



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2026 – 02:17 PM JST

PDB ID : 24HR / pdb_000024hr
Title : Human KRAS G12D (GDP-bound) in complex with macrocyclic peptide inhibitor AP6252
Authors : Yamano, T.; Chiyoda, A.; Fukami, T.A.; Tanada, M.; Irie, M.; Torizawa, T.
Deposited on : 2026-03-04
Resolution : 2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

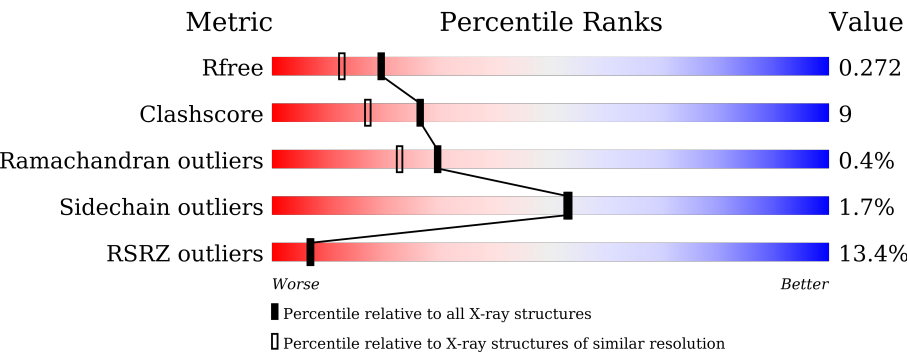
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.07 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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

Mol	Chain	Length	Quality of chain
1	A	179	<div><div>5%</div><div>84%</div><div>13%</div><div>..</div></div>
1	B	179	<div><div>2%</div><div>86%</div><div>9%</div><div>..</div></div>
1	C	179	<div><div>20%</div><div>67%</div><div>29%</div><div>..</div></div>
1	D	179	<div><div>25%</div><div>78%</div><div>18%</div><div>..</div></div>
2	I	12	<div><div>25%</div><div>58%</div><div>17%</div></div>
2	J	12	<div><div>17%</div><div>83%</div></div>

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Mol	Chain	Length	Quality of chain
2	K	12	
2	L	12	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FMT	B	210	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6254 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 Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1377	858	237	275	7			
1	B	174	Total	C	N	O	S	0	0	0
			1376	858	237	274	7			
1	C	173	Total	C	N	O	S	0	0	0
			1349	843	234	266	6			
1	D	172	Total	C	N	O	S	0	0	0
			1328	830	228	264	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P01116
A	-3	SER	-	expression tag	UNP P01116
A	-2	SER	-	expression tag	UNP P01116
A	-1	GLY	-	expression tag	UNP P01116
A	0	GLY	-	expression tag	UNP P01116
A	1	SER	-	expression tag	UNP P01116
A	12	ASP	GLY	engineered mutation	UNP P01116
B	-4	GLY	-	expression tag	UNP P01116
B	-3	SER	-	expression tag	UNP P01116
B	-2	SER	-	expression tag	UNP P01116
B	-1	GLY	-	expression tag	UNP P01116
B	0	GLY	-	expression tag	UNP P01116
B	1	SER	-	expression tag	UNP P01116
B	12	ASP	GLY	engineered mutation	UNP P01116
C	-4	GLY	-	expression tag	UNP P01116
C	-3	SER	-	expression tag	UNP P01116
C	-2	SER	-	expression tag	UNP P01116
C	-1	GLY	-	expression tag	UNP P01116
C	0	GLY	-	expression tag	UNP P01116
C	1	SER	-	expression tag	UNP P01116
C	12	ASP	GLY	engineered mutation	UNP P01116

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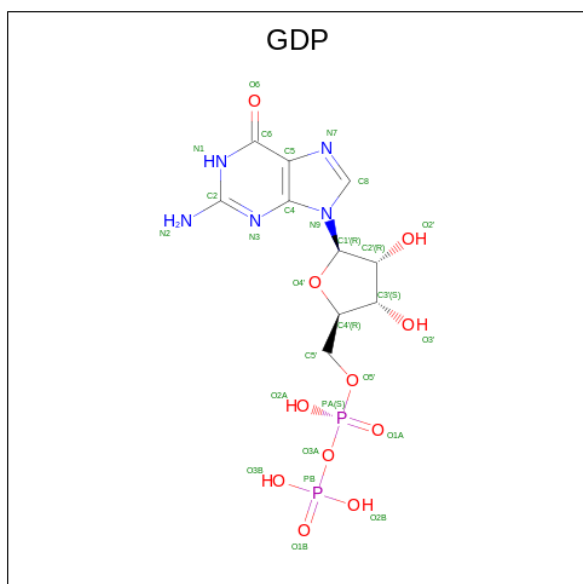
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	GLY	-	expression tag	UNP P01116
D	-3	SER	-	expression tag	UNP P01116
D	-2	SER	-	expression tag	UNP P01116
D	-1	GLY	-	expression tag	UNP P01116
D	0	GLY	-	expression tag	UNP P01116
D	1	SER	-	expression tag	UNP P01116
D	12	ASP	GLY	engineered mutation	UNP P01116

- Molecule 2 is a protein called AP6252.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	I	12	Total 100	C 71	Cl 1	F 4	N 12	O 12	0	0	0
2	J	12	Total 100	C 71	Cl 1	F 4	N 12	O 12	0	0	0
2	K	12	Total 100	C 71	Cl 1	F 4	N 12	O 12	0	0	0
2	L	12	Total 100	C 71	Cl 1	F 4	N 12	O 12	0	0	0

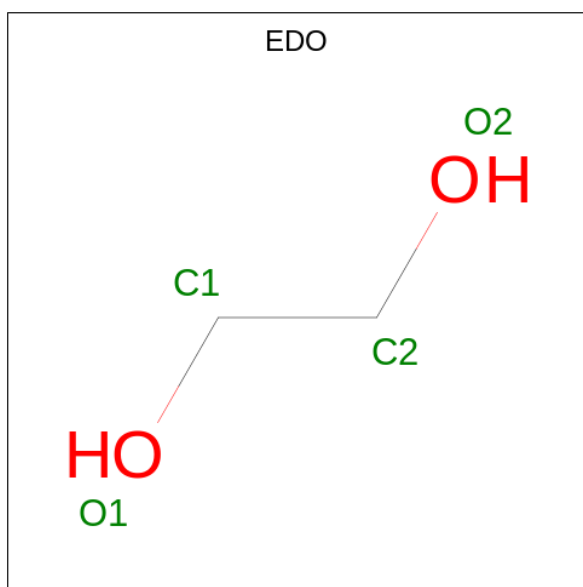
- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



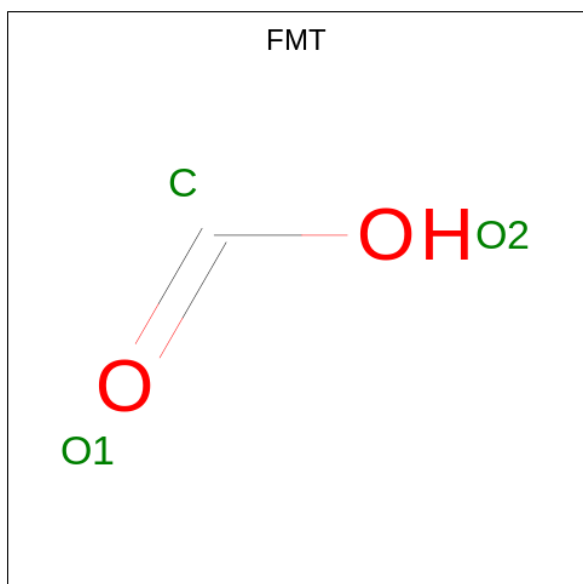
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

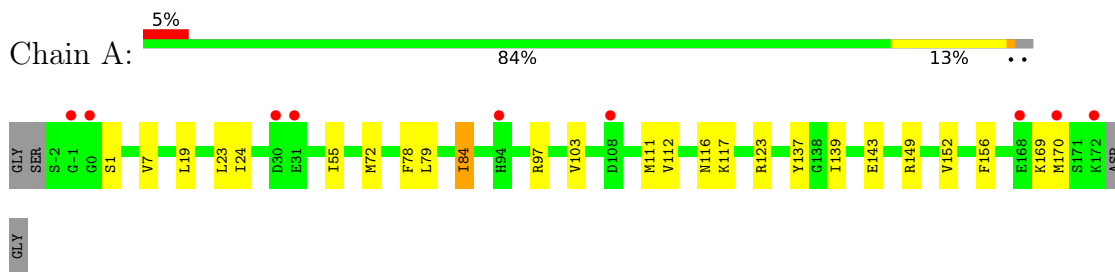
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	81	Total 81	O 81	0	0
7	B	57	Total 57	O 57	0	0
7	C	22	Total 22	O 22	0	0
7	D	26	Total 26	O 26	0	0
7	I	3	Total 3	O 3	0	0
7	J	1	Total 1	O 1	0	0

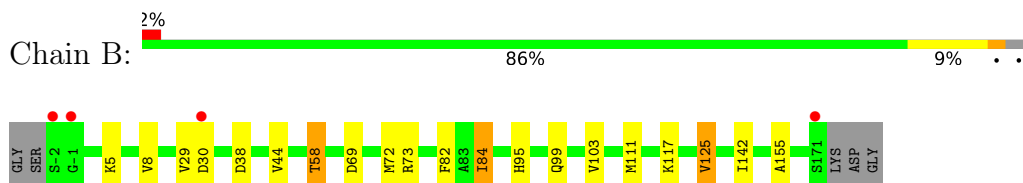
3 Residue-property plots [i](#)

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.

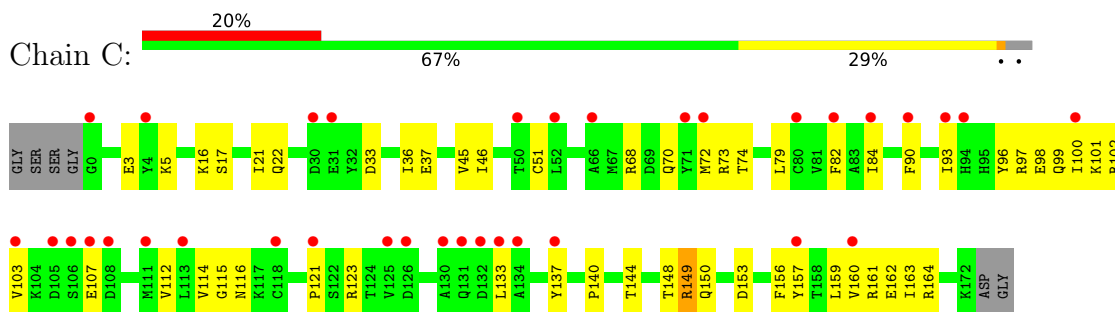
- Molecule 1: Isoform 2B of GTPase KRas



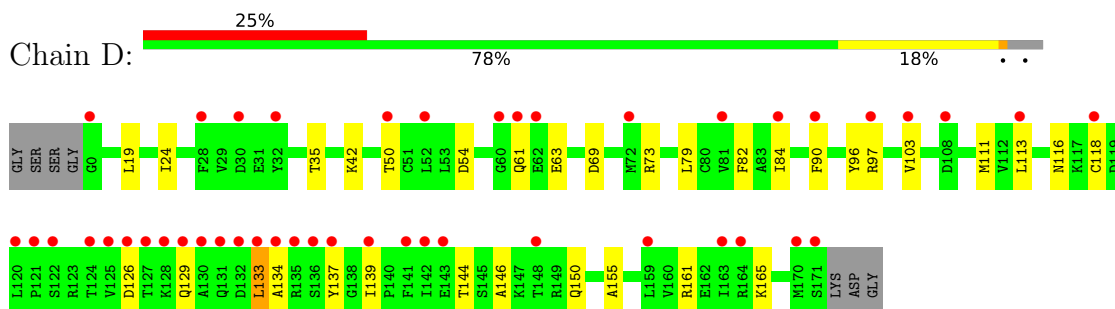
- Molecule 1: Isoform 2B of GTPase KRas



- Molecule 1: Isoform 2B of GTPase KRas



- Molecule 1: Isoform 2B of GTPase KRas



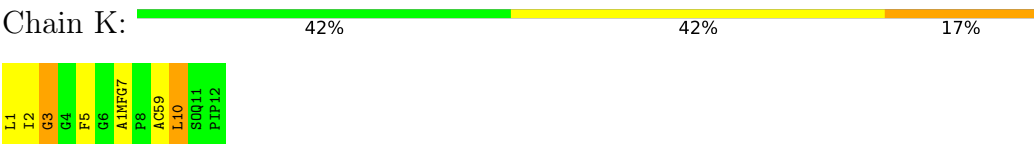
● Molecule 2: AP6252



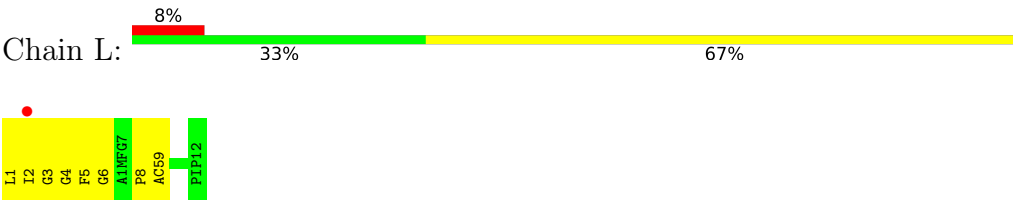
● Molecule 2: AP6252



● Molecule 2: AP6252



● Molecule 2: AP6252



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.48Å 111.48Å 201.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.07 – 2.07 62.07 – 2.07	Depositor EDS
% Data completeness (in resolution range)	59.7 (62.07-2.07) 55.5 (62.07-2.07)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.228 , 0.270 0.229 , 0.272	Depositor DCC
R_{free} test set	2305 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6254	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, SOQ, AC5, SAR, MG, MLE, FMT, GDP, 7T2, A1MFG, PIP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/1398	0.64	0/1886
1	B	0.42	0/1397	0.59	0/1883
1	C	0.35	0/1370	0.54	0/1852
1	D	0.35	0/1349	0.54	0/1828
2	I	0.29	0/14	1.50	0/16
2	J	0.44	0/14	1.34	0/16
2	K	0.32	0/14	1.01	0/16
2	L	0.25	0/14	0.88	0/16
All	All	0.39	0/5570	0.59	0/7513

There are no bond length outliers.

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	1377	0	1342	21	0
1	B	1376	0	1351	16	0
1	C	1349	0	1306	36	0
1	D	1328	0	1266	20	0
2	I	100	0	77	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	100	0	77	6	0
2	K	100	0	77	6	0
2	L	100	0	77	4	0
3	A	28	0	12	0	0
3	B	28	0	12	2	0
3	C	28	0	12	0	0
3	D	28	0	12	0	0
4	A	24	0	36	4	0
4	B	16	0	24	3	0
4	D	4	0	6	2	0
4	I	4	0	6	0	0
5	A	27	0	9	1	0
5	B	27	0	9	2	0
5	C	12	0	4	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
7	A	81	0	0	0	0
7	B	57	0	0	0	0
7	C	22	0	0	1	0
7	D	26	0	0	0	0
7	I	3	0	0	0	0
7	J	1	0	0	0	0
All	All	6254	0	5715	110	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 9.

All (110) 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:D:19:LEU:HD12	1:D:146:ALA:HB2	1.45	0.99
1:B:99:GLN:O	1:B:103:VAL:HG23	1.82	0.77
1:C:161:ARG:HA	1:C:164:ARG:HD2	1.68	0.76
5:A:212:FMT:H	1:C:45:VAL:HG12	1.69	0.73
1:A:72:MET:HE2	2:I:12:PIP:H41	1.73	0.71
1:C:22:GLN:CD	1:C:149:ARG:HG2	2.19	0.68
1:C:3:GLU:HB3	1:C:5:LYS:HE2	1.77	0.66
1:A:143:GLU:H	4:A:211:EDO:H21	1.60	0.65
1:D:126:ASP:HB2	1:D:129:GLN:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:MLE:HN3	2:I:2:ILE:HG13	1.80	0.63
1:C:101:LYS:HD2	1:C:107:GLU:HA	1.79	0.63
1:B:8:VAL:O	1:B:58:THR:HB	1.99	0.63
1:B:72:MET:HE3	1:B:103:VAL:HG12	1.82	0.61
1:A:84:ILE:HG23	1:A:123:ARG:HB2	1.84	0.59
1:A:149:ARG:NH2	4:A:203:EDO:H12	2.16	0.59
2:K:1:MLE:HN3	2:K:2:ILE:HG13	1.86	0.58
1:A:97:ARG:HD2	1:A:111:MET:HE1	1.86	0.57
1:C:96:TYR:O	1:C:100:ILE:HD13	2.03	0.57
1:C:84:ILE:HG23	1:C:123:ARG:HB2	1.87	0.56
1:D:61:GLN:HB3	1:D:63:GLU:HG3	1.85	0.56
1:C:82:PHE:HB3	1:C:93:ILE:HD11	1.86	0.56
1:A:23:LEU:HD22	1:A:156:PHE:CG	2.41	0.56
1:D:90:PHE:CE1	1:D:133:LEU:HD12	2.43	0.54
1:B:38:ASP:OD2	4:B:206:EDO:H22	2.08	0.54
1:B:142:ILE:HD12	1:B:155:ALA:HA	1.89	0.54
1:C:22:GLN:OE1	1:C:149:ARG:HG2	2.08	0.53
1:C:84:ILE:HD13	1:C:115:GLY:C	2.34	0.53
1:C:159:LEU:O	1:C:163:ILE:HG13	2.09	0.53
1:D:103:VAL:HG12	2:L:2:ILE:HD12	1.90	0.53
1:B:95:HIS:CD2	2:J:4:SAR:HA2	2.44	0.52
1:C:112:VAL:HG23	1:C:159:LEU:HD13	1.91	0.52
1:D:69:ASP:O	1:D:73:ARG:HG3	2.09	0.52
1:A:23:LEU:HD22	1:A:156:PHE:CD2	2.44	0.52
1:D:97:ARG:HD3	1:D:137:TYR:CE2	2.46	0.51
1:C:70:GLN:HG2	1:C:73:ARG:HH12	1.76	0.50
1:D:97:ARG:HD3	1:D:137:TYR:CD2	2.47	0.50
1:D:19:LEU:HD11	1:D:116:ASN:OD1	2.11	0.50
1:C:79:LEU:HD23	1:C:112:VAL:HB	1.92	0.50
1:C:90:PHE:CZ	1:C:133:LEU:HD12	2.46	0.49
1:B:44:VAL:HG12	4:B:202:EDO:H22	1.93	0.49
1:A:7:VAL:HB	1:A:78:PHE:CD2	2.48	0.49
4:A:202:EDO:H22	2:I:8:PRO:HD3	1.94	0.49
1:C:33:ASP:HB3	1:C:36:ILE:HG13	1.94	0.49
1:A:111:MET:HE2	1:A:139:ILE:HD13	1.94	0.49
4:B:206:EDO:H11	7:C:1014:HOH:O	2.13	0.49
1:A:24:ILE:HD11	1:A:55:ILE:HD12	1.95	0.48
1:B:69:ASP:O	1:B:73:ARG:HG3	2.13	0.48
1:D:19:LEU:CD1	1:D:146:ALA:HB2	2.32	0.48
1:D:84:ILE:HD13	1:D:118:CYS:HA	1.94	0.48
1:C:84:ILE:HD11	1:C:115:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:THR:HG21	1:D:155:ALA:HB2	1.97	0.47
1:C:99:GLN:O	1:C:103:VAL:HG22	2.15	0.47
1:B:5:LYS:HD3	5:B:210:FMT:O1	2.15	0.46
1:D:134:ALA:HB1	1:D:139:ILE:O	2.15	0.46
2:K:9:AC5:N	2:K:10:MLE:HN1	2.30	0.46
1:A:19:LEU:HD23	1:A:152:VAL:HG22	1.97	0.46
1:B:117:LYS:HG2	3:B:201:GDP:C6	2.51	0.46
1:C:153:ASP:HB3	1:C:157:TYR:CE2	2.50	0.46
1:D:35:THR:HG22	1:D:61:GLN:OE1	2.16	0.45
2:J:2:ILE:HA	2:J:3:SAR:HN1	1.59	0.45
1:D:97:ARG:HG3	1:D:111:MET:HE1	1.98	0.45
1:A:79:LEU:HD23	1:A:112:VAL:HB	1.99	0.45
1:A:169:LYS:HG3	1:A:170:MET:HE2	1.99	0.45
2:L:2:ILE:HA	2:L:3:SAR:HN1	1.59	0.45
1:C:140:PRO:HD3	1:C:162:GLU:OE2	2.18	0.44
2:J:1:MLE:HD22	2:J:1:MLE:HA	1.85	0.44
4:A:202:EDO:H22	2:I:8:PRO:CD	2.48	0.44
1:C:72:MET:HE3	1:C:73:ARG:HG3	1.98	0.44
1:C:97:ARG:HD3	1:C:137:TYR:CE2	2.52	0.44
2:J:10:MLE:C	2:J:12:PIP:H61	2.48	0.44
2:J:10:MLE:HA	2:J:10:MLE:HD23	1.86	0.44
1:C:116:ASN:HA	1:C:144:THR:O	2.18	0.43
1:C:156:PHE:O	1:C:160:VAL:HG23	2.18	0.43
2:K:2:ILE:HA	2:K:3:SAR:HN1	1.63	0.43
2:L:1:MLE:HN3	2:L:2:ILE:HG13	2.00	0.43
2:I:2:ILE:HA	2:I:3:SAR:HN1	1.41	0.43
1:A:84:ILE:HG23	1:A:123:ARG:CB	2.48	0.43
1:B:82:PHE:HE1	1:B:84:ILE:HD12	1.83	0.43
1:B:5:LYS:NZ	5:B:210:FMT:H	2.33	0.43
1:D:24:ILE:O	1:D:42:LYS:HE2	2.18	0.43
1:C:46:ILE:HG12	1:C:157:TYR:CE1	2.53	0.43
2:I:1:MLE:HD22	2:I:5:7T2:CL	2.56	0.43
1:D:96:TYR:OH	4:D:202:EDO:H12	2.18	0.43
1:C:37:GLU:OE2	1:C:68:ARG:HB2	2.19	0.43
1:A:72:MET:SD	1:A:103:VAL:HB	2.58	0.42
1:B:30:ASP:HA	3:B:201:GDP:O2'	2.19	0.42
1:B:111:MET:HE3	1:B:111:MET:HB2	1.73	0.42
4:D:202:EDO:H11	2:L:8:PRO:HD3	2.01	0.42
1:C:46:ILE:HD12	1:C:51:CYS:SG	2.59	0.42
1:A:97:ARG:HH11	1:A:111:MET:CE	2.33	0.42
1:C:150:GLN:HB2	1:D:150:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:VAL:HG11	2:K:10:MLE:HD11	2.01	0.41
1:C:148:THR:C	1:C:150:GLN:H	2.28	0.41
1:D:82:PHE:CD2	1:D:113:LEU:HD11	2.55	0.41
1:A:116:ASN:O	1:A:117:LYS:HB2	2.19	0.41
1:C:16:LYS:HB2	1:C:16:LYS:HE2	1.88	0.41
1:C:17:SER:O	1:C:21:ILE:HG12	2.20	0.41
1:A:137:TYR:HB2	1:A:139:ILE:HG12	2.02	0.41
1:C:98:GLU:O	1:C:102:ARG:HG2	2.21	0.41
1:C:103:VAL:HG12	2:K:2:ILE:HD12	2.02	0.41
1:C:33:ASP:HB3	1:C:36:ILE:CD1	2.51	0.41
1:A:169:LYS:HG3	1:A:170:MET:N	2.37	0.40
1:B:84:ILE:O	1:B:125:VAL:HG23	2.20	0.40
2:J:11:SOQ:N	2:J:12:PIP:H61	2.35	0.40
1:C:99:GLN:NE2	2:K:10:MLE:HD12	2.37	0.40
1:D:161:ARG:O	1:D:165:LYS:HG3	2.22	0.40
2:I:9:AC5:N	2:I:10:MLE:HN1	2.36	0.40
1:A:84:ILE:HA	1:A:84:ILE:HD12	1.80	0.40
1:A:169:LYS:CG	1:A:170:MET:HE2	2.51	0.40
1:B:29:VAL:O	1:B:29:VAL:HG23	2.22	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	173/179 (97%)	166 (96%)	6 (4%)	1 (1%)	21	13
1	B	172/179 (96%)	165 (96%)	7 (4%)	0	100	100
1	C	171/179 (96%)	164 (96%)	5 (3%)	2 (1%)	10	4
1	D	170/179 (95%)	162 (95%)	8 (5%)	0	100	100
2	I	2/12 (17%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	2/12 (17%)	2 (100%)	0	0	100	100
2	K	2/12 (17%)	2 (100%)	0	0	100	100
2	L	2/12 (17%)	2 (100%)	0	0	100	100
All	All	694/764 (91%)	665 (96%)	26 (4%)	3 (0%)	30	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	121	PRO
1	C	149	ARG
1	A	1	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	151/156 (97%)	150 (99%)	1 (1%)	76	79
1	B	152/156 (97%)	149 (98%)	3 (2%)	48	47
1	C	145/156 (93%)	143 (99%)	2 (1%)	59	60
1	D	141/156 (90%)	137 (97%)	4 (3%)	38	34
2	I	2/2 (100%)	2 (100%)	0	100	100
2	J	2/2 (100%)	2 (100%)	0	100	100
2	K	2/2 (100%)	2 (100%)	0	100	100
2	L	2/2 (100%)	2 (100%)	0	100	100
All	All	597/632 (94%)	587 (98%)	10 (2%)	53	53

