Full wwPDB X-ray Structure Validation Report (i)

Oct 6, 2026 – 07:34 pm BST

PDB ID	:	9QI0 / pdb_00009qi0
Title	:	Crystal Structure of human MLH1 N-terminal domain with ADP-BeF3
Authors	:	Thomsen, M.; Ganichkin, O.; Thieulin-Pardo, G.; Bandera, A.M.; Boudet, J.; Finley, M.; Felsenfeld, D.; Haque, T.; Prasad, B.C.; Monteagudo, E.; Vogt, T.; Stamford, A.
Deposited on	:	2025-03-17
Resolution	:	1.70 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 (i) 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 (1)) were used in the production of this report:

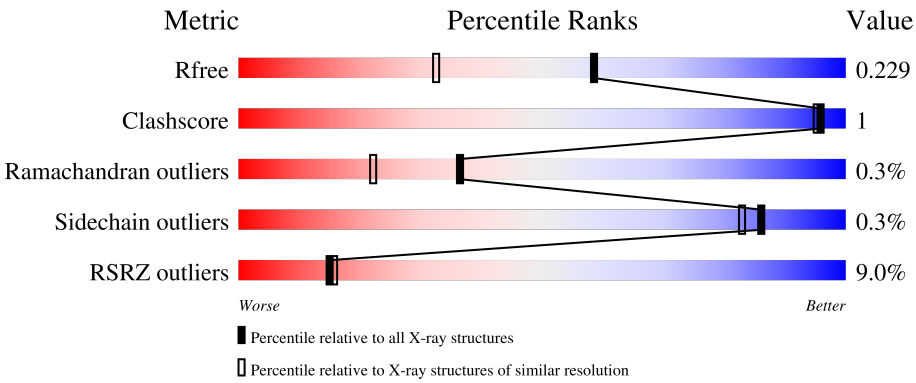
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	341	7% 95%
1	B	341	7% 96%
1	C	341	13% 96%
1	D	341	9% 94%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 12192 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.

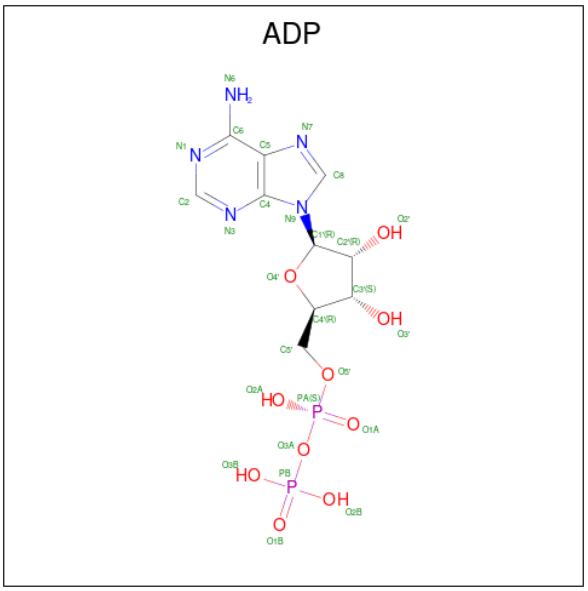
- Molecule 1 is a protein called DNA mismatch repair protein Mlh1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2726	1721	480	517	8	31	15	0
1	B	334	2675	1689	470	508	8	29	9	0
1	C	335	2691	1694	475	514	8	29	9	0
1	D	337	2717	1708	477	522	10	33	12	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P40692
B	0	GLY	-	expression tag	UNP P40692
C	0	GLY	-	expression tag	UNP P40692
D	0	GLY	-	expression tag	UNP P40692

