



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:12 PM UTC

PDB ID : 8FTY / pdb\_00008fty  
Title : Crystal structure of the carotenoid isomeroxygenase, NinaB  
Authors : Kiser, P.D.; Solano, Y.J.  
Deposited on : 2023-01-14  
Resolution : 1.95 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

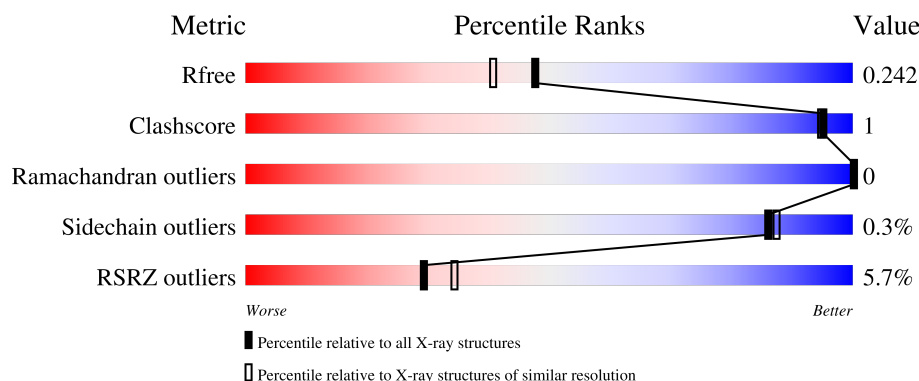
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	509	<div> <div>4%</div> <div>92%</div> <div>5%</div> </div>
1	B	509	<div> <div>6%</div> <div>95%</div> <div>• •</div> </div>
1	C	509	<div> <div>4%</div> <div>91%</div> <div>• 5%</div> </div>
1	D	509	<div> <div>7%</div> <div>94%</div> <div>• •</div> </div>
2	E	509	<div> <div>2%</div> <div>95%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	509	<div><div></div><div>2%</div><div>96%</div><div></div><div></div><div></div></div>
3	G	509	<div><div></div><div>13%</div><div>93%</div><div></div><div></div><div></div></div>
3	H	509	<div><div></div><div>8%</div><div>94%</div><div></div><div></div><div>5%</div></div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 33838 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 carotenoid isomeroxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	2	0
			3851	2453	653	715	30			
1	B	506	Total	C	N	O	S	0	3	0
			4039	2572	686	749	32			
1	C	482	Total	C	N	O	S	0	5	0
			3866	2460	658	716	32			
1	D	497	Total	C	N	O	S	0	5	0
			3976	2534	676	734	32			

- Molecule 2 is a protein called carotenoid isomeroxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	494	Total	C	N	O	S	0	4	0
			3957	2520	674	731	32			
2	F	501	Total	C	N	O	S	0	9	0
			4050	2579	691	746	34			

- Molecule 3 is a protein called carotenoid isomeroxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	490	Total	C	N	O	S	0	2	0
			3887	2472	663	721	31			
3	H	502	Total	C	N	O	S	0	3	0
			4004	2550	682	741	31			

- Molecule 4 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

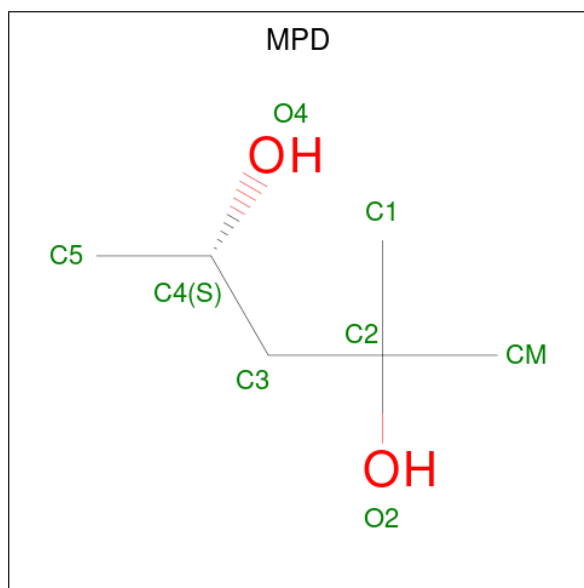
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Fe	0	0
			1	1		
4	C	1	Total	Fe	0	0
			1	1		
4	D	1	Total	Fe	0	0
			1	1		
4	E	1	Total	Fe	0	0
			1	1		
4	F	1	Total	Fe	0	0
			1	1		
4	G	1	Total	Fe	0	0
			1	1		
4	H	1	Total	Fe	0	0
			1	1		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula:  $C_6H_{14}O_2$ ) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	F	1	Total C O 8 6 2	0	0
5	F	1	Total C O 8 6 2	0	0
5	G	1	Total C O 8 6 2	0	0
5	G	1	Total C O 8 6 2	0	0
5	H	1	Total C O 8 6 2	0	0

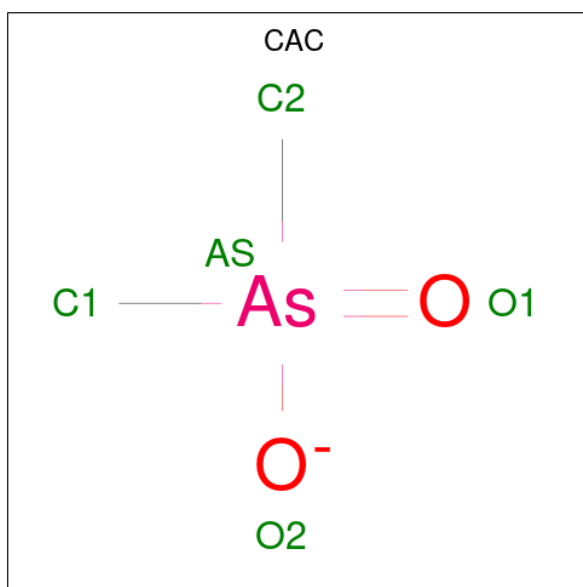
- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	D	1	Total Cl 1 1	0	0
6	E	1	Total Cl 1 1	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total Na 1 1	0	0

- Molecule 8 is CACODYLATE ION (CCD ID: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	1	Total	As	C	O	0	0
			5	1	2	2		

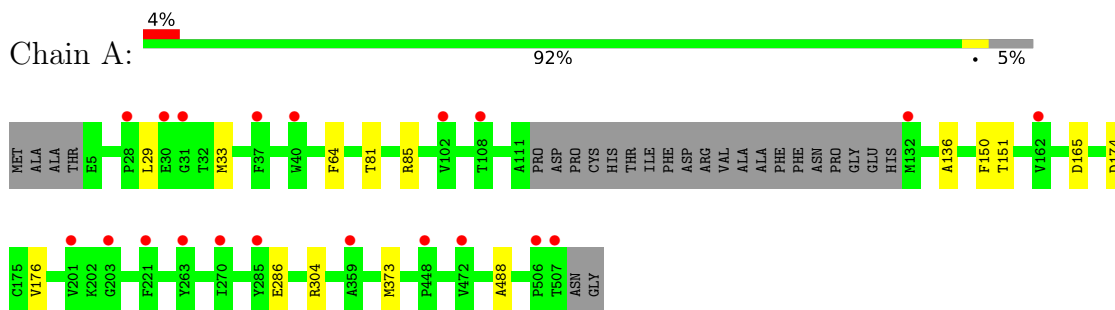
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	193	Total	O	0	0
			193	193		
9	B	314	Total	O	0	0
			314	314		
9	C	241	Total	O	0	0
			241	241		
9	D	242	Total	O	0	0
			242	242		
9	E	333	Total	O	0	0
			333	333		
9	F	337	Total	O	0	0
			337	337		
9	G	210	Total	O	0	0
			210	210		
9	H	201	Total	O	0	0
			201	201		

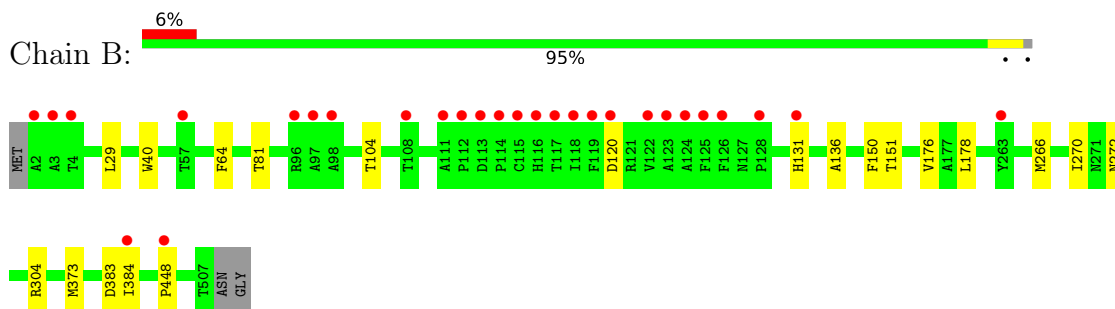
### 3 Residue-property plots [i](#)

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.

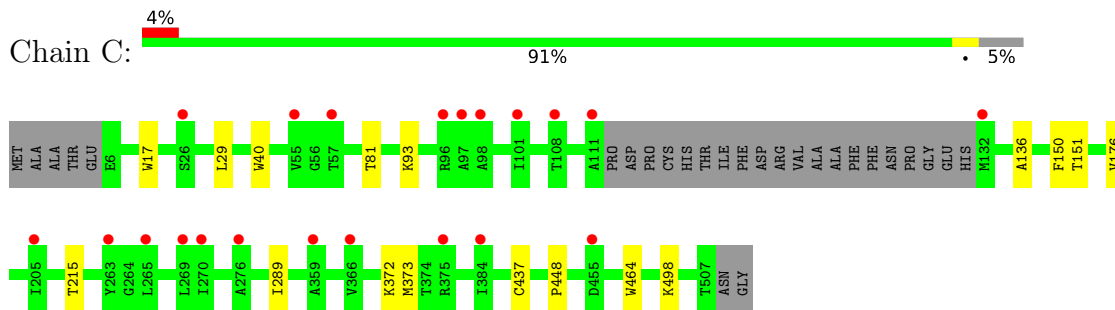
- Molecule 1: carotenoid isomeroxygenase



- Molecule 1: carotenoid isomeroxygenase



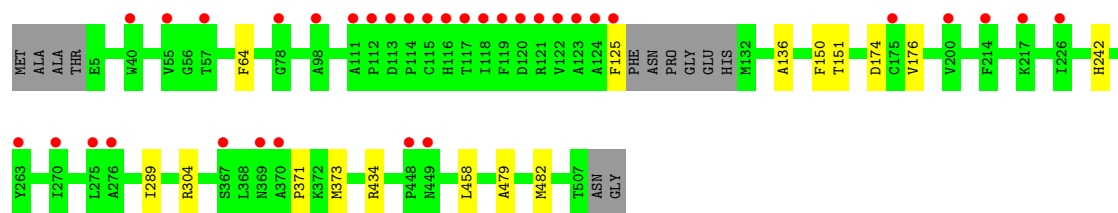
- Molecule 1: carotenoid isomeroxygenase



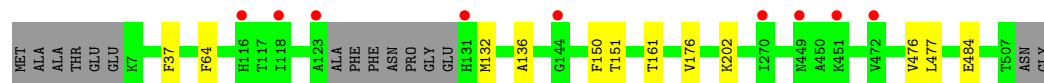
- Molecule 1: carotenoid isomeroxygenase



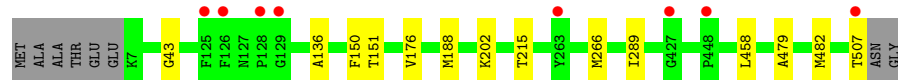




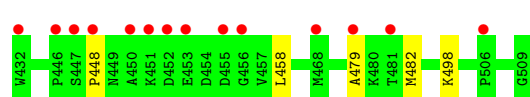
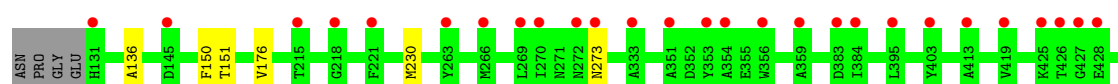
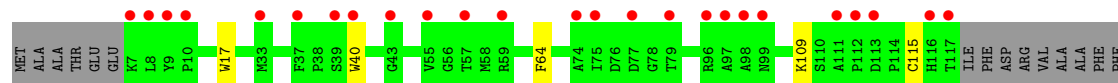
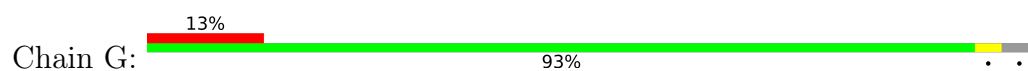
- Molecule 2: carotenoid isomeroxygenase



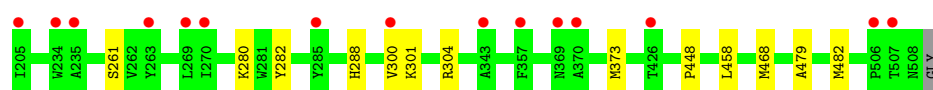
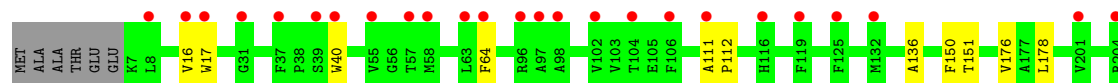
- Molecule 2: carotenoid isomeroxygenase



- Molecule 3: carotenoid isomeroxygenase



- Molecule 3: carotenoid isomeroxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	349.93Å 52.04Å 210.04Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	49.67 – 1.95 49.67 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.67-1.95) 98.7 (49.67-1.95)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, $R_{free}$	0.217 , 0.247 (Not available) , 0.242	Depositor DCC
$R_{free}$ test set	13352 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 32.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	33838	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8251e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, CL, CAC, FE2, CSD, NA, CSO

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	0/3949	0.71	0/5367
1	B	0.46	0/4146	0.73	0/5639
1	C	0.45	0/3964	0.72	0/5387
1	D	0.45	0/4080	0.71	0/5550
2	E	0.45	0/4052	0.73	0/5508
2	F	0.45	0/4150	0.72	0/5640
3	G	0.46	0/3981	0.72	0/5416
3	H	0.45	0/4105	0.72	0/5588
All	All	0.45	0/32427	0.72	0/44095

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	1
1	C	0	1
1	D	0	1
2	E	0	1
2	F	0	1
3	G	0	1
3	H	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	PHE	Peptide
1	B	150	PHE	Peptide
1	C	150	PHE	Peptide
1	D	150	PHE	Peptide
2	E	150	PHE	Peptide
2	F	150	PHE	Peptide
3	G	150	PHE	Peptide
3	H	150	PHE	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3851	0	3777	8	0
1	B	4039	0	3947	10	0
1	C	3866	0	3788	9	0
1	D	3976	0	3879	12	0
2	E	3957	0	3880	8	0
2	F	4050	0	3953	9	0
3	G	3887	0	3787	9	0
3	H	4004	0	3887	16	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	16	0	28	1	0
5	B	8	0	14	1	0
5	C	16	0	28	0	0
5	D	16	0	28	2	0
5	E	24	0	42	1	0
5	F	16	0	28	0	0
5	G	16	0	28	1	0
5	H	8	0	14	1	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1	0	0	0	0
7	D	1	0	0	0	0
8	F	5	0	0	0	0
9	A	193	0	0	0	0
9	B	314	0	0	0	0
9	C	241	0	0	1	0
9	D	242	0	0	1	0
9	E	333	0	0	0	0
9	F	337	0	0	1	0
9	G	210	0	0	0	0
9	H	201	0	0	0	0
All	All	33838	0	31108	76	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 1.

