



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 10:12 PM JST

PDB ID : 8JI8  
Title : Crystal Structure of Prophenoloxidase PPO6 chimeric mutant (F215EASNRAIVD224 to G215DGPDSVVR223) from *Aedes aegypti*  
Authors : Zhu, X.; Zhang, L.; Yang, X.; Bao, P.; Ren, D.; Han, Q.  
Deposited on : 2023-05-26  
Resolution : 2.65 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](mailto: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>.

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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

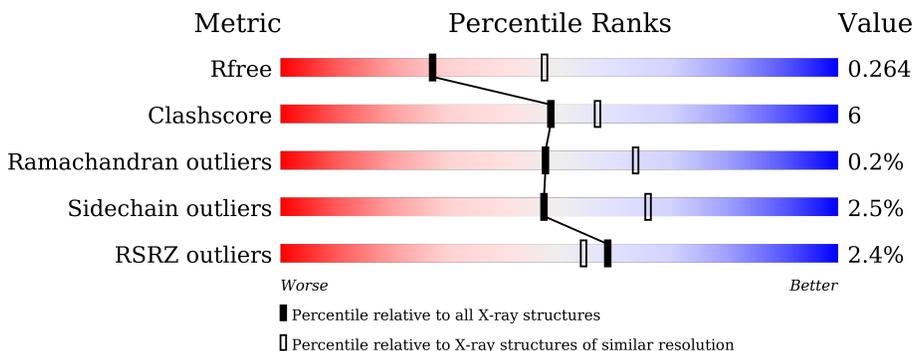
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	680	
1	B	680	
1	C	680	
1	D	680	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CU	A	702	-	-	-	X
2	CU	B	702	-	-	-	X
2	CU	C	702	-	-	-	X
2	CU	D	701	-	-	-	X
3	EDO	D	703	-	-	-	X
4	TRS	A	710	-	-	X	-
4	TRS	B	706	-	-	X	-
4	TRS	C	708	-	X	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22561 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 TK receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	658	5428	3452	979	971	26	0	1	0
1	B	657	5409	3442	974	967	26	0	0	0
1	C	658	5428	3452	979	971	26	0	1	0
1	D	658	5414	3441	976	971	26	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	GLY	PHE	engineered mutation	UNP Q16G28
A	216	ASP	GLU	engineered mutation	UNP Q16G28
A	217	GLY	ALA	engineered mutation	UNP Q16G28
A	218	PRO	SER	engineered mutation	UNP Q16G28
A	219	ASP	ASN	engineered mutation	UNP Q16G28
A	220	SER	ARG	engineered mutation	UNP Q16G28
A	221	VAL	ALA	engineered mutation	UNP Q16G28
A	222	VAL	ILE	engineered mutation	UNP Q16G28
A	223	ARG	VAL	engineered mutation	UNP Q16G28
A	?	-	ASP	deletion	UNP Q16G28
B	215	GLY	PHE	engineered mutation	UNP Q16G28
B	216	ASP	GLU	engineered mutation	UNP Q16G28
B	217	GLY	ALA	engineered mutation	UNP Q16G28
B	218	PRO	SER	engineered mutation	UNP Q16G28
B	219	ASP	ASN	engineered mutation	UNP Q16G28
B	220	SER	ARG	engineered mutation	UNP Q16G28
B	221	VAL	ALA	engineered mutation	UNP Q16G28
B	222	VAL	ILE	engineered mutation	UNP Q16G28
B	223	ARG	VAL	engineered mutation	UNP Q16G28
B	?	-	ASP	deletion	UNP Q16G28
C	215	GLY	PHE	engineered mutation	UNP Q16G28

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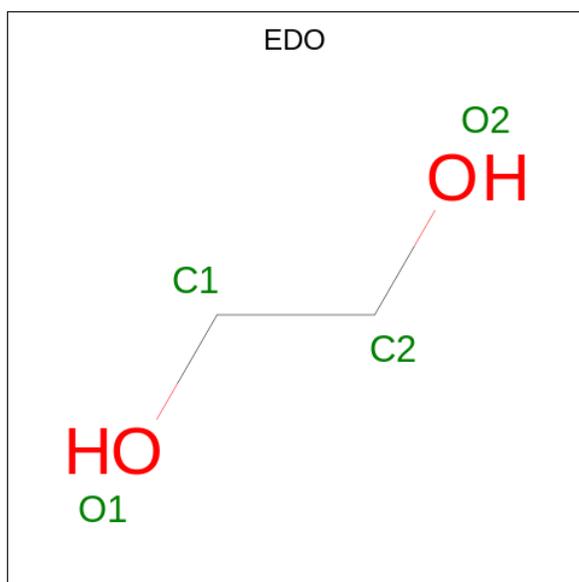
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Chain	Residue	Modelled	Actual	Comment	Reference
C	216	ASP	GLU	engineered mutation	UNP Q16G28
C	217	GLY	ALA	engineered mutation	UNP Q16G28
C	218	PRO	SER	engineered mutation	UNP Q16G28
C	219	ASP	ASN	engineered mutation	UNP Q16G28
C	220	SER	ARG	engineered mutation	UNP Q16G28
C	221	VAL	ALA	engineered mutation	UNP Q16G28
C	222	VAL	ILE	engineered mutation	UNP Q16G28
C	223	ARG	VAL	engineered mutation	UNP Q16G28
C	?	-	ASP	deletion	UNP Q16G28
D	215	GLY	PHE	engineered mutation	UNP Q16G28
D	216	ASP	GLU	engineered mutation	UNP Q16G28
D	217	GLY	ALA	engineered mutation	UNP Q16G28
D	218	PRO	SER	engineered mutation	UNP Q16G28
D	219	ASP	ASN	engineered mutation	UNP Q16G28
D	220	SER	ARG	engineered mutation	UNP Q16G28
D	221	VAL	ALA	engineered mutation	UNP Q16G28
D	222	VAL	ILE	engineered mutation	UNP Q16G28
D	223	ARG	VAL	engineered mutation	UNP Q16G28
D	?	-	ASP	deletion	UNP Q16G28

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



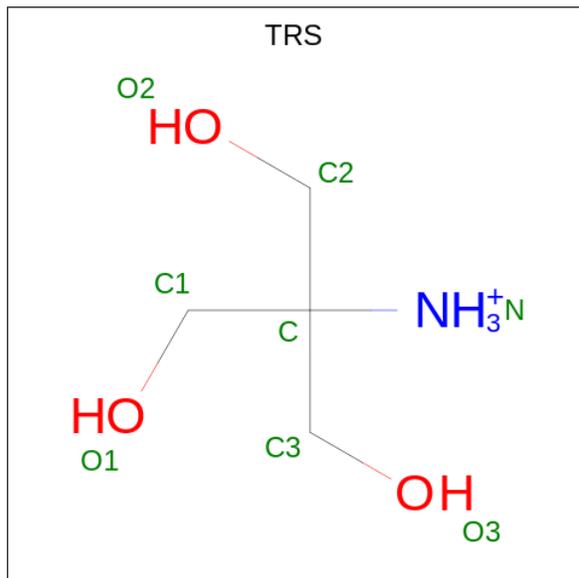
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0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

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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	222	Total O 222 222	0	0

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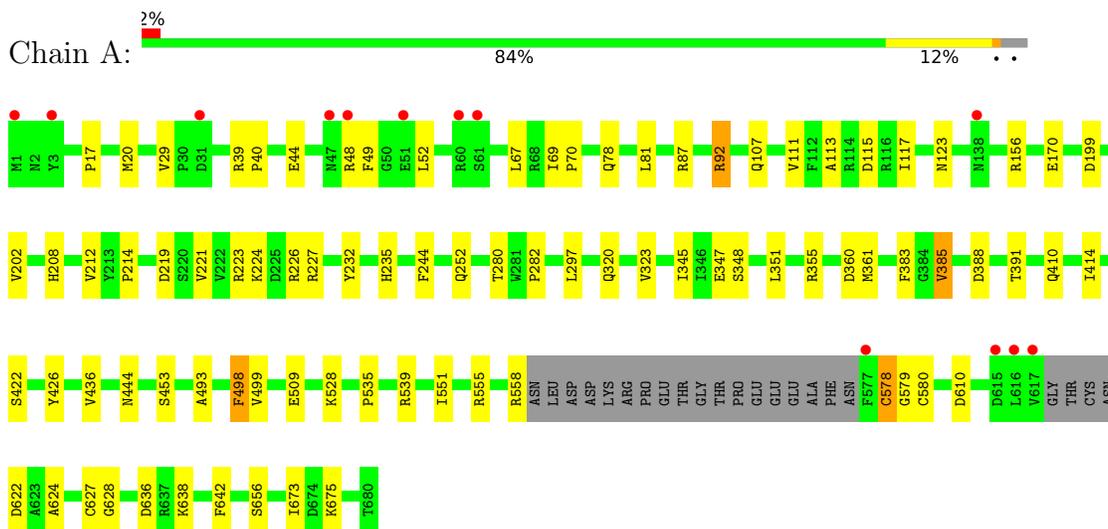
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	B	194	Total 194	O 194	0	0
5	C	159	Total 159	O 159	0	0
5	D	199	Total 199	O 199	0	0

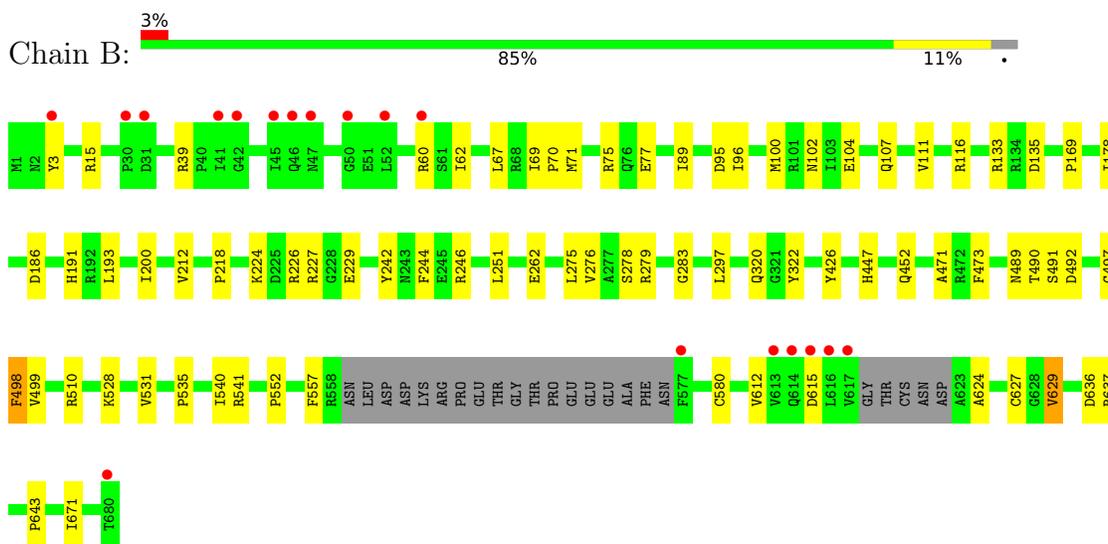
### 3 Residue-property plots [i](#)

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.

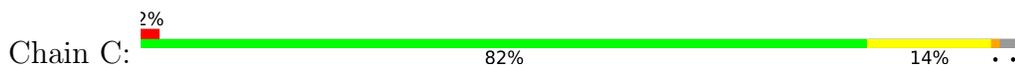
- Molecule 1: TK receptor



- Molecule 1: TK receptor



- Molecule 1: TK receptor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.57Å 153.66Å 223.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.69 – 2.65 47.65 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.69-2.65) 98.5 (47.65-2.65)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 2.65Å)	Xtrriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.176 , 0.261 0.183 , 0.264	Depositor DCC
$R_{free}$ test set	4600 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.1	Xtrriage
Anisotropy	0.542	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22561	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, EDO, CU

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	0.39	0/5565	0.74	1/7532 (0.0%)
1	B	0.37	0/5546	0.72	0/7507
1	C	0.38	0/5565	0.73	1/7532 (0.0%)
1	D	0.39	0/5550	0.76	0/7513
All	All	0.38	0/22226	0.74	2/30084 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	8
1	D	0	9
All	All	0	21

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	HIS	CB-CA-C	6.63	123.67	110.40
1	C	580	CYS	C-N-CA	5.01	132.82	122.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	539	ARG	Sidechain
1	B	39	ARG	Sidechain
1	B	510	ARG	Sidechain
1	B	75	ARG	Sidechain
1	C	13	ARG	Sidechain
1	C	134	ARG	Sidechain
1	C	226	ARG	Sidechain
1	C	295	ARG	Sidechain
1	C	313	ARG	Sidechain
1	C	355	ARG	Sidechain
1	C	37	ARG	Sidechain
1	C	520	ARG	Sidechain
1	D	156	ARG	Sidechain
1	D	173	ARG	Sidechain
1	D	192	ARG	Sidechain
1	D	226	ARG	Sidechain
1	D	313	ARG	Sidechain
1	D	37	ARG	Sidechain
1	D	394	ARG	Sidechain
1	D	56	ARG	Sidechain
1	D	75	ARG	Sidechain

