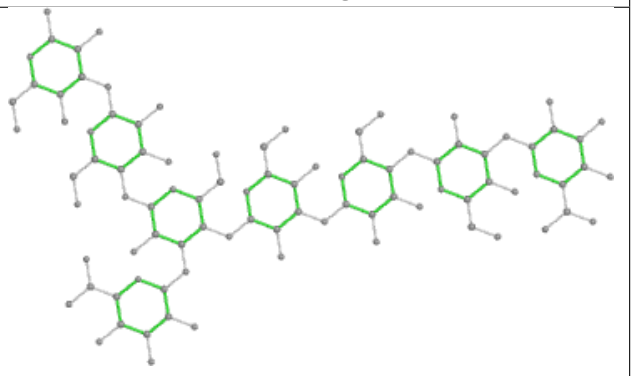
Bond lengths



Bond angles

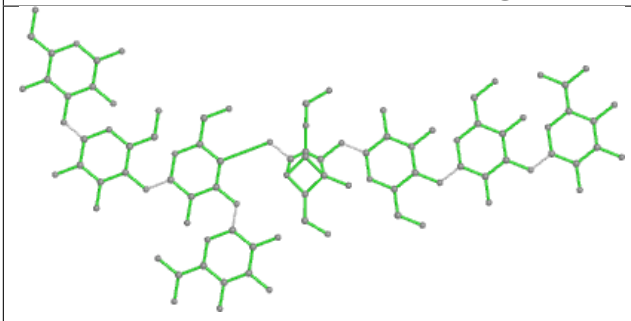


Torsions

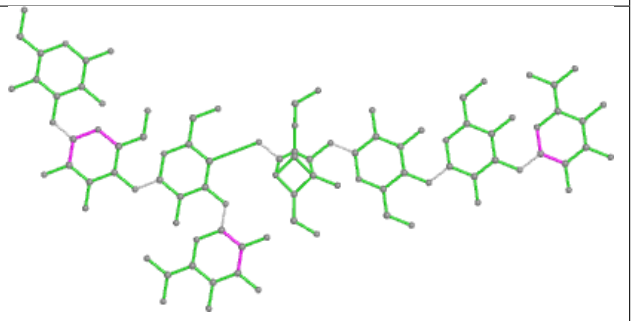


Rings

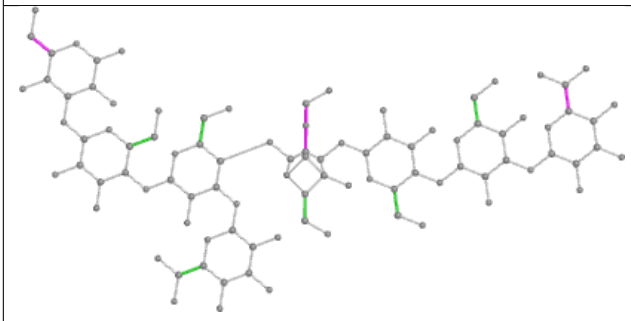
Oligosaccharide Chain F



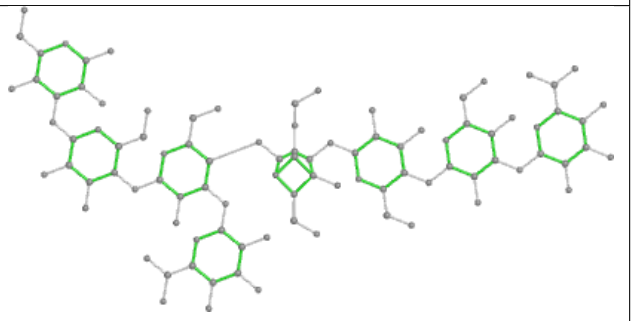
Bond lengths



Bond angles

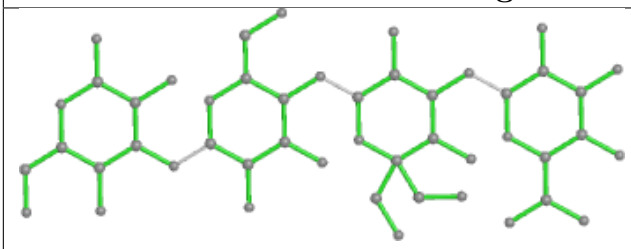


Torsions

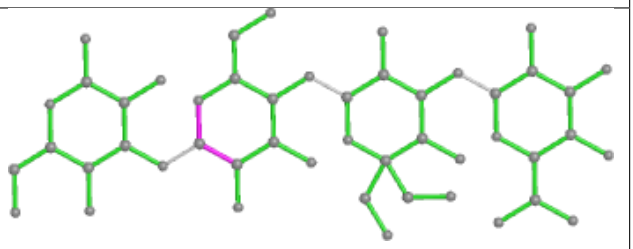


Rings

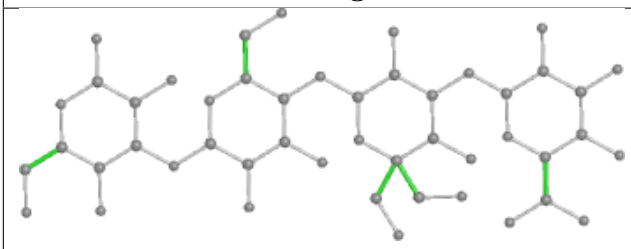
Oligosaccharide Chain E



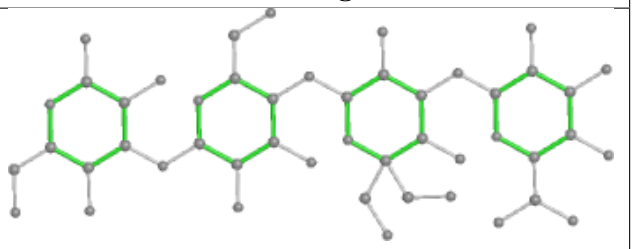
Bond lengths



Bond angles

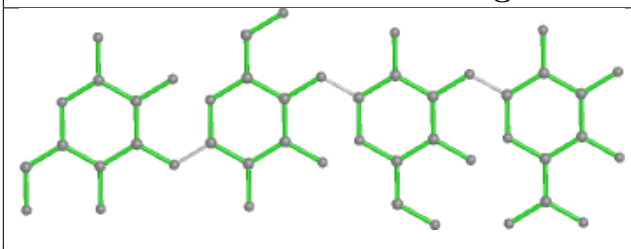


Torsions

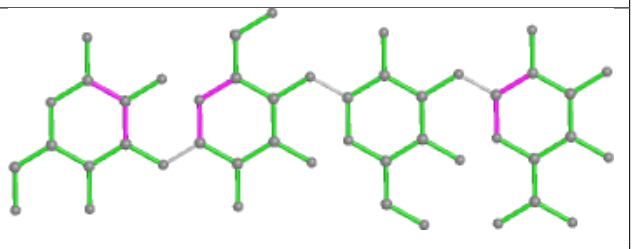


Rings

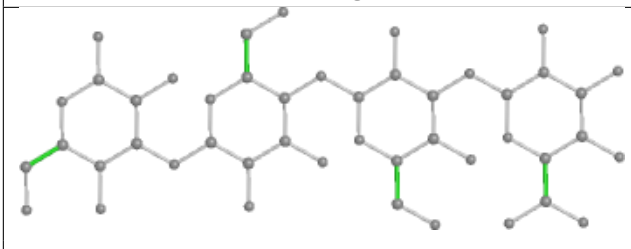
Oligosaccharide Chain G



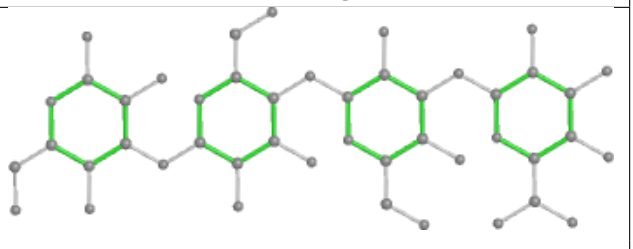
Bond lengths



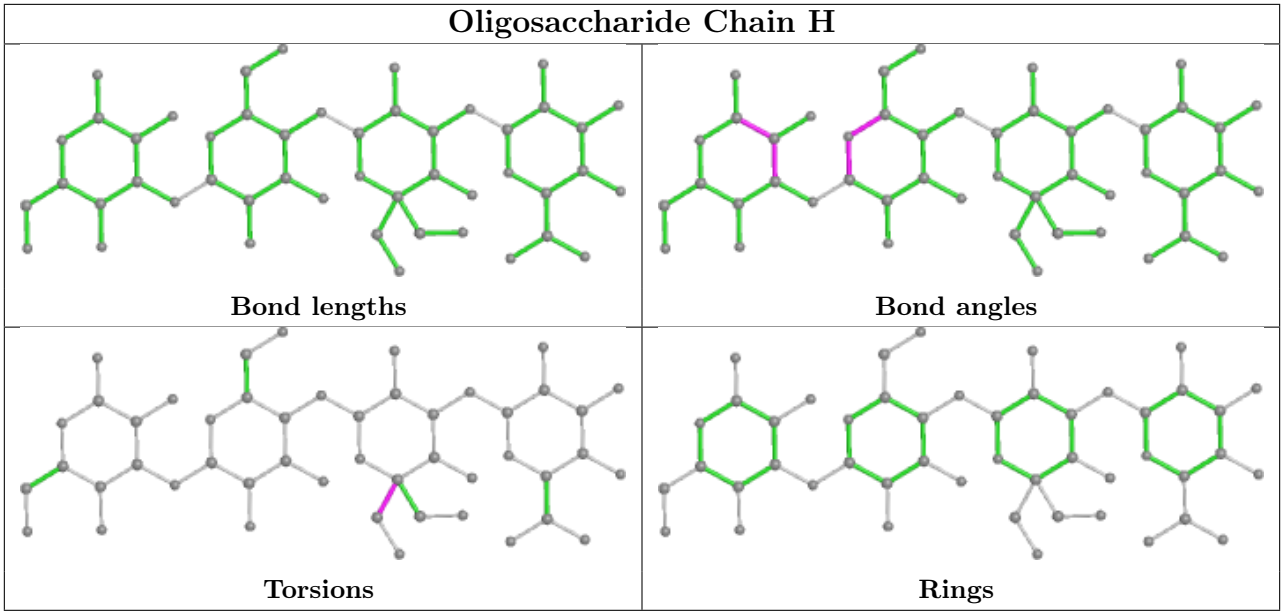
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

25 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	$\#\|Z\| > 2$
5	EDO	B	601[A]	-	3,3,3	0.40	0	2,2,2	0.23	0
5	EDO	B	603	-	3,3,3	0.41	0	2,2,2	0.52	0
5	EDO	A	606	-	3,3,3	0.39	0	2,2,2	0.67	0
5	EDO	C	604[B]	-	3,3,3	0.43	0	2,2,2	0.33	0
5	EDO	C	602	-	3,3,3	0.37	0	2,2,2	0.51	0
5	EDO	A	608	-	3,3,3	0.44	0	2,2,2	0.27	0
5	EDO	A	609	-	3,3,3	0.34	0	2,2,2	0.45	0
5	EDO	A	602[B]	-	3,3,3	0.44	0	2,2,2	0.60	0
5	EDO	A	603	-	3,3,3	0.58	0	2,2,2	0.50	0
5	EDO	B	605[B]	-	3,3,3	0.40	0	2,2,2	0.68	0
5	EDO	C	606[B]	-	3,3,3	0.38	0	2,2,2	0.49	0
5	EDO	B	602	-	3,3,3	0.53	0	2,2,2	0.42	0
5	EDO	C	603	-	3,3,3	0.39	0	2,2,2	0.51	0
5	EDO	A	605	-	3,3,3	0.41	0	2,2,2	0.30	0
5	EDO	C	604[A]	-	3,3,3	0.48	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	B	604	-	3,3,3	0.37	0	2,2,2	0.40	0
5	EDO	B	601[B]	-	3,3,3	0.29	0	2,2,2	0.54	0
4	ACE	A	601	2	1,2,2	0.60	0	1,1,1	0.36	0
5	EDO	A	604	-	3,3,3	0.32	0	2,2,2	0.44	0
4	ACE	C	601	2	1,2,2	0.61	0	1,1,1	0.24	0
5	EDO	C	605	-	3,3,3	0.41	0	2,2,2	0.54	0
5	EDO	A	602[A]	-	3,3,3	0.39	0	2,2,2	0.53	0
5	EDO	B	605[A]	-	3,3,3	0.44	0	2,2,2	0.44	0
5	EDO	A	607	-	3,3,3	0.38	0	2,2,2	0.86	0
5	EDO	C	606[A]	-	3,3,3	0.38	0	2,2,2	0.75	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
5	EDO	B	601[A]	-	-	0/1/1/1	-
5	EDO	B	603	-	-	0/1/1/1	-
5	EDO	A	606	-	-	0/1/1/1	-
5	EDO	C	604[B]	-	-	0/1/1/1	-
5	EDO	C	602	-	-	0/1/1/1	-
5	EDO	A	608	-	-	1/1/1/1	-
5	EDO	A	609	-	-	0/1/1/1	-
5	EDO	A	602[B]	-	-	0/1/1/1	-
5	EDO	A	603	-	-	0/1/1/1	-
5	EDO	B	605[B]	-	-	1/1/1/1	-
5	EDO	C	606[B]	-	-	1/1/1/1	-
5	EDO	B	602	-	-	0/1/1/1	-
5	EDO	C	603	-	-	0/1/1/1	-
5	EDO	A	605	-	-	0/1/1/1	-
5	EDO	C	604[A]	-	-	0/1/1/1	-
5	EDO	B	604	-	-	0/1/1/1	-
5	EDO	B	601[B]	-	-	0/1/1/1	-
5	EDO	A	604	-	-	1/1/1/1	-
5	EDO	C	605	-	-	1/1/1/1	-
5	EDO	A	602[A]	-	-	0/1/1/1	-
5	EDO	B	605[A]	-	-	1/1/1/1	-
5	EDO	A	607	-	-	0/1/1/1	-
5	EDO	C	606[A]	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	604	EDO	O1-C1-C2-O2
5	B	605[A]	EDO	O1-C1-C2-O2
5	C	606[A]	EDO	O1-C1-C2-O2
5	B	605[B]	EDO	O1-C1-C2-O2
5	C	606[B]	EDO	O1-C1-C2-O2
5	A	608	EDO	O1-C1-C2-O2
5	C	605	EDO	O1-C1-C2-O2

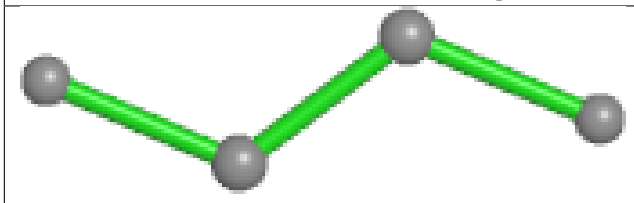
There are no ring outliers.

4 monomers are involved in 6 short contacts:

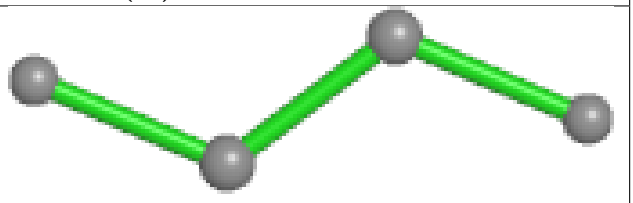
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	608	EDO	2	0
5	B	605[B]	EDO	1	0
5	C	606[B]	EDO	1	0
5	A	604	EDO	2	0

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 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.

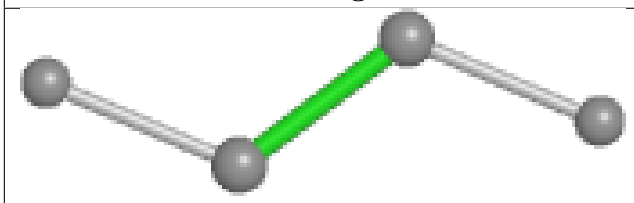
Ligand EDO B 601 (A)



