



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:08 PM UTC

PDB ID : 8VC9 / pdb_00008vc9
Title : Crystal structure of Rec-controlled histidine kinase LvrB, BeF3-activated
Authors : Mechaly, A.; Buschiazzi, A.
Deposited on : 2023-12-13
Resolution : 2.65 Å(reported)

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

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

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:

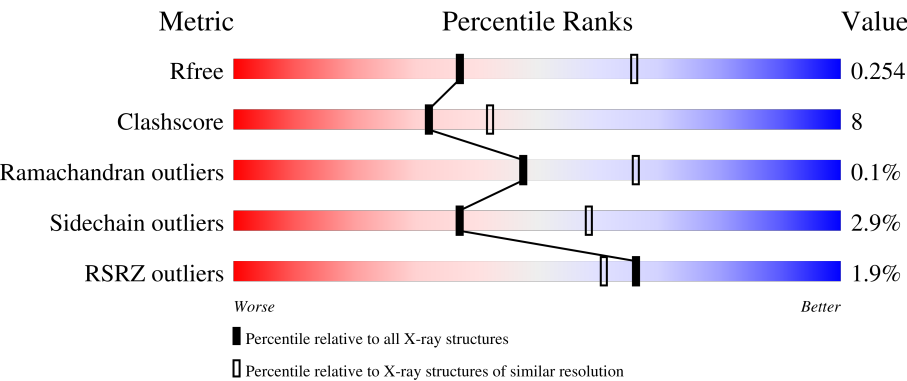
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	382	% 80% 18% ..
1	B	382	5% 77% 20% ..
1	C	382	% 79% 19% ..
1	D	382	% 76% 21% ..
1	E	382	2% 80% 17% ..

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Mol	Chain	Length	Quality of chain
1	F	382	2% 79% 19% ..

2 Entry composition [i](#)

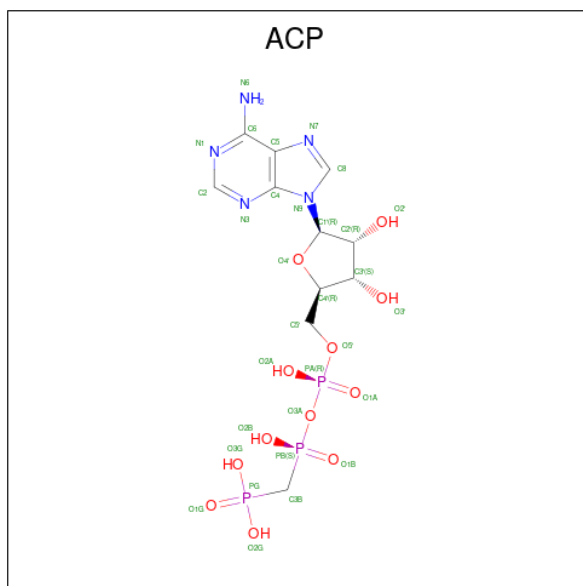
There are 6 unique types of molecules in this entry. The entry contains 18135 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 *Leptospira* virulence regulator B (LvrB).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2970	1895	494	572	9			
1	B	376	Total	C	N	O	S	0	0	0
			2942	1878	488	566	10			
1	C	378	Total	C	N	O	S	0	1	0
			3013	1921	505	577	10			
1	D	378	Total	C	N	O	S	0	0	0
			2986	1907	497	573	9			
1	E	376	Total	C	N	O	S	0	0	0
			2954	1886	491	568	9			
1	F	378	Total	C	N	O	S	0	0	0
			2992	1911	498	574	9			

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

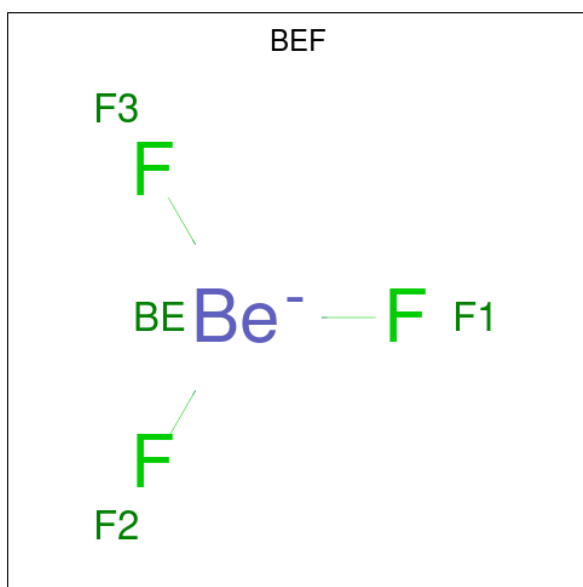


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	E	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		
3	F	2	Total	Mg	0	0
			2	2		

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Be	F	0	0
			4	1	3		
4	B	1	Total	Be	F	0	0
			4	1	3		
4	C	1	Total	Be	F	0	0
			4	1	3		
4	D	1	Total	Be	F	0	0
			4	1	3		
4	E	1	Total	Be	F	0	0
			4	1	3		
4	F	1	Total	Be	F	0	0
			4	1	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

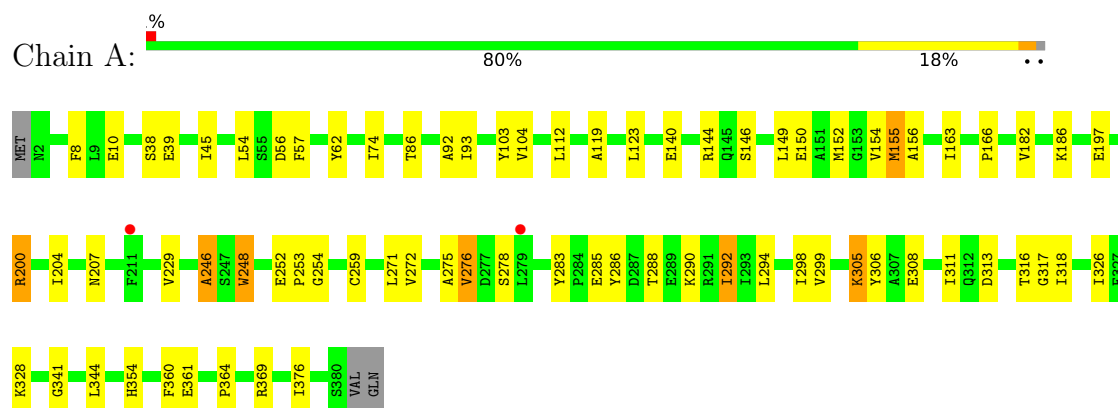
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		
6	B	6	Total	O	0	0
			6	6		
6	C	7	Total	O	0	0
			7	7		
6	D	7	Total	O	0	0
			7	7		
6	E	6	Total	O	0	0
			6	6		
6	F	5	Total	O	0	0
			5	5		

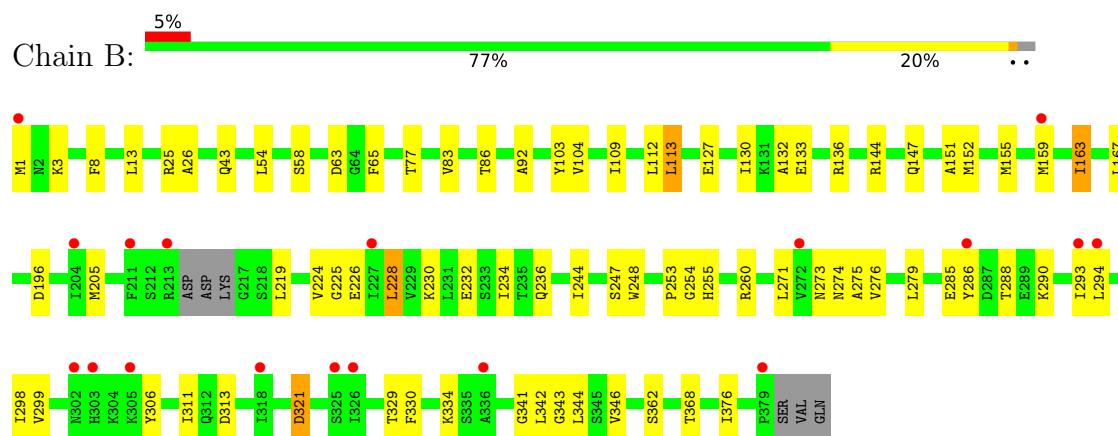
3 Residue-property plots

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.

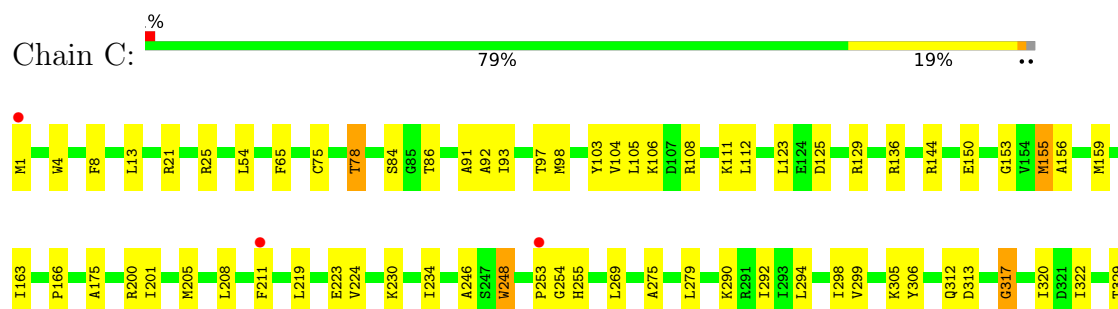
• Molecule 1: *Leptospira* virulence regulator B (LvrB)



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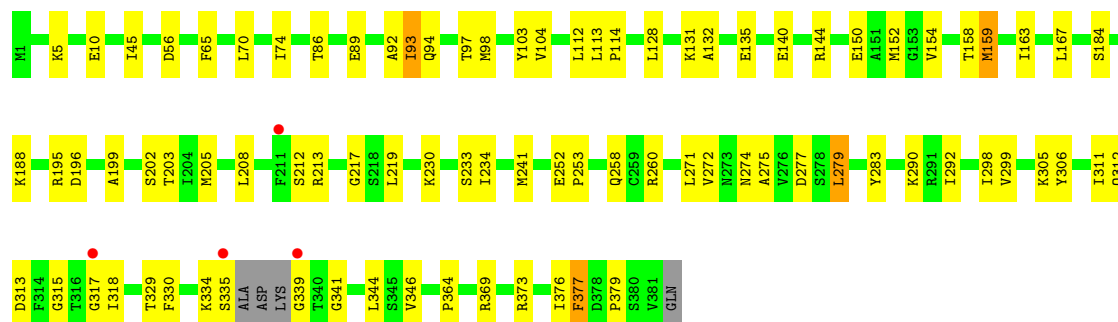
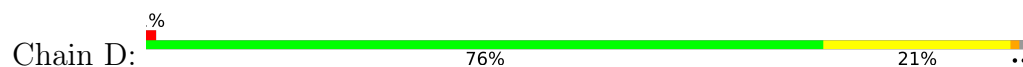


• Molecule 1: *Leptospira* virulence regulator B (LvrB)

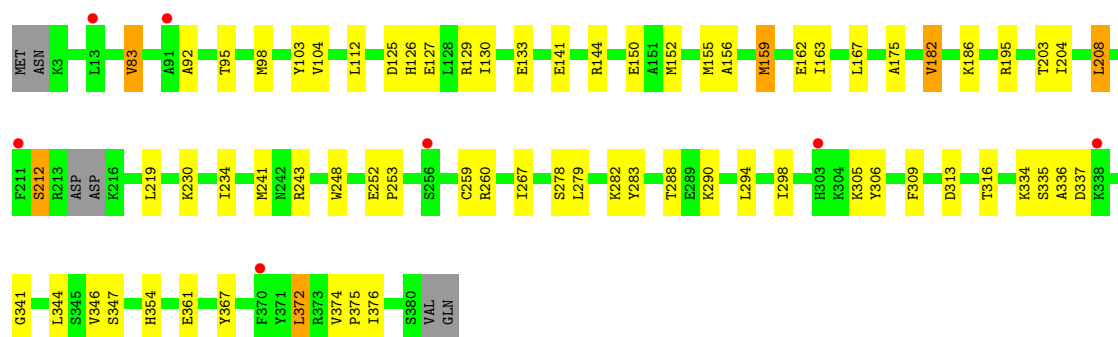
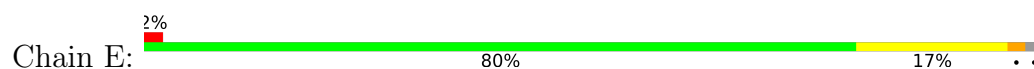




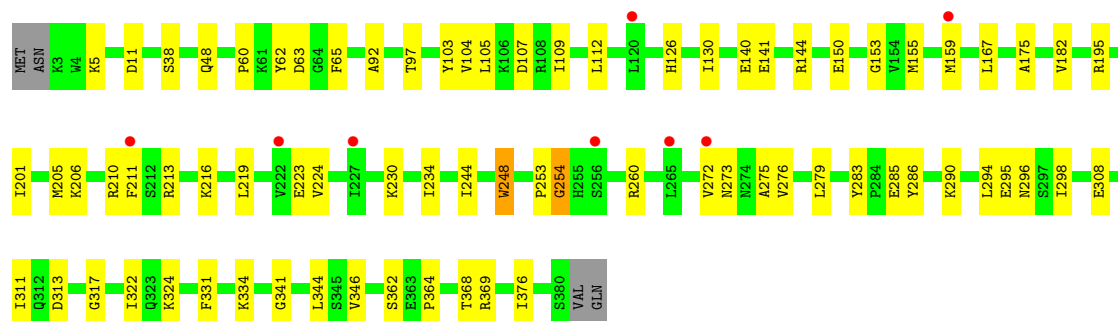
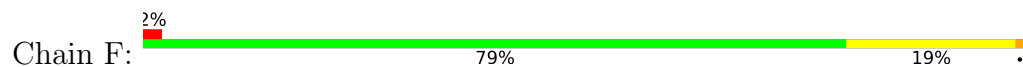
- Molecule 1: *Leptospira* virulence regulator B (LvrB)



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.07Å 102.33Å 184.48Å 90.00° 92.49° 90.00°	Depositor
Resolution (Å)	49.27 – 2.65 49.27 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.27-2.65) 99.7 (49.27-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.210 , 0.254 0.212 , 0.254	Depositor DCC
R_{free} test set	4651 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.007 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.010 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.012 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18135	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: ACP, BEF, MG, SO4

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	0.28	0/3025	0.74	5/4090 (0.1%)
1	B	0.28	0/2995	0.73	2/4048 (0.0%)
1	C	0.29	0/3070	0.74	4/4139 (0.1%)
1	D	0.31	0/3040	0.77	1/4103 (0.0%)
1	E	0.27	0/3008	0.72	0/4063
1	F	0.27	0/3047	0.72	3/4111 (0.1%)
All	All	0.28	0/18185	0.74	15/24554 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	TRP	N-CA-C	-6.44	98.40	108.90
1	C	246	ALA	CA-C-N	6.09	131.77	122.93
1	C	246	ALA	C-N-CA	6.09	131.77	122.93
1	A	254	GLY	CA-C-N	5.84	131.06	123.00
1	A	254	GLY	C-N-CA	5.84	131.06	123.00
1	D	377	PHE	N-CA-CB	-5.79	101.50	110.65
1	C	4	TRP	N-CA-C	5.76	118.62	110.50
1	B	254	GLY	CA-C-N	5.73	130.91	123.00
1	B	254	GLY	C-N-CA	5.73	130.91	123.00
1	C	248	TRP	N-CA-C	-5.44	100.03	108.90
1	F	254	GLY	CA-C-N	5.26	130.26	123.00
1	F	254	GLY	C-N-CA	5.26	130.26	123.00
1	A	246	ALA	CA-C-N	5.25	130.54	122.93
1	A	246	ALA	C-N-CA	5.25	130.54	122.93
1	F	248	TRP	N-CA-C	-5.16	100.49	108.90

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	2970	0	2935	52	0
1	B	2942	0	2908	51	0
1	C	3013	0	3028	62	0
1	D	2986	0	2985	66	0
1	E	2954	0	2928	54	0
1	F	2992	0	2999	57	0
2	A	31	0	14	4	0
2	B	31	0	14	5	0
2	C	31	0	14	4	0
2	D	31	0	14	5	0
2	E	31	0	14	2	0
2	F	31	0	14	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
5	A	5	0	0	0	0
5	E	15	0	0	0	0
6	A	5	0	0	0	0
6	B	6	0	0	0	0
6	C	7	0	0	0	0
6	D	7	0	0	0	0
6	E	6	0	0	0	0
6	F	5	0	0	0	0
All	All	18135	0	17867	289	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 8.