## 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	5428	0	5333	69	0
1	B	5409	0	5317	60	0
1	C	5428	0	5333	65	0
1	D	5414	0	5317	73	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	28	0	42	1	0
3	B	12	0	18	0	0
3	C	20	0	30	0	0
3	D	16	0	24	0	0
4	A	8	0	12	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	8	0	12	15	0
4	C	8	0	12	15	0
5	A	222	0	0	6	0
5	B	194	0	0	3	0
5	C	159	0	0	3	0
5	D	199	0	0	5	0
All	All	22561	0	21450	261	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 (261) 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:A:627:CYS:SG	4:A:710:TRS:C3	2.08	1.42
1:C:627:CYS:SG	4:C:708:TRS:C	2.13	1.36
1:C:627:CYS:SG	4:C:708:TRS:C3	2.16	1.33
1:C:627:CYS:SG	4:C:708:TRS:C1	2.23	1.25
1:A:627:CYS:SG	4:A:710:TRS:H31	1.83	1.12
1:A:627:CYS:SG	4:A:710:TRS:H32	1.81	1.10
1:B:627:CYS:SG	4:B:706:TRS:C1	2.40	1.08
1:B:627:CYS:SG	4:B:706:TRS:H11	1.94	1.08
1:C:627:CYS:SG	4:C:708:TRS:H11	1.91	1.06
1:B:627:CYS:SG	4:B:706:TRS:C3	2.46	1.04
1:C:627:CYS:SG	4:C:708:TRS:C2	2.46	1.02
1:C:627:CYS:SG	4:C:708:TRS:H32	1.99	0.97
1:A:627:CYS:SG	4:A:710:TRS:C	2.56	0.93
1:B:627:CYS:SG	4:B:706:TRS:C	2.56	0.93
1:A:627:CYS:HG	4:A:710:TRS:H32	1.20	0.93
1:D:227:ARG:NH1	1:D:347:GLU:OE1	2.03	0.92
1:C:627:CYS:SG	4:C:708:TRS:H31	2.11	0.90
1:A:627:CYS:SG	4:A:710:TRS:H11	2.18	0.84
1:A:675:LYS:NZ	5:A:801:HOH:O	2.11	0.81
1:A:81:LEU:O	1:A:87:ARG:HD2	1.83	0.78
1:C:627:CYS:SG	4:C:708:TRS:H21	2.24	0.78
1:C:258:ASN:HA	5:C:836:HOH:O	1.84	0.78
1:B:627:CYS:SG	4:B:706:TRS:H31	2.23	0.76
1:D:428:GLY:O	1:D:489:ASN:O	2.03	0.76
1:D:558:ARG:HH21	1:D:558:ARG:CG	1.99	0.75
1:B:580:CYS:HB3	4:B:706:TRS:O2	1.87	0.74
1:D:67:LEU:HB3	1:D:71:MET:HE3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:CYS:SG	4:A:710:TRS:C1	2.76	0.73
1:B:627:CYS:SG	4:B:706:TRS:H32	2.28	0.73
1:A:355:ARG:HG3	1:A:355:ARG:HH11	1.55	0.72
1:B:279:ARG:HD2	5:B:911:HOH:O	1.91	0.70
1:C:627:CYS:HG	4:C:708:TRS:H32	1.57	0.70
1:A:44:GLU:HG2	1:B:169:PRO:HG2	1.73	0.69
1:A:385:VAL:HG22	1:A:391:THR:HB	1.76	0.68
1:C:551:ILE:HG21	1:C:580:CYS:HA	1.75	0.68
1:D:78:GLN:HG3	1:D:383:PHE:CZ	2.29	0.68
1:D:1:MET:HA	5:D:949:HOH:O	1.93	0.67
1:B:77:GLU:OE1	5:B:801:HOH:O	2.13	0.66
1:A:627:CYS:CB	4:A:710:TRS:H11	2.25	0.66
1:A:48:ARG:HB3	5:A:830:HOH:O	1.95	0.65
1:A:226:ARG:NH2	1:A:636:ASP:O	2.29	0.65
1:B:627:CYS:SG	4:B:706:TRS:H21	2.35	0.65
1:A:48:ARG:CB	5:A:830:HOH:O	2.44	0.65
1:C:453:SER:HA	1:C:679:ARG:HD3	1.78	0.65
1:D:260:LEU:HD13	1:D:307:LEU:HD23	1.79	0.65
1:D:226:ARG:NH2	1:D:636:ASP:O	2.28	0.65
1:A:92:ARG:NH2	5:A:802:HOH:O	2.29	0.65
1:B:60:ARG:HD3	1:B:62:ILE:CG2	2.28	0.64
1:B:580:CYS:CB	4:B:706:TRS:O2	2.45	0.64
1:D:385:VAL:HG22	1:D:391:THR:HB	1.79	0.64
1:A:227[B]:ARG:HH21	1:A:227[B]:ARG:HG3	1.61	0.64
1:C:578:CYS:O	4:C:708:TRS:O1	2.13	0.63
1:C:113:ALA:HB1	1:C:117:ILE:HD12	1.80	0.63
1:A:78:GLN:HG3	1:A:383:PHE:CZ	2.33	0.63
1:C:4:LYS:HB3	1:C:139:LEU:HD13	1.82	0.62
1:C:320:GLN:HB3	1:C:322:TYR:CE1	2.35	0.62
1:C:348:SER:OG	1:C:355:ARG:NH1	2.33	0.62
1:C:60:ARG:HD3	1:C:104:GLU:OE2	1.99	0.61
1:C:438:SER:HB2	1:C:441:ALA:HB3	1.82	0.61
1:B:178:ILE:HD11	1:B:471:ALA:HB1	1.81	0.61
1:B:489:ASN:OD1	1:B:491:SER:HB3	2.01	0.61
1:B:627:CYS:SG	4:B:706:TRS:C2	2.88	0.61
1:D:212:VAL:O	1:D:224:LYS:NZ	2.34	0.60
1:D:457:LEU:O	1:D:461:MET:HG2	2.03	0.59
1:C:428:GLY:O	1:C:489:ASN:O	2.21	0.59
1:A:212:VAL:O	1:A:224:LYS:NZ	2.36	0.59
1:C:278:SER:HB3	1:D:156:ARG:HA	1.85	0.58
1:C:627:CYS:HA	4:C:708:TRS:H21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:627:CYS:SG	4:C:708:TRS:H12	2.38	0.58
1:C:325:ASP:HB3	1:C:331:ILE:HD11	1.85	0.58
1:C:607:TYR:O	1:C:611:ARG:HB2	2.04	0.58
1:D:385:VAL:CG2	1:D:391:THR:HB	2.34	0.58
1:A:579:GLY:HA2	4:A:710:TRS:O1	2.03	0.58
1:B:226:ARG:NH2	1:B:636:ASP:O	2.37	0.57
1:A:69:ILE:HB	1:A:70:PRO:HD3	1.86	0.57
1:B:200:ILE:HD11	1:B:557:PHE:CE1	2.39	0.57
1:A:580:CYS:N	4:A:710:TRS:HN2	2.02	0.57
1:B:67:LEU:HB2	1:B:71:MET:HE3	1.85	0.57
1:C:543:ARG:NH2	1:C:545:ASN:OD1	2.37	0.57
1:B:60:ARG:HD3	1:B:62:ILE:HG22	1.87	0.56
1:A:214:PRO:CG	1:A:221:VAL:HG12	2.35	0.56
1:A:219:ASP:OD1	1:A:223:ARG:NE	2.38	0.56
1:A:52:LEU:HG	1:A:52:LEU:O	2.05	0.56
1:D:425:THR:HG22	1:D:660:THR:HB	1.87	0.56
1:A:227[B]:ARG:HG3	1:A:227[B]:ARG:NH2	2.20	0.56
1:B:489:ASN:HB3	1:B:535:PRO:HA	1.87	0.56
1:C:26:VAL:HG23	1:C:53:ALA:HB2	1.89	0.55
1:C:208:HIS:ND1	1:C:580:CYS:HB3	2.21	0.55
1:D:558:ARG:HH21	1:D:558:ARG:HG3	1.69	0.55
1:B:540:ILE:HD13	1:B:540:ILE:N	2.20	0.55
1:B:186:ASP:HA	1:B:191:HIS:CE1	2.42	0.55
1:A:227[B]:ARG:NH2	1:A:347:GLU:OE1	2.40	0.55
1:B:497:GLY:O	1:B:531:VAL:HG12	2.07	0.54
1:A:208:HIS:CG	1:A:580:CYS:SG	3.00	0.54
1:A:555:ARG:HD2	1:A:578:CYS:O	2.07	0.54
1:D:648:ALA:HB1	1:D:652:VAL:HB	1.89	0.54
1:A:156:ARG:HA	1:B:278:SER:HB3	1.90	0.54
1:B:612:VAL:HG22	1:B:637:ARG:HG2	1.90	0.54
1:D:260:LEU:CD1	1:D:307:LEU:HD23	2.38	0.54
1:A:113:ALA:HB1	1:A:117:ILE:HD12	1.90	0.54
1:D:558:ARG:HH21	1:D:558:ARG:HG2	1.71	0.53
1:D:145:VAL:CG2	1:D:204:LEU:HD11	2.38	0.53
1:C:208:HIS:CG	1:C:580:CYS:HB3	2.44	0.53
1:A:17:PRO:HA	1:A:115:ASP:OD2	2.09	0.53
1:D:377:HIS:HD2	5:D:941:HOH:O	1.92	0.53
1:A:627:CYS:HB2	4:A:710:TRS:H11	1.91	0.53
1:B:627:CYS:SG	4:B:706:TRS:H12	2.46	0.53
1:D:616:LEU:O	1:D:617:VAL:C	2.47	0.52
1:D:144:VAL:HG21	1:D:207:TRP:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ILE:HA	1:D:22:LYS:HE2	1.91	0.52
1:B:320:GLN:HB3	1:B:322:TYR:CE1	2.45	0.52
1:B:627:CYS:HG	4:B:706:TRS:H32	1.73	0.52
1:B:15:ARG:HD3	1:B:276:VAL:HA	1.91	0.51
1:D:385:VAL:HG22	1:D:391:THR:CB	2.40	0.51
1:A:227[B]:ARG:NH1	1:A:347:GLU:OE1	2.43	0.51
1:B:212:VAL:O	1:B:224:LYS:NZ	2.43	0.51
1:C:580:CYS:N	4:C:708:TRS:N	2.58	0.51
1:A:436:VAL:HG22	1:A:444:ASN:HA	1.90	0.51
1:B:67:LEU:CB	1:B:71:MET:HE3	2.40	0.51
1:B:70:PRO:HA	1:B:89:ILE:HG23	1.93	0.51
1:C:67:LEU:HD23	1:C:96:ILE:HD13	1.92	0.51
1:D:551:ILE:HG13	1:D:552:PRO:HD2	1.92	0.51
1:A:579:GLY:O	1:A:580:CYS:HB2	2.11	0.51
1:A:627:CYS:SG	4:A:710:TRS:C2	2.98	0.51
1:D:437:GLN:HE21	1:D:482:GLN:HE21	1.59	0.50
1:A:385:VAL:HG22	1:A:391:THR:CB	2.41	0.50
1:B:3:TYR:OH	1:B:104:GLU:HG3	2.11	0.50
1:B:15:ARG:NH2	1:B:275:LEU:HB3	2.26	0.50
1:D:348:SER:HB2	1:D:360:ASP:HA	1.94	0.50
1:C:350:ILE:HD13	1:C:355:ARG:HH21	1.76	0.50
1:B:100:MET:HE2	1:B:100:MET:HA	1.93	0.50
1:C:295:ARG:HB3	5:C:864:HOH:O	2.12	0.50
1:B:60:ARG:CD	1:B:62:ILE:CG2	2.89	0.49
1:B:627:CYS:CB	4:B:706:TRS:H11	2.42	0.49
1:D:489:ASN:O	1:D:490:THR:HB	2.11	0.49
1:C:582:TRP:CD2	1:C:583:PRO:HD2	2.47	0.49
1:D:323:VAL:HG11	1:D:345:ILE:CD1	2.43	0.49
1:D:200:ILE:CD1	1:D:473:PHE:CE1	2.95	0.49
1:D:348:SER:CB	1:D:360:ASP:HA	2.43	0.49
1:C:453:SER:HA	1:C:679:ARG:HH21	1.78	0.49
1:A:107:GLN:O	1:A:111:VAL:HG23	2.13	0.49
1:B:69:ILE:HB	1:B:70:PRO:HD3	1.94	0.49
1:A:551:ILE:HG21	1:A:580:CYS:HA	1.95	0.49
1:D:200:ILE:HD13	1:D:473:PHE:CE1	2.48	0.49
1:D:78:GLN:CG	1:D:383:PHE:CZ	2.95	0.49
1:B:629:VAL:HG13	4:B:706:TRS:H31	1.95	0.48
1:C:78:GLN:HB3	1:C:383:PHE:CZ	2.48	0.48
1:B:3:TYR:CZ	1:B:104:GLU:HG3	2.48	0.48
1:A:638:LYS:HD2	1:A:642:PHE:CE2	2.49	0.48
1:C:317:ALA:HB1	1:C:323:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:CYS:CB	4:B:706:TRS:C1	2.91	0.48
1:D:431:VAL:HG22	1:D:487:ILE:HG12	1.95	0.48
1:D:200:ILE:CD1	1:D:473:PHE:CD1	2.96	0.48
1:D:313:ARG:NH2	5:D:807:HOH:O	2.47	0.48
1:A:227[B]:ARG:HD3	1:A:351:LEU:HD12	1.95	0.48
1:B:499:VAL:O	1:B:528:LYS:HA	2.14	0.48
1:A:627:CYS:SG	4:A:710:TRS:H21	2.53	0.47
1:C:348:SER:CB	1:C:360:ASP:HA	2.43	0.47
1:A:320:GLN:NE2	5:A:814:HOH:O	2.47	0.47
1:A:323:VAL:HG11	1:A:345:ILE:HD12	1.97	0.47
1:D:582:TRP:CD2	1:D:583:PRO:HD2	2.48	0.47
1:A:252:GLN:HA	1:A:509:GLU:HG2	1.96	0.47
1:A:638:LYS:HD2	1:A:642:PHE:CZ	2.50	0.47
1:B:262:GLU:HG2	5:B:980:HOH:O	2.15	0.47
1:C:323:VAL:HG11	1:C:345:ILE:CD1	2.43	0.47
1:C:579:GLY:HA3	4:C:708:TRS:N	2.30	0.47
1:C:377:HIS:CE1	1:C:380:LEU:HA	2.49	0.47
1:D:659:VAL:HG23	1:D:663:MET:CB	2.44	0.47
1:D:280:THR:OG1	1:D:281:TRP:N	2.48	0.47
1:B:227:ARG:HG3	1:B:227:ARG:HH11	1.80	0.47
3:A:708:EDO:H12	1:B:283:GLY:O	2.14	0.46
1:D:113:ALA:HB1	1:D:117:ILE:HD12	1.97	0.46
1:A:214:PRO:O	1:A:227[A]:ARG:NH2	2.48	0.46
1:C:348:SER:HB3	1:C:360:ASP:OD1	2.15	0.46
1:D:15:ARG:HG3	1:D:462:ASP:OD2	2.14	0.46
1:A:348:SER:CB	1:A:360:ASP:HA	2.45	0.46
1:B:226:ARG:HD2	1:B:229:GLU:OE1	2.16	0.46
1:D:348:SER:HB3	1:D:360:ASP:OD1	2.16	0.46
1:A:81:LEU:O	1:A:87:ARG:CD	2.58	0.46
1:C:242:TYR:CE2	1:C:246:ARG:HD2	2.50	0.46
1:D:186:ASP:HA	1:D:191:HIS:CD2	2.51	0.46
1:A:558:ARG:NH2	5:A:815:HOH:O	2.49	0.46
1:A:214:PRO:HG3	1:A:221:VAL:HG12	1.98	0.45
1:A:214:PRO:HG2	1:A:221:VAL:HG12	1.98	0.45
1:A:410:GLN:O	1:A:414:ILE:HG12	2.17	0.45
1:C:294:ASN:O	1:C:376:ASP:HA	2.17	0.45
1:D:659:VAL:HG23	1:D:663:MET:HB2	1.97	0.45
1:B:498:PHE:HE1	1:B:624:ALA:HB2	1.81	0.45
1:A:493:ALA:O	1:A:535:PRO:HG3	2.17	0.45
1:C:500:ARG:O	1:C:602:VAL:HA	2.16	0.45
1:B:491:SER:O	1:B:492:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:LEU:HD23	1:D:18:ILE:HD11	1.97	0.45
1:A:280:THR:O	1:A:282:PRO:HD3	2.17	0.45
1:B:193:LEU:HD21	1:B:251:LEU:HD12	1.98	0.45
1:C:39:ARG:N	1:C:40:PRO:CD	2.80	0.45
1:D:543:ARG:N	1:D:546:GLU:OE1	2.38	0.44
1:B:489:ASN:OD1	1:B:491:SER:CB	2.65	0.44
1:C:15:ARG:HD3	1:C:276:VAL:HA	1.99	0.44
1:A:628:GLY:H	4:A:710:TRS:H21	1.82	0.44
1:B:95:ASP:OD1	1:B:218:PRO:HG3	2.18	0.44
1:D:459:ARG:HH21	1:D:459:ARG:HG3	1.82	0.44
1:C:94:ILE:O	1:C:98:MET:HB2	2.16	0.44
1:D:10:LEU:CD2	1:D:18:ILE:HD11	2.48	0.44
1:D:426:TYR:CE2	1:D:606:ASN:HA	2.52	0.44
1:D:499:VAL:O	1:D:528:LYS:HA	2.17	0.44
1:C:81:LEU:O	1:C:87:ARG:HD2	2.18	0.44
1:C:318:VAL:O	1:C:415:LYS:HE2	2.18	0.44
1:A:20:MET:HG2	1:A:49:PHE:CE1	2.53	0.44
1:D:18:ILE:HD12	1:D:114:ARG:HD3	1.99	0.44
1:B:242:TYR:CE2	1:B:246:ARG:HD2	2.53	0.44
1:D:161:ILE:HG12	1:D:176:ILE:HG13	2.00	0.44
1:C:279:ARG:HG3	1:D:156:ARG:NH1	2.34	0.43
1:A:67:LEU:O	1:A:70:PRO:HD2	2.19	0.43
1:B:447:HIS:HA	1:B:671:ILE:O	2.18	0.43
1:A:39:ARG:N	1:A:40:PRO:CD	2.82	0.43
1:C:180:LYS:HE2	5:C:936:HOH:O	2.17	0.43
1:B:67:LEU:HD23	1:B:96:ILE:HD13	2.00	0.43
1:C:139:LEU:HD12	1:C:139:LEU:HA	1.88	0.43
1:C:317:ALA:HA	1:C:320:GLN:HE21	1.84	0.43
1:D:382:SER:OG	1:D:383:PHE:N	2.51	0.43
1:B:107:GLN:O	1:B:111:VAL:HG23	2.19	0.42
1:D:399:TYR:CD1	1:D:399:TYR:N	2.87	0.42
1:D:481:PHE:CE1	1:D:544:SER:HB3	2.54	0.42
1:C:145:VAL:HG23	1:C:204:LEU:HD21	2.02	0.42
1:C:156:ARG:HA	1:D:278:SER:HB2	2.02	0.42
1:A:214:PRO:HG3	1:A:221:VAL:CG1	2.49	0.42
1:D:78:GLN:HG3	1:D:383:PHE:HZ	1.79	0.42
1:D:541:ARG:HD2	5:D:960:HOH:O	2.19	0.42
1:D:39:ARG:N	1:D:40:PRO:CD	2.83	0.42
1:D:156:ARG:NH2	5:D:809:HOH:O	2.53	0.42
1:A:355:ARG:HG3	1:A:355:ARG:NH1	2.29	0.42
1:A:499:VAL:O	1:A:528:LYS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:PRO:HB3	1:C:457:LEU:HD22	2.02	0.42
1:C:162:ARG:HD3	1:D:162:ARG:NH1	2.35	0.42
1:D:209:TRP:CE2	1:D:234:MET:HE2	2.55	0.42
1:A:208:HIS:CD2	1:A:580:CYS:CB	3.03	0.41
1:D:659:VAL:CG2	1:D:663:MET:HB2	2.50	0.41
1:A:388:ASP:HB3	1:A:391:THR:OG1	2.20	0.41
1:B:71:MET:HE1	1:B:116:ARG:HD3	2.01	0.41
1:B:452:GLN:HA	1:B:473:PHE:O	2.20	0.41
1:C:70:PRO:HA	1:C:89:ILE:HG23	2.03	0.41
1:C:161:ILE:HG12	1:C:176:ILE:HG13	2.03	0.41
1:C:627:CYS:HB3	1:C:630:ARG:HB3	2.02	0.41
1:A:610:ASP:OD1	1:A:638:LYS:NZ	2.52	0.41
1:D:178:ILE:HD11	1:D:471:ALA:HB1	2.02	0.41
1:D:310:TRP:CE2	1:D:359:GLY:HA3	2.55	0.41
1:D:558:ARG:CG	1:D:558:ARG:NH2	2.69	0.41
1:D:310:TRP:CD2	1:D:359:GLY:HA3	2.56	0.41
1:B:133:ARG:HB3	1:B:135:ASP:OD1	2.21	0.41
1:C:316:GLU:O	1:C:320:GLN:HG3	2.21	0.41
1:D:607:TYR:O	1:D:611:ARG:HB2	2.21	0.41
1:A:673:ILE:HG22	1:A:675:LYS:HG2	2.03	0.41
1:C:67:LEU:C	1:C:70:PRO:HD2	2.41	0.41
1:D:88:LYS:HD2	1:D:88:LYS:HA	1.80	0.41
1:D:325:ASP:OD1	1:D:326:GLU:N	2.54	0.41
1:C:580:CYS:N	4:C:708:TRS:HN2	2.18	0.40
1:D:214:PRO:HG2	1:D:221:VAL:HG12	2.03	0.40
1:B:541:ARG:HD2	1:B:541:ARG:C	2.41	0.40
1:C:497:GLY:O	1:C:530:LEU:HD12	2.21	0.40
1:A:498:PHE:CE1	1:A:624:ALA:HB2	2.56	0.40
1:D:147:VAL:HG23	1:D:148:PHE:CD2	2.56	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	653/680 (96%)	628 (96%)	25 (4%)	0	100	100
1	B	651/680 (96%)	625 (96%)	24 (4%)	2 (0%)	41	56
1	C	653/680 (96%)	630 (96%)	22 (3%)	1 (0%)	47	64
1	D	652/680 (96%)	625 (96%)	26 (4%)	1 (0%)	47	64
All	All	2609/2720 (96%)	2508 (96%)	97 (4%)	4 (0%)	47	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	325	ASP
1	B	615	ASP
1	C	139	LEU
1	B	552	PRO

### 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	591/609 (97%)	573 (97%)	18 (3%)	41	59
1	B	589/609 (97%)	581 (99%)	8 (1%)	67	81
1	C	591/609 (97%)	575 (97%)	16 (3%)	44	63
1	D	590/609 (97%)	574 (97%)	16 (3%)	44	63
All	All	2361/2436 (97%)	2303 (98%)	58 (2%)	47	66

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	92	ARG
1	A	123	ASN
1	A	170	GLU
1	A	199	ASP
1	A	202	VAL
1	A	232	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	244	PHE
1	A	297	LEU
1	A	361	MET
1	A	385	VAL
1	A	422	SER
1	A	426	TYR
1	A	453	SER
1	A	498	PHE
1	A	578	CYS
1	A	622	ASP
1	A	656	SER
1	B	102	ASN
1	B	244	PHE
1	B	297	LEU
1	B	426	TYR
1	B	490	THR
1	B	498	PHE
1	B	629	VAL
1	B	643	PRO
1	C	2	ASN
1	C	3	TYR
1	C	134	ARG
1	C	177	VAL
1	C	236	SER
1	C	244	PHE
1	C	300	ILE
1	C	302	GLN
1	C	329	ASN
1	C	407	ASP
1	C	426	TYR
1	C	436	VAL
1	C	439	GLU
1	C	498	PHE
1	C	608	GLU
1	C	643	PRO
1	D	26	VAL
1	D	45	ILE
1	D	143	SER
1	D	170	GLU
1	D	191	HIS
1	D	244	PHE
1	D	297	LEU

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Mol	Chain	Res	Type
1	D	337	LYS
1	D	371	TYR
1	D	426	TYR
1	D	469	VAL
1	D	490	THR
1	D	558	ARG
1	D	617	VAL
1	D	629	VAL
1	D	657	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	208	HIS
1	A	452	GLN
1	C	2	ASN
1	D	437	GLN
1	D	614	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	709	-	3,3,3	0.13	0	2,2,2	0.22	0
3	EDO	A	704	-	3,3,3	0.24	0	2,2,2	0.24	0
3	EDO	A	707	-	3,3,3	0.27	0	2,2,2	0.41	0
3	EDO	D	706	-	3,3,3	0.16	0	2,2,2	0.05	0
3	EDO	B	703	-	3,3,3	0.28	0	2,2,2	0.35	0
3	EDO	A	703	-	3,3,3	0.19	0	2,2,2	0.23	0
3	EDO	D	703	-	3,3,3	0.59	0	2,2,2	0.56	0
4	TRS	A	710	-	7,7,7	0.53	0	9,9,9	0.77	0
4	TRS	C	708	-	7,7,7	0.56	0	9,9,9	1.17	1 (11%)
4	TRS	B	706	-	7,7,7	0.27	0	9,9,9	0.53	0
3	EDO	B	705	-	3,3,3	0.07	0	2,2,2	0.13	0
3	EDO	C	705	-	3,3,3	0.14	0	2,2,2	0.43	0
3	EDO	A	708	-	3,3,3	0.35	0	2,2,2	0.34	0
3	EDO	B	704	-	3,3,3	0.39	0	2,2,2	0.75	0
3	EDO	D	704	-	3,3,3	0.14	0	2,2,2	0.18	0
3	EDO	D	705	-	3,3,3	0.31	0	2,2,2	0.49	0
3	EDO	C	706	-	3,3,3	0.33	0	2,2,2	0.33	0
3	EDO	C	703	-	3,3,3	0.33	0	2,2,2	0.31	0
3	EDO	A	706	-	3,3,3	0.18	0	2,2,2	0.26	0
3	EDO	C	704	-	3,3,3	0.26	0	2,2,2	0.72	0
3	EDO	A	705	-	3,3,3	0.24	0	2,2,2	0.42	0
3	EDO	C	707	-	3,3,3	0.12	0	2,2,2	0.06	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	EDO	A	709	-	-	1/1/1/1	-
3	EDO	A	704	-	-	1/1/1/1	-
3	EDO	A	707	-	-	0/1/1/1	-
3	EDO	D	706	-	-	1/1/1/1	-
3	EDO	B	703	-	-	1/1/1/1	-
3	EDO	A	703	-	-	1/1/1/1	-
3	EDO	D	703	-	-	1/1/1/1	-
4	TRS	A	710	-	-	3/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRS	C	708	-	-	9/9/9/9	-
4	TRS	B	706	-	-	6/9/9/9	-
3	EDO	B	705	-	-	1/1/1/1	-
3	EDO	C	705	-	-	1/1/1/1	-
3	EDO	A	708	-	-	1/1/1/1	-
3	EDO	B	704	-	-	0/1/1/1	-
3	EDO	D	704	-	-	1/1/1/1	-
3	EDO	D	705	-	-	1/1/1/1	-
3	EDO	C	706	-	-	1/1/1/1	-
3	EDO	C	703	-	-	0/1/1/1	-
3	EDO	A	706	-	-	1/1/1/1	-
3	EDO	C	704	-	-	1/1/1/1	-
3	EDO	A	705	-	-	1/1/1/1	-
3	EDO	C	707	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	708	TRS	C2-C-N	-2.76	99.75	107.98

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	710	TRS	C1-C-C3-O3
4	A	710	TRS	C2-C-C3-O3
4	A	710	TRS	N-C-C3-O3
4	B	706	TRS	C2-C-C1-O1
4	B	706	TRS	C3-C-C1-O1
4	B	706	TRS	N-C-C1-O1
4	B	706	TRS	C1-C-C3-O3
4	C	708	TRS	C2-C-C1-O1
4	C	708	TRS	C3-C-C2-O2
4	C	708	TRS	C1-C-C3-O3
4	C	708	TRS	C2-C-C3-O3
4	C	708	TRS	N-C-C3-O3
3	A	703	EDO	O1-C1-C2-O2
3	A	704	EDO	O1-C1-C2-O2
3	B	703	EDO	O1-C1-C2-O2
3	C	704	EDO	O1-C1-C2-O2