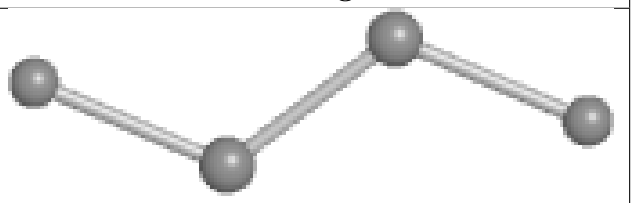
Bond lengths



Bond angles

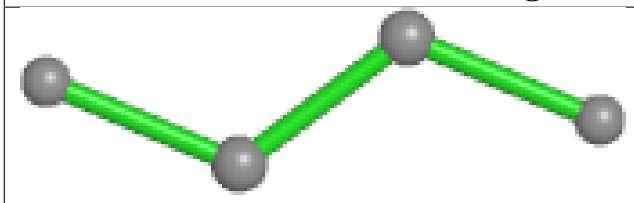


Torsions

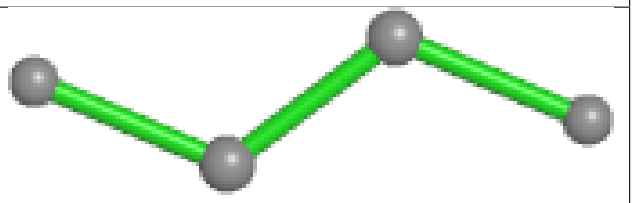


Rings

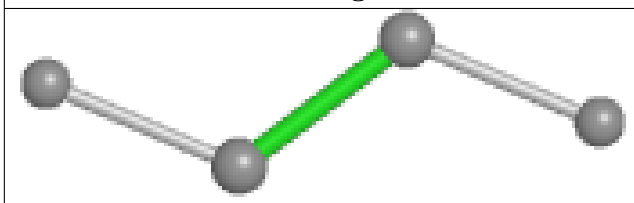
Ligand EDO B 603



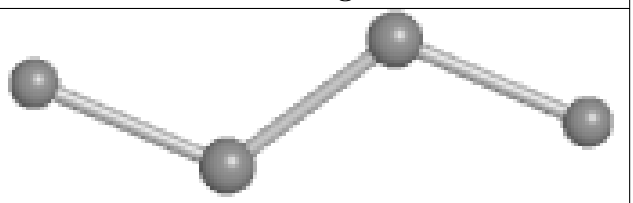
Bond lengths



Bond angles

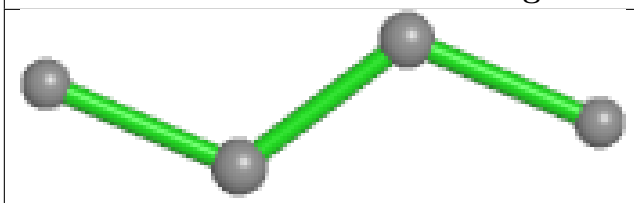


Torsions

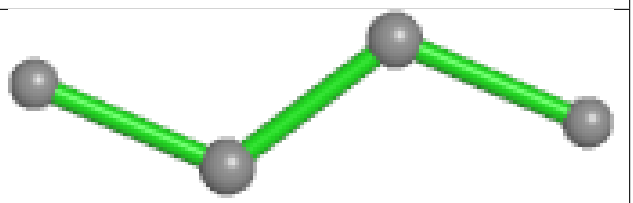


Rings

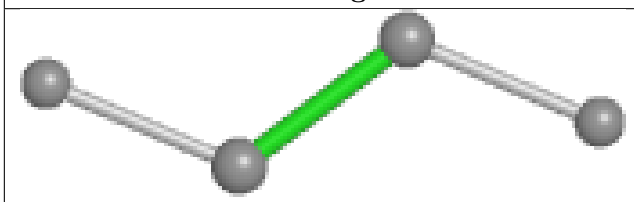
Ligand EDO A 606



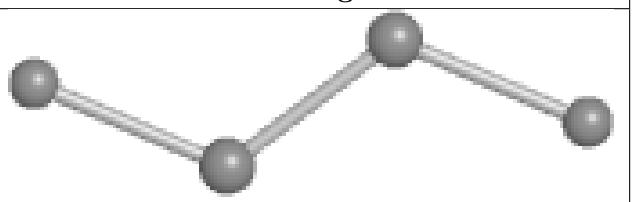
Bond lengths



Bond angles

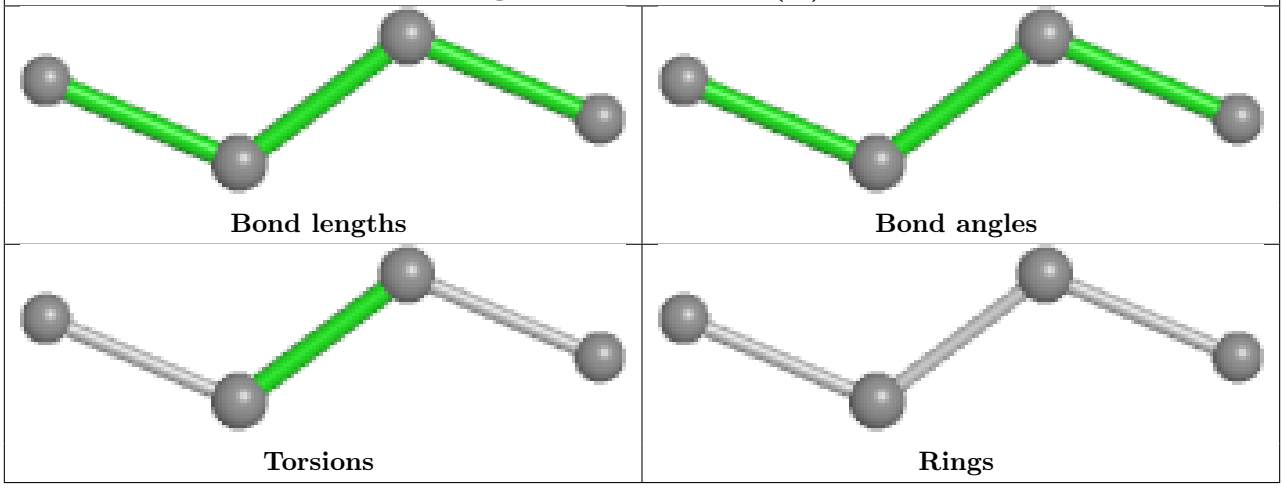


Torsions

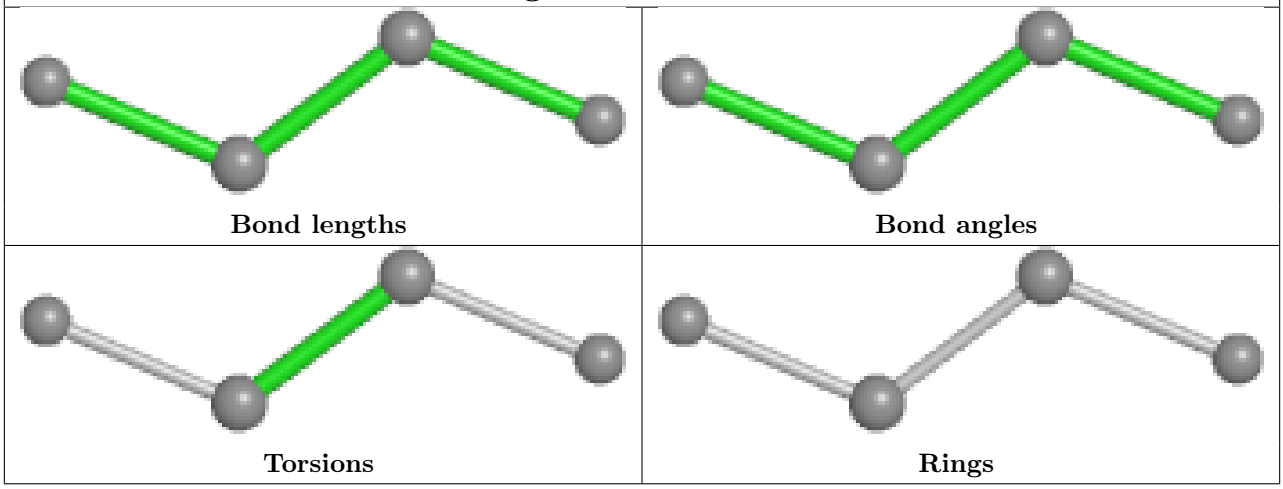


Rings

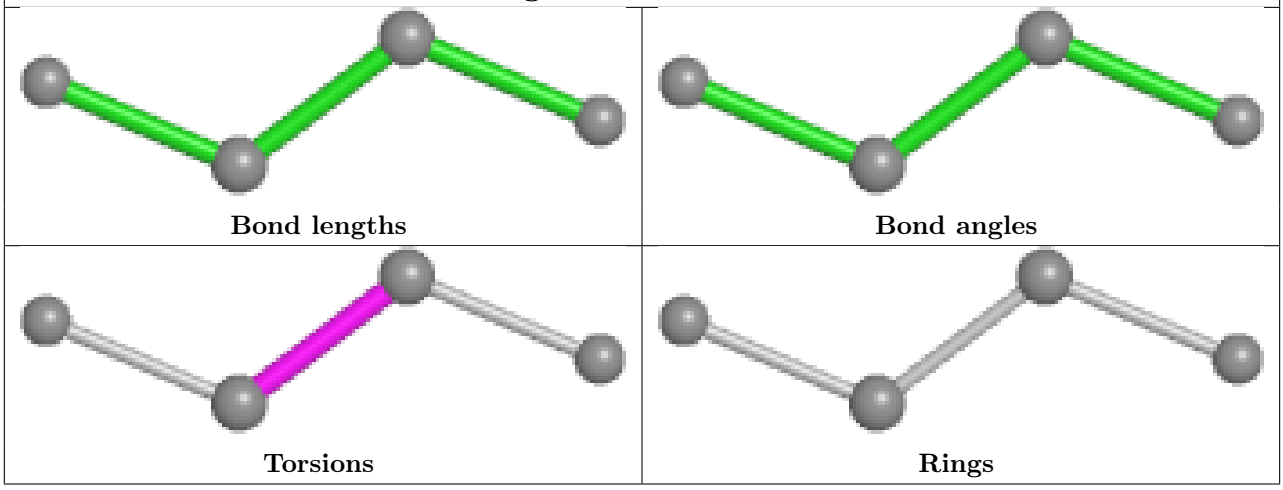
Ligand EDO C 604 (B)



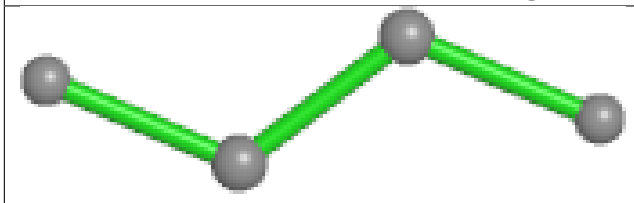
Ligand EDO C 602



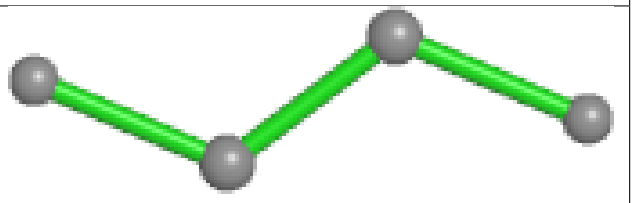
Ligand EDO A 608



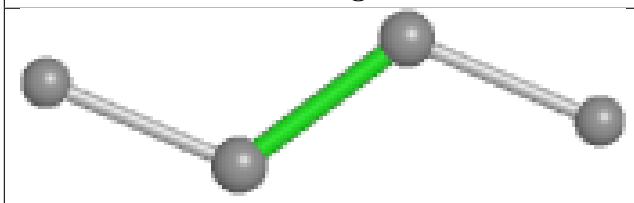
Ligand EDO A 609



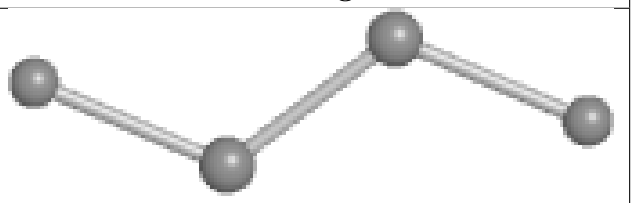
Bond lengths



Bond angles

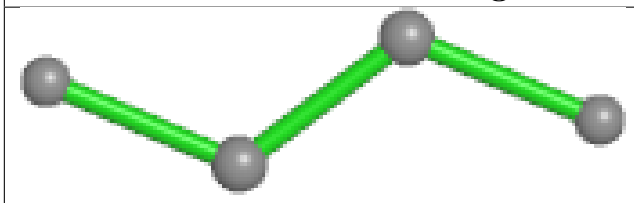


Torsions

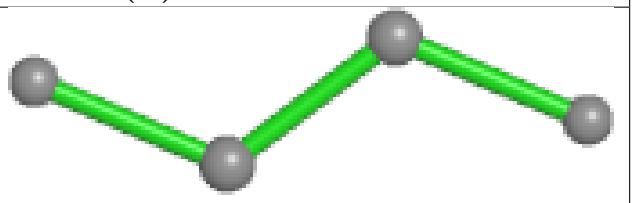


Rings

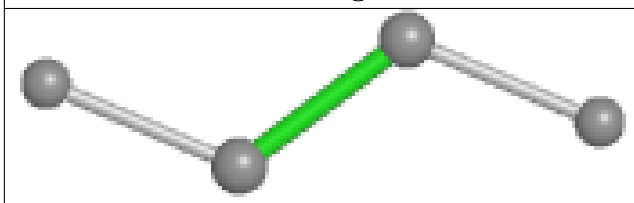
Ligand EDO A 602 (B)



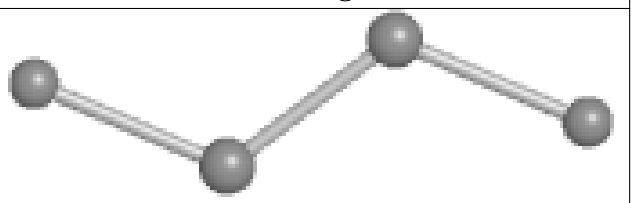
Bond lengths



Bond angles

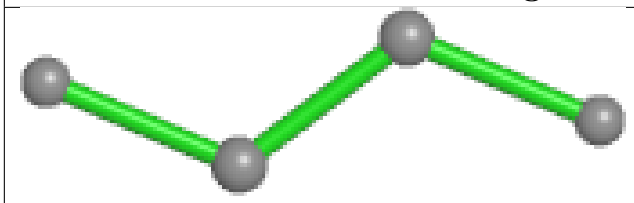


Torsions

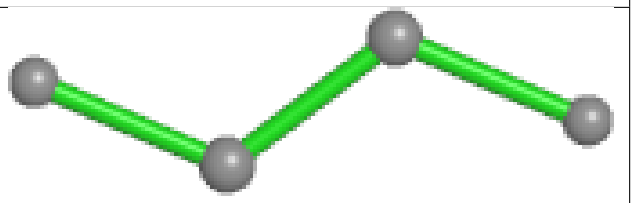


Rings

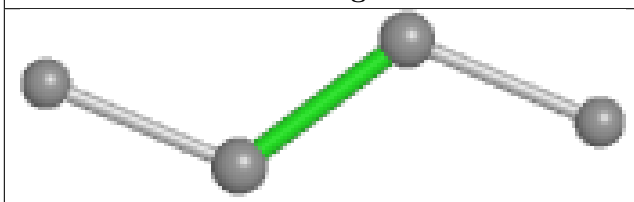
Ligand EDO A 603



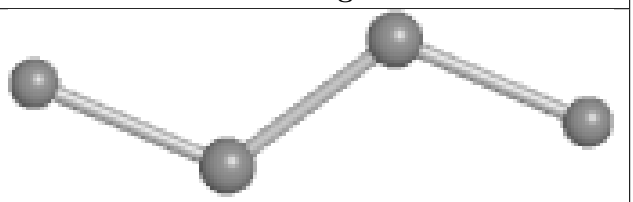
Bond lengths



Bond angles

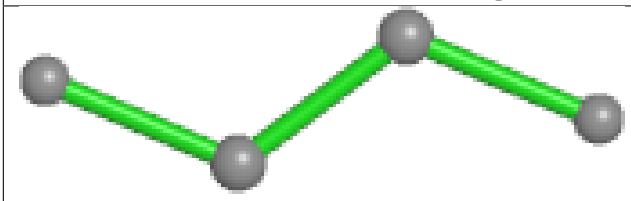


Torsions

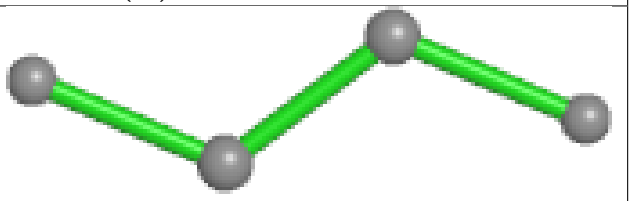


Rings

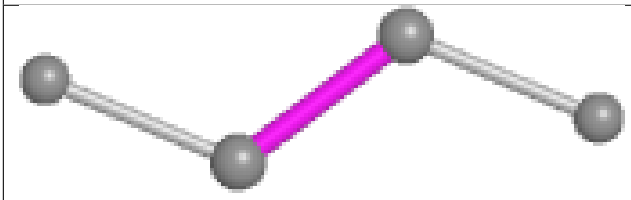
Ligand EDO B 605 (B)



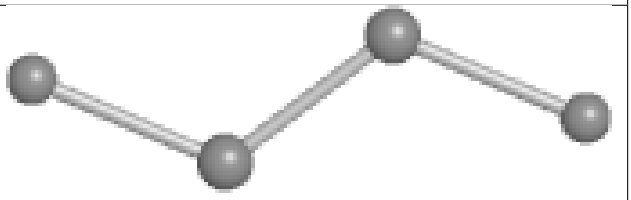
Bond lengths



Bond angles

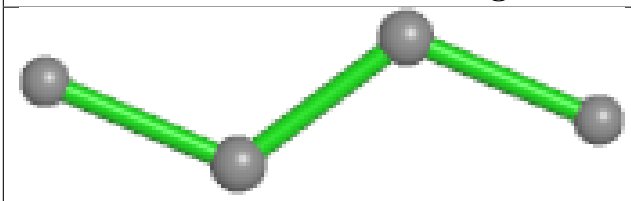


Torsions

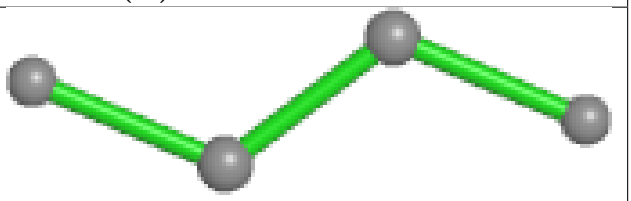


Rings

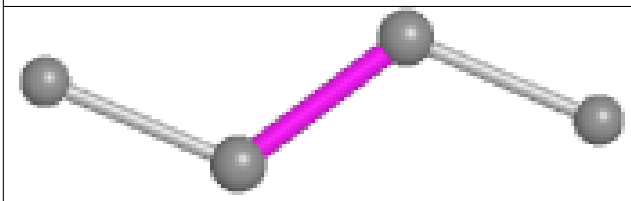
Ligand EDO C 606 (B)



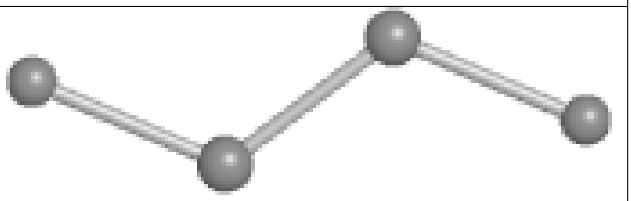
Bond lengths



Bond angles

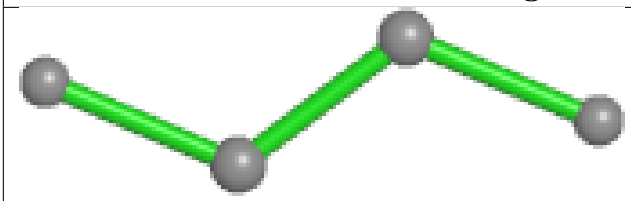


Torsions

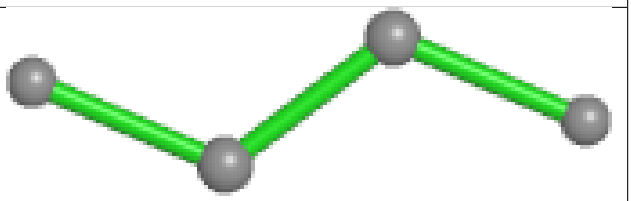


Rings

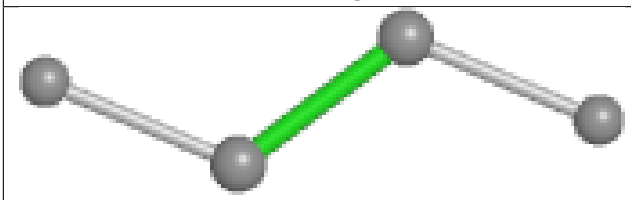
Ligand EDO B 602



Bond lengths



Bond angles



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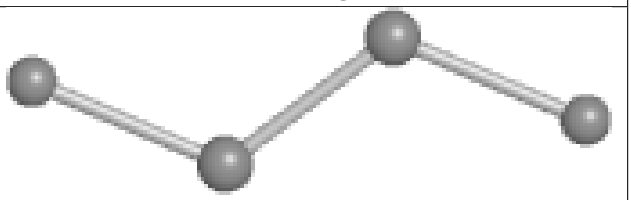
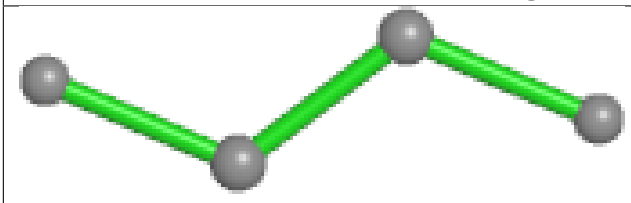
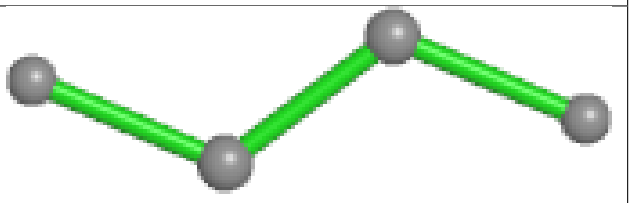


Rings

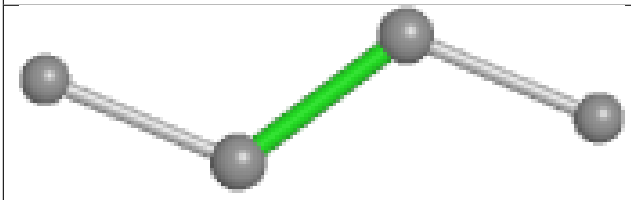
Ligand EDO C 603



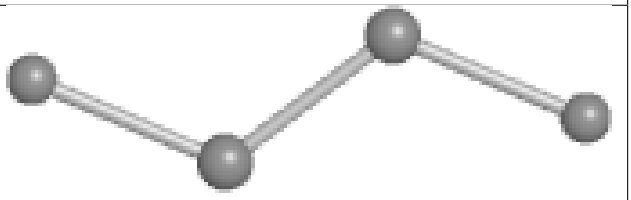
Bond lengths



Bond angles

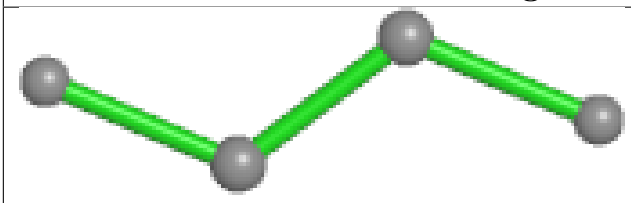


Torsions

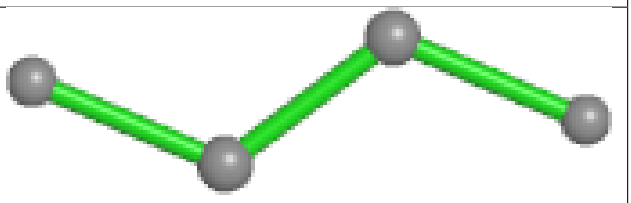


Rings

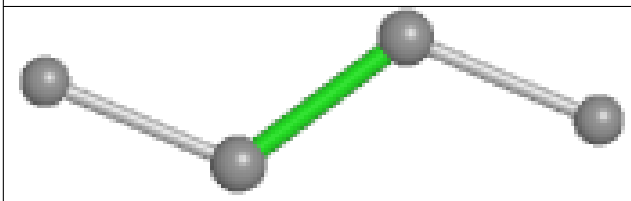
Ligand EDO A 605



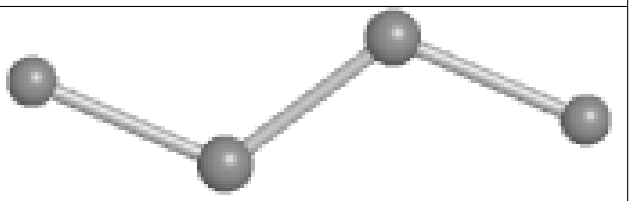
Bond lengths



Bond angles

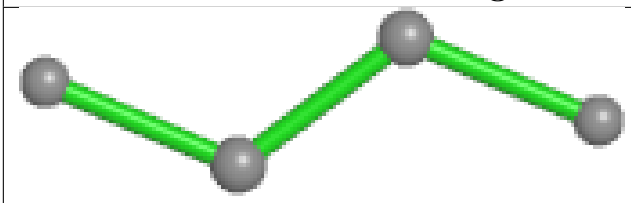


Torsions

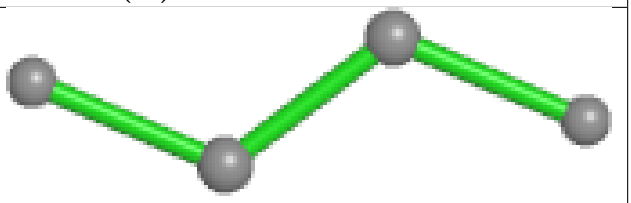


Rings

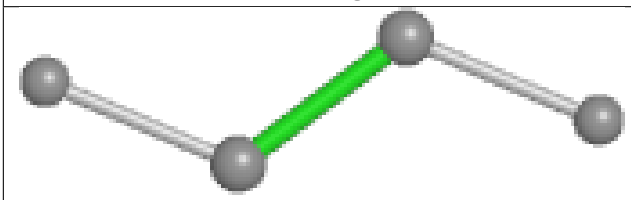
Ligand EDO C 604 (A)