All (289) 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:298:ILE:HD12	1:D:376:ILE:HD11	1.52	0.92
1:D:252:GLU:HG2	1:D:298:ILE:HG12	1.51	0.89
1:A:298:ILE:HD12	1:A:376:ILE:HD11	1.57	0.86
1:A:197:GLU:OE2	1:A:200:ARG:NH2	2.12	0.83
1:E:163:ILE:HD11	1:F:205:MET:HG3	1.62	0.80
1:A:144:ARG:HD2	1:B:144:ARG:HD2	1.64	0.78
1:F:341:GLY:H	2:F:401:ACP:H3B1	1.51	0.76
1:F:298:ILE:HD12	1:F:376:ILE:HD11	1.66	0.75
1:B:86:THR:HB	1:D:253:PRO:HB2	1.68	0.75
1:C:344:LEU:HD12	2:C:401:ACP:H5'1	1.71	0.72
1:E:298:ILE:HD12	1:E:376:ILE:HD11	1.71	0.71
1:E:159:MET:HG3	1:E:208:LEU:HD23	1.72	0.70
1:F:317:GLY:HA3	1:F:364:PRO:HA	1.73	0.69
1:B:253:PRO:HB2	1:D:86:THR:HB	1.73	0.69
1:C:298:ILE:HD12	1:C:376:ILE:HD11	1.73	0.69
1:D:341:GLY:H	2:D:401:ACP:H3B1	1.56	0.69
1:E:279:LEU:HD12	1:E:290:LYS:HG3	1.75	0.68
1:C:223:GLU:OE2	1:C:254:GLY:N	2.23	0.68
1:F:344:LEU:HD12	2:F:401:ACP:H5'1	1.76	0.67
1:A:308:GLU:OE2	1:A:369:ARG:NH2	2.28	0.67
1:F:283:TYR:HB2	1:F:290:LYS:HD3	1.76	0.66
1:F:308:GLU:OE2	1:F:369:ARG:NH2	2.27	0.66
1:E:267:ILE:HG21	1:E:372:LEU:HD12	1.76	0.66
1:E:279:LEU:HD21	1:E:313:ASP:HB2	1.77	0.65
1:C:104:VAL:HG21	1:C:112:LEU:HA	1.79	0.65
1:A:93:ILE:HG12	1:D:132:ALA:HB2	1.79	0.65
1:A:253:PRO:HB2	1:C:86:THR:HB	1.79	0.65
1:C:341:GLY:H	2:C:401:ACP:H3B1	1.61	0.65
1:C:279:LEU:HD21	1:C:313:ASP:HB2	1.80	0.63
1:E:156:ALA:HB2	1:F:155:MET:HE1	1.81	0.63
1:F:285:GLU:HG2	1:F:286:TYR:H	1.64	0.63
1:A:344:LEU:HD12	2:A:401:ACP:H5'1	1.82	0.62
1:E:344:LEU:HD11	2:E:401:ACP:H8	1.81	0.62
1:F:92:ALA:HB1	1:F:103:TYR:CD1	2.35	0.62
1:A:86:THR:HB	1:C:253:PRO:HB2	1.82	0.61
1:A:341:GLY:H	2:A:401:ACP:H3B1	1.65	0.61
1:B:321:ASP:N	1:B:321:ASP:OD1	2.31	0.61
1:E:212:SER:HB3	1:F:153:GLY:HA2	1.83	0.61
1:A:39:GLU:N	1:A:39:GLU:OE1	2.33	0.61
1:C:234:ILE:HD12	1:D:140:GLU:HG3	1.82	0.60
1:E:150:GLU:HG2	1:F:346:VAL:HG11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:LEU:HD11	2:F:401:ACP:H8	1.82	0.60
1:B:285:GLU:HG2	1:B:286:TYR:H	1.65	0.60
1:C:21:ARG:HE	1:C:25:ARG:HH21	1.49	0.60
1:F:334:LYS:HE2	2:F:401:ACP:H3B2	1.83	0.60
1:E:144:ARG:CD	1:F:144:ARG:HD2	2.32	0.59
1:B:224:VAL:HG23	1:B:255:HIS:O	2.01	0.59
1:E:346:VAL:HG11	1:F:150:GLU:HG2	1.83	0.59
1:F:38:SER:HB2	1:F:62:TYR:CE1	2.37	0.59
1:B:104:VAL:HG21	1:B:112:LEU:HA	1.84	0.59
1:D:92:ALA:HB1	1:D:103:TYR:CD1	2.36	0.59
1:B:244:ILE:HD13	1:B:290:LYS:HG2	1.84	0.59
1:A:140:GLU:HG3	1:B:234:ILE:HD12	1.85	0.59
1:F:224:VAL:HG23	1:F:253:PRO:HA	1.84	0.59
1:C:136:ARG:NE	1:D:233:SER:HB2	2.17	0.59
1:B:247:SER:HB2	1:B:293:ILE:HD13	1.86	0.58
1:D:344:LEU:HD12	2:D:401:ACP:H5'1	1.85	0.58
1:A:154:VAL:HG21	1:B:346:VAL:HG22	1.85	0.58
1:C:279:LEU:CD2	1:C:313:ASP:HB2	2.34	0.58
1:C:125:ASP:OD2	1:C:129:ARG:NH1	2.34	0.58
1:C:224:VAL:HG23	1:C:255:HIS:O	2.03	0.57
1:B:92:ALA:HB1	1:B:103:TYR:CD1	2.39	0.57
1:C:346:VAL:HG11	1:D:150:GLU:HG2	1.85	0.57
1:D:335:SER:O	1:D:339:GLY:N	2.37	0.57
1:C:159:MET:CE	1:D:159:MET:HE3	2.35	0.57
1:C:305:LYS:HB3	1:C:376:ILE:HD12	1.84	0.57
1:C:136:ARG:HE	1:D:233:SER:HB2	1.68	0.57
1:C:205:MET:HG3	1:D:163:ILE:HD11	1.87	0.57
1:E:92:ALA:HB1	1:E:103:TYR:CD1	2.40	0.57
1:B:127:GLU:O	1:B:130:ILE:HG13	2.05	0.56
1:C:340:THR:OG1	2:C:401:ACP:O2G	2.22	0.56
1:D:159:MET:HG3	1:D:208:LEU:HD22	1.88	0.56
1:A:144:ARG:HD2	1:B:144:ARG:CD	2.33	0.55
1:B:271:LEU:HB2	1:B:311:ILE:HD12	1.87	0.55
1:E:95:THR:HA	1:E:98:MET:HE2	1.88	0.55
1:F:273:ASN:HA	1:F:276:VAL:HG12	1.87	0.55
1:D:275:ALA:HB1	1:D:313:ASP:HB3	1.87	0.55
1:F:230:LYS:O	1:F:234:ILE:HG12	2.06	0.55
1:C:144:ARG:HD3	1:D:144:ARG:CD	2.37	0.54
1:B:232:GLU:OE1	1:B:236:GLN:NE2	2.39	0.54
1:E:133:GLU:HB3	1:E:241:MET:HE2	1.90	0.54
1:D:104:VAL:HG21	1:D:112:LEU:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ALA:HB1	1:C:103:TYR:CD1	2.43	0.54
1:E:159:MET:HE3	1:F:159:MET:SD	2.47	0.53
1:A:92:ALA:HB1	1:A:103:TYR:CD1	2.43	0.53
1:F:141:GLU:HG2	1:F:144:ARG:HH21	1.74	0.53
1:A:163:ILE:HD11	1:B:205:MET:SD	2.49	0.53
1:C:230:LYS:O	1:C:234:ILE:HG12	2.09	0.53
1:B:132:ALA:HB2	1:C:93:ILE:HG12	1.91	0.52
1:E:152:MET:HB3	1:F:155:MET:HG3	1.89	0.52
1:F:223:GLU:OE2	1:F:254:GLY:N	2.38	0.52
1:E:283:TYR:HB2	1:E:290:LYS:HD2	1.92	0.52
1:A:38:SER:HB2	1:A:62:TYR:CE1	2.45	0.51
1:A:8:PHE:CE2	1:A:54:LEU:HD12	2.45	0.51
1:A:283:TYR:HB2	1:A:290:LYS:HD2	1.91	0.51
2:A:401:ACP:O3'	2:A:401:ACP:O1B	2.29	0.51
1:A:156:ALA:HA	1:B:159:MET:HE1	1.92	0.51
1:C:65:PHE:CD1	1:C:98:MET:HE1	2.46	0.51
1:D:219:LEU:HB3	1:D:258:GLN:HG2	1.91	0.51
1:A:104:VAL:HG21	1:A:112:LEU:HA	1.90	0.51
1:C:211:PHE:CZ	1:D:330:PHE:HB3	2.46	0.51
1:D:159:MET:HG2	1:D:205:MET:SD	2.51	0.51
1:E:309:PHE:HD1	1:E:372:LEU:HD22	1.76	0.51
1:A:166:PRO:HG3	1:A:200:ARG:HD2	1.93	0.51
1:F:126:HIS:O	1:F:130:ILE:HG12	2.11	0.51
1:E:144:ARG:HD2	1:F:144:ARG:HD2	1.93	0.51
1:E:195:ARG:HD2	1:F:175:ALA:HA	1.93	0.51
1:B:344:LEU:HD12	2:B:401:ACP:H5'1	1.92	0.51
1:C:317:GLY:HA3	1:C:364:PRO:HA	1.93	0.51
1:B:244:ILE:HD12	1:B:279:LEU:HD13	1.91	0.50
1:F:362:SER:HB2	1:F:368:THR:HG23	1.93	0.50
1:D:305:LYS:HB3	1:D:376:ILE:HD12	1.92	0.50
1:E:104:VAL:HG21	1:E:112:LEU:HA	1.93	0.50
1:C:150:GLU:HG2	1:D:346:VAL:HG11	1.93	0.50
1:A:299:VAL:HG23	1:A:306:TYR:HB2	1.93	0.50
1:B:255:HIS:CE1	1:B:298:ILE:HG13	2.47	0.50
1:E:219:LEU:HD23	1:E:260:ARG:HG3	1.93	0.50
1:F:210:ARG:HA	1:F:213:ARG:HG2	1.94	0.50
1:F:206:LYS:O	1:F:210:ARG:HB2	2.11	0.50
1:A:285:GLU:HG2	1:A:286:TYR:H	1.76	0.50
1:D:283:TYR:HB2	1:D:290:LYS:HD2	1.93	0.50
1:A:57:PHE:CE2	1:C:253:PRO:HG3	2.47	0.49
1:D:131:LYS:HE2	1:D:135:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:ALA:HB2	1:F:155:MET:CE	2.41	0.49
1:E:162:GLU:HB3	1:E:204:ILE:HD13	1.95	0.49
1:C:75:CYS:HB2	1:C:78:THR:OG1	2.12	0.49
1:E:309:PHE:CD1	1:E:372:LEU:HD22	2.48	0.49
1:F:272:VAL:HG23	1:F:311:ILE:HD13	1.94	0.49
1:A:248:TRP:HA	1:A:294:LEU:O	2.12	0.49
1:B:8:PHE:CE1	1:B:54:LEU:HD12	2.48	0.49
1:A:253:PRO:CB	1:C:86:THR:HB	2.42	0.49
1:B:26:ALA:HB2	1:B:113:LEU:HD11	1.95	0.49
1:E:267:ILE:CG2	1:E:372:LEU:HD12	2.42	0.49
1:F:219:LEU:HD23	1:F:260:ARG:HG3	1.94	0.49
1:E:282:LYS:HB2	1:E:316:THR:HG22	1.94	0.49
1:F:63:ASP:OD2	1:F:65:PHE:HB2	2.13	0.48
1:B:274:ASN:HB3	2:B:401:ACP:N7	2.28	0.48
1:B:248:TRP:HA	1:B:294:LEU:O	2.13	0.48
1:C:144:ARG:HD3	1:D:144:ARG:HD2	1.94	0.48
1:C:312:GLN:HB2	1:C:369:ARG:HG3	1.94	0.48
1:C:111:LYS:O	1:C:111:LYS:HG2	2.12	0.48
1:A:204:ILE:HA	1:A:207:ASN:ND2	2.28	0.48
1:B:58:SER:HB2	1:D:253:PRO:HG2	1.94	0.48
1:B:341:GLY:H	2:B:401:ACP:H3B1	1.79	0.48
1:C:159:MET:HG3	1:C:208:LEU:HD12	1.94	0.48
1:B:299:VAL:HG23	1:B:306:TYR:HB2	1.96	0.47
1:C:84:SER:HA	1:C:106:LYS:HE3	1.96	0.47
1:C:163:ILE:HD11	1:D:205:MET:HG3	1.96	0.47
1:E:167:LEU:HD11	1:F:201:ILE:HG22	1.96	0.47
1:D:65:PHE:CD1	1:D:98:MET:HE1	2.49	0.47
1:F:104:VAL:HG21	1:F:112:LEU:HA	1.95	0.47
1:A:361:GLU:HG2	1:A:369:ARG:HB3	1.97	0.47
1:F:275:ALA:HB1	1:F:313:ASP:HB3	1.95	0.47
1:A:229:VAL:HG11	1:C:91:ALA:O	2.14	0.47
1:C:329:THR:HG22	1:C:330:PHE:CD2	2.50	0.47
1:D:113:LEU:HB3	1:D:114:PRO:HD3	1.97	0.47
1:D:199:ALA:O	1:D:203:THR:HG23	2.14	0.47
1:B:329:THR:HG22	1:B:330:PHE:CD2	2.50	0.47
1:E:282:LYS:HB2	1:E:316:THR:CG2	2.44	0.47
1:A:182:VAL:HB	1:A:186:LYS:HB3	1.96	0.47
1:B:159:MET:HE2	1:B:159:MET:HB2	1.82	0.47
1:D:377:PHE:CE2	1:D:379:PRO:HG3	2.50	0.46
1:E:125:ASP:O	1:E:129:ARG:HG3	2.15	0.46
1:E:150:GLU:HG2	1:F:346:VAL:CG1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:GLU:OE2	1:E:367:TYR:OH	2.33	0.46
1:E:230:LYS:O	1:E:234:ILE:HG12	2.15	0.46
1:C:255:HIS:CE1	1:C:298:ILE:HG13	2.50	0.46
1:D:299:VAL:HG21	1:D:373:ARG:NE	2.31	0.46
1:E:372:LEU:HD21	1:E:374:VAL:HG23	1.98	0.46
1:A:246:ALA:HA	1:A:292:ILE:HG22	1.97	0.46
1:A:152:MET:SD	1:B:151:ALA:HB1	2.56	0.45
1:D:299:VAL:HG23	1:D:306:TYR:HB2	1.98	0.45
1:B:273:ASN:HA	1:B:276:VAL:HG12	1.96	0.45
1:F:279:LEU:HD22	1:F:290:LYS:HG3	1.98	0.45
1:C:159:MET:HE2	1:D:159:MET:HE3	1.97	0.45
1:B:275:ALA:HB1	1:B:313:ASP:HB3	1.98	0.45
1:F:105:LEU:HB3	1:F:107:ASP:OD1	2.17	0.45
1:B:230:LYS:O	1:B:234:ILE:HG12	2.17	0.45
1:A:119:ALA:O	1:A:123:LEU:HD13	2.17	0.45
1:D:317:GLY:HA3	1:D:364:PRO:HA	1.98	0.45
1:E:127:GLU:OE1	1:E:243:ARG:NH1	2.50	0.45
1:A:271:LEU:HB2	1:A:311:ILE:HD12	1.99	0.45
1:C:159:MET:HG3	1:C:208:LEU:CD1	2.47	0.45
1:A:272:VAL:O	1:A:276:VAL:HG13	2.17	0.44
1:C:248:TRP:HA	1:C:294:LEU:O	2.17	0.44
1:D:5:LYS:HB2	1:D:5:LYS:HE3	1.72	0.44
1:A:326:ILE:HD11	1:A:360:PHE:CE1	2.51	0.44
1:E:175:ALA:HA	1:F:195:ARG:HD2	1.99	0.44
1:C:156:ALA:HA	1:D:159:MET:HE1	1.98	0.44
1:C:279:LEU:HD12	1:C:290:LYS:HG3	1.99	0.44
1:D:89:GLU:O	1:D:93:ILE:HG12	2.18	0.44
1:A:317:GLY:HA3	1:A:364:PRO:HA	1.99	0.44
1:A:344:LEU:HD11	2:A:401:ACP:H8	1.99	0.44
1:E:126:HIS:O	1:E:130:ILE:HG12	2.18	0.44
1:B:83:VAL:HA	1:B:104:VAL:O	2.17	0.44
1:B:232:GLU:HG3	1:D:65:PHE:CE2	2.52	0.44
1:C:166:PRO:HG3	1:C:200:ARG:HD3	2.00	0.44
1:C:299:VAL:HG23	1:C:306:TYR:HB2	1.99	0.44
1:D:217:GLY:O	1:D:260:ARG:HD3	2.18	0.44
1:A:10:GLU:OE1	1:A:56:ASP:HB2	2.18	0.44
1:A:146:SER:O	1:A:150:GLU:HG2	2.18	0.44
1:B:285:GLU:HG2	1:B:286:TYR:N	2.32	0.44
1:D:329:THR:HG22	1:D:330:PHE:CD2	2.53	0.44
1:E:259:CYS:HA	1:E:354:HIS:CD2	2.52	0.44
1:E:279:LEU:CD2	1:E:313:ASP:HB2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:ILE:HG12	1:E:347:SER:HA	2.00	0.43
1:F:104:VAL:HG11	1:F:112:LEU:HB2	2.00	0.43
1:B:109:ILE:HD12	1:B:109:ILE:HA	1.89	0.43
1:E:141:GLU:OE2	1:E:144:ARG:NH2	2.36	0.43
1:E:305:LYS:HE3	1:E:305:LYS:HB2	1.69	0.43
1:E:372:LEU:CD2	1:E:374:VAL:HG23	2.48	0.43
1:A:253:PRO:HB2	1:C:86:THR:CB	2.48	0.43
1:B:342:LEU:N	2:B:401:ACP:O2G	2.52	0.43
1:B:247:SER:HB2	1:B:293:ILE:CD1	2.47	0.43
1:D:45:ILE:HD12	1:D:74:ILE:HD11	2.00	0.43
1:D:272:VAL:HG23	1:D:311:ILE:HD13	2.00	0.43
1:B:63:ASP:OD2	1:B:65:PHE:HB2	2.17	0.43
1:C:201:ILE:HG22	1:D:167:LEU:HD11	2.01	0.43
1:F:155:MET:HE3	1:F:155:MET:HB3	1.56	0.43
1:B:225:GLY:HA2	1:B:228:LEU:HD22	2.00	0.43
1:C:105:LEU:HD12	1:C:108[B]:ARG:NH2	2.34	0.43
1:C:320:ILE:HD12	1:C:320:ILE:H	1.84	0.43
1:E:252:GLU:N	1:E:253:PRO:HD3	2.34	0.43
1:B:219:LEU:HD23	1:B:260:ARG:HG3	2.01	0.43
1:E:334:LYS:O	1:E:336:ALA:N	2.50	0.43
1:F:109:ILE:HD12	1:F:109:ILE:HA	1.94	0.43
1:B:236:GLN:NE2	1:D:98:MET:HE3	2.34	0.43
1:D:230:LYS:O	1:D:234:ILE:HG12	2.19	0.43
1:E:182:VAL:HG13	1:E:186:LYS:HB3	2.01	0.43
1:F:167:LEU:HD23	1:F:167:LEU:HA	1.91	0.43
1:F:285:GLU:HG2	1:F:286:TYR:N	2.33	0.43
1:B:343:GLY:N	2:B:401:ACP:O2G	2.50	0.43
1:E:341:GLY:H	2:E:401:ACP:H3B1	1.83	0.43
1:D:167:LEU:HD23	1:D:167:LEU:HA	1.92	0.42
1:E:234:ILE:HG22	1:F:140:GLU:HG3	2.01	0.42
1:A:197:GLU:CD	1:A:200:ARG:NH2	2.78	0.42
1:F:224:VAL:CG2	1:F:253:PRO:HA	2.49	0.42
1:F:322:ILE:HG23	1:F:331:PHE:CZ	2.54	0.42
1:D:271:LEU:HB2	1:D:311:ILE:HD12	2.02	0.42
1:F:11:ASP:CG	1:F:60:PRO:HD3	2.44	0.42
1:A:93:ILE:CD1	1:D:128:LEU:HD22	2.49	0.42
1:C:1:MET:HE3	1:C:1:MET:HB2	1.85	0.42
1:D:154:VAL:O	1:D:158:THR:HG23	2.20	0.42
1:D:377:PHE:CZ	1:D:379:PRO:HG3	2.54	0.42
1:F:324:LYS:HD3	1:F:324:LYS:HA	1.86	0.42
1:D:94:GLN:O	1:D:98:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:ACP:O1B	2:D:401:ACP:O3'	2.35	0.42
1:D:219:LEU:HD23	1:D:260:ARG:HG3	2.01	0.42
1:F:295:GLU:HG2	1:F:296:ASN:N	2.35	0.42
1:C:334:LYS:H	1:C:334:LYS:HG2	1.64	0.42
1:D:279:LEU:HD13	1:D:315:GLY:CA	2.50	0.42
1:E:83:VAL:HA	1:E:104:VAL:O	2.20	0.42
1:F:159:MET:SD	1:F:205:MET:HE1	2.60	0.42
1:A:252:GLU:N	1:A:253:PRO:HD3	2.35	0.41
1:B:163:ILE:HD12	1:B:167:LEU:HD22	2.02	0.41
1:C:153:GLY:HA2	1:D:212:SER:OG	2.20	0.41
1:C:175:ALA:HA	1:D:195:ARG:HD2	2.01	0.41
1:F:248:TRP:HA	1:F:294:LEU:O	2.19	0.41
1:D:312:GLN:HB2	1:D:369:ARG:HG3	2.02	0.41
1:F:140:GLU:HB3	1:F:144:ARG:NH1	2.35	0.41
1:F:244:ILE:HD11	1:F:276:VAL:HG23	2.01	0.41
1:A:229:VAL:HB	1:C:91:ALA:HB1	2.03	0.41
1:A:275:ALA:HB1	1:A:313:ASP:HB3	2.02	0.41
1:A:305:LYS:HE3	1:A:305:LYS:H	1.83	0.41
1:D:274:ASN:HB3	2:D:401:ACP:N7	2.35	0.41
1:A:45:ILE:HG21	1:A:74:ILE:HG13	2.02	0.41
1:C:275:ALA:HB1	1:C:313:ASP:HB3	2.02	0.41
1:B:13:LEU:HD13	1:B:13:LEU:HA	1.92	0.41
1:D:10:GLU:OE1	1:D:56:ASP:HB2	2.21	0.41
1:A:155:MET:HE3	1:B:152:MET:HE3	2.02	0.41
1:C:8:PHE:CE1	1:C:54:LEU:HD12	2.55	0.41
1:A:278:SER:O	1:A:316:THR:HG23	2.20	0.41
1:D:184:SER:O	1:D:188:LYS:HG3	2.20	0.41
1:E:248:TRP:HA	1:E:294:LEU:O	2.21	0.41
1:E:278:SER:O	1:E:316:THR:HG23	2.21	0.41
1:C:13:LEU:HD13	1:C:13:LEU:HA	1.83	0.41
1:C:155:MET:HE3	1:D:152:MET:HE3	2.03	0.41
1:C:340:THR:N	2:C:401:ACP:H3B1	2.36	0.41
1:D:277:ASP:OD2	1:D:334:LYS:HE3	2.20	0.41
1:E:159:MET:HE2	1:E:159:MET:HB2	1.94	0.41
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.94	0.41
1:B:133:GLU:HG2	1:B:136:ARG:NH2	2.36	0.41
1:E:306:TYR:CD1	1:E:375:PRO:HA	2.56	0.41
1:B:362:SER:HB2	1:B:368:THR:HG23	2.03	0.40
1:D:334:LYS:HE2	2:D:401:ACP:O2B	2.21	0.40
1:A:259:CYS:HA	1:A:354:HIS:CD2	2.55	0.40
1:C:340:THR:O	1:C:342:LEU:HD12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:LEU:CD2	1:D:313:ASP:HB2	2.51	0.40
1:F:5:LYS:NZ	1:F:48:GLN:O	2.39	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	377/382 (99%)	369 (98%)	8 (2%)	0	100	100
1	B	372/382 (97%)	364 (98%)	7 (2%)	1 (0%)	36	52
1	C	377/382 (99%)	368 (98%)	8 (2%)	1 (0%)	36	52
1	D	374/382 (98%)	368 (98%)	6 (2%)	0	100	100
1	E	372/382 (97%)	362 (97%)	9 (2%)	1 (0%)	36	52
1	F	376/382 (98%)	368 (98%)	8 (2%)	0	100	100
All	All	2248/2292 (98%)	2199 (98%)	46 (2%)	3 (0%)	48	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	335	SER
1	B	3	LYS
1	C	317	GLY