All (76) 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:64:PHE:CZ	5:A:602:MPD:H31	2.36	0.60
1:A:174:ASP:O	2:E:202:LYS:HA	2.04	0.58
3:H:64:PHE:CZ	5:H:1001:MPD:H31	2.40	0.56
2:F:482[A]:MET:HA	2:F:482[A]:MET:HE2	1.88	0.54
1:A:286:GLU:OE1	1:A:304:ARG:HD2	2.07	0.54
1:D:434:ARG:NH2	9:D:2102:HOH:O	2.40	0.54
1:B:64:PHE:CZ	5:B:1001:MPD:H31	2.43	0.53
1:D:242:HIS:CE1	5:D:602:MPD:O2	2.62	0.53
3:H:482[A]:MET:HA	3:H:482[A]:MET:HE2	1.90	0.51
3:G:482:MET:HE2	3:G:482:MET:HA	1.93	0.51
2:E:64:PHE:CZ	5:E:602:MPD:H31	2.46	0.51
3:H:111:ALA:HB1	3:H:112:PRO:HD2	1.93	0.51
1:B:29:LEU:O	1:B:81:THR:HA	2.11	0.50
3:H:288:HIS:CE1	3:H:373:MET:HE1	2.47	0.50
1:A:304:ARG:HD3	1:A:373:MET:HE3	1.92	0.50
3:G:458:LEU:CD1	3:G:482:MET:HE1	2.42	0.50
3:H:261:SER:HB2	3:H:280:LYS:HD2	1.94	0.50
1:D:174:ASP:O	2:F:202:LYS:HA	2.11	0.50
1:C:29:LEU:O	1:C:81:THR:HA	2.11	0.50
1:D:458:LEU:CD1	1:D:482[A]:MET:HE1	2.41	0.50
1:B:104:THR:OG1	1:B:272:ASN:OD1	2.24	0.49
1:C:437[B]:CYS:SG	1:C:464:TRP:NE1	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:458:LEU:CD1	2:F:482[A]:MET:HE1	2.43	0.48
1:D:64:PHE:CZ	5:D:602:MPD:H31	2.49	0.48
1:D:479:ALA:HA	1:D:482[A]:MET:CE	2.44	0.48
1:D:482[A]:MET:HA	1:D:482[A]:MET:HE2	1.95	0.47
1:B:266:MET:O	1:B:270:ILE:HG12	2.14	0.47
1:B:176:VAL:HG13	1:B:178:LEU:HG	1.96	0.47
3:H:176:VAL:HG22	3:H:176:VAL:O	2.15	0.47
3:H:458:LEU:CD1	3:H:482[A]:MET:HE1	2.45	0.47
2:E:37:PHE:CE2	2:E:476[A]:VAL:HG21	2.49	0.47
3:H:280:LYS:HD3	3:H:282:TYR:OH	2.16	0.46
1:B:40:TRP:CD2	1:B:448:PRO:HD3	2.51	0.46
1:D:304:ARG:HD3	1:D:373:MET:HE3	1.98	0.46
1:B:304:ARG:CG	1:B:373:MET:HE3	2.46	0.46
3:H:136:ALA:HA	3:H:151:THR:HB	1.98	0.46
3:H:304:ARG:HD3	3:H:373:MET:HE3	1.97	0.46
1:C:17:TRP:CZ2	1:C:498:LYS:HE3	2.51	0.45
3:H:176:VAL:HG13	3:H:178:LEU:HG	1.96	0.45
1:C:437[B]:CYS:HG	1:C:464:TRP:NE1	2.15	0.45
2:E:37:PHE:CE2	2:E:476[A]:VAL:CG2	2.99	0.45
3:G:109:LYS:HG3	3:G:273:ASN:HA	1.98	0.45
3:H:300:VAL:HG12	3:H:301:LYS:HG3	1.99	0.45
1:B:136:ALA:HA	1:B:151:THR:HB	1.99	0.44
3:G:17:TRP:CZ2	3:G:498:LYS:HE3	2.53	0.44
1:D:371:PRO:HB2	3:H:468:MET:CE	2.47	0.44
2:F:136:ALA:HA	2:F:151:THR:HB	2.00	0.44
3:H:40:TRP:CD2	3:H:448:PRO:HD3	2.52	0.44
2:E:136:ALA:HA	2:E:151:THR:HB	2.00	0.43
1:A:85:ARG:NH1	1:A:165:ASP:OD1	2.47	0.43
1:D:136:ALA:HA	1:D:151:THR:HB	2.00	0.43
3:G:64:PHE:CZ	5:G:602:MPD:H31	2.53	0.43
2:F:188:MET:HE2	9:F:1357:HOH:O	2.18	0.43
1:A:136:ALA:HA	1:A:151:THR:HB	2.00	0.42
3:G:136:ALA:HA	3:G:151:THR:HB	2.01	0.42
1:C:372:LYS:O	1:C:373:MET:HB2	2.19	0.42
2:E:161:THR:H	3:G:115:CSD:HD2	1.60	0.42
2:F:43:GLY:HA2	2:F:507:THR:HG22	2.02	0.42
2:E:37:PHE:CZ	2:E:476[A]:VAL:HG23	2.55	0.42
2:E:477:LEU:HD23	2:E:484:GLU:HA	2.01	0.42
3:H:479:ALA:HA	3:H:482[A]:MET:CE	2.50	0.42
2:F:479:ALA:HA	2:F:482[A]:MET:CE	2.50	0.42
1:A:29:LEU:O	1:A:81:THR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ASP:O	1:B:384:ILE:HG23	2.19	0.42
1:D:125:PHE:HB3	2:F:266[B]:MET:HE3	2.02	0.42
1:C:136:ALA:HA	1:C:151:THR:HB	2.00	0.42
3:H:16:VAL:HG22	3:H:17[B]:TRP:CE3	2.55	0.42
1:A:33:MET:HE1	1:A:488:ALA:HB2	2.02	0.41
1:B:120:ASP:OD1	1:B:131:HIS:NE2	2.46	0.41
1:C:40:TRP:CD2	1:C:448:PRO:HD3	2.55	0.41
3:G:479:ALA:HA	3:G:482:MET:CE	2.50	0.41
1:C:289:ILE:HD12	1:C:289:ILE:N	2.36	0.41
3:G:40:TRP:CD2	3:G:448:PRO:HD3	2.55	0.41
2:F:289:ILE:HD12	2:F:289:ILE:N	2.36	0.41
1:C:93:LYS:HG3	9:C:1310:HOH:O	2.20	0.40
1:D:289:ILE:HD12	1:D:289:ILE:N	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	481/509 (94%)	467 (97%)	14 (3%)	0	100	100
1	B	507/509 (100%)	492 (97%)	15 (3%)	0	100	100
1	C	483/509 (95%)	469 (97%)	14 (3%)	0	100	100
1	D	498/509 (98%)	481 (97%)	17 (3%)	0	100	100
2	E	493/509 (97%)	479 (97%)	14 (3%)	0	100	100
2	F	507/509 (100%)	491 (97%)	16 (3%)	0	100	100
3	G	487/509 (96%)	472 (97%)	15 (3%)	0	100	100
3	H	502/509 (99%)	487 (97%)	15 (3%)	0	100	100
All	All	3958/4072 (97%)	3838 (97%)	120 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	425/444 (96%)	424 (100%)	1 (0%)	87	89
1	B	445/444 (100%)	445 (100%)	0	100	100
1	C	427/444 (96%)	425 (100%)	2 (0%)	81	82
1	D	437/444 (98%)	436 (100%)	1 (0%)	87	89
2	E	437/443 (99%)	435 (100%)	2 (0%)	81	82
2	F	445/443 (100%)	443 (100%)	2 (0%)	84	85
3	G	426/443 (96%)	424 (100%)	2 (0%)	81	82
3	H	438/443 (99%)	438 (100%)	0	100	100
All	All	3480/3548 (98%)	3470 (100%)	10 (0%)	86	87

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

Mol	Chain	Res	Type
1	A	176	VAL
1	C	176	VAL
1	C	215	THR
1	D	176	VAL
2	E	132	MET
2	E	176	VAL
2	F	176	VAL
2	F	215	THR
3	G	176	VAL
3	G	230	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	HIS

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Mol	Chain	Res	Type
1	B	90	ASN
1	B	99	ASN
1	B	169	GLN
1	C	90	ASN
1	C	99	ASN
1	C	169	GLN
2	E	90	ASN
2	E	169	GLN
2	E	491	ASN
3	G	273	ASN
3	H	90	ASN
3	H	99	ASN
3	H	157	HIS
3	H	169	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z  > 2$
3	CSD	G	115	3	4,7,8	0.67	0	1,8,10	0.27	0
2	CSO	E	115	2	3,6,7	0.70	0	1,6,8	0.39	0
2	CSO	F	115	2	3,6,7	0.74	0	1,6,8	0.41	0
3	CSD	H	115	3	4,7,8	0.84	0	1,8,10	0.49	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	CSD	G	115	3	-	1/2/6/8	-
2	CSO	E	115	2	-	1/1/5/7	-
2	CSO	F	115	2	-	0/1/5/7	-
3	CSD	H	115	3	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	115	CSO	N-CA-CB-SG
3	G	115	CSD	CA-CB-SG-OD1
3	H	115	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	115	CSD	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 12 are monoatomic - leaving 16 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	MPD	A	602	-	7,7,7	0.17	0	9,10,10	0.34	0
5	MPD	G	602	-	7,7,7	0.16	0	9,10,10	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MPD	F	1001	-	7,7,7	0.11	0	9,10,10	0.38	0
5	MPD	E	602	-	7,7,7	0.16	0	9,10,10	0.34	0
5	MPD	E	604	-	7,7,7	0.12	0	9,10,10	0.36	0
5	MPD	C	602	-	7,7,7	0.13	0	9,10,10	0.37	0
5	MPD	D	603	-	7,7,7	0.14	0	9,10,10	0.34	0
5	MPD	F	1002	-	7,7,7	0.16	0	9,10,10	0.34	0
5	MPD	B	1001	-	7,7,7	0.15	0	9,10,10	0.32	0
5	MPD	G	603	-	7,7,7	0.13	0	9,10,10	0.36	0
5	MPD	C	603	-	7,7,7	0.15	0	9,10,10	0.39	0
5	MPD	E	603	-	7,7,7	0.14	0	9,10,10	0.38	0
8	CAC	F	1003	-	2,4,4	2.91	2 (100%)	4,6,6	1.35	1 (25%)
5	MPD	H	1001	-	7,7,7	0.15	0	9,10,10	0.32	0
5	MPD	A	604	-	7,7,7	0.15	0	9,10,10	0.29	0
5	MPD	D	602	-	7,7,7	0.15	0	9,10,10	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	A	602	-	-	0/5/5/5	-
5	MPD	G	602	-	-	1/5/5/5	-
5	MPD	F	1001	-	-	0/5/5/5	-
5	MPD	E	602	-	-	0/5/5/5	-
5	MPD	E	604	-	-	0/5/5/5	-
5	MPD	C	602	-	-	0/5/5/5	-
5	MPD	D	603	-	-	0/5/5/5	-
5	MPD	F	1002	-	-	0/5/5/5	-
5	MPD	B	1001	-	-	0/5/5/5	-
5	MPD	G	603	-	-	2/5/5/5	-
5	MPD	C	603	-	-	2/5/5/5	-
5	MPD	E	603	-	-	0/5/5/5	-
5	MPD	H	1001	-	-	0/5/5/5	-
5	MPD	A	604	-	-	0/5/5/5	-
5	MPD	D	602	-	-	0/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	1003	CAC	AS-C1	2.93	1.97	1.90
8	F	1003	CAC	AS-C2	2.88	1.97	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
8	F	1003	CAC	O1-AS-C1	-2.01	109.00	111.50

There are no chirality outliers.

All (5) torsion outliers are listed below:

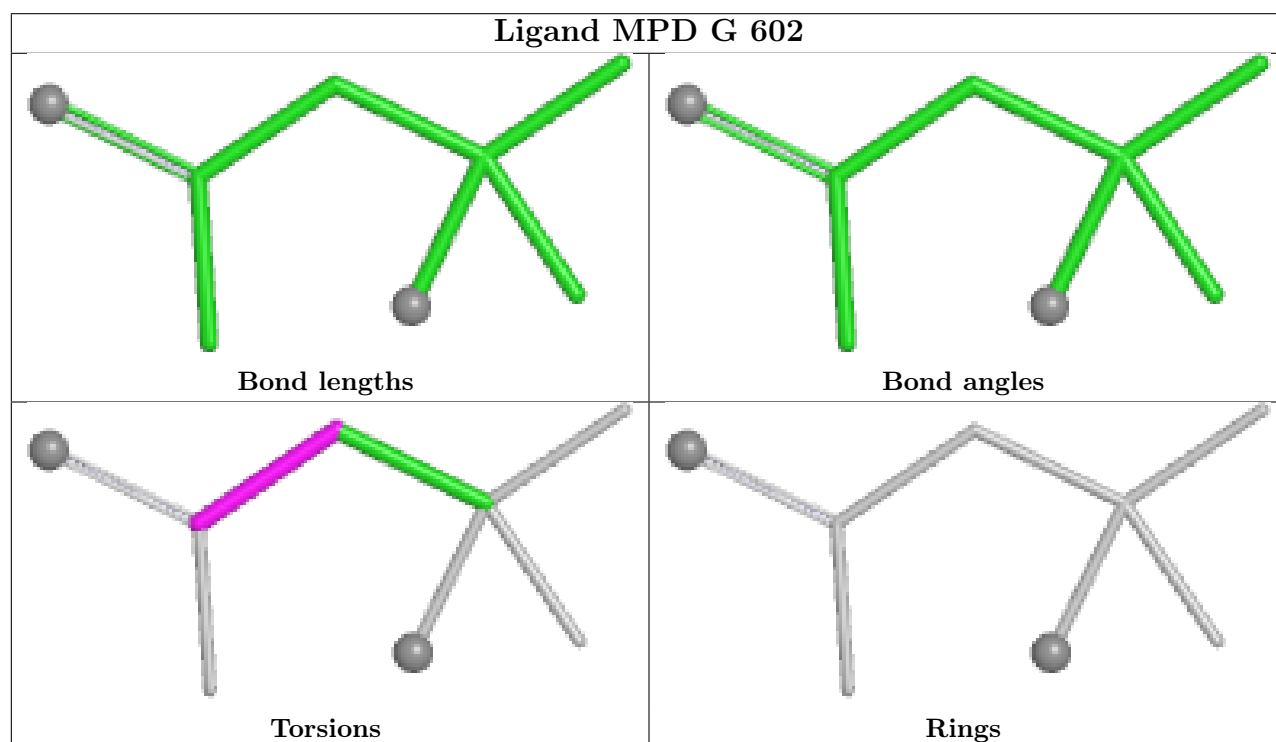
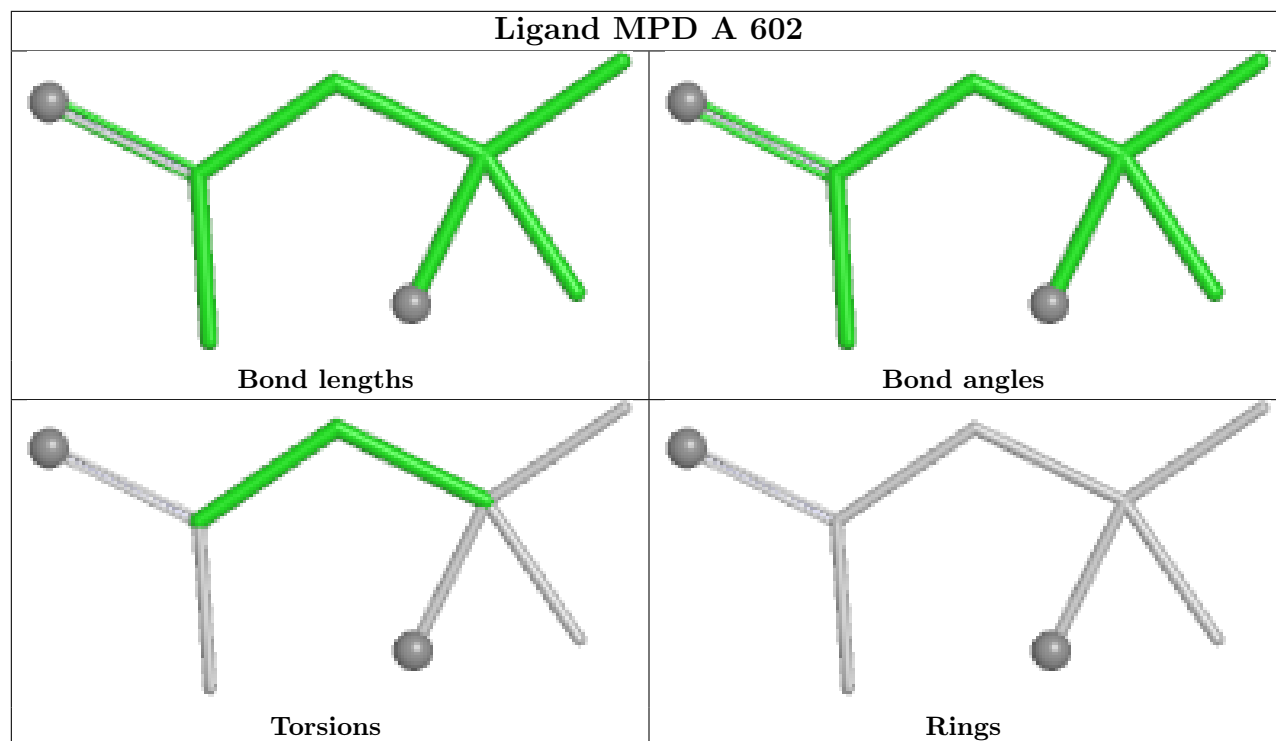
Mol	Chain	Res	Type	Atoms
5	G	603	MPD	C2-C3-C4-C5
5	G	603	MPD	O2-C2-C3-C4
5	G	602	MPD	C2-C3-C4-O4
5	C	603	MPD	C1-C2-C3-C4
5	C	603	MPD	CM-C2-C3-C4