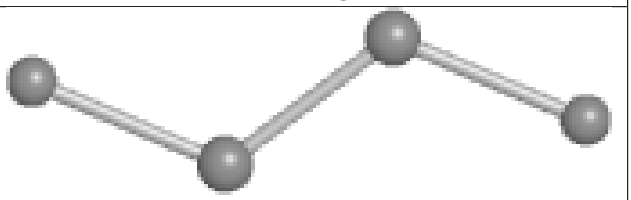
Bond lengths



Bond angles

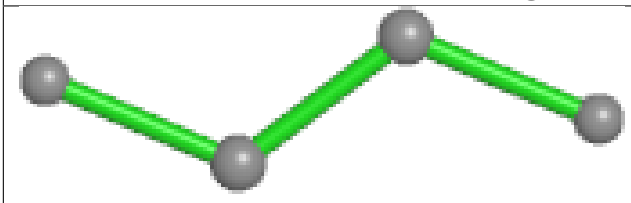


Torsions

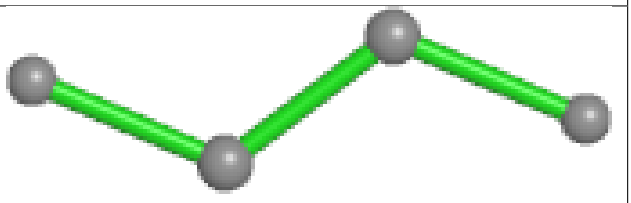


Rings

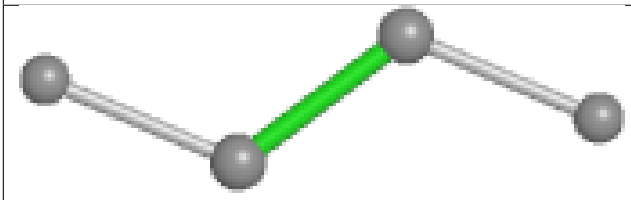
Ligand EDO B 604



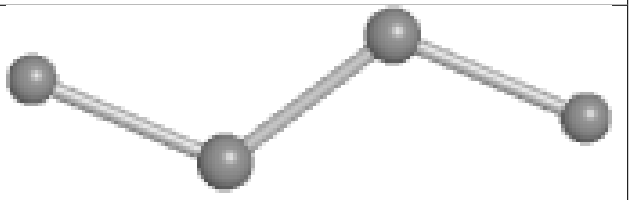
Bond lengths



Bond angles

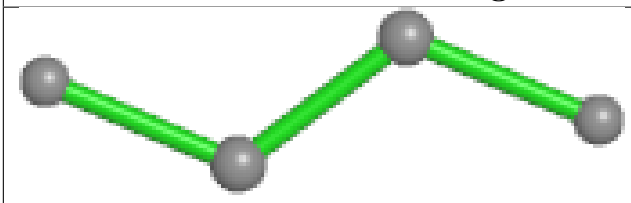


Torsions

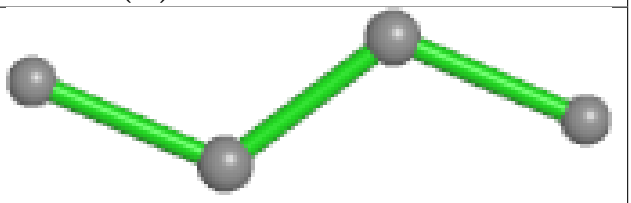


Rings

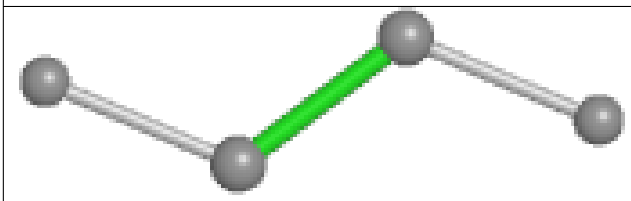
Ligand EDO B 601 (B)



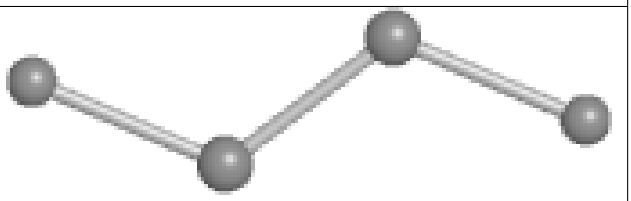
Bond lengths



Bond angles

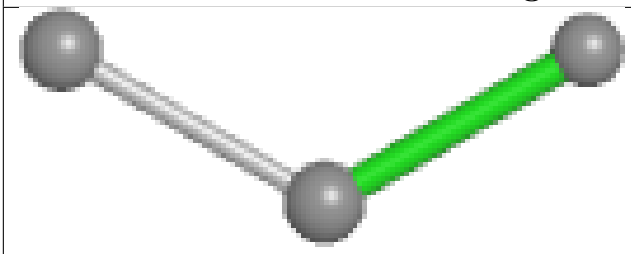


Torsions

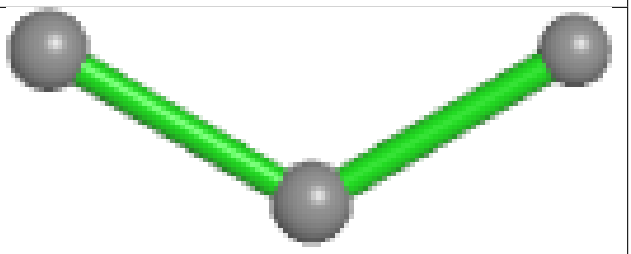


Rings

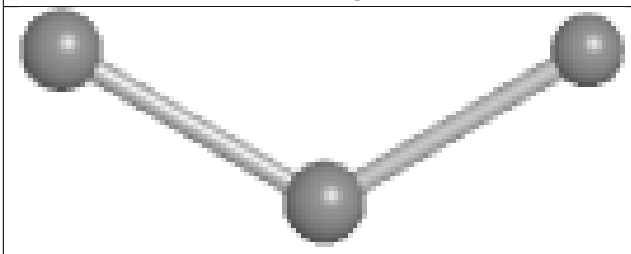
Ligand ACE A 601



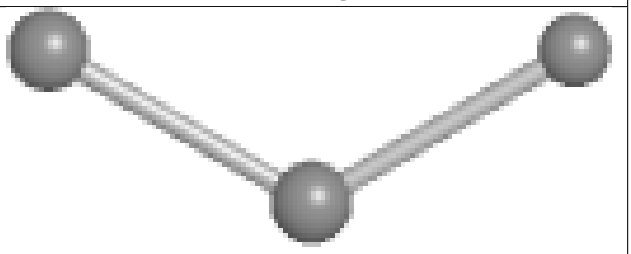
Bond lengths



Bond angles

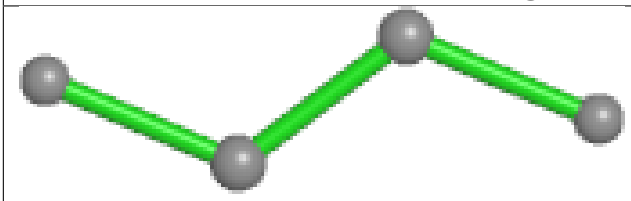


Torsions

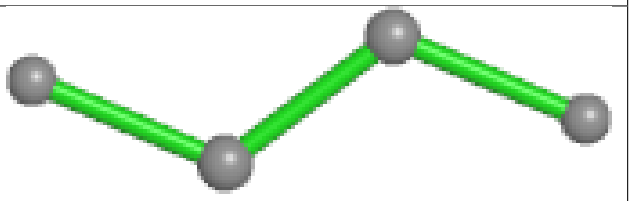


Rings

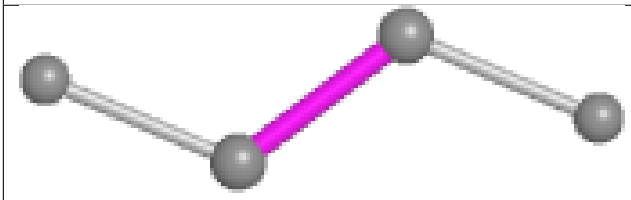
Ligand EDO A 604



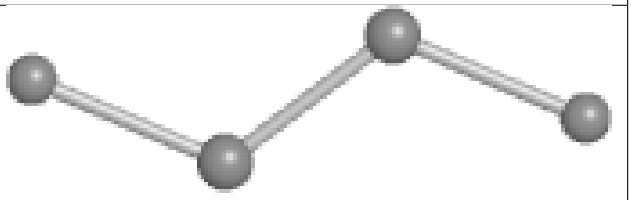
Bond lengths



Bond angles

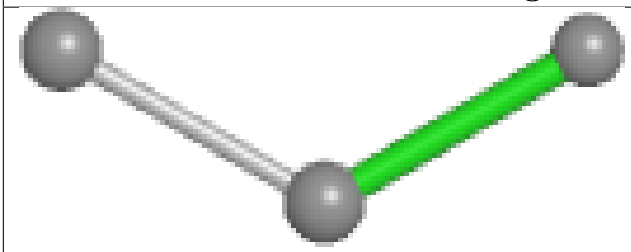


Torsions

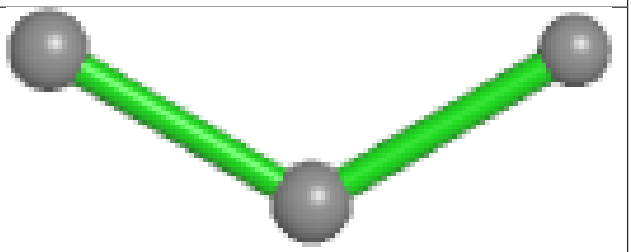


Rings

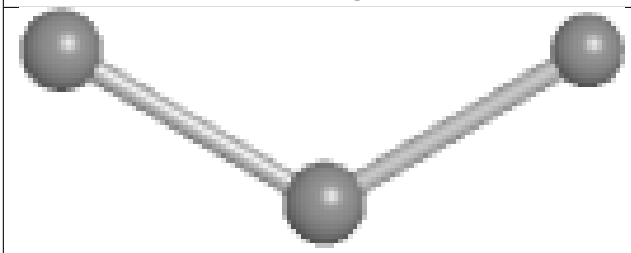
Ligand ACE C 601



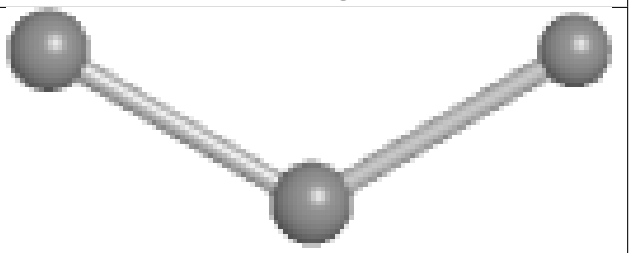
Bond lengths



Bond angles

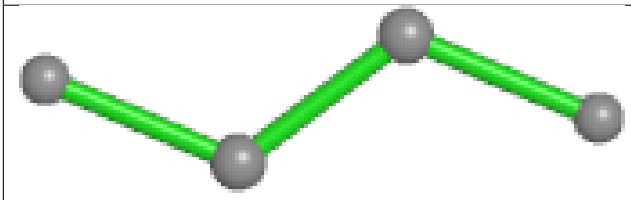


Torsions

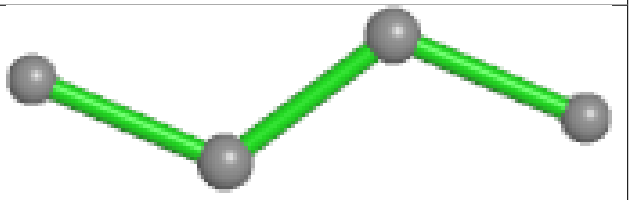


Rings

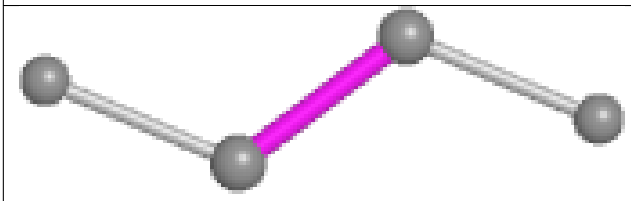
Ligand EDO C 605



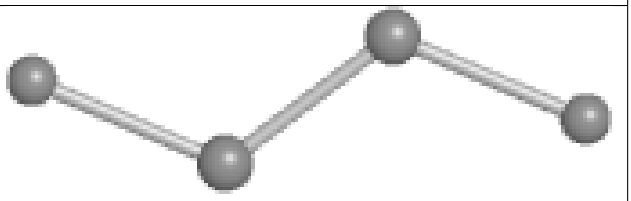
Bond lengths



Bond angles

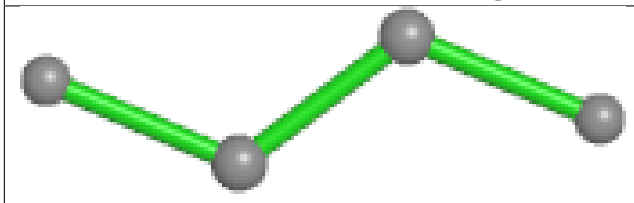


Torsions

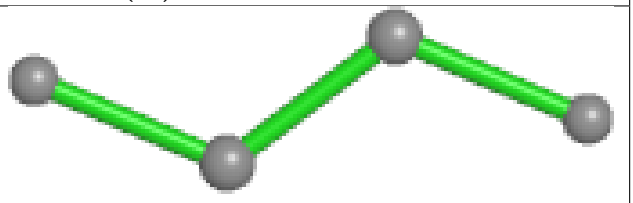


Rings

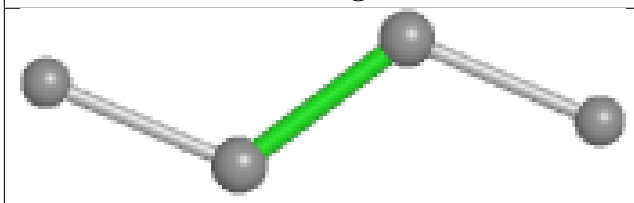
Ligand EDO A 602 (A)



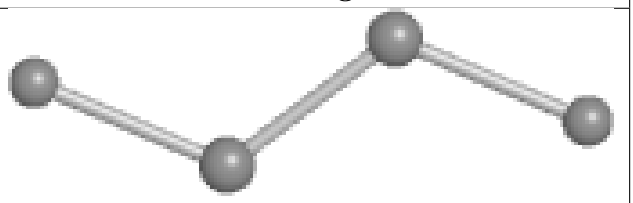
Bond lengths



Bond angles

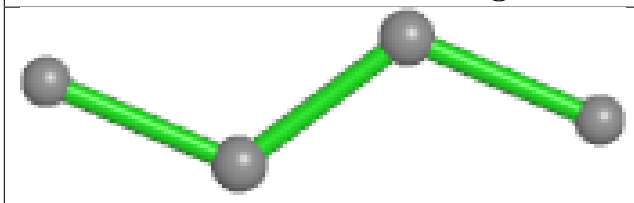


Torsions

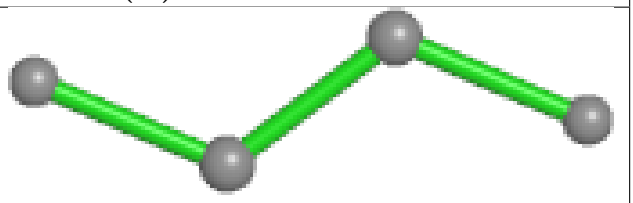


Rings

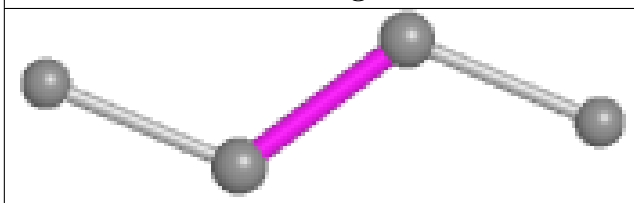
Ligand EDO B 605 (A)



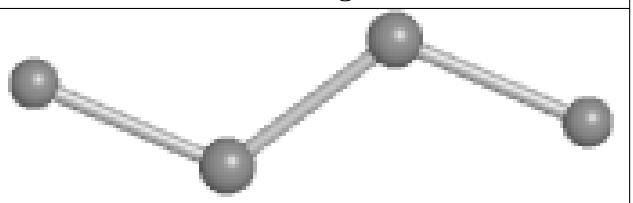
Bond lengths



Bond angles

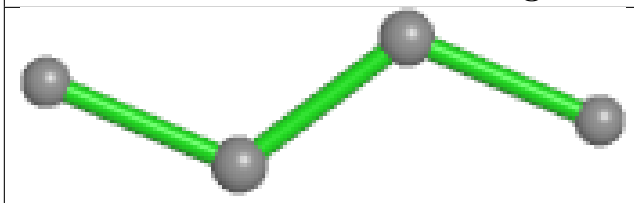


Torsions

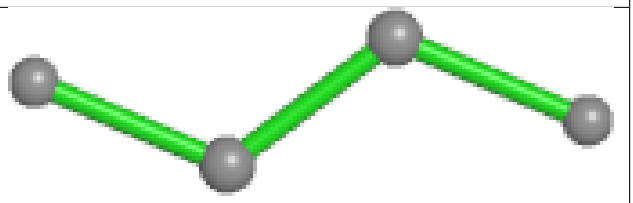


Rings

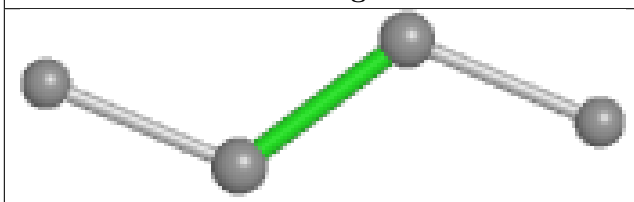
Ligand EDO A 607



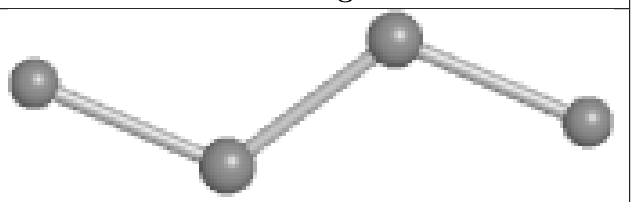
Bond lengths



Bond angles

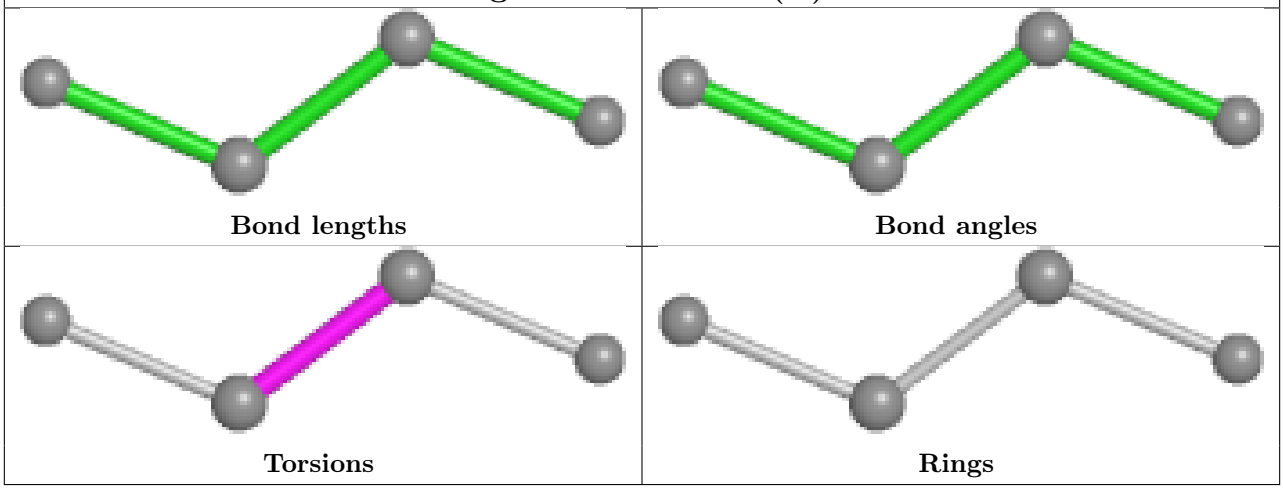


Torsions



Rings

Ligand EDO C 606 (A)