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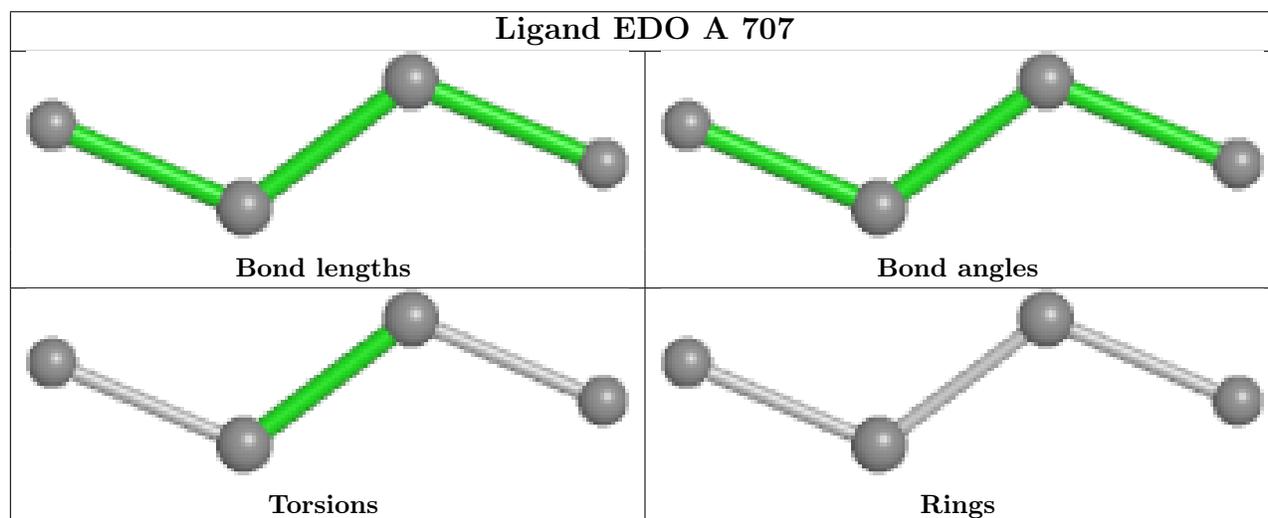
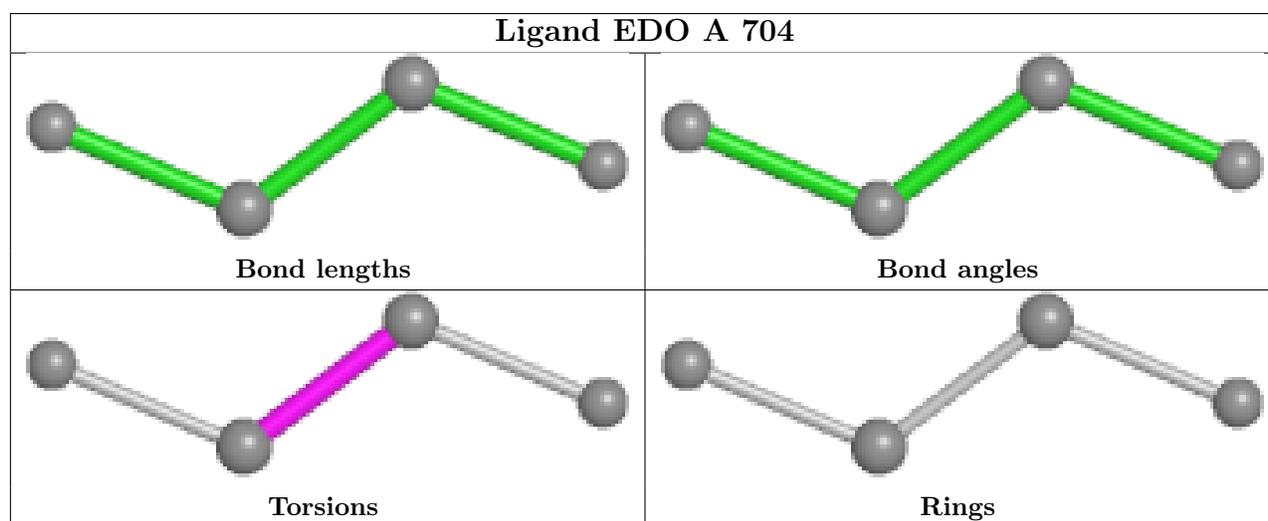
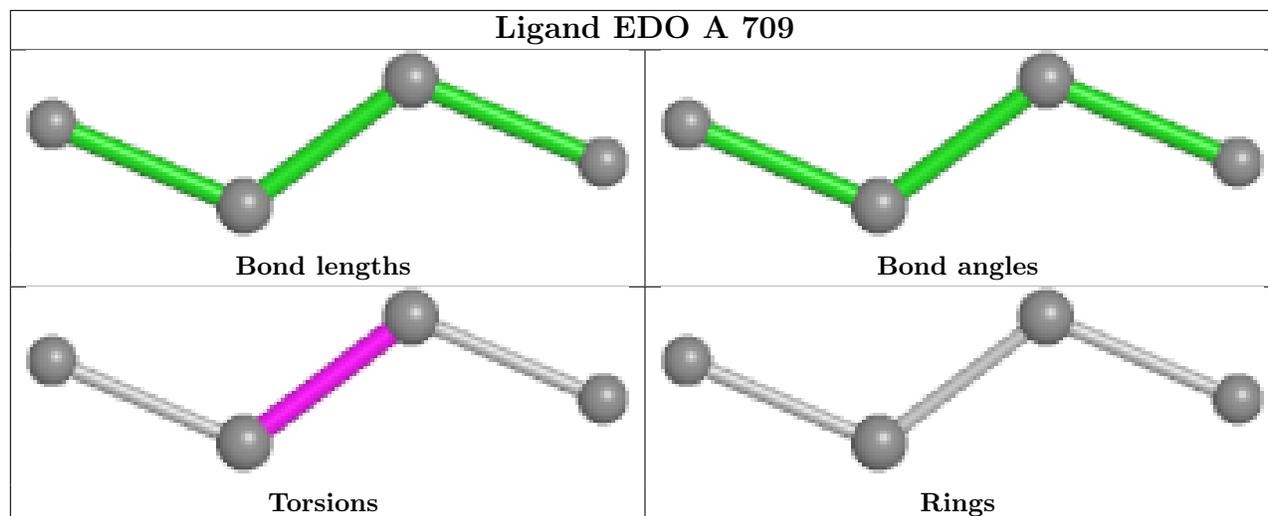
Mol	Chain	Res	Type	Atoms
3	D	703	EDO	O1-C1-C2-O2
4	B	706	TRS	C2-C-C3-O3
4	C	708	TRS	C3-C-C1-O1
3	C	706	EDO	O1-C1-C2-O2
3	D	705	EDO	O1-C1-C2-O2
3	D	706	EDO	O1-C1-C2-O2
4	B	706	TRS	N-C-C3-O3
4	C	708	TRS	C1-C-C2-O2
3	C	705	EDO	O1-C1-C2-O2
3	A	706	EDO	O1-C1-C2-O2
3	B	705	EDO	O1-C1-C2-O2
3	C	707	EDO	O1-C1-C2-O2
3	D	704	EDO	O1-C1-C2-O2
3	A	708	EDO	O1-C1-C2-O2
3	A	709	EDO	O1-C1-C2-O2
4	C	708	TRS	N-C-C1-O1
4	C	708	TRS	N-C-C2-O2
3	A	705	EDO	O1-C1-C2-O2

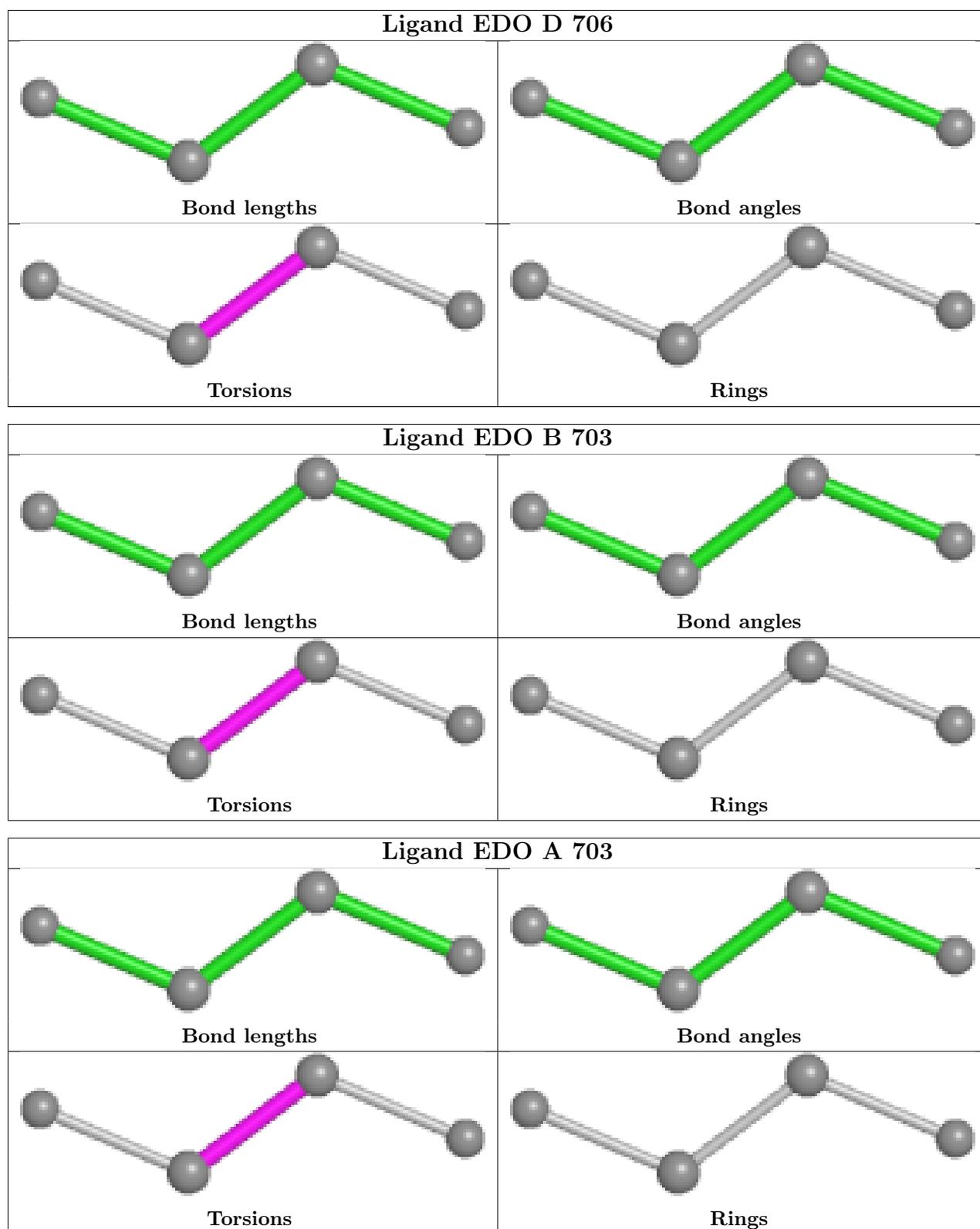
There are no ring outliers.

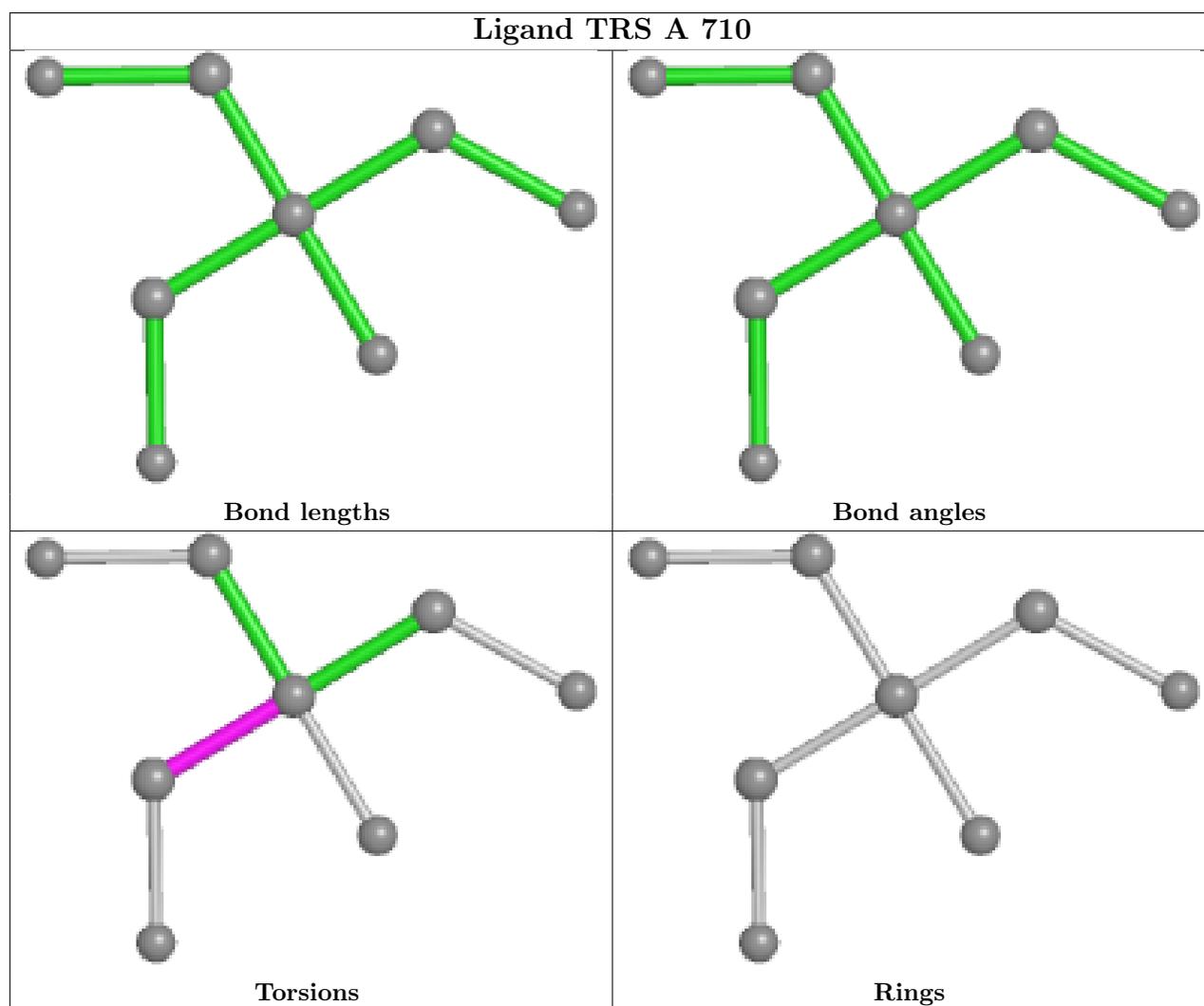
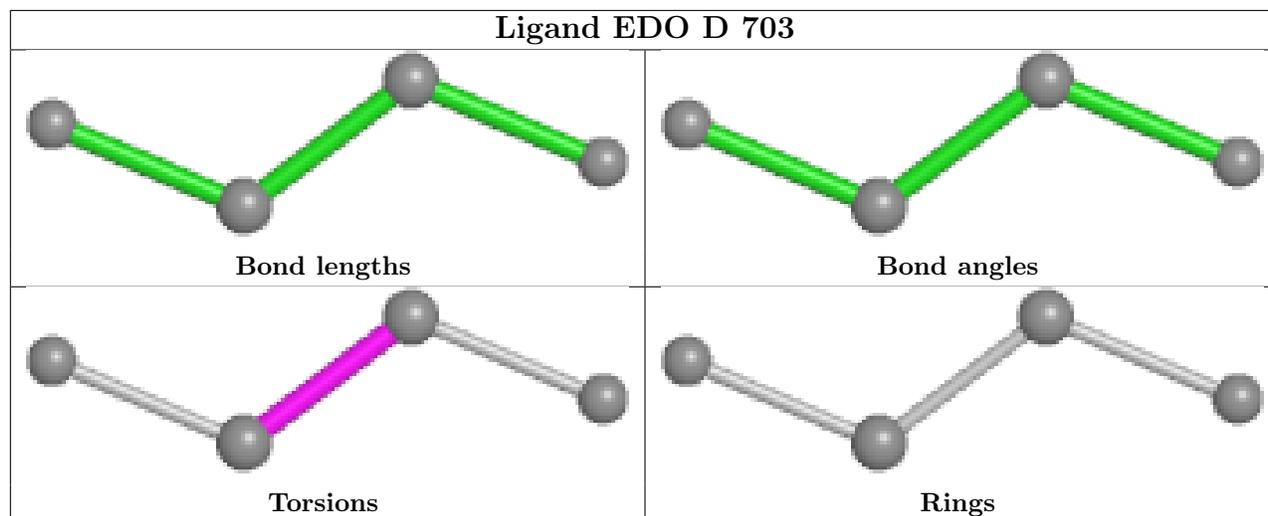
4 monomers are involved in 45 short contacts:

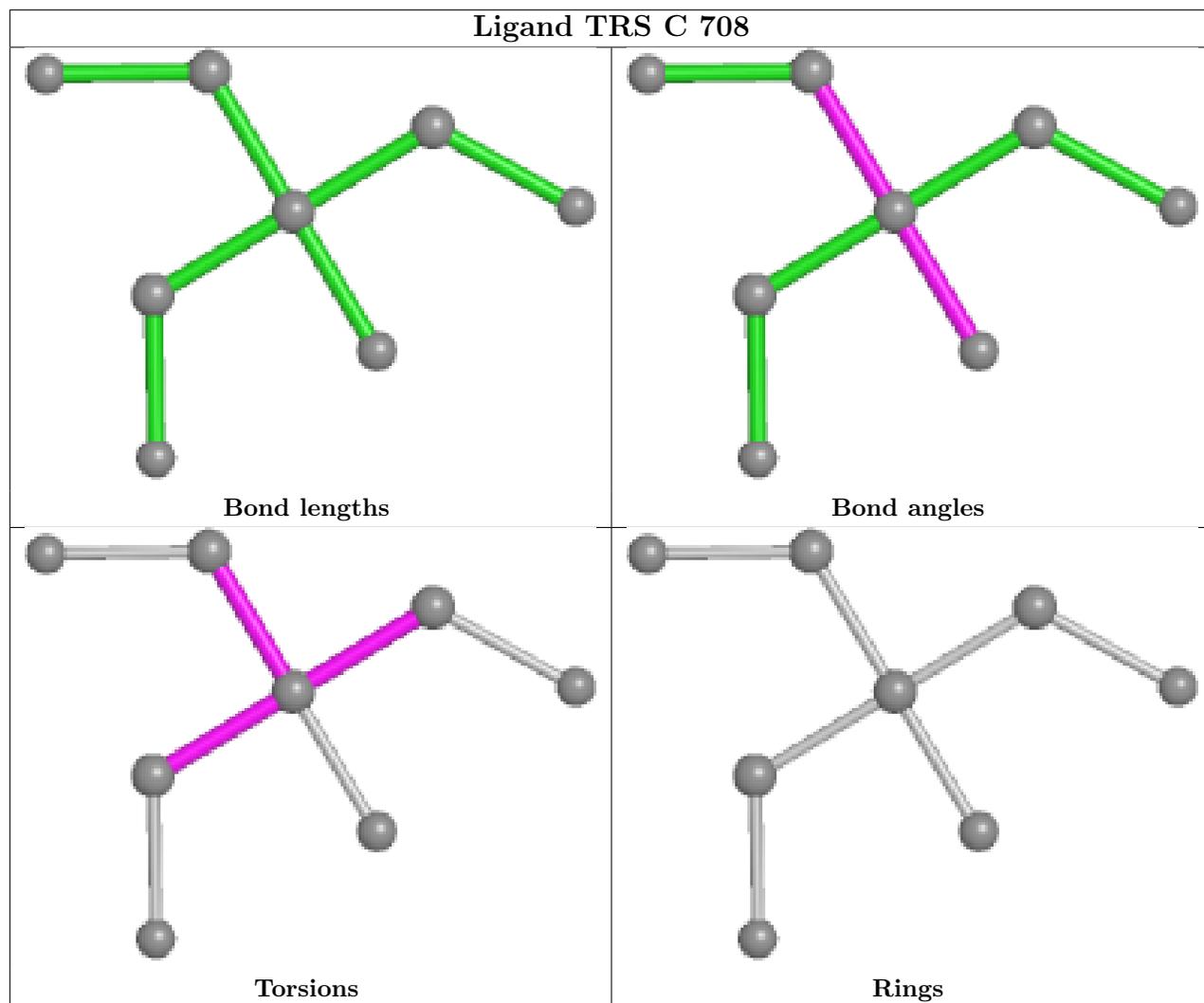
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	710	TRS	14	0
4	C	708	TRS	15	0
4	B	706	TRS	15	0
3	A	708	EDO	1	0

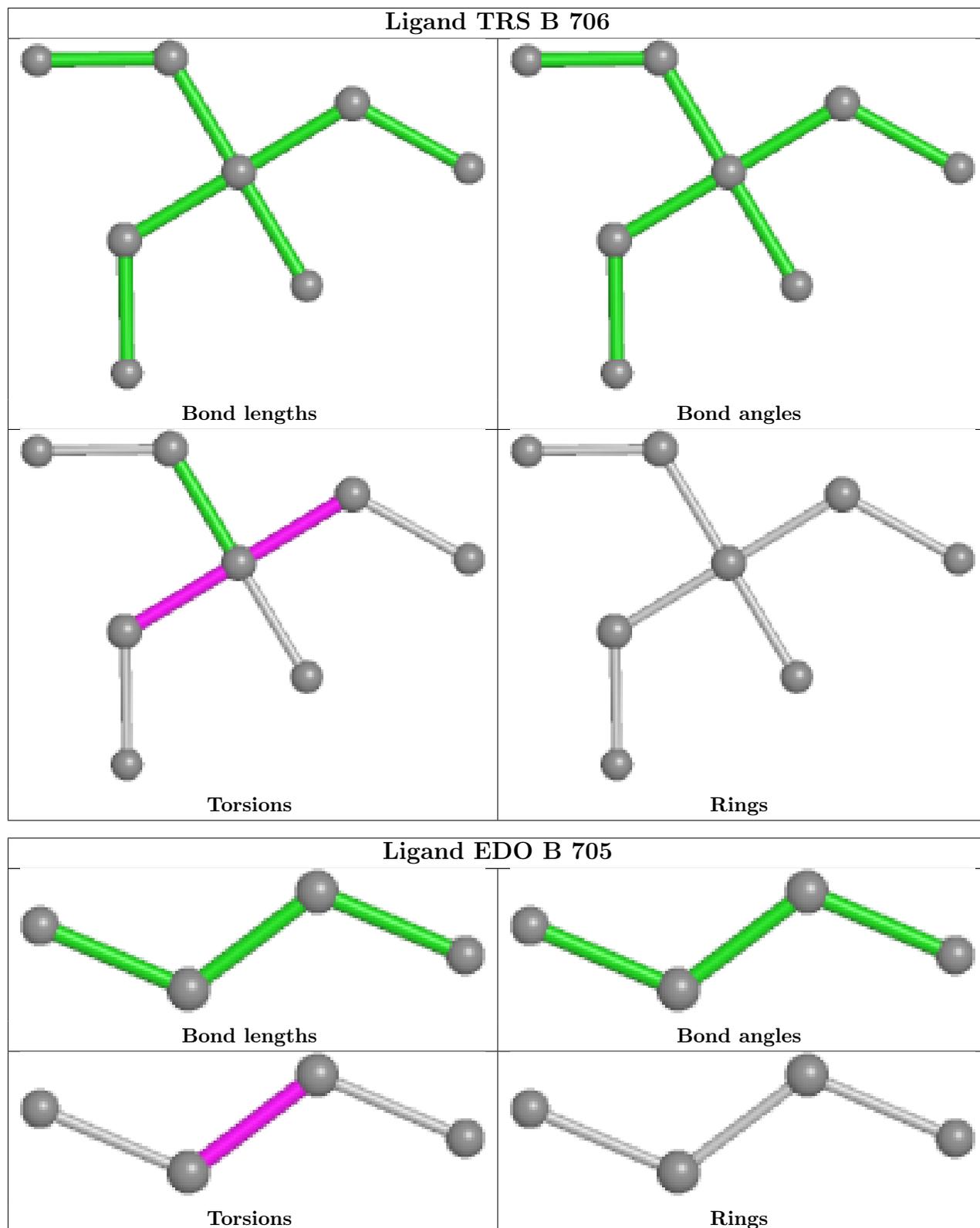
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