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	319/336 (95%)	311 (98%)	8 (2%)	42	64
1	B	315/336 (94%)	300 (95%)	15 (5%)	23	39
1	C	329/336 (98%)	321 (98%)	8 (2%)	43	65
1	D	325/336 (97%)	314 (97%)	11 (3%)	32	53
1	E	318/336 (95%)	308 (97%)	10 (3%)	35	56
1	F	326/336 (97%)	322 (99%)	4 (1%)	63	79
All	All	1932/2016 (96%)	1876 (97%)	56 (3%)	37	58

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	MET
1	A	200	ARG
1	A	276	VAL
1	A	288	THR
1	A	292	ILE
1	A	305	LYS
1	A	318	ILE
1	A	328	LYS
1	B	1	MET
1	B	25	ARG
1	B	43	GLN
1	B	77	THR
1	B	113	LEU
1	B	147	GLN
1	B	155	MET
1	B	163	ILE
1	B	196	ASP
1	B	226	GLU
1	B	228	LEU
1	B	288	THR
1	B	321	ASP
1	B	334	LYS
1	B	376	ILE
1	C	78	THR
1	C	97	THR
1	C	123	LEU
1	C	155	MET
1	C	219	LEU

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Mol	Chain	Res	Type
1	C	269	LEU
1	C	292	ILE
1	C	322	ILE
1	D	70	LEU
1	D	93	ILE
1	D	97	THR
1	D	159	MET
1	D	196	ASP
1	D	202	SER
1	D	213	ARG
1	D	241	MET
1	D	279	LEU
1	D	292	ILE
1	D	318	ILE
1	E	83	VAL
1	E	155	MET
1	E	159	MET
1	E	182	VAL
1	E	203	THR
1	E	208	LEU
1	E	212	SER
1	E	288	THR
1	E	337	ASP
1	E	372	LEU
1	F	97	THR
1	F	182	VAL
1	F	211	PHE
1	F	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	250	ASN
1	A	263	GLN
1	B	2	ASN
1	B	189	GLN
1	C	236	GLN
1	C	255	HIS
1	C	258	GLN
1	D	94	GLN
1	D	189	GLN

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Mol	Chain	Res	Type
1	D	255	HIS
1	E	126	HIS
1	E	145	GLN
1	E	237	GLN
1	E	359	ASN
1	F	258	GLN
1	F	273	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	SO4	E	406	-	4,4,4	0.23	0	6,6,6	0.20	0
2	ACP	F	401	3	31,33,33	0.71	1 (3%)	47,52,52	0.98	2 (4%)
4	BEF	D	403	1	0,3,3	-	-	-		
4	BEF	B	403	1	0,3,3	-	-	-		
5	SO4	A	405	-	4,4,4	0.25	0	6,6,6	0.09	0
4	BEF	E	403	1	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACP	C	401	3	31,33,33	0.54	1 (3%)	47,52,52	0.98	1 (2%)
2	ACP	A	401	3	31,33,33	0.54	1 (3%)	47,52,52	0.99	1 (2%)
5	SO4	E	405	-	4,4,4	0.27	0	6,6,6	0.16	0
5	SO4	E	407	-	4,4,4	0.21	0	6,6,6	0.22	0
4	BEF	F	403	1	0,3,3	-	-	-	-	-
2	ACP	B	401	3	31,33,33	0.64	1 (3%)	47,52,52	0.97	1 (2%)
2	ACP	E	401	3	31,33,33	0.63	1 (3%)	47,52,52	1.07	1 (2%)
4	BEF	C	403	1	0,3,3	-	-	-	-	-
2	ACP	D	401	3	31,33,33	0.93	2 (6%)	47,52,52	0.87	1 (2%)
4	BEF	A	403	1	0,3,3	-	-	-	-	-

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	ACP	F	401	3	-	2/19/38/38	0/3/3/3
2	ACP	C	401	3	-	8/19/38/38	0/3/3/3
2	ACP	A	401	3	-	3/19/38/38	0/3/3/3
2	ACP	B	401	3	-	5/19/38/38	0/3/3/3
2	ACP	E	401	3	-	1/19/38/38	0/3/3/3
2	ACP	D	401	3	-	5/19/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ACP	PB-O3A	4.19	1.63	1.58
2	F	401	ACP	PB-O3A	3.79	1.62	1.58
2	B	401	ACP	PB-O3A	3.29	1.62	1.58
2	E	401	ACP	PB-O3A	3.29	1.62	1.58
2	D	401	ACP	PA-O3A	2.87	1.62	1.59
2	A	401	ACP	PB-O3A	2.77	1.61	1.58
2	C	401	ACP	PB-O3A	2.75	1.61	1.58

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	ACP	PB-O3A-PA	-6.87	109.94	132.37
2	A	401	ACP	PB-O3A-PA	-6.49	111.18	132.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	ACP	PB-O3A-PA	-6.18	112.19	132.37
2	C	401	ACP	PB-O3A-PA	-6.10	112.45	132.37
2	F	401	ACP	PB-O3A-PA	-6.03	112.70	132.37
2	D	401	ACP	PB-O3A-PA	-5.52	114.37	132.37
2	F	401	ACP	O5'-PA-O1A	2.17	117.55	108.94

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	ACP	C5'-O5'-PA-O2A
2	C	401	ACP	C5'-O5'-PA-O1A
2	C	401	ACP	C5'-O5'-PA-O2A
2	C	401	ACP	C5'-O5'-PA-O3A
2	E	401	ACP	PB-O3A-PA-O5'
2	D	401	ACP	C3'-C4'-C5'-O5'
2	C	401	ACP	O4'-C4'-C5'-O5'
2	C	401	ACP	C3'-C4'-C5'-O5'
2	D	401	ACP	O4'-C4'-C5'-O5'
2	F	401	ACP	C3'-C4'-C5'-O5'
2	B	401	ACP	C3'-C4'-C5'-O5'
2	F	401	ACP	O4'-C4'-C5'-O5'
2	A	401	ACP	O4'-C4'-C5'-O5'
2	A	401	ACP	C3'-C4'-C5'-O5'
2	B	401	ACP	O4'-C4'-C5'-O5'
2	A	401	ACP	PB-O3A-PA-O5'
2	C	401	ACP	PB-O3A-PA-O5'
2	D	401	ACP	PB-O3A-PA-O5'
2	B	401	ACP	C5'-O5'-PA-O1A
2	B	401	ACP	C5'-O5'-PA-O3A
2	C	401	ACP	PB-C3B-PG-O2G
2	C	401	ACP	PB-C3B-PG-O3G
2	D	401	ACP	C5'-O5'-PA-O1A
2	D	401	ACP	C5'-O5'-PA-O2A

There are no ring outliers.

6 monomers are involved in 24 short contacts:

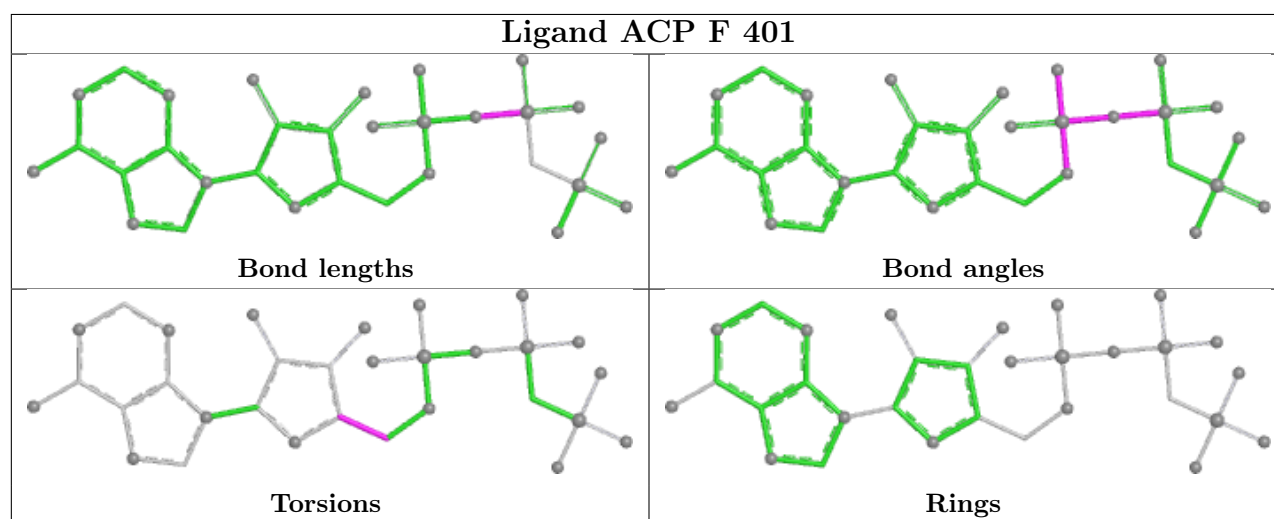
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	ACP	4	0
2	C	401	ACP	4	0

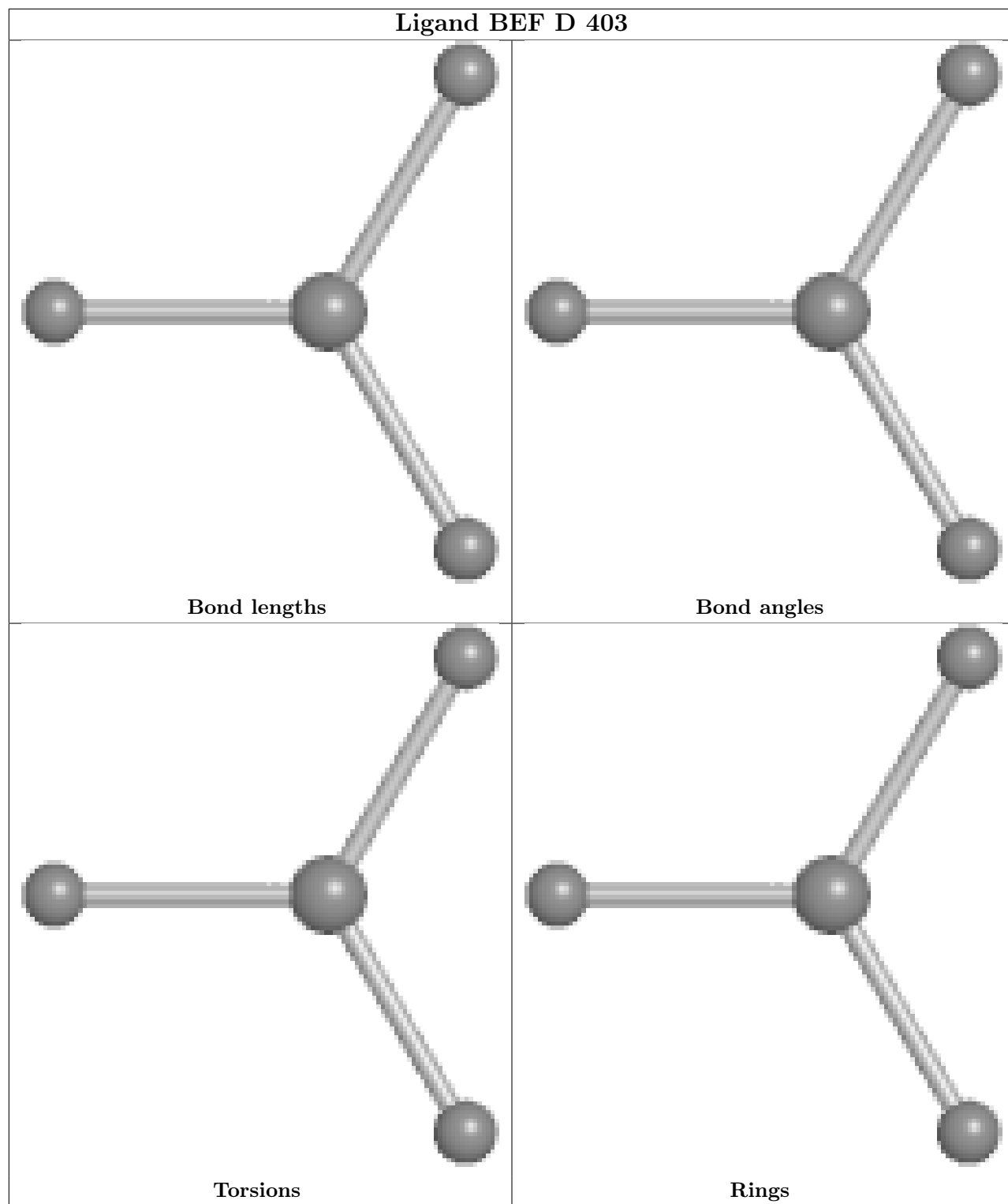
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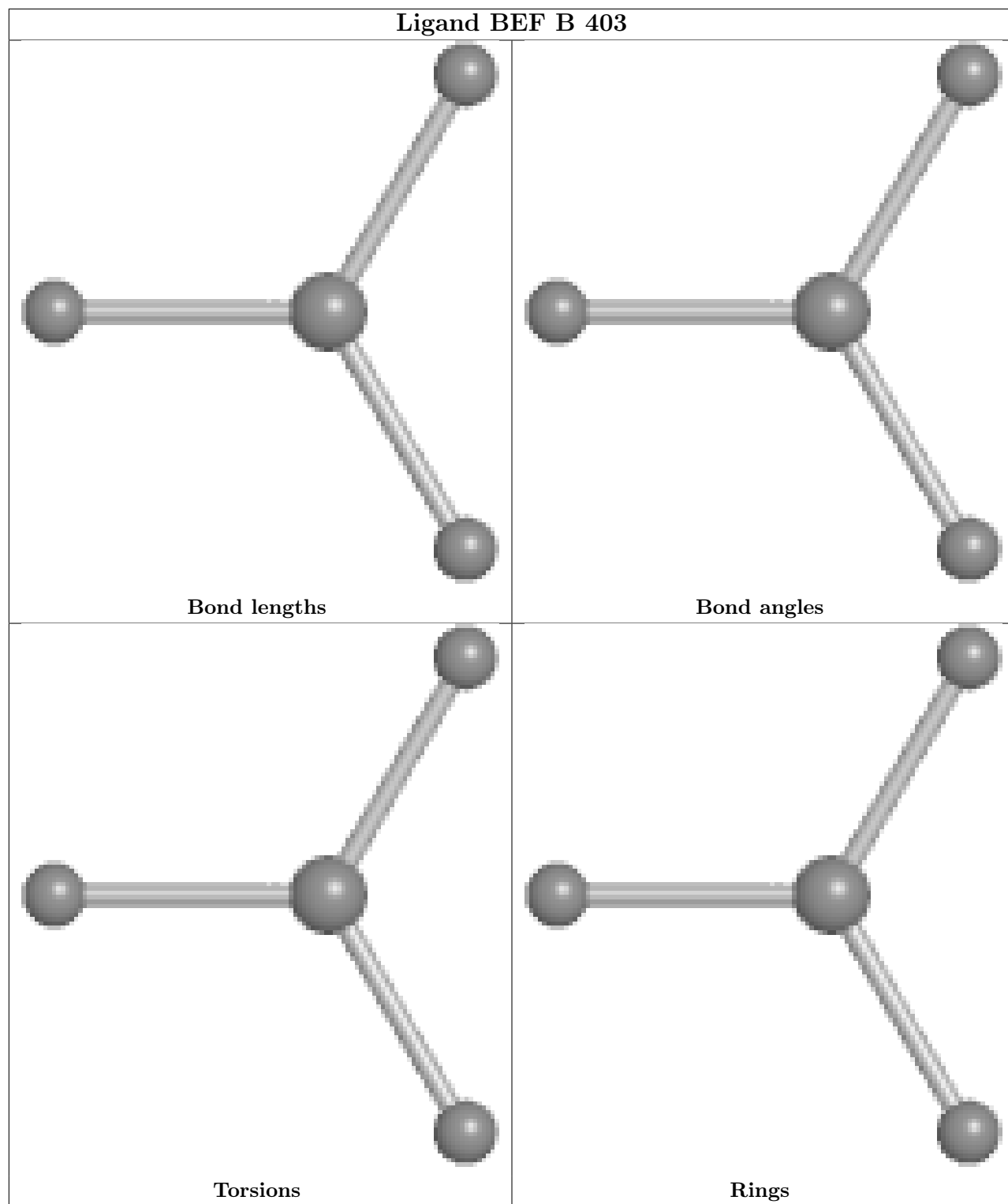
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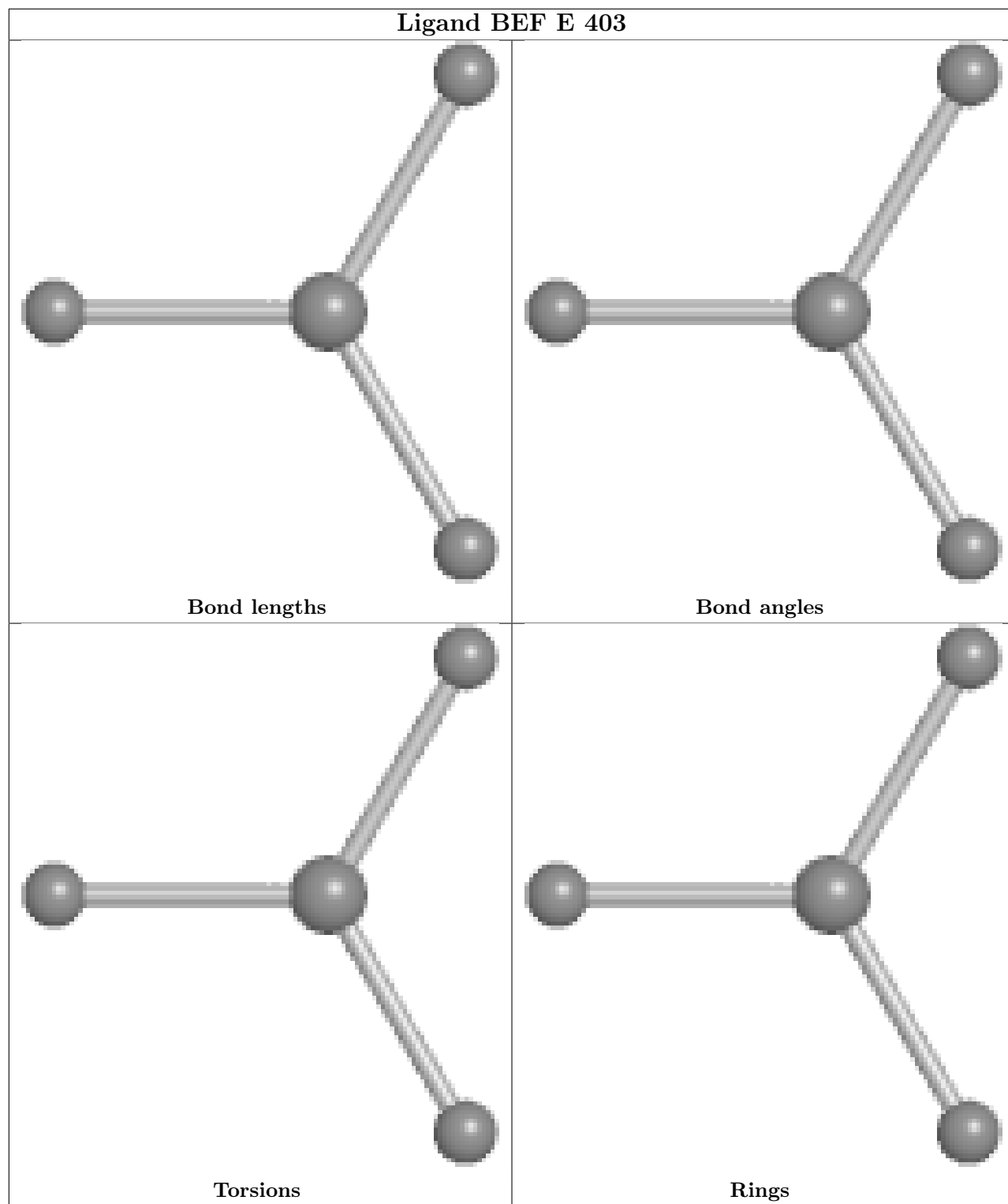
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ACP	4	0
2	B	401	ACP	5	0
2	E	401	ACP	2	0
2	D	401	ACP	5	0