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	565/612 (92%)	-0.45	6 (1%) 80 82	10, 16, 29, 69	0
1	B	563/612 (91%)	0.25	66 (11%) 4 4	11, 18, 79, 118	0
1	C	565/612 (92%)	-0.28	10 (1%) 68 70	10, 18, 35, 62	0
All	All	1693/1836 (92%)	-0.16	82 (4%) 30 30	10, 17, 53, 118	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	473	VAL	8.9
1	B	449	THR	8.3
1	B	475	VAL	8.2
1	B	470	VAL	8.2
1	B	471	ALA	8.0
1	B	453	VAL	7.8
1	B	474	SER	7.7
1	B	447	THR	7.6
1	B	561	VAL	7.2
1	B	451	SER	7.0
1	B	450	SER	6.8
1	B	500	ALA	6.7
1	A	16	TYR	6.5
1	B	452	VAL	5.8
1	B	456	LEU	5.7
1	B	504	GLY	5.6
1	B	448	GLY	5.5
1	B	455	TYR	5.4
1	B	477	THR	5.3
1	B	446	GLY	5.3
1	B	549	ILE	5.1
1	B	502	THR	5.0
1	B	499	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	531	THR	4.8
1	B	445	LYS	4.8
1	B	562	ALA	4.5
1	B	443	VAL	4.4
1	B	507	GLY	4.2
1	B	566	VAL	4.2
1	B	563	GLY	4.2
1	B	560	THR	4.2
1	B	16	TYR	4.2
1	B	503	PRO	4.0
1	B	559	GLN	4.0
1	B	472	PRO	3.9
1	B	564	ALA	3.9
1	B	530	GLY	3.9
1	B	15	GLU	3.9
1	B	476	GLY	3.8
1	B	468	MET	3.6
1	B	505	ASN	3.6
1	B	568	TYR	3.5
1	B	501	THR	3.5
1	C	449	THR	3.5
1	A	579	LEU	3.5
1	C	16	TYR	3.3
1	B	437	ASN	3.2
1	A	449	THR	3.1
1	B	550	GLY	3.1
1	B	487	ASN	3.1
1	B	441	TRP	3.1
1	A	15	GLU	3.1
1	B	533	THR	3.0
1	C	463	GLY	2.9
1	B	479	VAL	2.9
1	B	467	ALA	2.8
1	B	469	ARG	2.8
1	B	522	PRO	2.8
1	B	558	ILE	2.7
1	B	439	ASN	2.7
1	B	428	PHE	2.7
1	B	534	GLY	2.6
1	B	480	SER	2.6
1	B	433	PHE	2.6
1	C	15	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	517	ALA	2.5
1	C	448	GLY	2.5
1	B	435	TYR	2.4
1	C	475	VAL	2.4
1	A	522	PRO	2.4
1	B	572	LEU	2.4
1	B	528	ASN	2.4
1	C	523	GLY	2.2
1	C	450	SER	2.2
1	C	446	GLY	2.2
1	B	488	PRO	2.1
1	C	522	PRO	2.1
1	B	440	ALA	2.1
1	B	516	ALA	2.1
1	B	486	THR	2.1
1	B	208	SER	2.0
1	B	434	GLY	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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GCU	F	7	12/13	0.71	0.39	52,62,71,73	0
2	GCU	D	7	12/13	0.73	0.34	52,59,62,78	0
2	BMA	D	6	11/12	0.80	0.18	36,43,51,53	0
2	BGC	D	1	12/12	0.82	0.41	49,60,64,68	0
2	BGC	F	1	12/12	0.84	0.40	41,56,66,70	0
2	BMA	F	6	11/12	0.86	0.18	28,43,56,56	0
2	GCU	D	8	12/13	0.87	0.21	23,29,42,44	0
2	GCU	F	8	12/13	0.90	0.17	24,29,47,49	0
2	GLC	D	2	11/12	0.91	0.26	25,39,43,45	0
2	BGC	D	4	11/12	0.91	0.12	19,23,26,28	0
2	GLC	F	5	11/12	0.91	0.10	21,22,27,27	0

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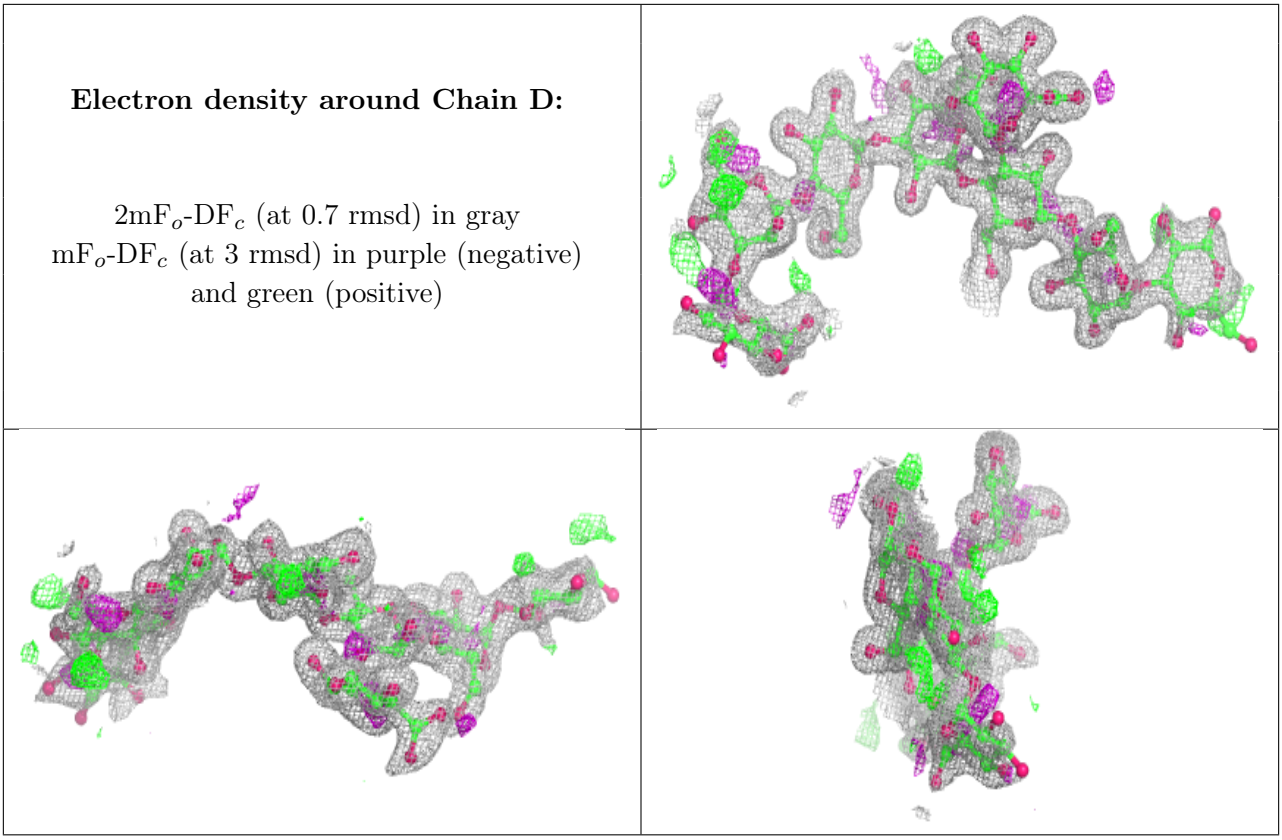
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	F	4[A]	11/12	0.92	0.12	18,19,25,25	3
2	BGC	F	4[B]	11/12	0.92	0.12	16,19,25,25	3
2	GLC	D	5	11/12	0.92	0.09	19,23,26,31	0
2	GLC	F	2	11/12	0.93	0.19	25,33,42,42	0
2	BMA	D	3	11/12	0.94	0.20	21,25,28,31	0
2	BMA	F	3	11/12	0.94	0.16	20,23,25,25	0
3	GLC	H	2	11/12	0.94	0.09	15,18,24,25	0
3	BGC	G	1	12/12	0.95	0.07	17,19,21,23	0
3	BGC	E	1	12/12	0.96	0.06	16,18,19,20	0
3	GCU	E	4	12/13	0.96	0.09	16,21,24,25	0
3	GCU	H	4	12/13	0.96	0.15	19,23,27,29	0
3	BMA	G	3	11/12	0.97	0.09	16,19,24,25	0
3	GCU	G	4	12/13	0.97	0.10	18,20,24,26	0
3	BGC	H	1	12/12	0.97	0.06	18,20,21,21	0
3	GLC	E	2	11/12	0.97	0.06	14,17,22,22	0
3	GLC	G	2	11/12	0.97	0.06	13,18,22,25	0
3	BMA	H	3[B]	11/12	0.98	0.12	18,20,22,24	2
3	BMA	H	3[A]	11/12	0.98	0.12	18,20,21,24	2
3	BMA	E	3[A]	11/12	0.99	0.05	16,19,22,22	2
3	BMA	E	3[B]	11/12	0.99	0.05	16,18,20,22	2

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

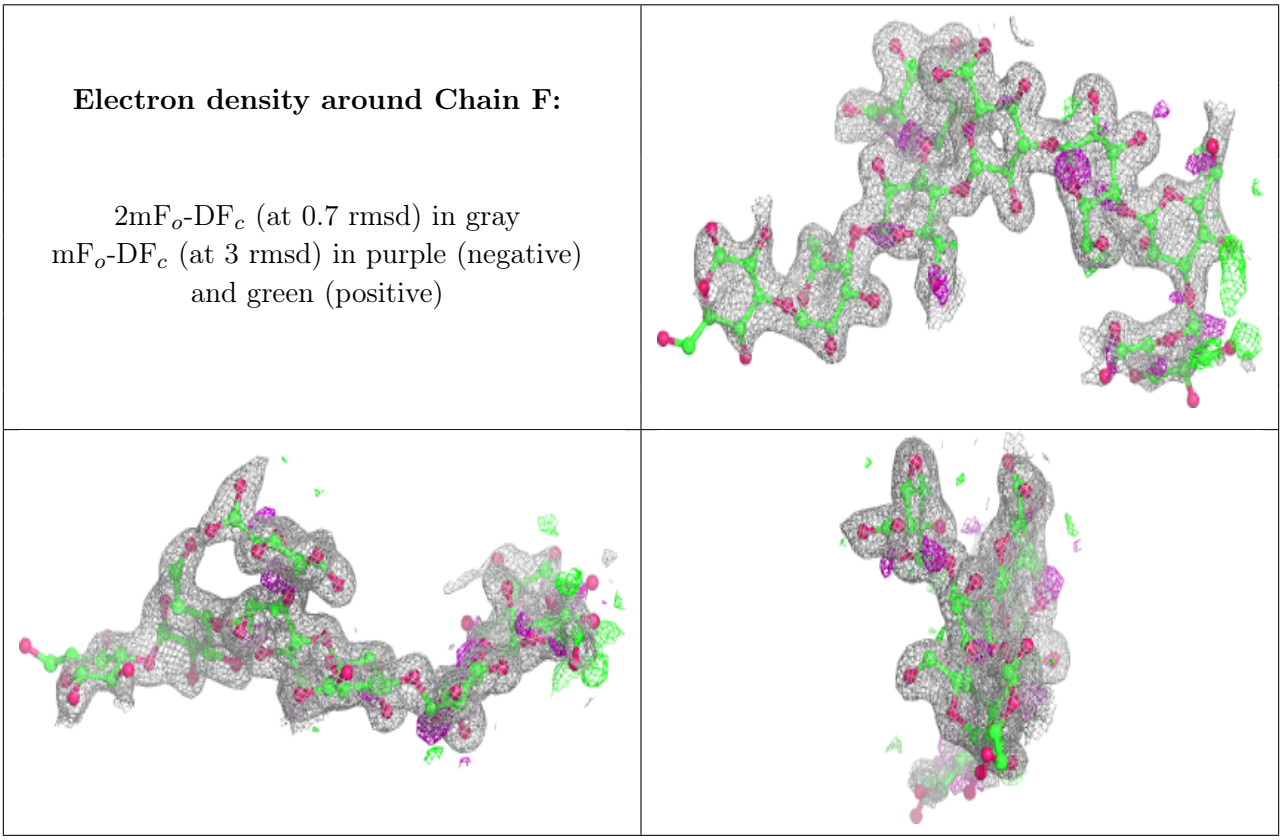
Electron density around Chain D:

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



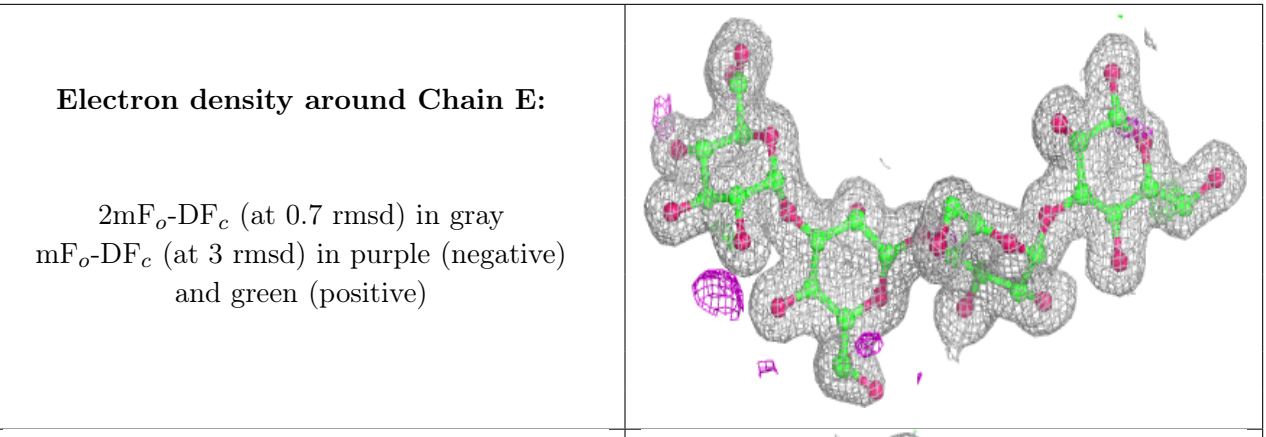
Electron density around Chain F:

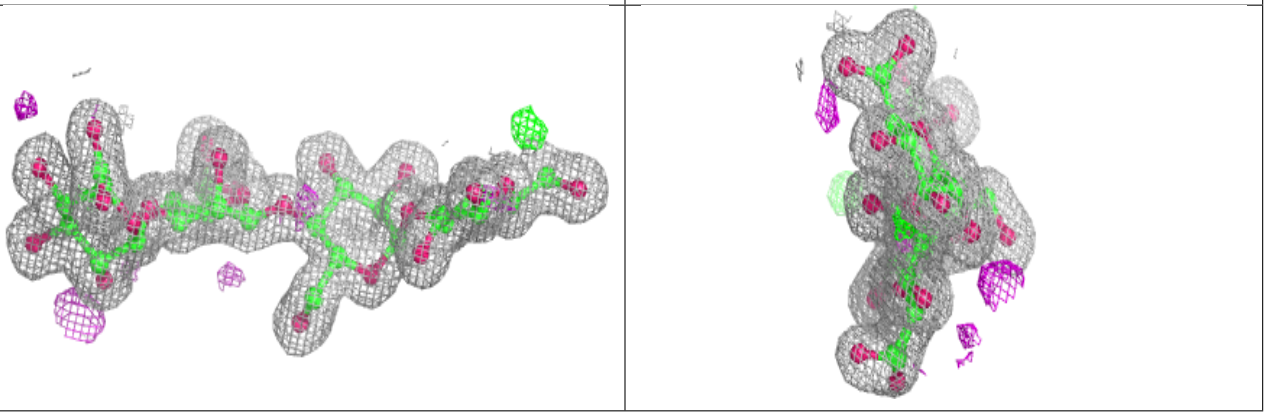
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain E:

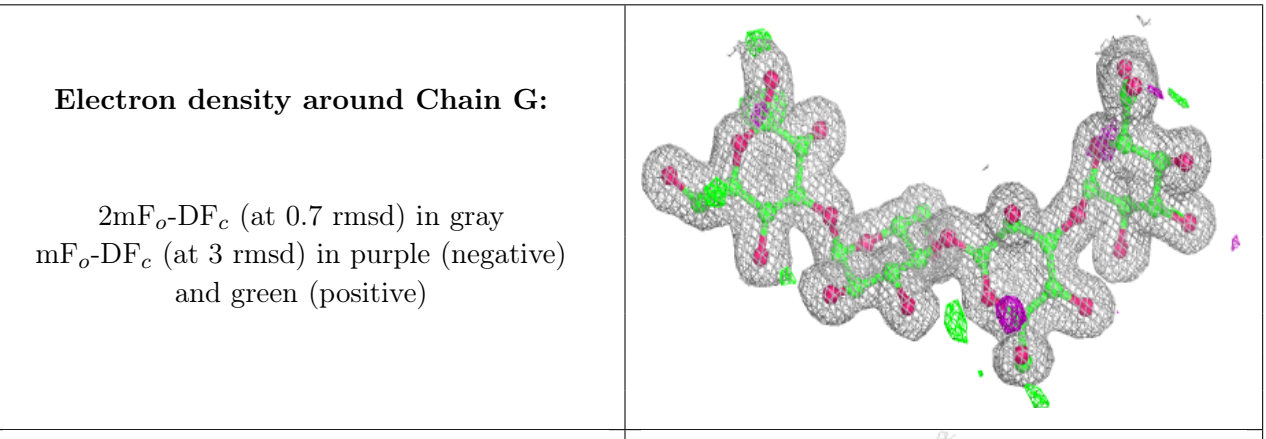
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

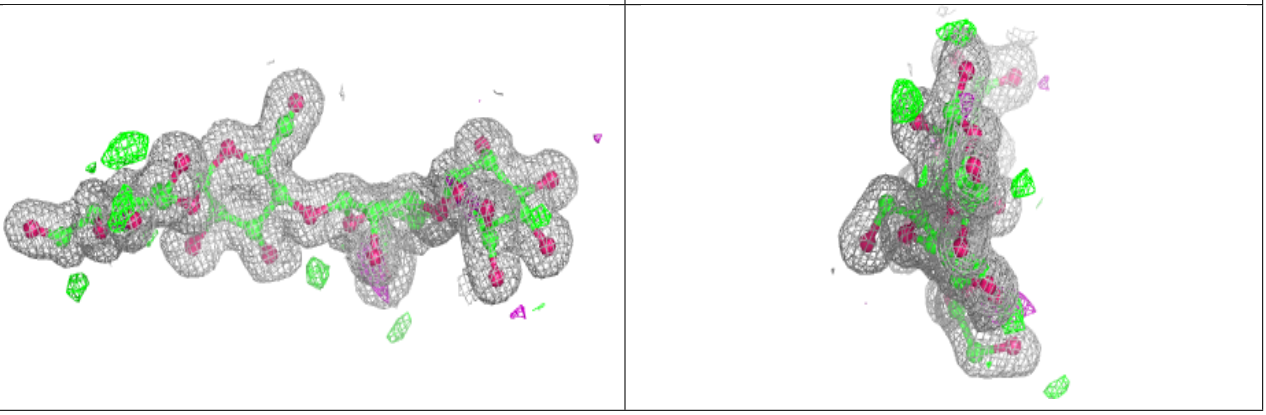




Electron density around Chain G:

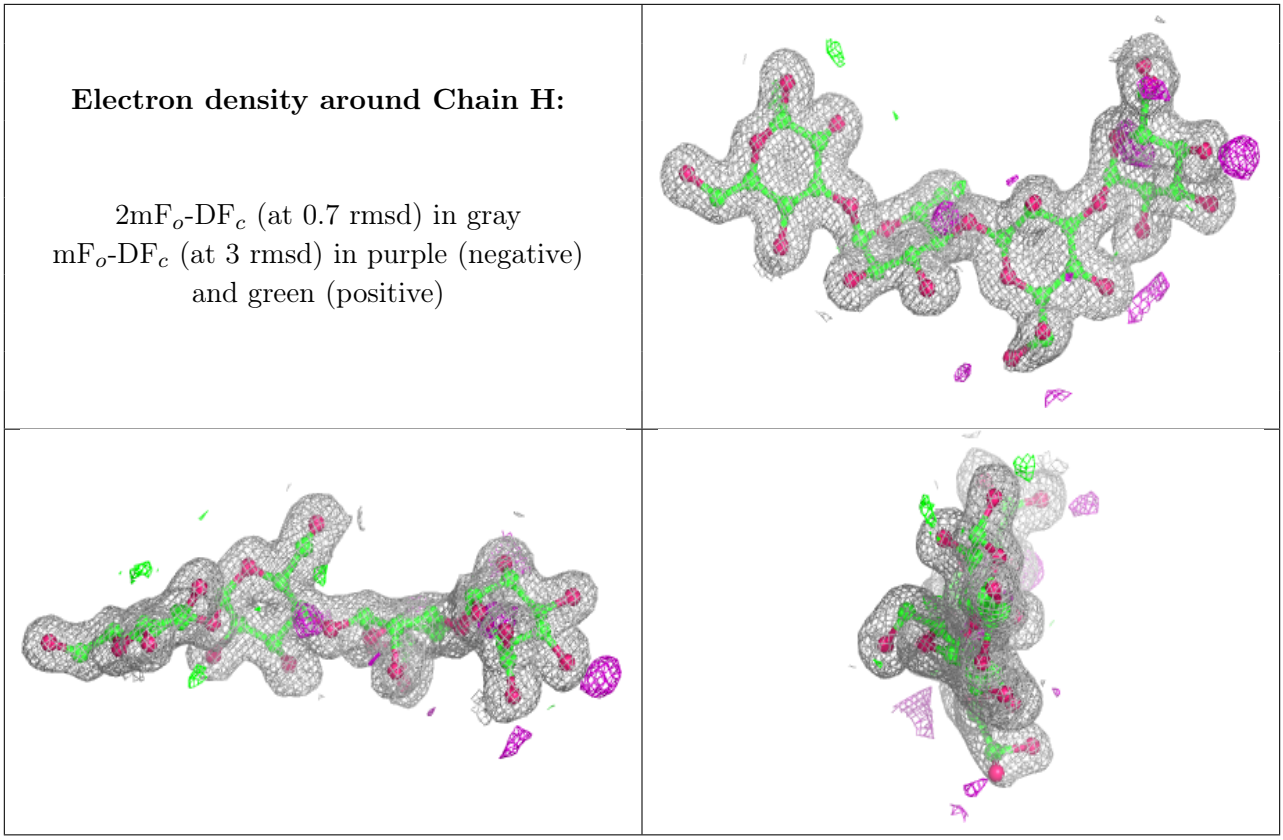
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around Chain H:

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



6.4 Ligands

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
5	EDO	B	605[A]	4/4	0.86	0.23	25,25,34,37	4
5	EDO	B	605[B]	4/4	0.86	0.23	20,21,30,33	4
5	EDO	C	605	4/4	0.91	0.37	32,45,47,51	0
5	EDO	A	608	4/4	0.93	0.23	32,35,41,43	0
4	ACE	A	601	3/3	0.93	0.13	27,27,28,30	0
5	EDO	C	603	4/4	0.94	0.11	31,35,37,47	0
5	EDO	C	606[A]	4/4	0.94	0.17	21,24,25,29	4
5	EDO	C	606[B]	4/4	0.94	0.17	19,27,27,28	4
5	EDO	A	606	4/4	0.95	0.14	23,25,31,33	0
4	ACE	C	601	3/3	0.95	0.09	31,31,32,33	0
5	EDO	B	604	4/4	0.95	0.11	31,31,33,37	0
5	EDO	B	601[B]	4/4	0.96	0.11	17,25,27,28	2
5	EDO	A	603	4/4	0.96	0.08	17,17,18,19	0
5	EDO	A	605	4/4	0.96	0.09	23,29,30,33	0