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ILE
1	B	58	THR
1	B	84	ILE

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Mol	Chain	Res	Type
1	B	125	VAL
1	C	74	THR
1	C	114	VAL
1	D	50	THR
1	D	54	ASP
1	D	79	LEU
1	D	133	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	95	HIS
1	A	129	GLN
1	B	25	GLN
1	B	61	GLN
1	B	95	HIS
1	B	166	HIS
1	C	150	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

32 non-standard protein/DNA/RNA residues 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	MLE	J	1	2	7,8,9	0.59	0	6,9,11	1.01	0
2	SAR	J	4	2	4,4,5	0.66	0	1,3,5	1.92	0
2	SAR	K	3	2	4,4,5	0.69	0	1,3,5	2.08	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AC5	K	9	2	6,8,9	0.48	0	5,11,13	0.66	0
2	MLE	I	1	2	7,8,9	0.57	0	6,9,11	1.21	1 (16%)
2	SAR	L	4	2	4,4,5	0.70	0	1,3,5	2.10	1 (100%)
2	AC5	I	9	2	6,8,9	0.50	0	5,11,13	1.23	0
2	MLE	L	1	2	7,8,9	0.45	0	6,9,11	0.81	0
2	SAR	K	4	2	4,4,5	0.76	0	1,3,5	1.39	0
2	MLE	K	10	2	7,8,9	0.39	0	6,9,11	1.00	1 (16%)
2	SAR	I	4	2	4,4,5	0.77	0	1,3,5	1.62	0
2	7T2	I	5	2	12,13,14	0.32	0	15,16,18	0.87	1 (6%)
2	7T2	L	5	2	12,13,14	0.31	0	15,16,18	1.35	3 (20%)
2	7T2	K	5	2	12,13,14	0.30	0	15,16,18	1.04	1 (6%)
2	MLE	I	10	2	7,8,9	0.47	0	6,9,11	0.77	0
2	SAR	K	6	2	4,4,5	0.64	0	1,3,5	1.53	0
2	A1MFG	K	7	2	16,17,18	0.38	0	19,24,26	0.93	2 (10%)
2	MLE	K	1	2	7,8,9	0.47	0	6,9,11	0.83	0
2	SAR	J	3	2	4,4,5	0.76	0	1,3,5	1.69	0
2	A1MFG	I	7	2	16,17,18	0.51	0	19,24,26	1.11	2 (10%)
2	SAR	I	3	2	4,4,5	0.74	0	1,3,5	1.74	0
2	SAR	L	3	2	4,4,5	0.75	0	1,3,5	1.64	0
2	A1MFG	L	7	2	16,17,18	0.40	0	19,24,26	0.67	0
2	AC5	J	9	2	6,8,9	0.63	0	5,11,13	1.42	1 (20%)
2	SAR	J	6	2	4,4,5	0.81	0	1,3,5	1.00	0
2	MLE	J	10	2	7,8,9	0.39	0	6,9,11	0.90	0
2	7T2	J	5	2	12,13,14	0.32	0	15,16,18	1.53	4 (26%)
2	AC5	L	9	2	6,8,9	0.63	0	5,11,13	1.79	2 (40%)
2	A1MFG	J	7	2	16,17,18	0.40	0	19,24,26	0.96	1 (5%)
2	SAR	L	6	2	4,4,5	0.81	0	1,3,5	2.28	1 (100%)
2	SAR	I	6	2	4,4,5	0.66	0	1,3,5	0.72	0
2	MLE	L	10	2	7,8,9	0.45	0	6,9,11	0.58	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	MLE	J	1	2	-	0/5/8/10	-
2	SAR	J	4	2	-	1/1/2/3	-
2	SAR	K	3	2	-	1/1/2/3	-
2	AC5	K	9	2	-	0/2/12/15	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLE	I	1	2	-	2/5/8/10	-
2	SAR	L	4	2	-	1/1/2/3	-
2	AC5	I	9	2	-	0/2/12/15	0/1/1/1
2	MLE	L	1	2	-	1/5/8/10	-
2	SAR	K	4	2	-	1/1/2/3	-
2	MLE	K	10	2	-	0/5/8/10	-
2	SAR	I	4	2	-	1/1/2/3	-
2	7T2	I	5	2	-	0/5/8/10	0/1/1/1
2	7T2	L	5	2	-	2/5/8/10	0/1/1/1
2	7T2	K	5	2	-	0/5/8/10	0/1/1/1
2	MLE	I	10	2	-	0/5/8/10	-
2	SAR	K	6	2	-	1/1/2/3	-
2	A1MFG	K	7	2	-	0/12/13/15	0/1/1/1
2	MLE	K	1	2	-	0/5/8/10	-
2	SAR	J	3	2	-	1/1/2/3	-
2	A1MFG	I	7	2	-	0/12/13/15	0/1/1/1
2	SAR	I	3	2	-	1/1/2/3	-
2	SAR	L	3	2	-	1/1/2/3	-
2	A1MFG	L	7	2	-	3/12/13/15	0/1/1/1
2	AC5	J	9	2	-	0/2/12/15	0/1/1/1
2	SAR	J	6	2	-	1/1/2/3	-
2	MLE	J	10	2	-	1/5/8/10	-
2	7T2	J	5	2	-	0/5/8/10	0/1/1/1
2	AC5	L	9	2	-	0/2/12/15	0/1/1/1
2	A1MFG	J	7	2	-	0/12/13/15	0/1/1/1
2	SAR	L	6	2	-	1/1/2/3	-
2	SAR	I	6	2	-	1/1/2/3	-
2	MLE	L	10	2	-	0/5/8/10	-

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	5	7T2	CG-CB-CA	-3.86	108.11	113.63
2	K	5	7T2	CG-CB-CA	-3.43	108.72	113.63
2	L	9	AC5	CB2-CG2-CG1	-2.97	97.83	105.79
2	L	5	7T2	CB-CA-N	2.90	115.15	110.65
2	L	5	7T2	CG-CB-CA	-2.89	109.49	113.63
2	J	5	7T2	CB-CA-N	2.72	114.88	110.65
2	J	5	7T2	O-C-CA	-2.68	117.75	124.78
2	K	7	A1MFG	CB-CG-CD	-2.66	103.93	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	5	7T2	CG-CB-CA	-2.42	110.16	113.63
2	L	5	7T2	O-C-CA	-2.38	118.55	124.78
2	J	7	A1MFG	CB-CG-CD	-2.33	105.10	113.18
2	J	5	7T2	CM-N-CA	2.29	120.78	113.64
2	I	7	A1MFG	CB-CG-CD	-2.29	105.21	113.18
2	K	10	MLE	O-C-CA	-2.29	118.78	124.78
2	L	6	SAR	O-C-CA	-2.28	118.81	125.42
2	I	1	MLE	CD2-CG-CB	-2.28	102.72	111.11
2	J	9	AC5	CB2-CG2-CG1	-2.25	99.76	105.79
2	L	9	AC5	CB1-CG1-CG2	-2.22	99.83	105.79
2	K	7	A1MFG	CZ2-CH-CT	2.13	122.38	118.12
2	L	4	SAR	O-C-CA	-2.10	119.34	125.42
2	K	3	SAR	O-C-CA	-2.08	119.39	125.42
2	I	7	A1MFG	CZ2-CH-CT	2.01	122.13	118.12

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	3	SAR	C-CA-N-CN
2	J	3	SAR	C-CA-N-CN
2	K	3	SAR	C-CA-N-CN
2	L	3	SAR	C-CA-N-CN
2	I	4	SAR	C-CA-N-CN
2	J	4	SAR	C-CA-N-CN
2	K	4	SAR	C-CA-N-CN
2	L	4	SAR	C-CA-N-CN
2	I	6	SAR	C-CA-N-CN
2	J	6	SAR	C-CA-N-CN
2	K	6	SAR	C-CA-N-CN
2	L	6	SAR	C-CA-N-CN
2	L	7	A1MFG	CZ1-CH-CT-FT2
2	L	7	A1MFG	CZ1-CH-CT-FT3
2	L	7	A1MFG	CZ1-CH-CT-FT1
2	L	5	7T2	CA-CB-CG-CD1
2	I	1	MLE	C-CA-CB-CG
2	L	5	7T2	CA-CB-CG-CD2
2	L	1	MLE	CA-CB-CG-CD1
2	I	1	MLE	N-CA-CB-CG
2	J	10	MLE	N-CA-CB-CG

There are no ring outliers.

15 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	MLE	1	0
2	J	4	SAR	1	0
2	K	3	SAR	1	0
2	K	9	AC5	1	0
2	I	1	MLE	2	0
2	I	9	AC5	1	0
2	L	1	MLE	1	0
2	K	10	MLE	3	0
2	I	5	7T2	1	0
2	I	10	MLE	1	0
2	K	1	MLE	1	0
2	J	3	SAR	1	0
2	I	3	SAR	1	0
2	L	3	SAR	1	0
2	J	10	MLE	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 8 are monoatomic - leaving 38 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	$\# Z > 2$
5	FMT	B	209	-	2,2,2	0.68	0	1,1,1	0.30	0
5	FMT	A	208	-	2,2,2	0.66	0	1,1,1	0.35	0
3	GDP	A	201	6	28,30,30	1.27	5 (17%)	44,47,47	1.65	6 (13%)
5	FMT	C	905	-	2,2,2	0.64	0	1,1,1	0.25	0
5	FMT	C	904	-	2,2,2	0.63	0	1,1,1	0.33	0
3	GDP	D	201	6	28,30,30	1.18	3 (10%)	44,47,47	1.72	8 (18%)
4	EDO	A	204	-	3,3,3	0.34	0	2,2,2	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	206	-	3,3,3	0.36	0	2,2,2	0.03	0
4	EDO	B	212	-	3,3,3	0.26	0	2,2,2	0.21	0
4	EDO	A	214	-	3,3,3	0.25	0	2,2,2	0.32	0
5	FMT	A	209	-	2,2,2	0.75	0	1,1,1	0.46	0
4	EDO	D	202	-	3,3,3	0.33	0	2,2,2	0.17	0
5	FMT	A	212	-	2,2,2	0.59	0	1,1,1	0.31	0
5	FMT	B	204	-	2,2,2	0.62	0	1,1,1	0.26	0
4	EDO	A	203	-	3,3,3	0.44	0	2,2,2	0.26	0
5	FMT	B	214	-	2,2,2	0.68	0	1,1,1	0.32	0
5	FMT	A	215	-	2,2,2	0.61	0	1,1,1	0.35	0
5	FMT	B	213	-	2,2,2	0.61	0	1,1,1	0.19	0
4	EDO	A	202	-	3,3,3	0.43	0	2,2,2	0.10	0
3	GDP	B	201	6	28,30,30	1.19	1 (3%)	44,47,47	1.80	8 (18%)
4	EDO	A	211	-	3,3,3	0.47	0	2,2,2	0.28	0
5	FMT	A	205	-	2,2,2	0.67	0	1,1,1	0.31	0
4	EDO	B	208	-	3,3,3	0.27	0	2,2,2	0.24	0
5	FMT	C	901	-	2,2,2	0.67	0	1,1,1	0.29	0
5	FMT	A	210	-	2,2,2	0.63	0	1,1,1	0.29	0
5	FMT	B	203	-	2,2,2	0.63	0	1,1,1	0.24	0
5	FMT	B	211	-	2,2,2	0.69	0	1,1,1	0.43	0
5	FMT	A	207	-	2,2,2	0.65	0	1,1,1	0.37	0
4	EDO	I	1501	-	3,3,3	0.53	0	2,2,2	0.33	0
5	FMT	A	213	-	2,2,2	0.63	0	1,1,1	0.36	0
5	FMT	B	210	-	2,2,2	0.66	0	1,1,1	0.26	0
5	FMT	A	216	-	2,2,2	0.70	0	1,1,1	0.01	0
5	FMT	B	205	-	2,2,2	0.69	0	1,1,1	0.33	0
5	FMT	B	207	-	2,2,2	0.69	0	1,1,1	0.29	0
4	EDO	B	206	-	3,3,3	0.35	0	2,2,2	0.37	0
3	GDP	C	902	6	28,30,30	1.10	3 (10%)	44,47,47	1.81	9 (20%)
4	EDO	B	202	-	3,3,3	0.28	0	2,2,2	0.41	0
5	FMT	C	903	-	2,2,2	0.65	0	1,1,1	0.33	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
4	EDO	B	208	-	-	0/1/1/1	-
4	EDO	A	214	-	-	1/1/1/1	-
3	GDP	A	201	6	-	0/16/32/32	0/3/3/3
4	EDO	I	1501	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	206	-	-	0/1/1/1	-
4	EDO	D	202	-	-	0/1/1/1	-
4	EDO	A	203	-	-	1/1/1/1	-
3	GDP	D	201	6	-	4/16/32/32	0/3/3/3
4	EDO	A	202	-	-	0/1/1/1	-
3	GDP	B	201	6	-	5/16/32/32	0/3/3/3
4	EDO	A	204	-	-	1/1/1/1	-
4	EDO	B	206	-	-	0/1/1/1	-
4	EDO	A	211	-	-	1/1/1/1	-
3	GDP	C	902	6	-	4/16/32/32	0/3/3/3
4	EDO	B	202	-	-	0/1/1/1	-
4	EDO	B	212	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	GDP	C5-C4	3.55	1.48	1.38
3	D	201	GDP	C5-C4	3.09	1.47	1.38
3	C	902	GDP	C5-C4	2.97	1.47	1.38
3	A	201	GDP	C6-N1	-2.63	1.34	1.38
3	D	201	GDP	C6-N1	-2.61	1.34	1.38
3	A	201	GDP	C5-C4	2.55	1.45	1.38
3	C	902	GDP	C6-N1	-2.38	1.34	1.38
3	D	201	GDP	C5-N7	-2.36	1.34	1.39
3	A	201	GDP	C5-N7	-2.24	1.34	1.39
3	A	201	GDP	PA-O2A	-2.16	1.45	1.55
3	C	902	GDP	C5-N7	-2.06	1.35	1.39
3	A	201	GDP	C4-N9	-2.02	1.32	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	GDP	C5-C4-N3	-5.81	119.04	128.46
3	C	902	GDP	C5-C4-N3	-5.66	119.28	128.46
3	B	201	GDP	C5-C4-N3	-5.61	119.36	128.46
3	A	201	GDP	C5-C4-N3	-5.29	119.87	128.46
3	B	201	GDP	C2-N3-C4	4.63	120.55	112.30
3	C	902	GDP	C2-N3-C4	4.61	120.51	112.30
3	D	201	GDP	N9-C4-N3	4.57	135.12	125.94
3	D	201	GDP	C2-N3-C4	4.57	120.43	112.30
3	B	201	GDP	N9-C4-N3	4.46	134.88	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	GDP	N9-C4-N3	4.21	134.40	125.94
3	A	201	GDP	C2-N3-C4	4.11	119.62	112.30
3	A	201	GDP	N9-C4-N3	4.06	134.10	125.94
3	C	902	GDP	C6-C5-N7	3.46	136.67	130.25
3	B	201	GDP	C6-C5-N7	3.40	136.58	130.25
3	C	902	GDP	PA-O3A-PB	-3.19	121.87	132.83
3	A	201	GDP	C6-C5-N7	3.01	135.85	130.25
3	C	902	GDP	C4-C5-N7	-2.93	106.09	110.72
3	D	201	GDP	C6-C5-N7	2.90	135.64	130.25
3	A	201	GDP	O6-C6-C5	-2.67	119.53	126.60
3	B	201	GDP	C5'-C4'-C3'	-2.66	105.22	115.18
3	B	201	GDP	C4-C5-N7	-2.50	106.77	110.72
3	D	201	GDP	O6-C6-C5	-2.50	119.98	126.60
3	B	201	GDP	PA-O3A-PB	-2.33	124.81	132.83
3	C	902	GDP	C8-N7-C5	2.32	108.44	104.24
3	B	201	GDP	O6-C6-C5	-2.26	120.60	126.60
3	C	902	GDP	O3B-PB-O3A	2.21	112.05	104.64
3	C	902	GDP	O6-C6-C5	-2.18	120.82	126.60
3	A	201	GDP	C4-C5-N7	-2.14	107.33	110.72
3	D	201	GDP	PA-O3A-PB	-2.10	125.63	132.83
3	D	201	GDP	C4-C5-N7	-2.08	107.43	110.72
3	D	201	GDP	C5-C6-N1	2.06	118.43	113.19

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	GDP	C5'-O5'-PA-O1A
3	B	201	GDP	C5'-O5'-PA-O2A
3	B	201	GDP	O4'-C4'-C5'-O5'
3	B	201	GDP	C3'-C4'-C5'-O5'
4	A	211	EDO	O1-C1-C2-O2
3	D	201	GDP	PA-O3A-PB-O1B
3	C	902	GDP	C5'-O5'-PA-O3A
3	C	902	GDP	C5'-O5'-PA-O1A
3	C	902	GDP	C5'-O5'-PA-O2A
3	D	201	GDP	O4'-C4'-C5'-O5'
4	A	203	EDO	O1-C1-C2-O2
4	A	204	EDO	O1-C1-C2-O2
4	A	214	EDO	O1-C1-C2-O2
4	B	212	EDO	O1-C1-C2-O2
4	I	1501	EDO	O1-C1-C2-O2

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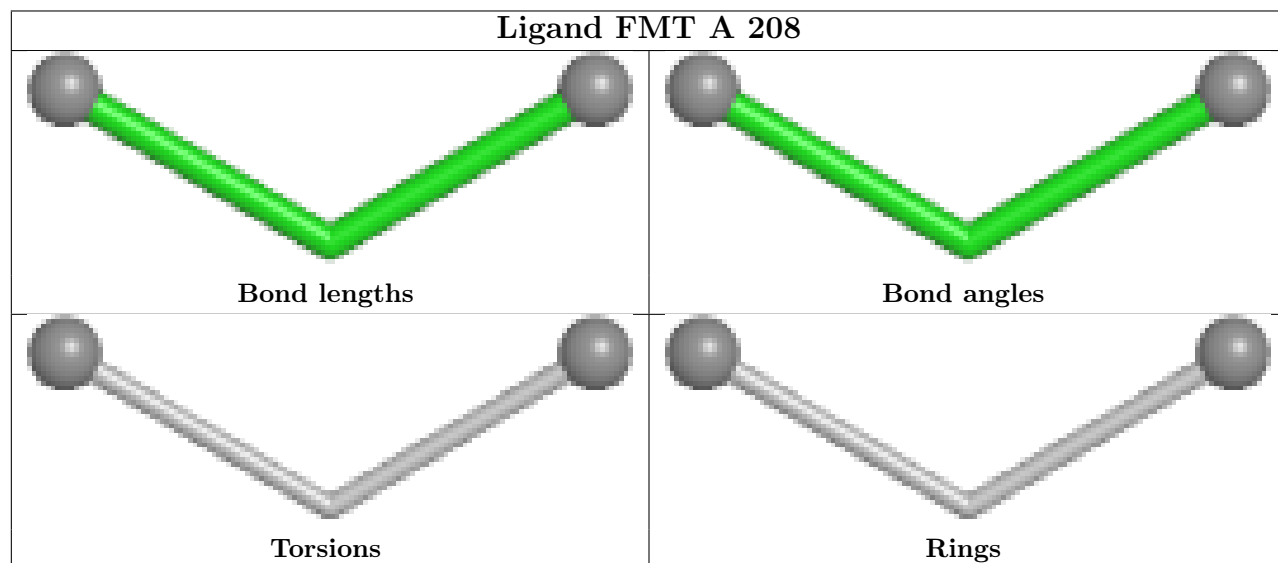
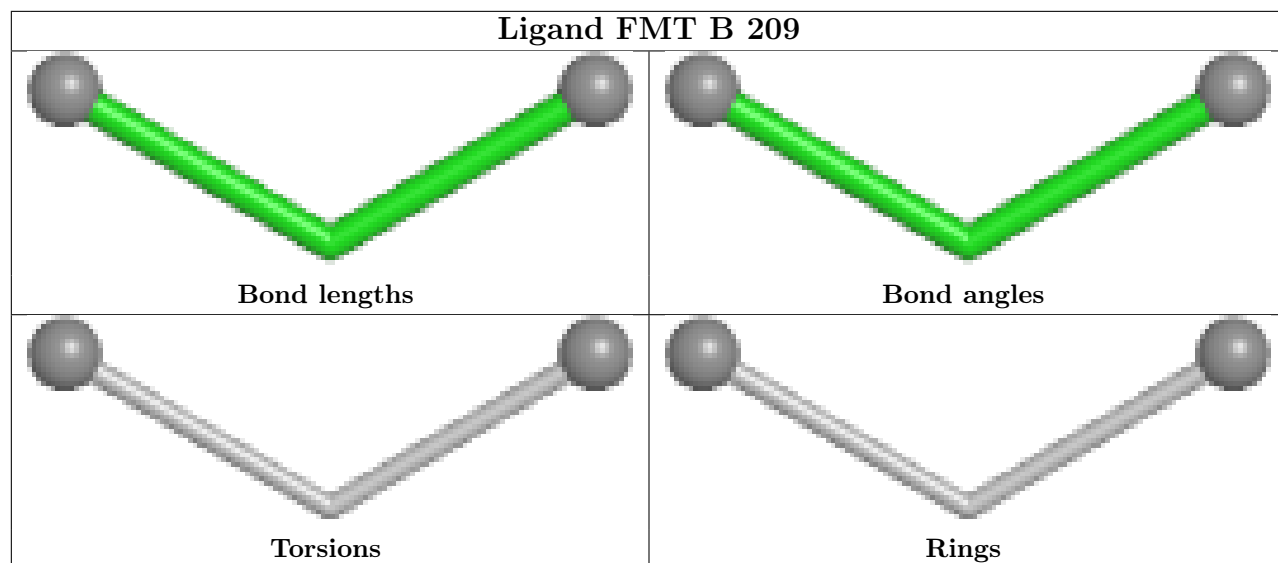
Mol	Chain	Res	Type	Atoms
3	D	201	GDP	PA-O3A-PB-O2B
3	D	201	GDP	PA-O3A-PB-O3B
3	B	201	GDP	C5'-O5'-PA-O3A
3	C	902	GDP	O4'-C4'-C5'-O5'