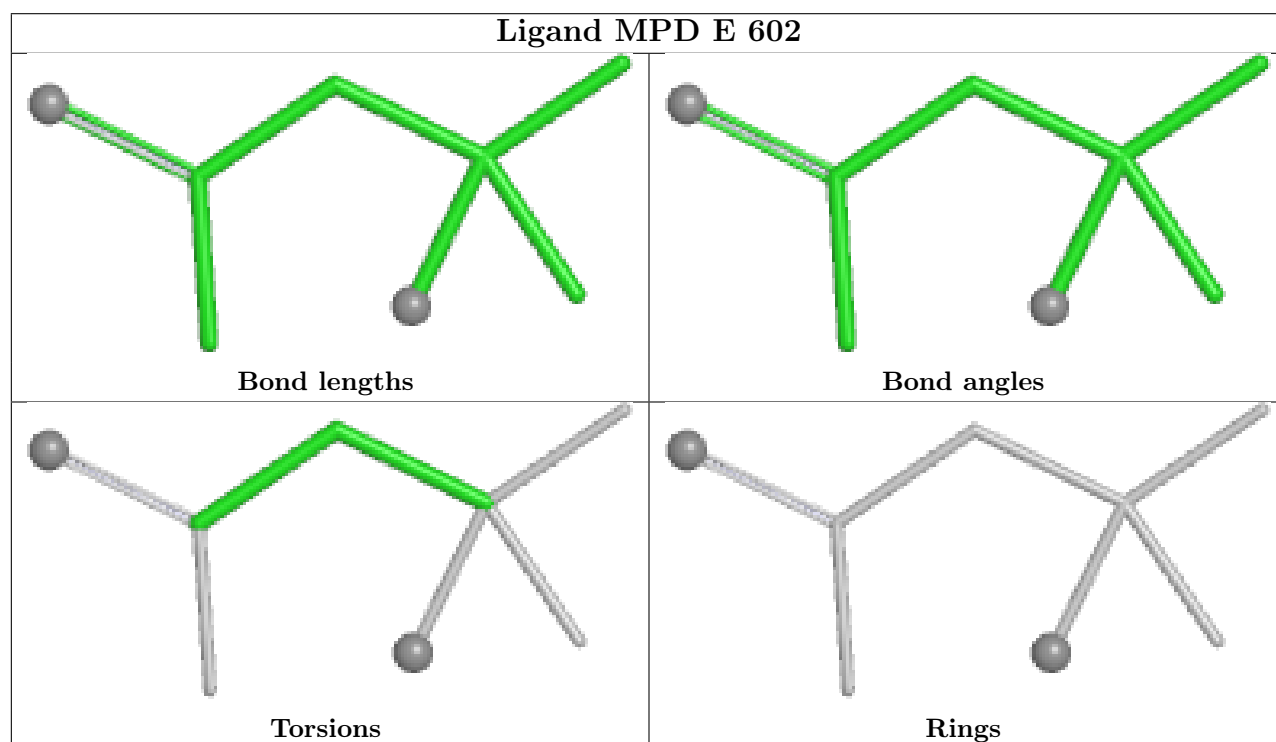
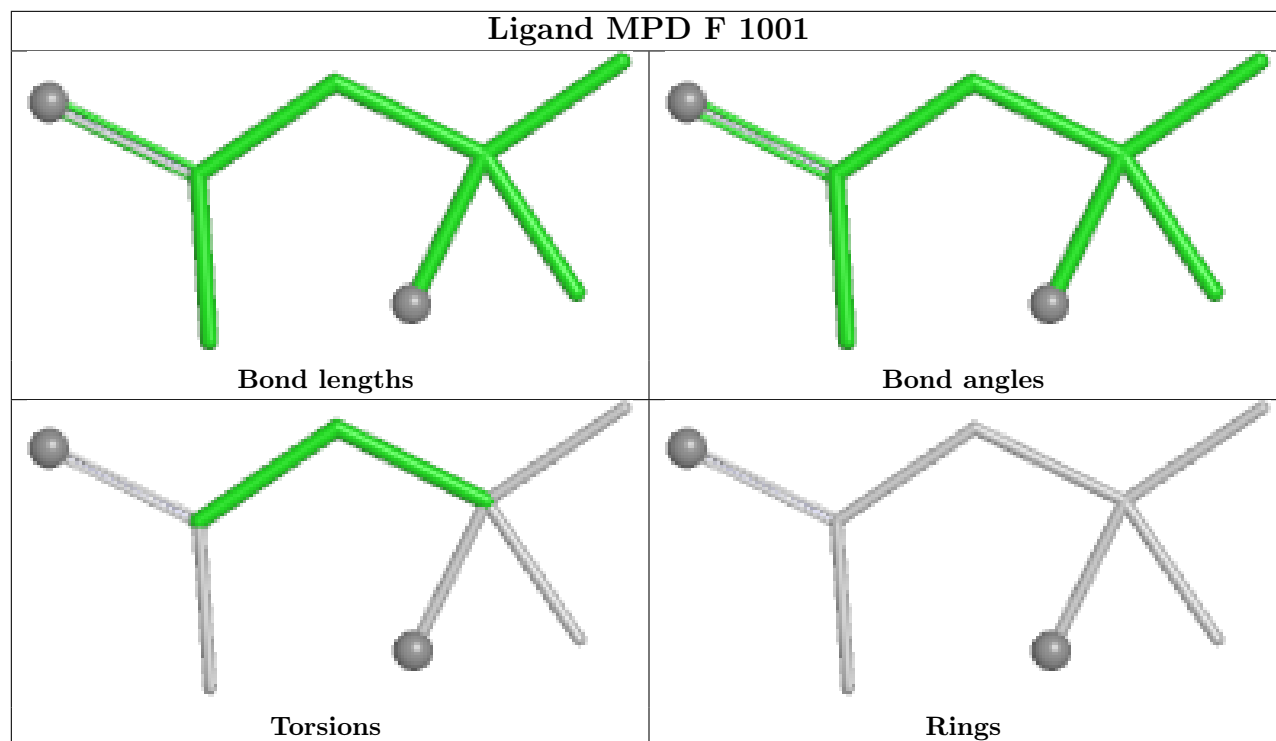
There are no ring outliers.

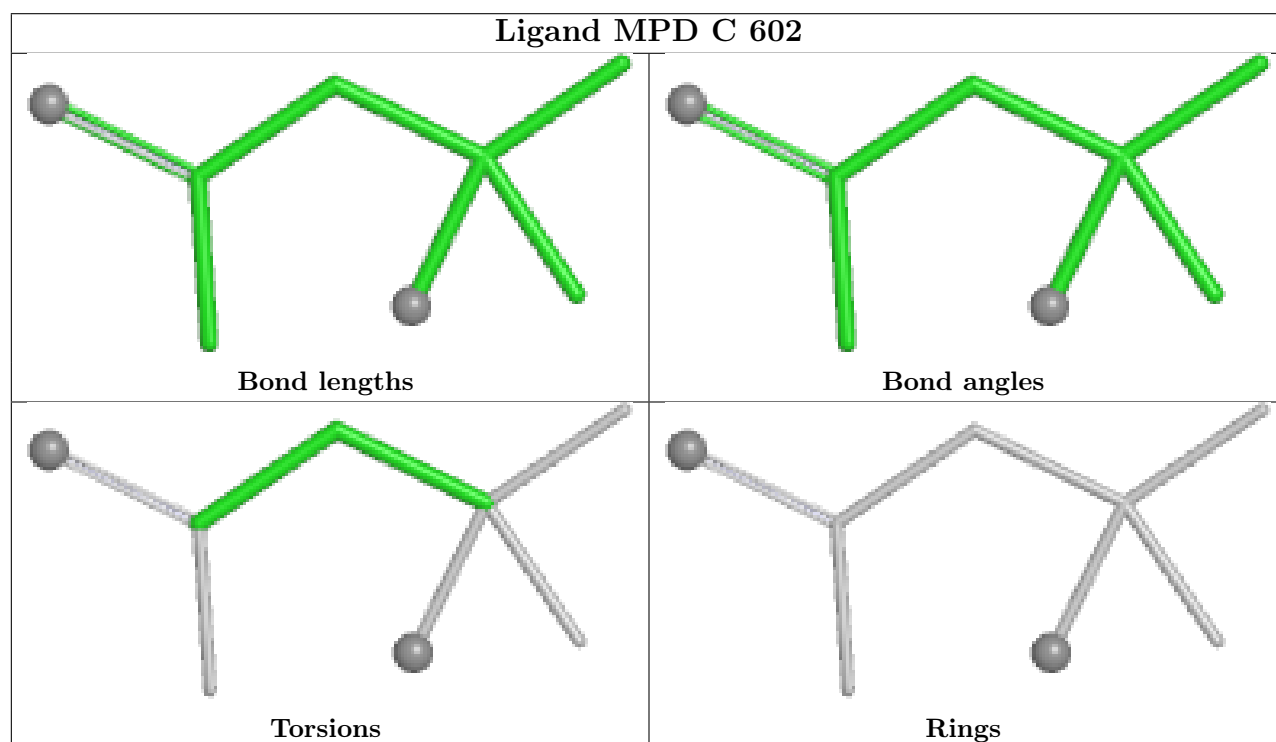
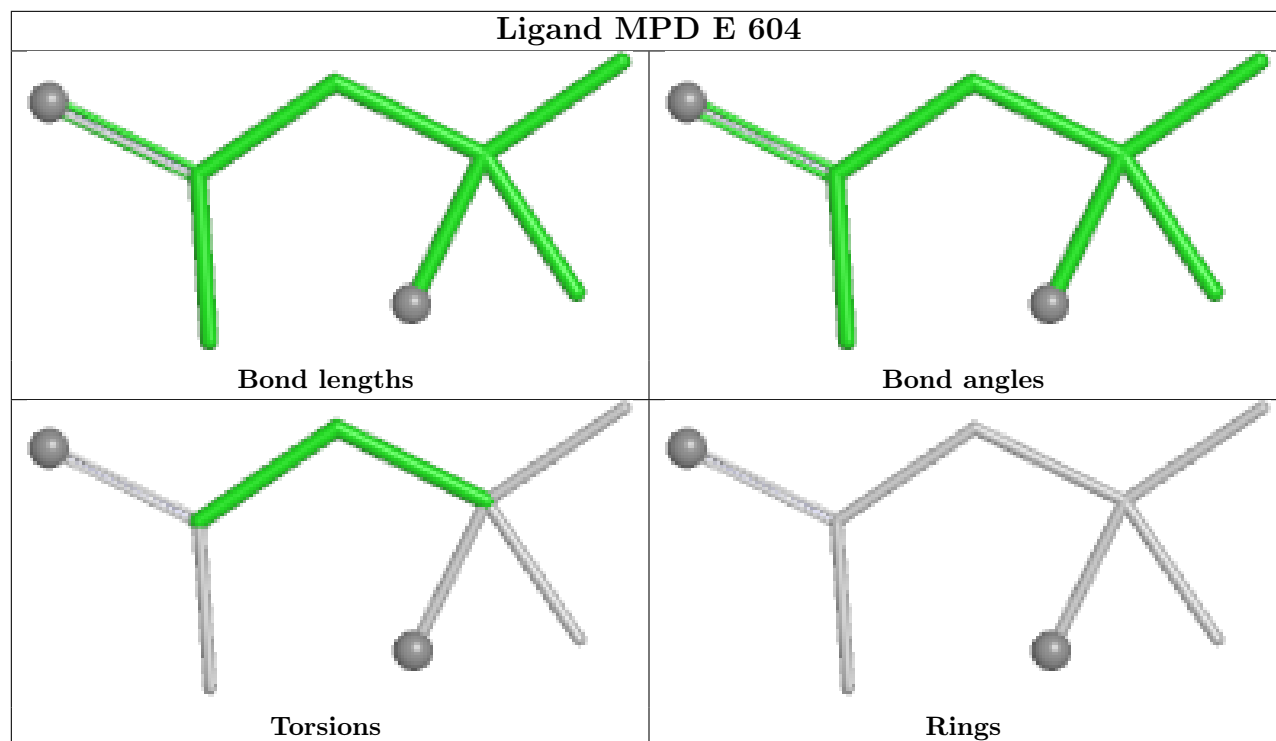
6 monomers are involved in 7 short contacts:

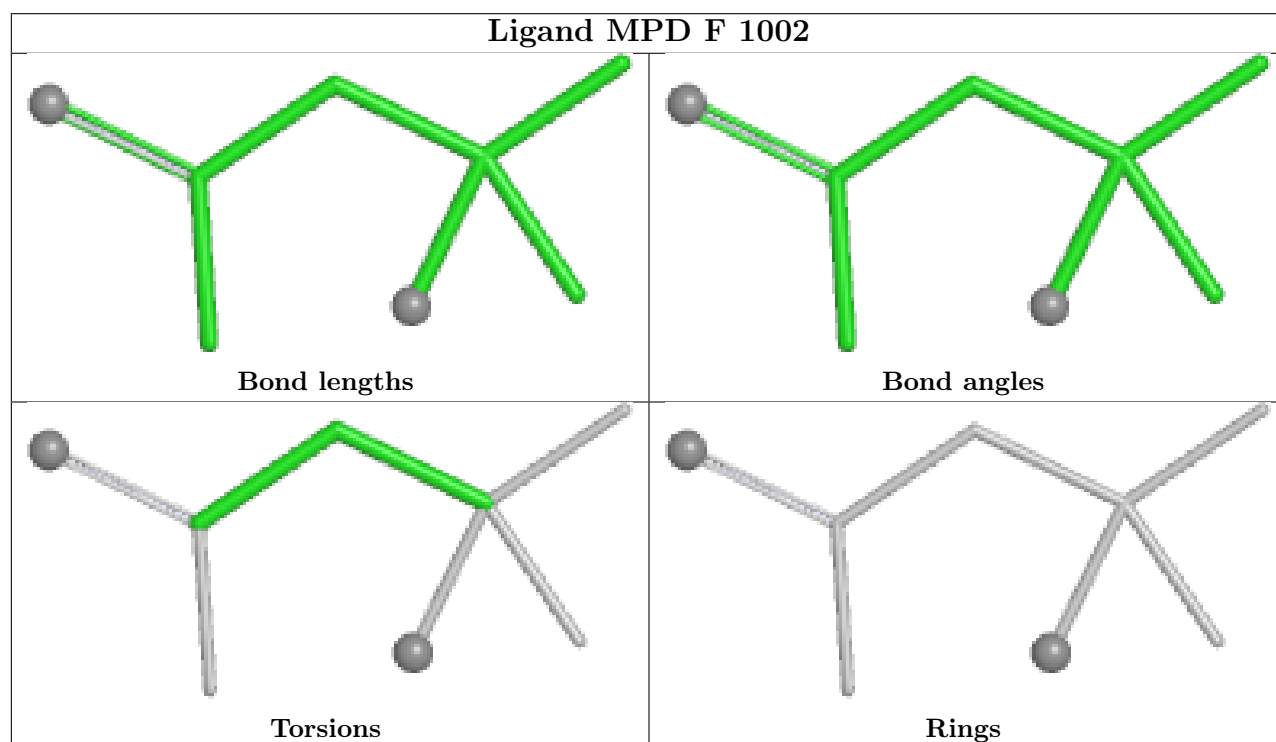
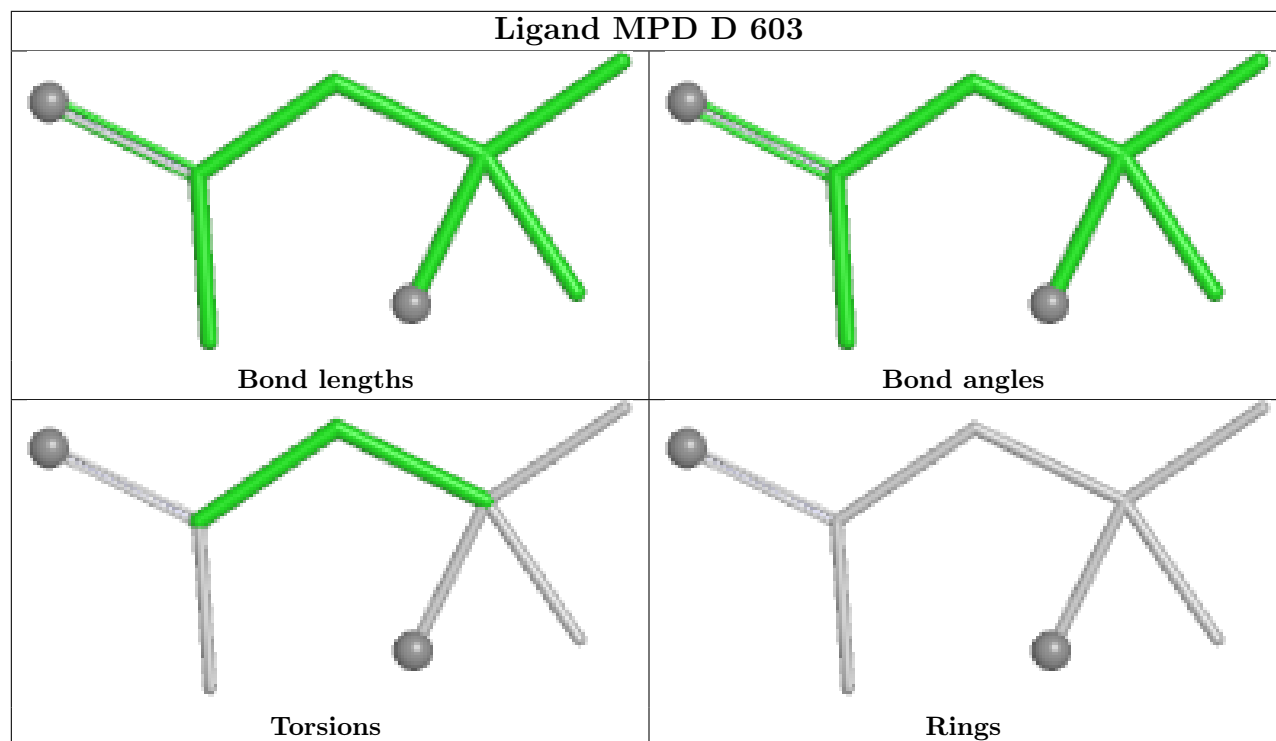
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	MPD	1	0
5	G	602	MPD	1	0
5	E	602	MPD	1	0
5	B	1001	MPD	1	0
5	H	1001	MPD	1	0
5	D	602	MPD	2	0