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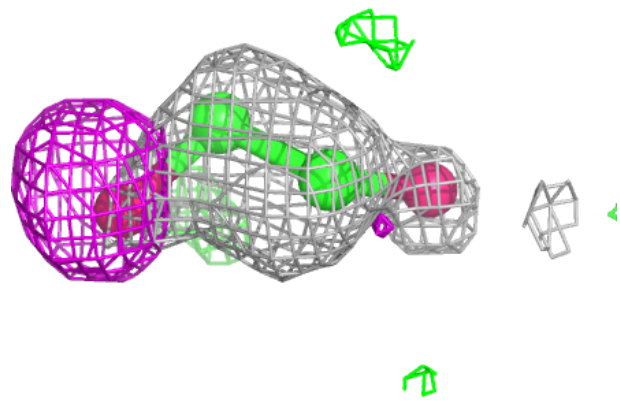
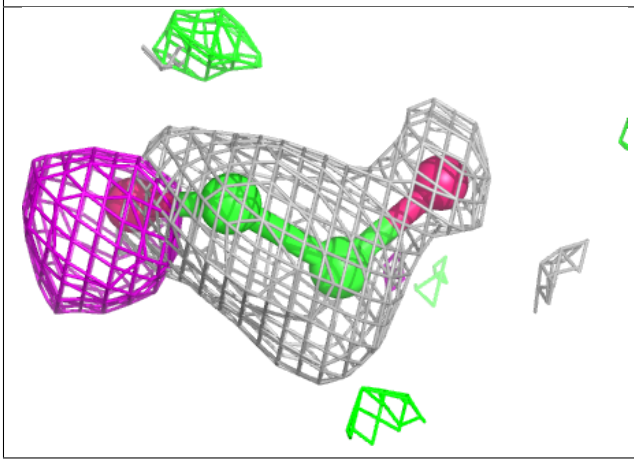
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	B	601[A]	4/4	0.96	0.11	17,22,25,29	2
5	EDO	A	609	4/4	0.97	0.13	21,26,39,47	0
5	EDO	A	607	4/4	0.97	0.07	19,21,24,31	0
5	EDO	A	604	4/4	0.97	0.10	21,26,28,37	0
5	EDO	C	602	4/4	0.97	0.15	25,29,31,39	0
5	EDO	A	602[B]	4/4	0.98	0.07	17,17,18,18	2
5	EDO	C	604[A]	4/4	0.98	0.07	18,19,21,22	2
5	EDO	C	604[B]	4/4	0.98	0.07	19,21,24,26	2
5	EDO	A	602[A]	4/4	0.98	0.07	15,17,17,17	2
5	EDO	B	602	4/4	0.98	0.07	22,24,25,28	0
5	EDO	B	603	4/4	0.98	0.04	18,22,23,25	0

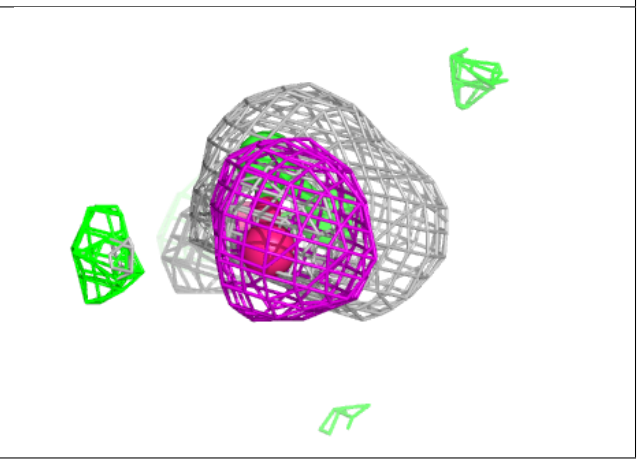
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EDO B 605 (A):

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

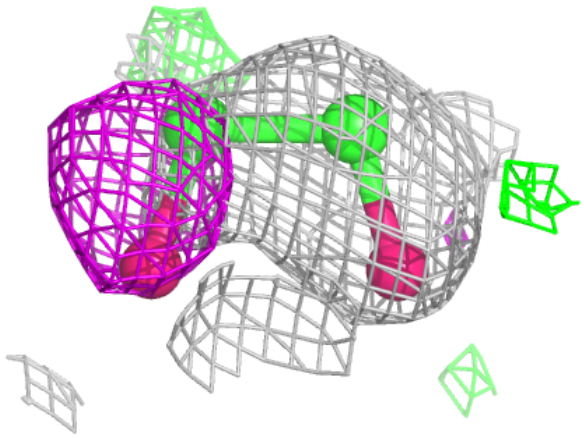


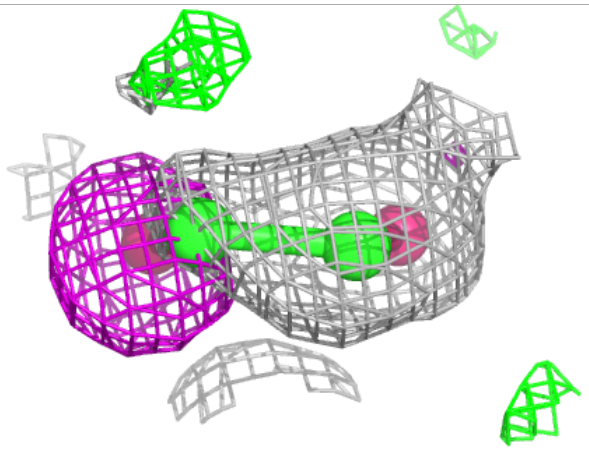


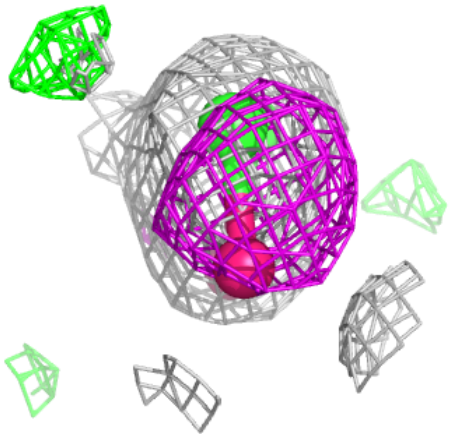


Electron density around EDO B 605 (B):

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

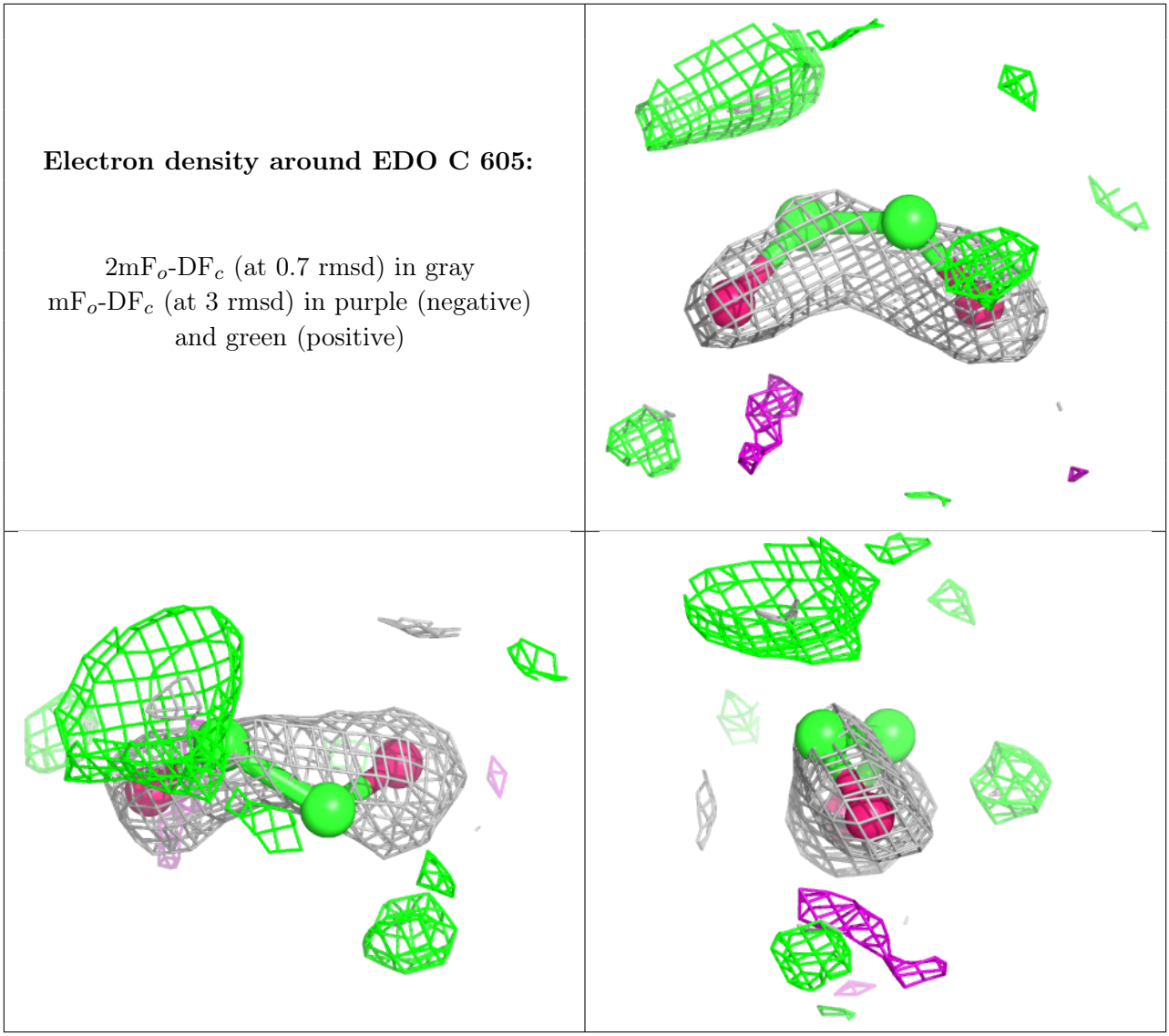






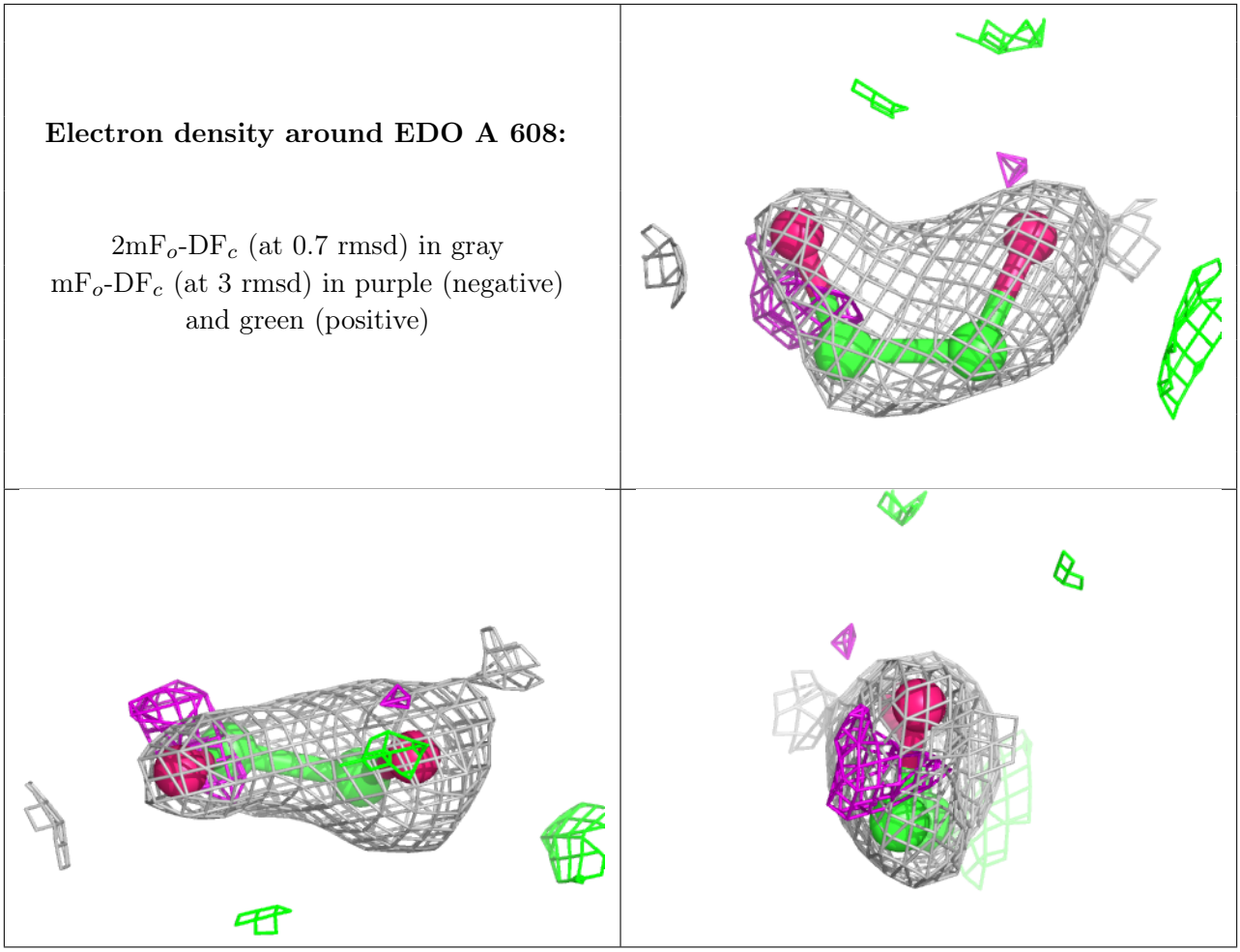
Electron density around EDO C 605:

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



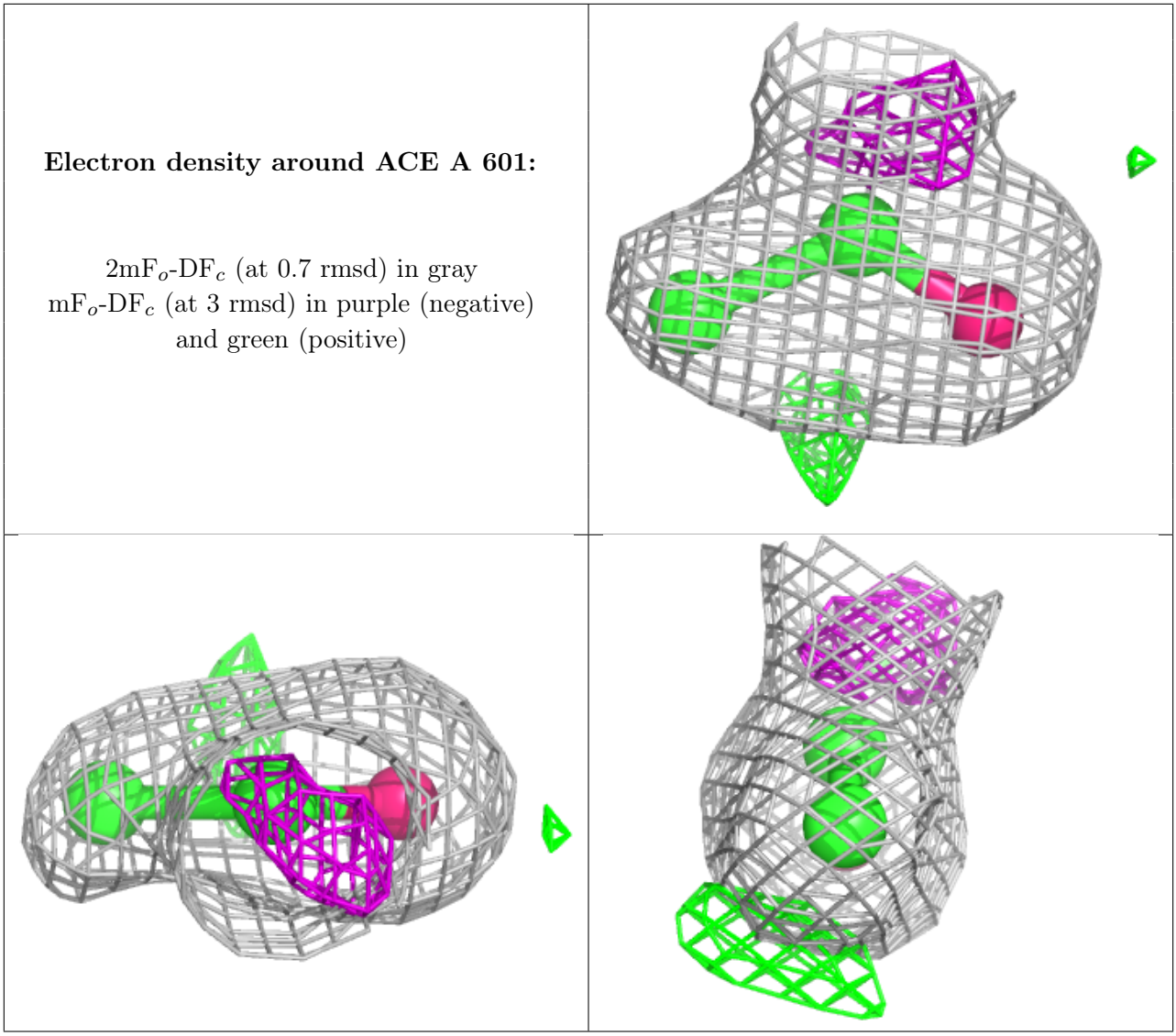
Electron density around EDO A 608:

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



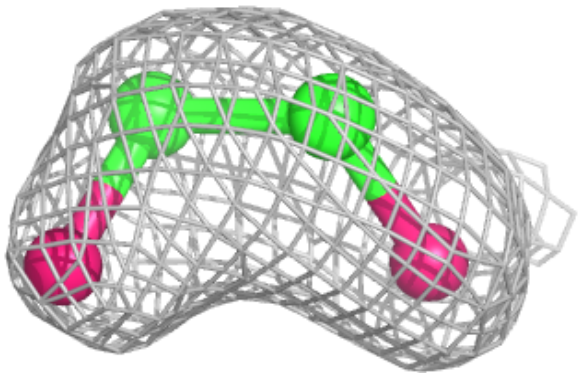
Electron density around ACE A 601:

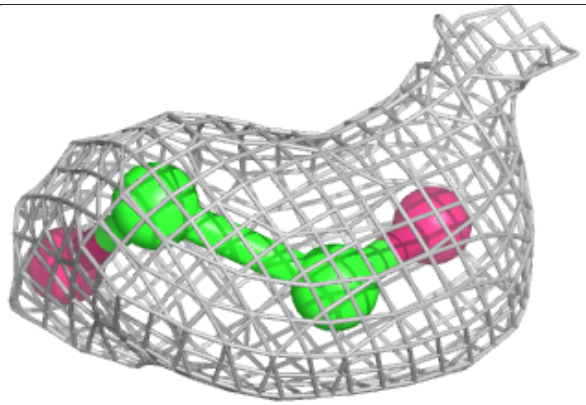
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

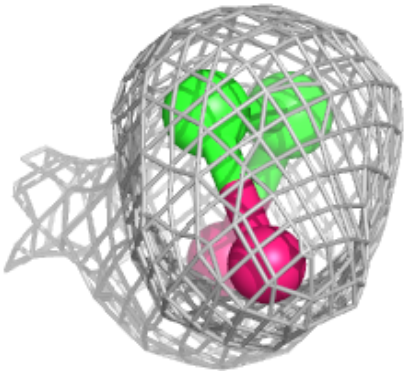


Electron density around EDO C 603:

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

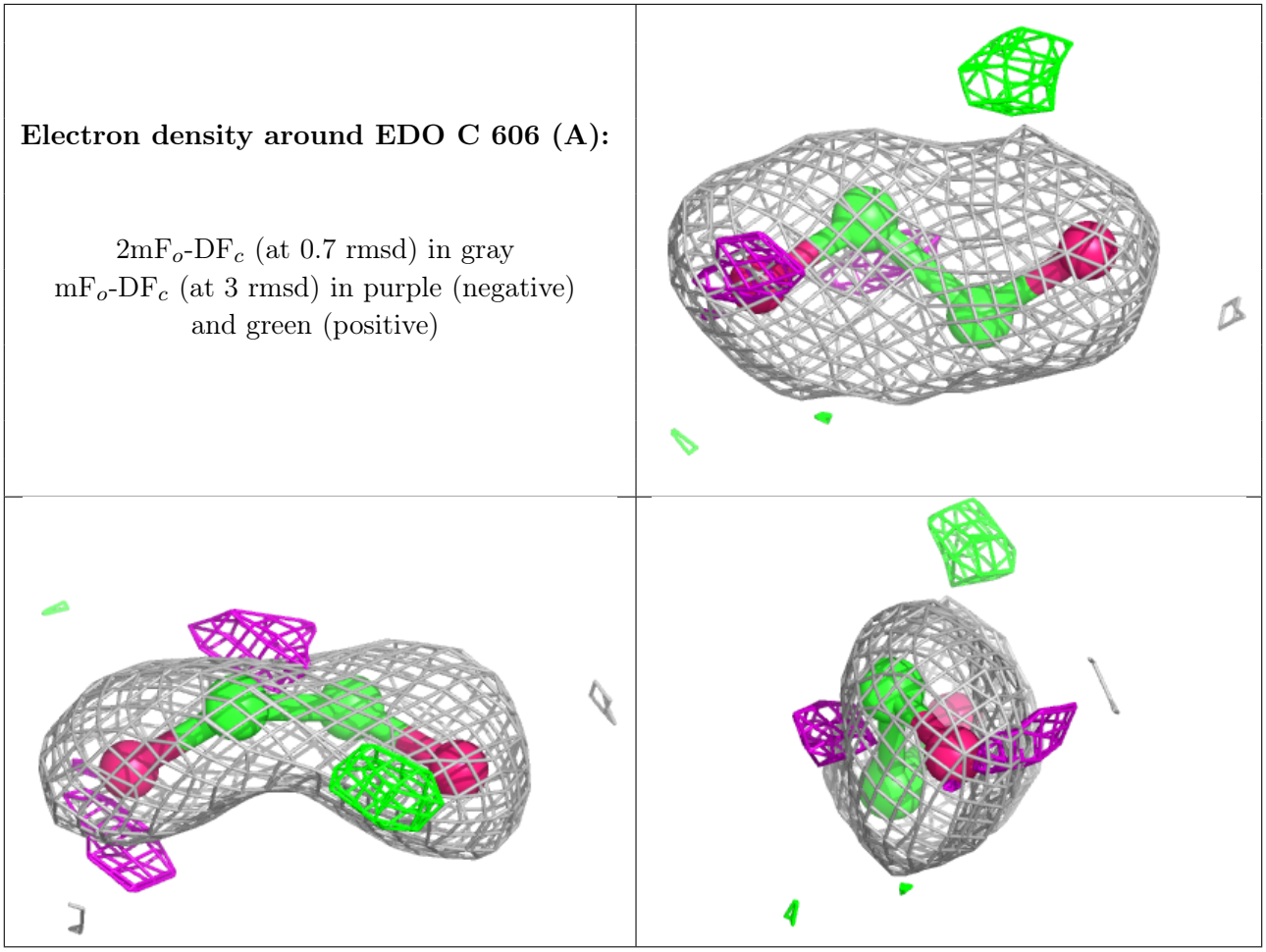






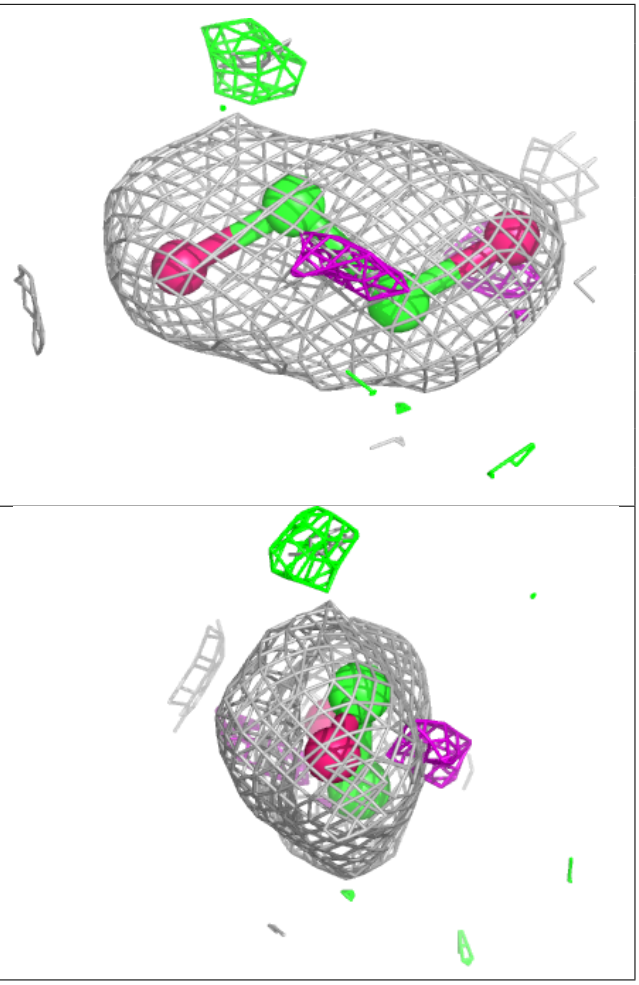
Electron density around EDO C 606 (A):

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



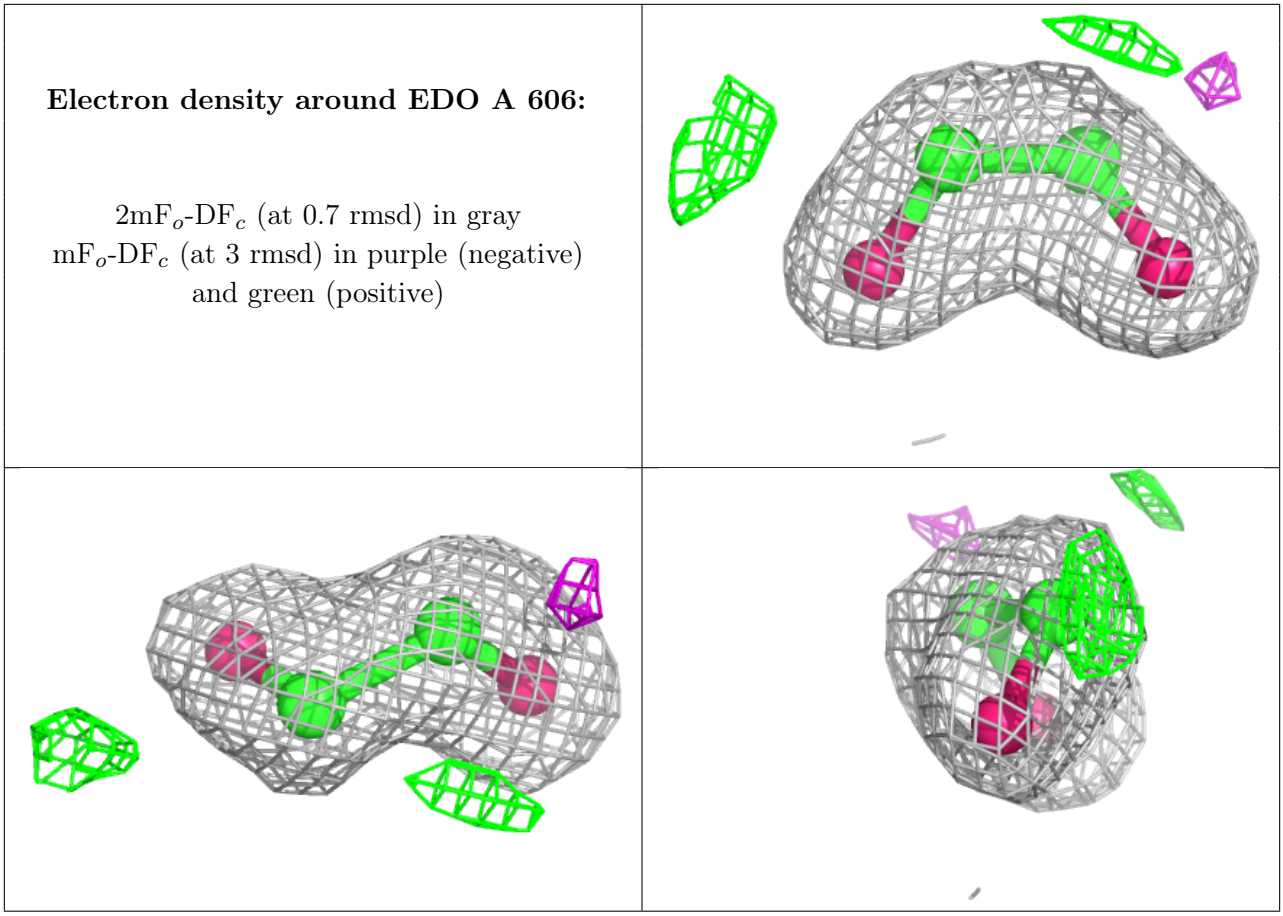
Electron density around EDO C 606 (B):

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



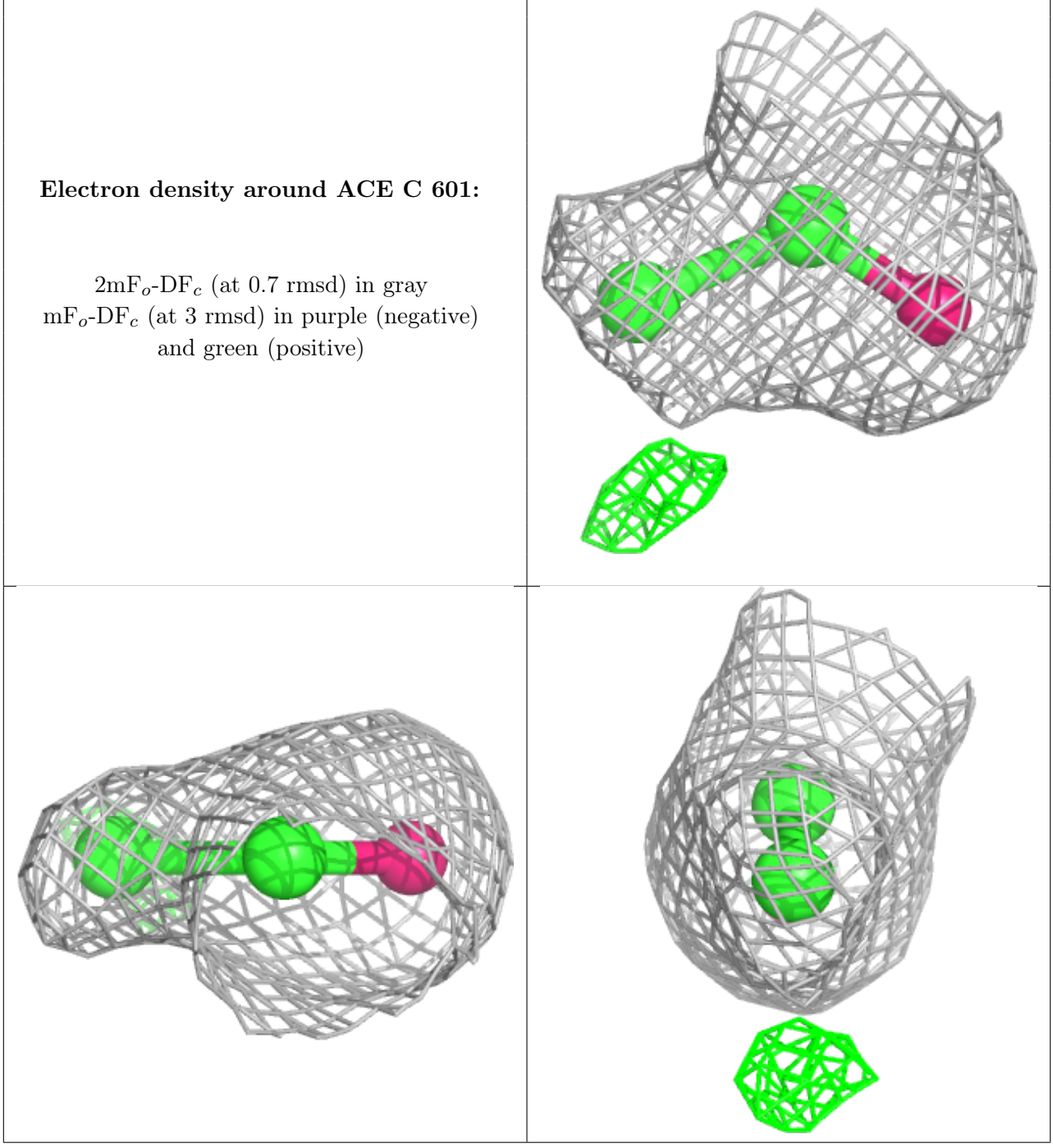
Electron density around EDO A 606:

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



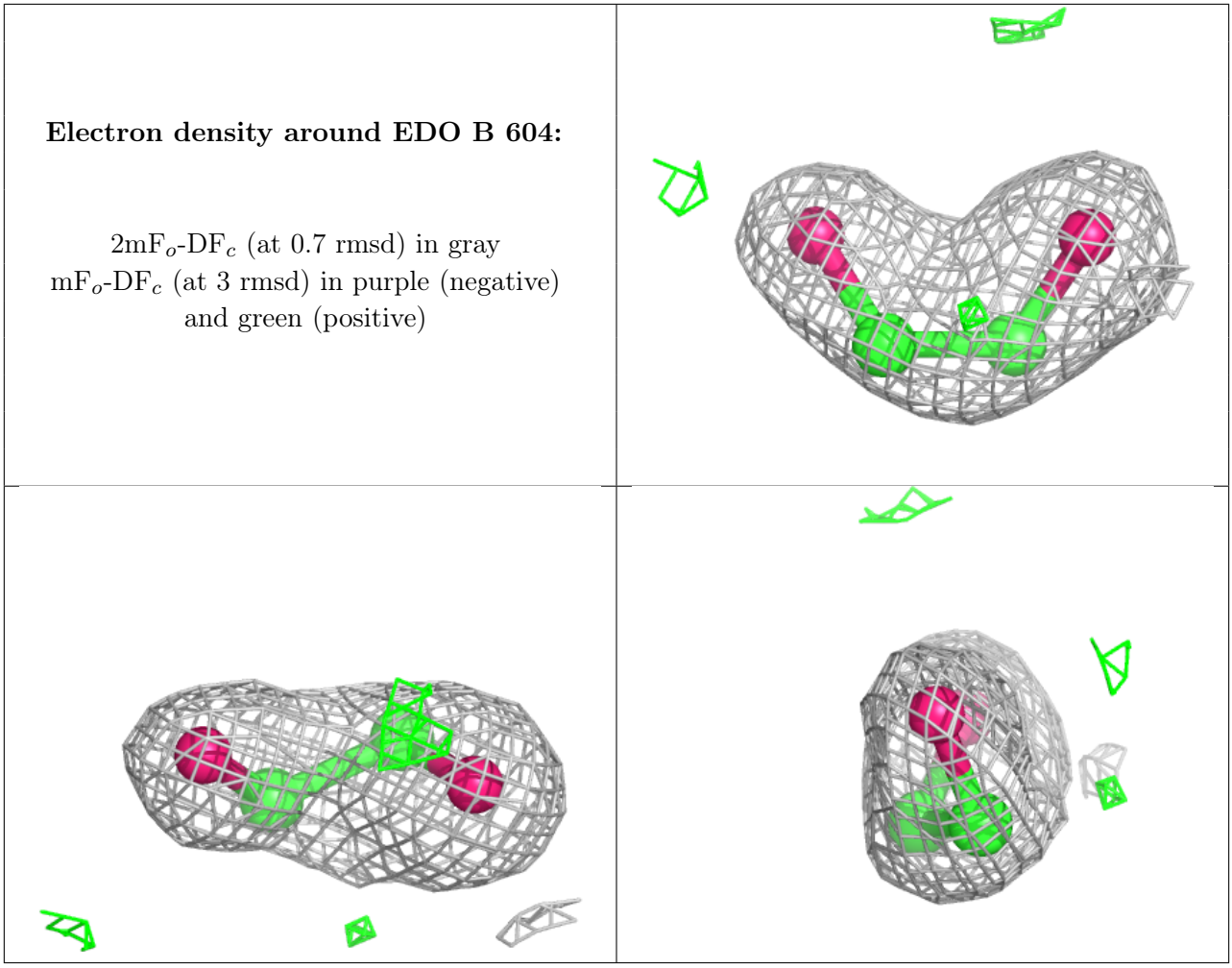
Electron density around ACE C 601:

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



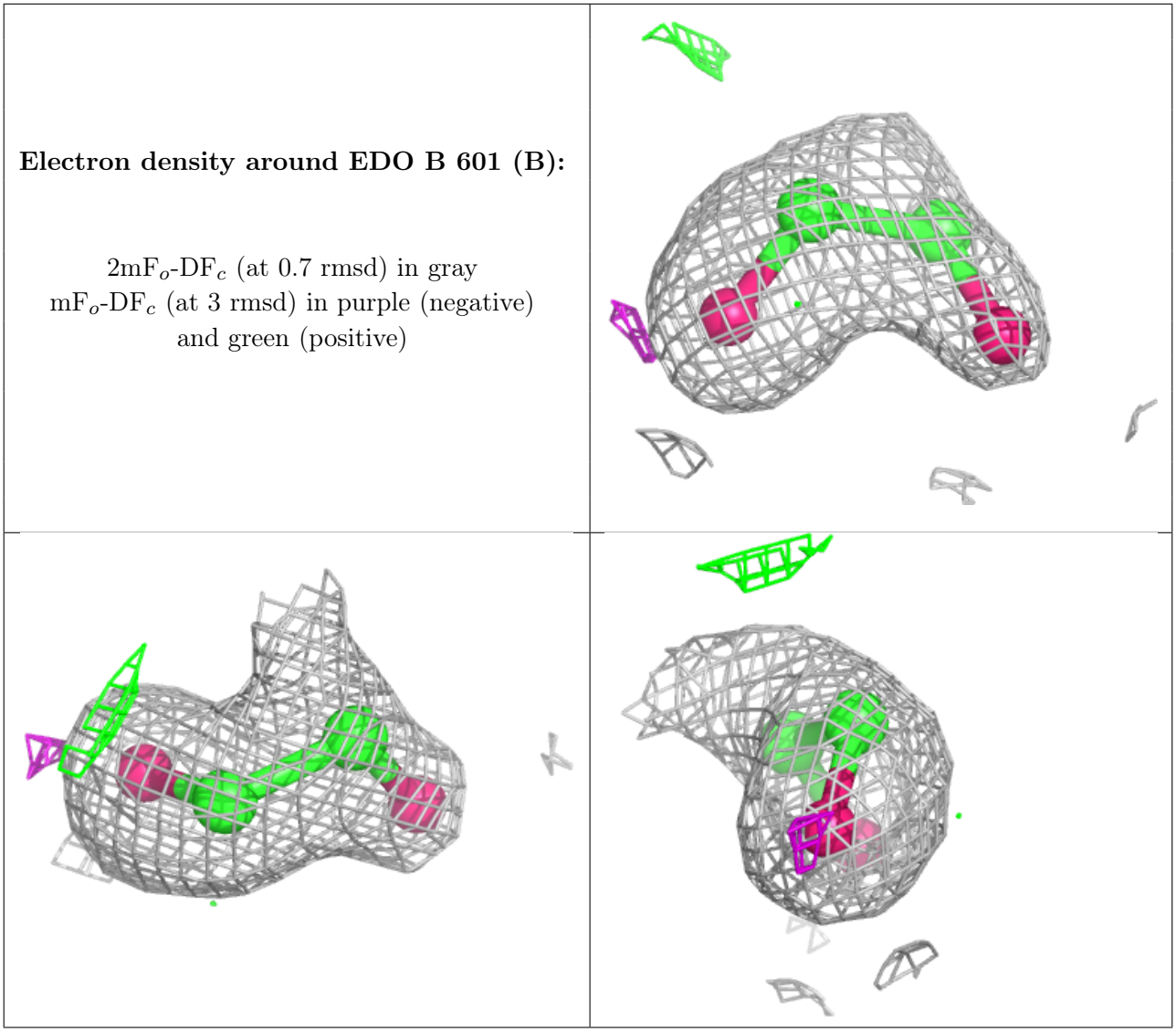
Electron density around EDO B 604:

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



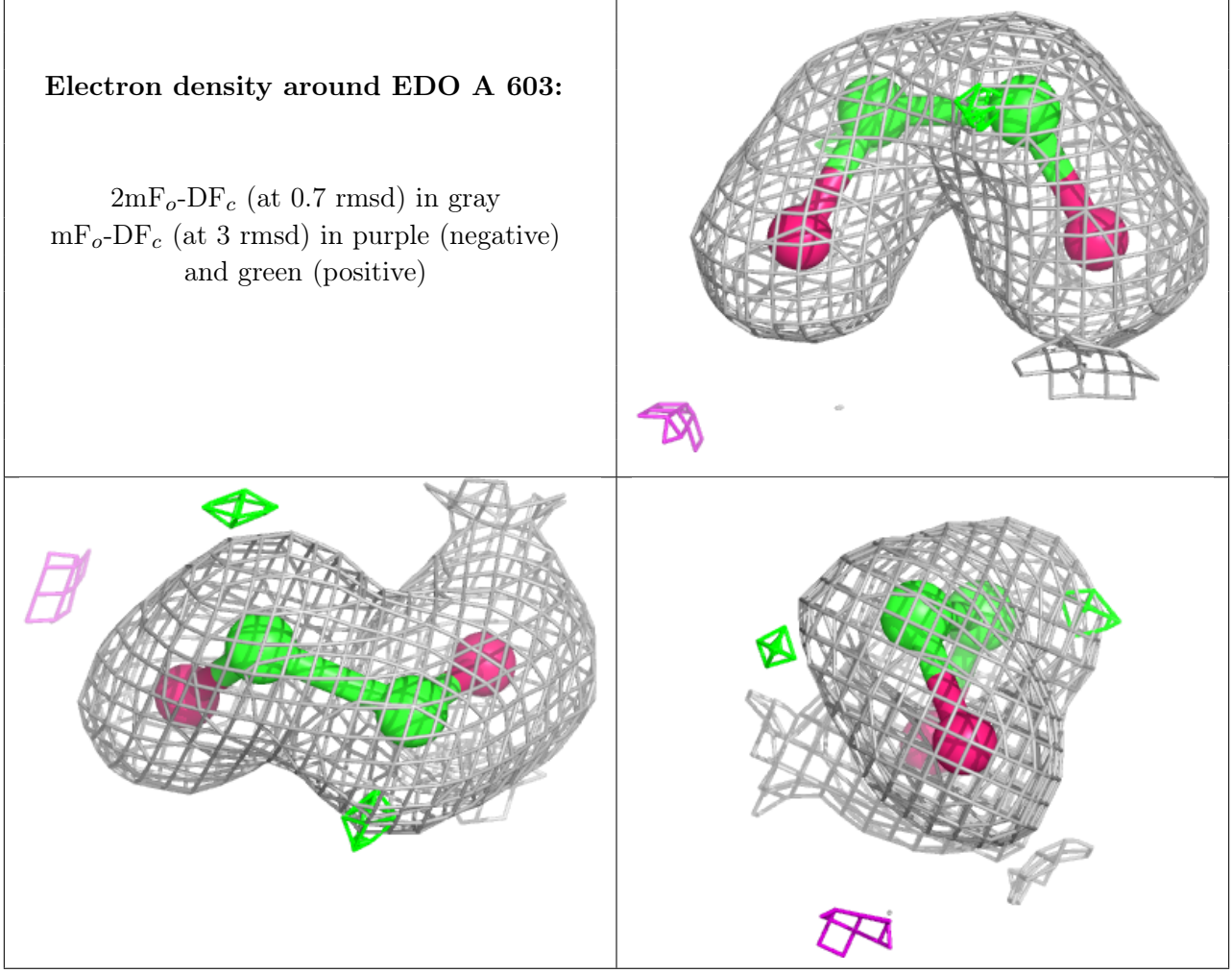
Electron density around EDO B 601 (B):