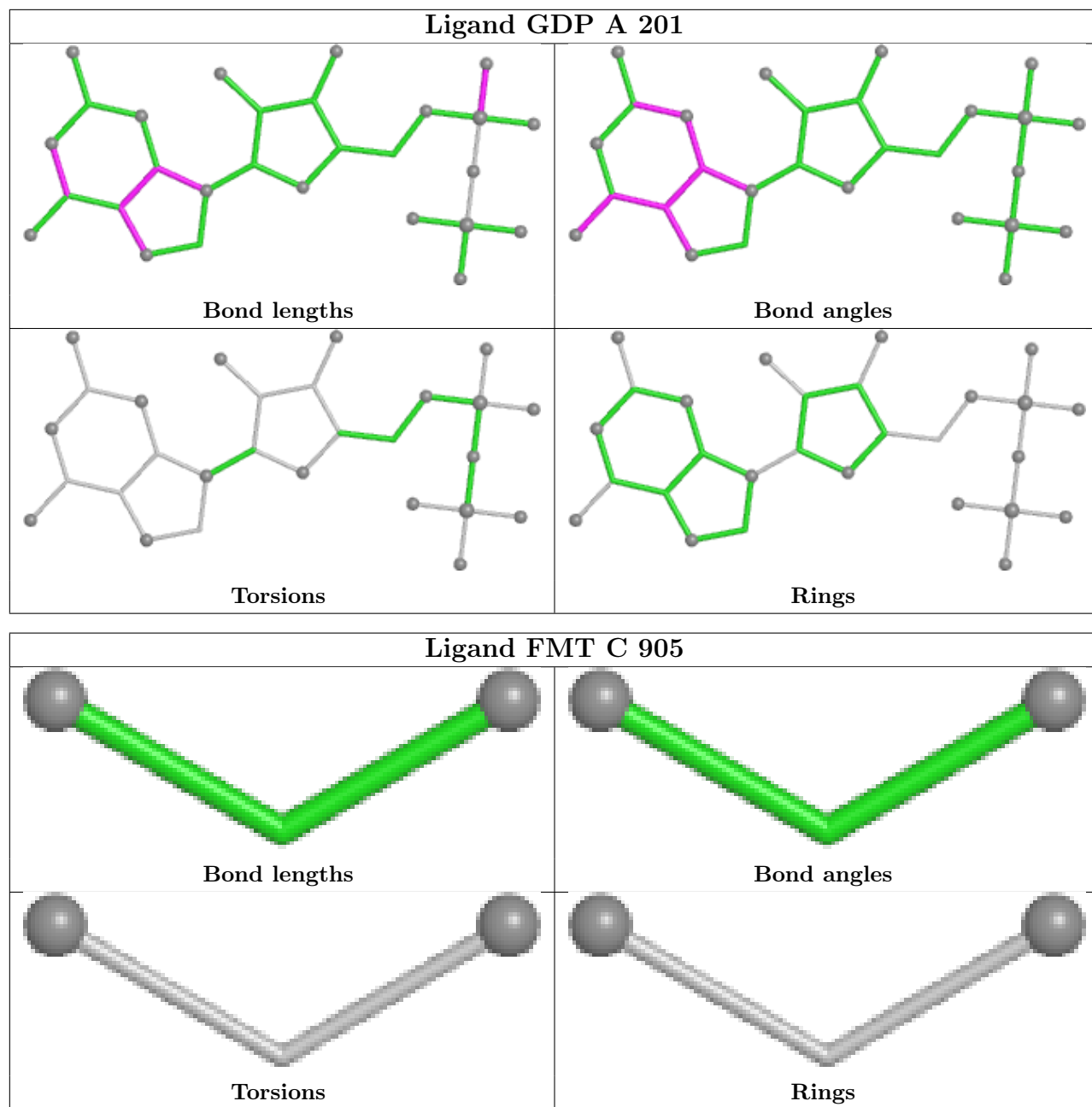
There are no ring outliers.

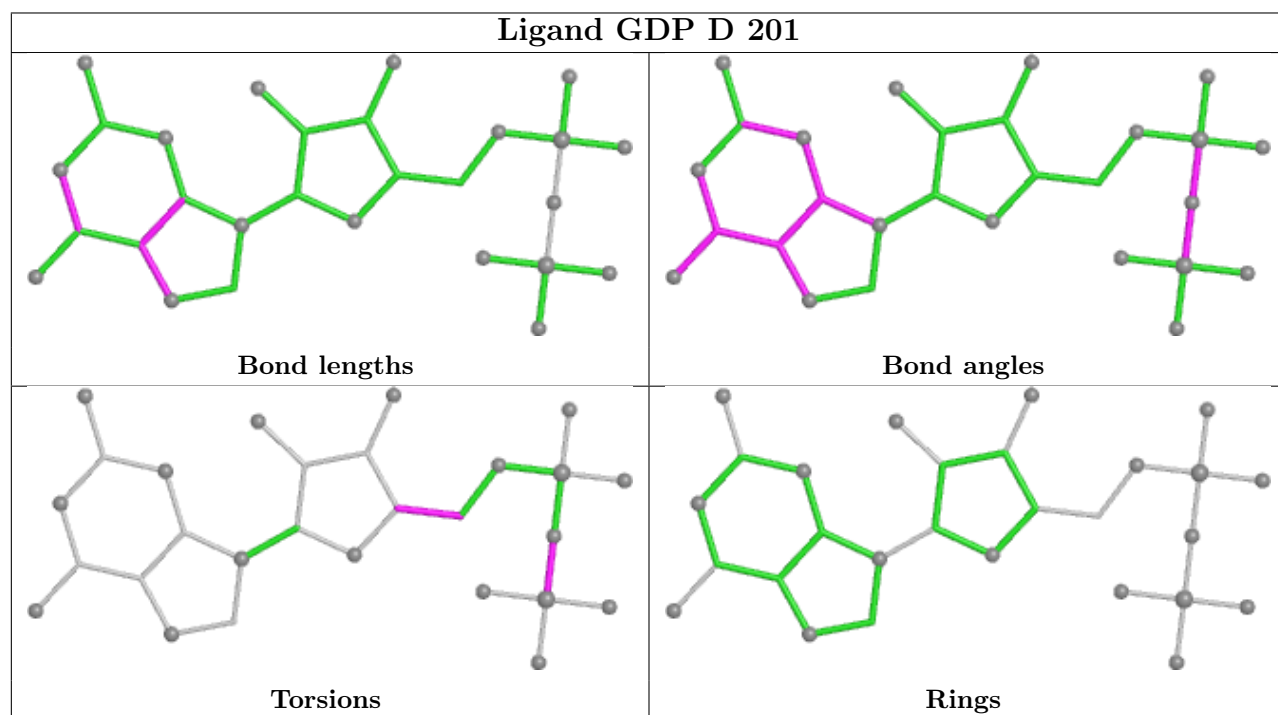
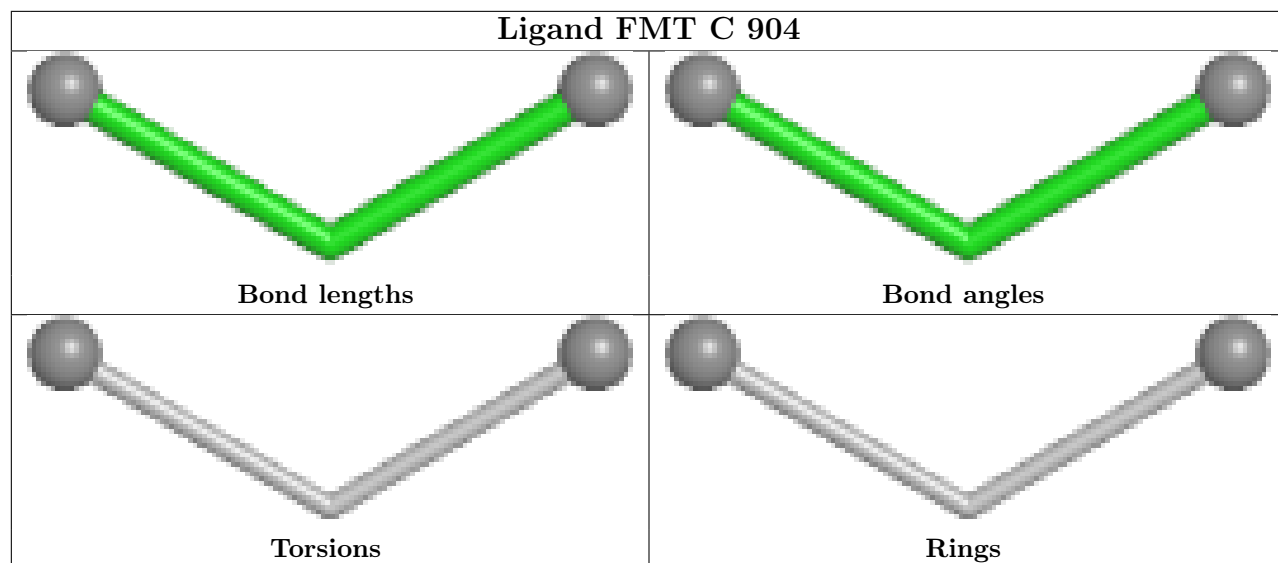
9 monomers are involved in 14 short contacts:

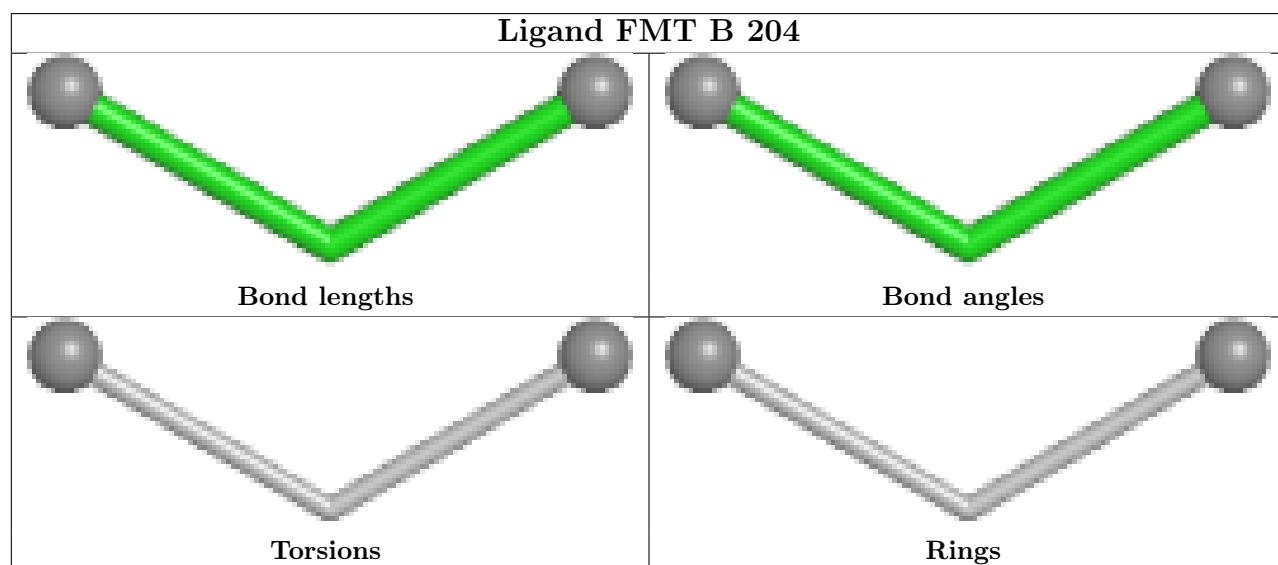
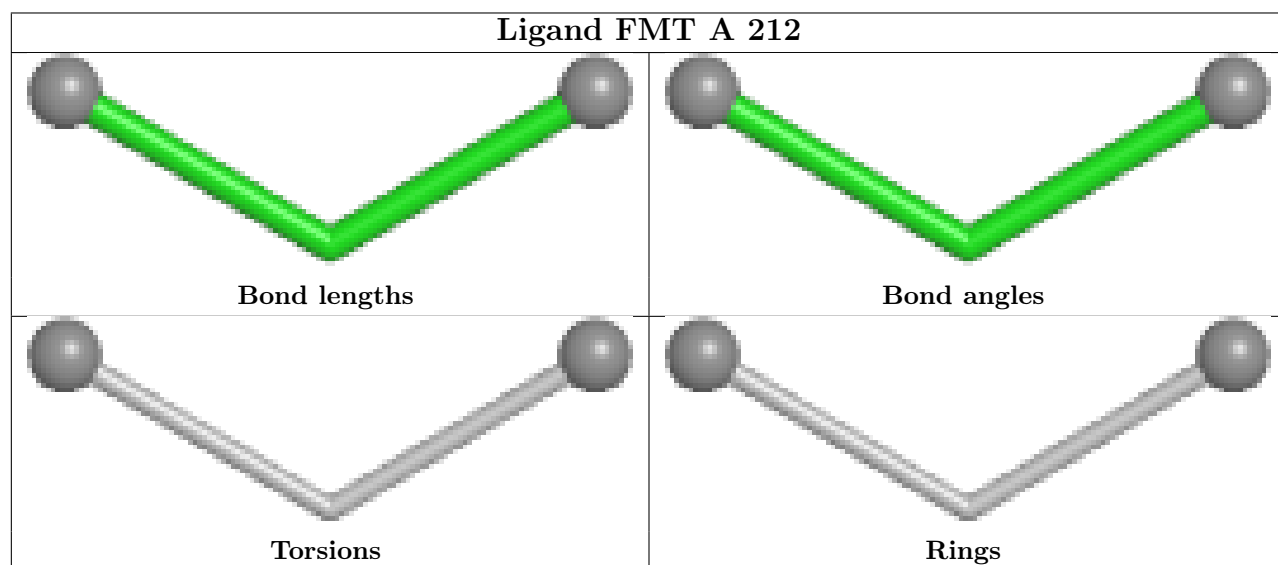
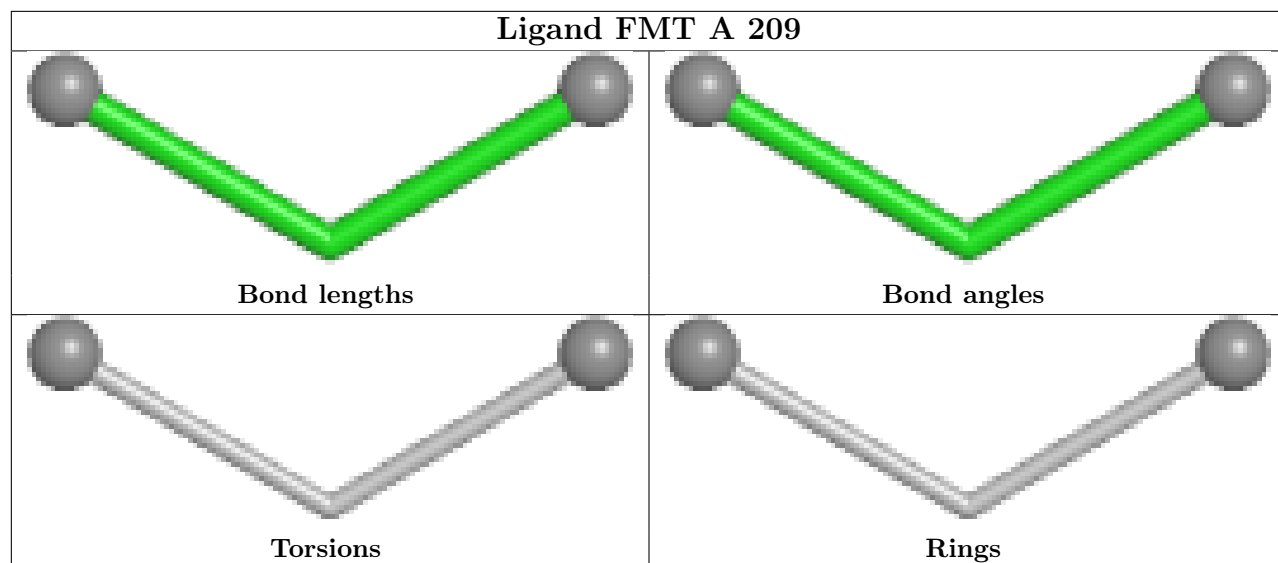
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	202	EDO	2	0
5	A	212	FMT	1	0
4	A	203	EDO	1	0
4	A	202	EDO	2	0
3	B	201	GDP	2	0
4	A	211	EDO	1	0
5	B	210	FMT	2	0
4	B	206	EDO	2	0
4	B	202	EDO	1	0

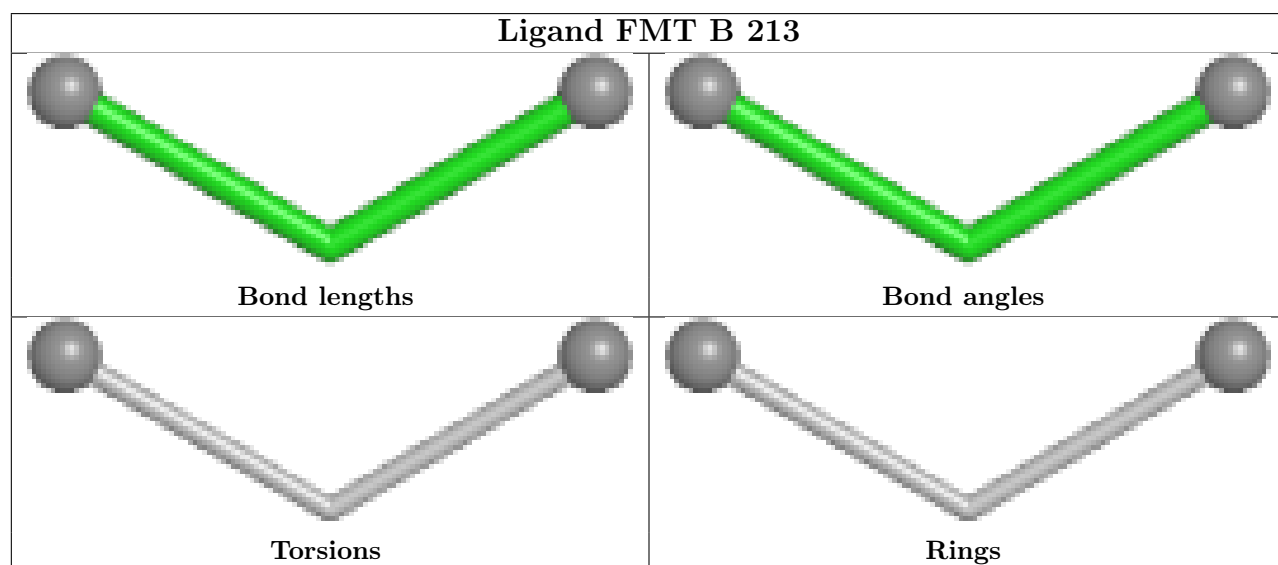
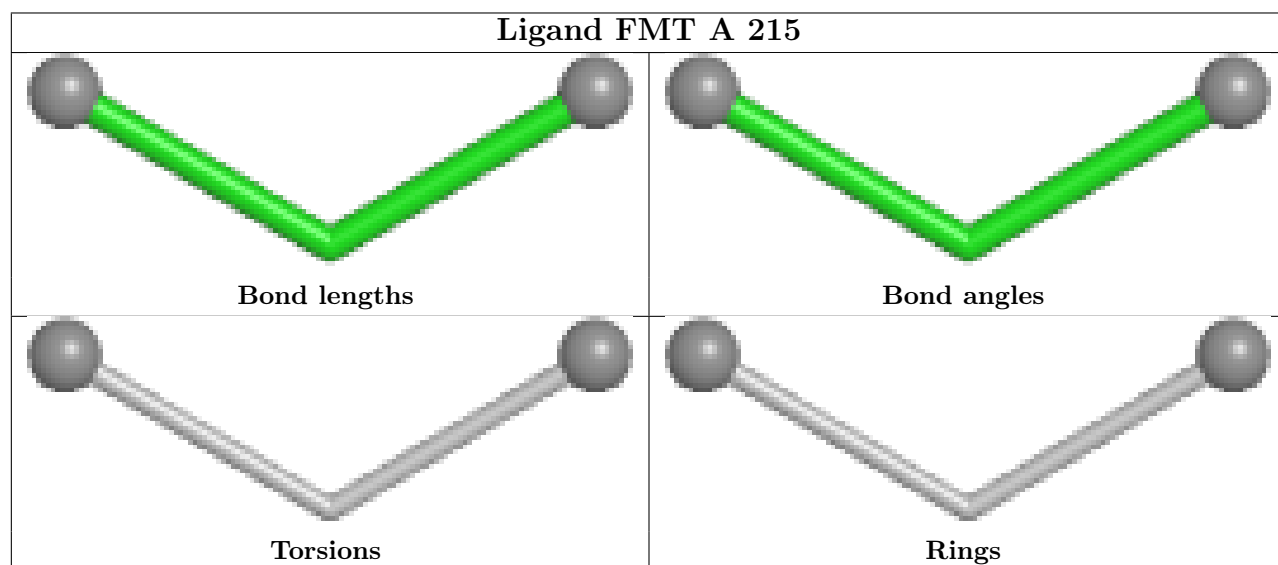
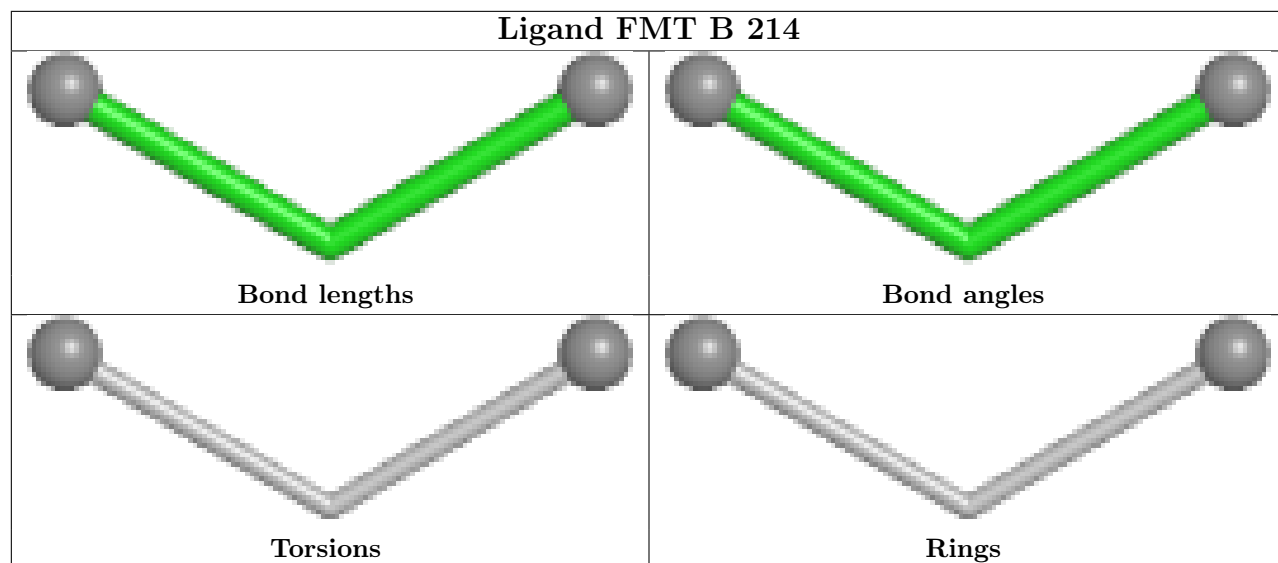
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