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

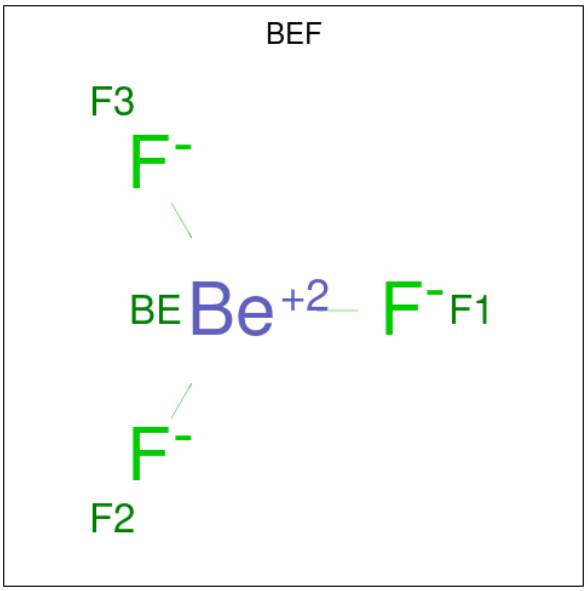


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	A	1	1	1	0	0
5	B	1	1	1	0	0
5	C	1	1	1	0	0
5	D	1	1	1	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	A	2	2	2	0	0

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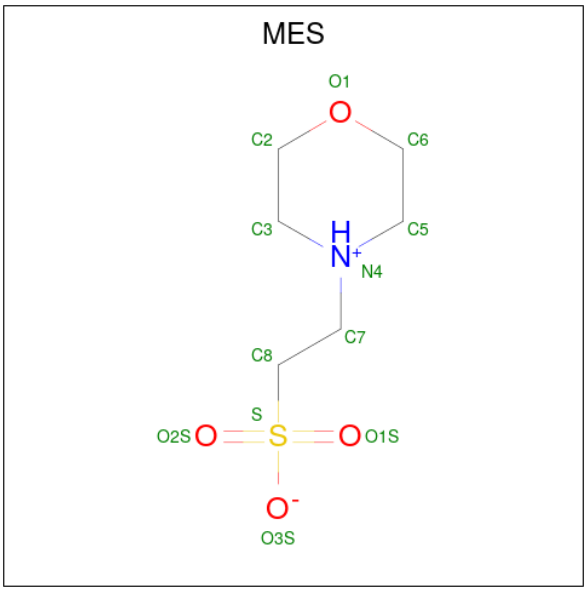
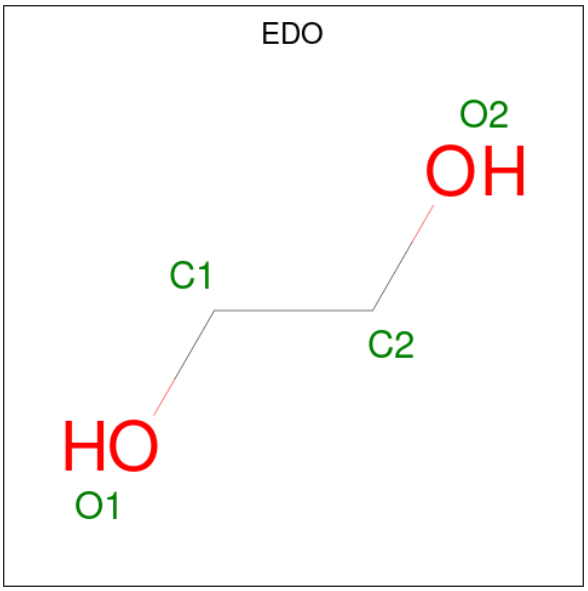
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0
6	C	2	Total Ca 2 2	0	0
6	D	1	Total Ca 1 1	0	0

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



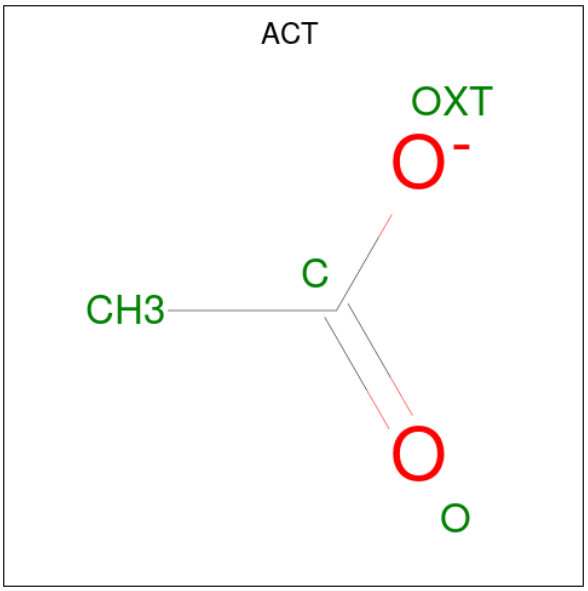
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O S 12 6 1 4 1	0	0
7	B	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