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.

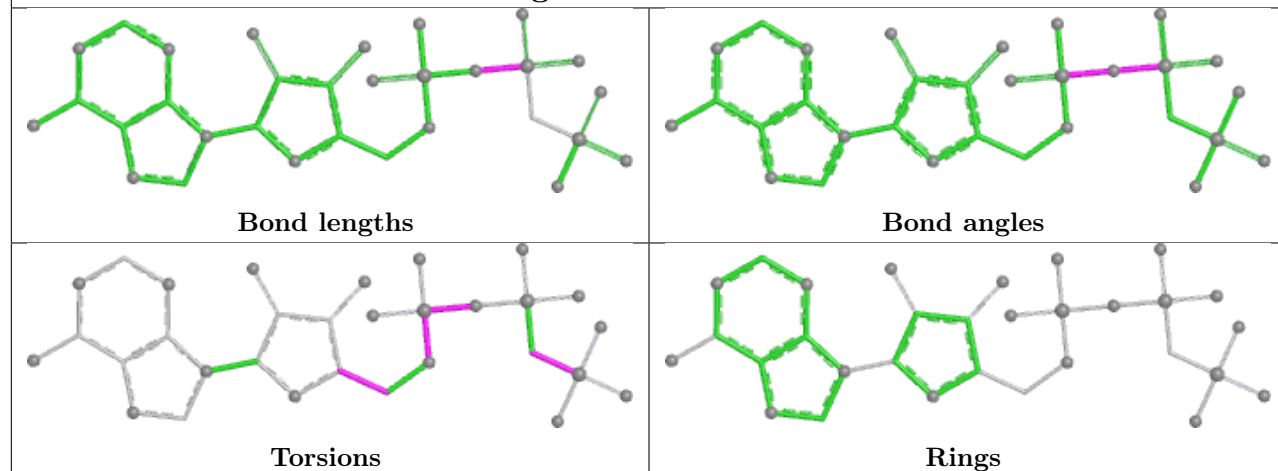




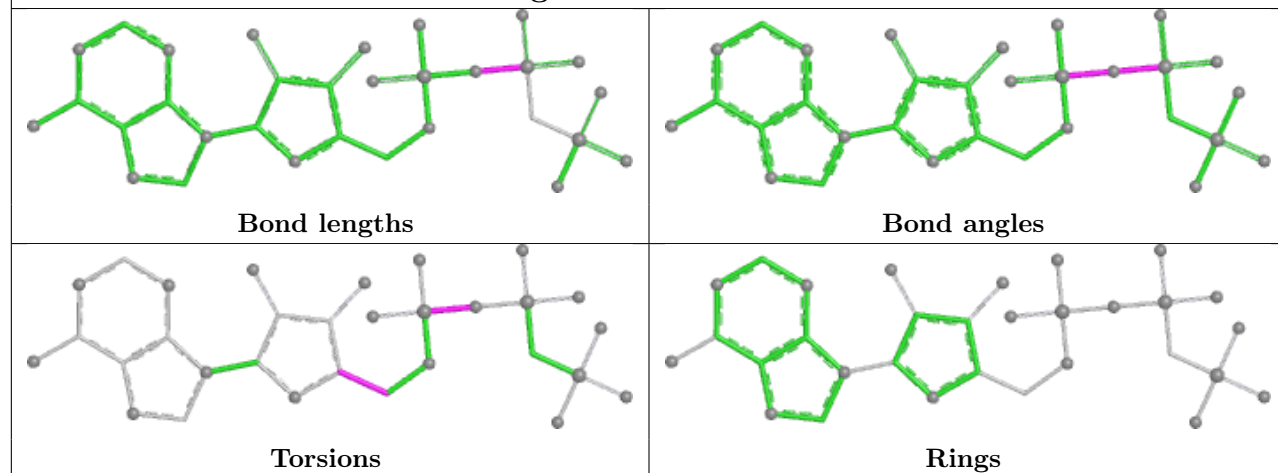


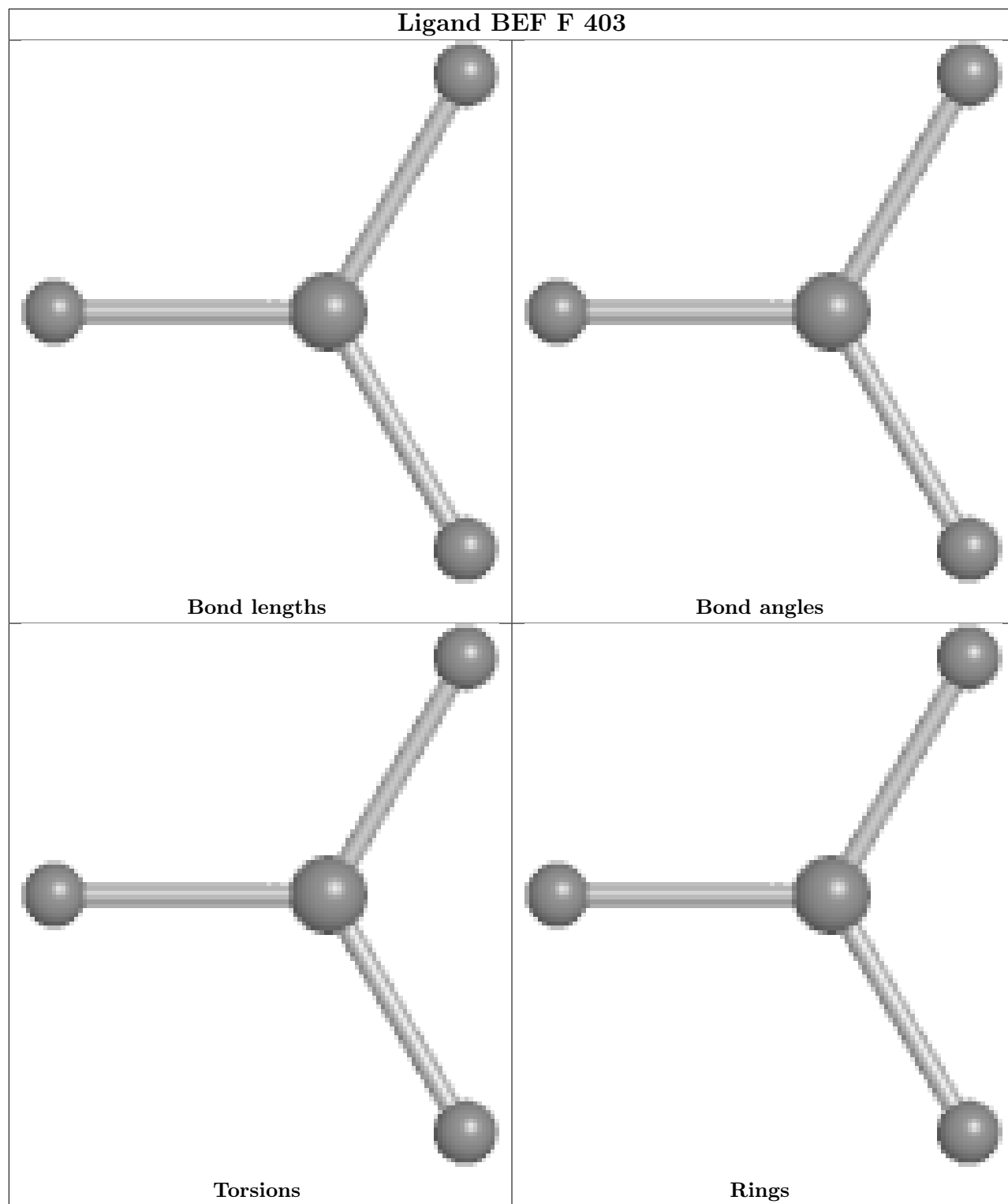


Ligand ACP C 401

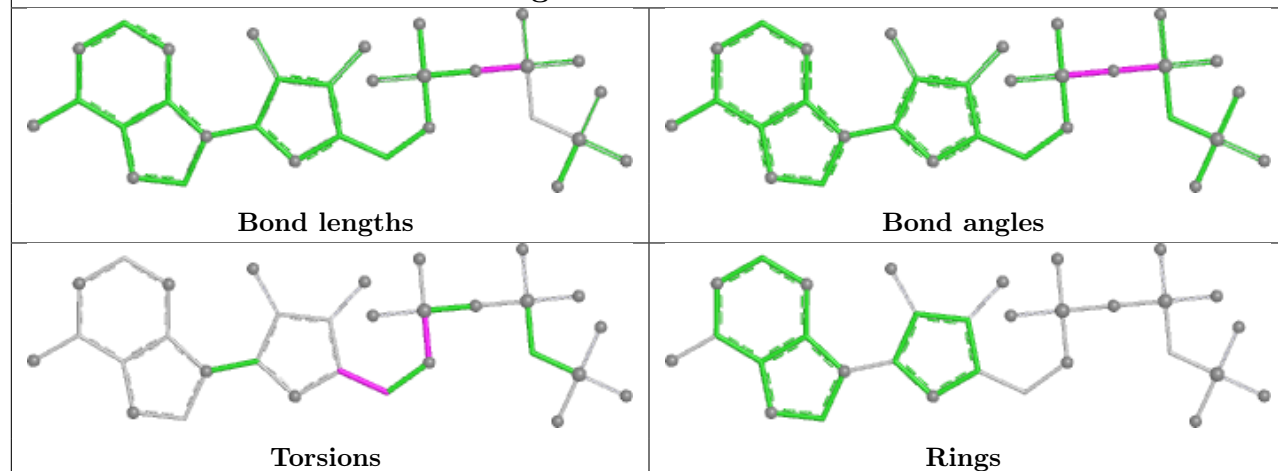


Ligand ACP A 401

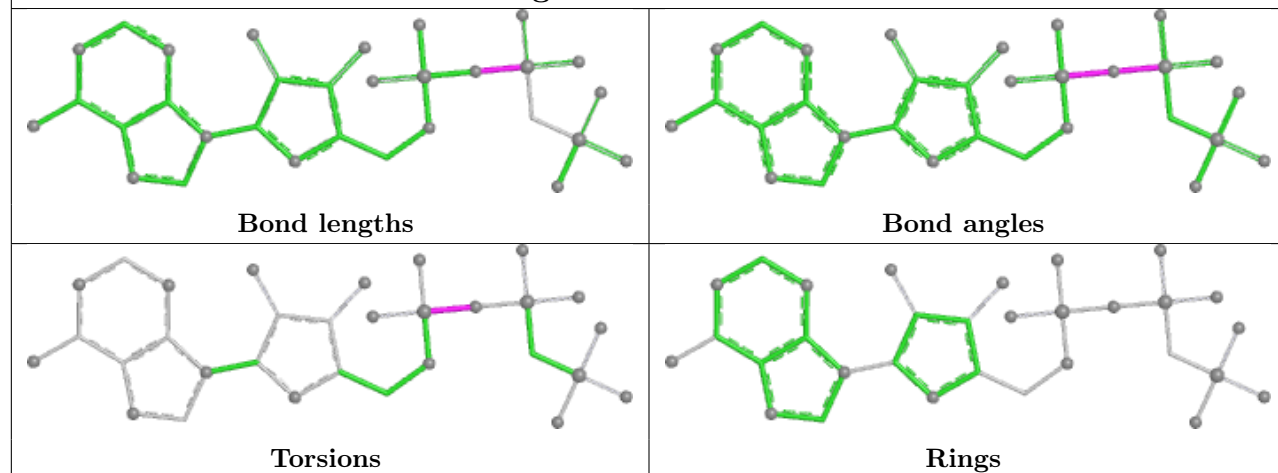


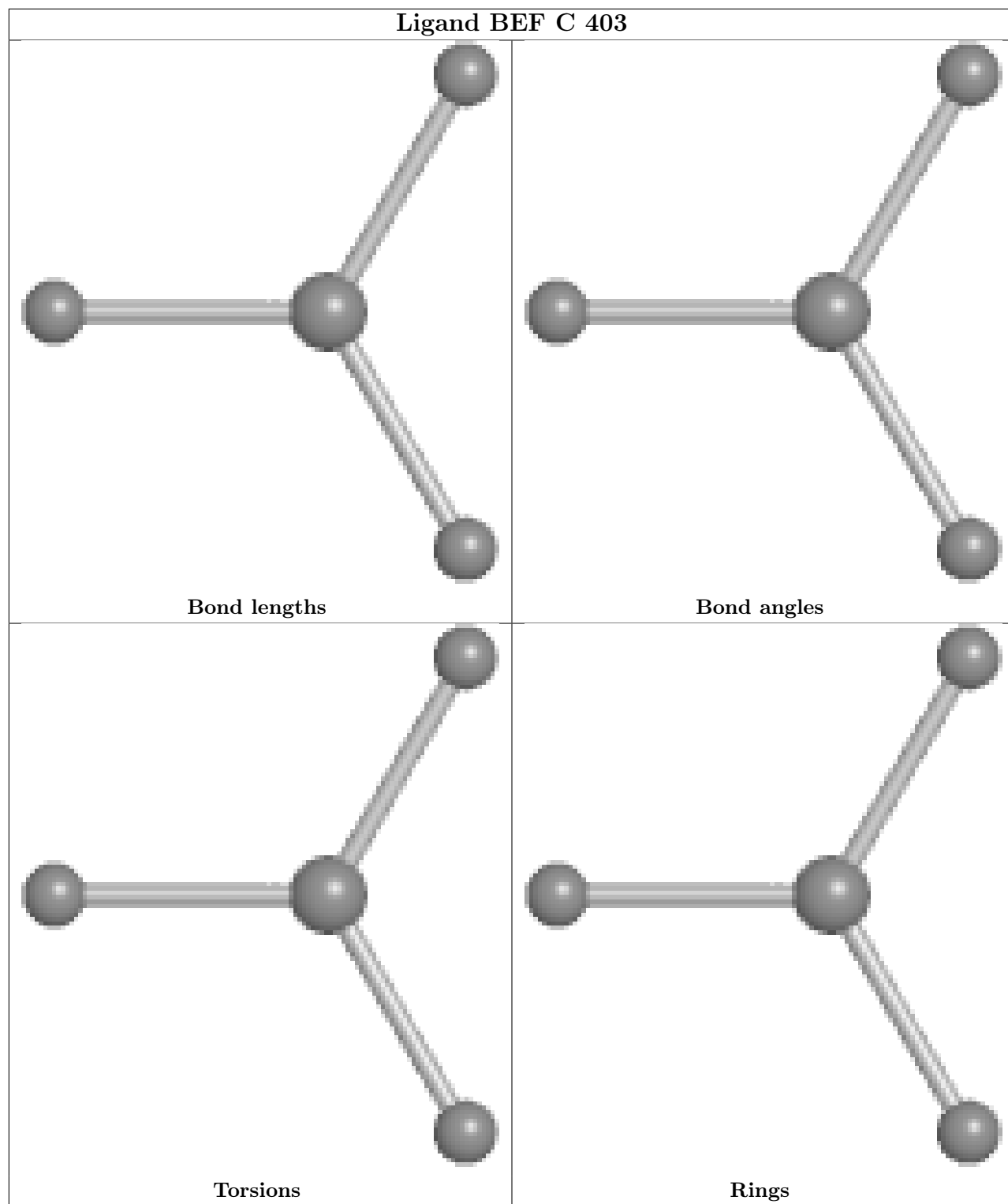


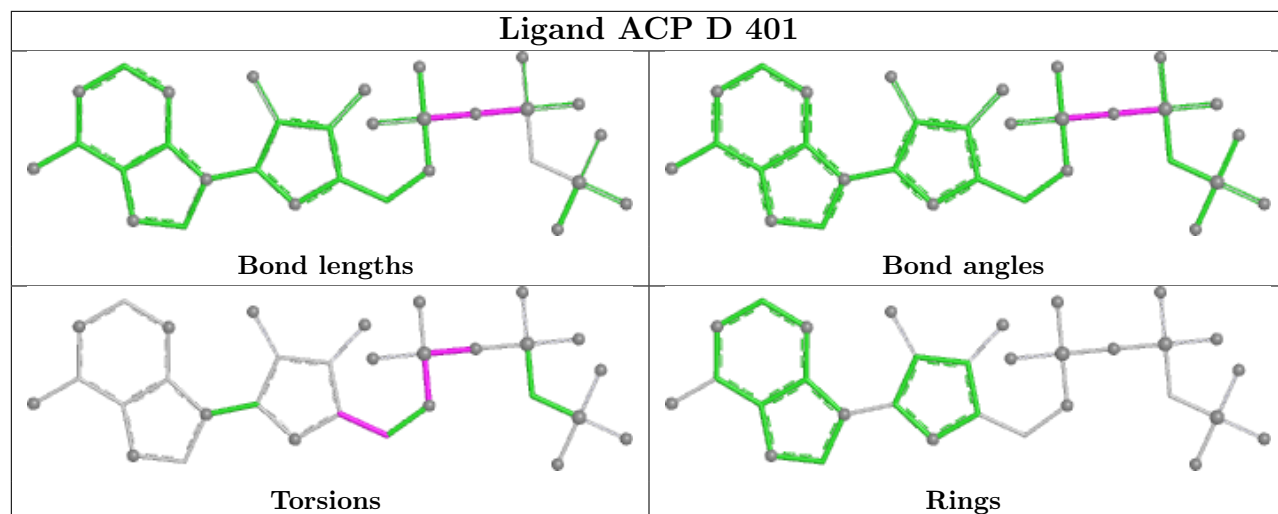
Ligand ACP B 401

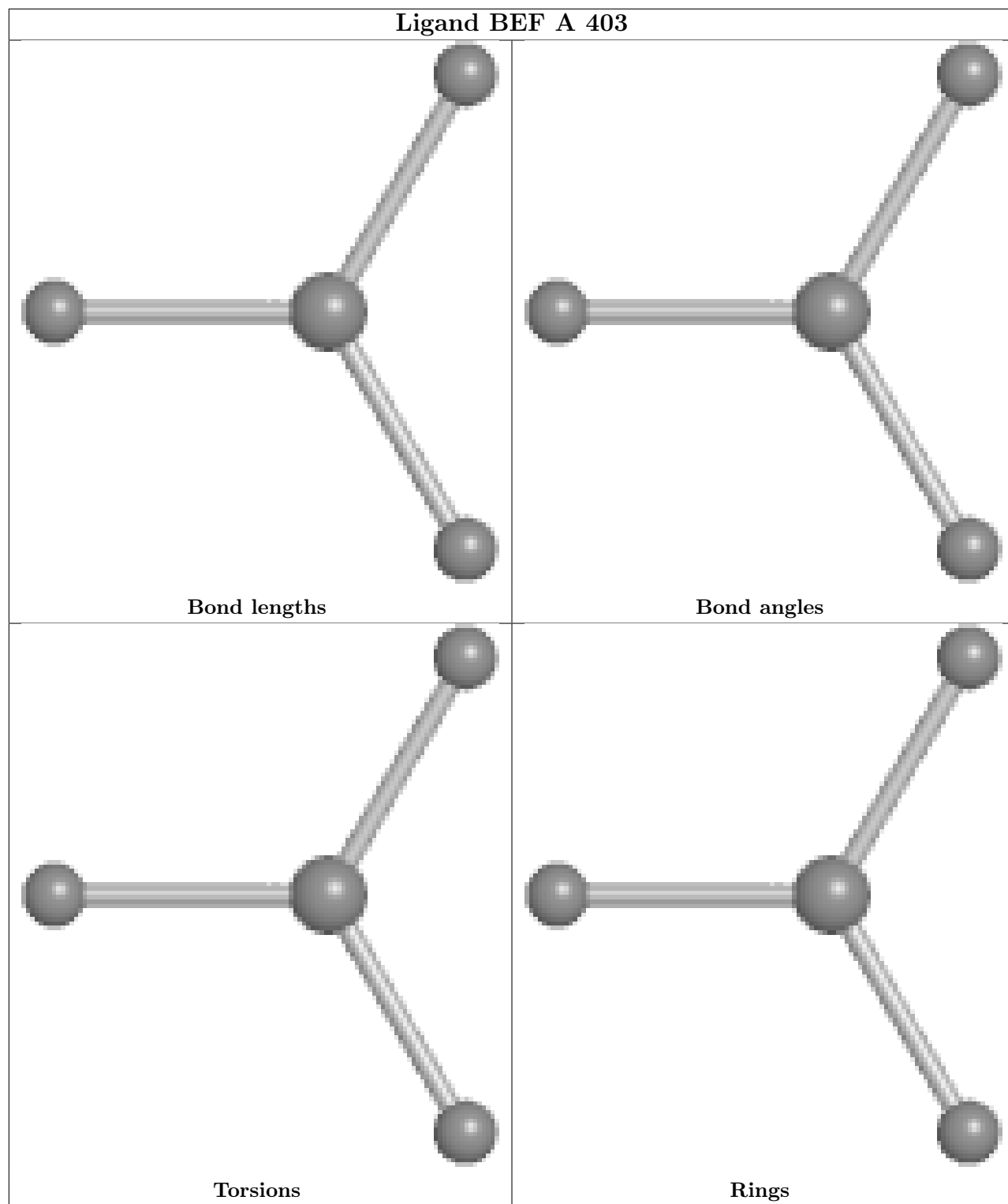


Ligand ACP E 401









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	379/382 (99%)	0.10	2 (0%) 87 85	61, 97, 148, 207	0
1	B	376/382 (98%)	0.27	18 (4%) 35 28	50, 108, 170, 203	0
1	C	378/382 (98%)	0.05	4 (1%) 78 75	56, 86, 133, 188	1 (0%)
1	D	378/382 (98%)	-0.04	4 (1%) 78 75	53, 82, 118, 205	0
1	E	376/382 (98%)	0.23	7 (1%) 66 61	62, 108, 151, 202	0
1	F	378/382 (98%)	0.28	8 (2%) 63 57	55, 110, 157, 224	0
All	All	2265/2292 (98%)	0.15	43 (1%) 66 61	50, 98, 152, 224	1 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	326	ILE	4.5
1	D	335	SER	3.7
1	A	211	PHE	3.5
1	D	211	PHE	3.2
1	C	211	PHE	3.0
1	B	286	TYR	2.9
1	B	211	PHE	2.9
1	B	293	ILE	2.8
1	C	1	MET	2.8
1	E	370	PHE	2.8
1	A	279	LEU	2.7
1	E	303	HIS	2.7
1	F	272	VAL	2.6
1	B	272	VAL	2.6
1	B	302	ASN	2.6
1	F	211	PHE	2.6
1	B	227	ILE	2.5
1	B	318	ILE	2.5
1	B	294	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	159	MET	2.4
1	E	338	LYS	2.4
1	D	317	GLY	2.4
1	F	120	LEU	2.3
1	B	303	HIS	2.3
1	B	325	SER	2.3
1	B	1	MET	2.3
1	B	213	ARG	2.3
1	B	336	ALA	2.2
1	F	256	SER	2.2
1	B	204	ILE	2.2
1	C	339	GLY	2.2
1	D	339	GLY	2.2
1	E	211	PHE	2.2
1	E	91	ALA	2.1
1	C	253	PRO	2.1
1	F	222	VAL	2.1
1	F	227	ILE	2.1
1	E	13	LEU	2.1
1	B	379	PRO	2.1
1	E	256	SER	2.1
1	F	265	LEU	2.1
1	B	305	LYS	2.0
1	F	159	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

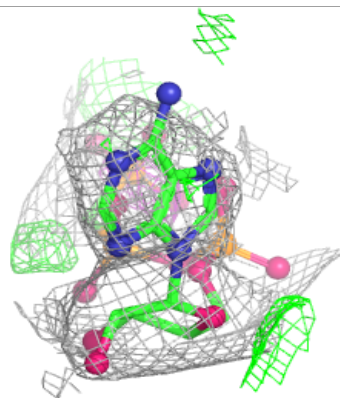
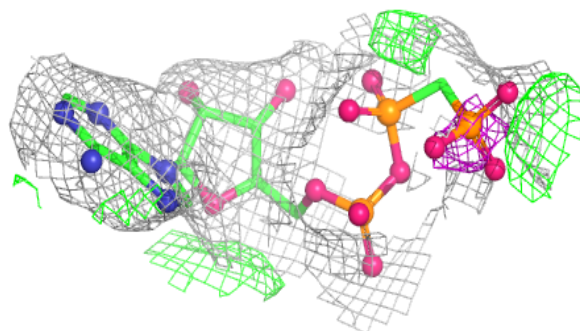
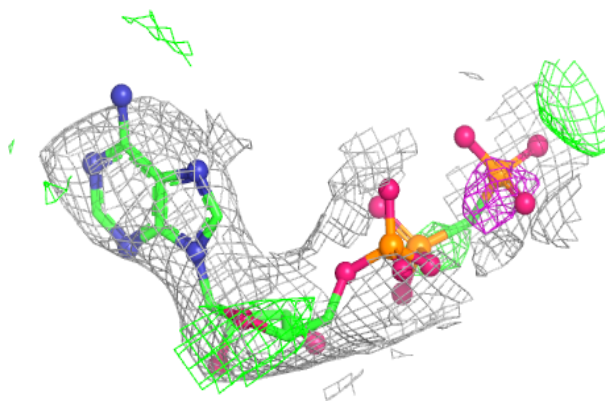