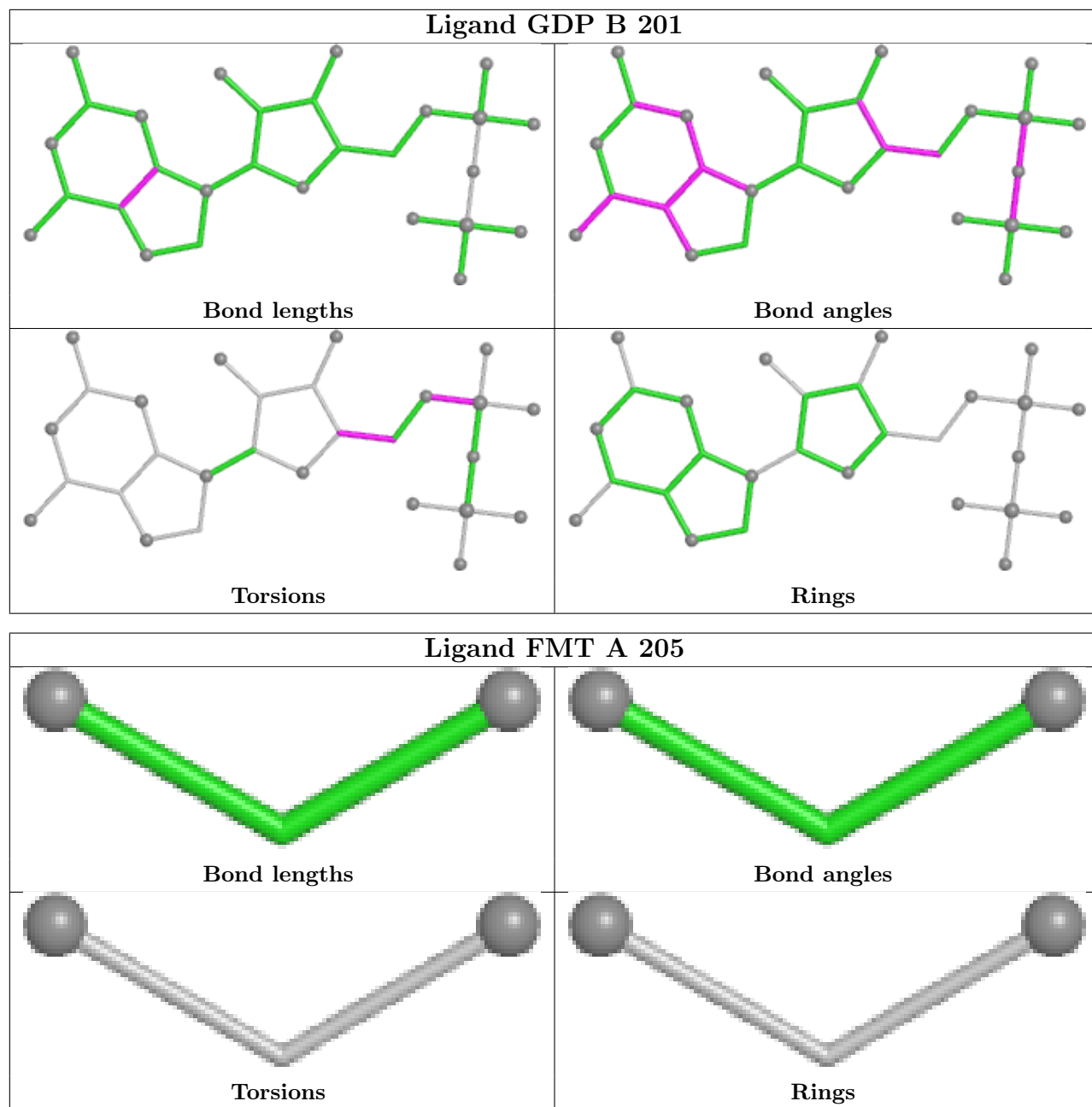


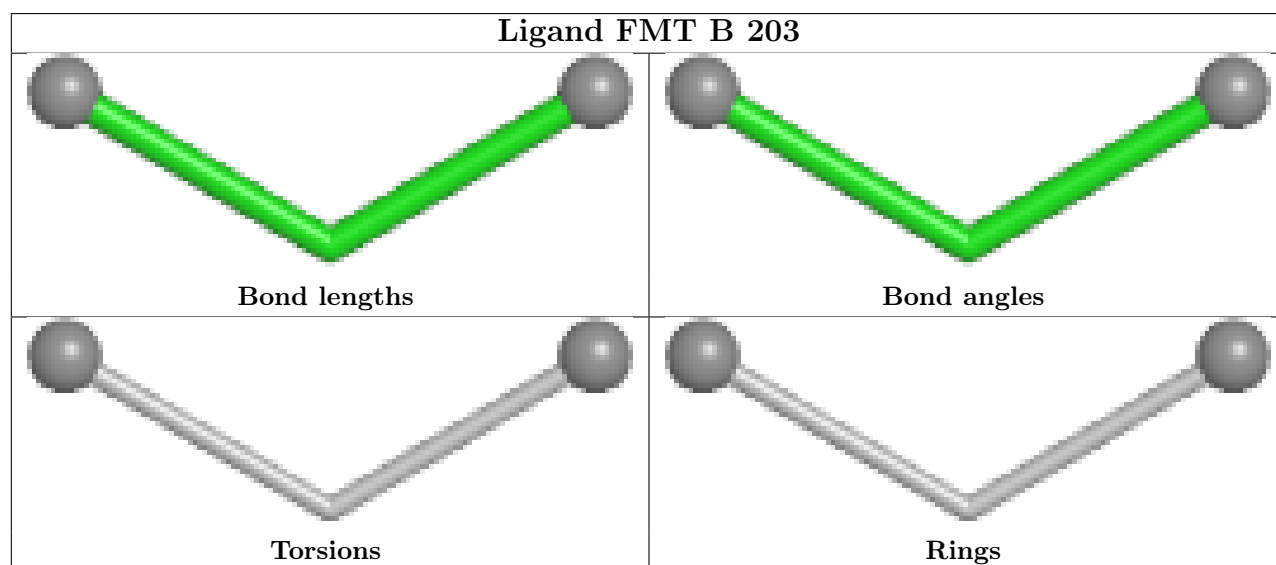
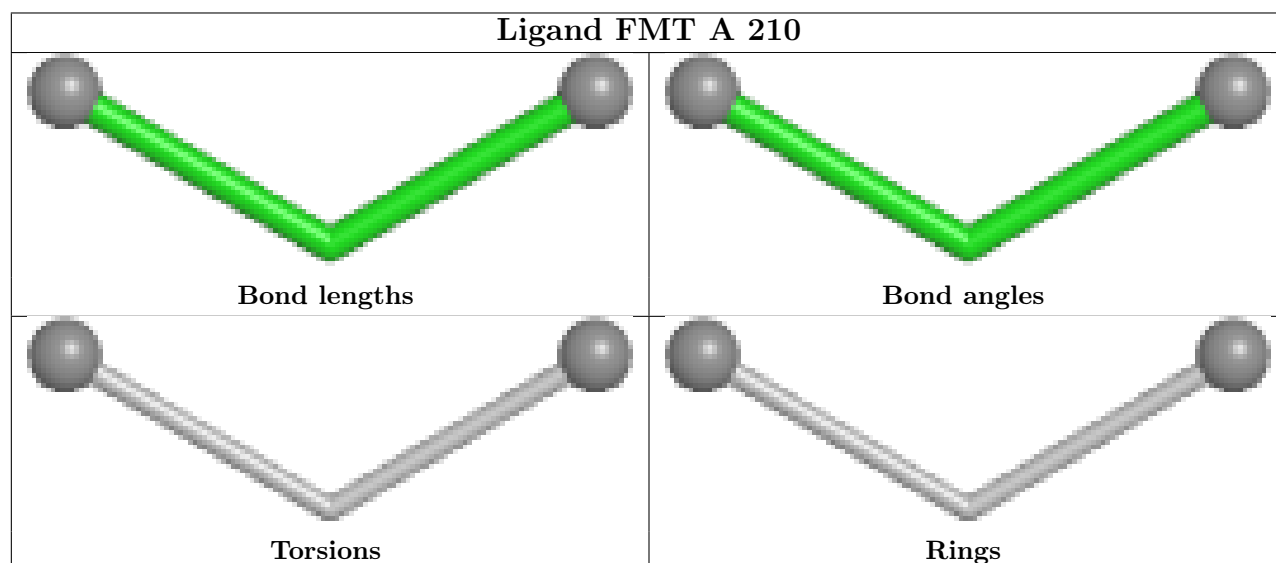
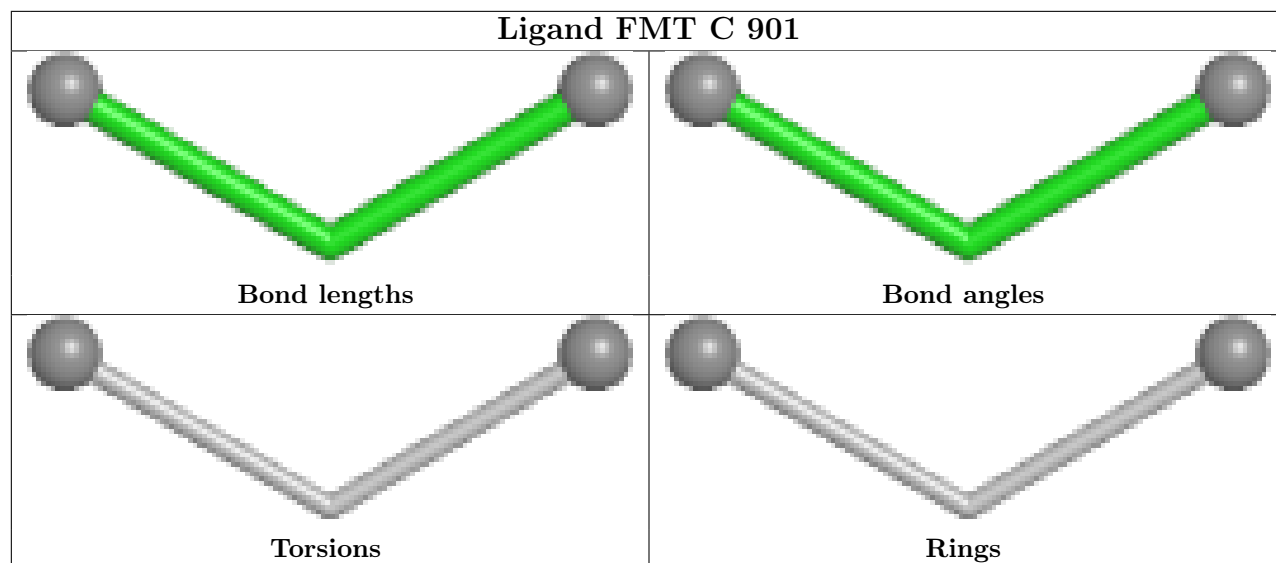


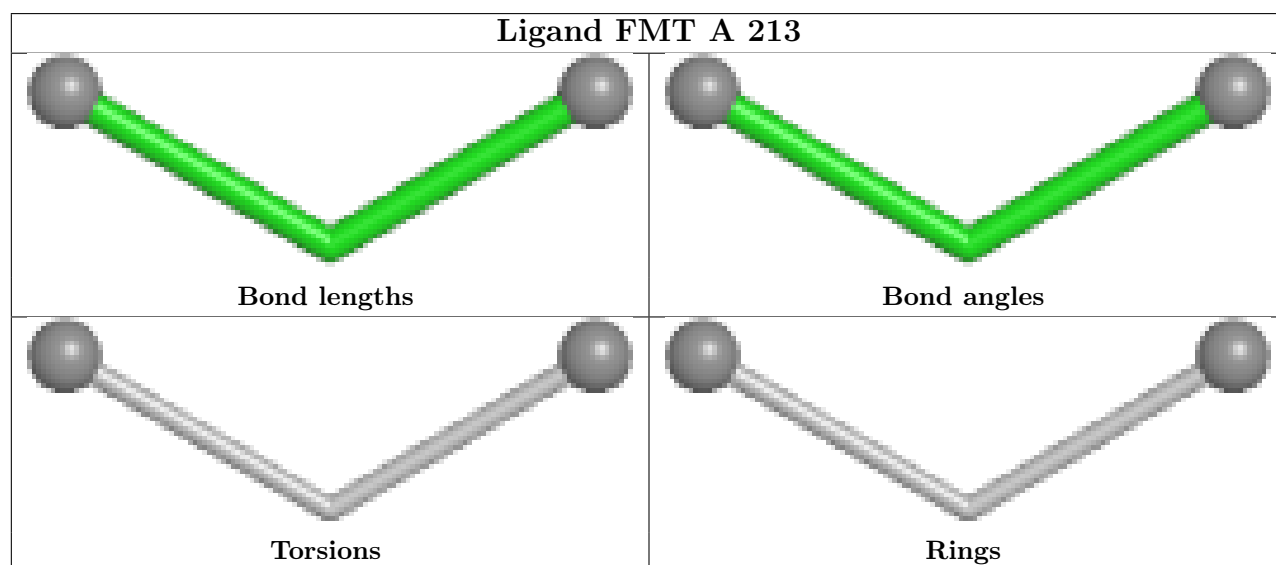
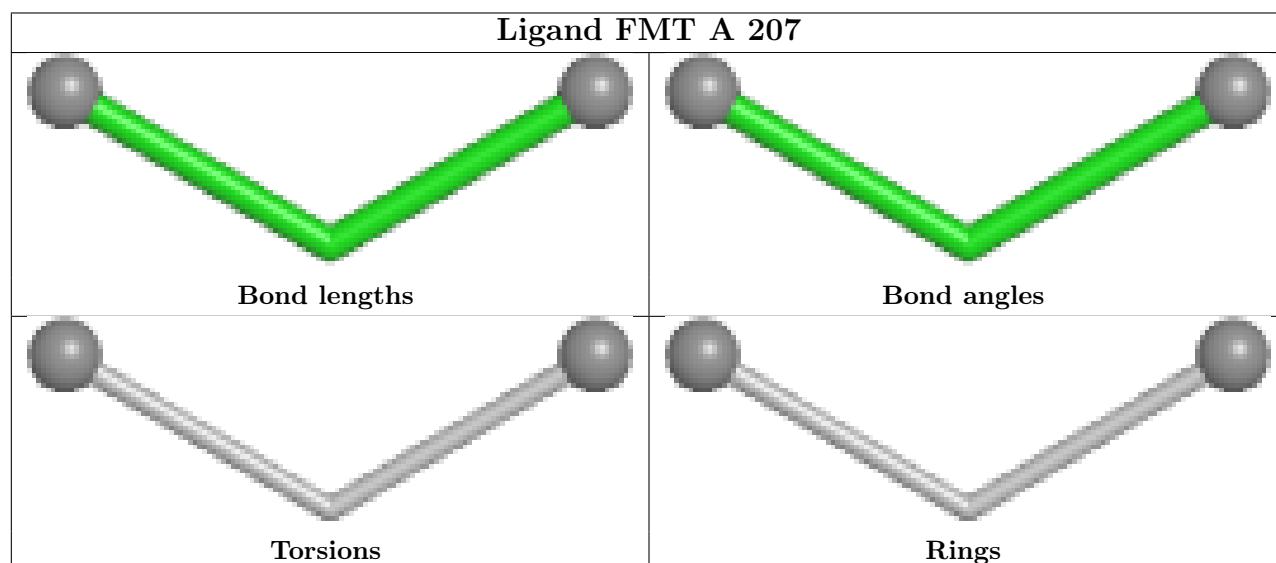
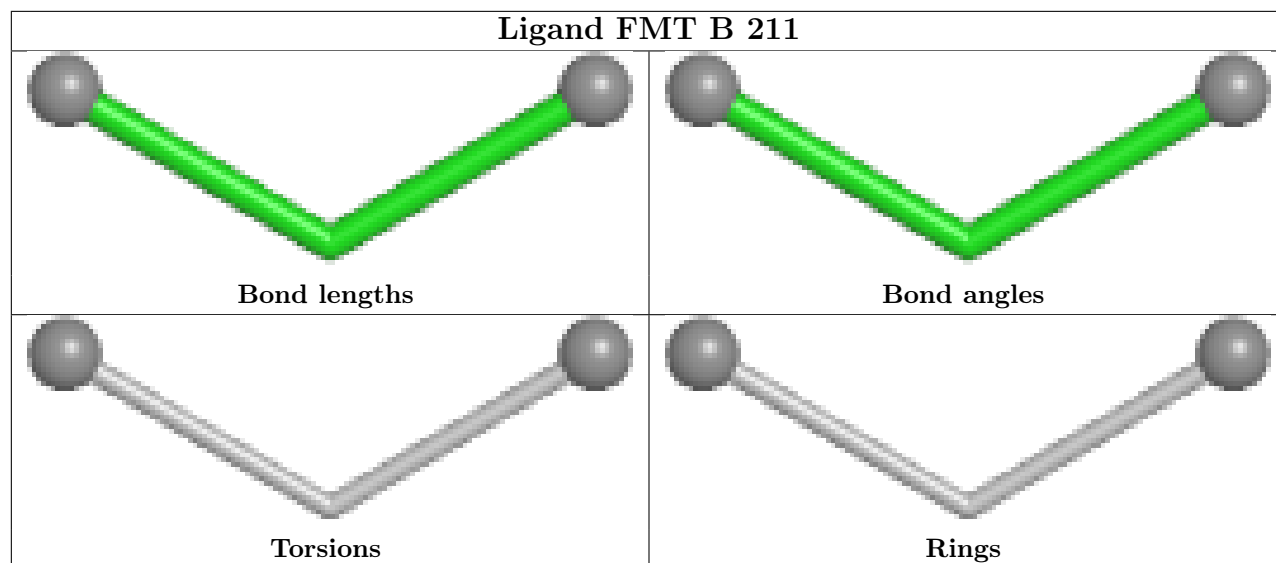


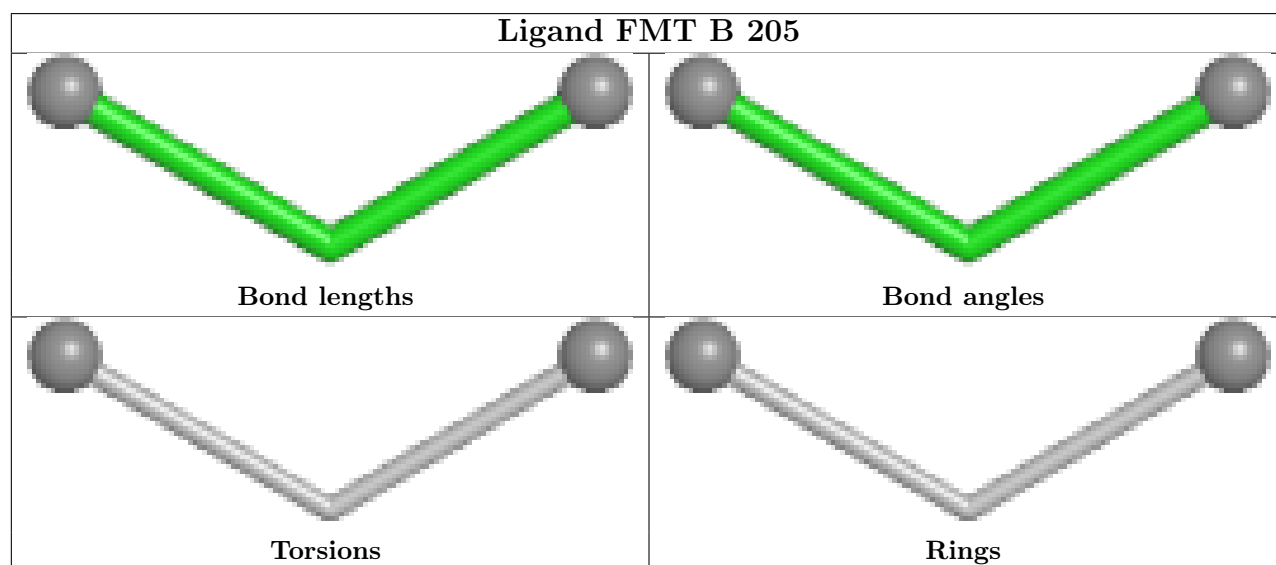
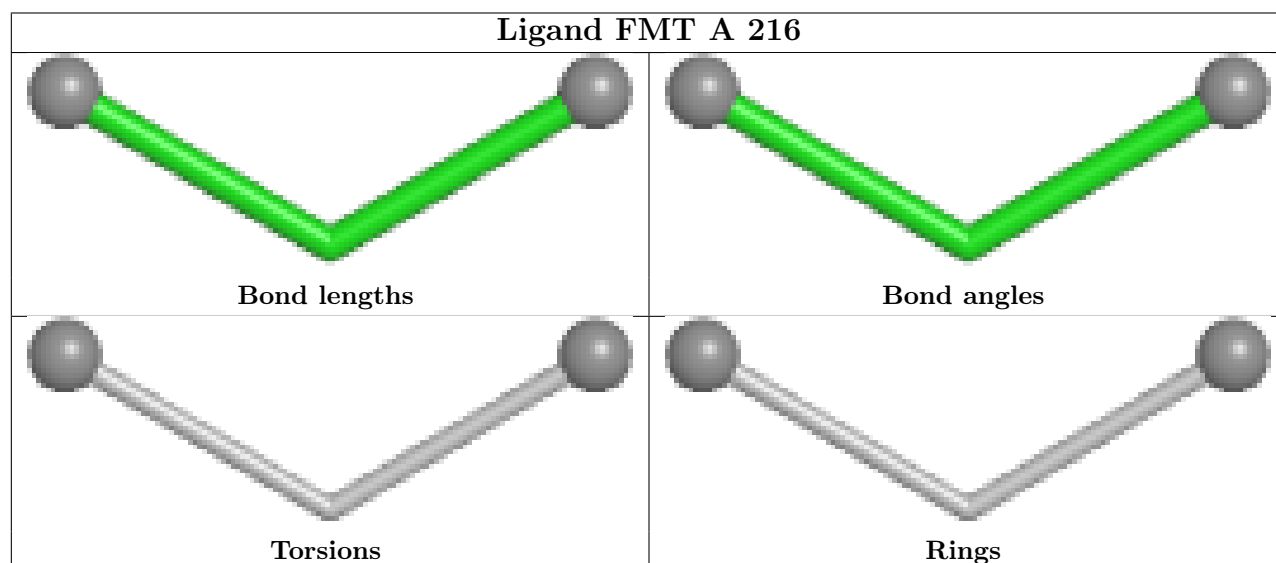
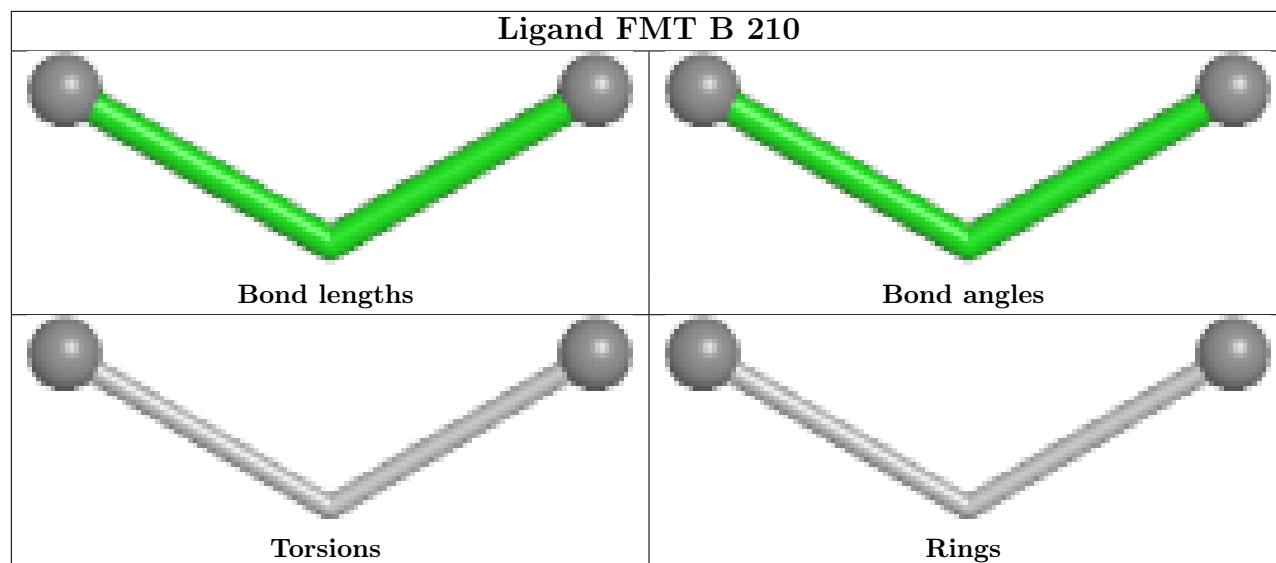