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



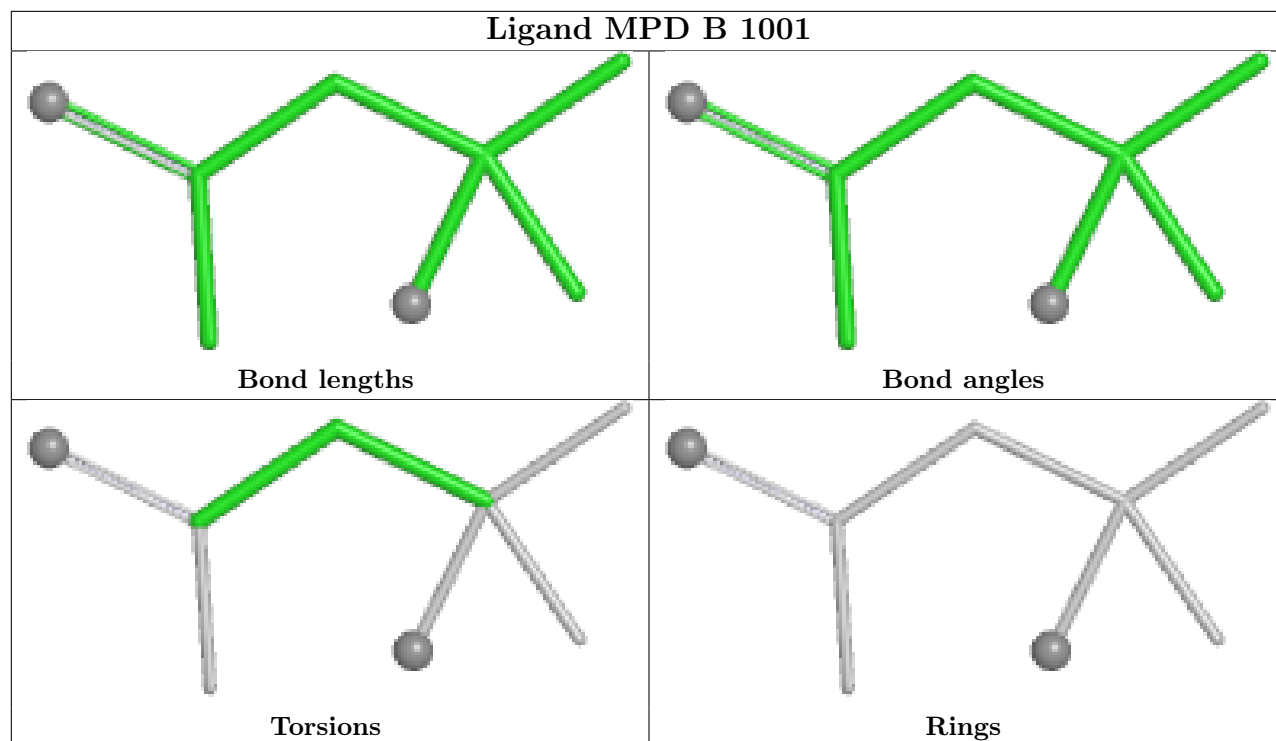




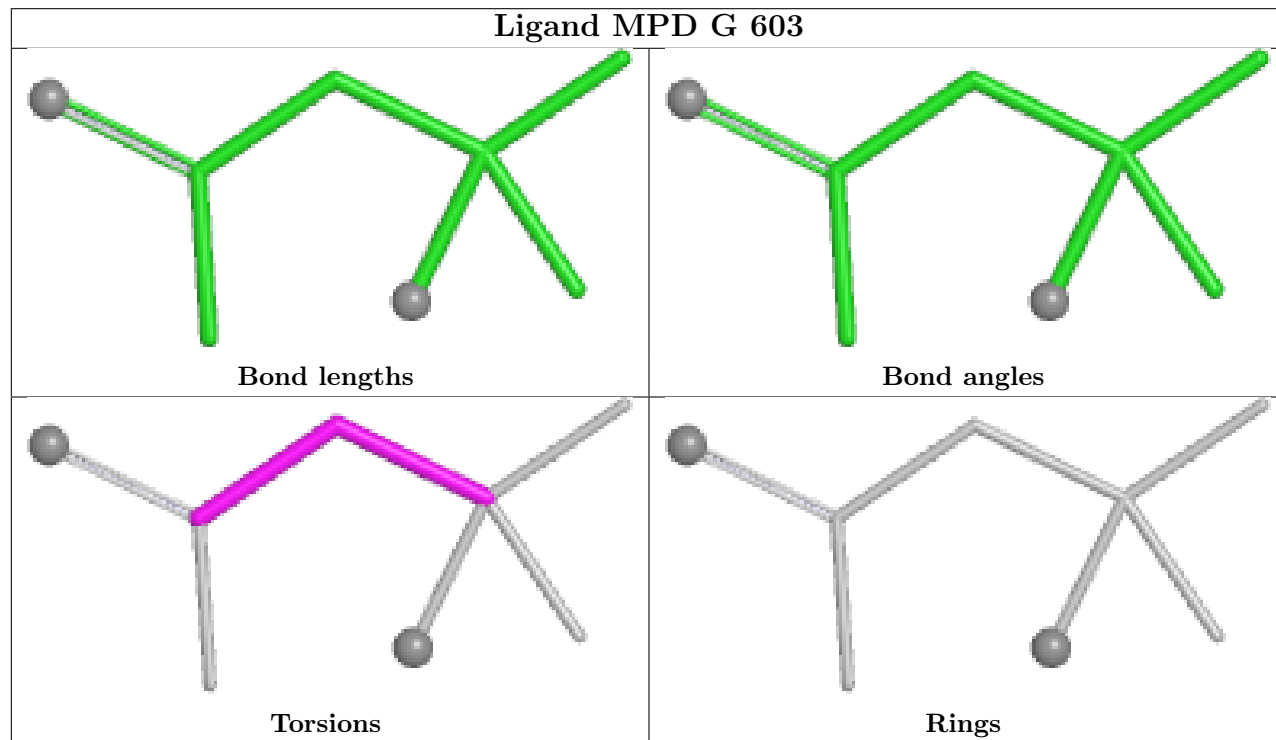


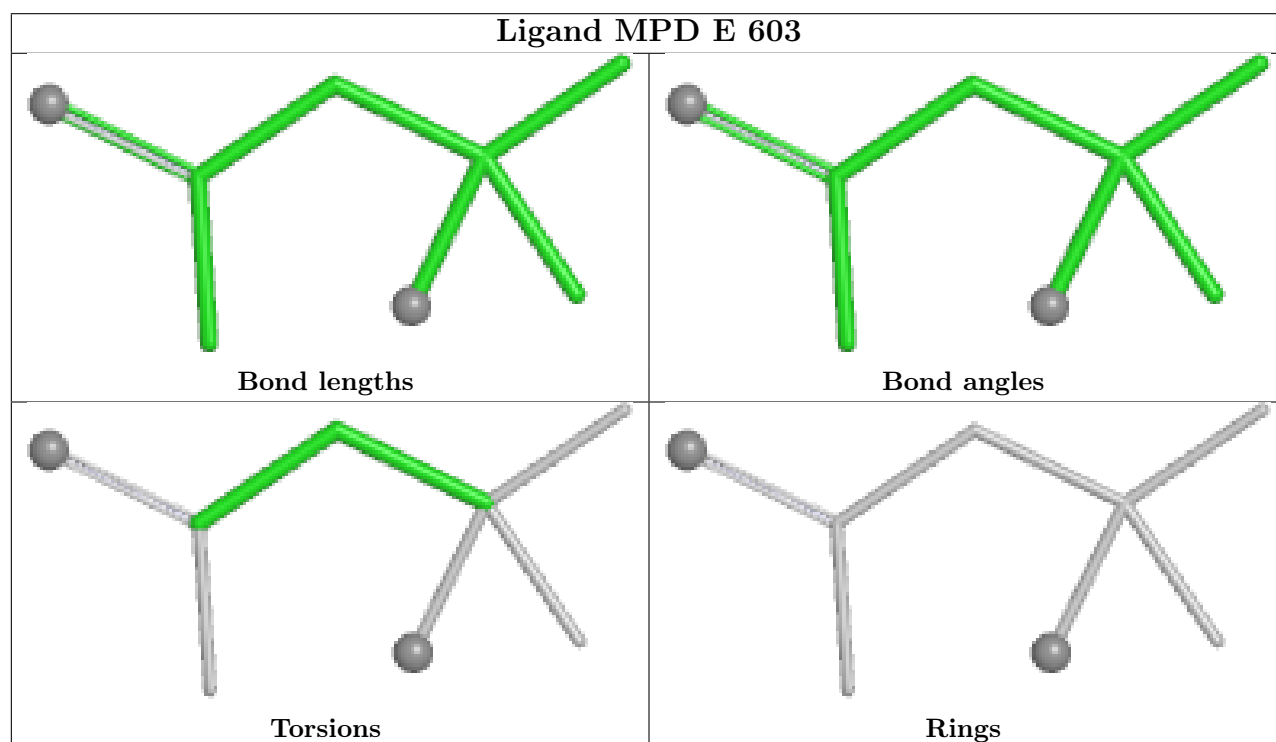
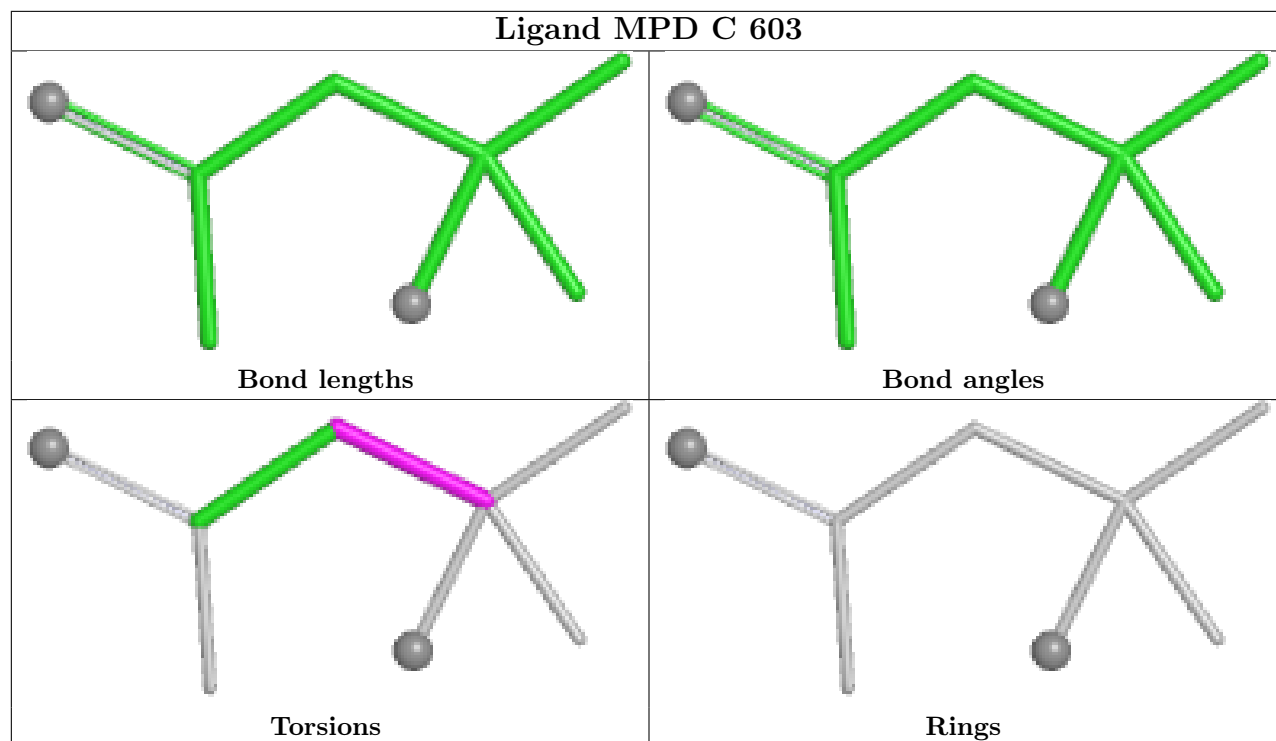