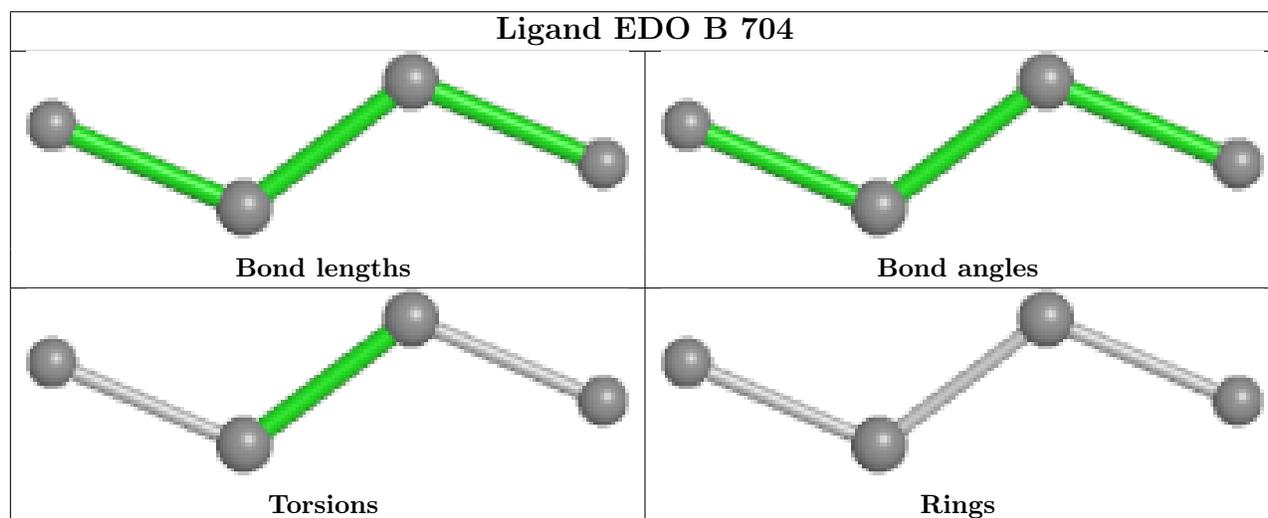
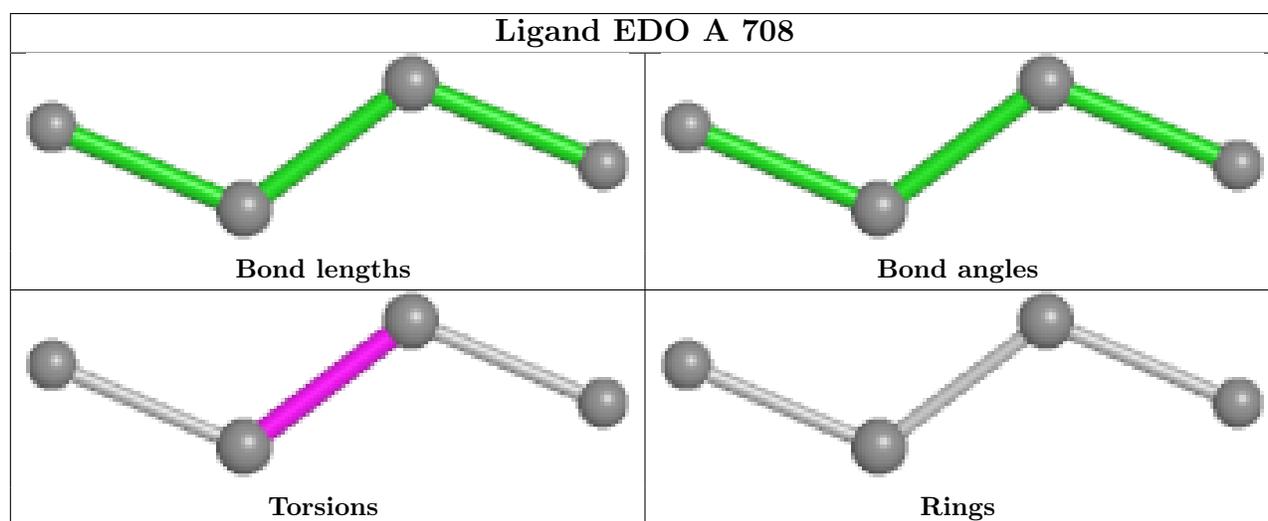
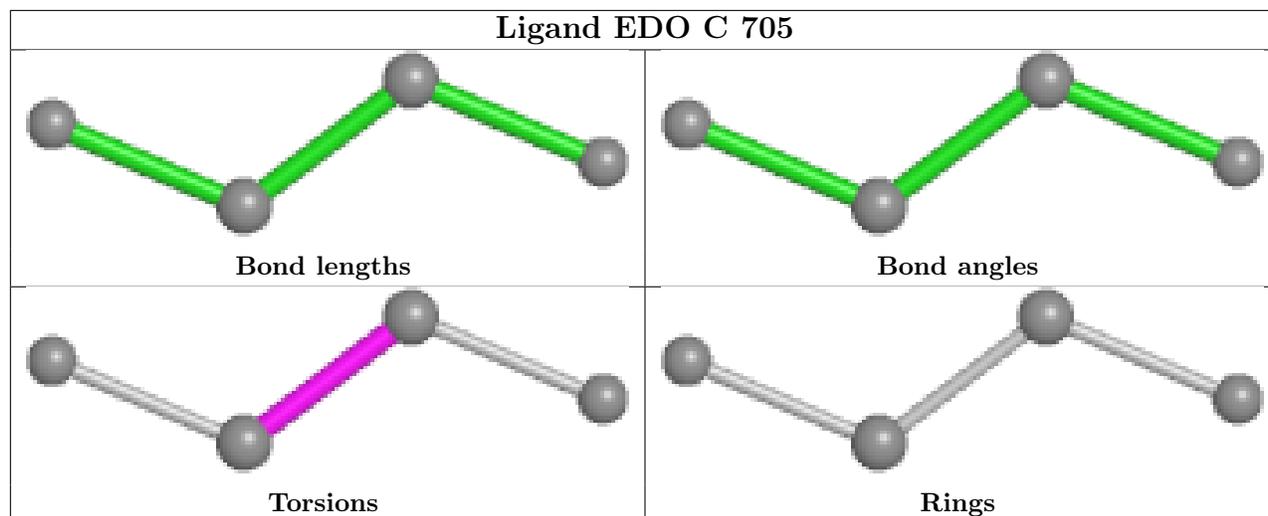


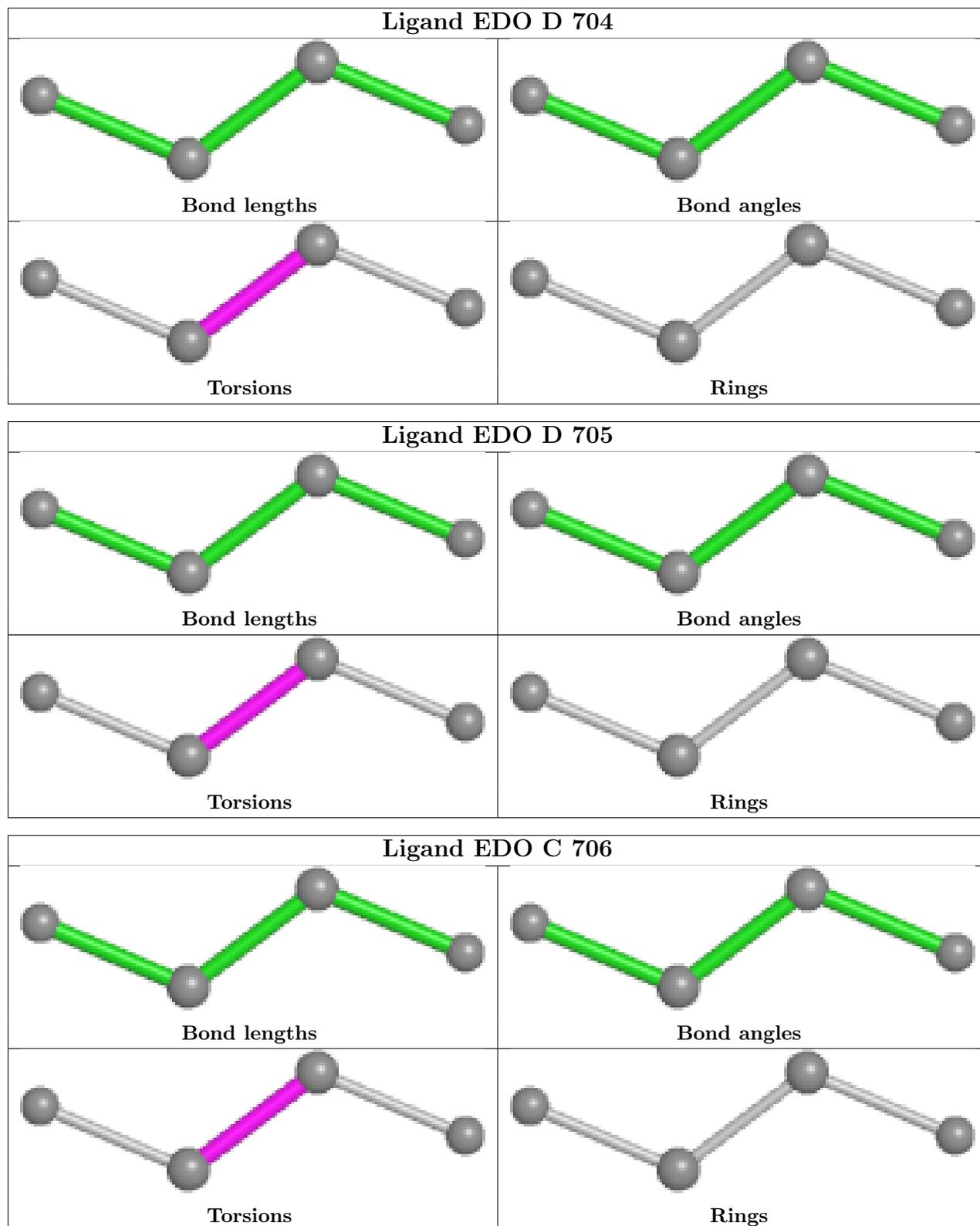


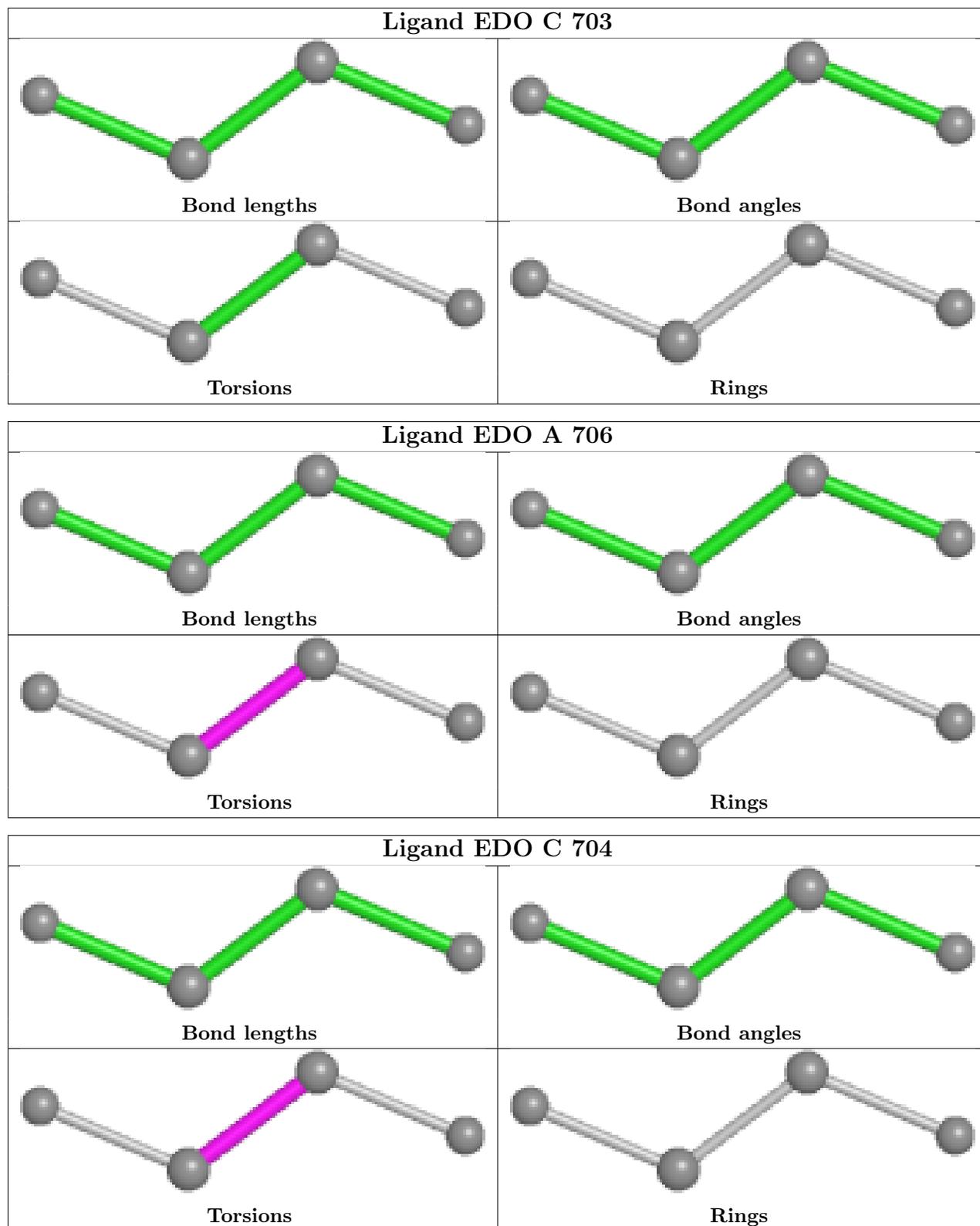


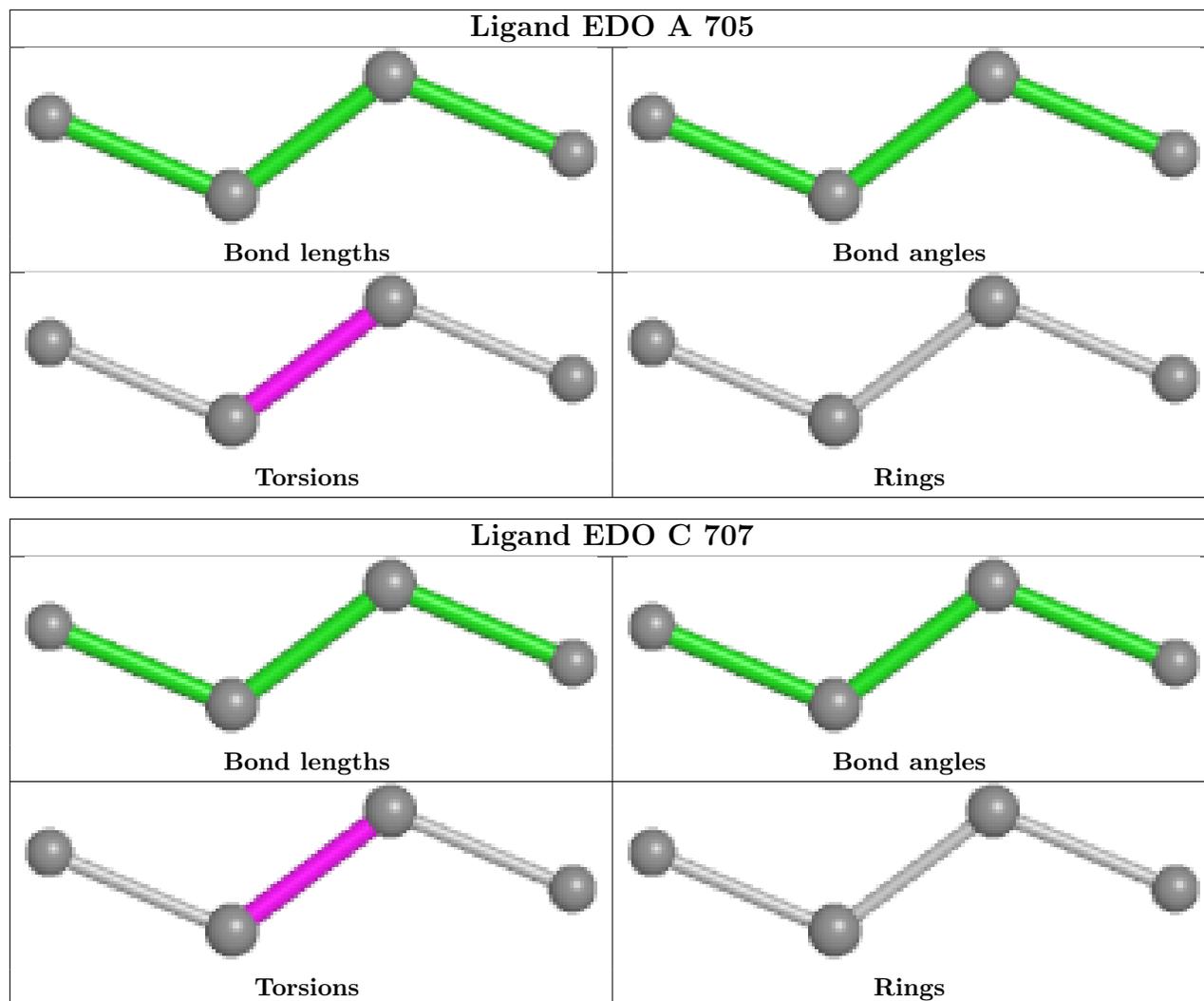












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	658/680 (96%)	-0.27	13 (1%) 65 60	23, 40, 75, 133	0
1	B	657/680 (96%)	-0.21	18 (2%) 54 50	25, 42, 86, 152	0
1	C	658/680 (96%)	-0.23	15 (2%) 60 56	25, 43, 80, 140	0
1	D	658/680 (96%)	-0.14	18 (2%) 54 50	25, 42, 90, 161	0
All	All	2631/2720 (96%)	-0.21	64 (2%) 59 54	23, 42, 82, 161	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	577	PHE	7.3
1	B	616	LEU	5.4
1	B	617	VAL	5.2
1	A	1	MET	5.1
1	C	678	PRO	5.1
1	A	616	LEU	5.0
1	A	617	VAL	4.8
1	D	631	ASP	4.7
1	A	615	ASP	4.6
1	D	553	PHE	4.6
1	C	615	ASP	4.5
1	C	51	GLU	4.4
1	A	47	ASN	4.3
1	D	630	ARG	4.0
1	B	615	ASP	3.9
1	D	615	ASP	3.9
1	C	50	GLY	3.8
1	D	678	PRO	3.8
1	B	31	ASP	3.6
1	D	616	LEU	3.6
1	C	614	GLN	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	558	ARG	3.5
1	A	48	ARG	3.5
1	B	614	GLN	3.3
1	C	577	PHE	3.3
1	B	680	THR	3.3
1	C	617	VAL	3.2
1	D	554	GLU	3.2
1	C	613	VAL	3.1
1	A	138	ASN	3.0
1	D	680	THR	3.0
1	A	51	GLU	3.0
1	D	45	ILE	2.9
1	D	617	VAL	2.9
1	B	41	ILE	2.9
1	D	31	ASP	2.8
1	B	46	GLN	2.8
1	B	50	GLY	2.8
1	B	3	TYR	2.7
1	C	679	ARG	2.7
1	C	23	GLY	2.6
1	D	47	ASN	2.5
1	C	24	LYS	2.5
1	B	577	PHE	2.5
1	C	53	ALA	2.4
1	A	60	ARG	2.4
1	D	629	VAL	2.4
1	A	31	ASP	2.4
1	D	679	ARG	2.3
1	D	613	VAL	2.3
1	C	580	CYS	2.3
1	D	557	PHE	2.3
1	B	42	GLY	2.3
1	B	613	VAL	2.3
1	A	61	SER	2.2
1	B	30	PRO	2.2
1	D	580	CYS	2.2
1	A	3	TYR	2.1
1	B	52	LEU	2.1
1	C	2	ASN	2.1
1	B	45	ILE	2.1
1	B	60	ARG	2.1
1	C	52	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	47	ASN	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CU	B	702	1/1	0.20	0.49	164,164,164,164	0
2	CU	D	701	1/1	0.27	0.93	183,183,183,183	0
2	CU	A	702	1/1	0.42	0.47	170,170,170,170	0
2	CU	C	701	1/1	0.68	0.24	128,128,128,128	0
2	CU	D	702	1/1	0.70	0.26	131,131,131,131	0
2	CU	A	701	1/1	0.76	0.20	118,118,118,118	0
3	EDO	D	703	4/4	0.78	0.57	44,47,48,51	0
2	CU	C	702	1/1	0.79	0.65	157,157,157,157	0
3	EDO	C	703	4/4	0.84	0.21	55,57,62,63	0
3	EDO	D	705	4/4	0.85	0.25	53,55,59,61	0
3	EDO	C	706	4/4	0.86	0.19	52,55,60,61	0
3	EDO	A	703	4/4	0.87	0.27	50,50,51,51	0
3	EDO	A	709	4/4	0.87	0.17	50,52,53,53	0
2	CU	B	701	1/1	0.87	0.26	116,116,116,116	0
3	EDO	D	706	4/4	0.88	0.15	63,64,64,64	0
3	EDO	A	707	4/4	0.89	0.18	48,49,50,53	0
3	EDO	A	706	4/4	0.90	0.28	56,59,59,65	0
3	EDO	D	704	4/4	0.90	0.12	53,55,57,58	0
3	EDO	C	705	4/4	0.90	0.17	62,67,67,69	0
3	EDO	B	704	4/4	0.90	0.29	43,45,51,53	0
3	EDO	A	708	4/4	0.92	0.27	43,48,48,50	0
3	EDO	A	705	4/4	0.92	0.12	48,54,54,56	0