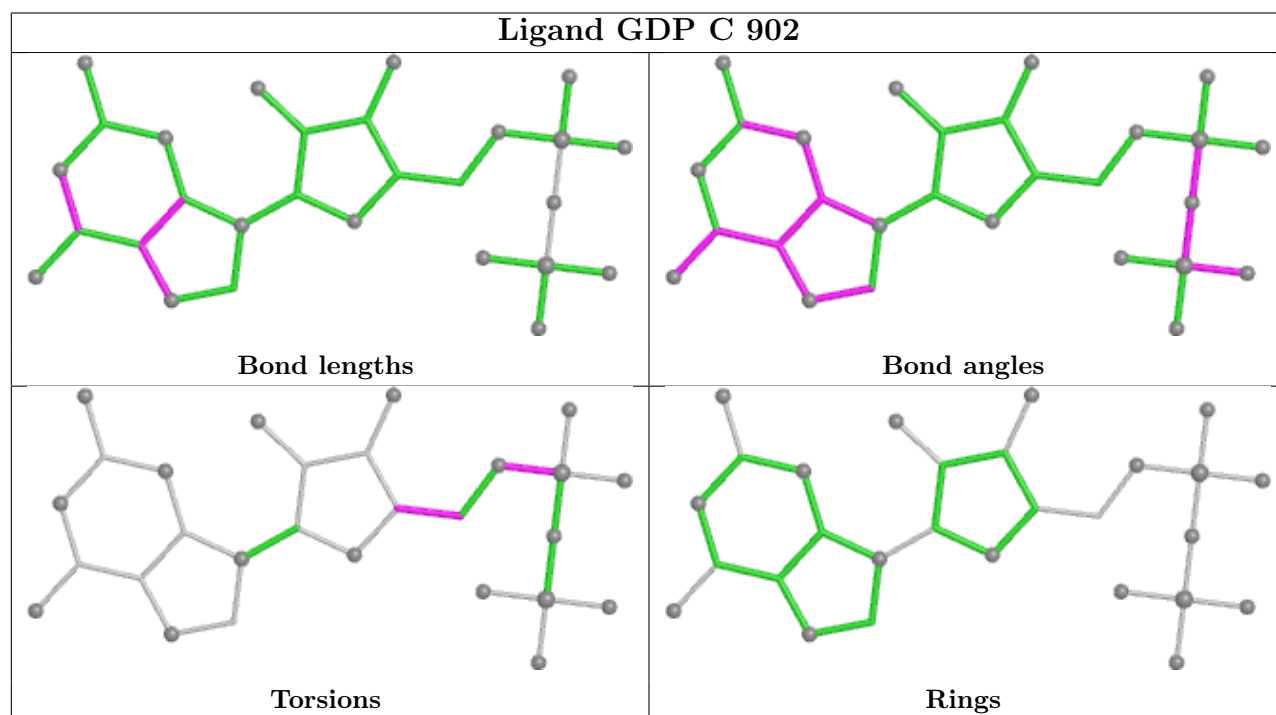
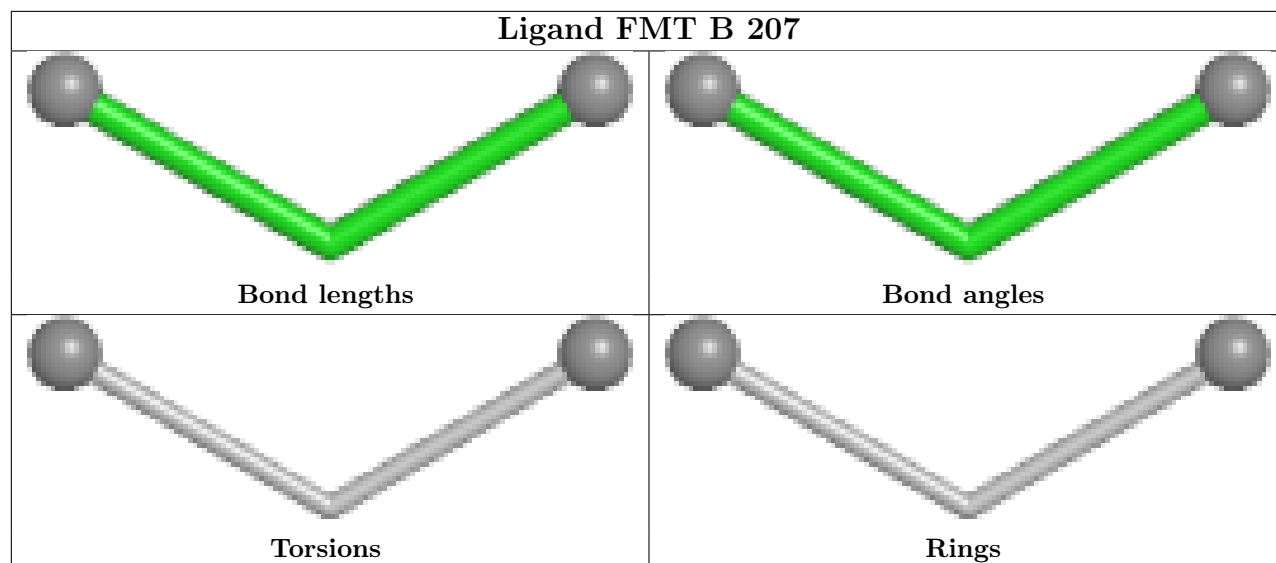


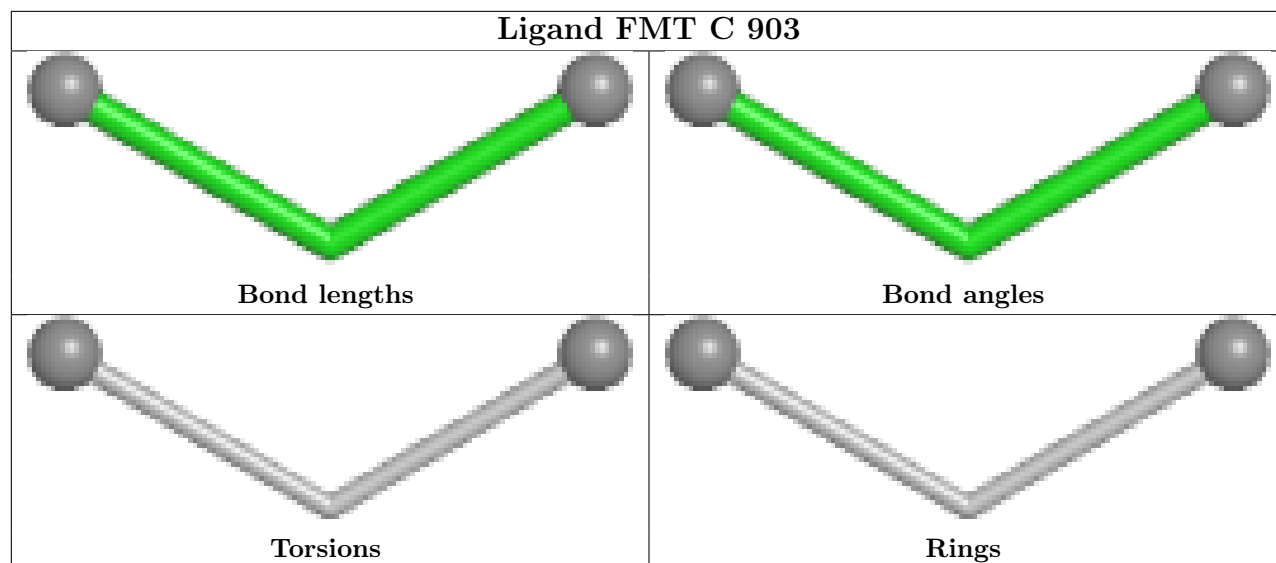












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	175/179 (97%)	0.12	9 (5%) 33 33	21, 30, 48, 59	0
1	B	174/179 (97%)	0.15	4 (2%) 61 63	20, 31, 49, 62	0
1	C	173/179 (96%)	1.39	35 (20%) 3 2	33, 47, 66, 73	0
1	D	172/179 (96%)	1.58	45 (26%) 1 1	34, 49, 67, 79	0
2	I	2/12 (16%)	-0.08	0 100 100	28, 28, 28, 32	0
2	J	2/12 (16%)	0.76	0 100 100	32, 32, 32, 34	0
2	K	2/12 (16%)	1.47	0 100 100	42, 42, 42, 44	0
2	L	2/12 (16%)	2.38	1 (50%) 0 0	46, 46, 46, 51	0
All	All	702/764 (91%)	0.81	94 (13%) 7 7	20, 40, 63, 79	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	171	SER	4.9
1	D	62	GLU	4.0
1	A	-1	GLY	3.9
1	C	133	LEU	3.8
1	D	124	THR	3.8
1	D	137	TYR	3.7
1	B	-1	GLY	3.7
1	C	157	TYR	3.6
1	D	170	MET	3.5
1	D	118	CYS	3.5
1	C	137	TYR	3.5
1	D	164	ARG	3.5
1	D	125	VAL	3.4
1	C	100	ILE	3.4
1	B	-2	SER	3.4
1	C	71	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	60	GLY	3.2
1	D	121	PRO	3.2
1	D	130	ALA	3.2
1	D	120	LEU	3.2
1	C	108	ASP	3.1
1	D	143	GLU	3.1
1	C	130	ALA	3.1
1	D	133	LEU	3.1
1	D	108	ASP	3.0
1	C	94	HIS	3.0
1	C	84	ILE	3.0
1	D	103	VAL	3.0
2	L	2	ILE	3.0
1	C	31	GLU	2.9
1	C	126	ASP	2.9
1	D	132	ASP	2.9
1	D	52	LEU	2.8
1	D	126	ASP	2.8
1	C	90	PHE	2.8
1	C	4	TYR	2.8
1	D	72	MET	2.8
1	D	61	GLN	2.7
1	C	134	ALA	2.6
1	C	118	CYS	2.6
1	C	131	GLN	2.6
1	C	50	THR	2.6
1	C	125	VAL	2.6
1	D	148	THR	2.6
1	D	90	PHE	2.6
1	D	163	ILE	2.6
1	C	93	ILE	2.5
1	A	170	MET	2.5
1	D	135	ARG	2.5
1	D	122	SER	2.5
1	B	30	ASP	2.5
1	D	131	GLN	2.5
1	D	128	LYS	2.5
1	D	0	GLY	2.5
1	C	72	MET	2.4
1	C	113	LEU	2.4
1	D	127	THR	2.4
1	C	0	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	82	PHE	2.3
1	D	134	ALA	2.3
1	A	94	HIS	2.3
1	D	142	ILE	2.3
1	C	160	VAL	2.3
1	D	50	THR	2.3
1	D	84	ILE	2.3
1	C	103	VAL	2.3
1	A	172	LYS	2.3
1	C	105	ASP	2.3
1	C	52	LEU	2.3
1	C	66	ALA	2.2
1	C	106	SER	2.2
1	D	81	VAL	2.2
1	C	30	ASP	2.2
1	D	113	LEU	2.2
1	C	111	MET	2.2
1	D	30	ASP	2.2
1	C	107	GLU	2.2
1	C	80	CYS	2.2
1	A	30	ASP	2.2
1	C	121	PRO	2.1
1	A	168	GLU	2.1
1	D	28	PHE	2.1
1	D	141	PHE	2.1
1	D	136	SER	2.1
1	A	31	GLU	2.1
1	A	108	ASP	2.1
1	C	132	ASP	2.1
1	D	32	TYR	2.1
1	D	129	GLN	2.1
1	D	97	ARG	2.1
1	A	0	GLY	2.1
1	D	159	LEU	2.0
1	D	139	ILE	2.0
1	B	171	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	7T2	L	5	13/14	0.76	0.19	46,49,58,79	0
2	MLE	L	1	9/10	0.78	0.18	39,47,55,61	0
2	7T2	J	5	13/14	0.83	0.17	30,33,40,57	0
2	AC5	J	9	8/9	0.85	0.14	35,36,39,40	0
2	SAR	L	3	5/6	0.87	0.16	48,48,55,55	0
2	7T2	K	5	13/14	0.87	0.15	41,46,51,64	0
2	AC5	L	9	8/9	0.88	0.14	50,52,54,54	0
2	SAR	L	6	5/6	0.90	0.13	44,44,46,46	0
2	SAR	K	4	5/6	0.90	0.12	42,45,47,48	0
2	MLE	K	1	9/10	0.90	0.15	43,46,50,51	0
2	SAR	K	6	5/6	0.91	0.11	39,41,43,44	0
2	SAR	L	4	5/6	0.91	0.14	45,45,47,47	0
2	SAR	K	3	5/6	0.92	0.13	41,42,44,46	0
2	AC5	K	9	8/9	0.92	0.13	41,43,45,48	0
2	A1MFG	L	7	17/18	0.92	0.12	40,44,52,55	0
2	A1MFG	K	7	17/18	0.93	0.10	38,42,48,50	0
2	MLE	I	1	9/10	0.93	0.10	32,34,38,38	0
2	SAR	J	6	5/6	0.93	0.09	31,32,34,35	0
2	MLE	J	1	9/10	0.93	0.09	25,32,39,39	0
2	SAR	J	3	5/6	0.93	0.10	34,36,38,41	0
2	MLE	I	10	9/10	0.93	0.10	25,26,33,43	0
2	MLE	K	10	9/10	0.93	0.11	40,42,46,48	0
2	MLE	L	10	9/10	0.93	0.15	45,47,50,51	0
2	A1MFG	J	7	17/18	0.94	0.08	24,27,31,34	0
2	SAR	I	3	5/6	0.94	0.10	29,29,32,32	0
2	SAR	J	4	5/6	0.94	0.10	33,34,36,37	0
2	MLE	J	10	9/10	0.95	0.09	25,29,32,41	0
2	A1MFG	I	7	17/18	0.95	0.07	20,24,32,34	0
2	SAR	I	4	5/6	0.95	0.08	25,26,28,28	0
2	AC5	I	9	8/9	0.96	0.07	20,23,28,30	0
2	7T2	I	5	13/14	0.96	0.10	25,27,32,107	0
2	SAR	I	6	5/6	0.98	0.05	22,23,25,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

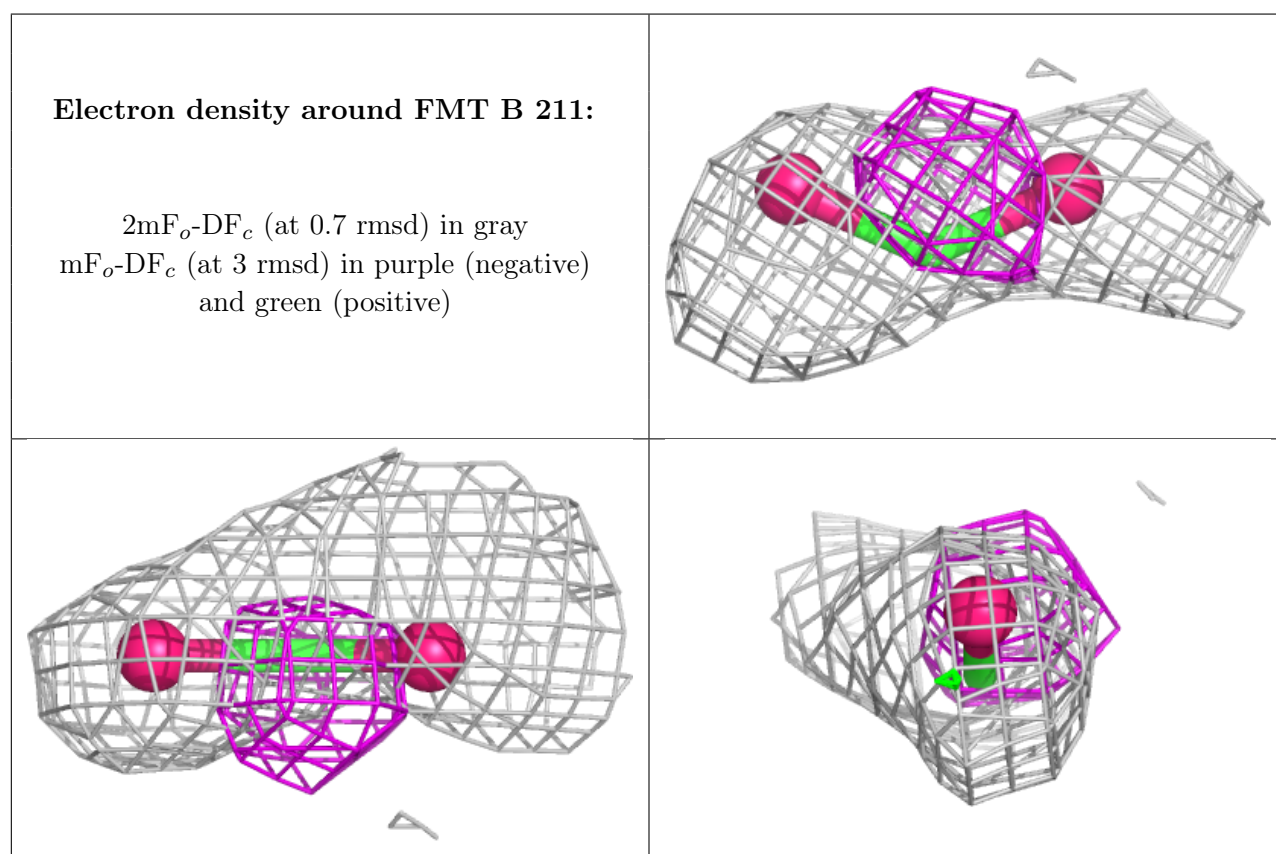
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	206	4/4	0.60	0.22	44,48,50,53	0
4	EDO	A	203	4/4	0.74	0.19	34,34,40,40	0
4	EDO	A	202	4/4	0.74	0.18	30,31,33,33	0
4	EDO	B	206	4/4	0.74	0.17	36,43,44,55	0
4	EDO	B	208	4/4	0.77	0.17	39,41,49,50	0
5	FMT	B	211	3/3	0.80	0.23	40,40,45,45	0
5	FMT	A	205	3/3	0.81	0.18	39,39,46,47	0
4	EDO	I	1501	4/4	0.82	0.21	39,39,39,40	0
5	FMT	A	209	3/3	0.83	0.15	36,36,37,42	0
5	FMT	B	207	3/3	0.83	0.12	46,46,47,47	0
4	EDO	D	202	4/4	0.83	0.26	48,54,54,61	0
4	EDO	A	211	4/4	0.84	0.14	29,36,36,39	0
5	FMT	A	215	3/3	0.84	0.15	47,47,47,50	0
5	FMT	C	903	3/3	0.86	0.20	43,43,44,44	0
5	FMT	C	905	3/3	0.86	0.19	42,42,45,47	0
5	FMT	B	205	3/3	0.87	0.20	45,45,48,51	0
4	EDO	A	204	4/4	0.88	0.14	39,40,41,44	0
5	FMT	B	203	3/3	0.88	0.13	46,46,47,49	0
5	FMT	B	209	3/3	0.88	0.13	34,34,41,44	0
5	FMT	B	210	3/3	0.89	0.19	41,41,42,44	0
5	FMT	B	204	3/3	0.90	0.13	38,38,43,43	0
6	MG	C	907	1/1	0.90	0.07	42,42,42,42	0
6	MG	D	204	1/1	0.90	0.08	47,47,47,47	0
5	FMT	A	208	3/3	0.91	0.14	31,31,37,38	0
4	EDO	B	212	4/4	0.91	0.13	40,41,43,49	0
5	FMT	A	213	3/3	0.92	0.19	44,44,45,49	0
5	FMT	A	210	3/3	0.92	0.09	34,34,39,41	0
5	FMT	A	212	3/3	0.92	0.10	40,40,45,46	0
5	FMT	B	214	3/3	0.92	0.10	37,37,38,41	0
4	EDO	B	202	4/4	0.93	0.13	37,38,38,44	0
5	FMT	B	213	3/3	0.93	0.10	32,32,33,35	0
5	FMT	C	904	3/3	0.93	0.11	44,44,50,50	0
5	FMT	C	901	3/3	0.94	0.09	39,39,41,41	0
4	EDO	A	214	4/4	0.94	0.11	31,37,37,37	0
5	FMT	A	216	3/3	0.95	0.07	34,34,35,36	0
5	FMT	A	207	3/3	0.95	0.12	42,42,43,46	0
3	GDP	B	201	28/28	0.96	0.09	27,37,42,55	0
3	GDP	C	902	28/28	0.96	0.07	35,39,43,48	0
3	GDP	D	201	28/28	0.96	0.09	35,45,51,52	0
3	GDP	A	201	28/28	0.97	0.07	19,25,33,43	0
6	MG	A	218	1/1	0.97	0.03	28,28,28,28	0

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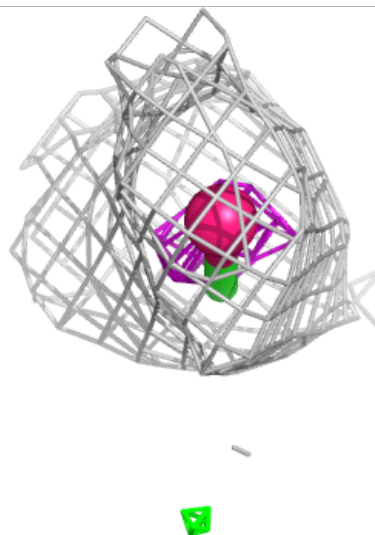
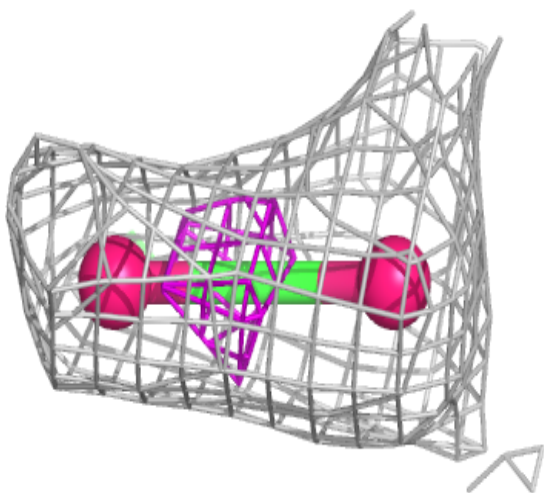
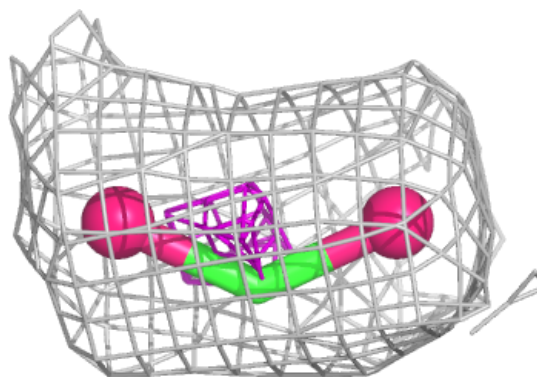
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	B	216	1/1	0.98	0.06	34,34,34,34	0
6	MG	A	217	1/1	0.99	0.03	22,22,22,22	0
6	MG	D	203	1/1	0.99	0.03	41,41,41,41	0
6	MG	C	906	1/1	0.99	0.05	38,38,38,38	0
6	MG	B	215	1/1	1.00	0.02	32,32,32,32	0

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.