## Ligand MPD B 1001

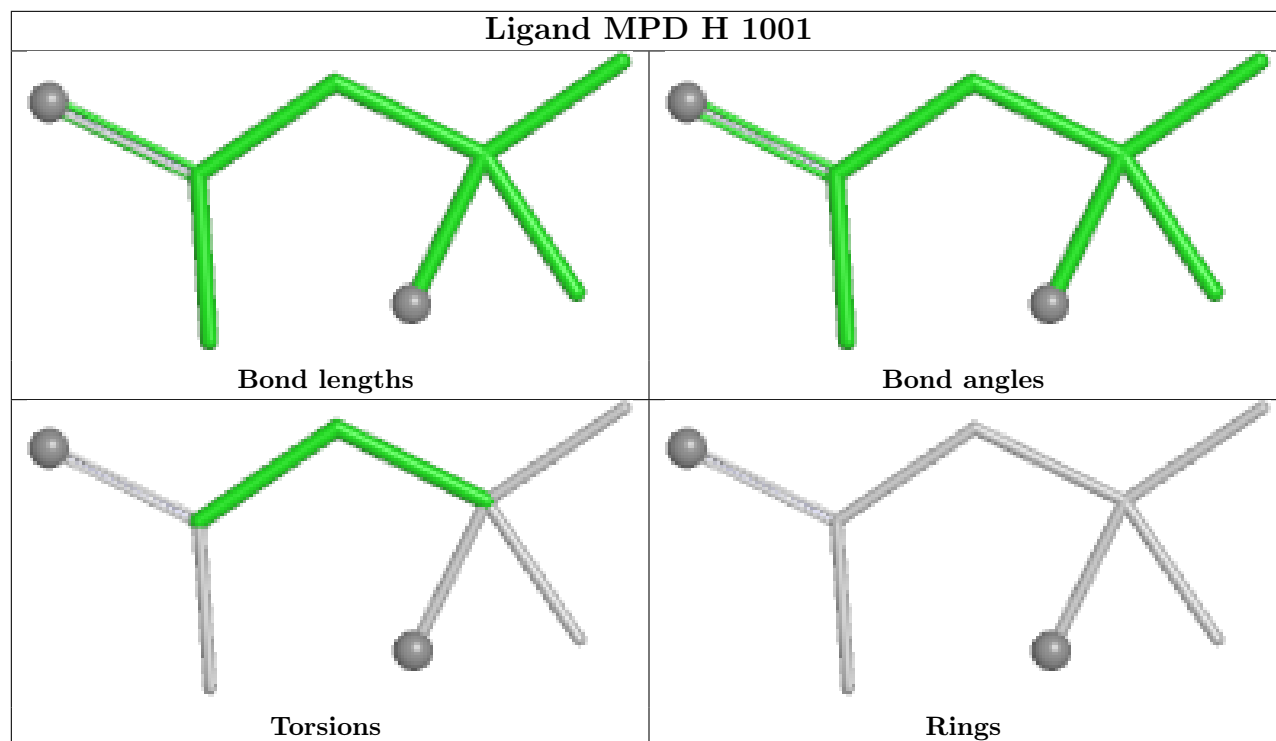


## Ligand MPD G 603

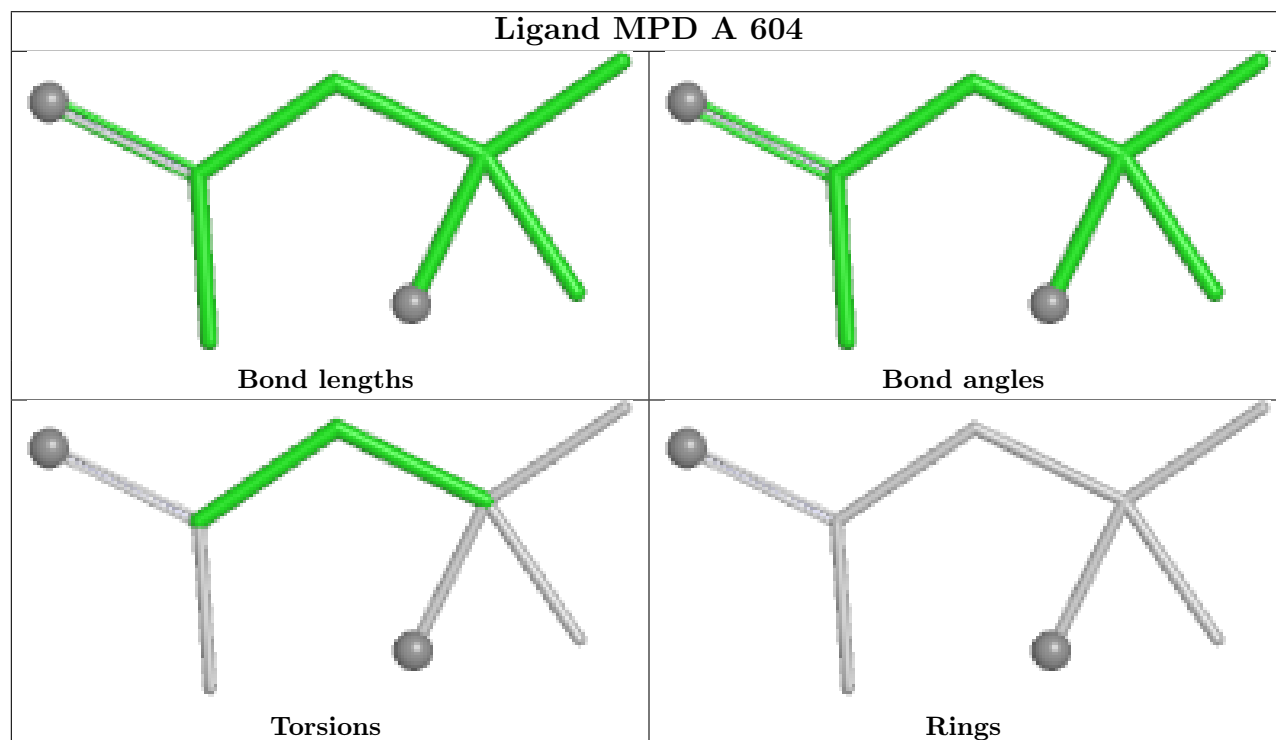


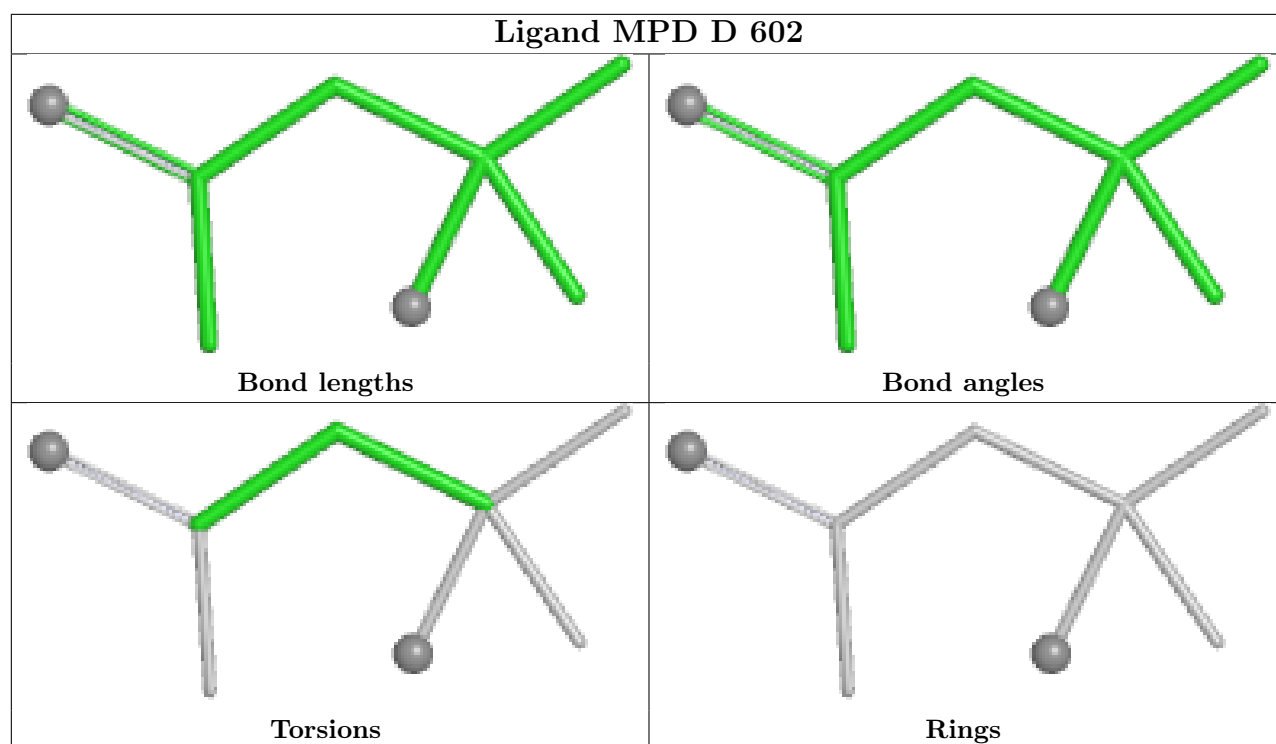


## Ligand MPD H 1001



## Ligand MPD A 604





## 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	483/509 (94%)	0.67	20 (4%)	41	48	19, 39, 59, 78	2 (0%)
1	B	506/509 (99%)	0.49	28 (5%)	30	36	15, 33, 66, 126	3 (0%)
1	C	482/509 (94%)	0.64	21 (4%)	39	45	14, 36, 58, 80	5 (1%)
1	D	497/509 (97%)	0.62	34 (6%)	23	27	14, 37, 59, 118	5 (1%)
2	E	493/509 (96%)	0.40	9 (1%)	67	75	14, 32, 49, 77	4 (0%)
2	F	500/509 (98%)	0.23	8 (1%)	70	77	13, 31, 48, 71	9 (1%)
3	G	489/509 (96%)	0.93	66 (13%)	7	7	17, 40, 63, 87	2 (0%)
3	H	501/509 (98%)	0.85	40 (7%)	18	21	18, 40, 66, 83	3 (0%)
All	All	3951/4072 (97%)	0.60	226 (5%)	29	34	13, 36, 60, 126	33 (0%)

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	118	ILE	8.0
1	B	119	PHE	5.1
1	D	448	PRO	5.0
3	H	40	TRP	4.9
1	C	375[A]	ARG	4.8
1	D	119	PHE	4.6
1	B	2	ALA	4.4
1	D	121	ARG	4.3
3	H	17[A]	TRP	4.3
1	B	125	PHE	4.2
1	B	118	ILE	4.2
3	H	97	ALA	4.1
3	H	119	PHE	4.1
1	D	125	PHE	4.0
1	B	263	TYR	4.0
1	C	263	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	122	VAL	4.0
1	C	97	ALA	3.9
3	H	300	VAL	3.9
3	G	117	THR	3.8
3	G	270	ILE	3.8
3	G	425	LYS	3.6
3	H	55	VAL	3.5
1	D	114	PRO	3.4
3	H	57	THR	3.4
1	D	117	THR	3.4
1	D	115	CYS	3.4
1	C	111	ALA	3.3
1	C	265	LEU	3.3
1	D	124	ALA	3.3
3	G	75	ILE	3.2
3	H	269	LEU	3.2
1	C	270	ILE	3.2
3	G	446	PRO	3.2
1	A	203	GLY	3.1
1	C	269	LEU	3.1
2	E	118	ILE	3.1
1	B	123	ALA	3.1
3	G	131	HIS	3.1
3	G	74	ALA	3.1
1	A	162	VAL	3.0
3	G	456	GLY	3.0
3	H	205	ILE	3.0
2	F	126	PHE	3.0
3	G	37	PHE	3.0
3	G	57	THR	3.0
1	B	120	ASP	3.0
3	G	43	GLY	3.0
1	B	113	ASP	3.0
3	G	384	ILE	3.0
1	B	115	CYS	2.9
3	H	235	ALA	2.9
3	G	221	PHE	2.9
3	H	37	PHE	2.9
3	H	125	PHE	2.9
3	G	351	ALA	2.9
1	D	116	HIS	2.9
1	A	263	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
3	G	112	PRO	2.9
3	G	98	ALA	2.9
3	G	113	ASP	2.9
3	H	234	TRP	2.9
3	G	266	MET	2.9
1	A	28	PRO	2.8
3	H	270	ILE	2.8
2	F	128	PRO	2.8
1	C	26	SER	2.8
3	G	97	ALA	2.8
2	F	129	GLY	2.8
3	G	116	HIS	2.8
1	A	201	VAL	2.8
3	G	7	LYS	2.8
3	H	506	PRO	2.8
3	G	356	TRP	2.8
3	H	16	VAL	2.8
3	H	102	VAL	2.8
3	G	263	TYR	2.7
3	G	96	ARG	2.7
1	C	96	ARG	2.7
1	A	285	TYR	2.7
1	B	124	ALA	2.7
1	C	455	ASP	2.7
3	G	8	LEU	2.7
3	H	98	ALA	2.7
3	H	370	ALA	2.7
3	G	269	LEU	2.7
1	B	3	ALA	2.6
1	B	97	ALA	2.6
1	A	132	MET	2.6
1	D	217	LYS	2.6
1	B	116	HIS	2.6
1	A	270	ILE	2.6
1	C	101	ILE	2.6
1	A	102	VAL	2.6
1	B	111	ALA	2.6
3	H	343	ALA	2.6
1	B	112	PRO	2.6
3	H	357	PHE	2.6
3	G	40	TRP	2.6
1	A	30	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	H	63	LEU	2.5
1	C	384	ILE	2.5
1	D	226[A]	ILE	2.5
2	E	123	ALA	2.5
3	G	450	ALA	2.5
1	A	472	VAL	2.5
1	B	122	VAL	2.5
1	B	4	THR	2.5
3	G	79	THR	2.5
3	G	145	ASP	2.5
3	H	285	TYR	2.5
1	A	37	PHE	2.5
3	G	55	VAL	2.5
3	G	481	THR	2.5
3	H	64	PHE	2.5
3	H	96	ARG	2.5
1	B	98	ALA	2.5
3	G	413	ALA	2.5
1	B	114	PRO	2.5
3	G	403	TYR	2.4
3	H	263	TYR	2.4
3	G	447	SER	2.4
3	G	426	THR	2.4
3	G	99	ASN	2.4
3	G	9	TYR	2.4
1	C	57	THR	2.4
3	G	215	THR	2.4
3	G	59	ARG	2.4
1	B	448	PRO	2.4
3	G	448	PRO	2.4
3	G	428	GLU	2.4
1	B	108	THR	2.4
3	H	507	THR	2.4
3	H	31	GLY	2.4
3	H	111	ALA	2.3
1	A	448	PRO	2.3
1	B	128	PRO	2.3
1	B	131	HIS	2.3
1	D	112	PRO	2.3
2	E	131	HIS	2.3
1	D	78	GLY	2.3
1	A	507	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	117	THR	2.3
3	G	479	ALA	2.3
3	G	419	VAL	2.3
1	B	57	THR	2.3
1	D	214	PHE	2.3
1	D	370	ALA	2.3
1	B	384	ILE	2.3
1	D	120	ASP	2.3
3	G	383	ASP	2.3
2	E	472	VAL	2.3
3	G	33	MET	2.3
2	F	427	GLY	2.2
3	G	111	ALA	2.2
1	C	366	VAL	2.2
3	H	104	THR	2.2
3	H	426	THR	2.2
3	G	395	LEU	2.2
3	G	39	SER	2.2
3	G	218	GLY	2.2
3	G	354	ALA	2.2
3	G	359	ALA	2.2
2	F	125	PHE	2.2
1	C	132	MET	2.2
3	H	369	ASN	2.2
1	D	275	LEU	2.2
1	A	506	PRO	2.2
1	C	98	ALA	2.2
1	D	98	ALA	2.2
1	D	111	ALA	2.2
1	B	126	PHE	2.2
1	D	270	ILE	2.2
1	A	40	TRP	2.2
1	D	40	TRP	2.2
2	E	449	ASN	2.2
3	G	273	ASN	2.2
1	D	367	SER	2.2
1	A	31	GLY	2.2
2	E	144	GLY	2.2
3	H	8	LEU	2.2
1	C	276	ALA	2.2
1	D	123	ALA	2.2
1	D	276	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	96	ARG	2.2
3	H	116	HIS	2.1
1	A	221	PHE	2.1
3	G	432	TRP	2.1
1	A	108	THR	2.1
3	G	455	ASP	2.1
1	D	369	ASN	2.1
1	C	205	ILE	2.1
2	F	263	TYR	2.1
1	C	108	THR	2.1
1	C	55	VAL	2.1
2	F	448	PRO	2.1
1	A	359	ALA	2.1
3	H	106	PHE	2.1
3	G	353	TYR	2.1
3	H	204	ARG	2.1
3	G	468	MET	2.1
2	E	116	HIS	2.1
1	D	55	VAL	2.1
1	D	200	VAL	2.1
1	D	449	ASN	2.1
3	G	272	ASN	2.1
3	G	506	PRO	2.1
1	D	175	CYS	2.1
1	D	113	ASP	2.1
3	G	77	ASP	2.1
3	H	39	SER	2.0
1	D	57	THR	2.0
3	H	58	MET	2.0
1	C	359	ALA	2.0
3	G	333	ALA	2.0
3	G	452	ASP	2.0
3	G	453	GLU	2.0
2	E	451	LYS	2.0
3	G	451	LYS	2.0
3	H	132	MET	2.0
2	E	270	ILE	2.0
2	F	507	THR	2.0
3	G	427	GLY	2.0
1	D	263	TYR	2.0
3	G	10	PRO	2.0
3	H	201	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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	CSO	E	115	7/8	0.78	0.13	59,64,70,73	0
2	CSO	F	115	7/8	0.87	0.12	50,53,58,61	0
3	CSD	G	115	8/9	0.93	0.10	44,48,54,55	0
3	CSD	H	115	8/9	0.94	0.10	44,47,50,52	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, 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
5	MPD	A	602	8/8	0.77	0.14	50,52,53,54	0
5	MPD	C	603	8/8	0.79	0.15	48,52,53,55	0
5	MPD	G	603	8/8	0.81	0.17	61,62,63,65	0
7	NA	D	605	1/1	0.81	0.21	47,47,47,47	1
5	MPD	C	602	8/8	0.82	0.16	48,51,52,52	0
5	MPD	D	602	8/8	0.83	0.15	51,53,54,54	0
5	MPD	E	603	8/8	0.84	0.14	49,52,53,55	0
5	MPD	H	1001	8/8	0.84	0.14	47,49,49,51	0
5	MPD	F	1002	8/8	0.84	0.12	41,44,45,47	0
5	MPD	E	602	8/8	0.85	0.13	42,46,48,48	0
5	MPD	F	1001	8/8	0.85	0.15	45,47,48,49	0
5	MPD	D	603	8/8	0.86	0.13	44,47,49,51	0
5	MPD	A	604	8/8	0.86	0.13	45,50,58,59	0
8	CAC	F	1003	5/5	0.87	0.16	71,71,75,76	0
5	MPD	B	1001	8/8	0.88	0.11	45,47,48,49	0
5	MPD	E	604	8/8	0.88	0.12	47,48,49,50	0
5	MPD	G	602	8/8	0.90	0.14	46,48,51,52	0
6	CL	E	605	1/1	0.94	0.08	57,57,57,57	0

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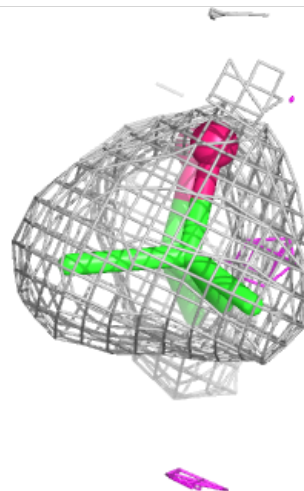
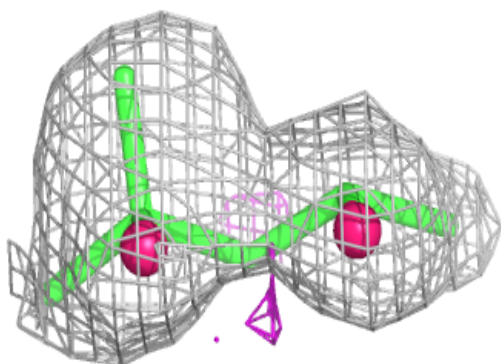
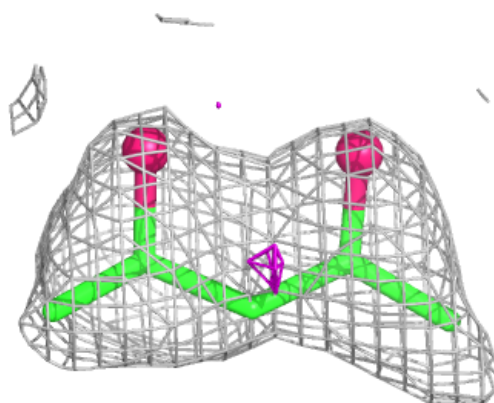
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CL	D	604	1/1	0.98	0.08	32,32,32,32	1
4	FE2	B	1000	1/1	0.99	0.04	27,27,27,27	0
6	CL	A	603	1/1	0.99	0.08	35,35,35,35	1
4	FE2	H	1000	1/1	1.00	0.03	28,28,28,28	0
4	FE2	A	601	1/1	1.00	0.02	34,34,34,34	0
4	FE2	C	601	1/1	1.00	0.02	25,25,25,25	0
4	FE2	D	601	1/1	1.00	0.01	31,31,31,31	0
4	FE2	E	601	1/1	1.00	0.01	26,26,26,26	0
4	FE2	F	1000	1/1	1.00	0.02	23,23,23,23	0
4	FE2	G	601	1/1	1.00	0.05	24,24,24,24	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.