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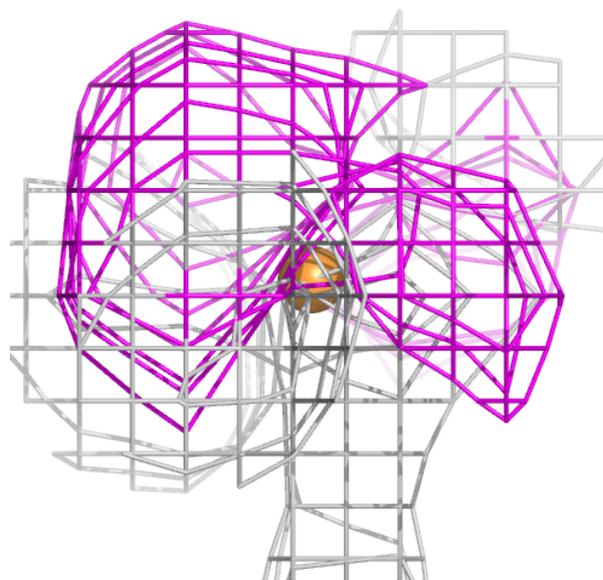
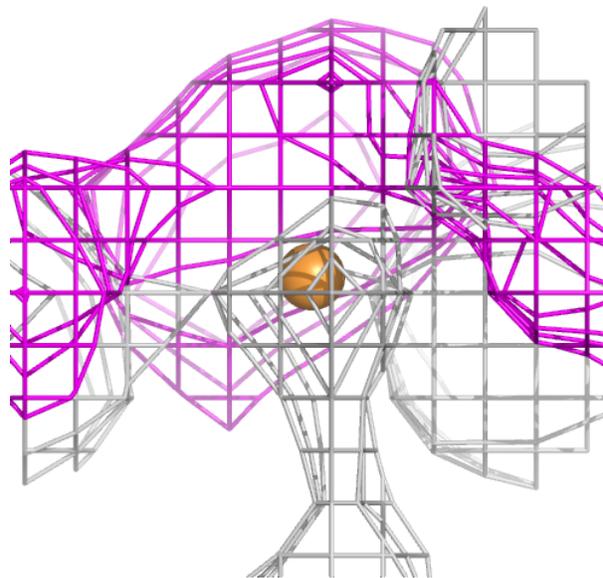
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	C	704	4/4	0.92	0.22	43,45,48,50	0
3	EDO	B	705	4/4	0.93	0.12	52,53,57,61	0
4	TRS	A	710	8/8	0.93	0.25	28,30,43,48	0
4	TRS	B	706	8/8	0.94	0.20	36,39,52,61	0
4	TRS	C	708	8/8	0.94	0.26	23,27,29,34	0
3	EDO	C	707	4/4	0.95	0.27	61,62,64,64	0
3	EDO	B	703	4/4	0.95	0.17	39,46,47,48	0
3	EDO	A	704	4/4	0.96	0.23	45,46,53,54	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.

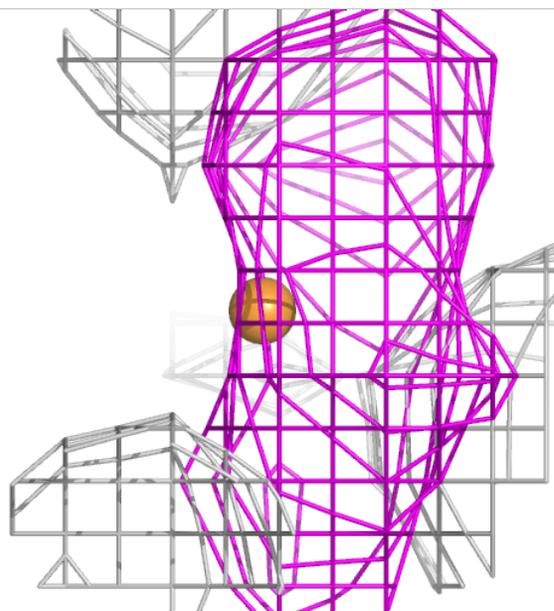
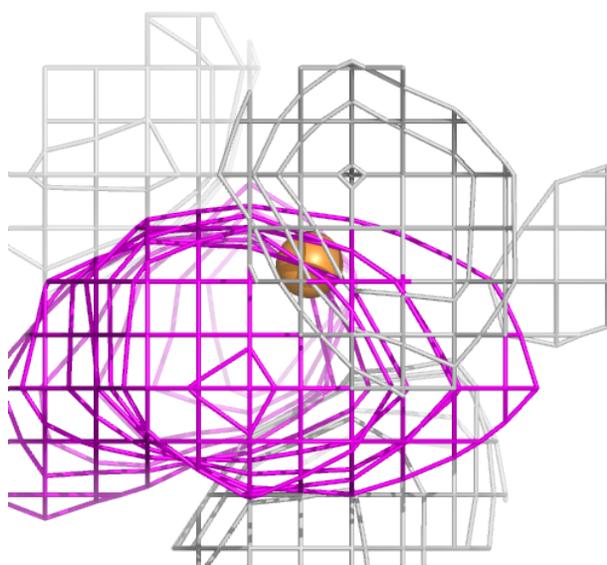
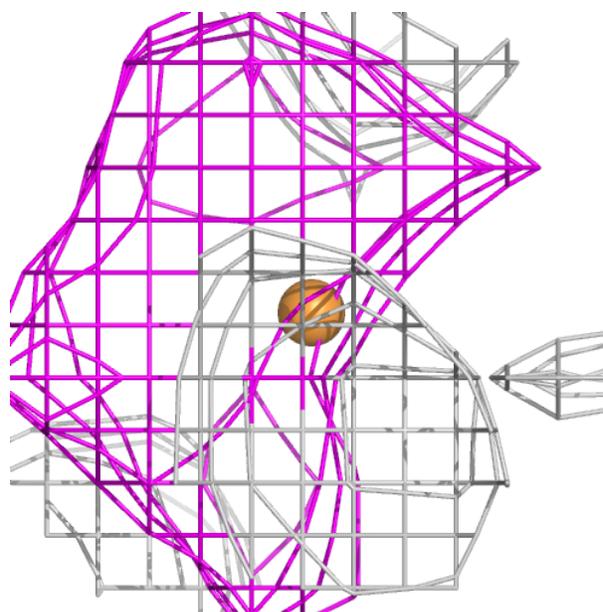
**Electron density around CU B 702:**

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



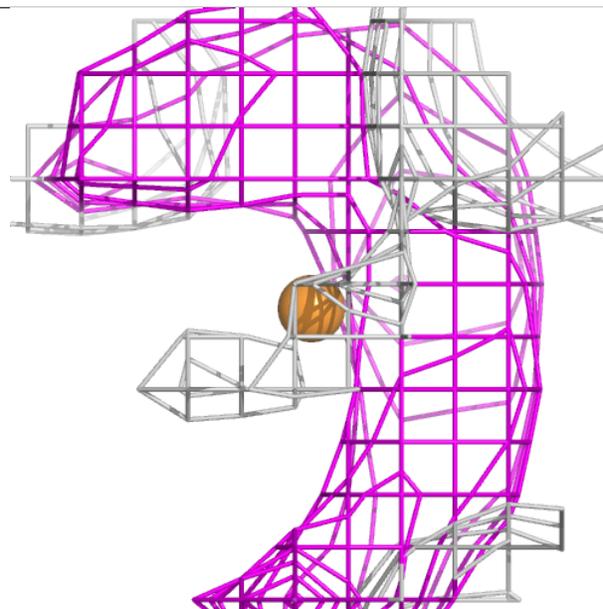
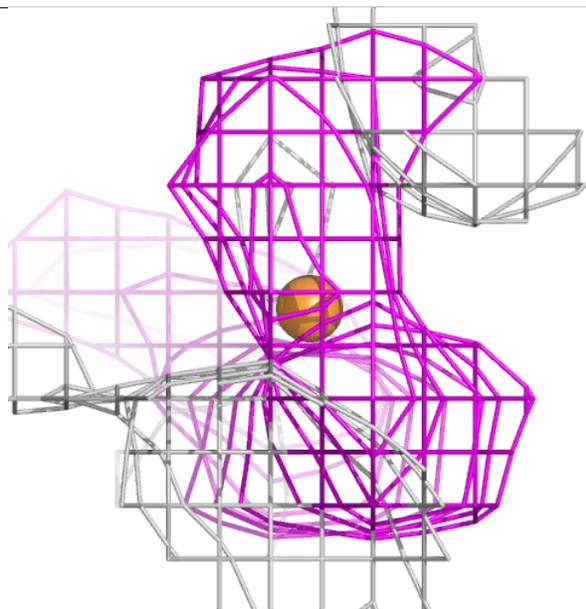
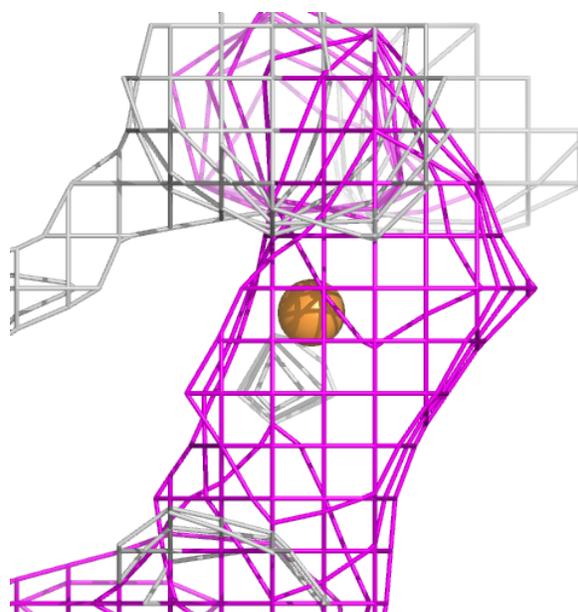
**Electron density around CU D 701:**

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



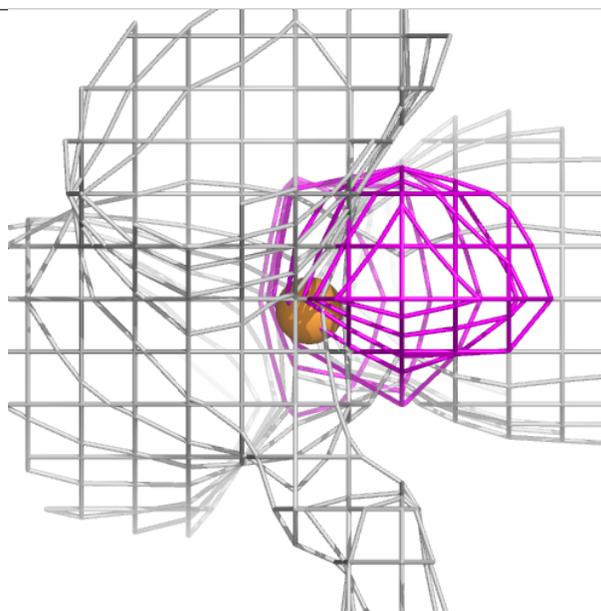
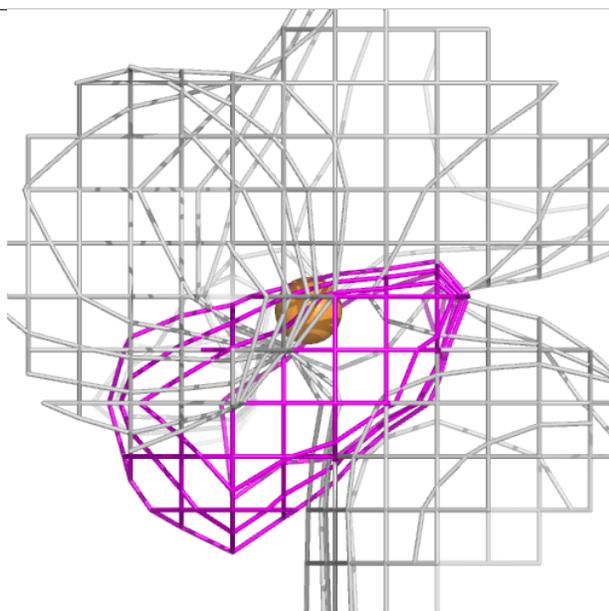
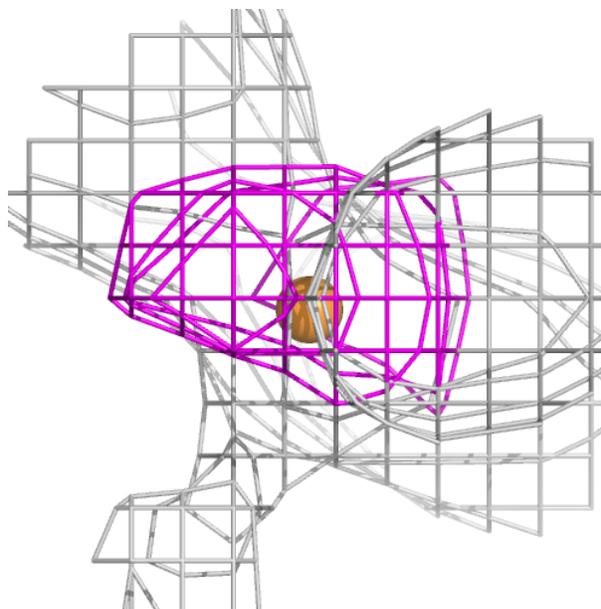
**Electron density around CU A 702:**

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



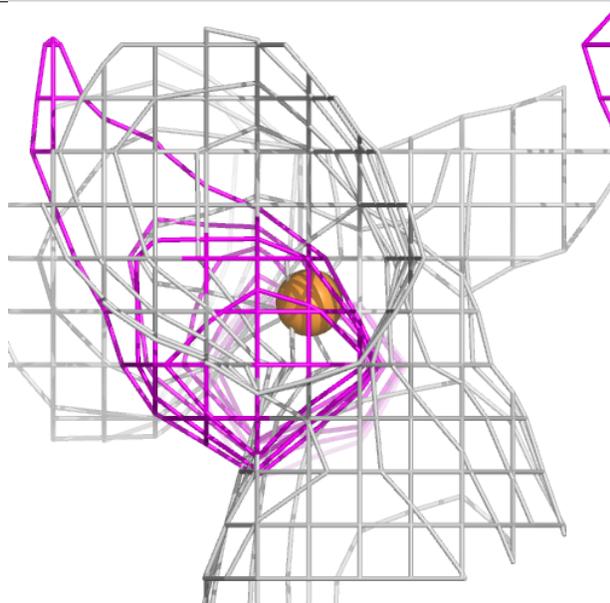
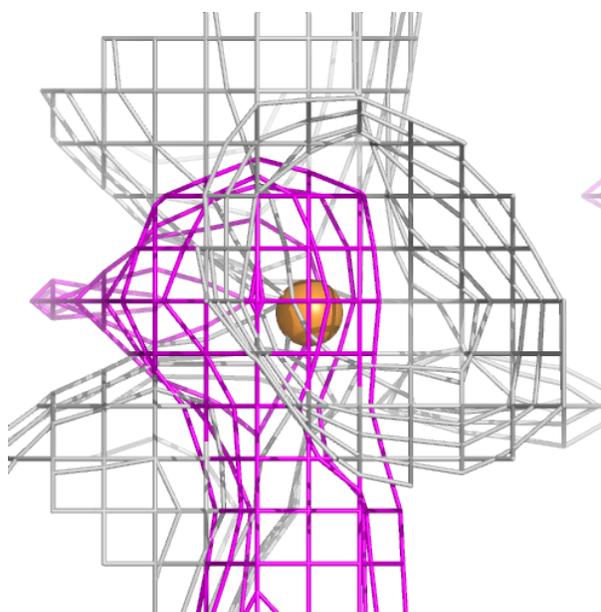
**Electron density around CU C 701:**

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



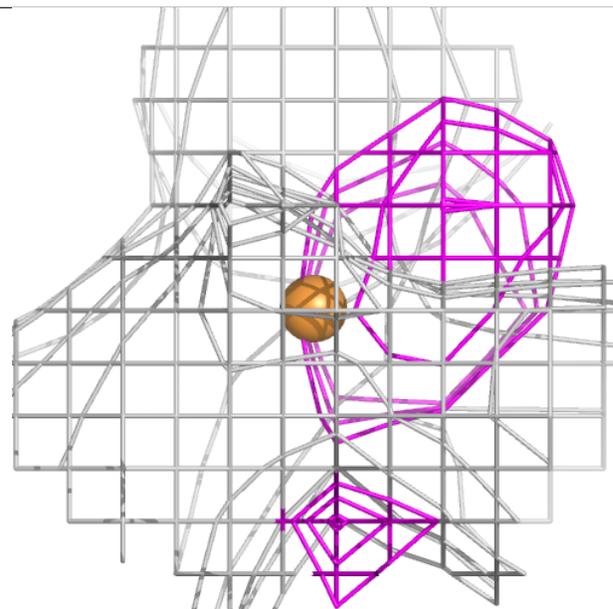
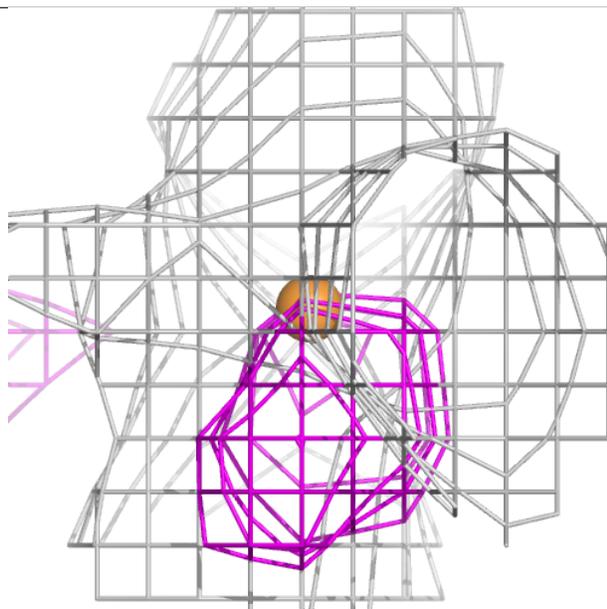
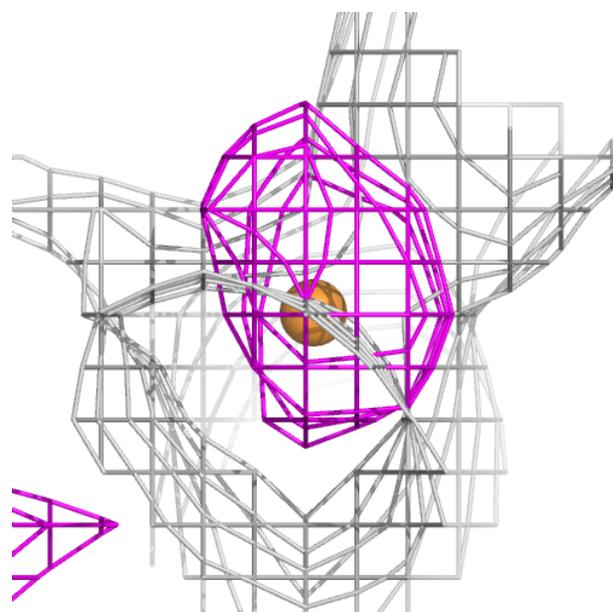
**Electron density around CU D 702:**