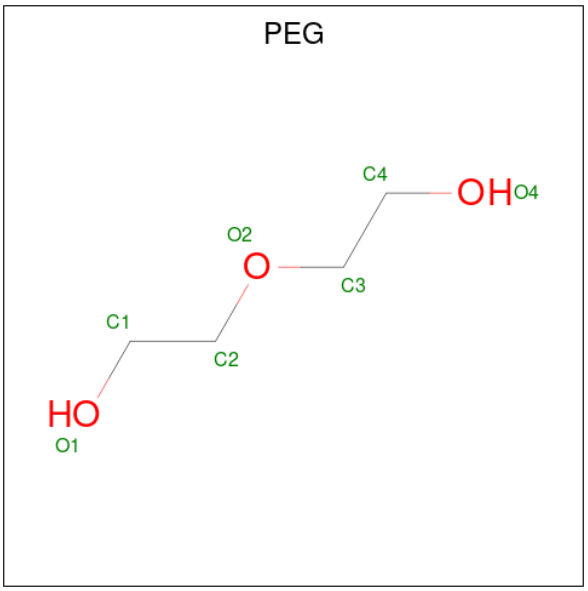
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	4	2	2	0	0
8	A	1	4	2	2	0	0
8	A	1	4	2	2	0	0
8	B	1	4	2	2	0	0
8	B	1	4	2	2	0	0
8	C	1	4	2	2	0	0
8	C	1	4	2	2	0	0
8	D	1	4	2	2	0	0

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



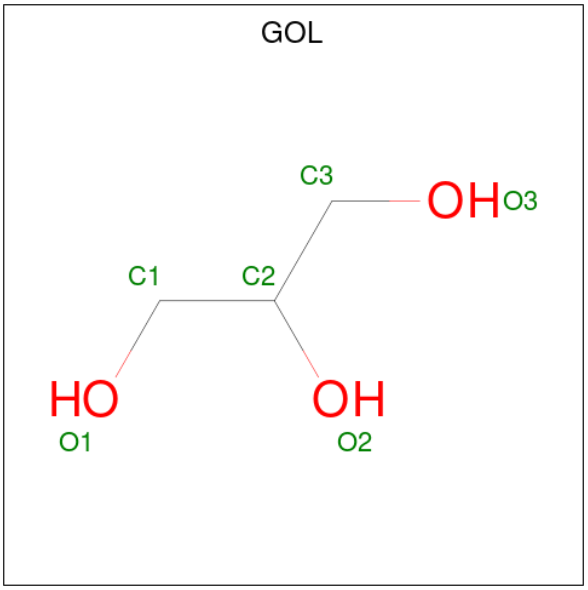
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	4	2	2	0	0
			Total	C	O		
9	A	1	4	2	2	0	0
			Total	C	O		
9	A	1	4	2	2	0	0
			Total	C	O		
9	B	1	4	2	2	0	0
			Total	C	O		
9	C	1	4	2	2	0	0
			Total	C	O		
9	D	1	4	2	2	0	0
			Total	C	O		
9	D	1	4	2	2	0	0

- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	A	1	7	4	3	0	0

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	A	1	6	3	3	0	0
11	A	1	6	3	3	0	0
11	C	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	D	1	6	3	3	0	0

- Molecule 12 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
12	B	2	2	2	0	0

- Molecule 13 is water.