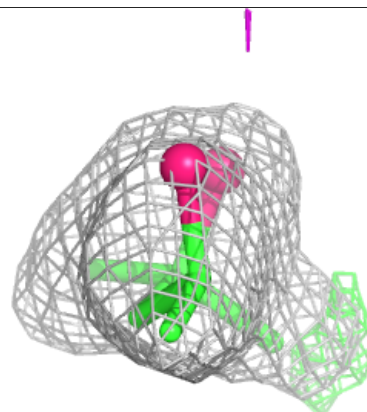
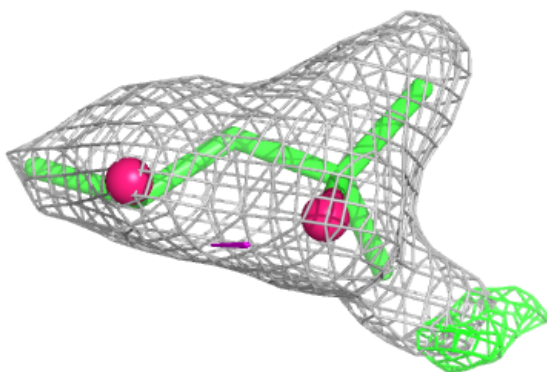
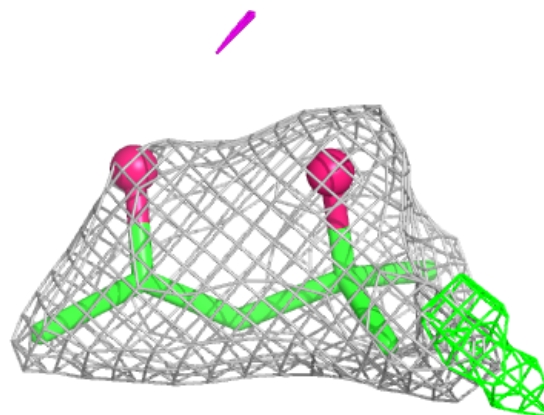
#### Electron density around MPD A 602:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

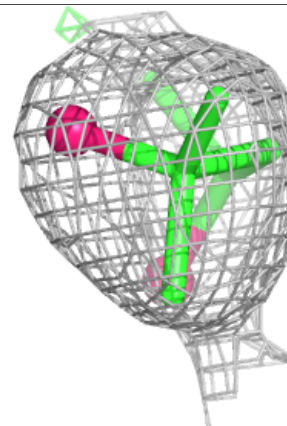
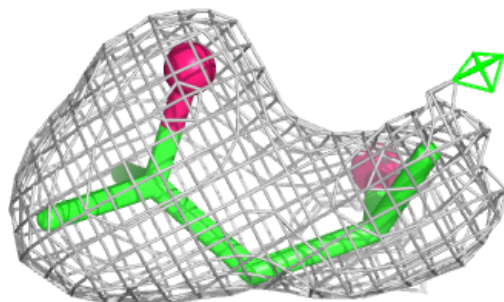
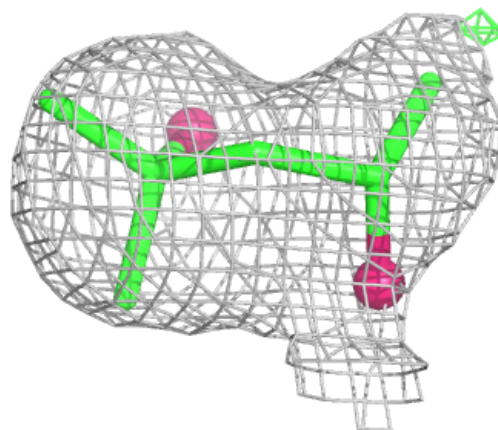


**Electron density around MPD C 603:**

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

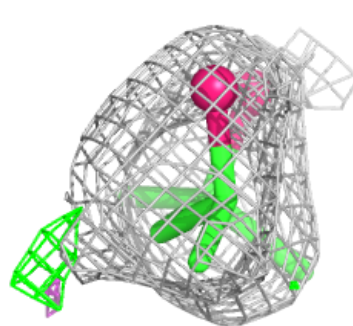
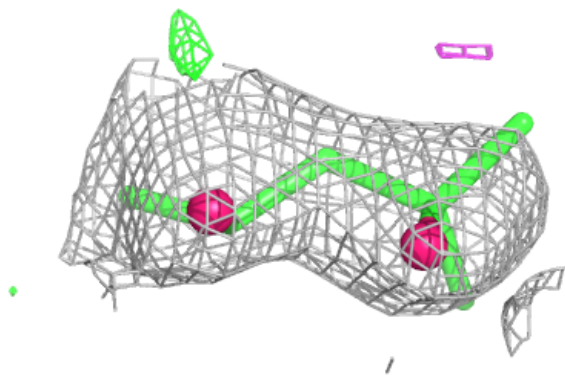
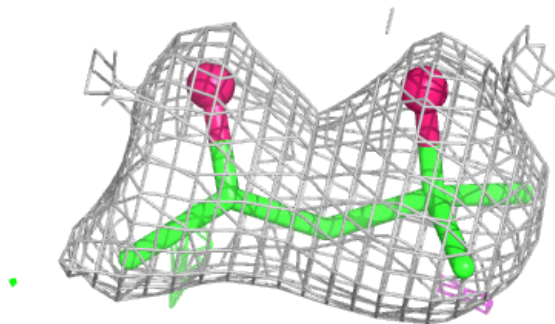
**Electron density around MPD G 603:**

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



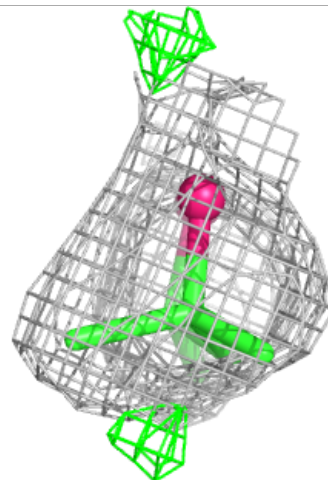
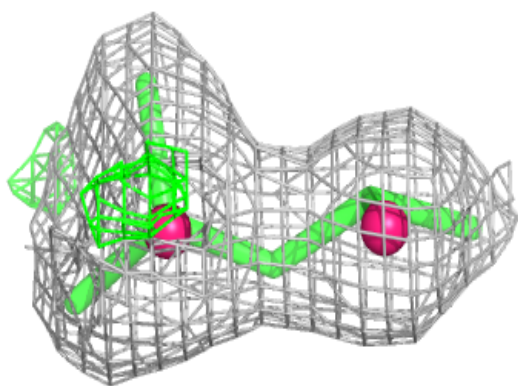
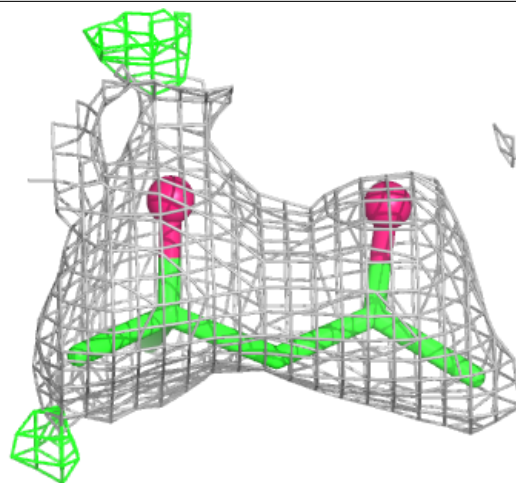
**Electron density around MPD C 602:**

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



**Electron density around MPD D 602:**

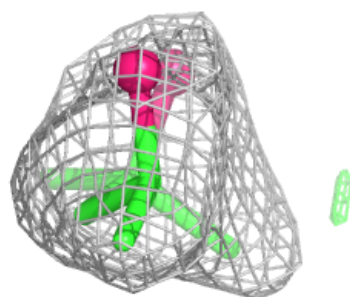
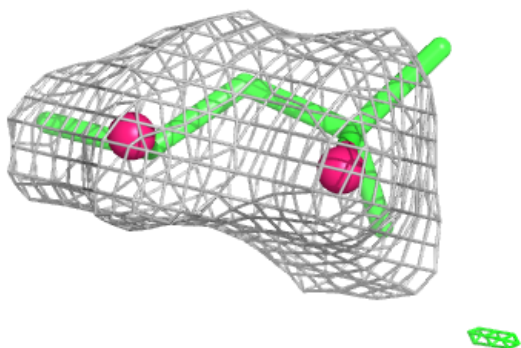
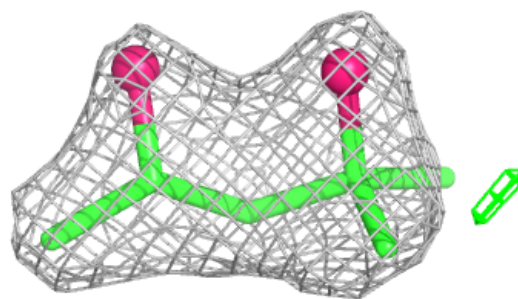
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



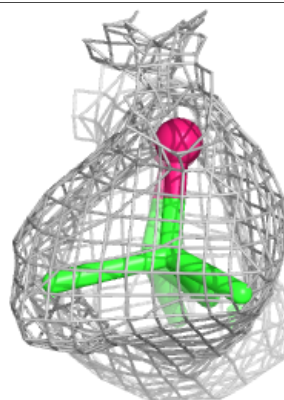
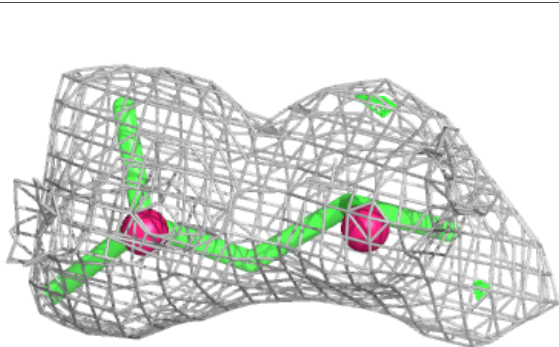
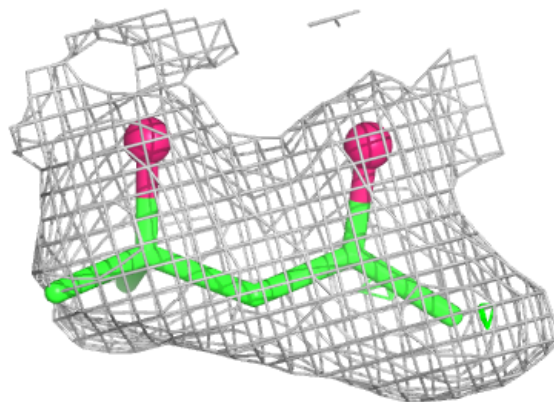


**Electron density around MPD E 603:**

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and green (positive)

**Electron density around MPD H 1001:**

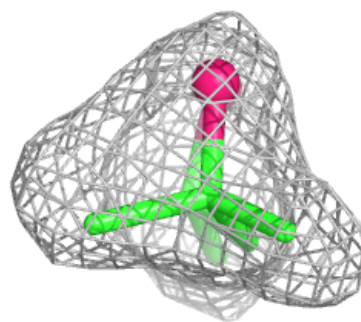
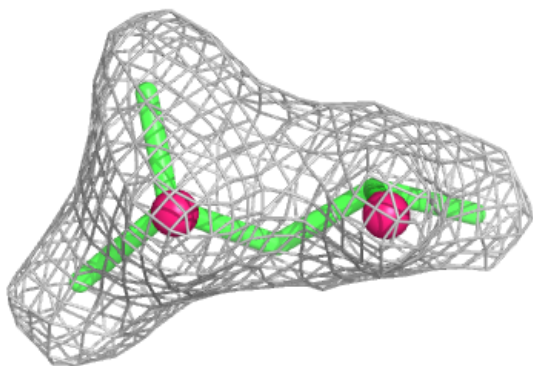
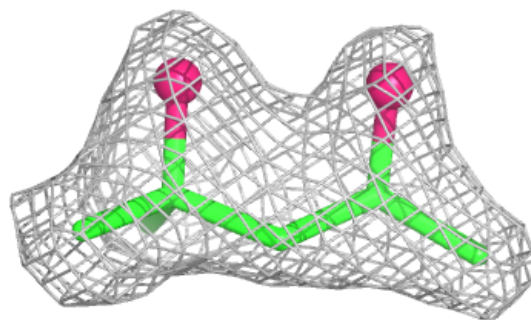
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and green (positive)





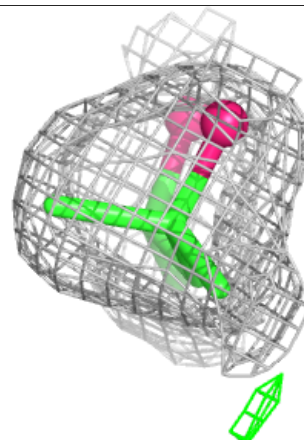
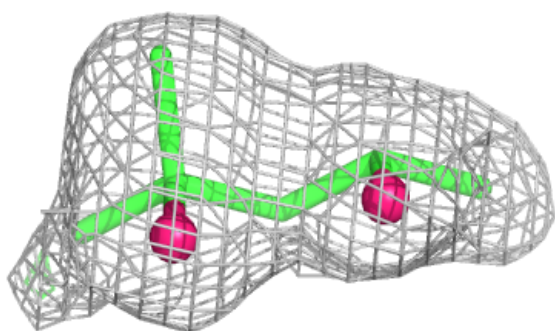
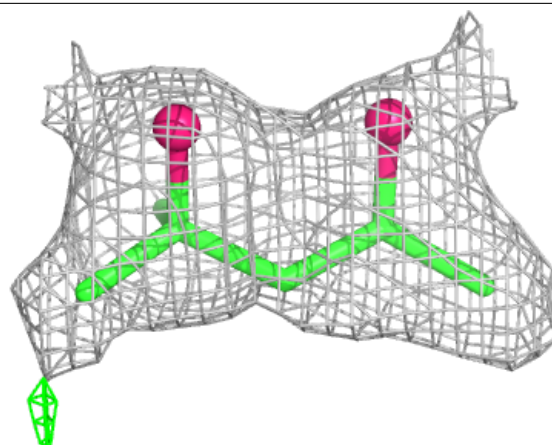
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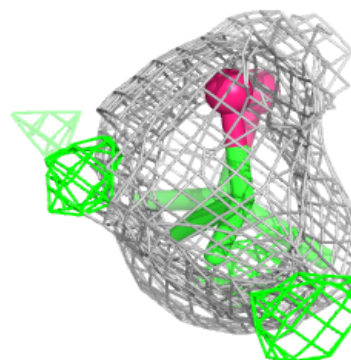
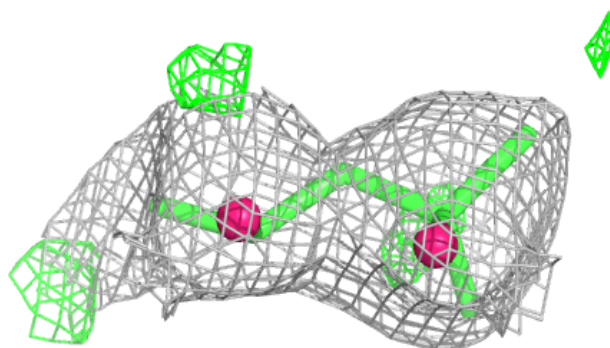
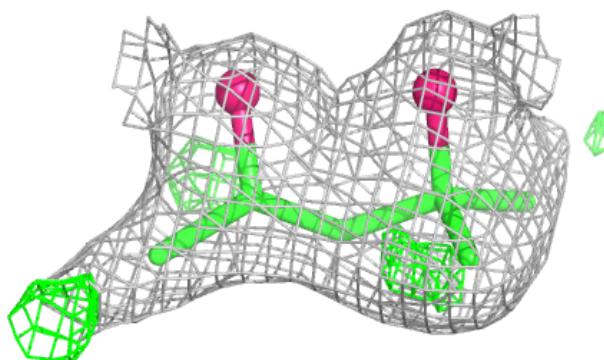


**Electron density around MPD E 602:**

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and green (positive)

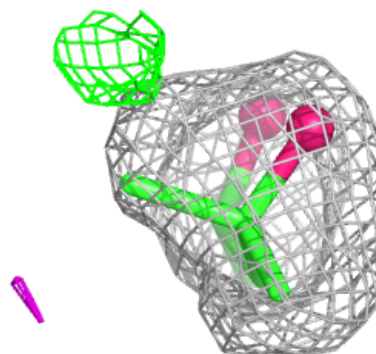
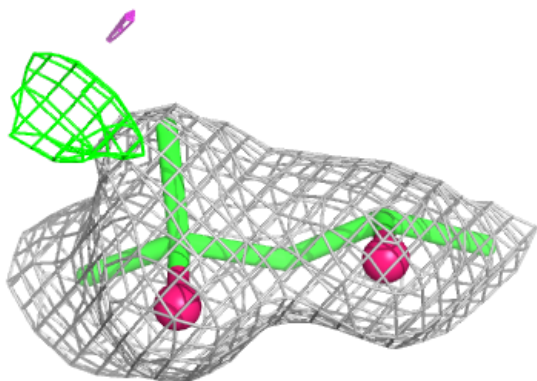
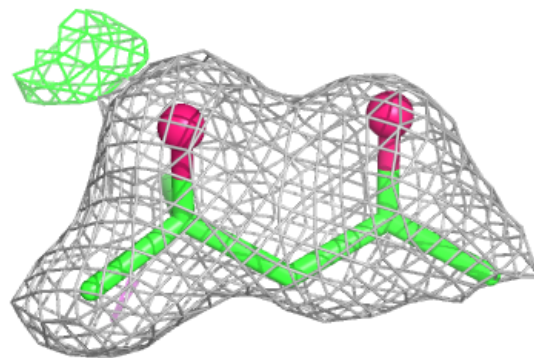
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and green (positive)