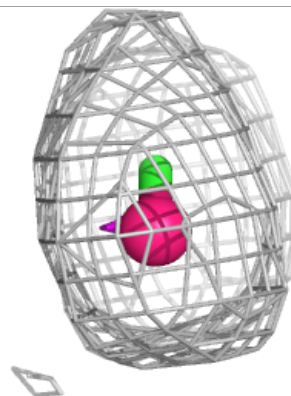
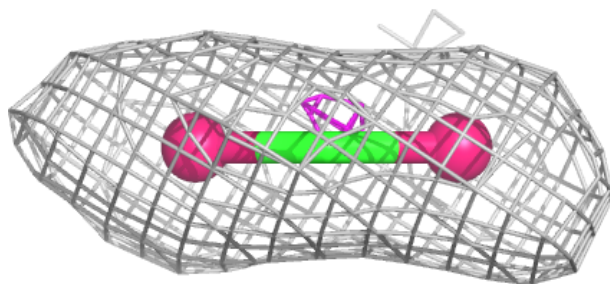
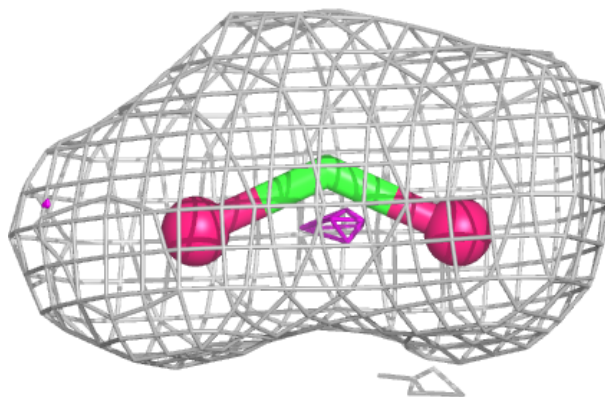
Electron density around FMT A 205:

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



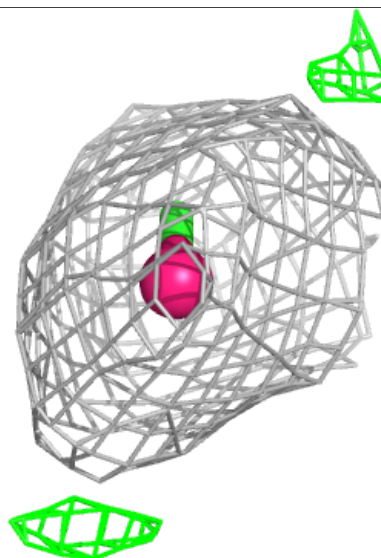
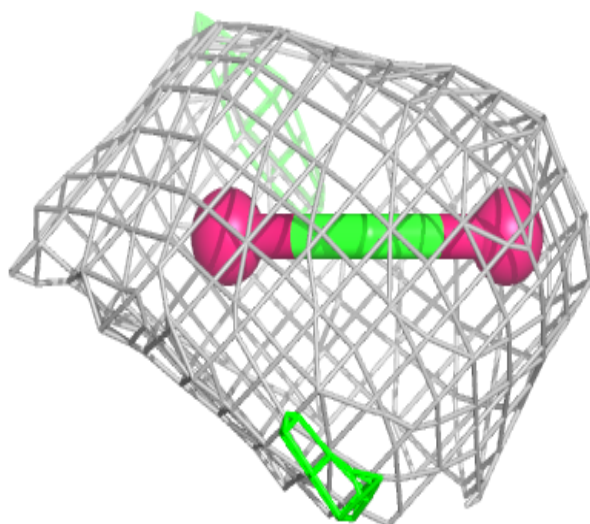
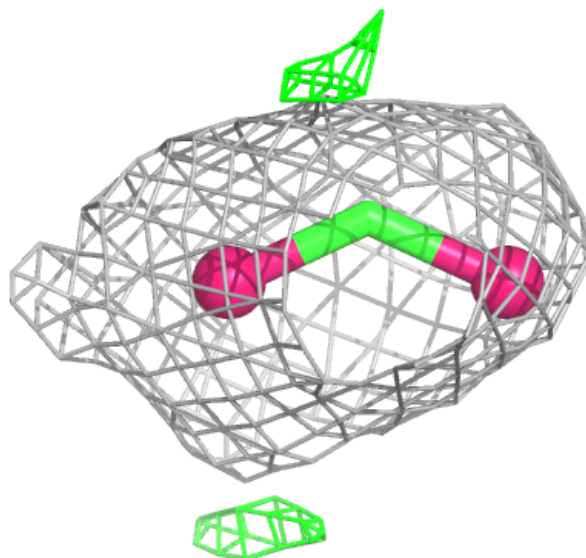
Electron density around FMT A 209:

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



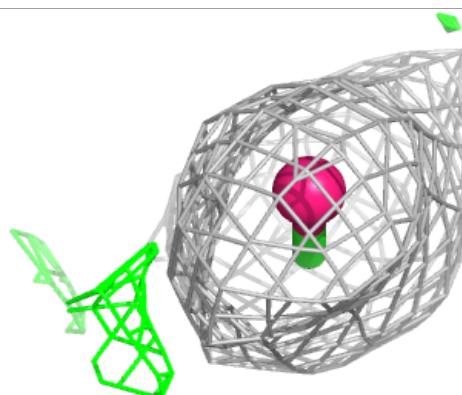
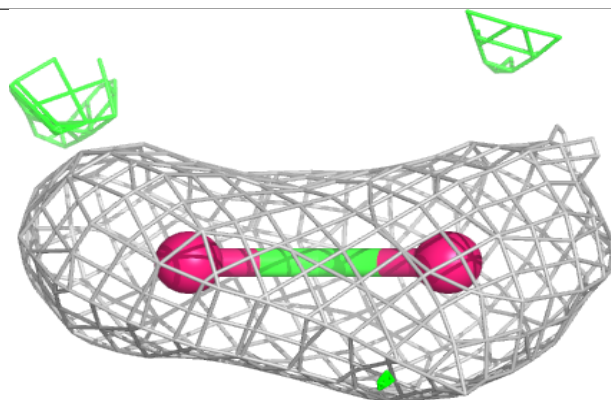
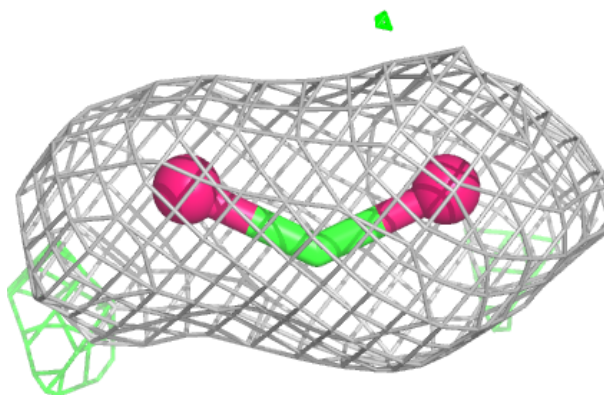
Electron density around FMT B 207:

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



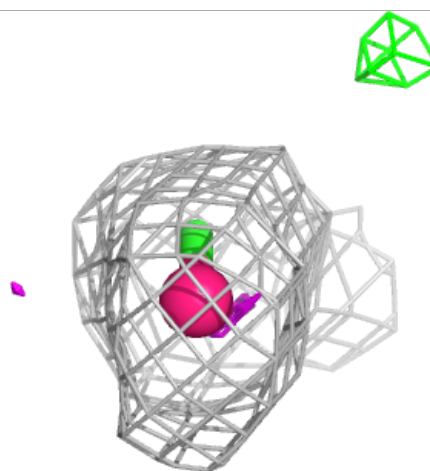
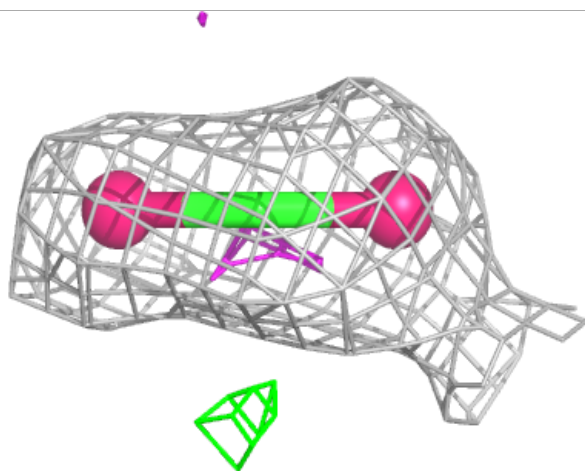
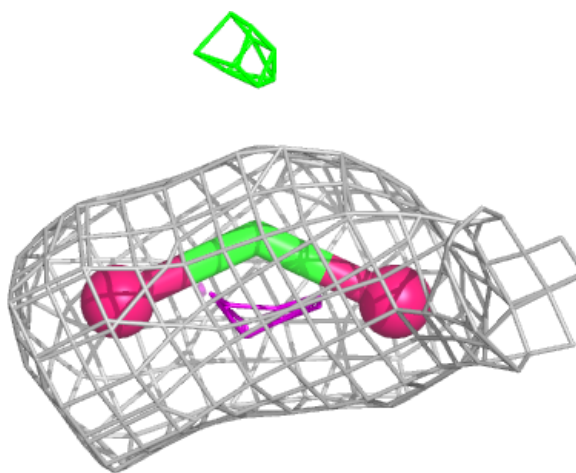
Electron density around FMT A 215:

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



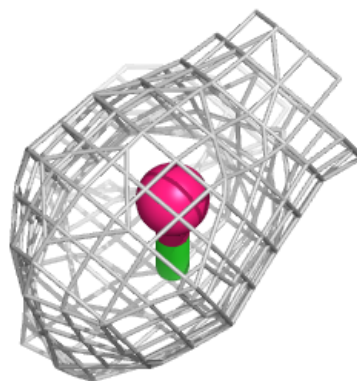
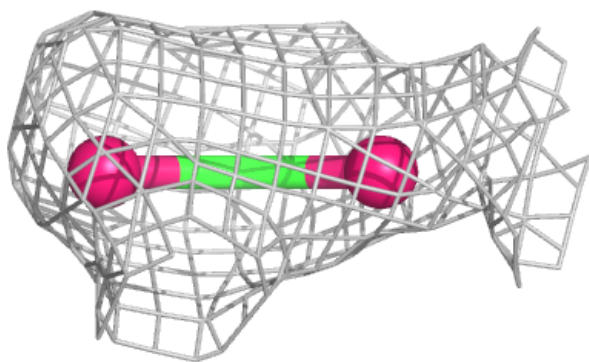
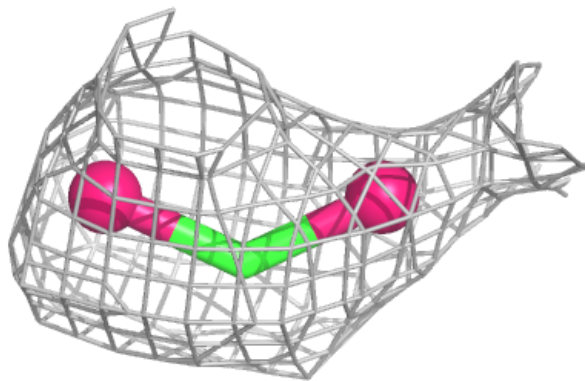
Electron density around FMT C 903:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

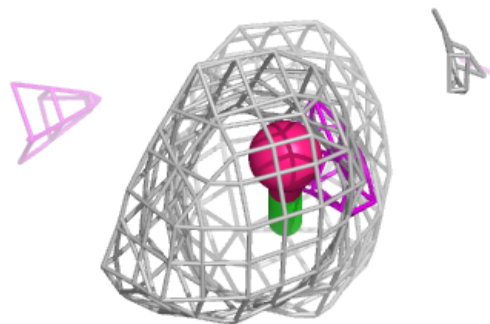
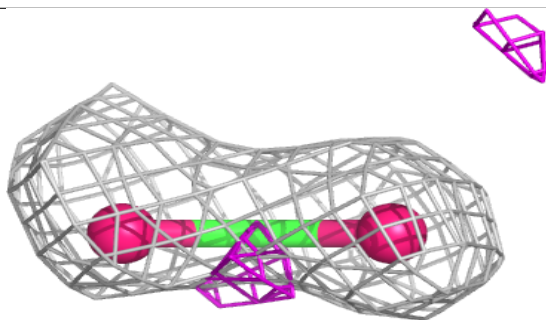
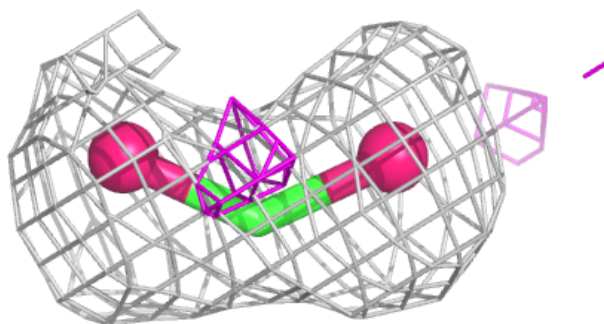


Electron density around FMT C 905:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

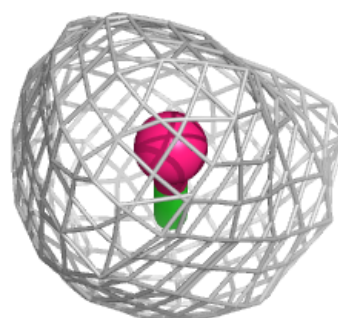
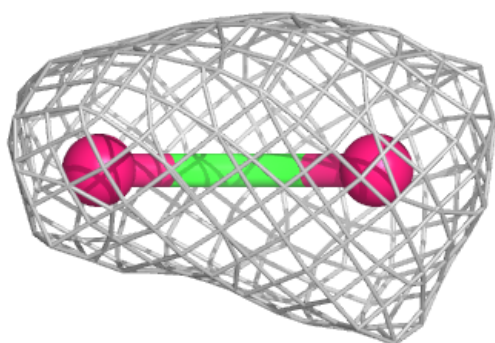
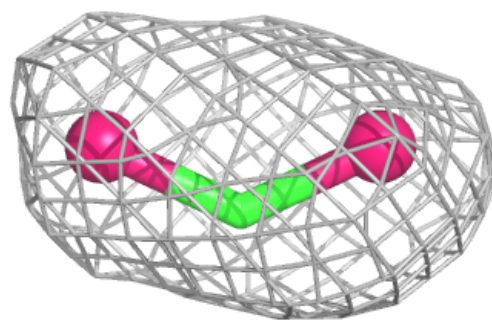
**Electron density around FMT B 205:**

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

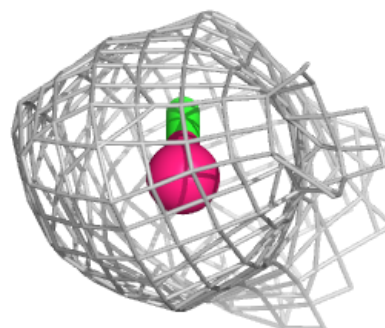
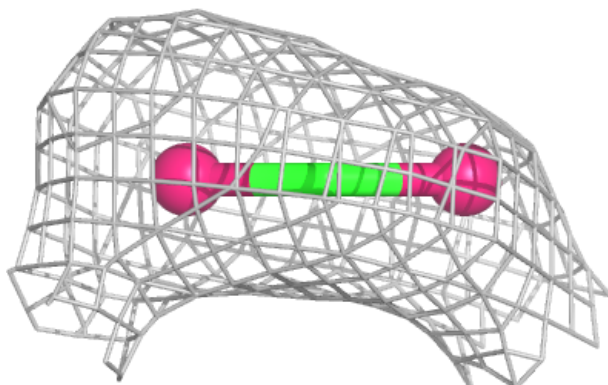
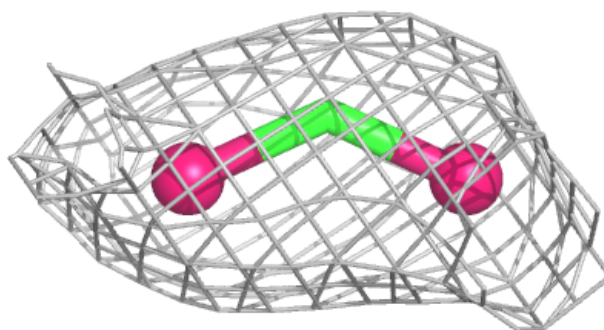


Electron density around FMT B 203:

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

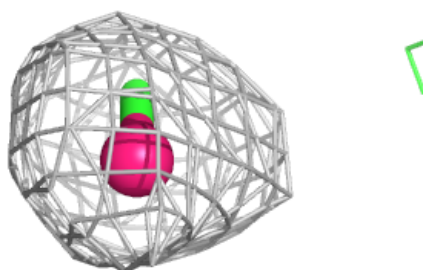
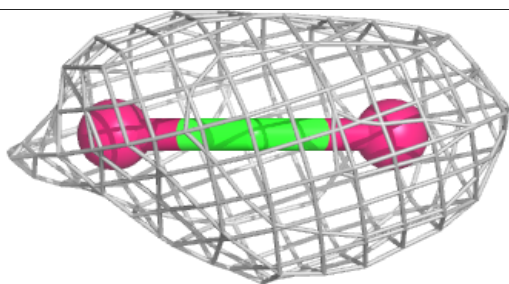
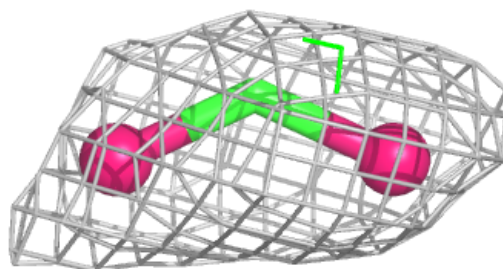
**Electron density around FMT B 209:**

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

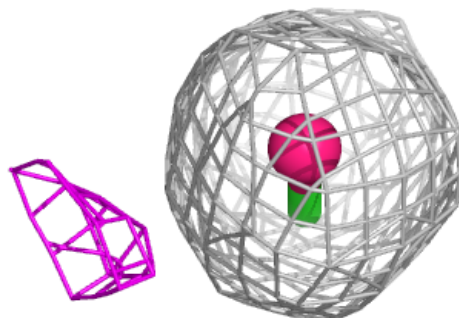
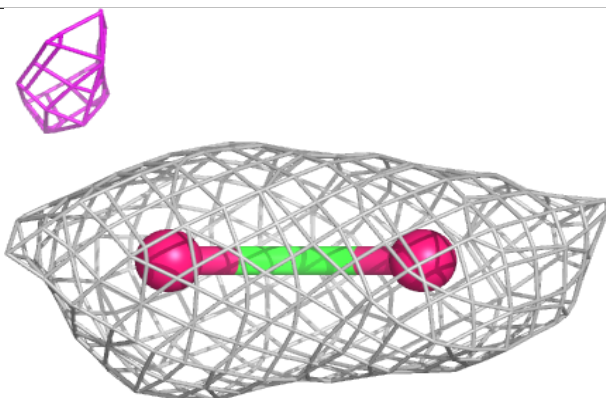
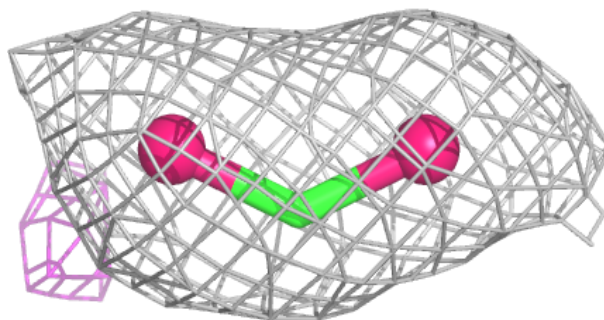


Electron density around FMT B 210:

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

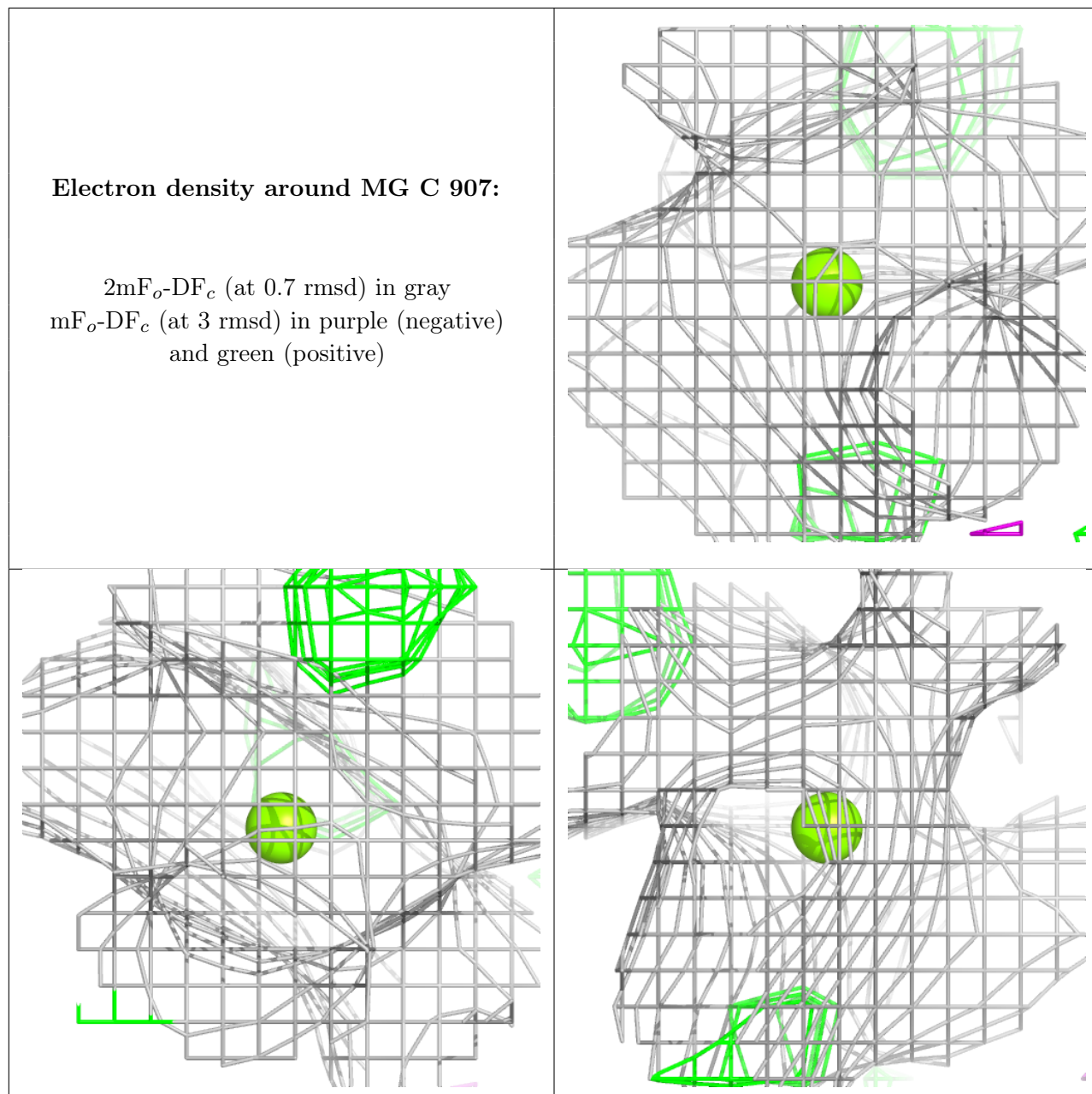
**Electron density around FMT B 204:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