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



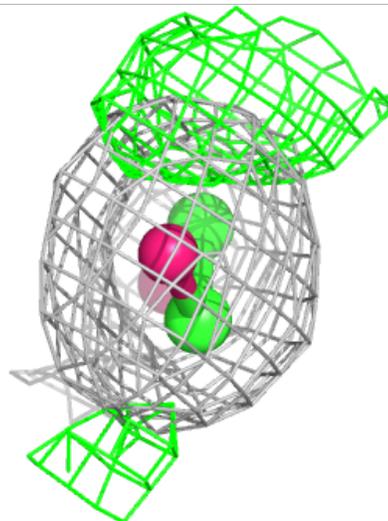
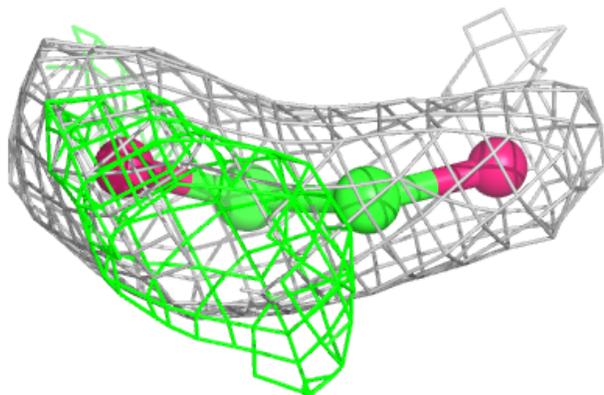
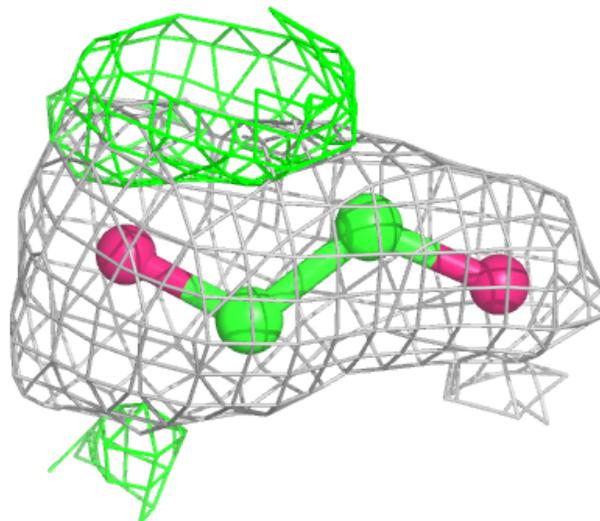
**Electron density around CU A 701:**

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



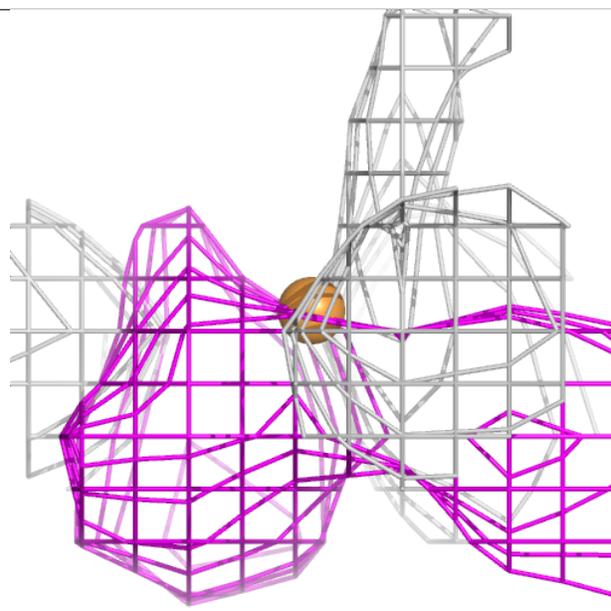
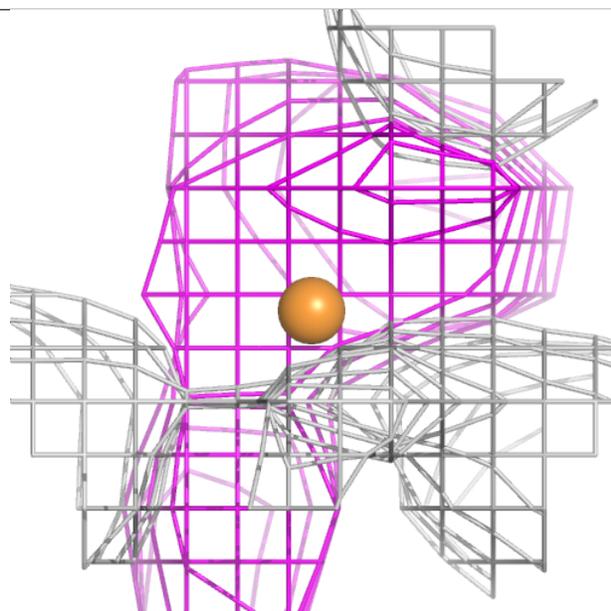
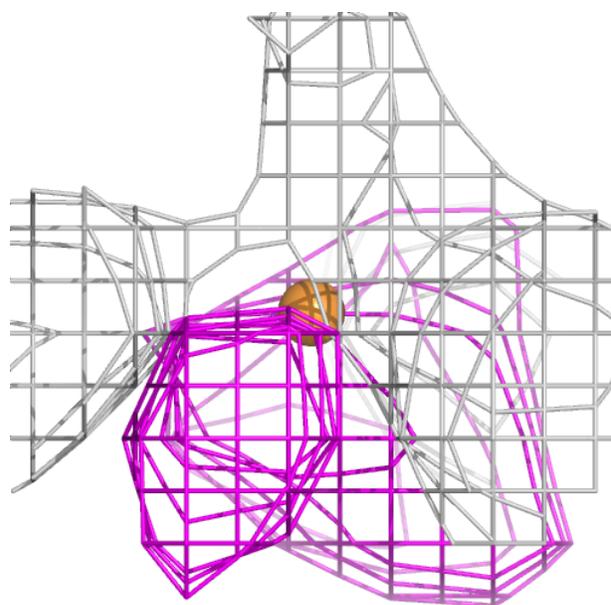
**Electron density around EDO D 703:**

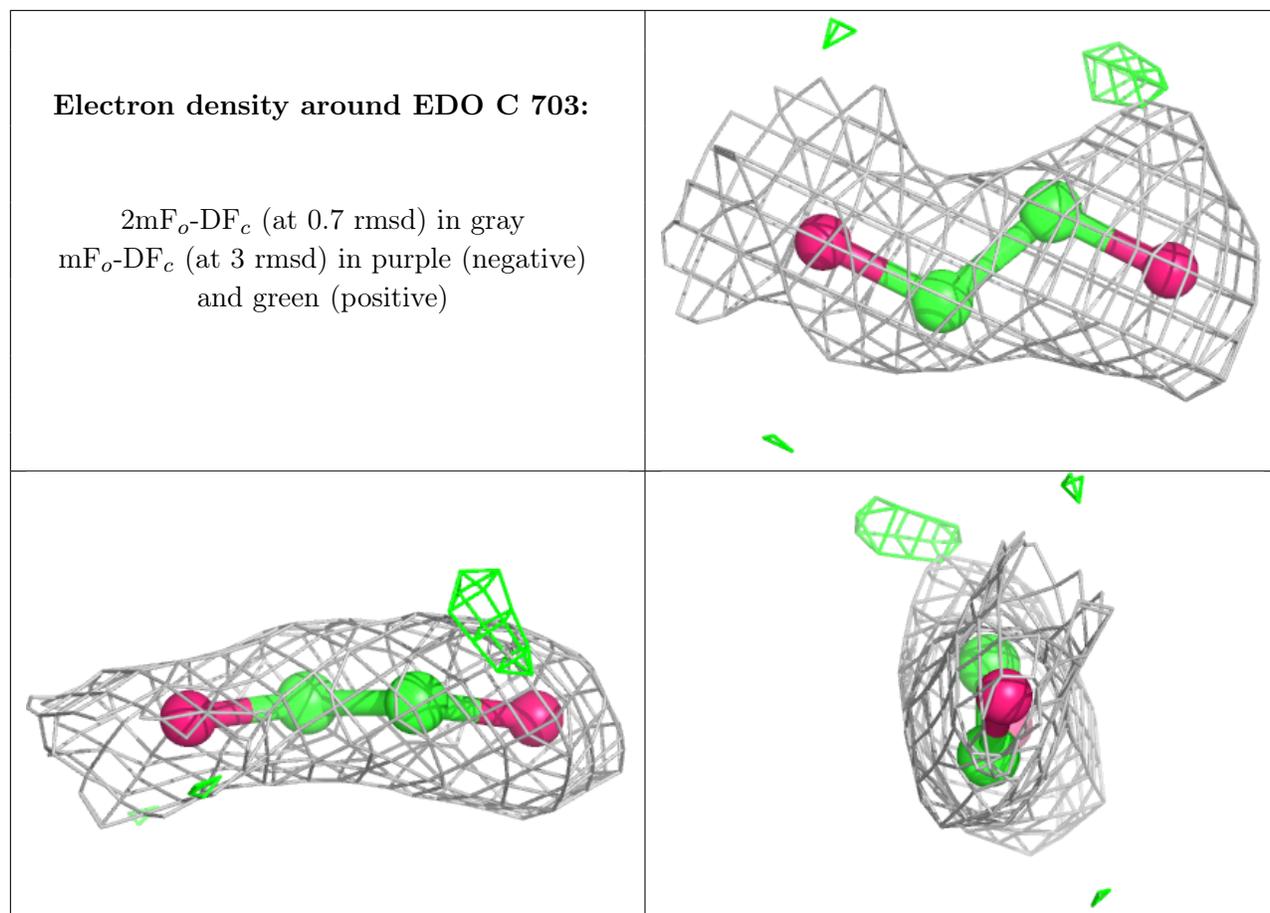
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CU C 702:**

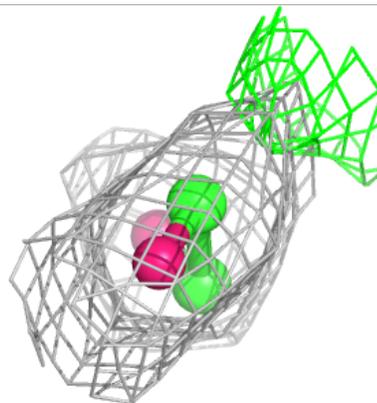
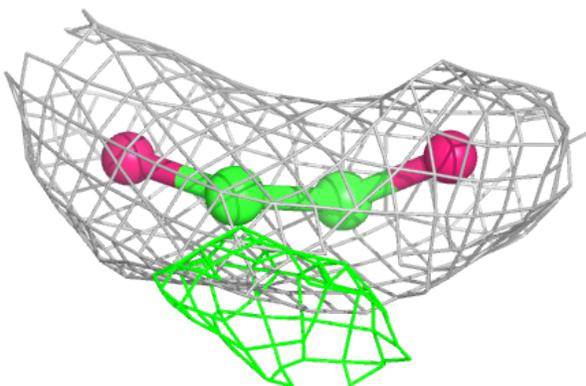
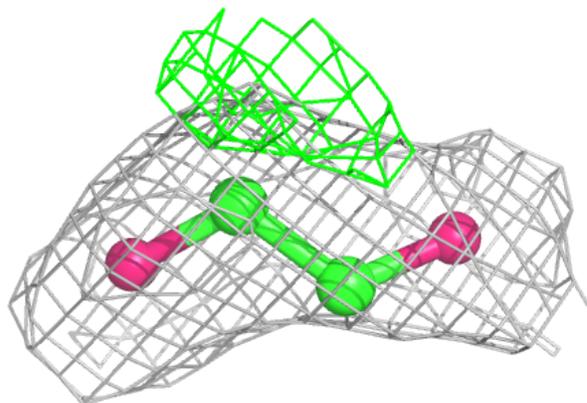
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





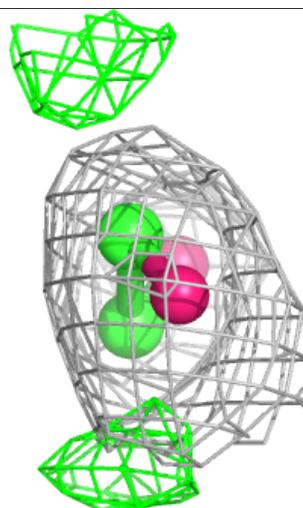
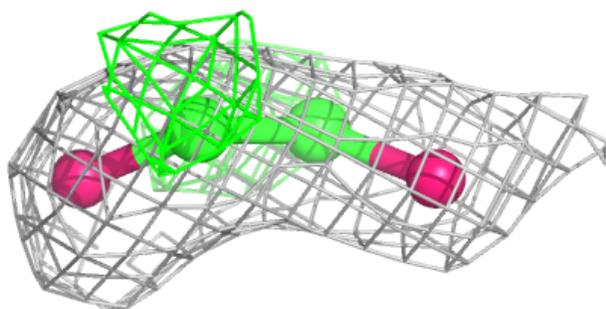
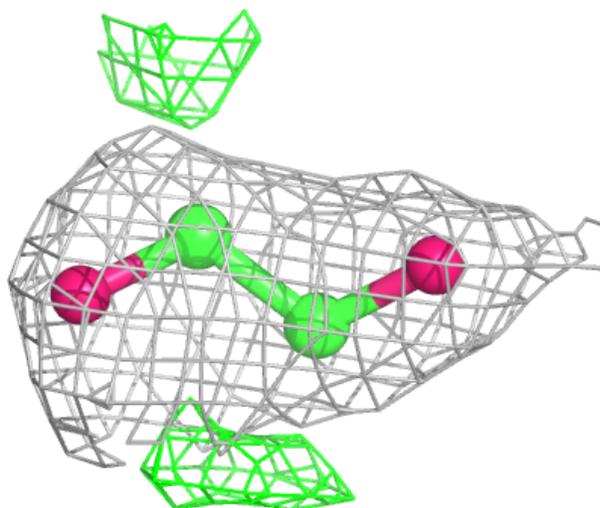
**Electron density around EDO D 705:**

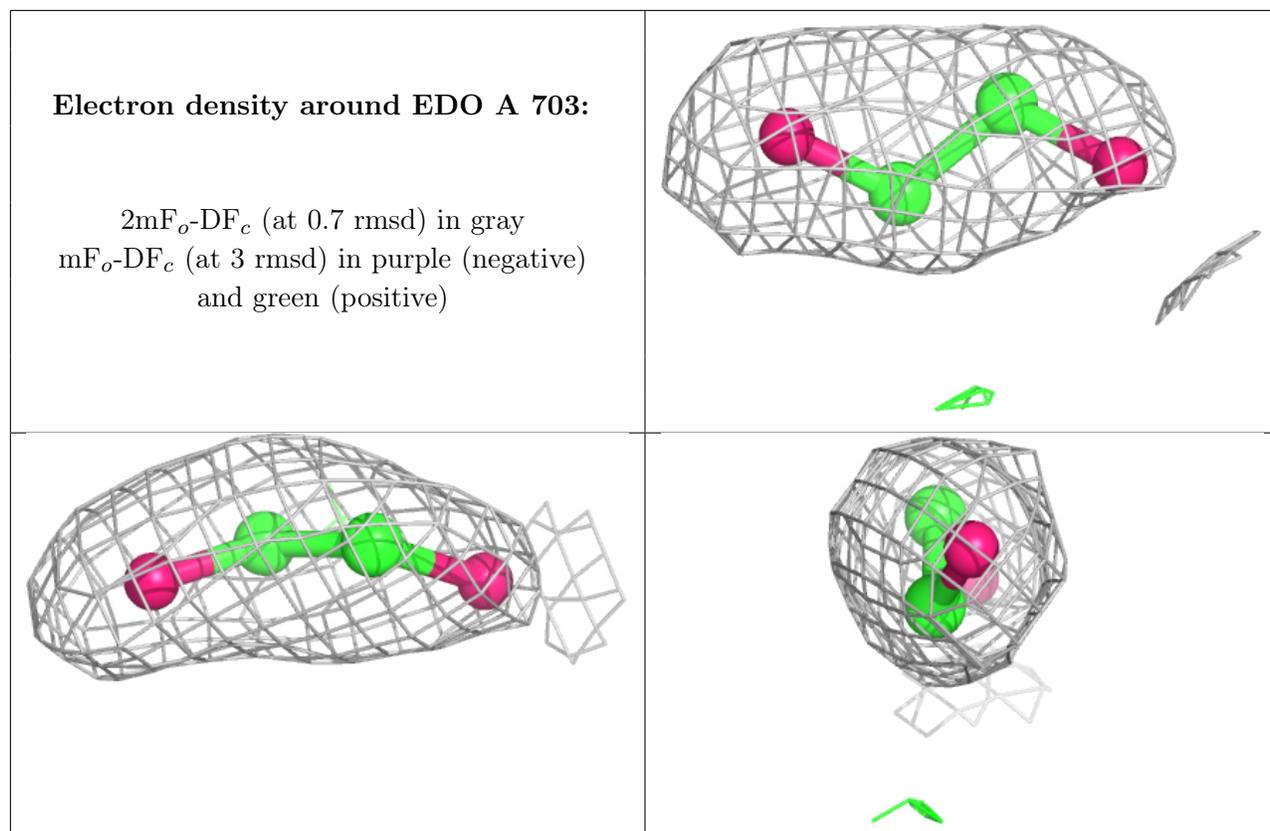
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around EDO C 706:**

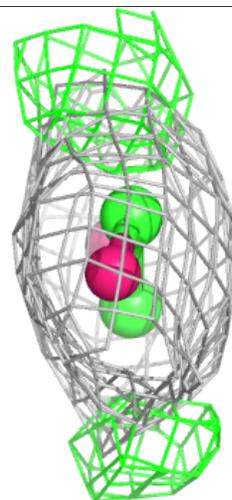
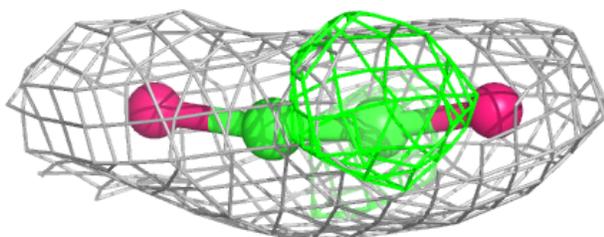
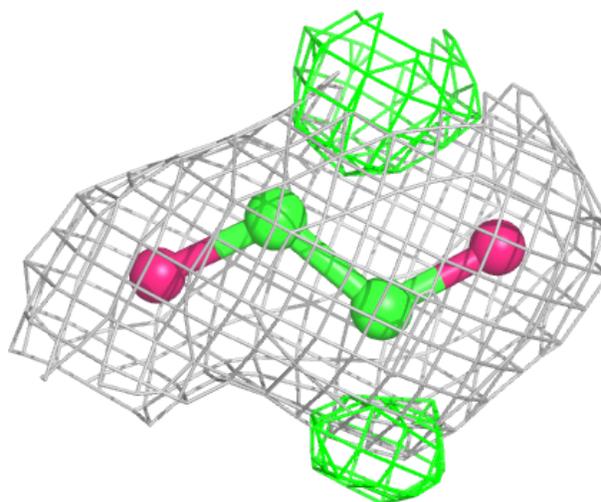
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





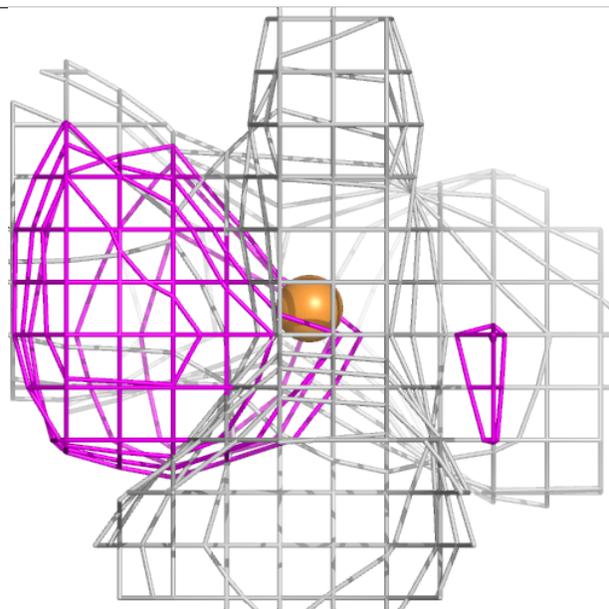
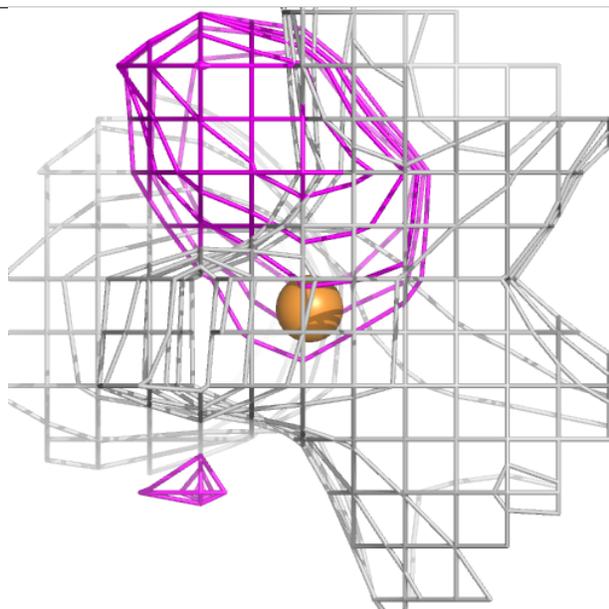
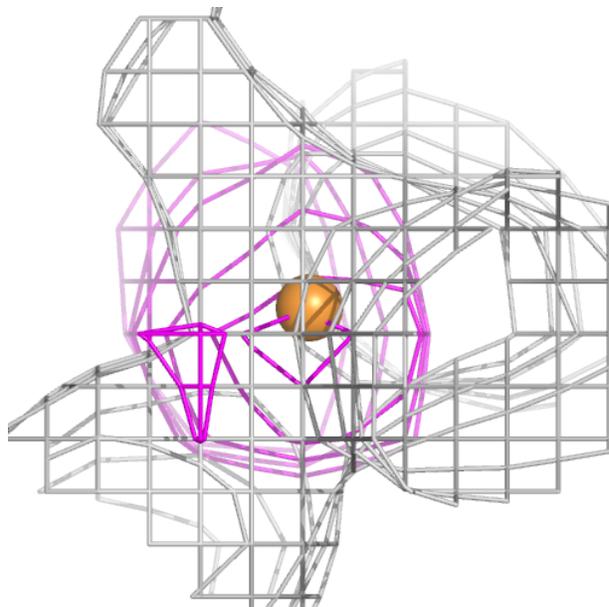
**Electron density around EDO A 709:**