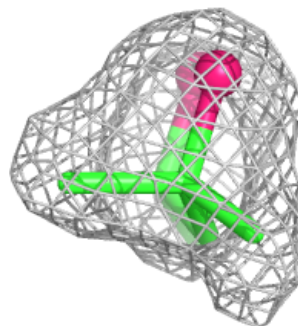
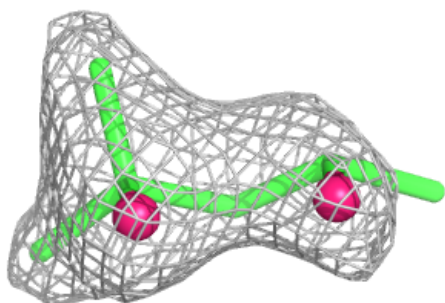
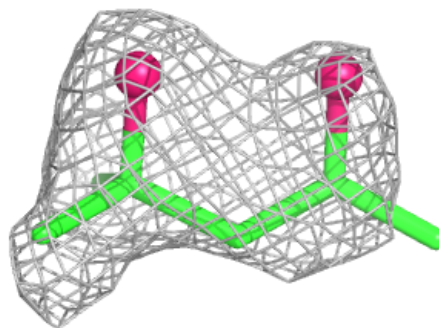


**Electron density around MPD D 603:**

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and green (positive)

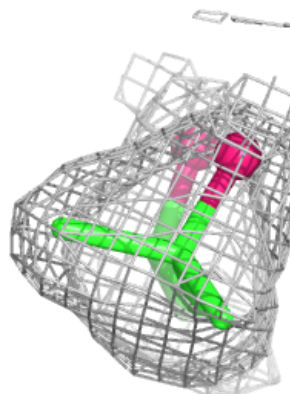
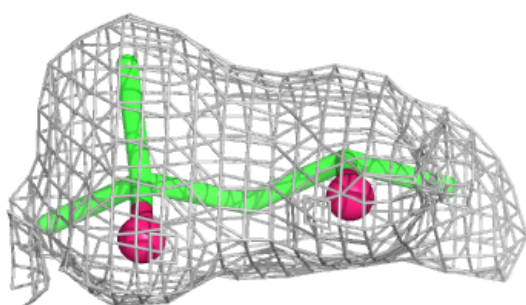
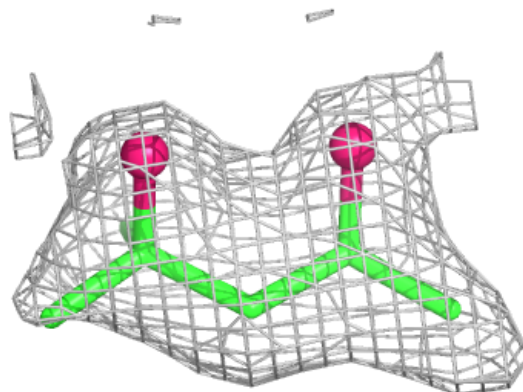
**Electron density around MPD A 604:**

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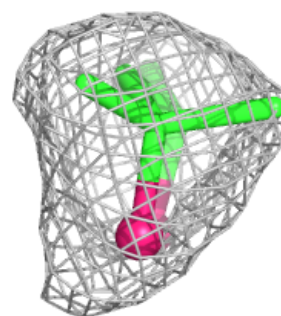
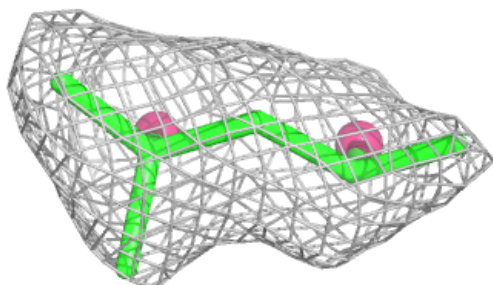
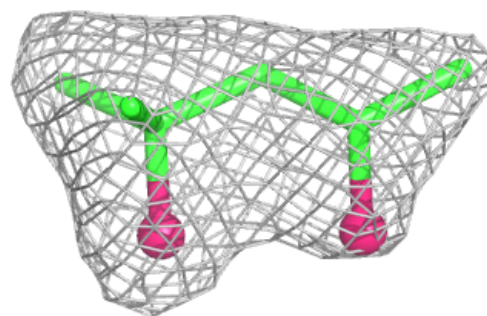


**Electron density around MPD B 1001:**

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

**Electron density around MPD E 604:**

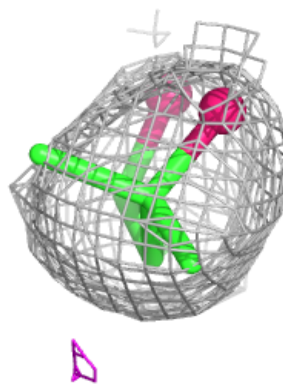
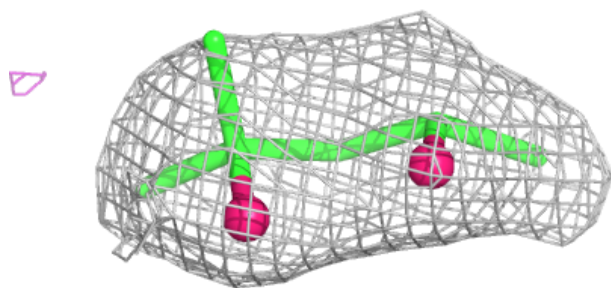
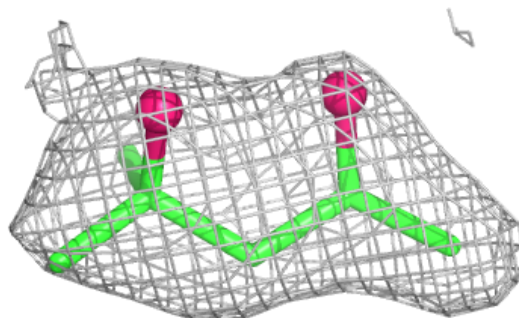
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and green (positive)





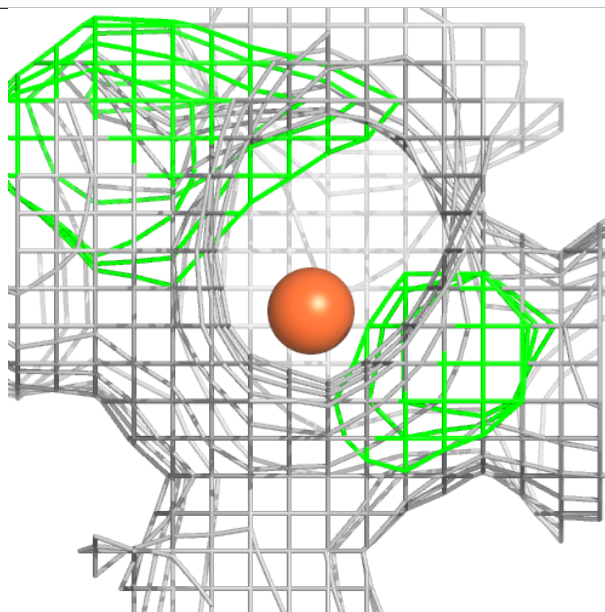
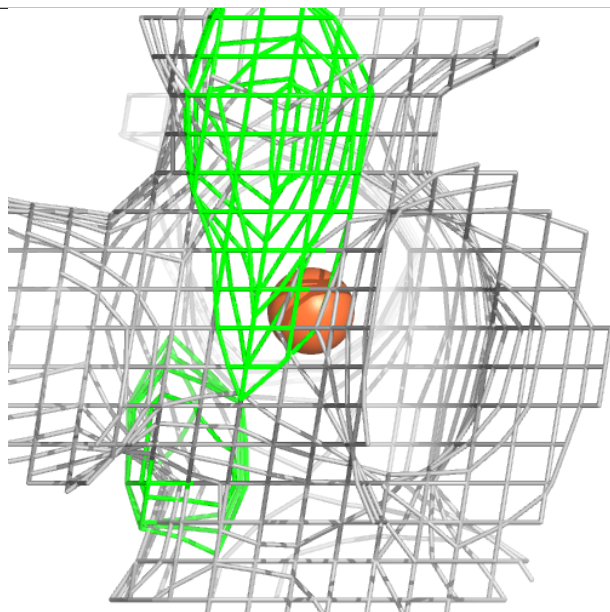
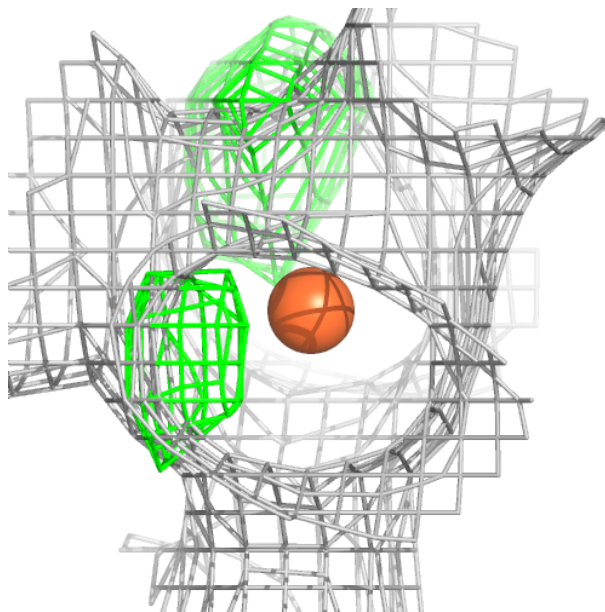
**Electron density around MPD G 602:**

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



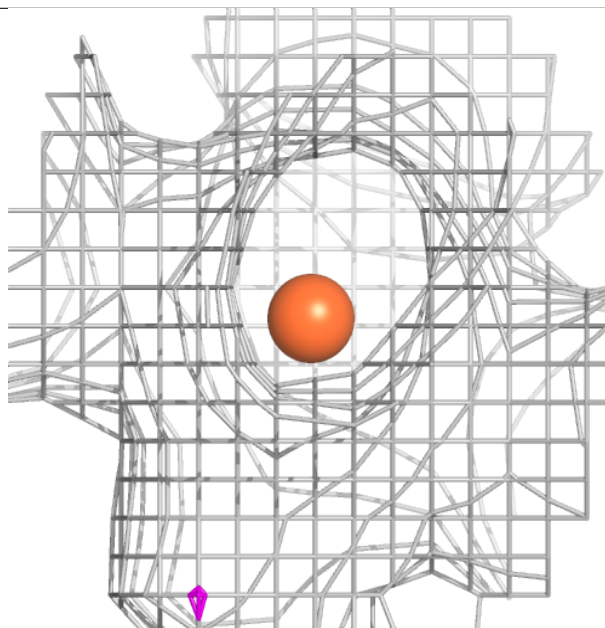
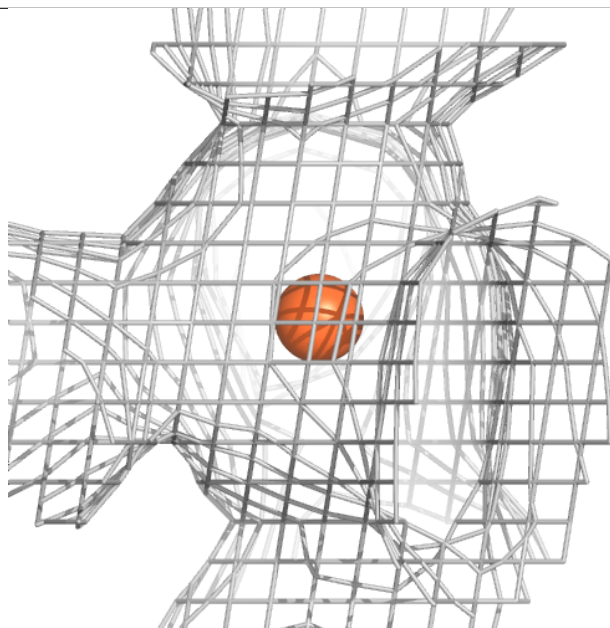
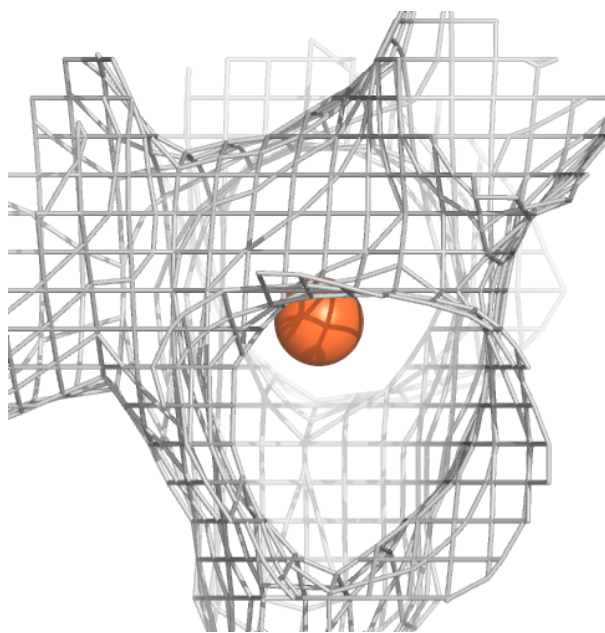
**Electron density around FE2 B 1000:**

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



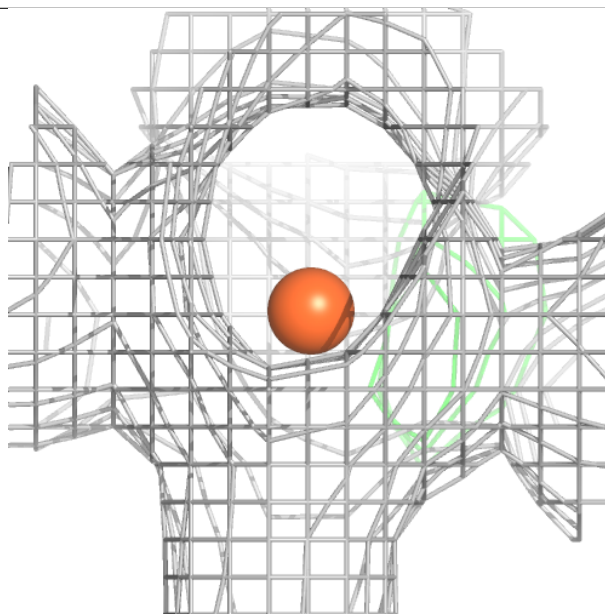
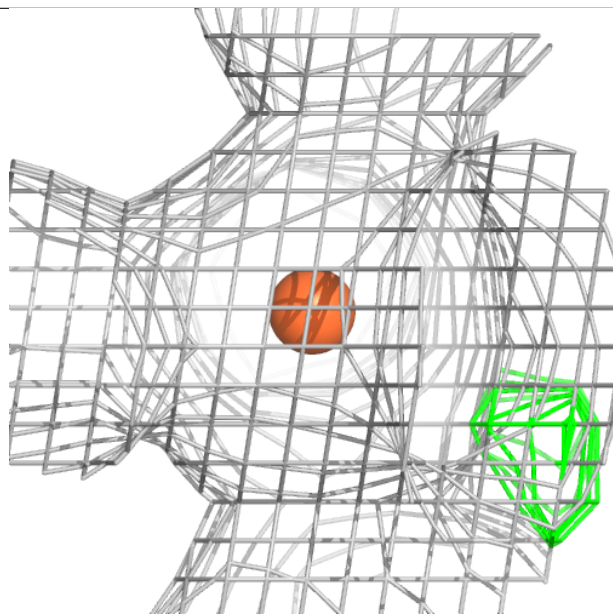
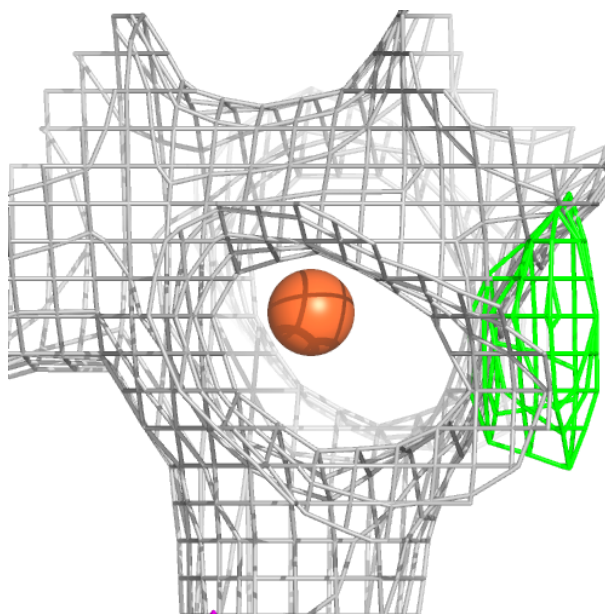
**Electron density around FE2 H 1000:**