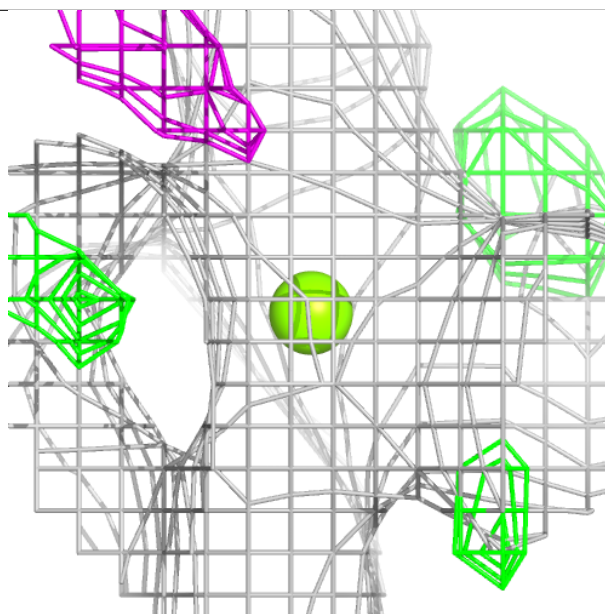
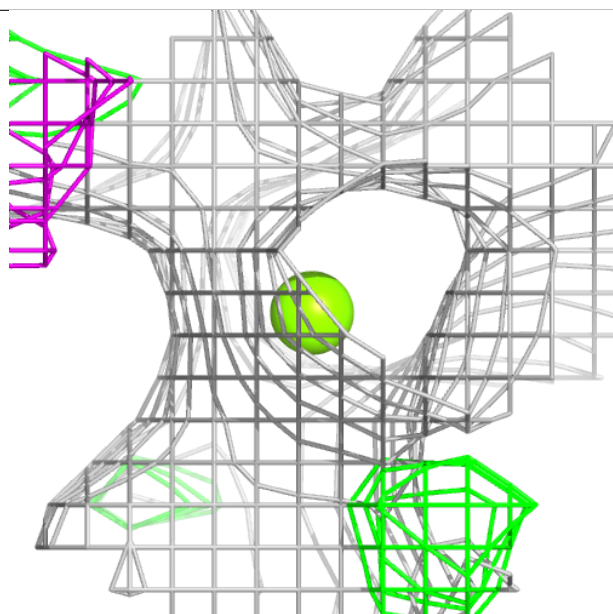
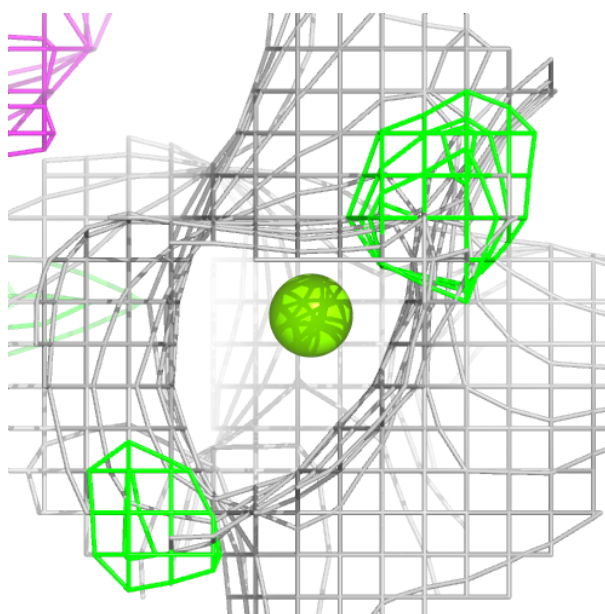
Electron density around MG C 907:

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and green (positive)



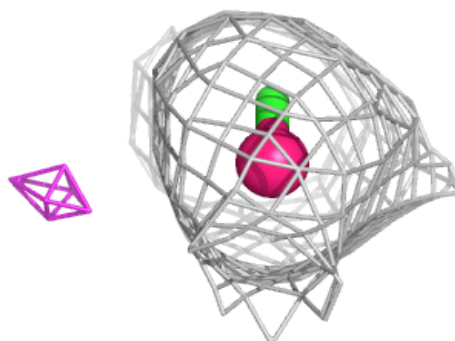
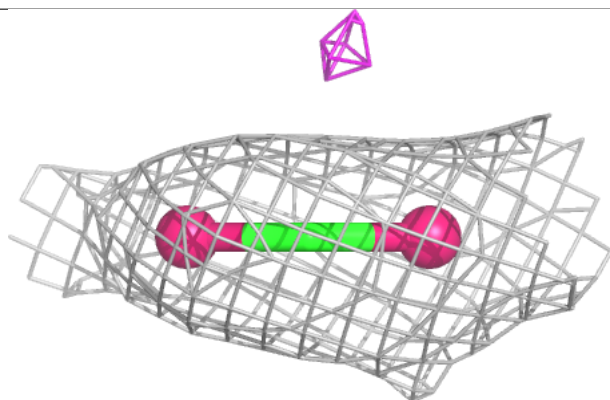
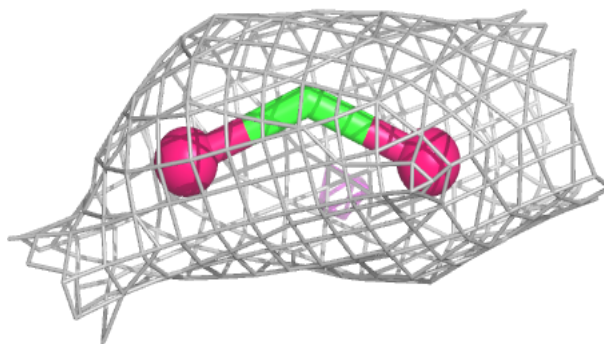
Electron density around MG D 204:

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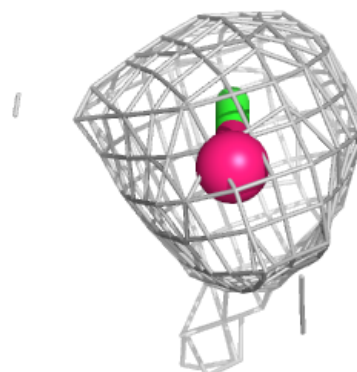
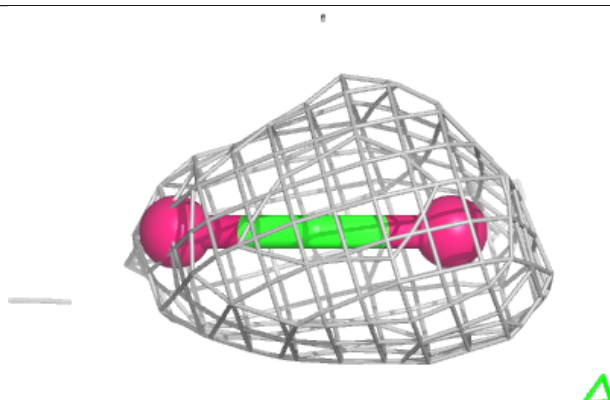
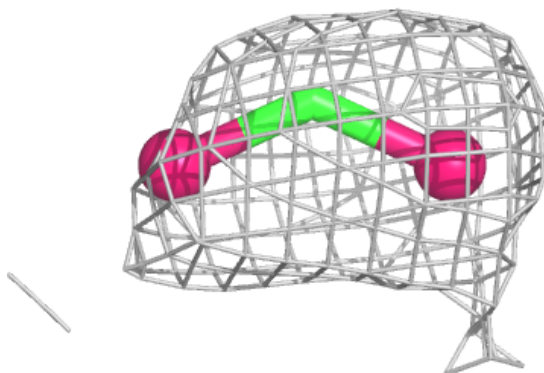


Electron density around FMT A 208:

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

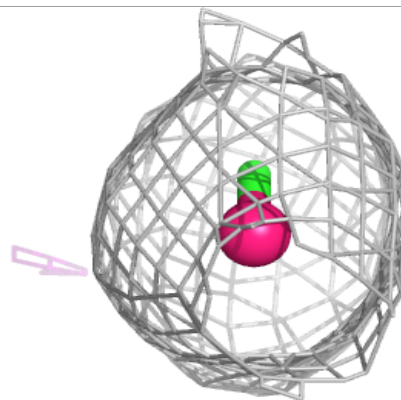
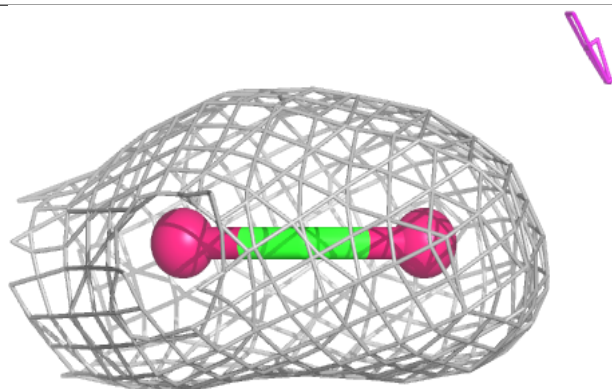
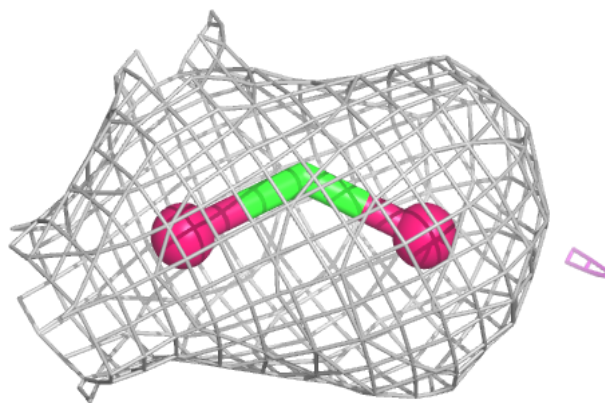
**Electron density around FMT A 213:**

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



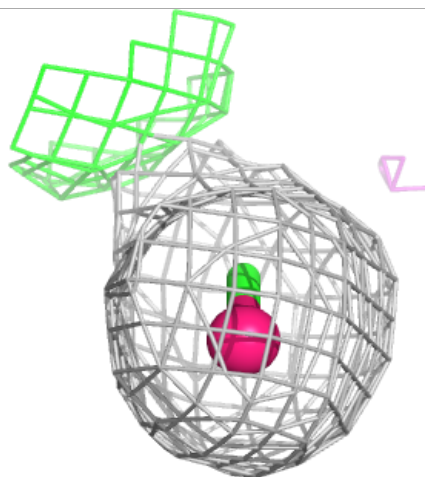
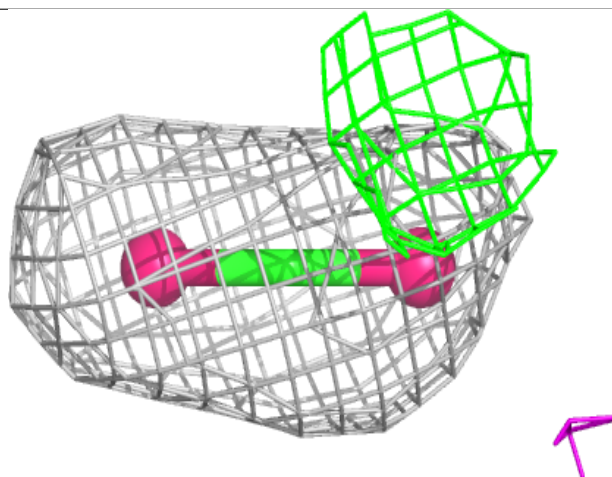
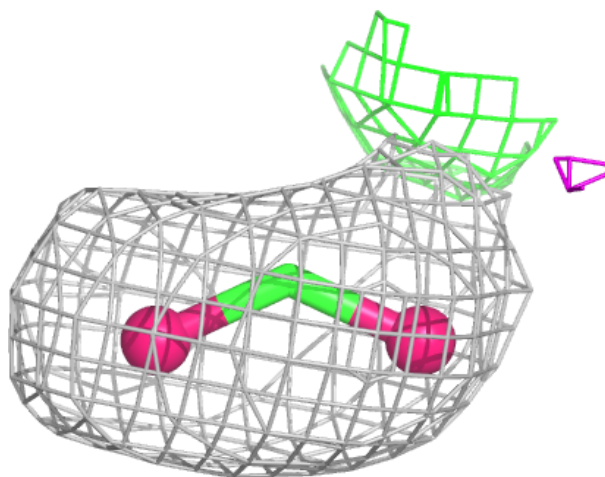
Electron density around FMT A 210:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



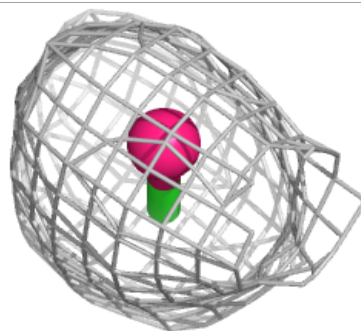
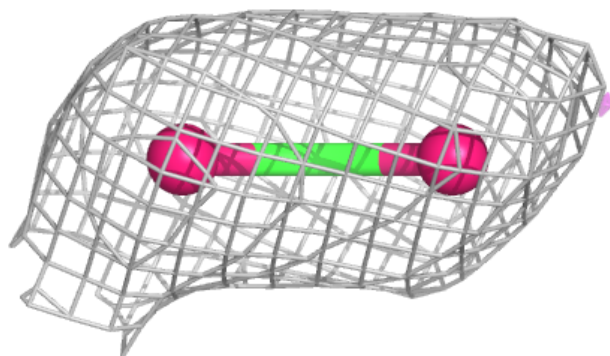
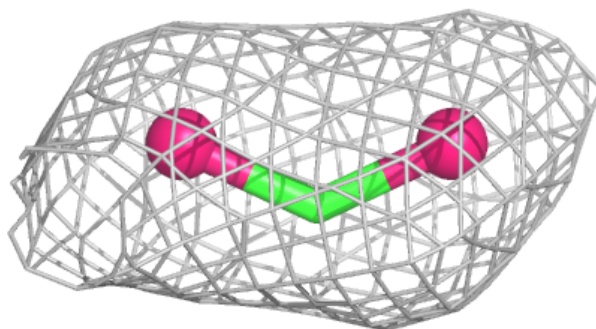
Electron density around FMT A 212:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

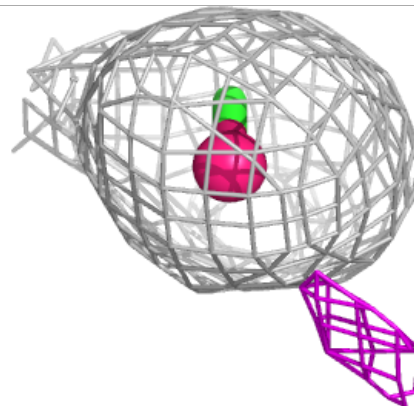
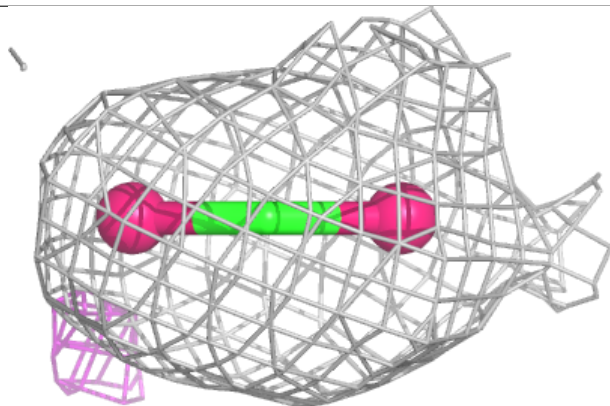
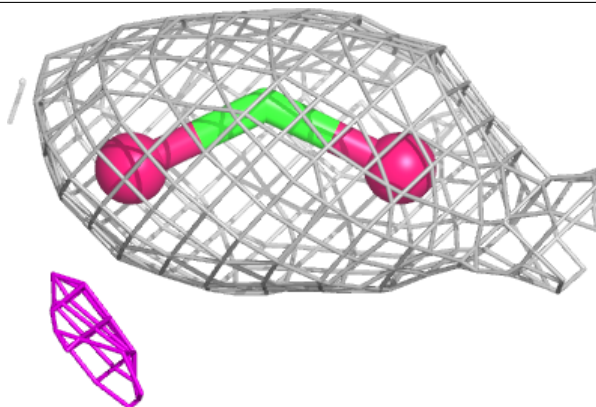


Electron density around FMT B 214:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

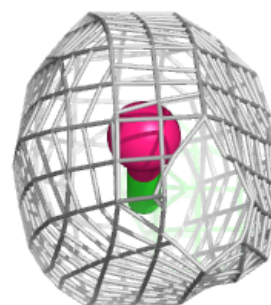
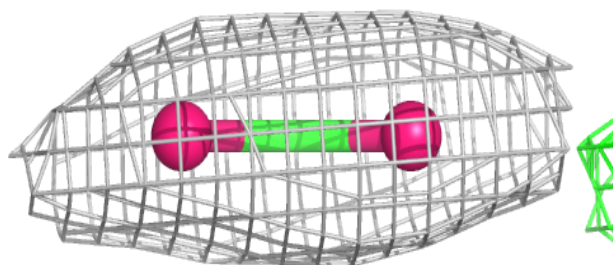
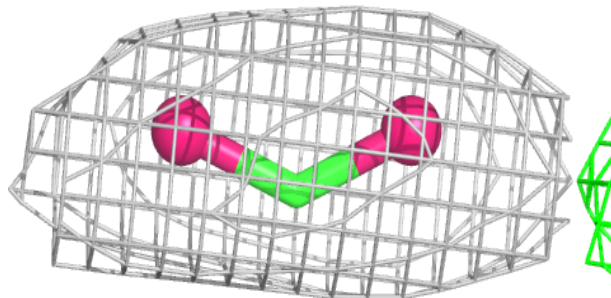
**Electron density around FMT B 213:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

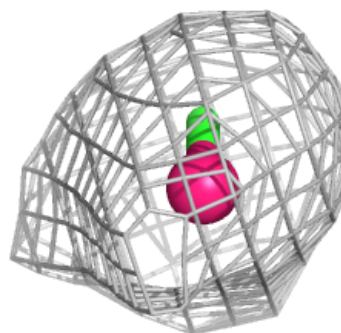
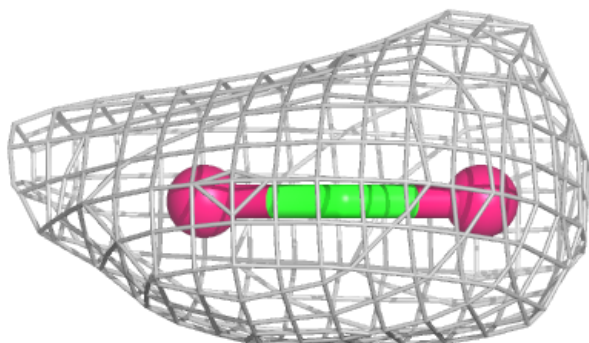
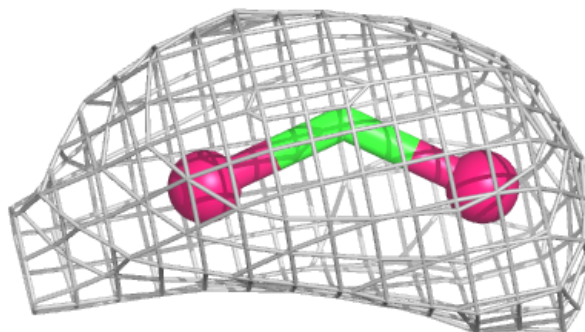


Electron density around FMT C 904:

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

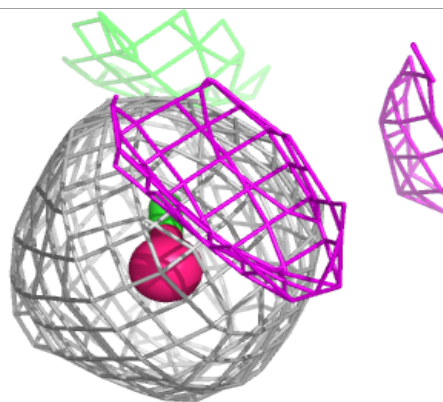
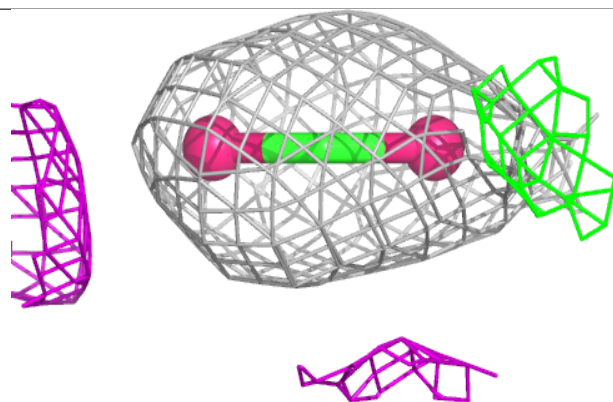
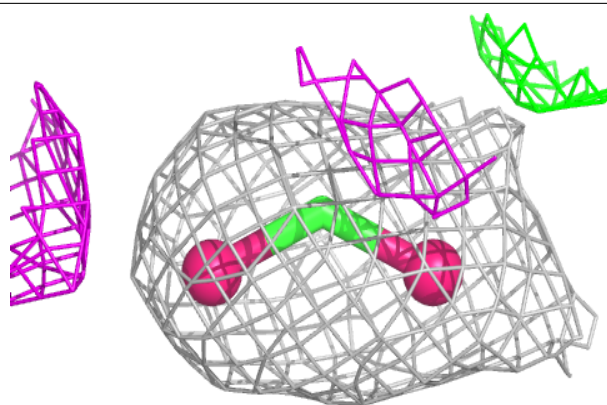
**Electron density around FMT C 901:**

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

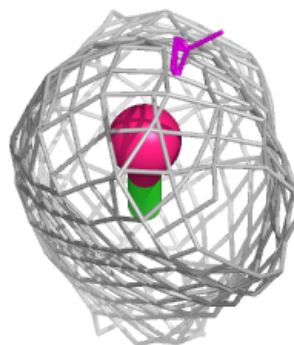
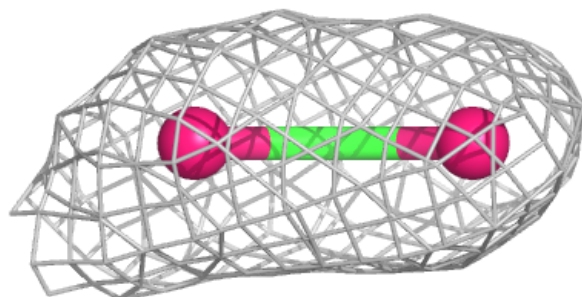
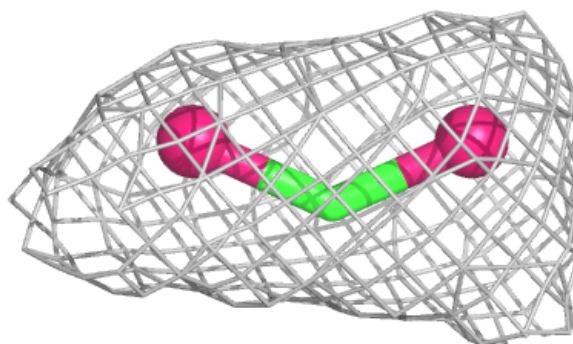


Electron density around FMT A 216:

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

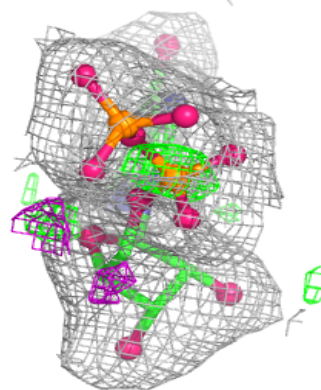
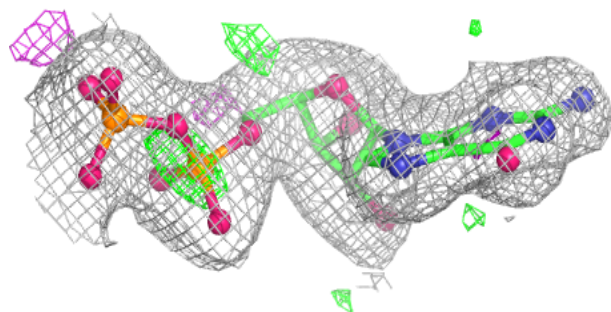
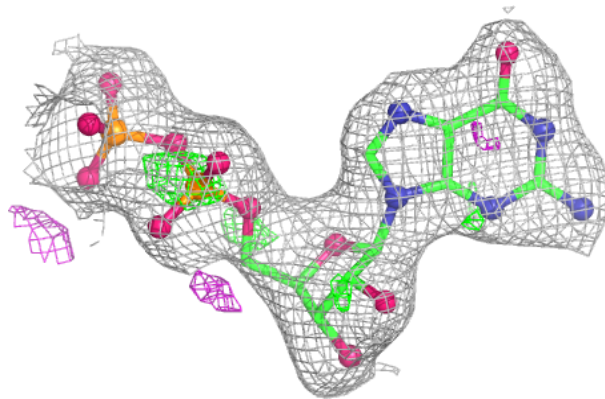
**Electron density around FMT A 207:**