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



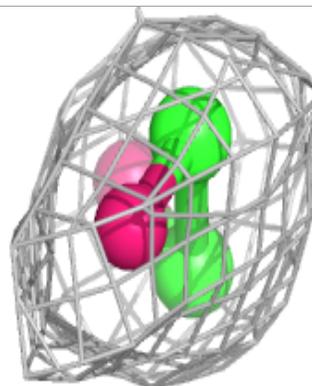
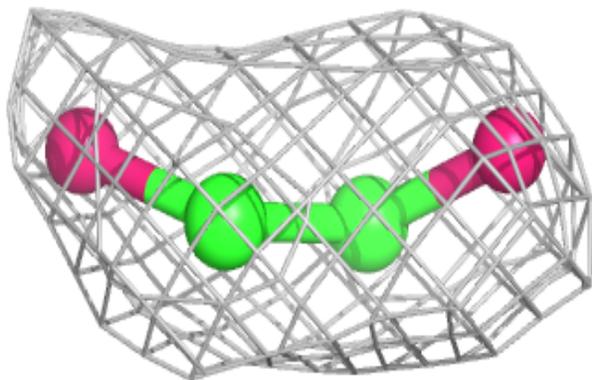
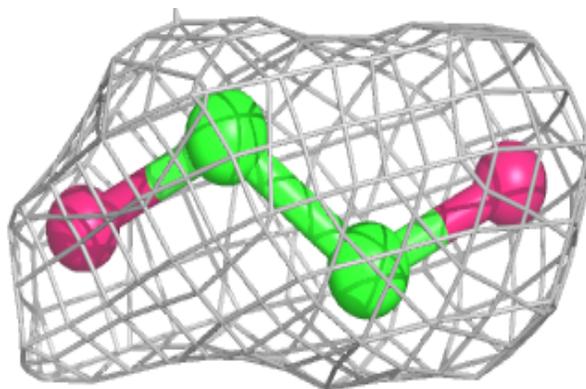
**Electron density around CU B 701:**

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



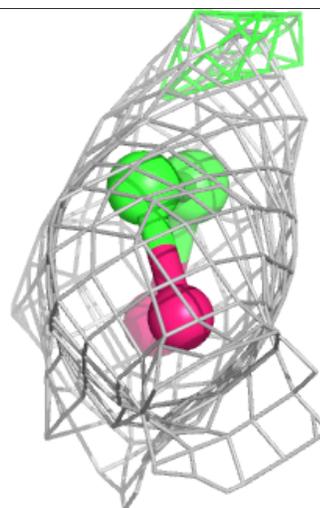
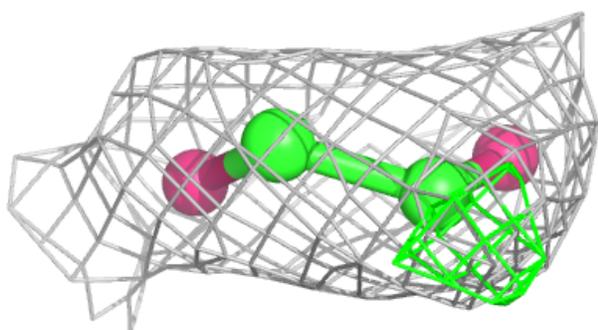
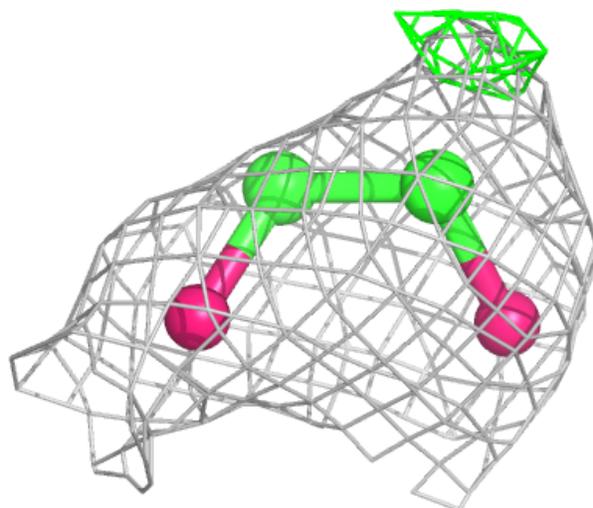
**Electron density around EDO D 706:**

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



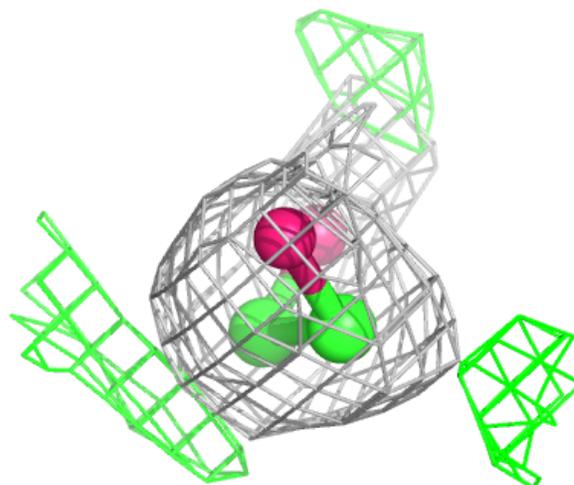
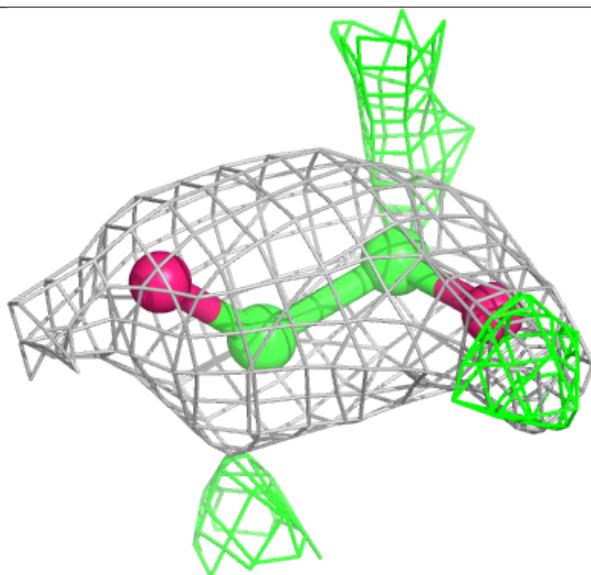
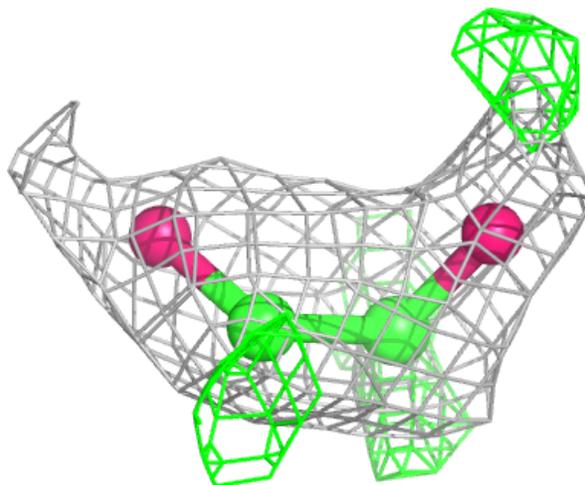
**Electron density around EDO A 707:**

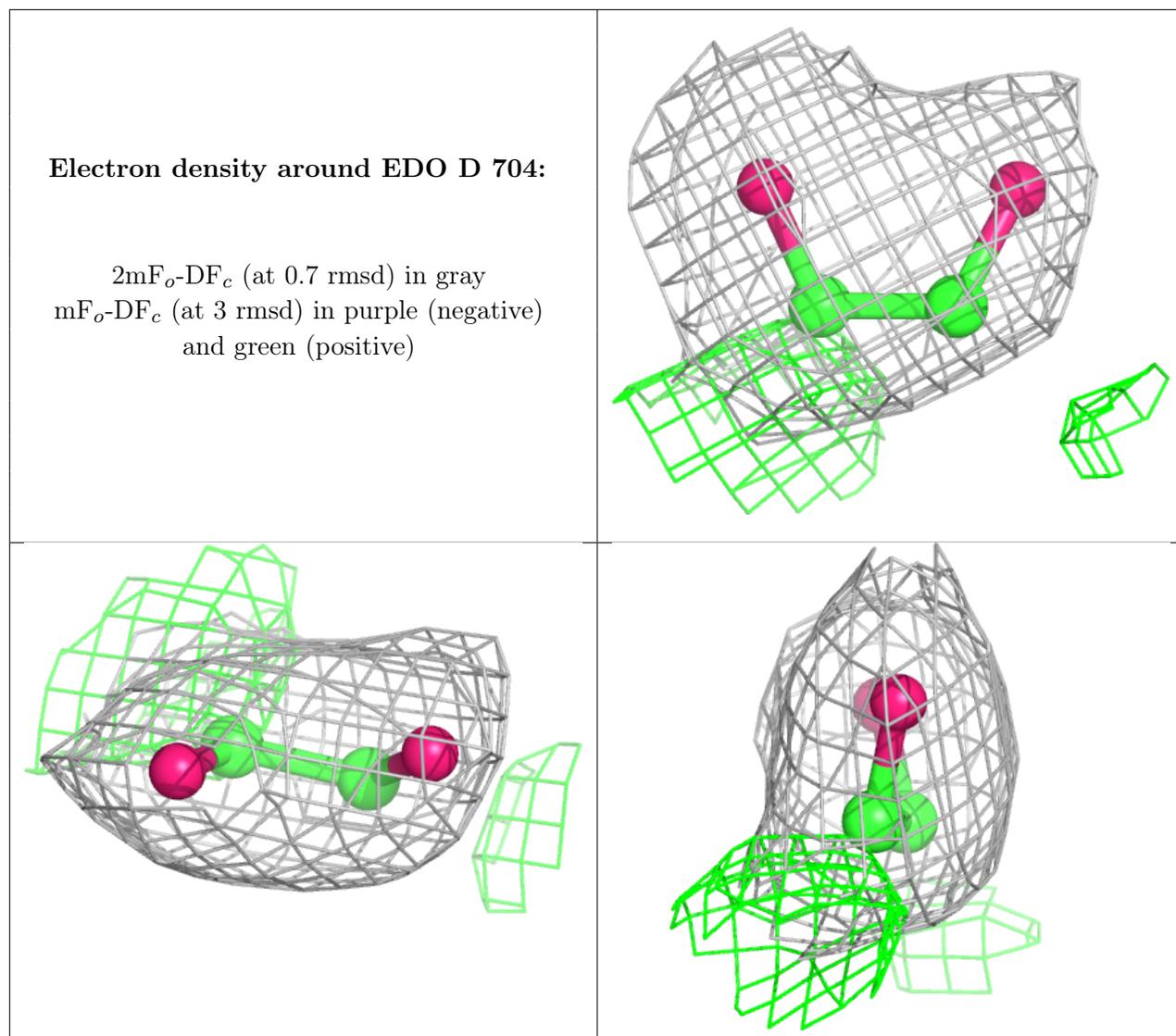
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

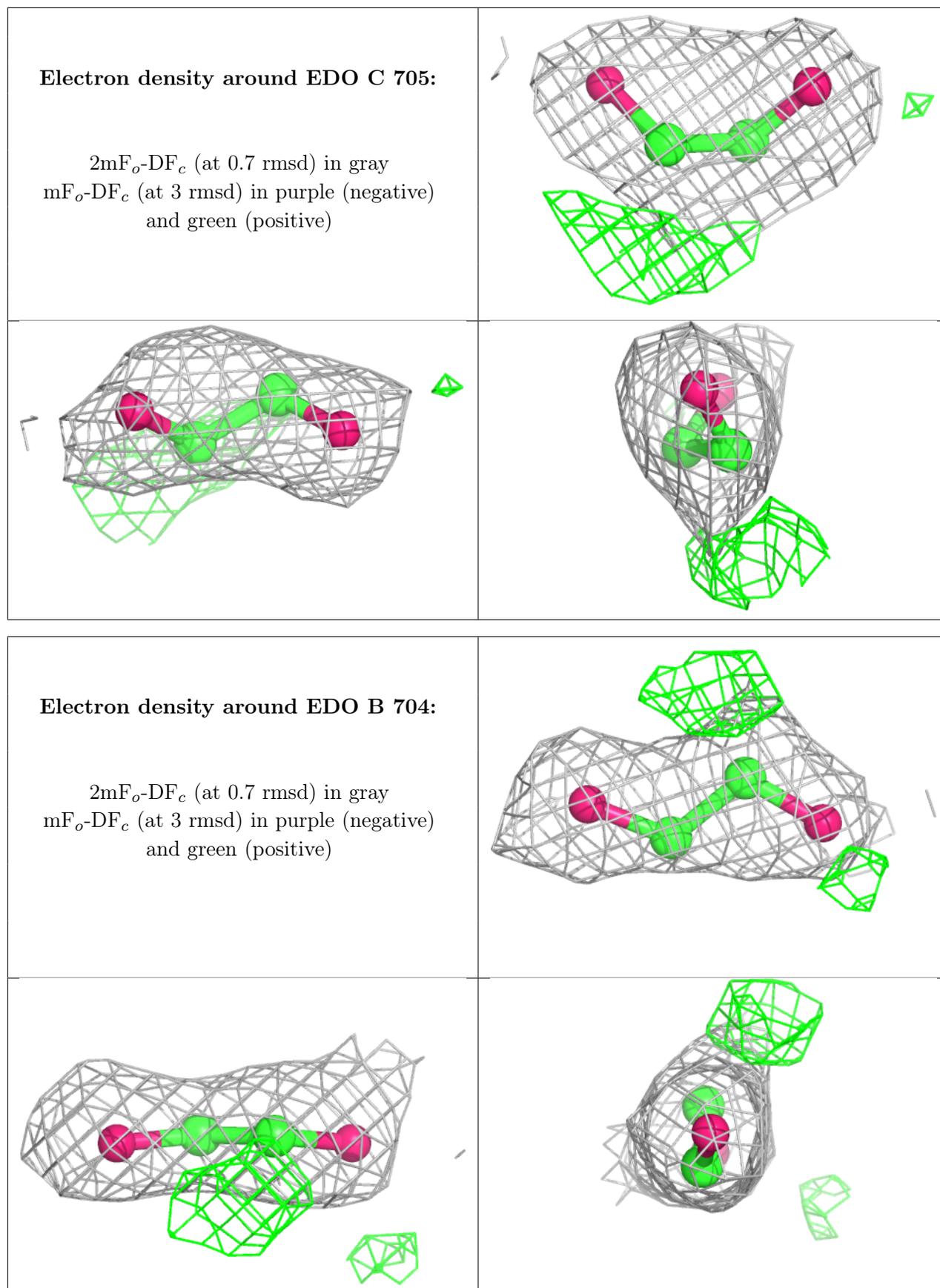


**Electron density around EDO A 706:**

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

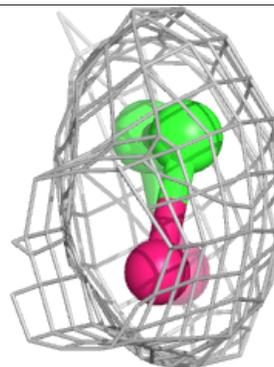
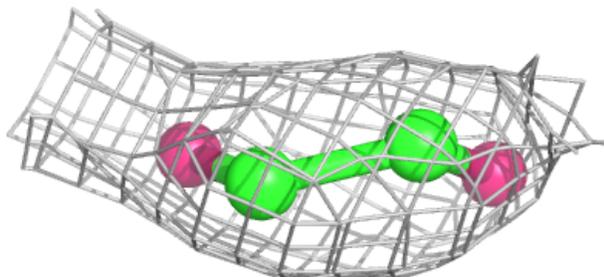
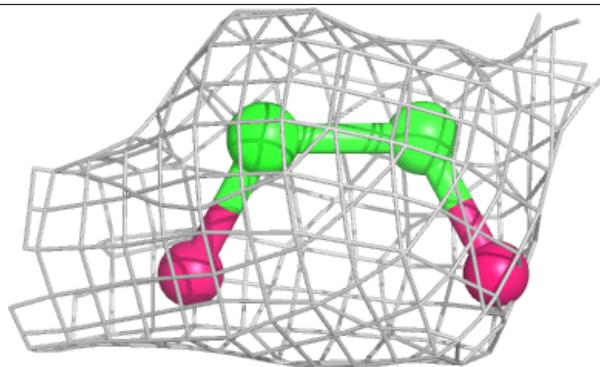