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



**Electron density around FE2 A 601:**

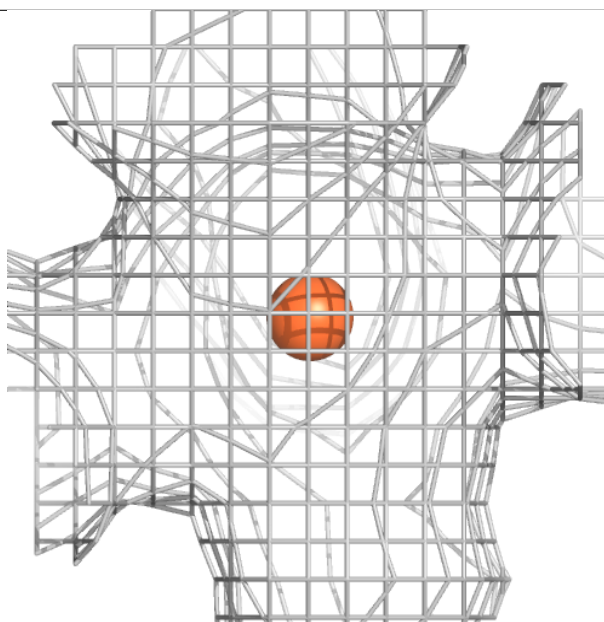
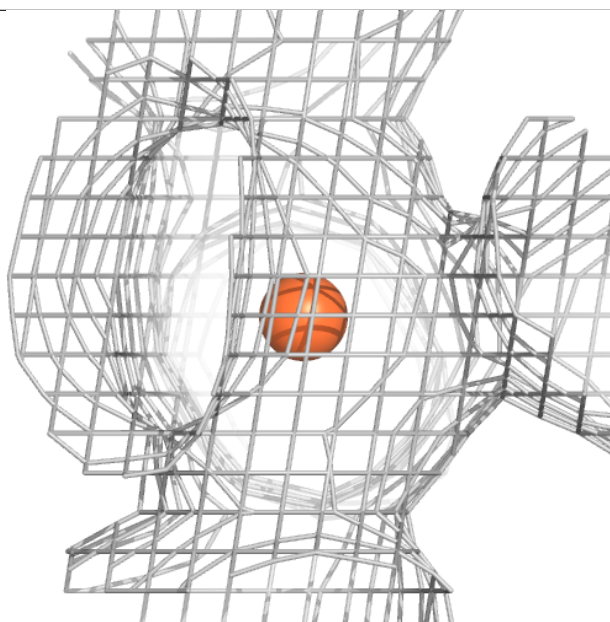
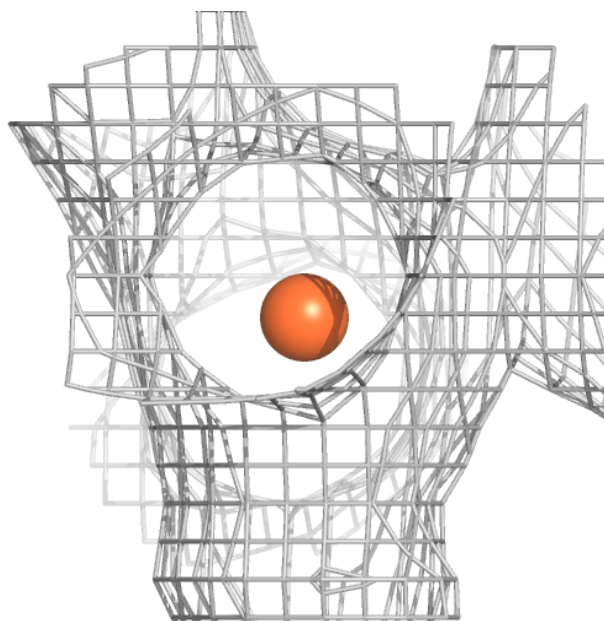
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





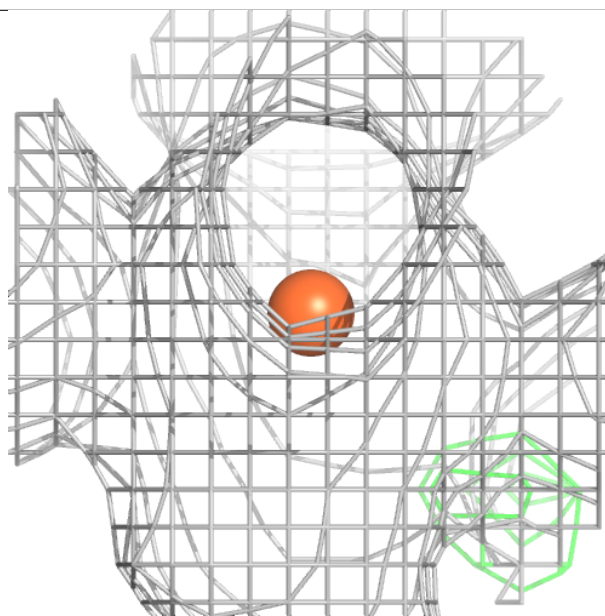
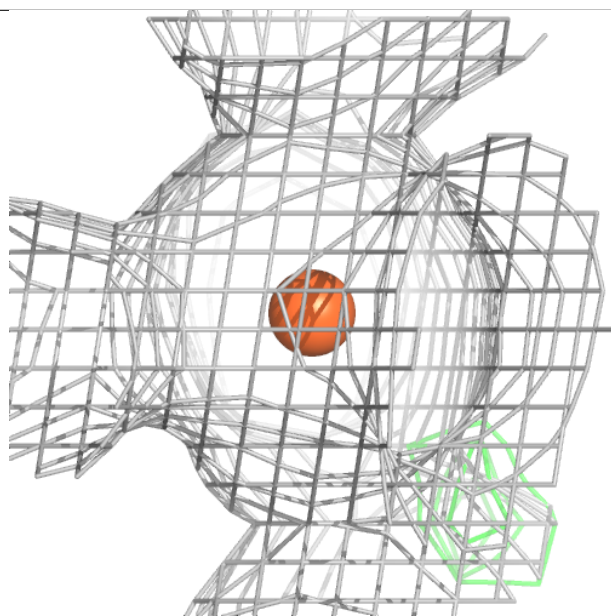
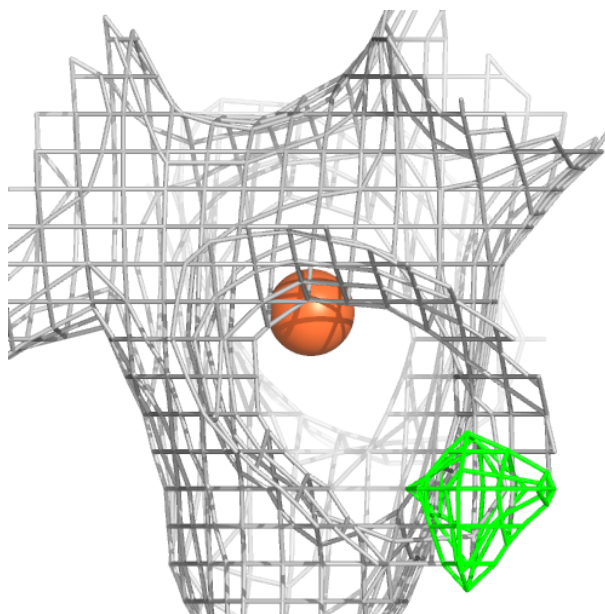
**Electron density around FE2 C 601:**

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



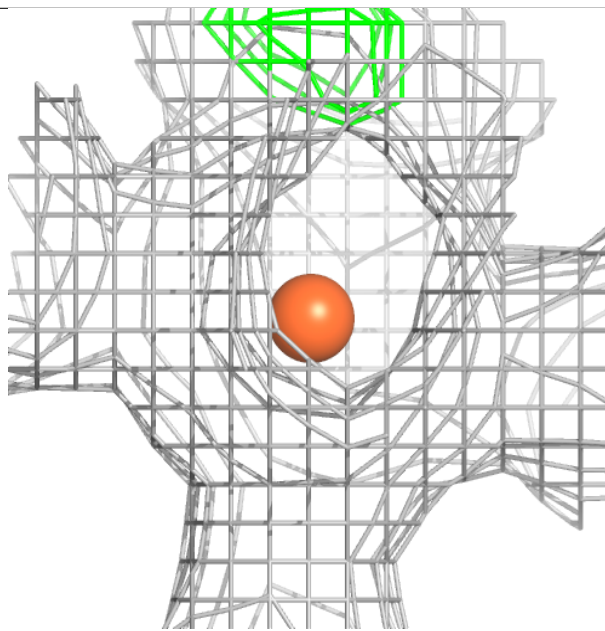
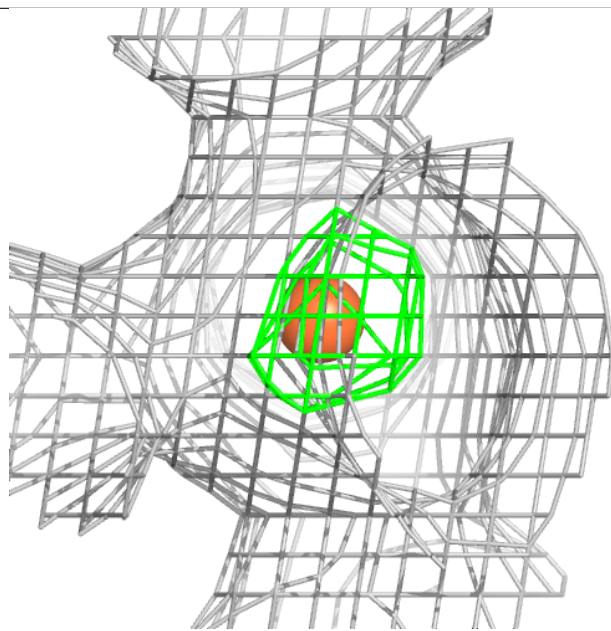
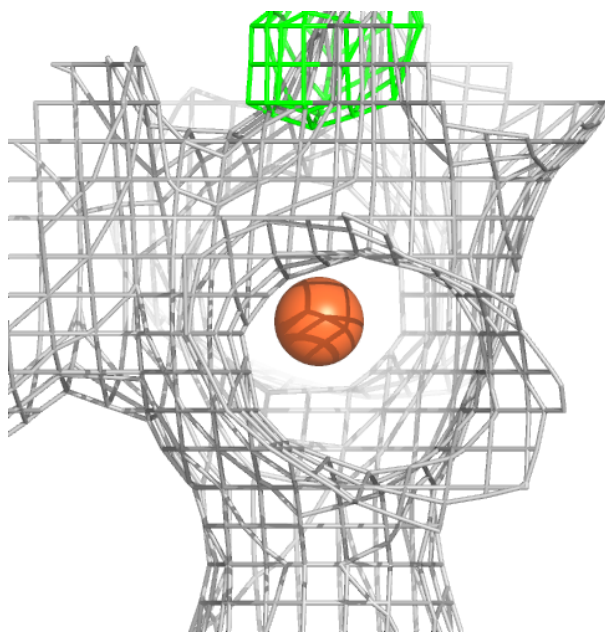
**Electron density around FE2 D 601:**

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



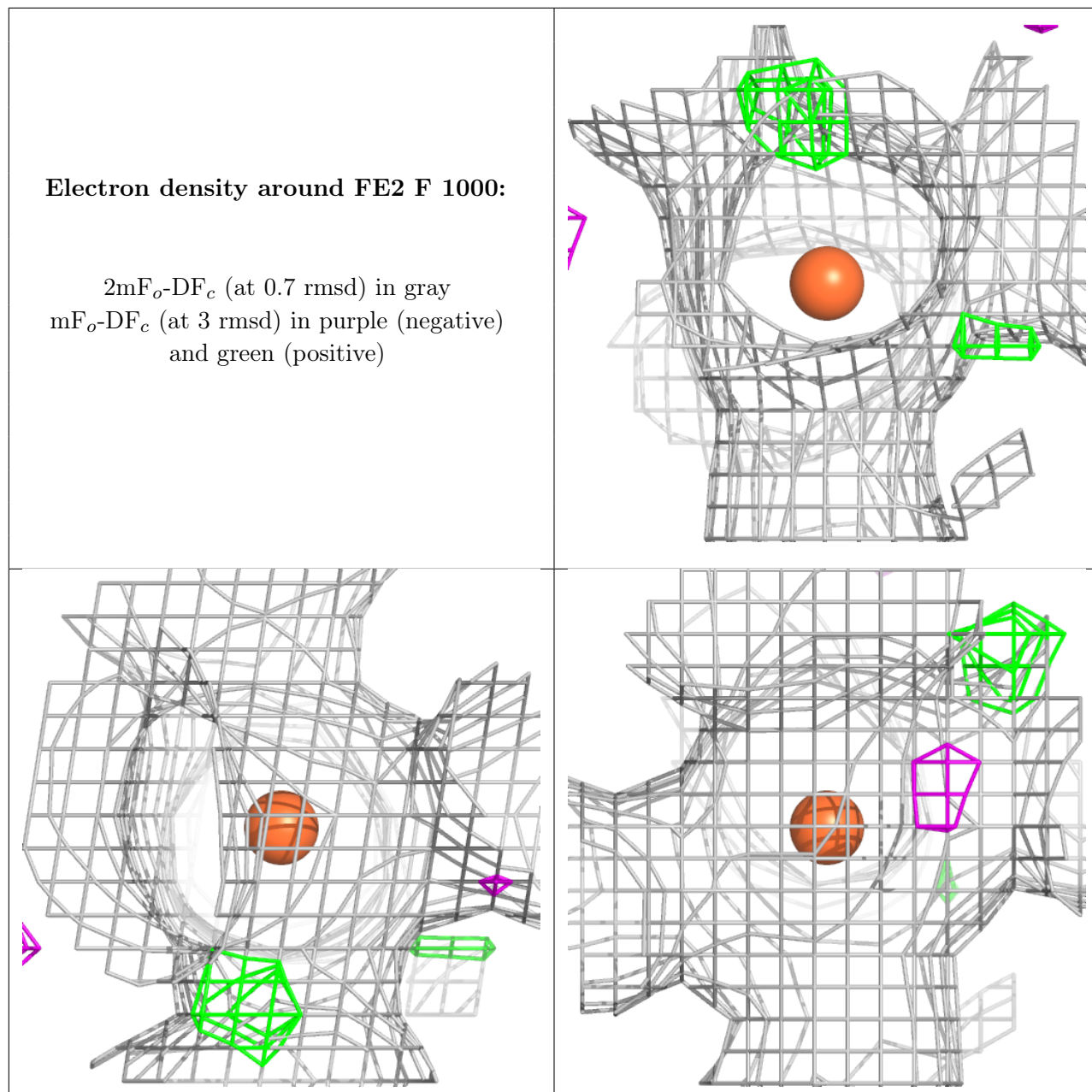
**Electron density around FE2 E 601:**

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



**Electron density around FE2 F 1000:**

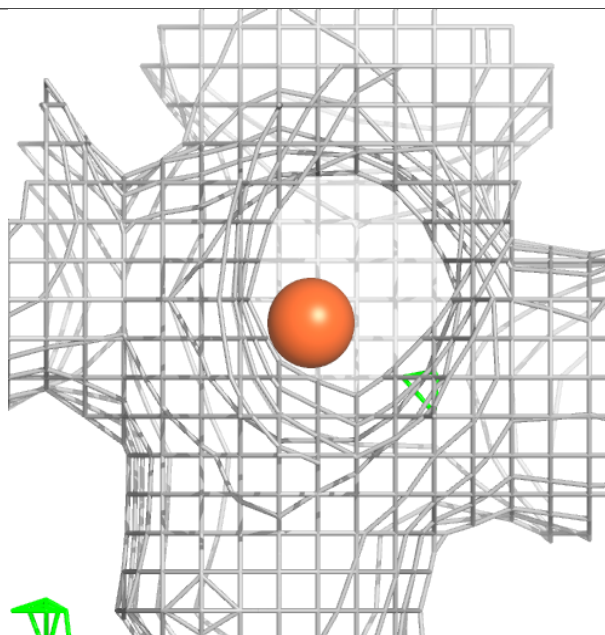
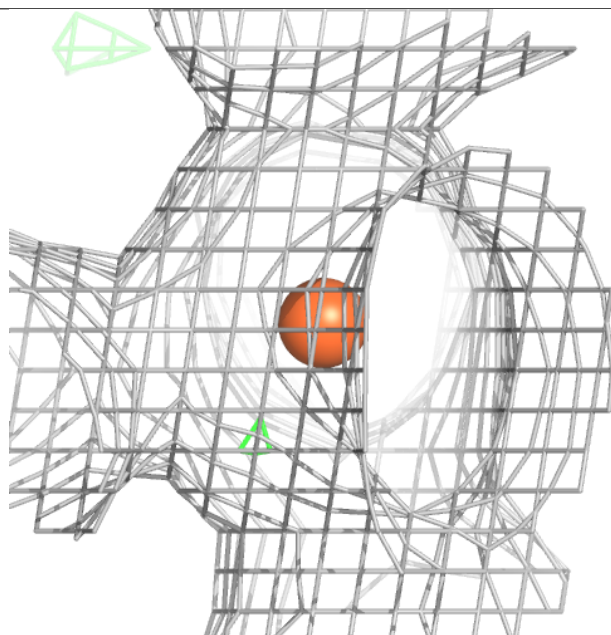
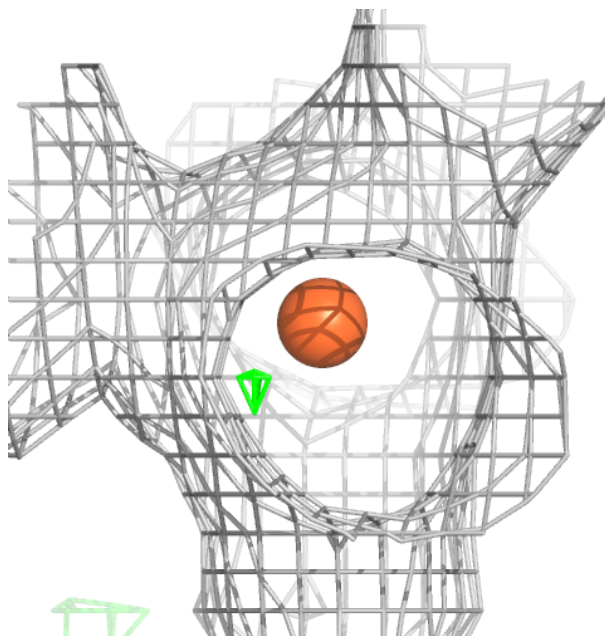
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around FE2 G 601:**

$2mF_o-DF_c$  (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.