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	A	405	5/5	0.64	0.11	125,150,162,230	0
5	SO4	E	407	5/5	0.70	0.10	139,140,152,230	0
5	SO4	E	406	5/5	0.80	0.07	110,110,136,182	0
2	ACP	B	401	31/31	0.88	0.10	115,136,141,150	0
2	ACP	E	401	31/31	0.89	0.11	107,119,132,143	0
2	ACP	F	401	31/31	0.90	0.10	103,121,134,142	0
3	MG	E	404	1/1	0.93	0.14	122,122,122,122	0
5	SO4	E	405	5/5	0.93	0.12	83,84,95,98	0
3	MG	F	404	1/1	0.94	0.08	117,117,117,117	0
4	BEF	F	403	4/4	0.94	0.06	82,84,85,89	0
2	ACP	D	401	31/31	0.95	0.08	67,80,103,122	0
2	ACP	A	401	31/31	0.95	0.08	83,103,116,125	0
4	BEF	E	403	4/4	0.95	0.06	93,97,100,101	0
2	ACP	C	401	31/31	0.95	0.07	78,90,109,126	0
4	BEF	B	403	4/4	0.97	0.05	55,56,58,58	0
4	BEF	D	403	4/4	0.97	0.04	66,72,72,74	0
4	BEF	C	403	4/4	0.98	0.04	56,62,63,63	0
3	MG	C	404	1/1	0.98	0.05	87,87,87,87	0
4	BEF	A	403	4/4	0.98	0.04	75,77,78,79	0
3	MG	B	404	1/1	0.98	0.04	125,125,125,125	0
3	MG	E	402	1/1	0.99	0.03	104,104,104,104	0
3	MG	B	402	1/1	0.99	0.04	61,61,61,61	0
3	MG	F	402	1/1	0.99	0.03	88,88,88,88	0
3	MG	A	402	1/1	0.99	0.05	82,82,82,82	0
3	MG	A	404	1/1	0.99	0.03	92,92,92,92	0
3	MG	D	402	1/1	0.99	0.02	77,77,77,77	0
3	MG	D	404	1/1	0.99	0.02	78,78,78,78	0
3	MG	C	402	1/1	1.00	0.02	60,60,60,60	0

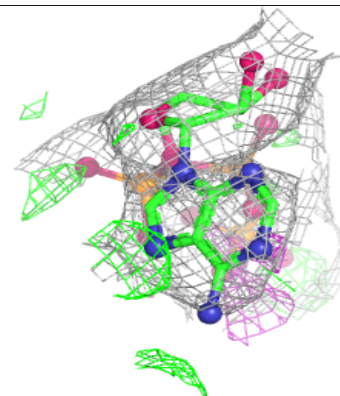
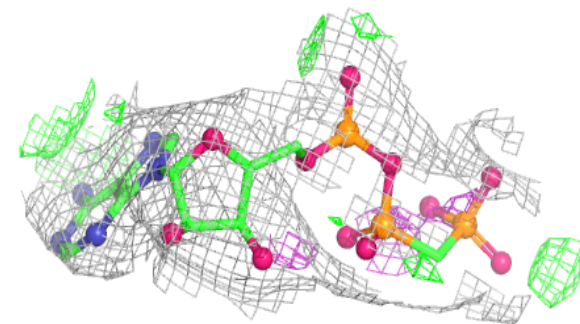
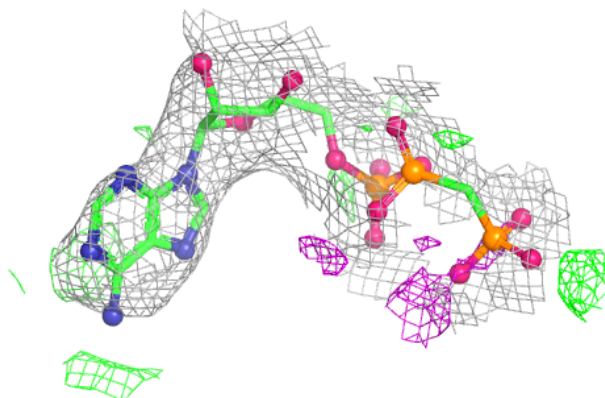
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP B 401:

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

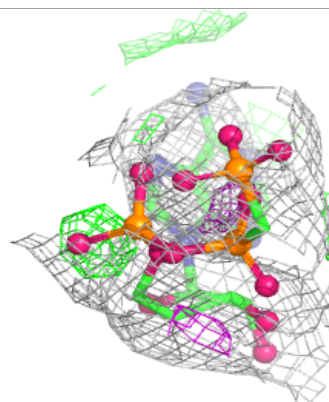
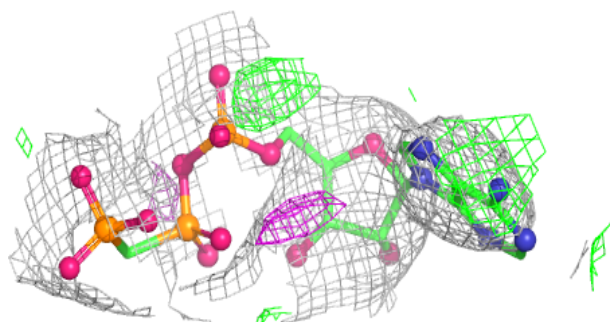
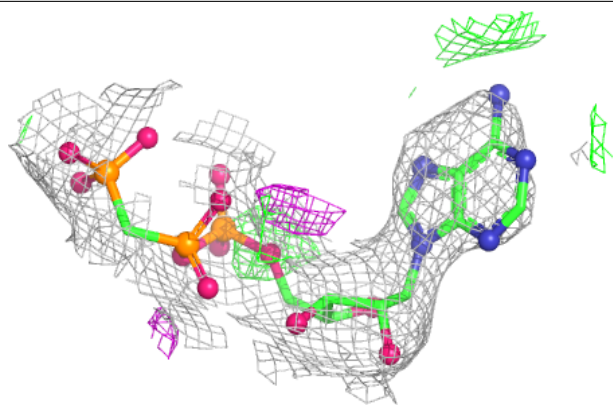
**Electron density around ACP E 401:**

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



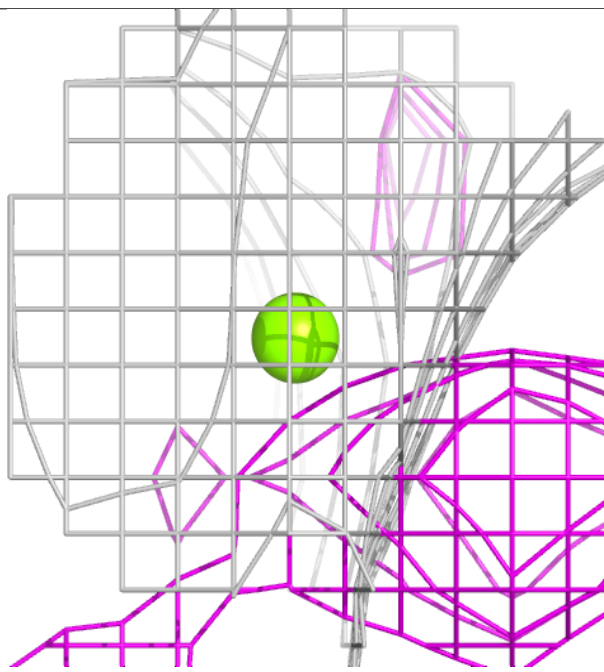
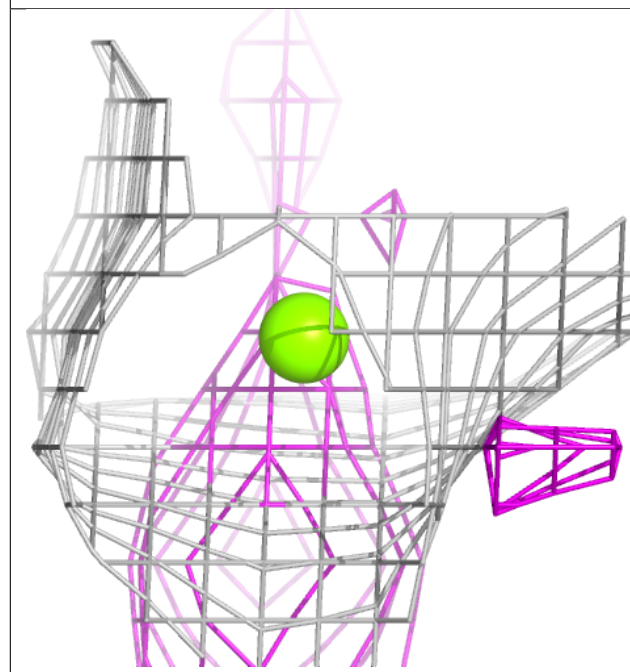
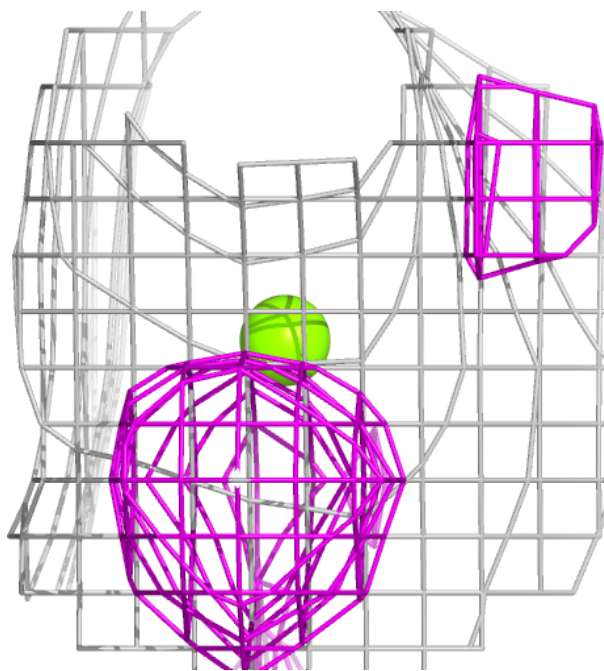
Electron density around ACP F 401:

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



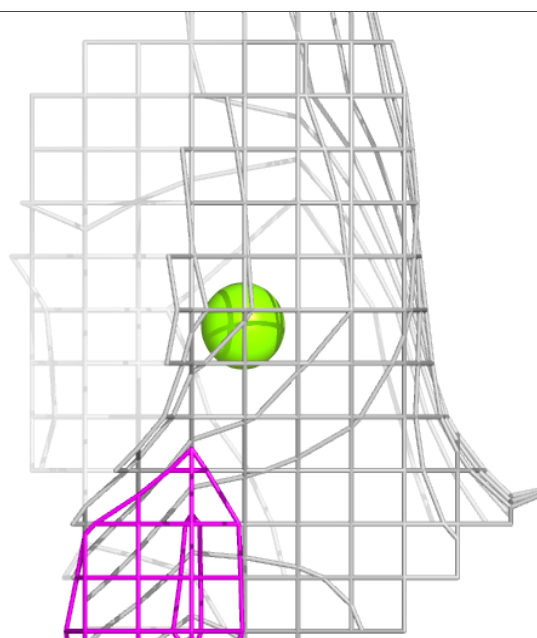
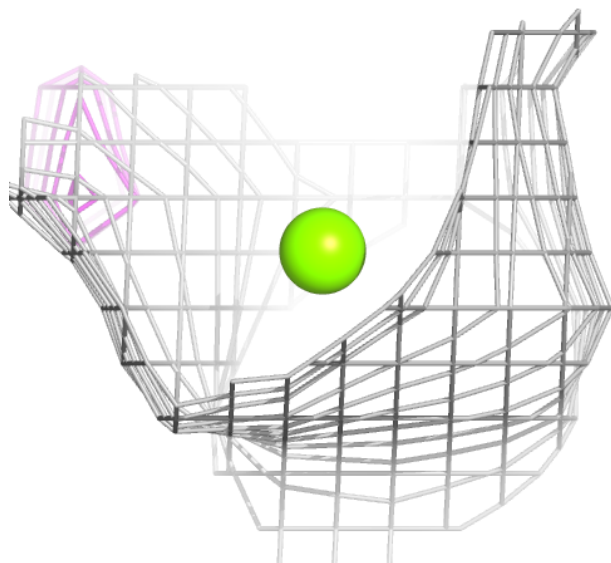
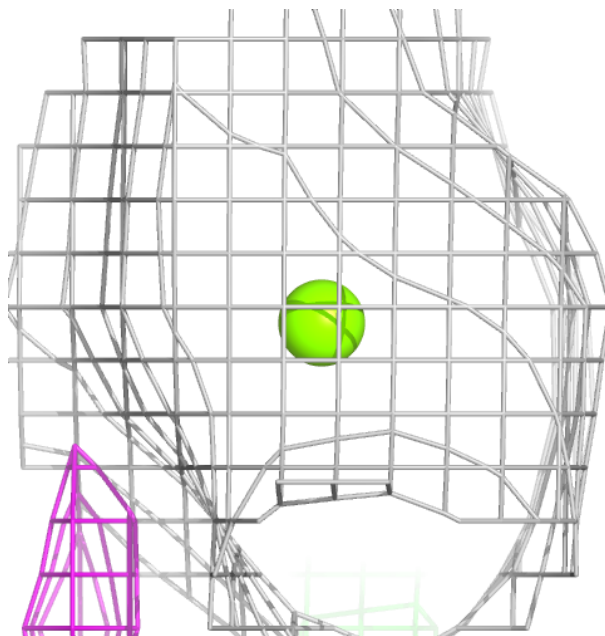
Electron density around MG E 404:

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



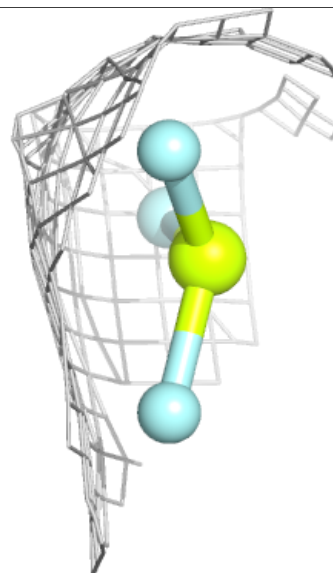
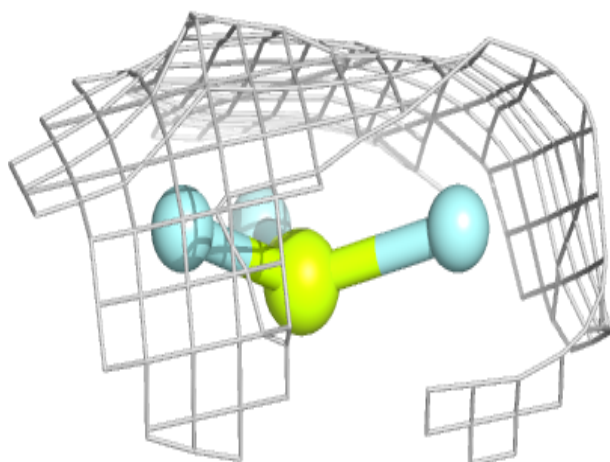
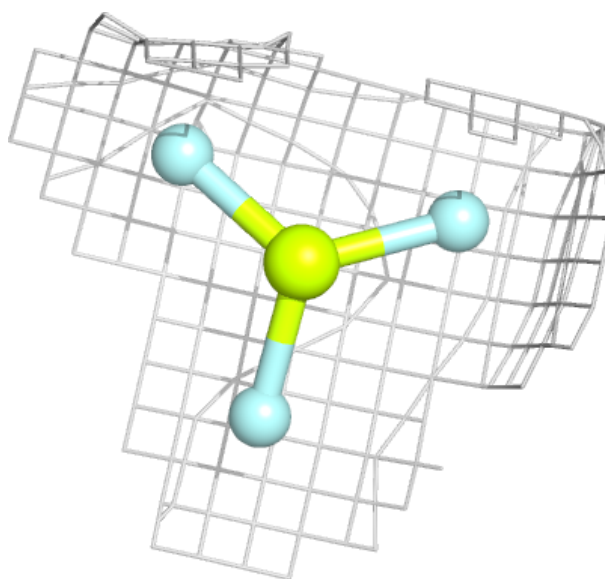
Electron density around MG F 404:

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



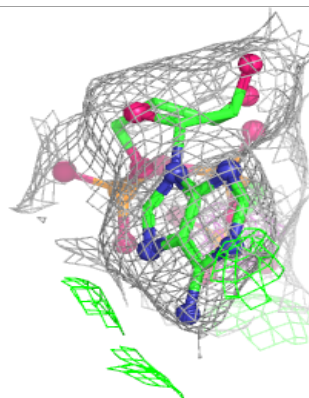
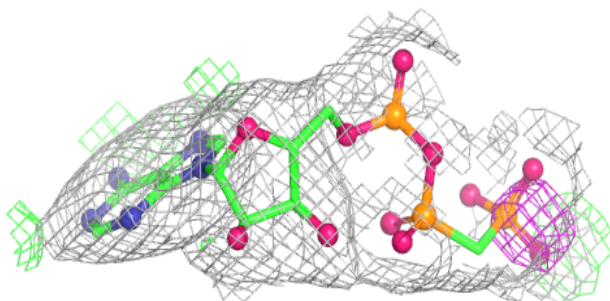
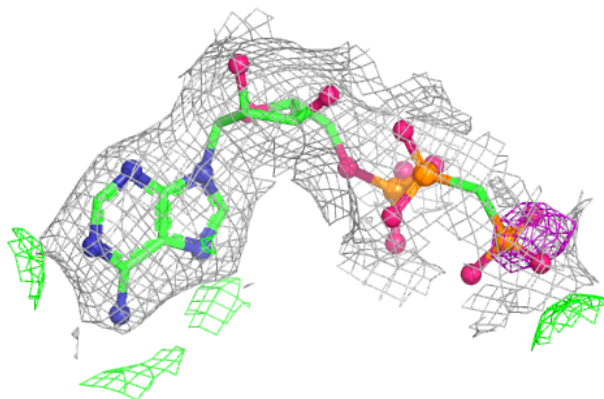
Electron density around BEF F 403:

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

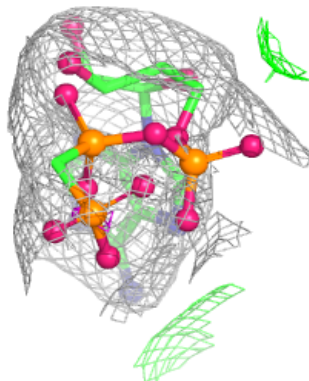
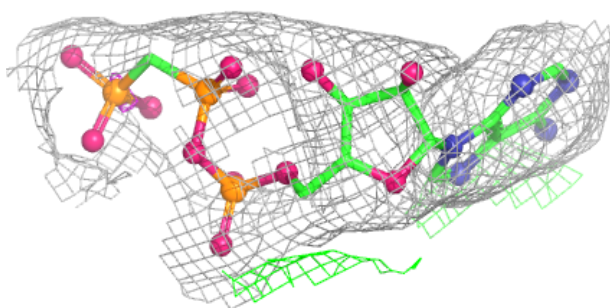
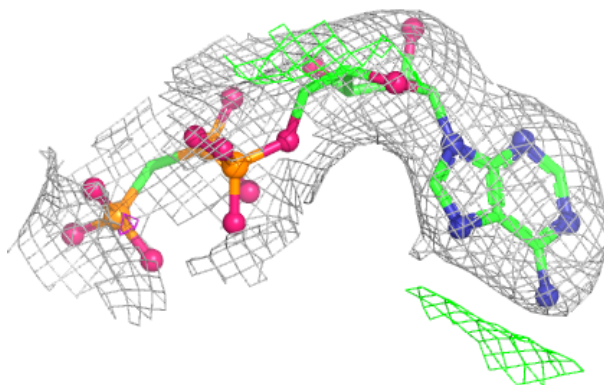


Electron density around ACP D 401:

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

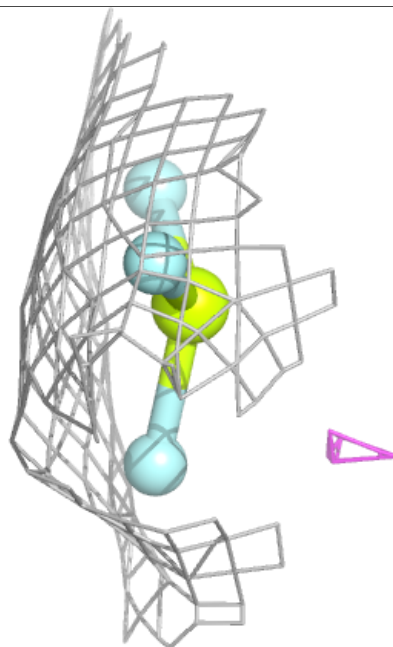
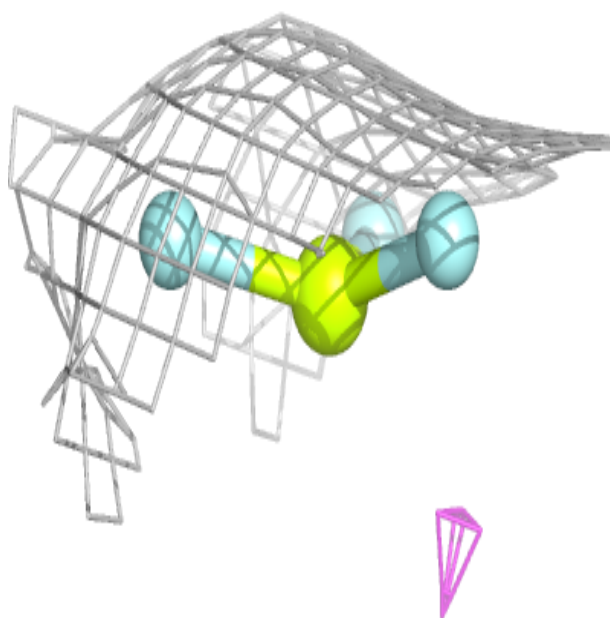
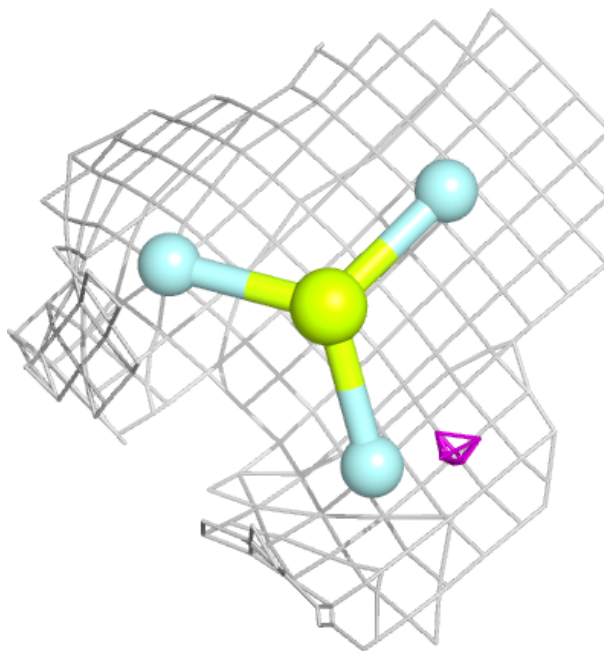
**Electron density around ACP A 401:**

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



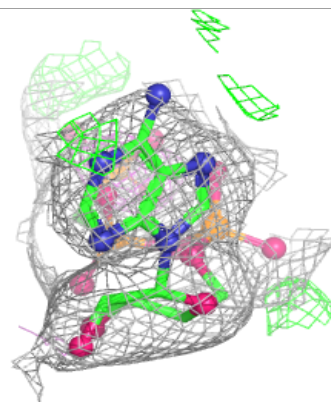
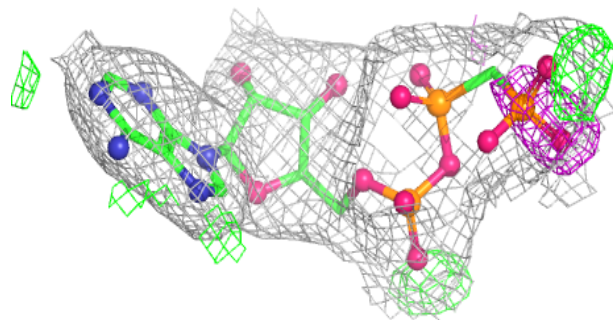
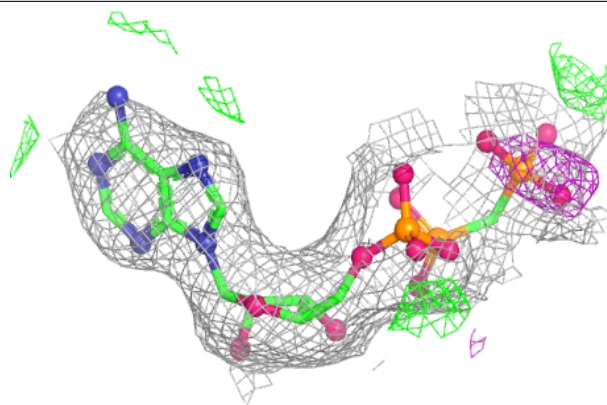
Electron density around BEF E 403:

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



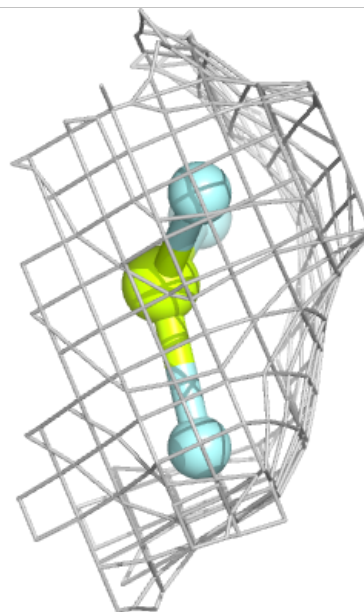
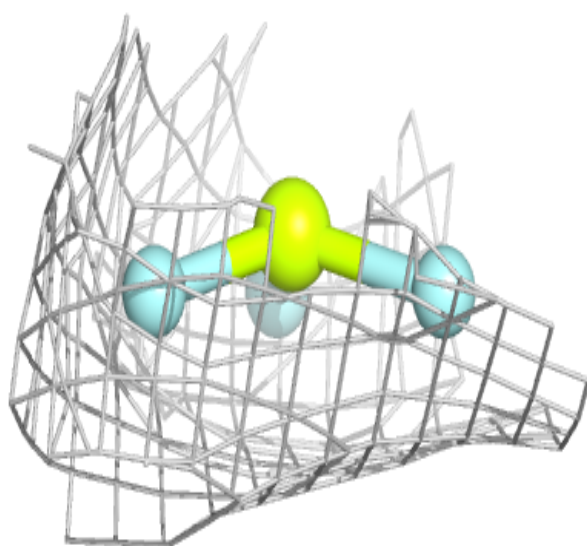
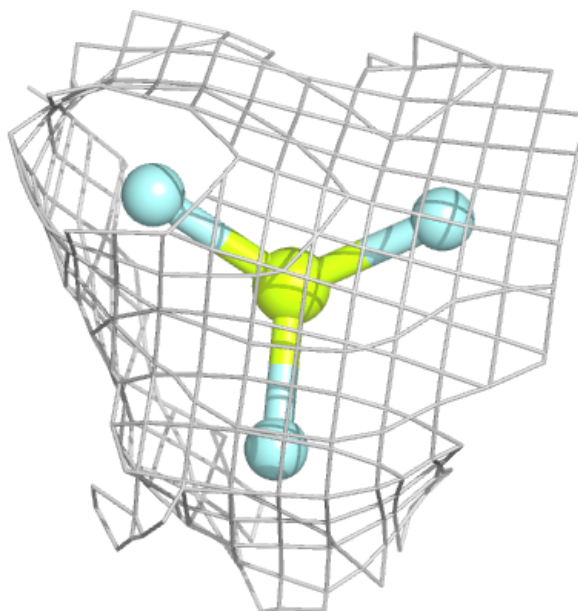
Electron density around ACP C 401:

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



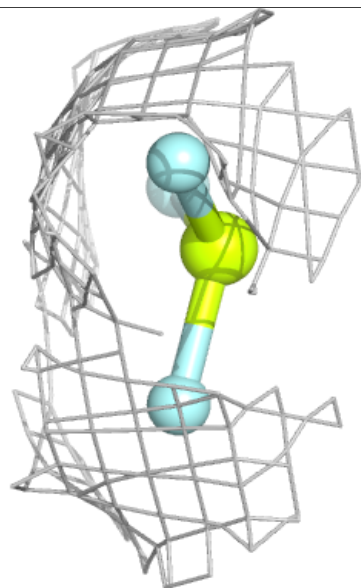
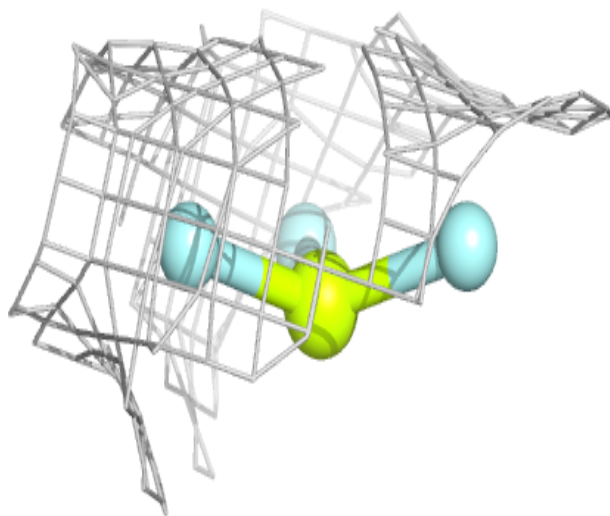
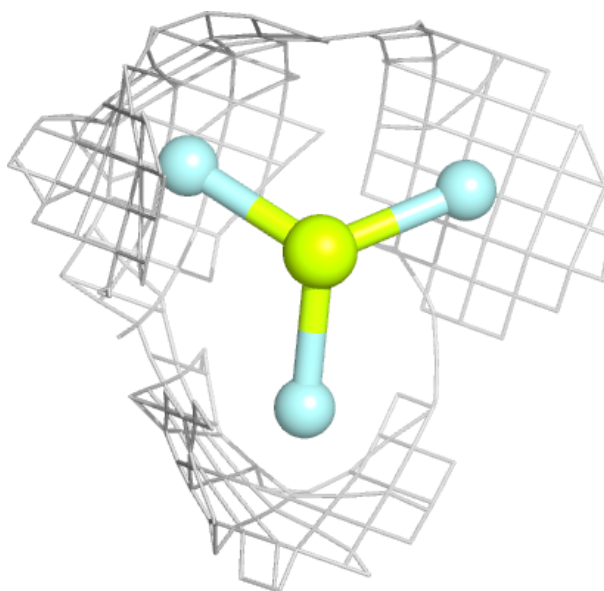
Electron density around BEF B 403:

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



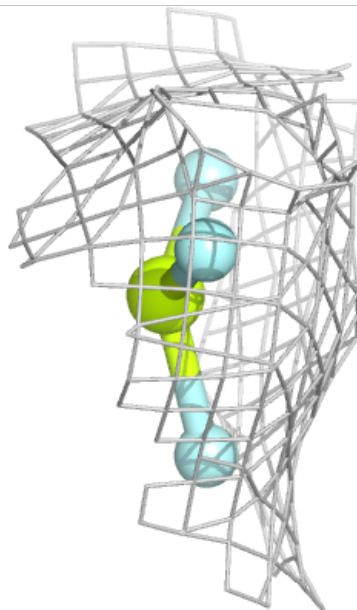
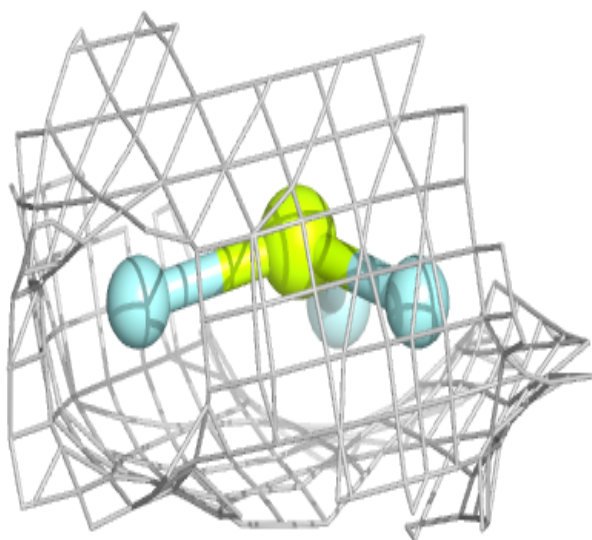
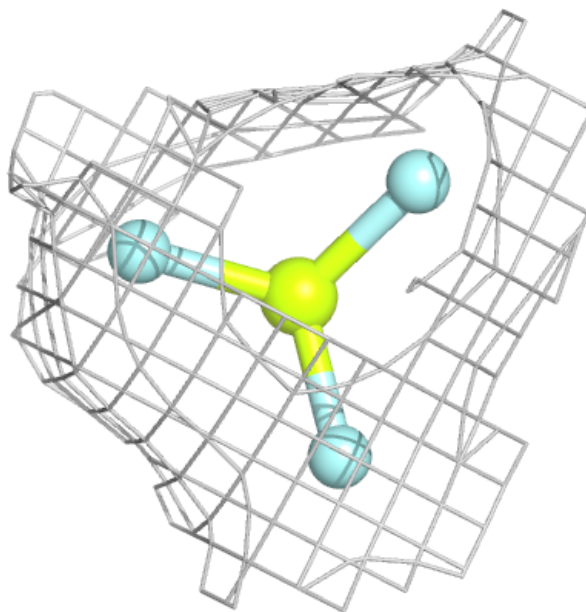
Electron density around BEF D 403:

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



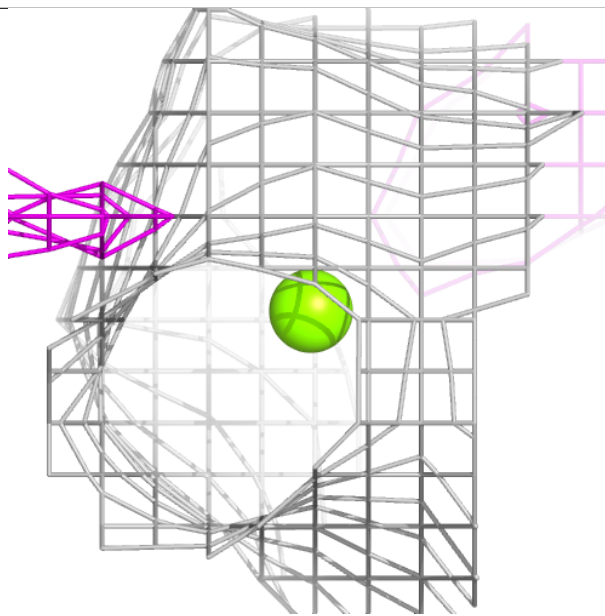
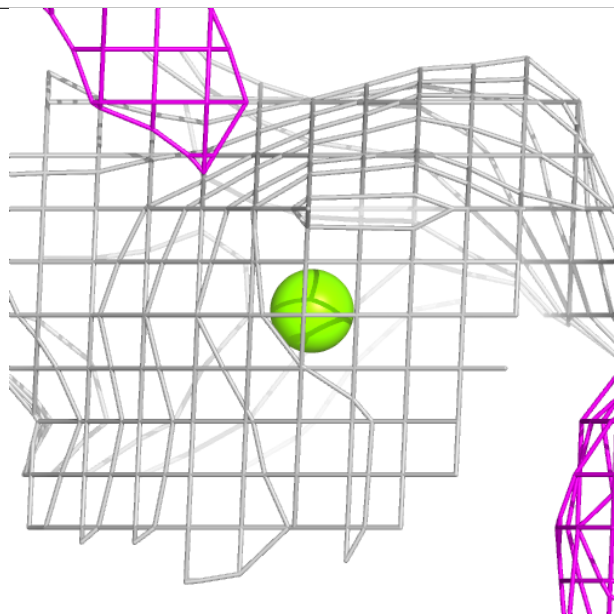
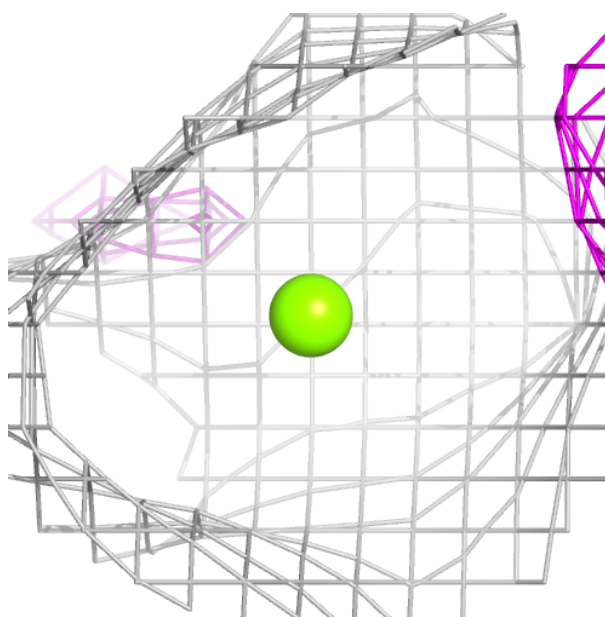
Electron density around BEF C 403:

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



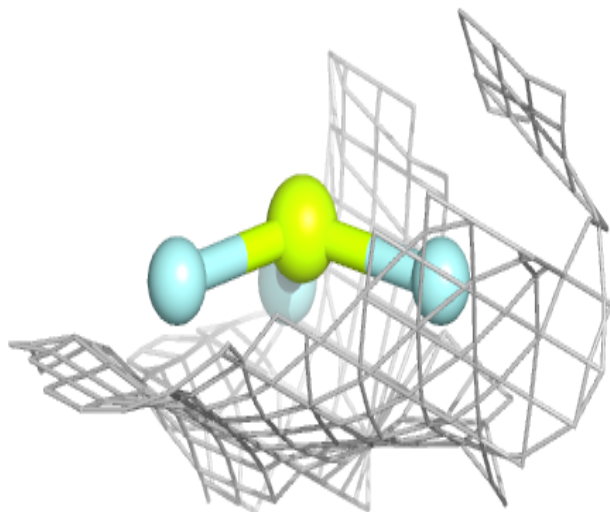
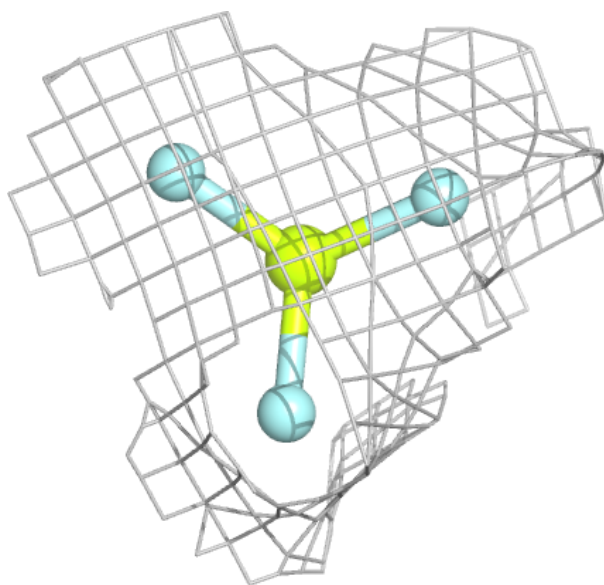
Electron density around MG C 404:

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



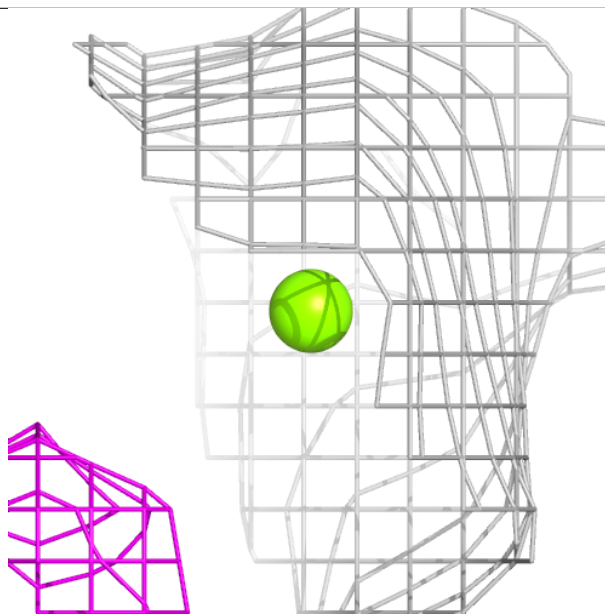
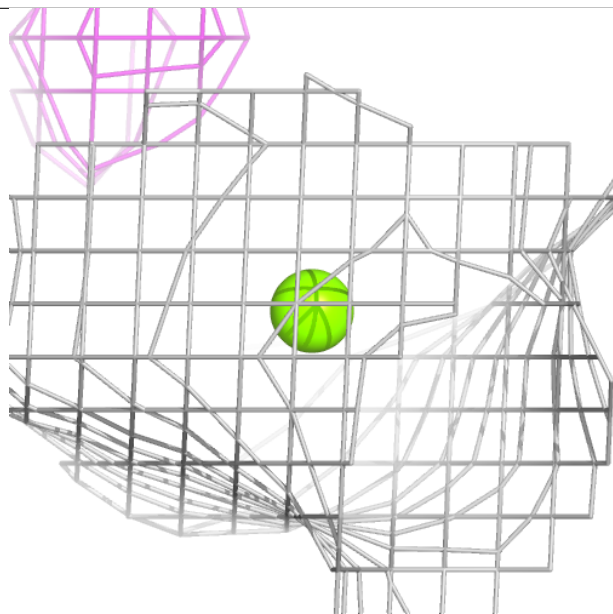
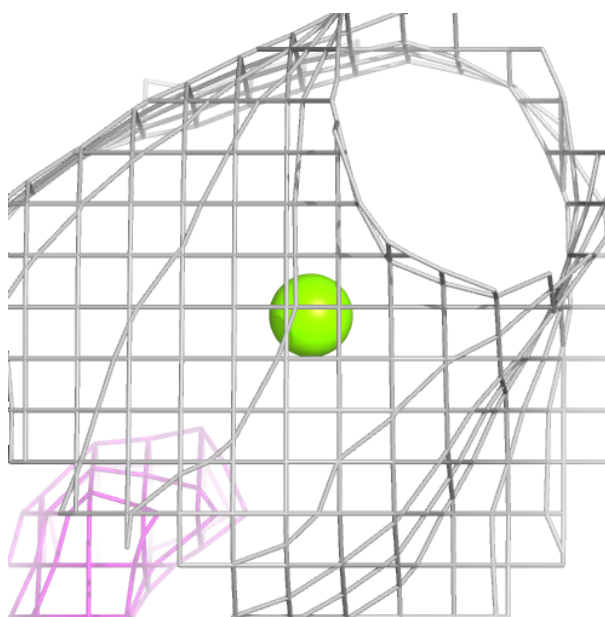
Electron density around BEF A 403:

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



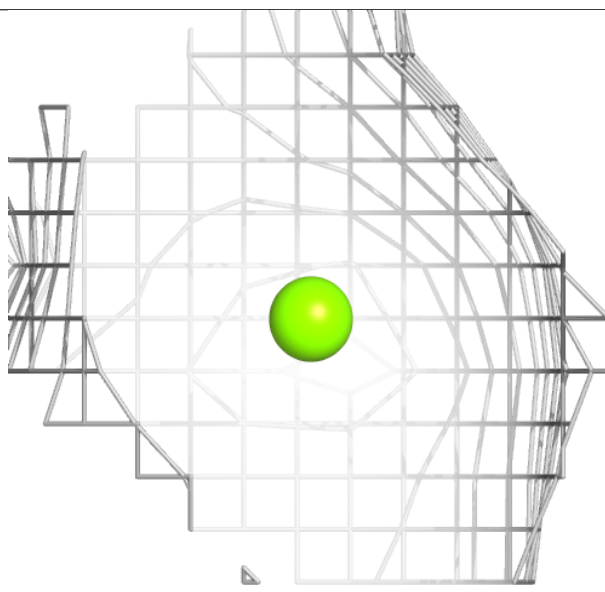
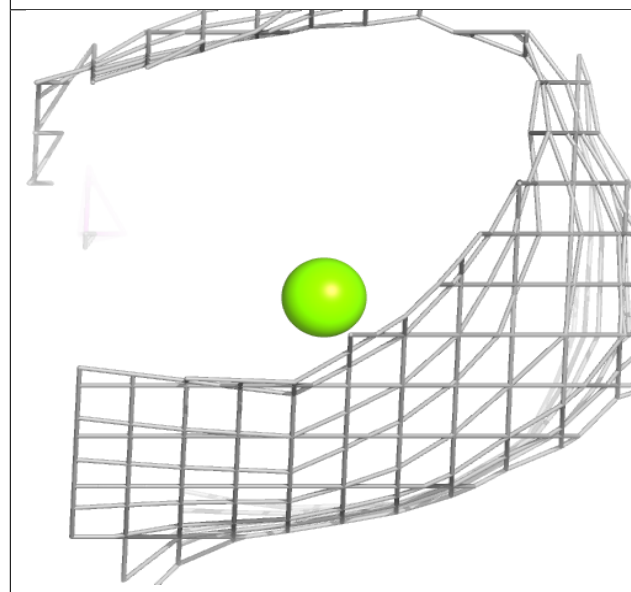
Electron density around MG B 404:

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



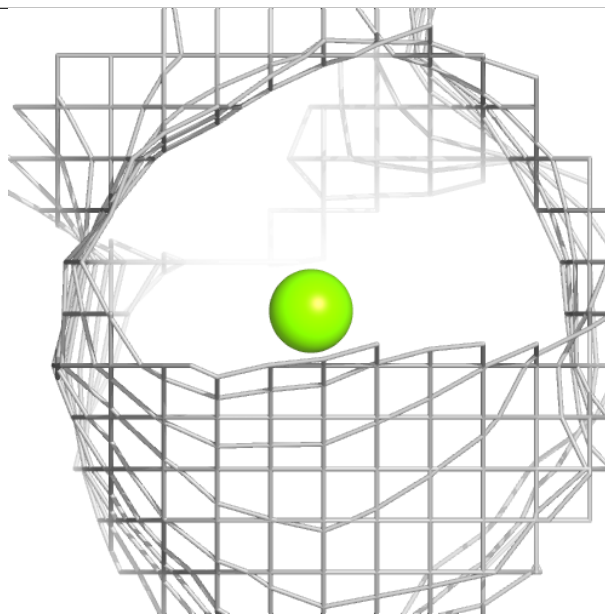
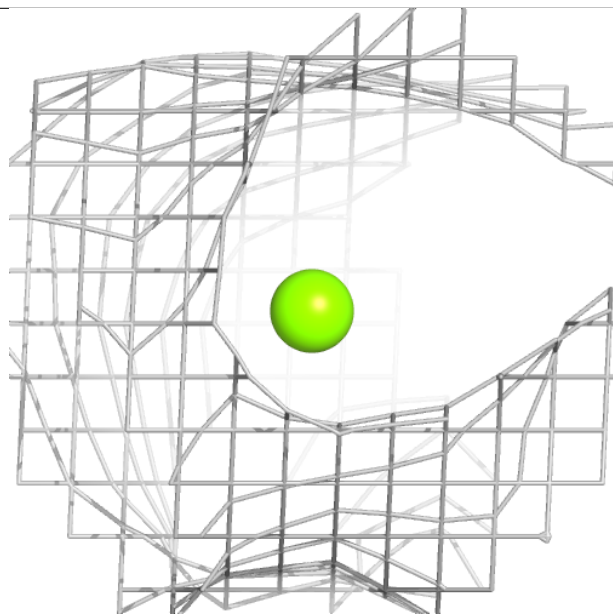
Electron density around MG E 402:

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



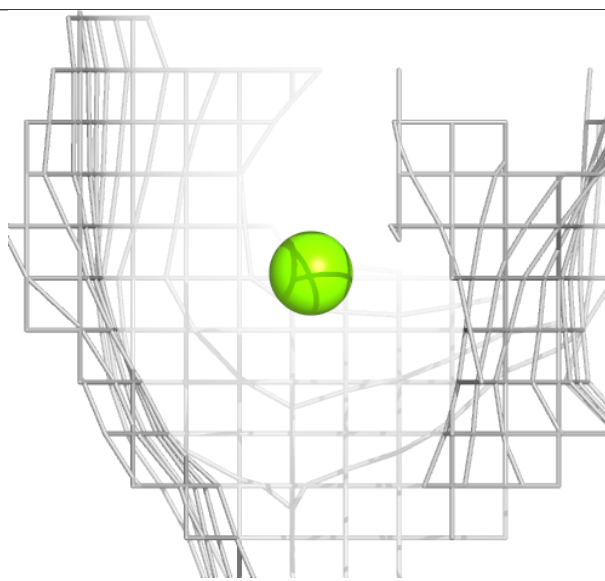
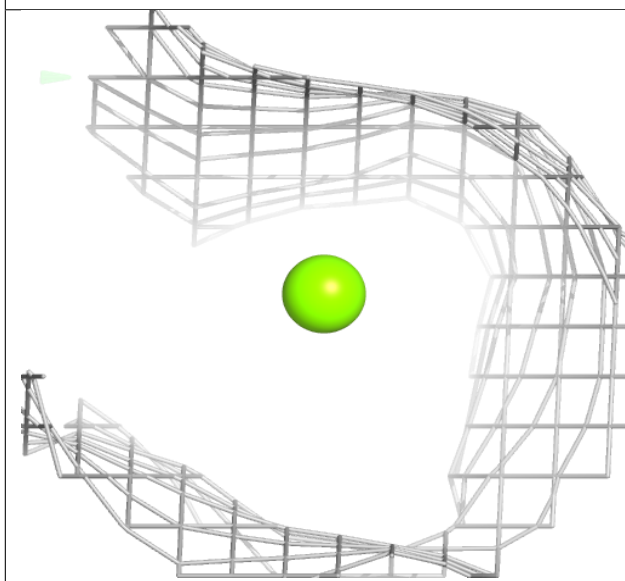
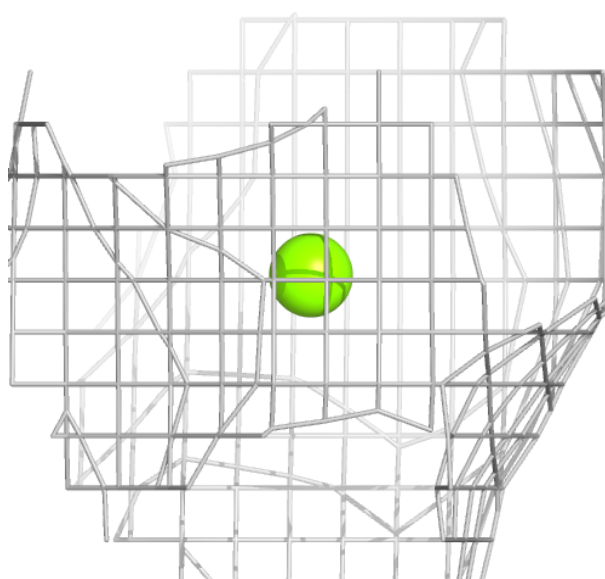
Electron density around MG B 402:

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



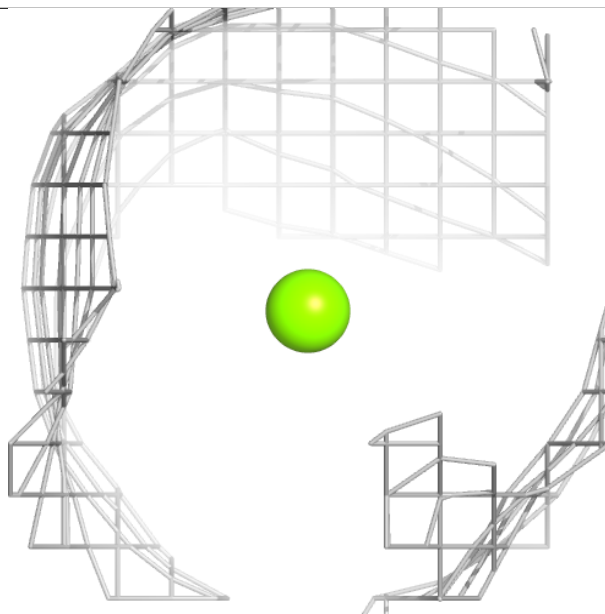
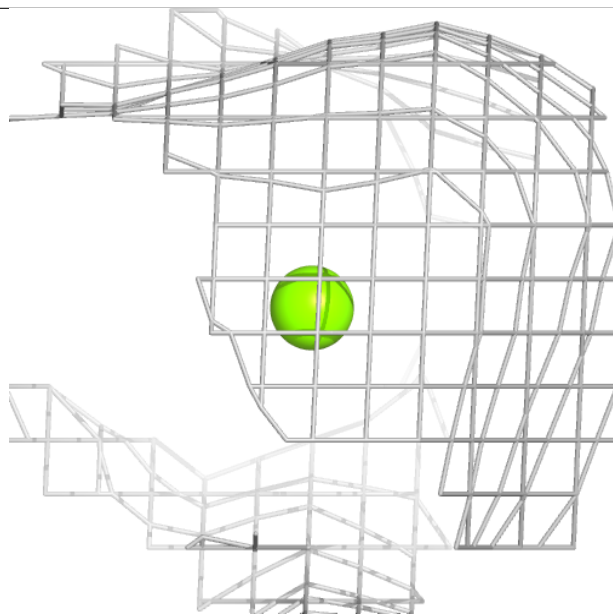
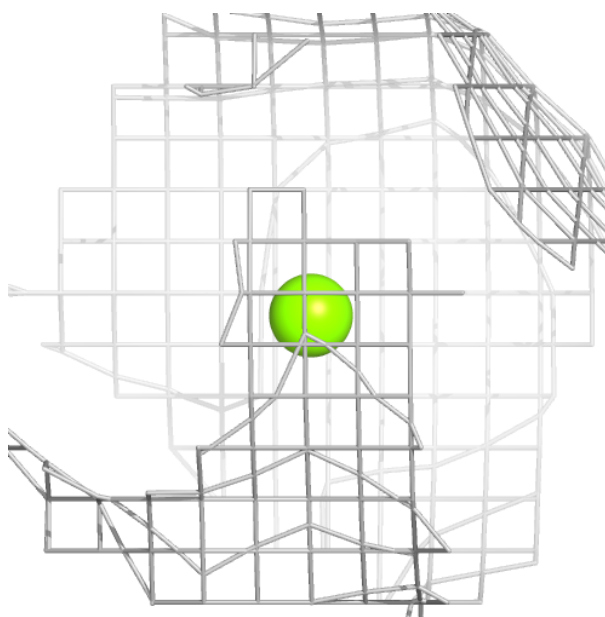
Electron density around MG F 402:

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



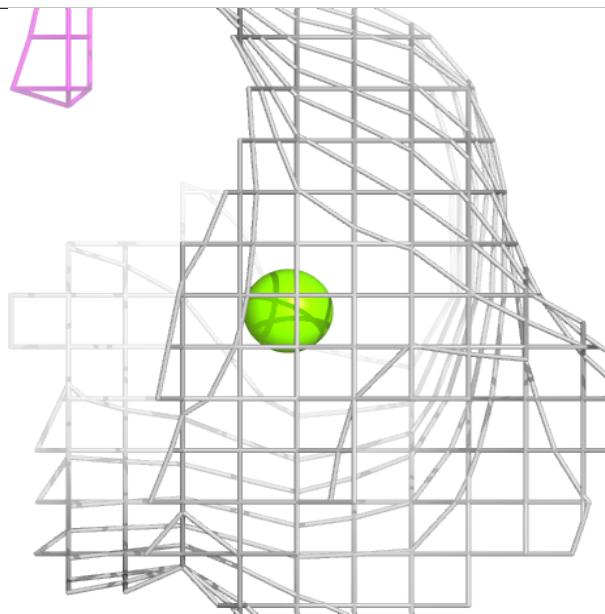
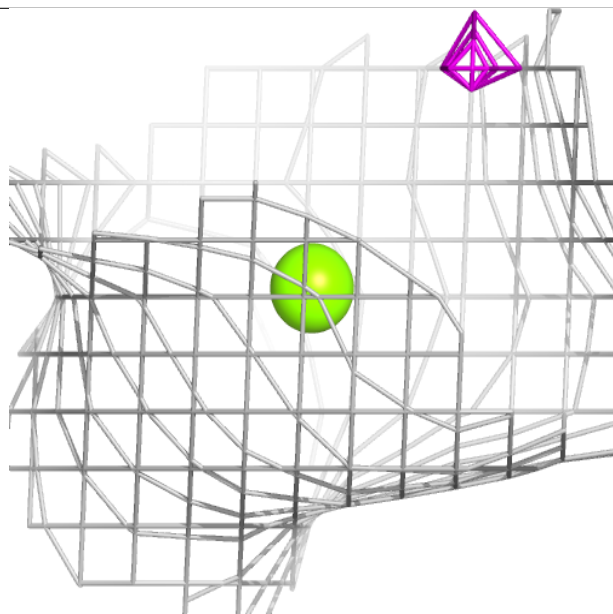
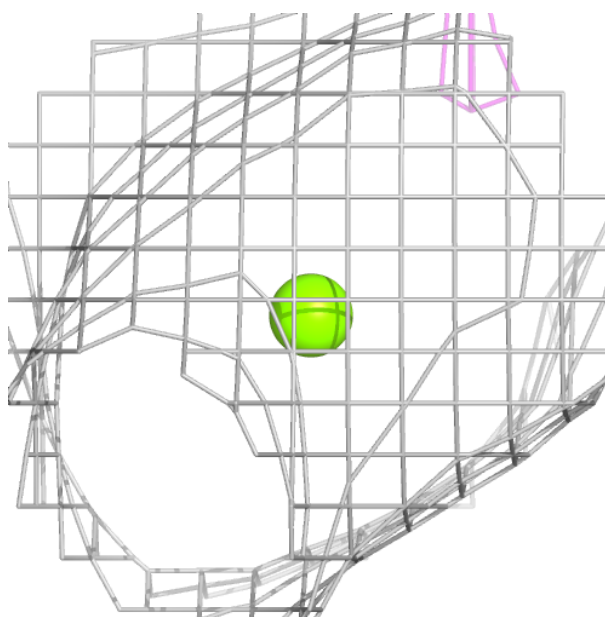
Electron density around MG A 402:

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



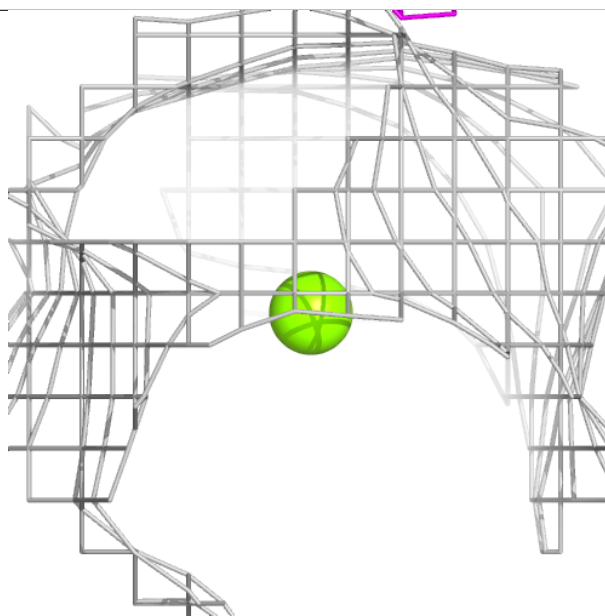
Electron density around MG A 404:

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



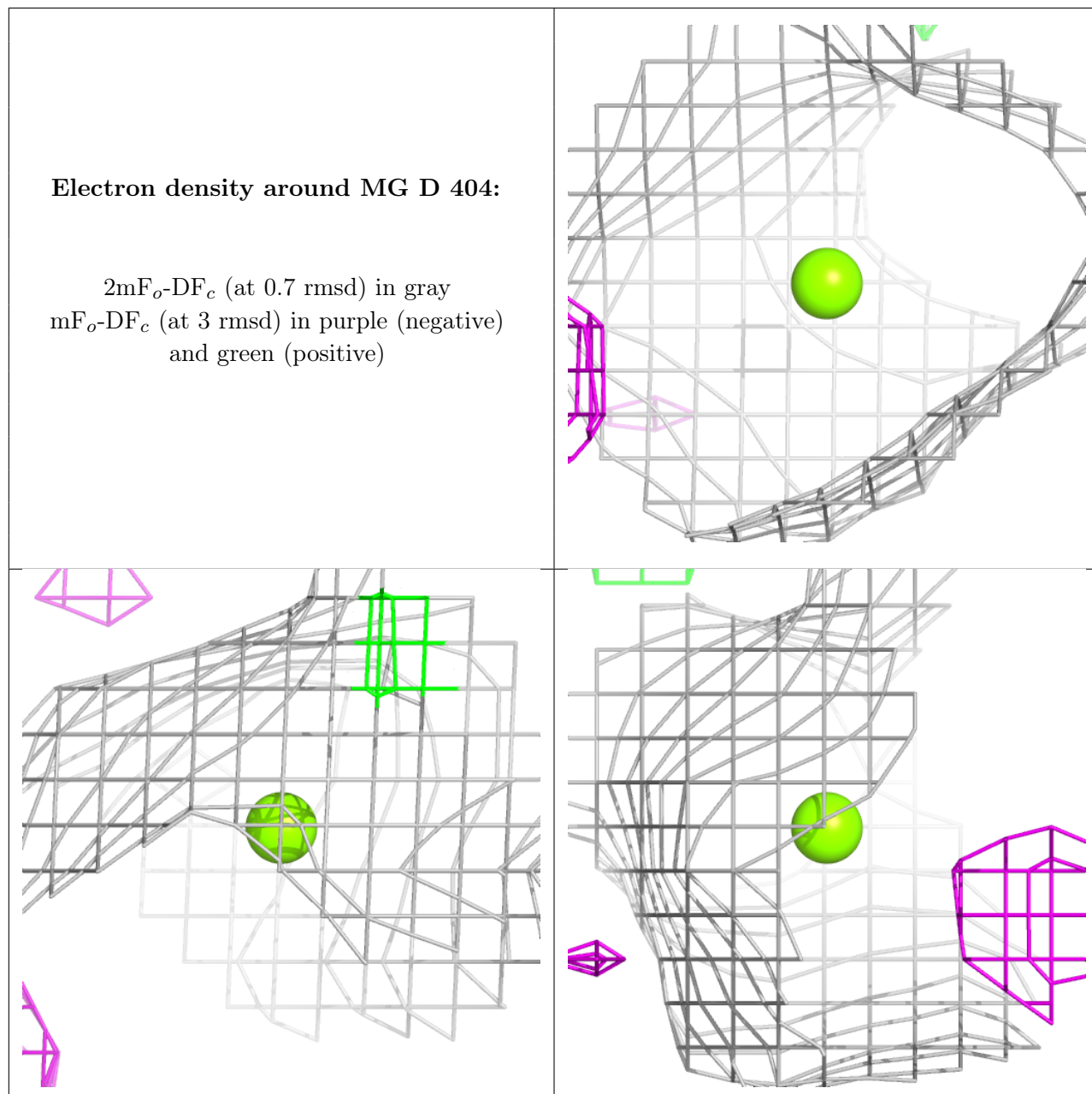
Electron density around MG D 402:

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



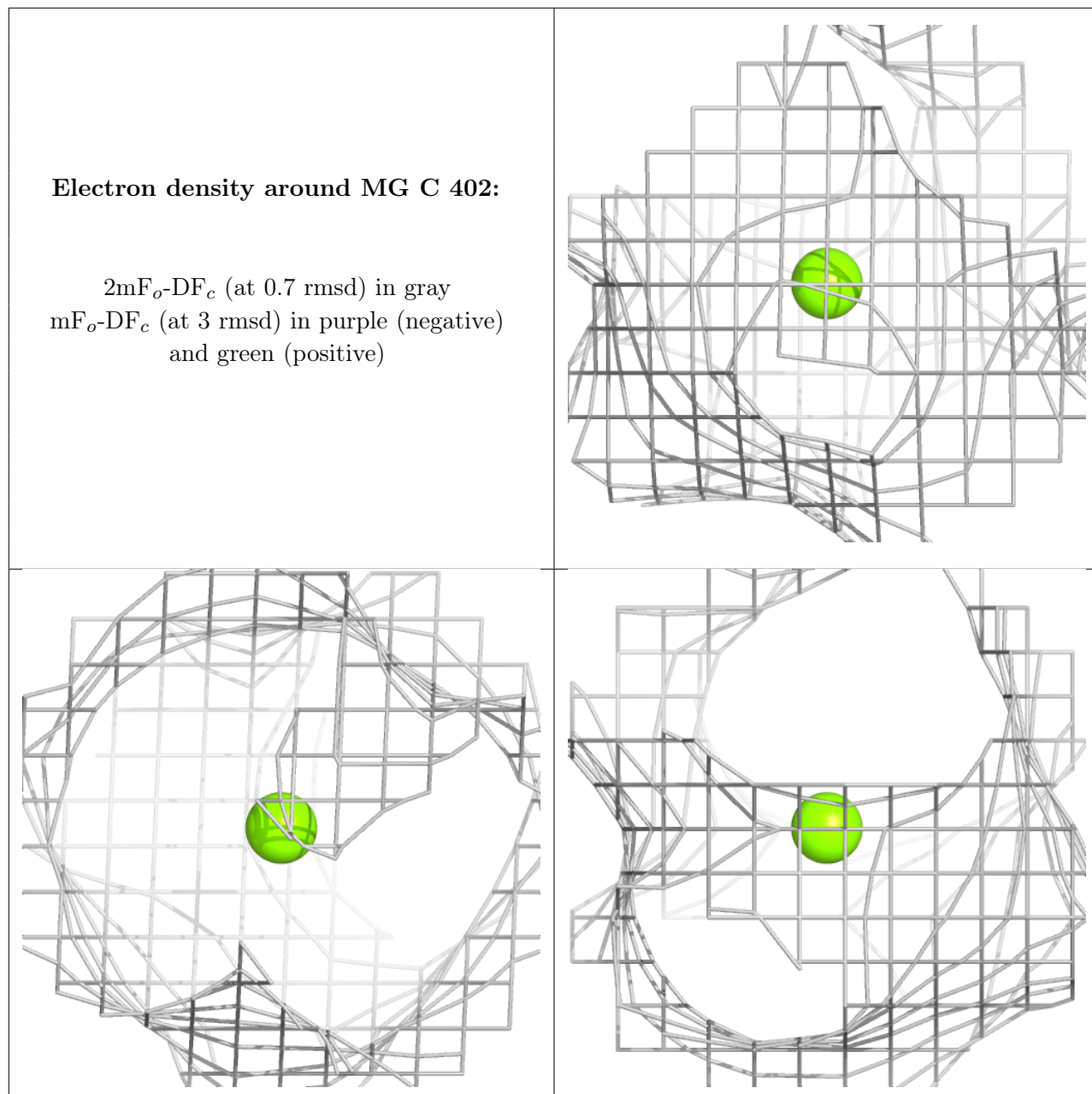
Electron density around MG D 404:

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



Electron density around MG C 402:

$2mF_o-DF_c$ (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.