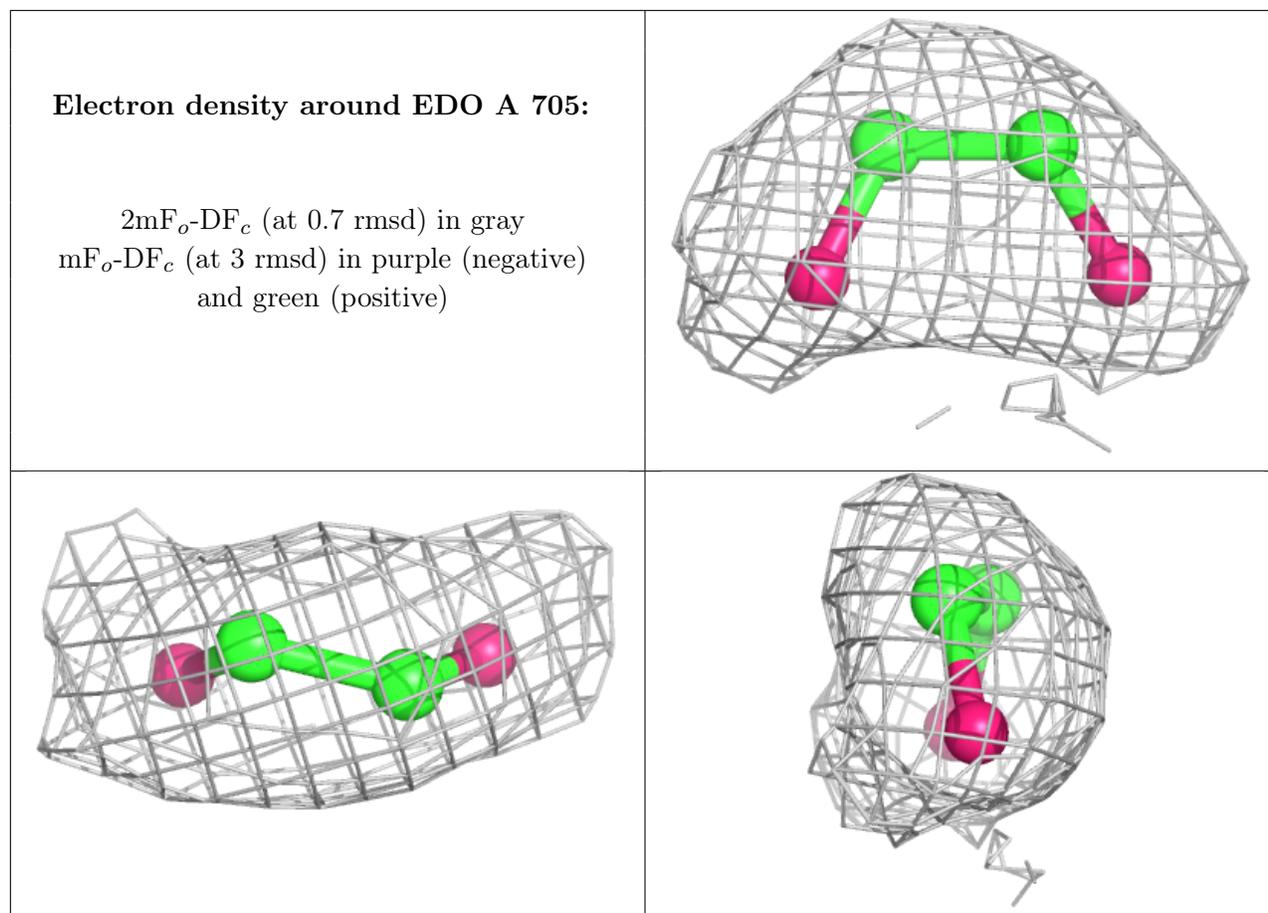


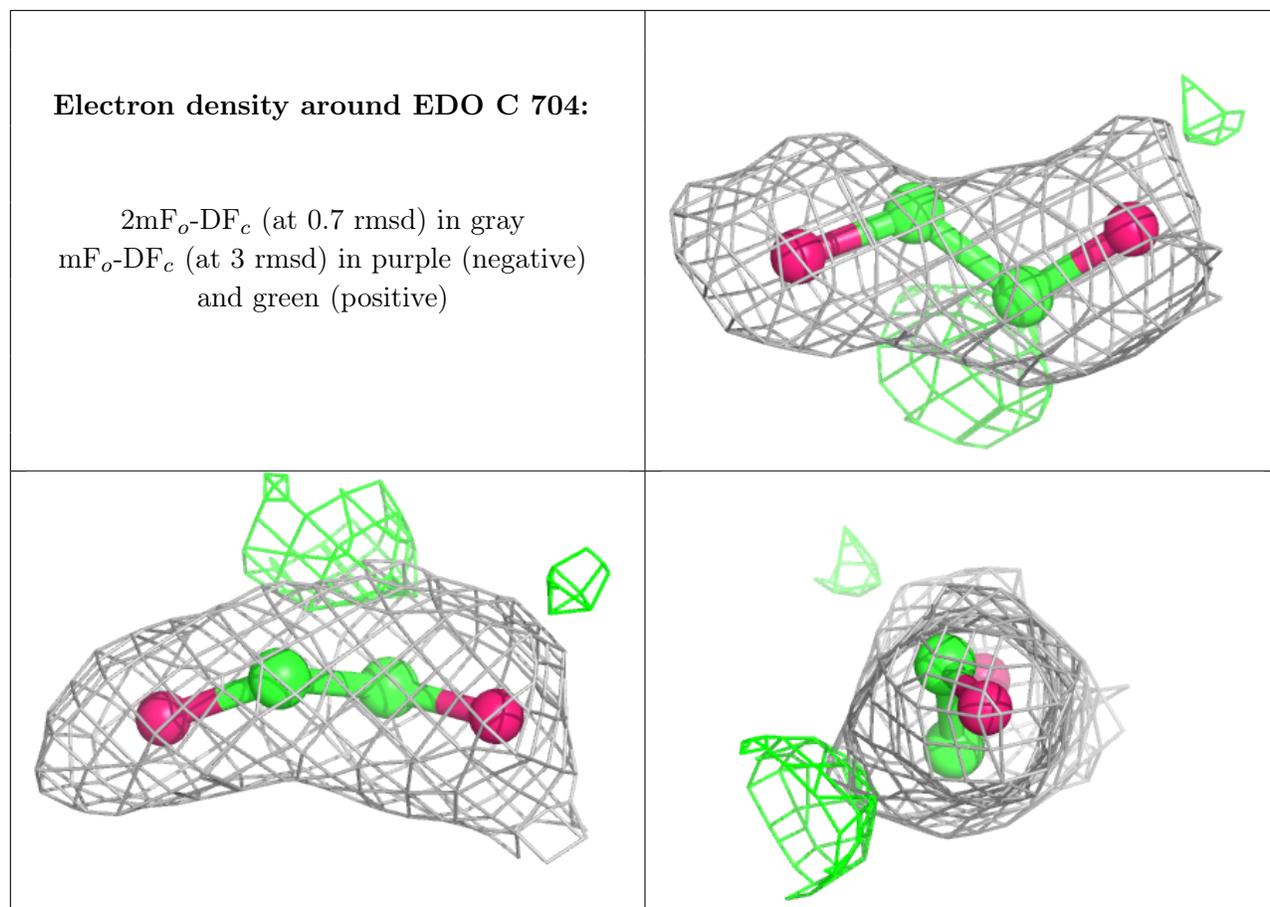


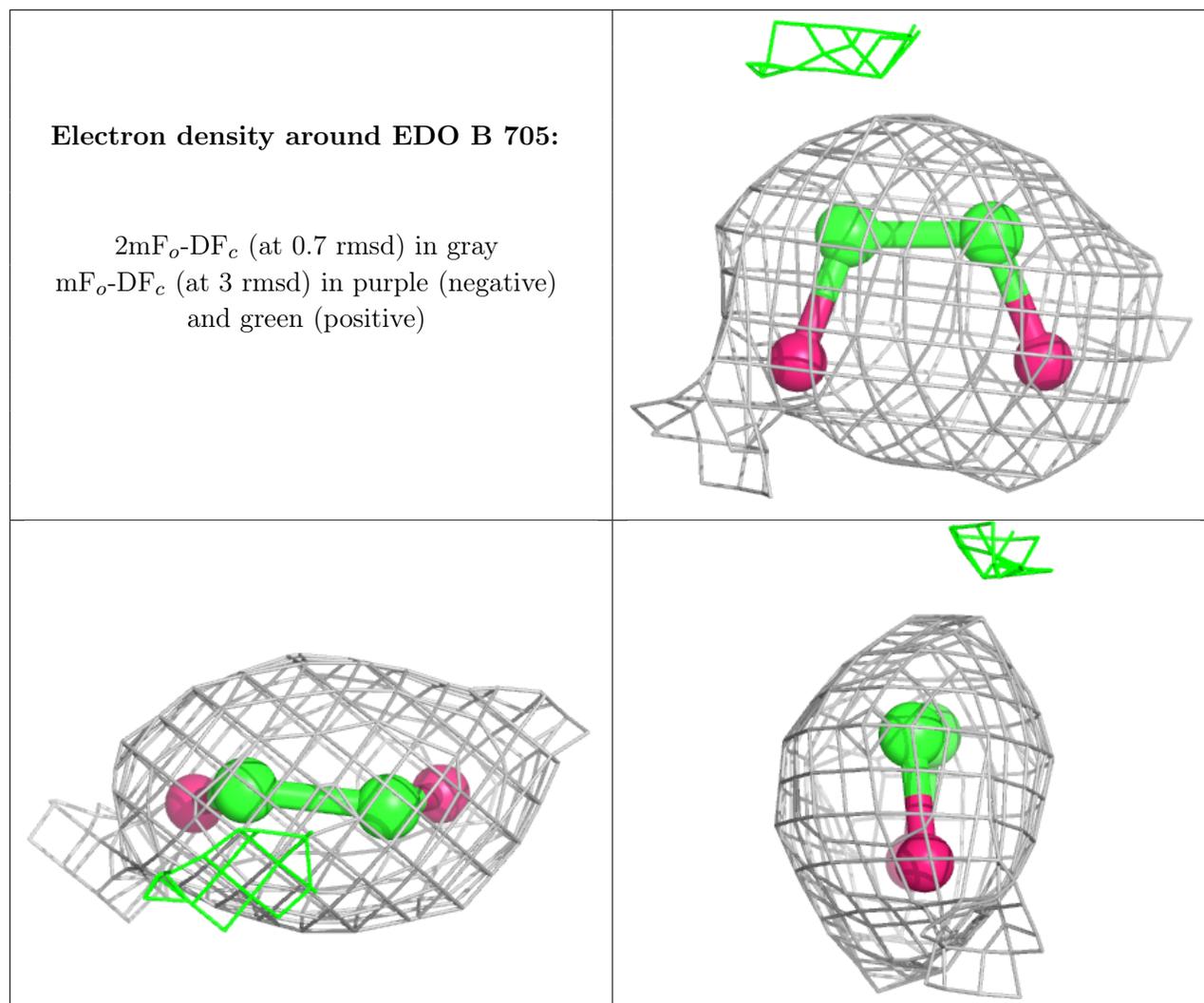
**Electron density around EDO A 708:**

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



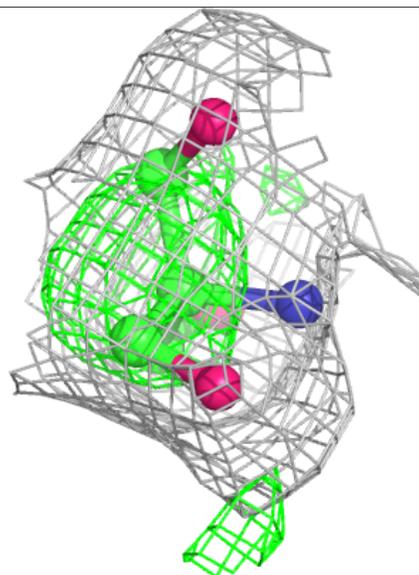
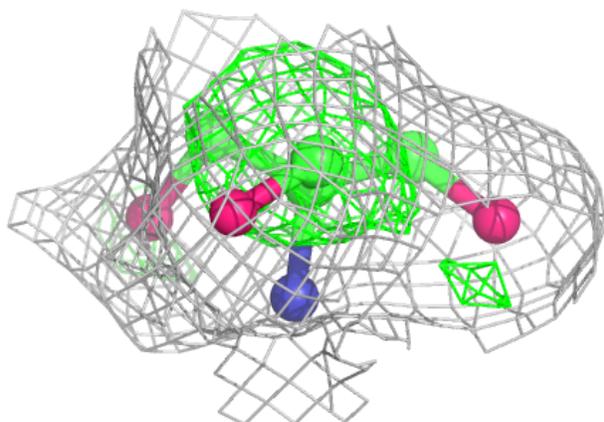
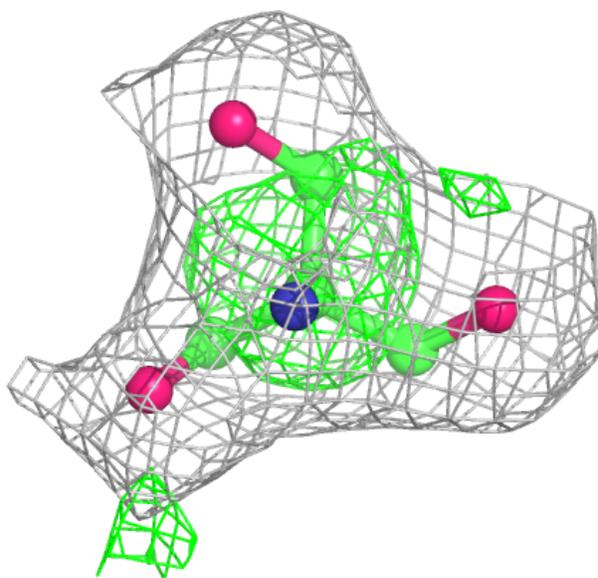






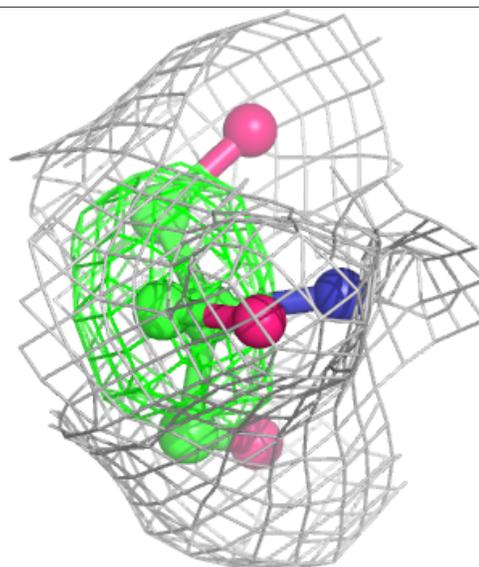
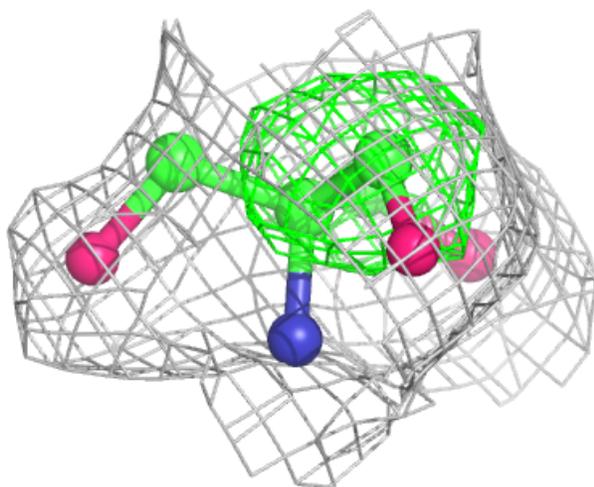
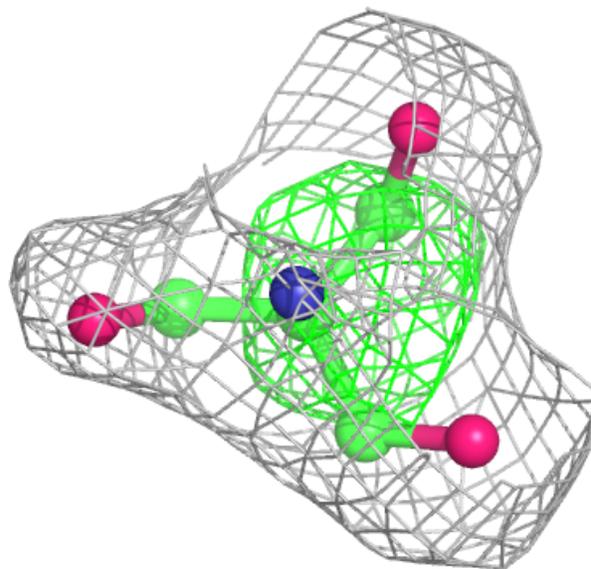
**Electron density around TRS A 710:**

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



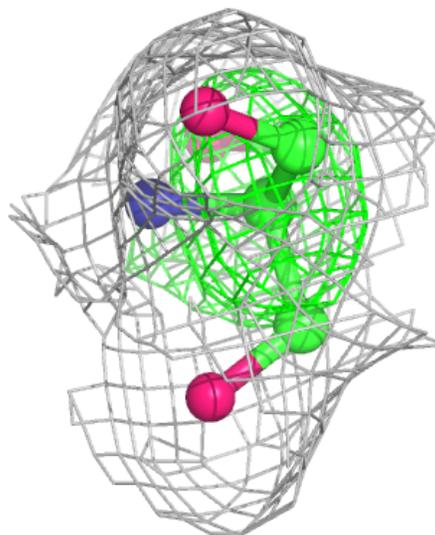
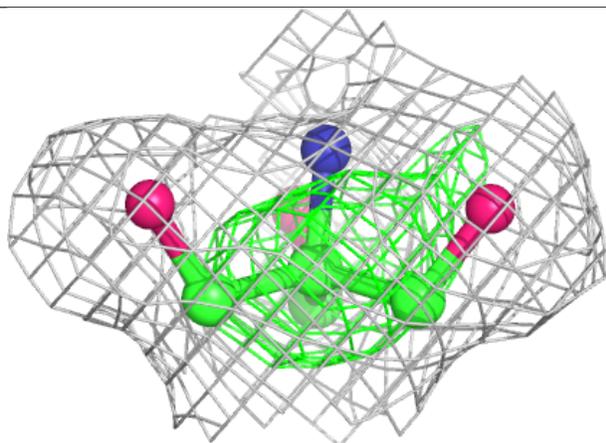
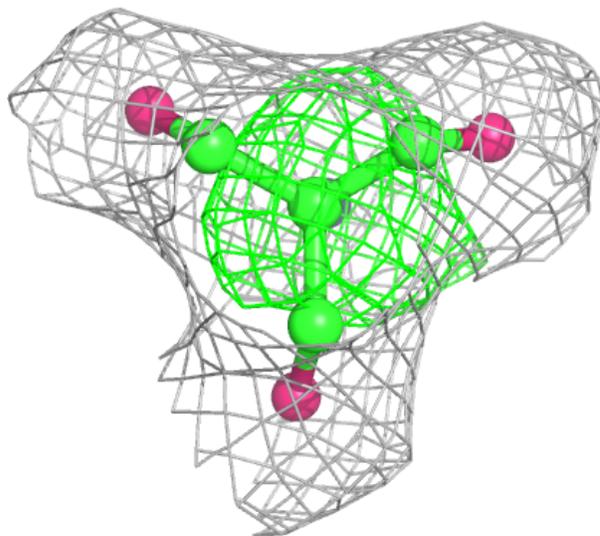
**Electron density around TRS B 706:**

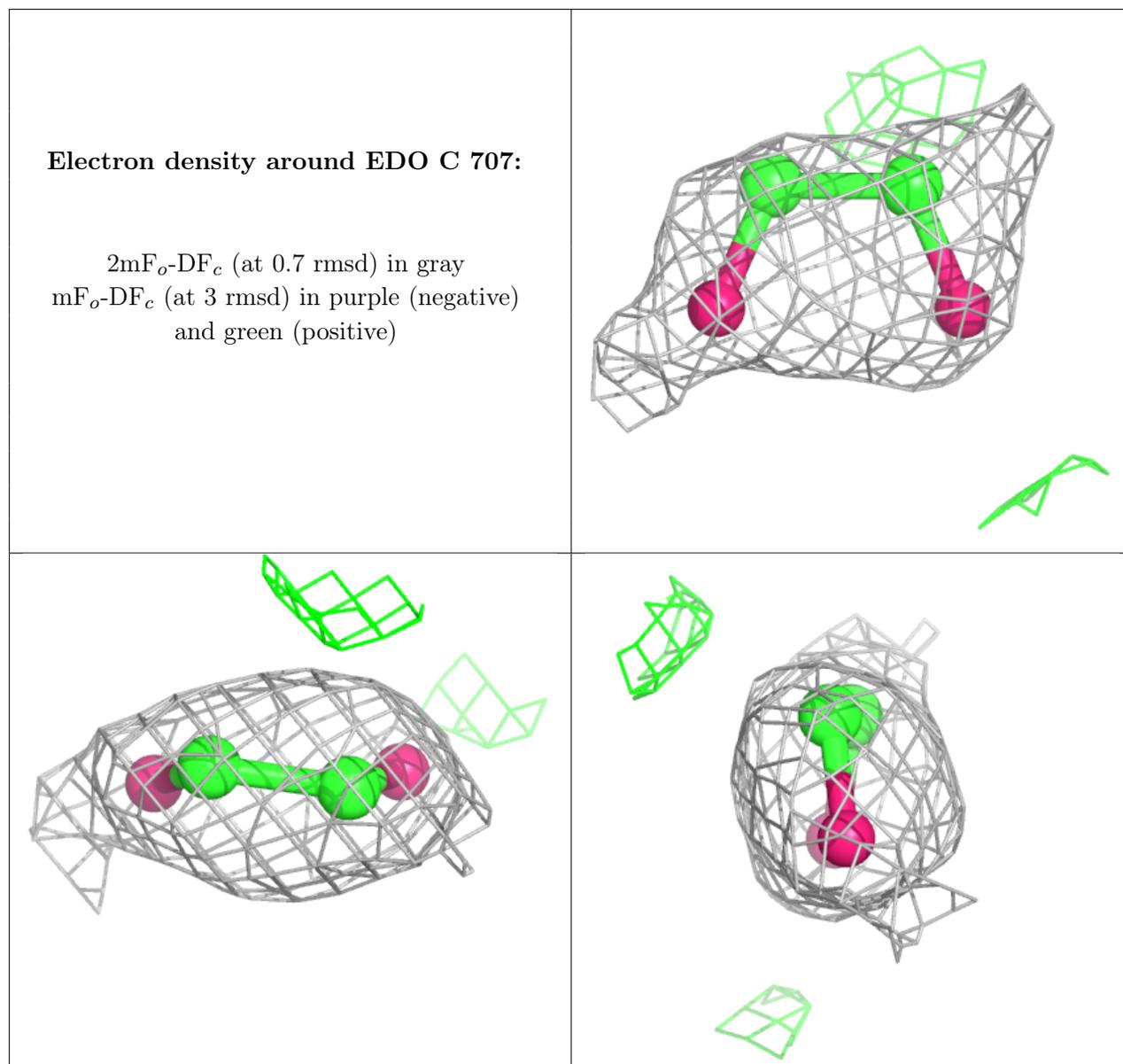
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around TRS C 708:**

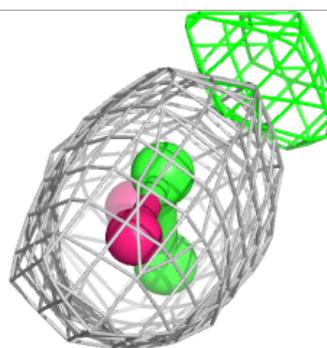
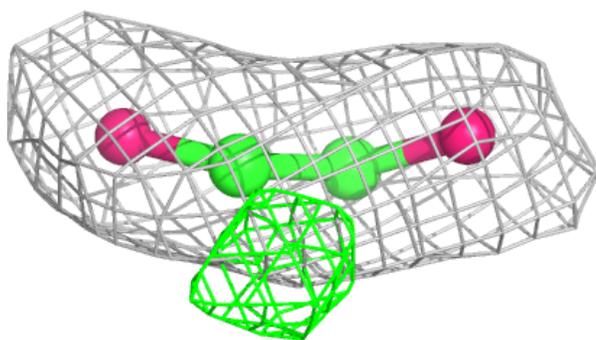
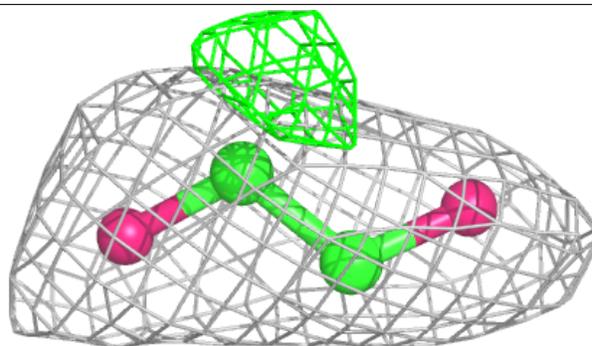
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



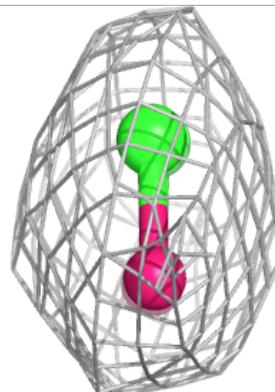
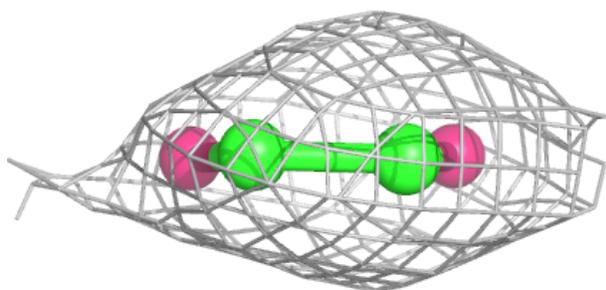
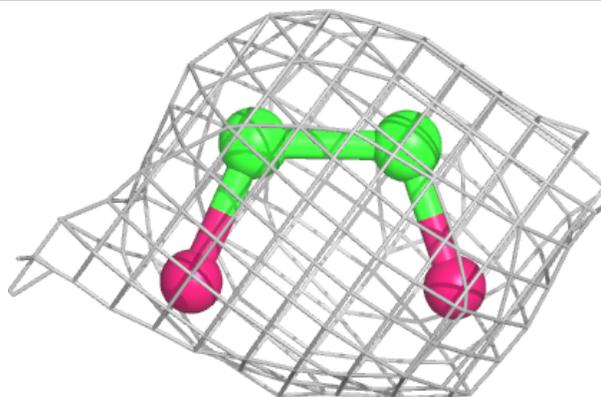


**Electron density around EDO B 703:**

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

**Electron density around EDO A 704:**

$2mF_o-DF_c$  (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.