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

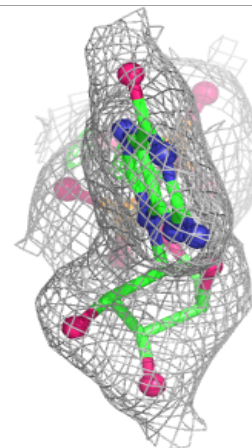
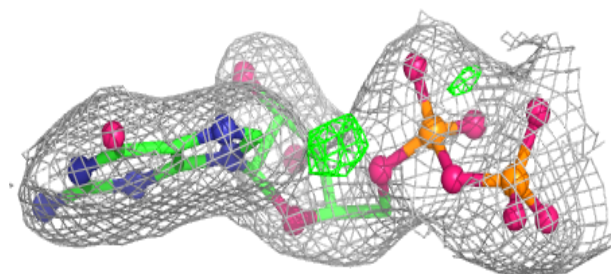
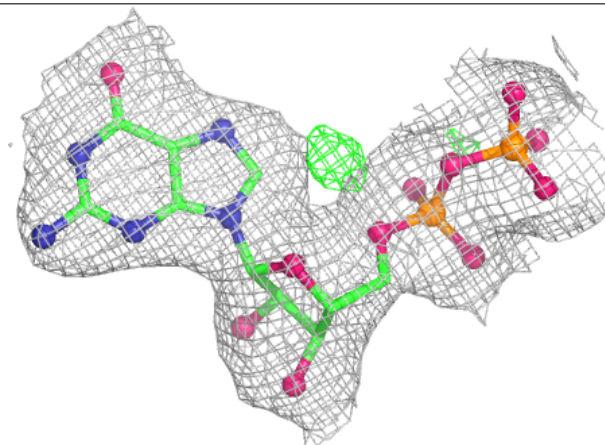


Electron density around GDP B 201:

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

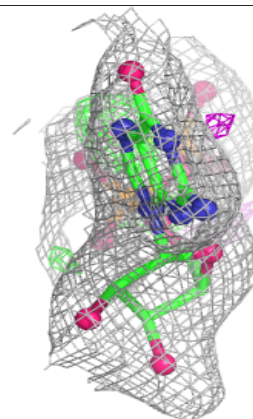
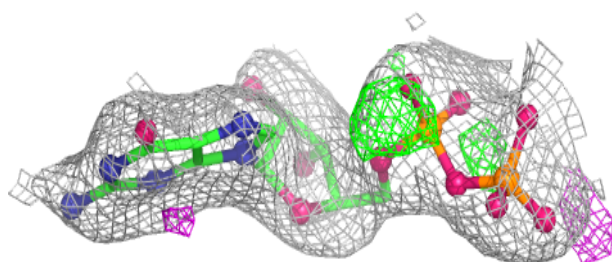
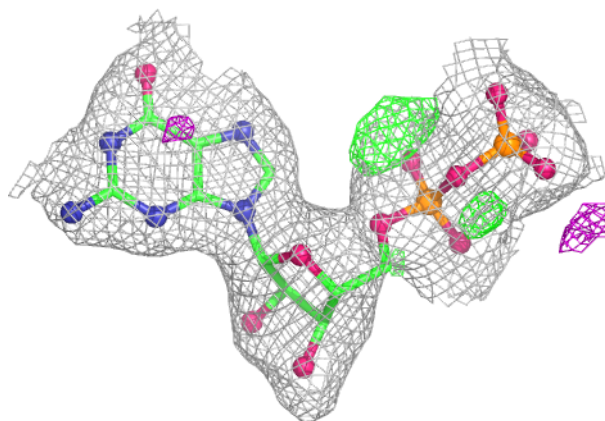
**Electron density around GDP C 902:**

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

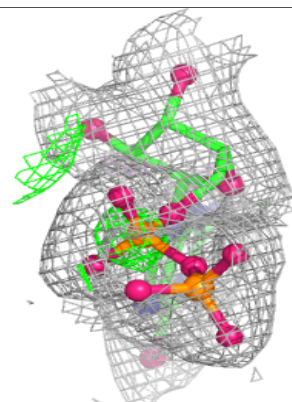
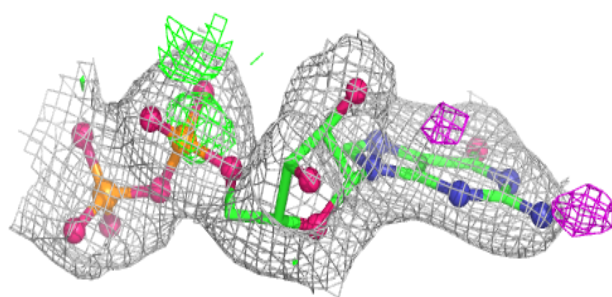
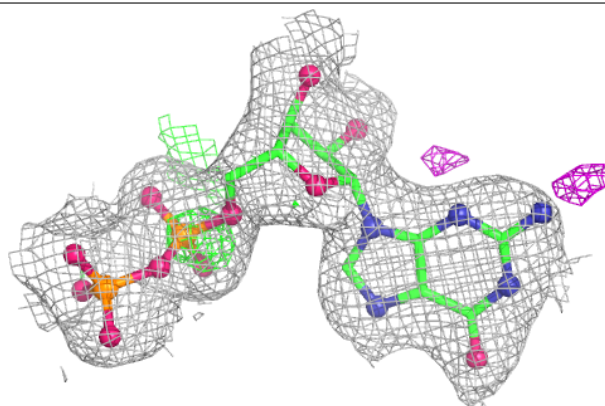


Electron density around GDP D 201:

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

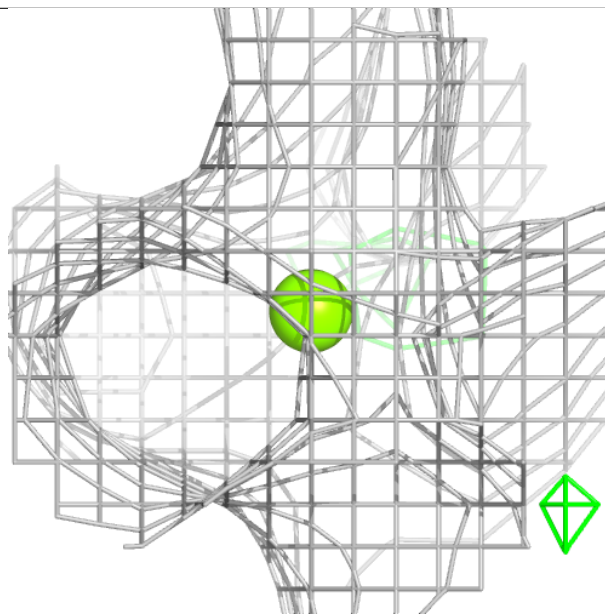
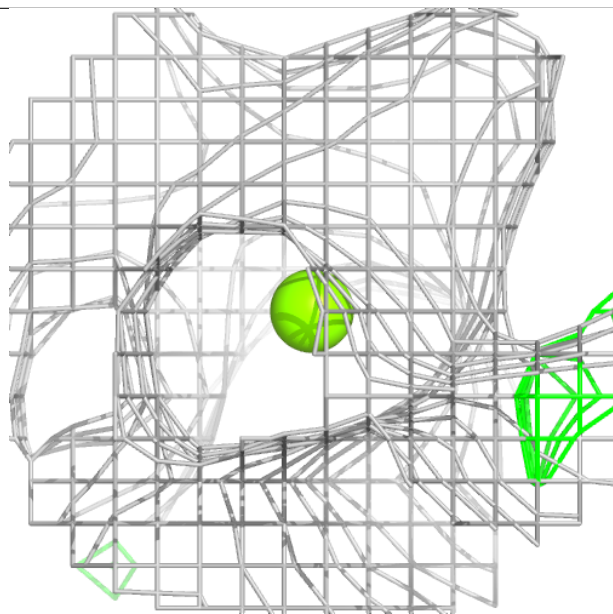
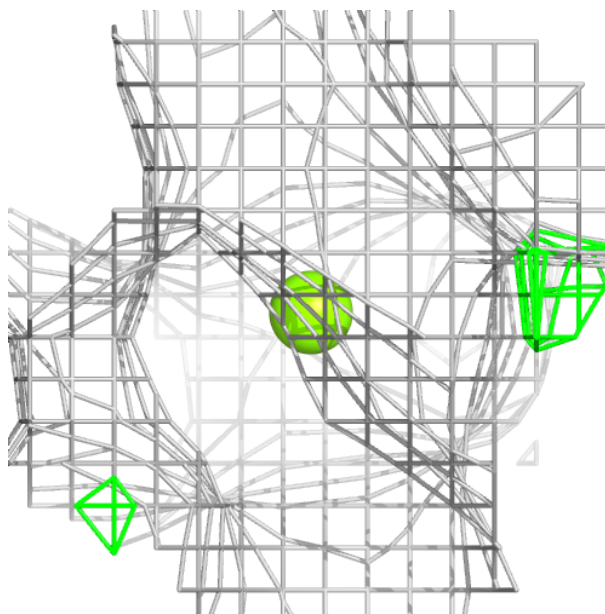
**Electron density around GDP A 201:**

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



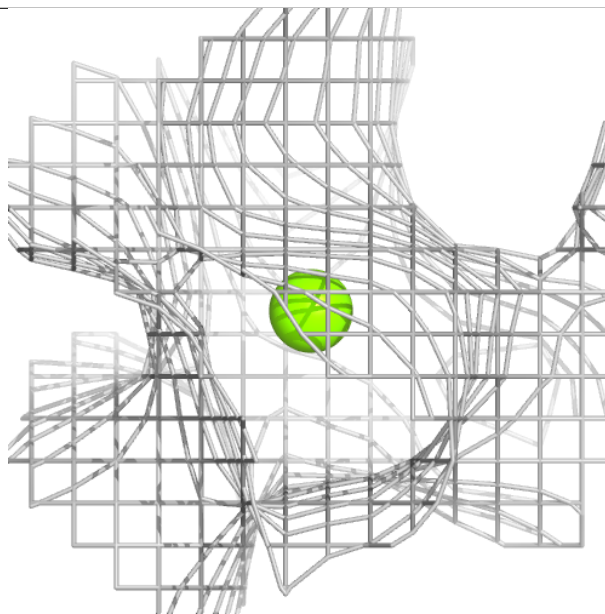
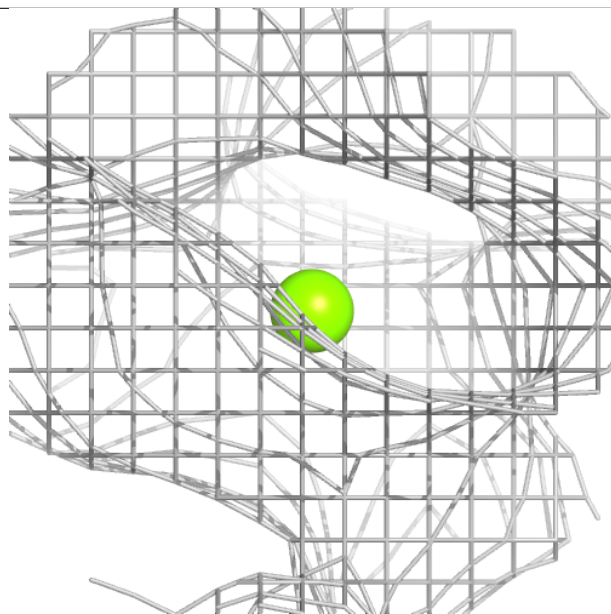
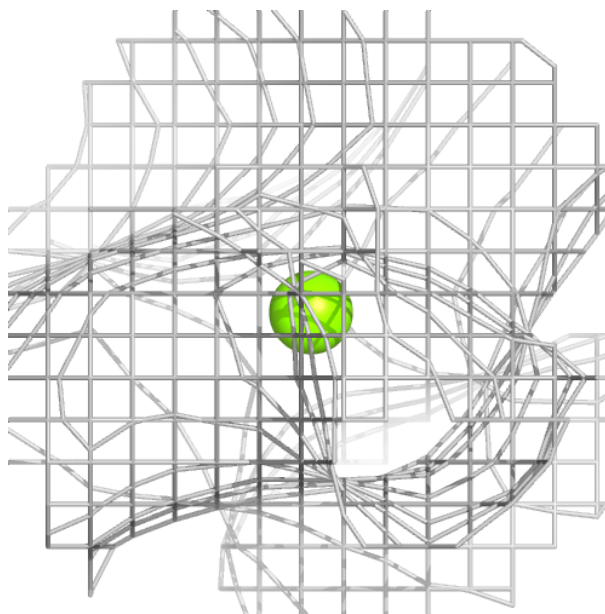
Electron density around MG A 218:

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



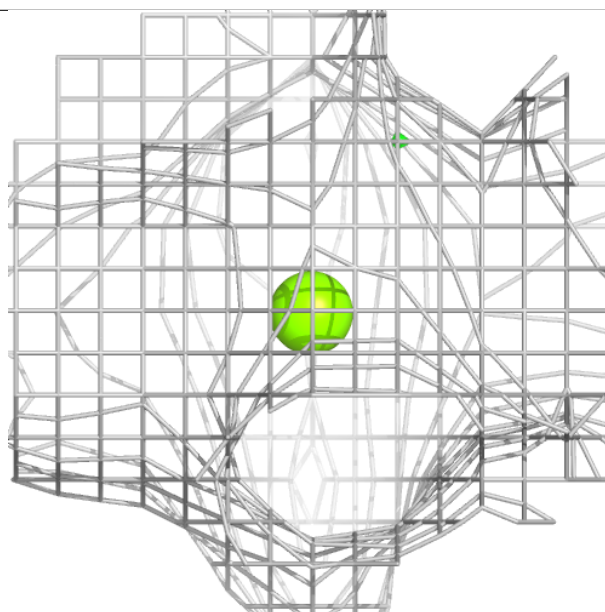
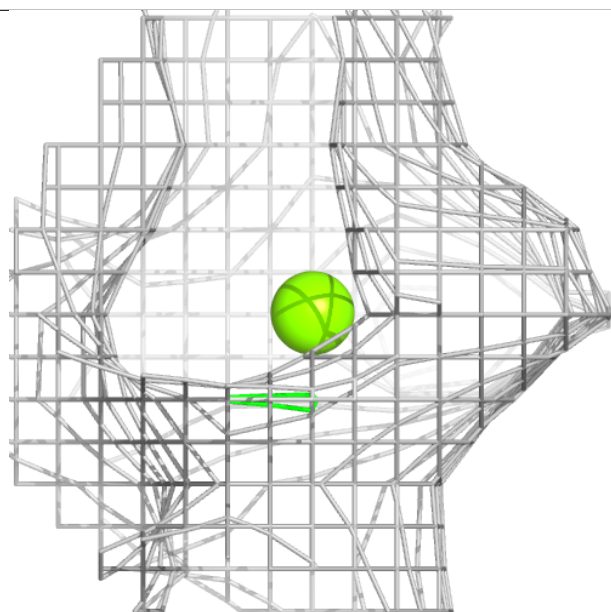
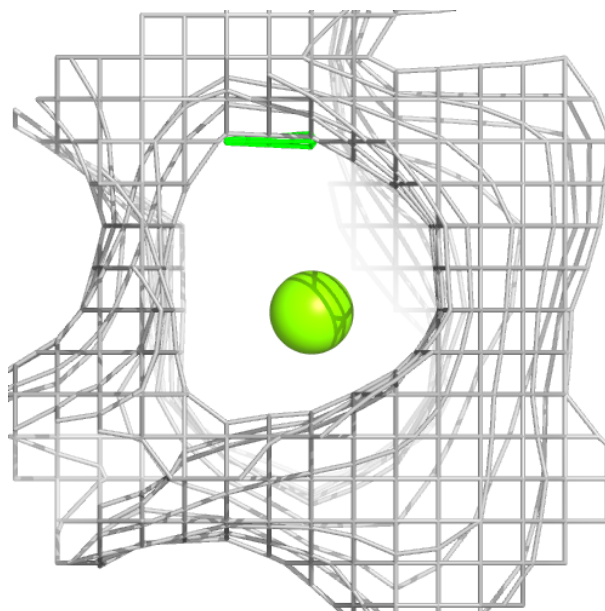
Electron density around MG B 216:

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



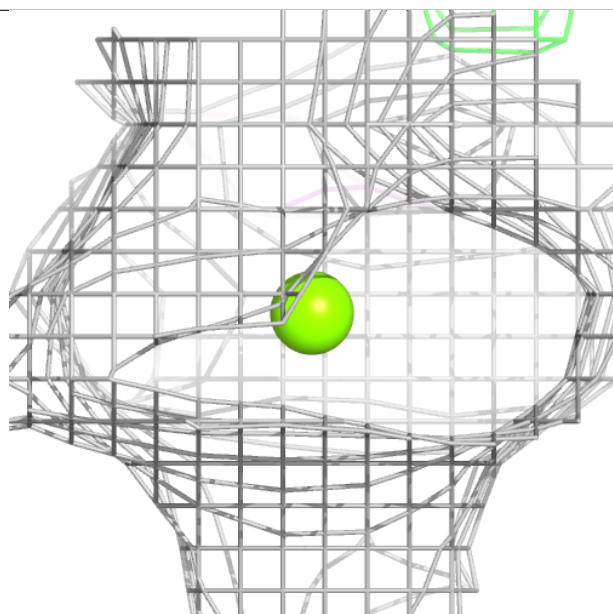
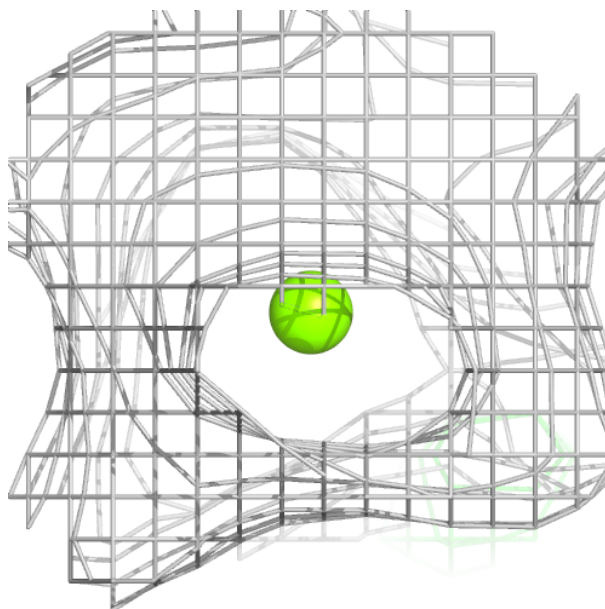
Electron density around MG A 217:

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



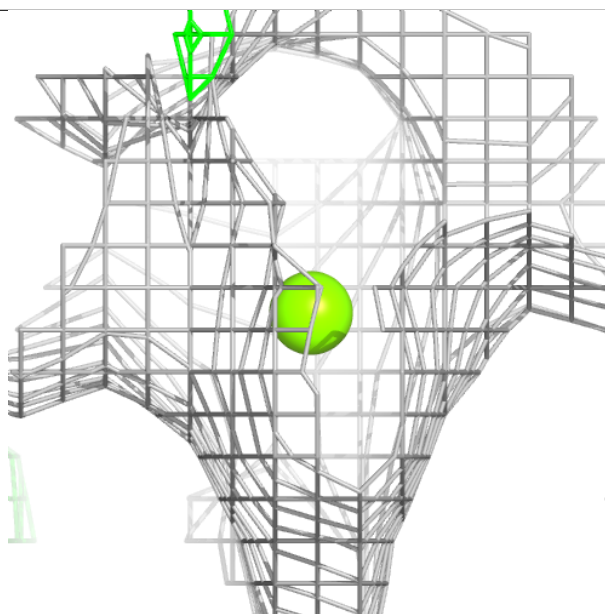
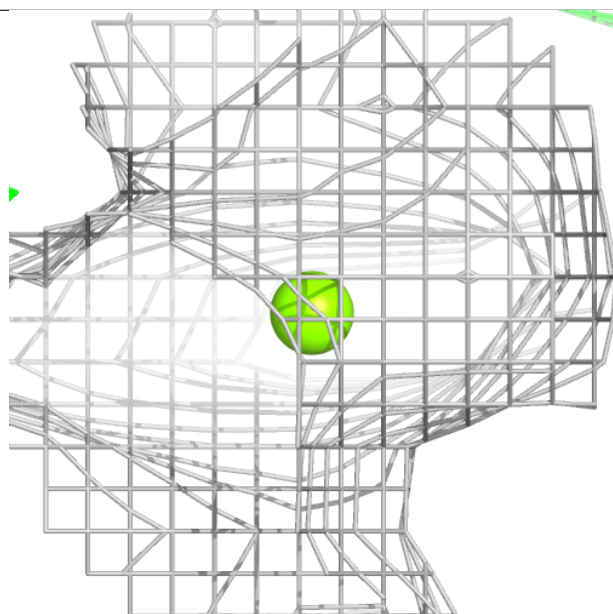
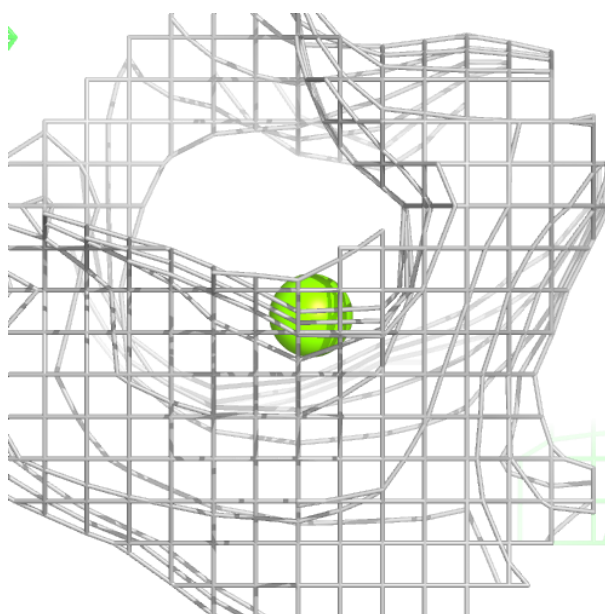
Electron density around MG D 203:

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



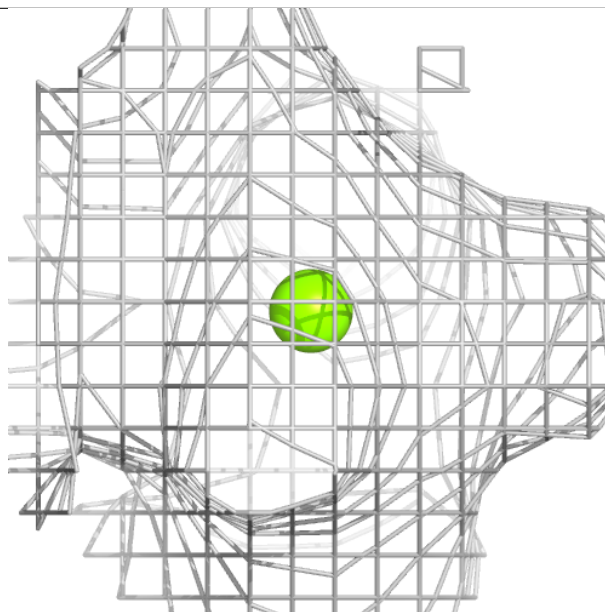
Electron density around MG C 906:

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



Electron density around MG B 215:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.