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



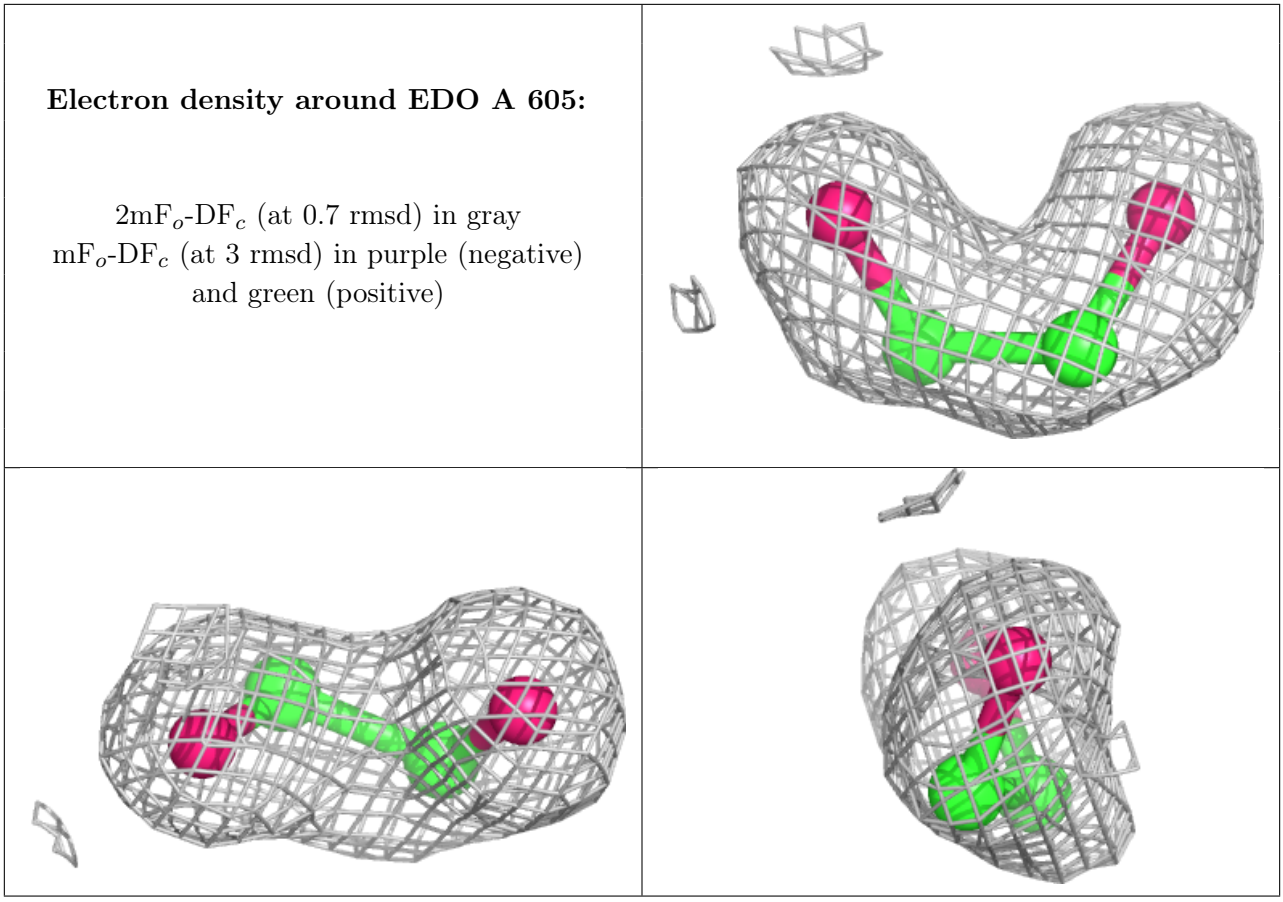
Electron density around EDO A 603:

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



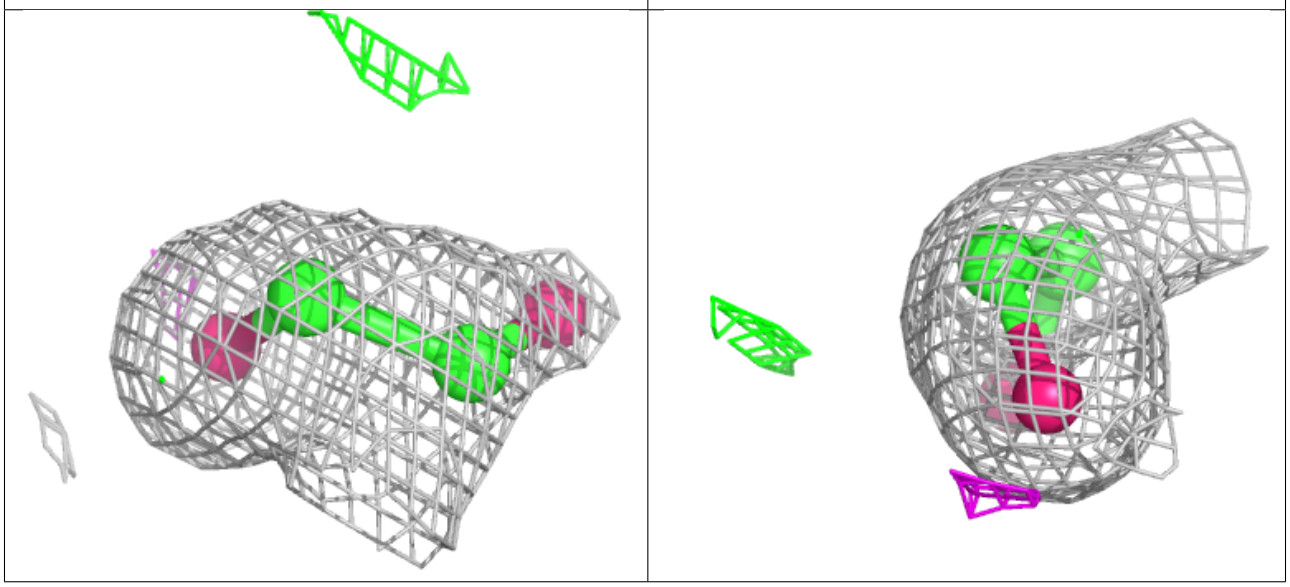
Electron density around EDO A 605:

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



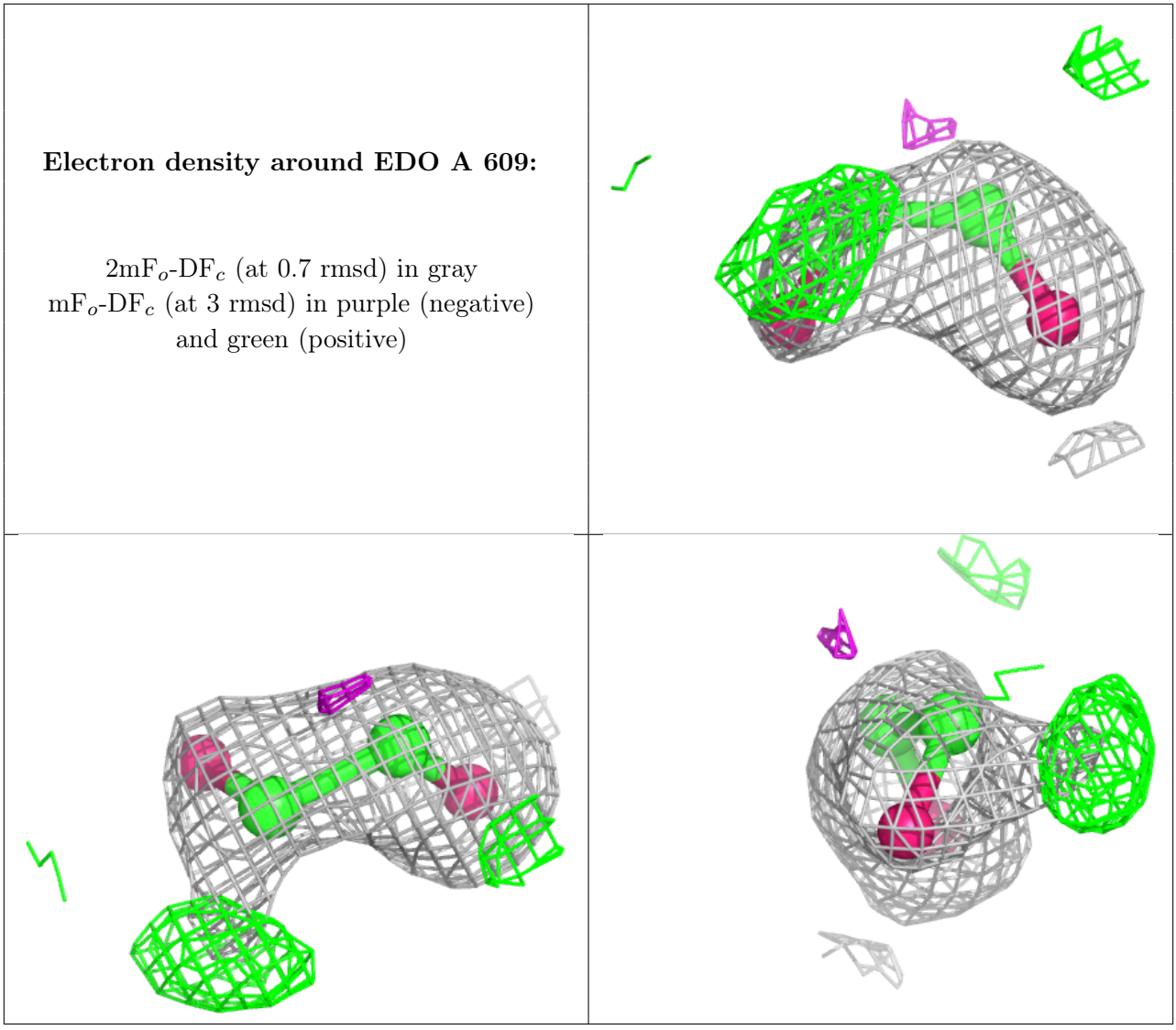
Electron density around EDO B 601 (A):

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



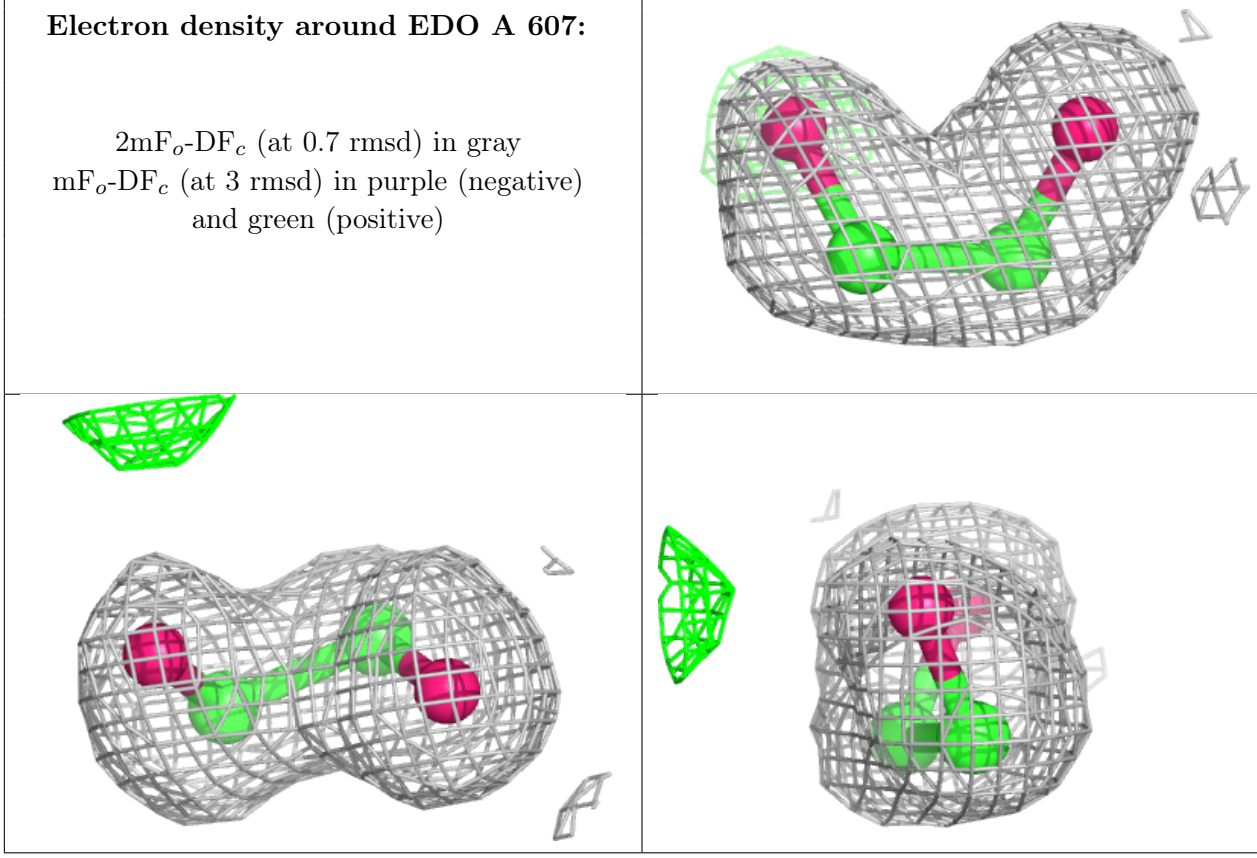
Electron density around EDO A 609:

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



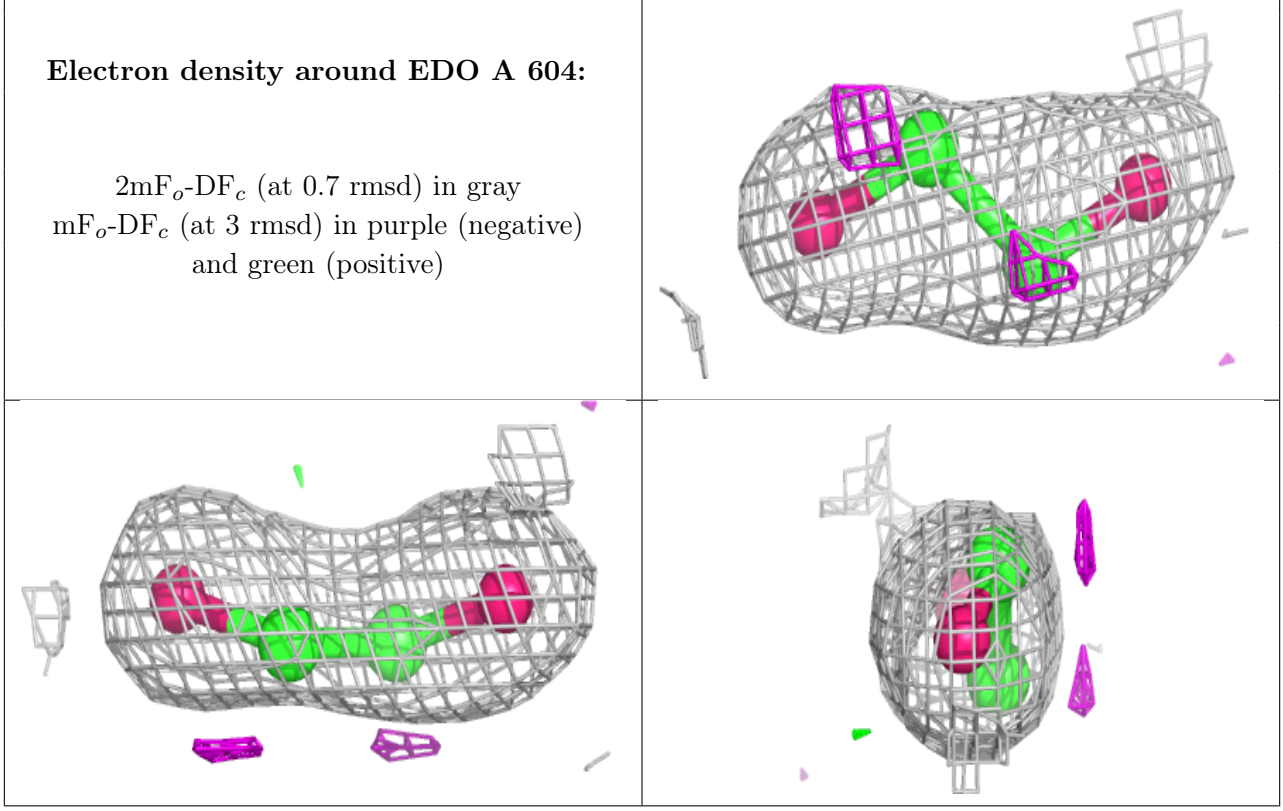
Electron density around EDO A 607:

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



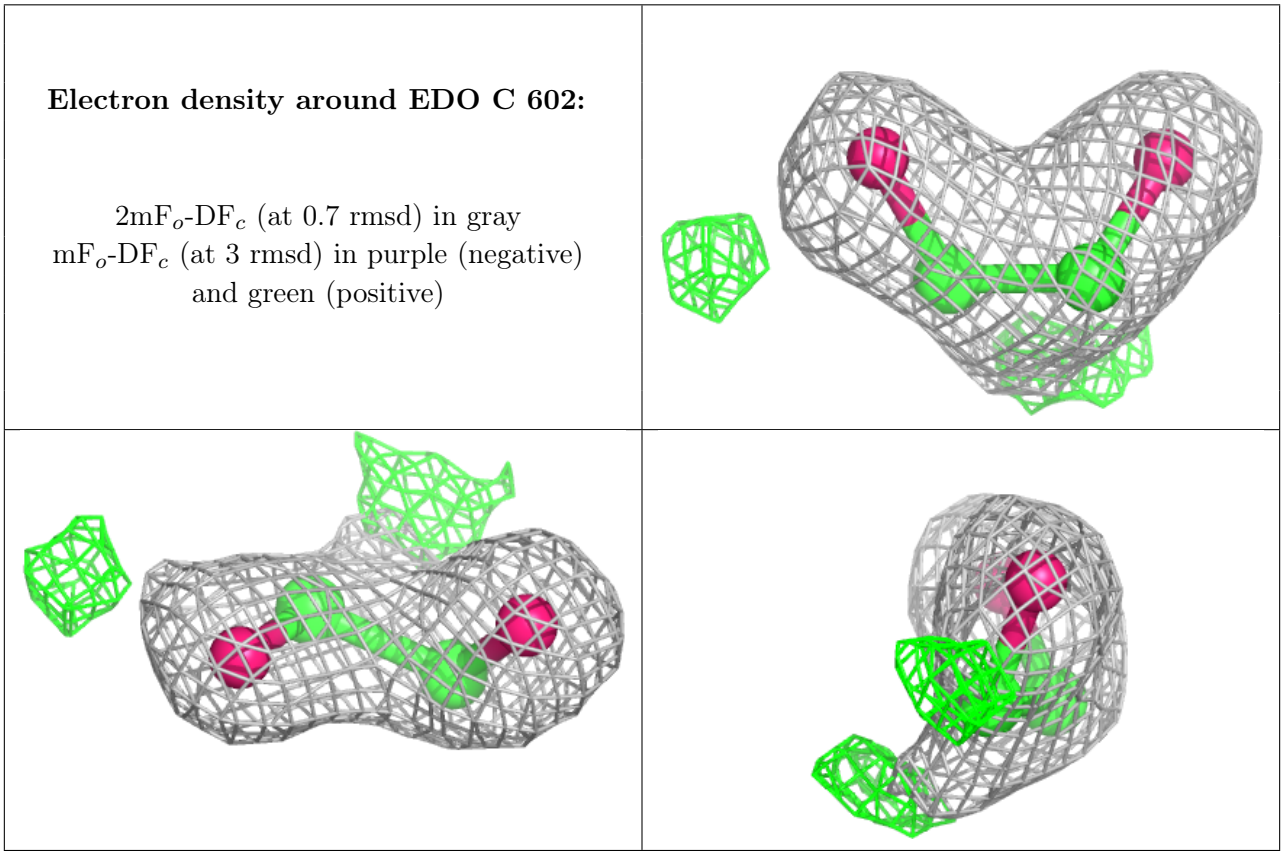
Electron density around EDO A 604:

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



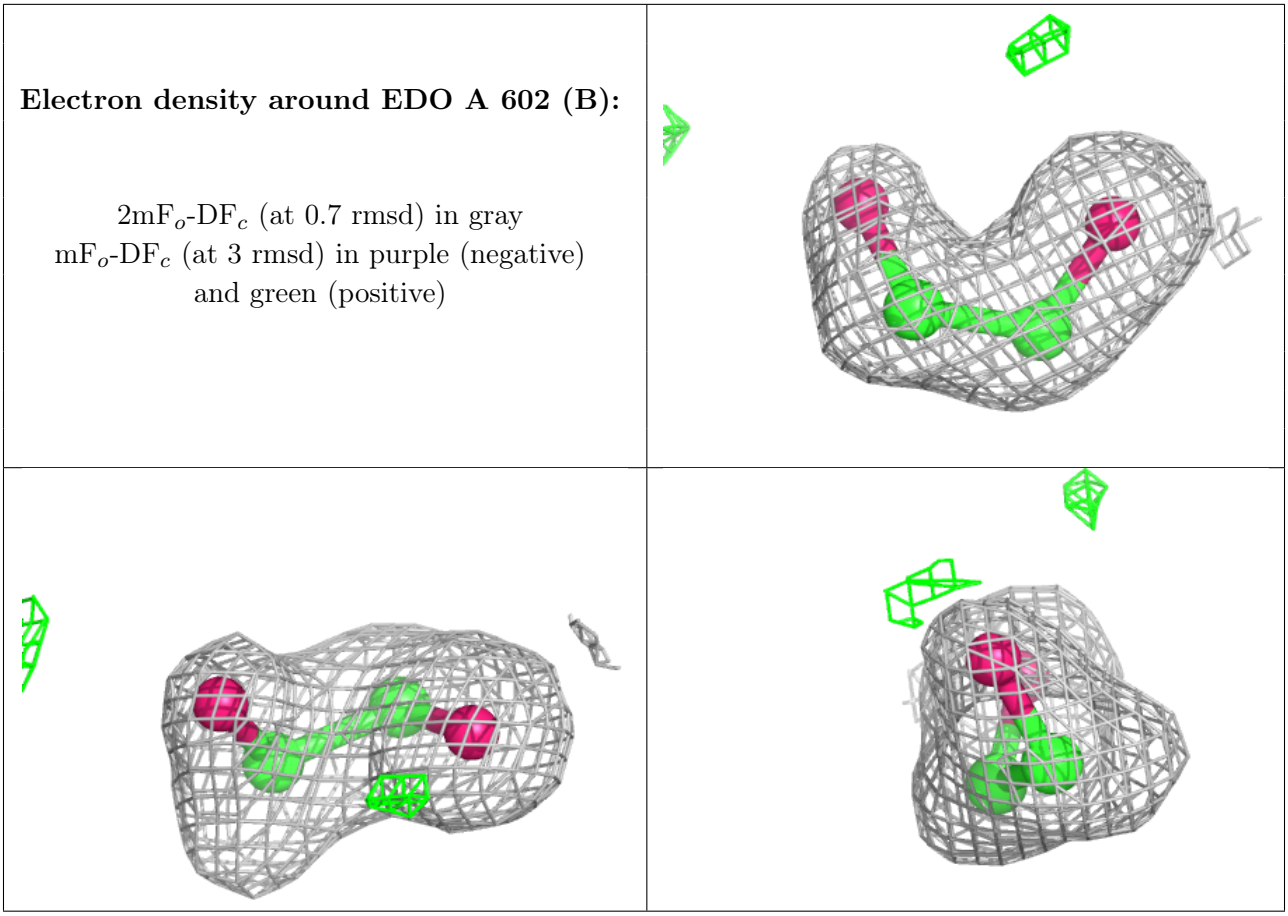
Electron density around EDO C 602:

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



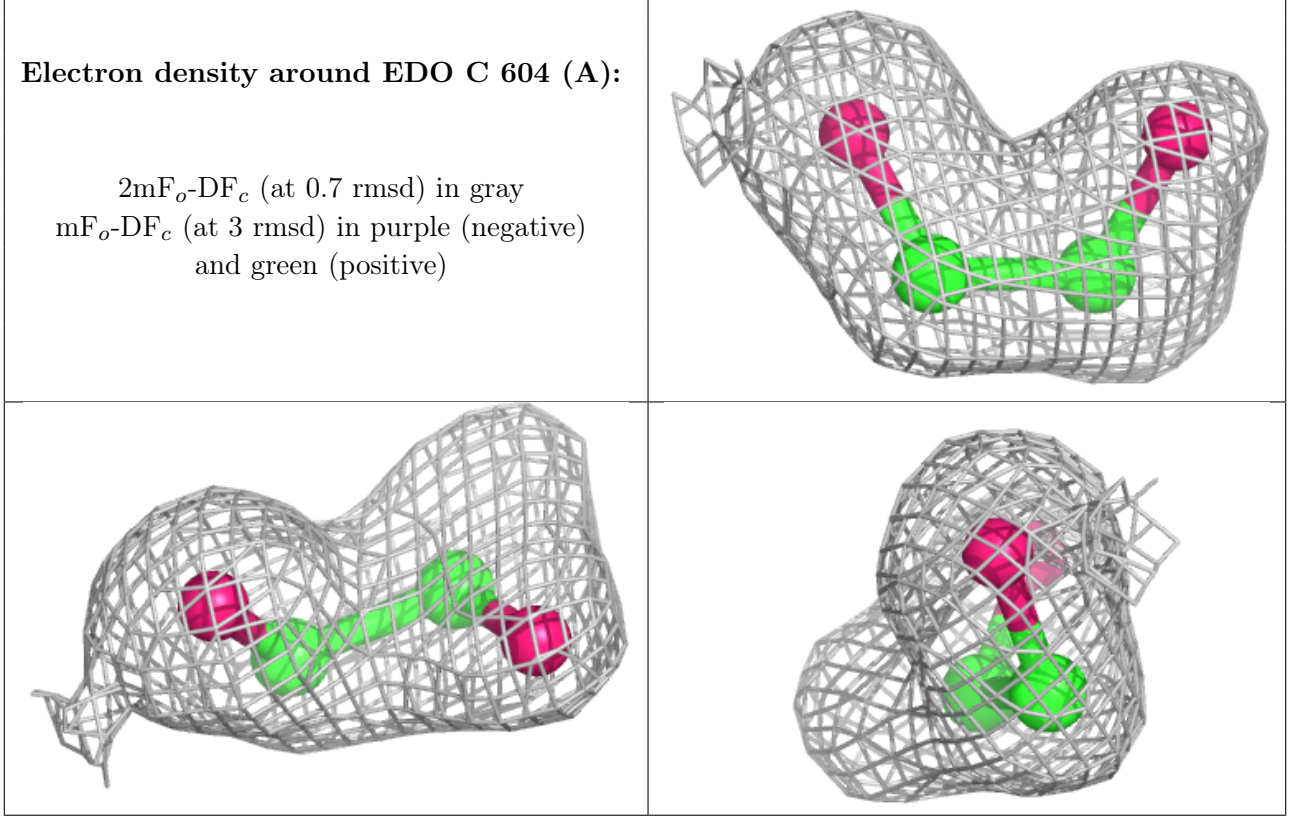
Electron density around EDO A 602 (B):

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



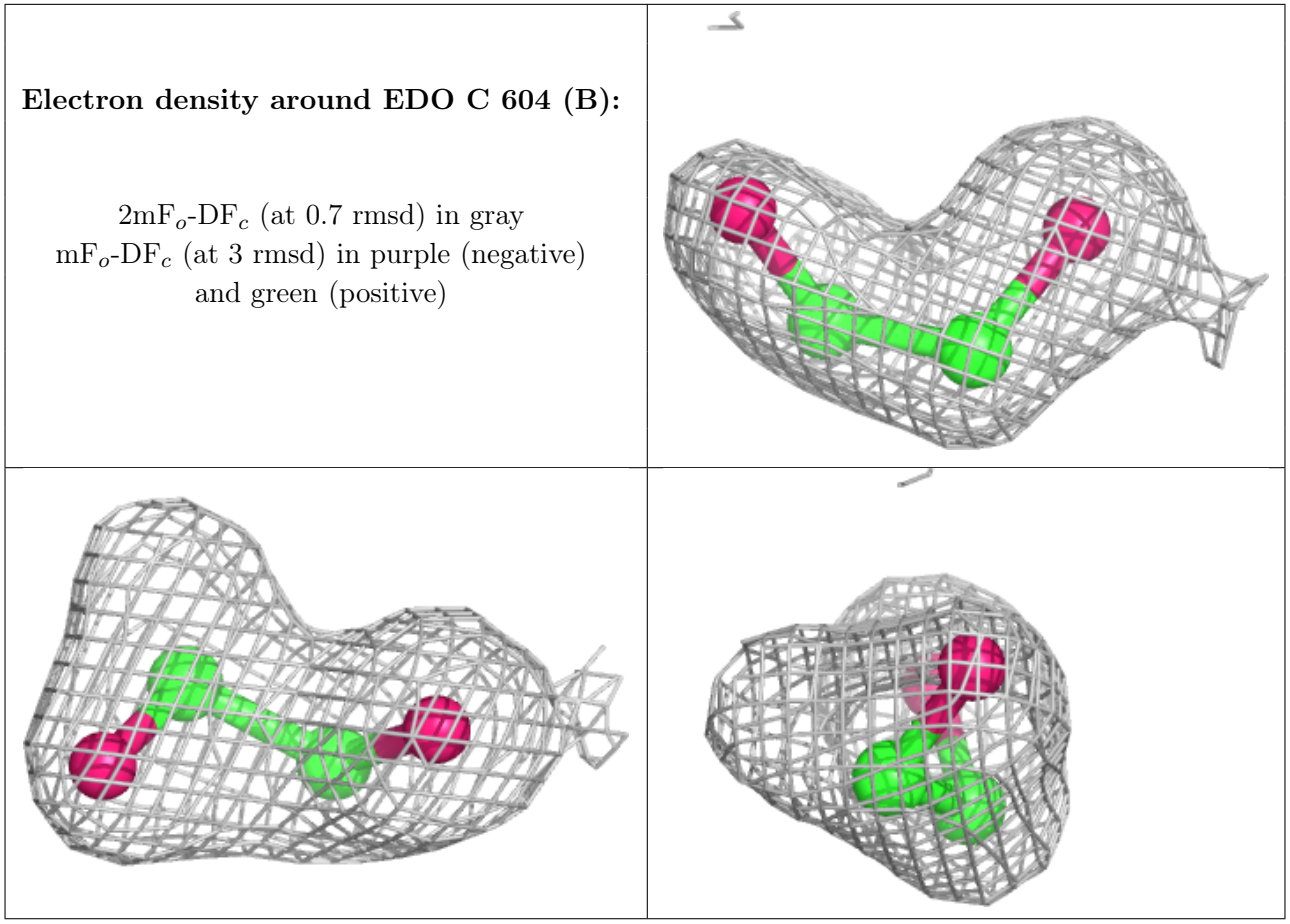
Electron density around EDO C 604 (A):

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



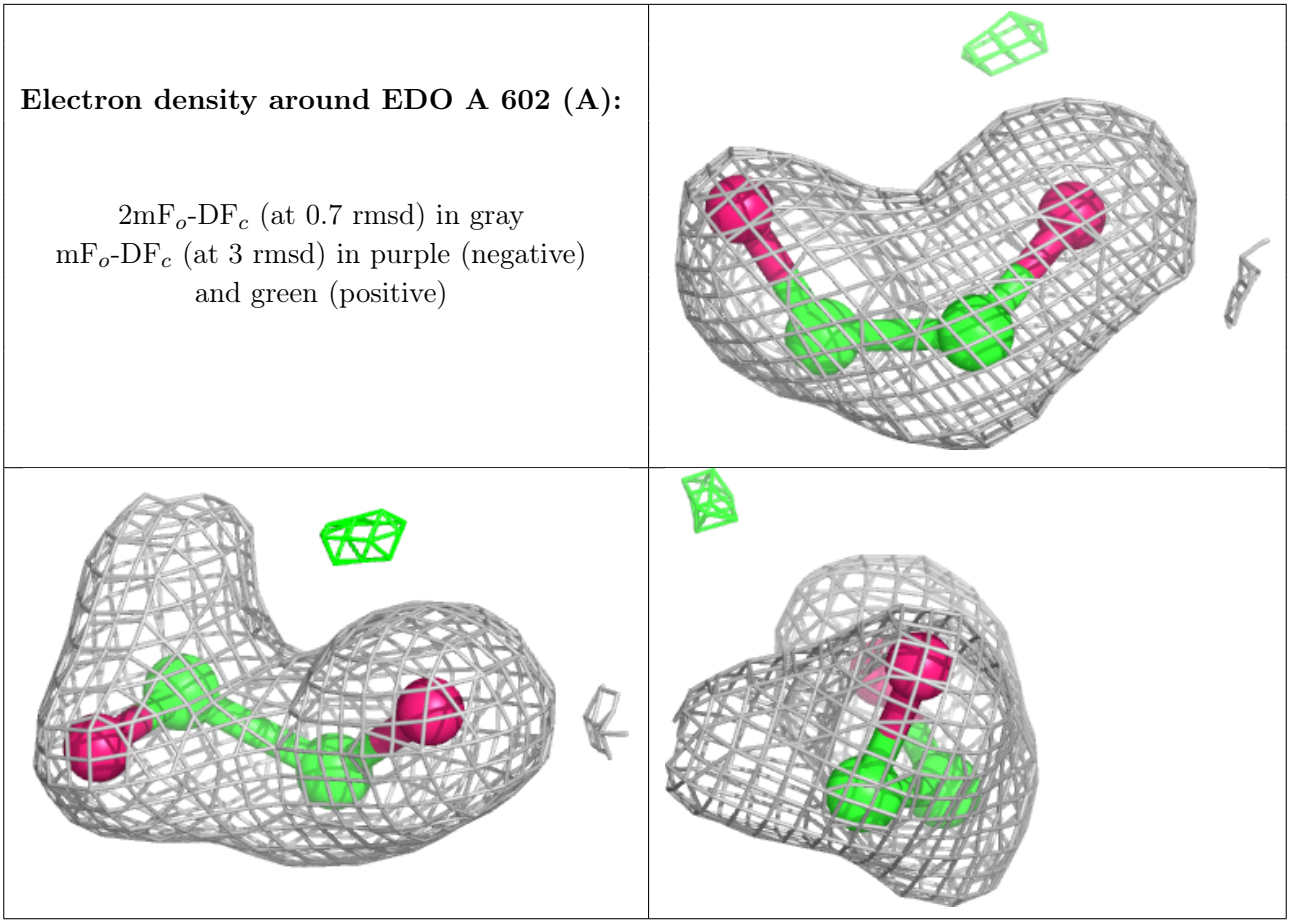
Electron density around EDO C 604 (B):

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



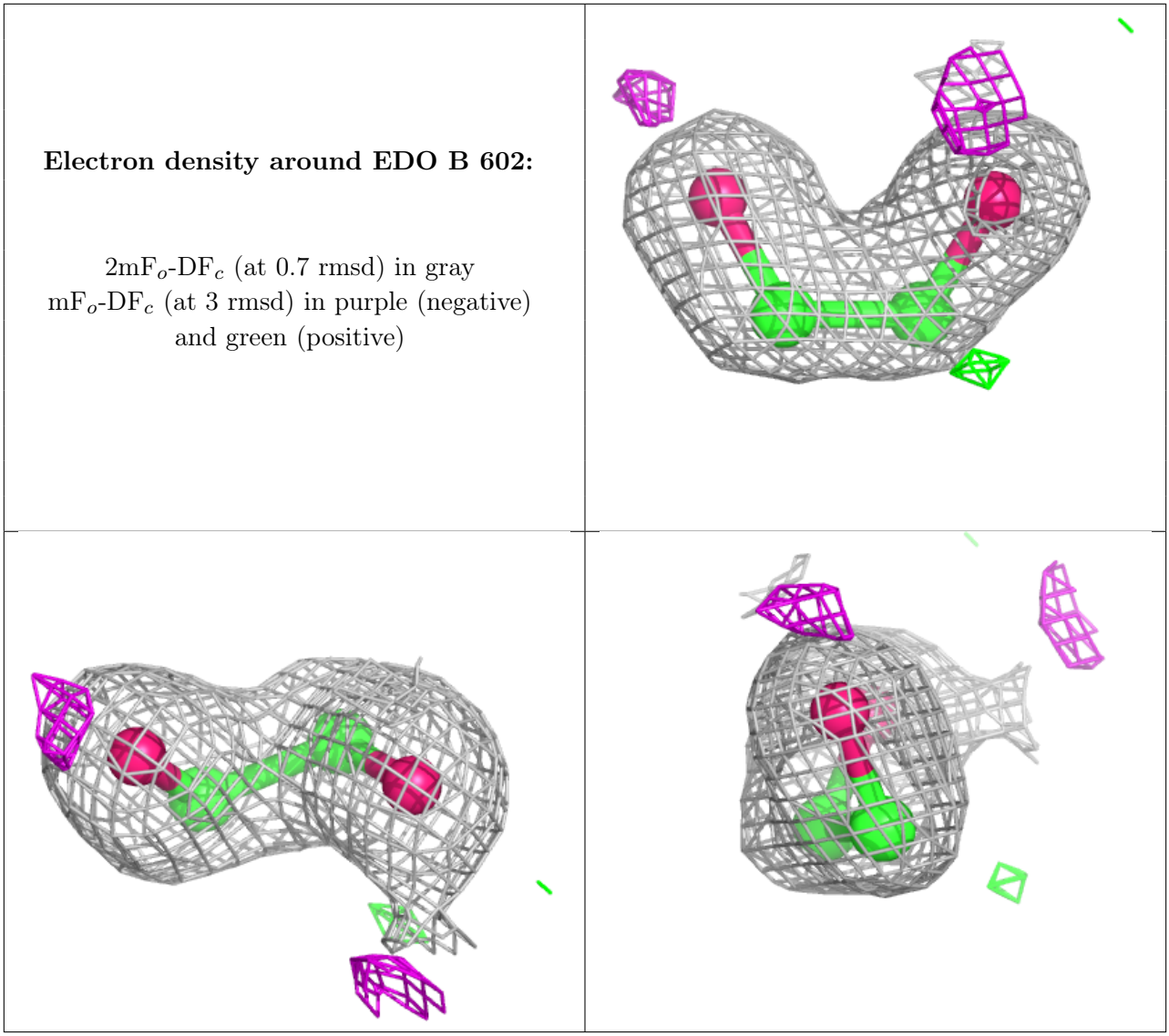
Electron density around EDO A 602 (A):

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



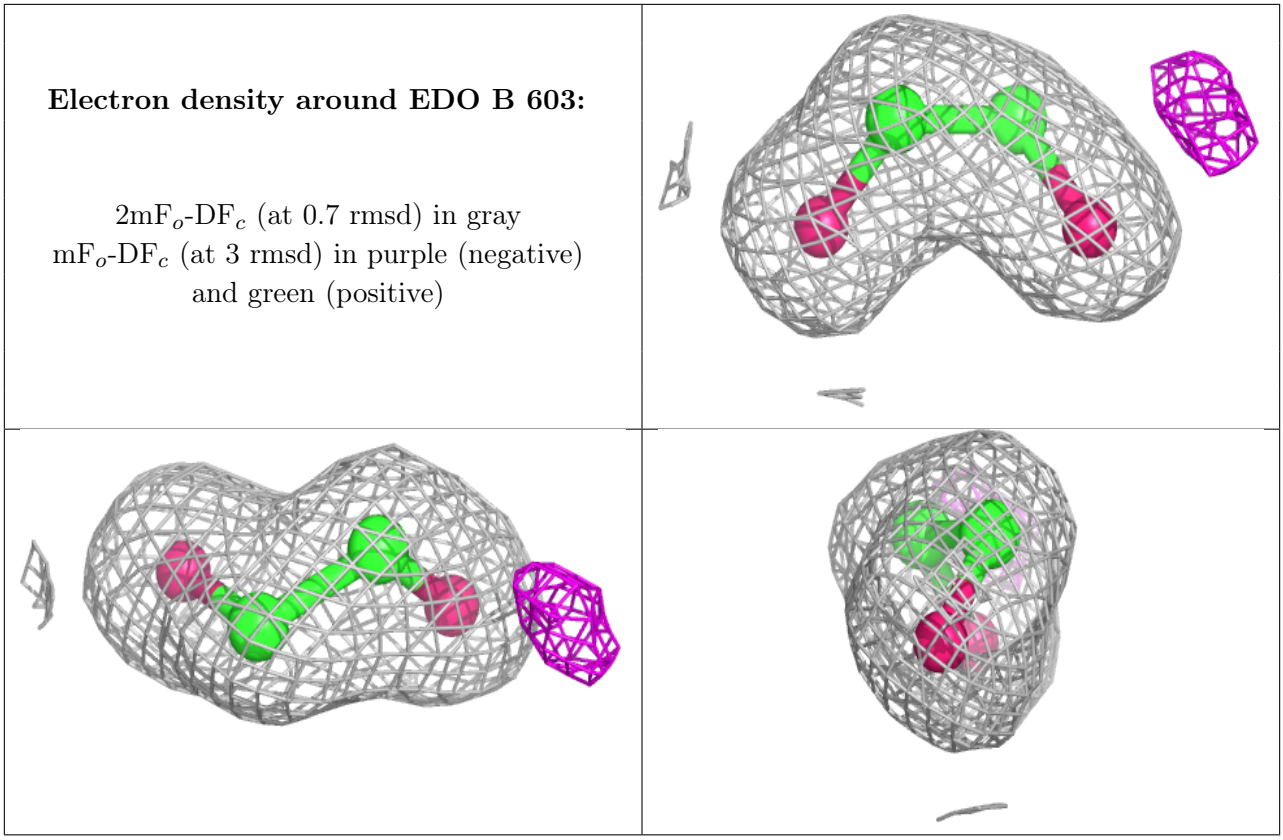
Electron density around EDO B 602:

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



Electron density around EDO 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)



6.5 Other polymers (i)

There are no such residues in this entry.