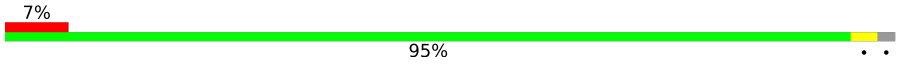
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	324	324	324	0	0
			Total	O		
13	B	281	281	281	0	0
			Total	O		
13	C	252	252	252	0	0
			Total	O		
13	D	271	271	271	0	0

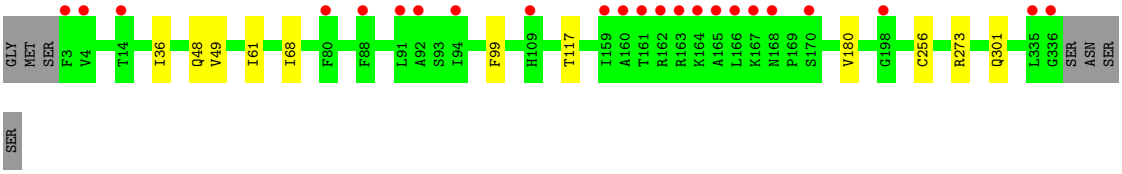
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA mismatch repair protein Mlh1

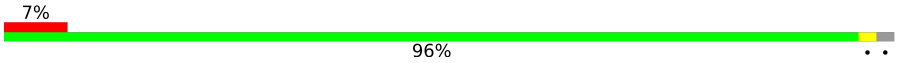
Chain A:

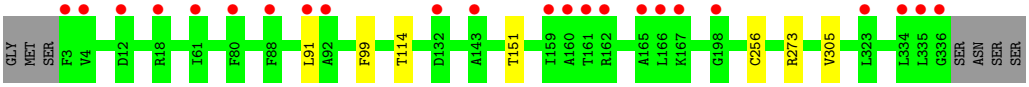




• Molecule 1: DNA mismatch repair protein Mlh1

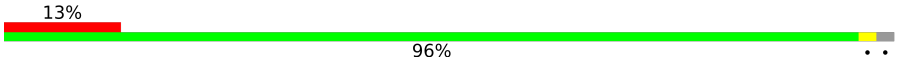
Chain B:

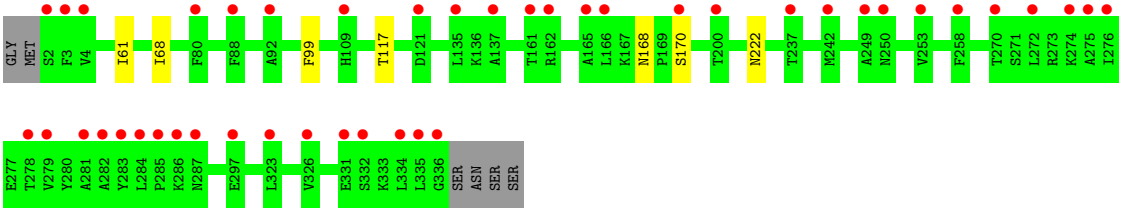




• Molecule 1: DNA mismatch repair protein Mlh1

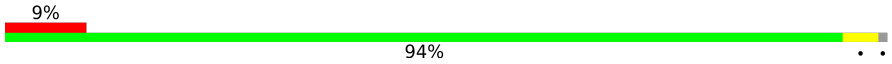
Chain C:

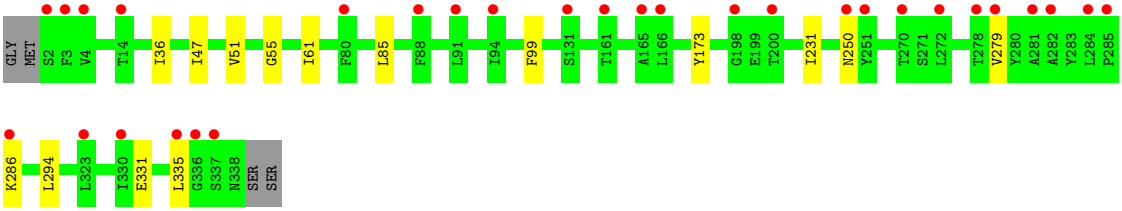




• Molecule 1: DNA mismatch repair protein Mlh1

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.21Å 179.48Å 73.35Å 90.00° 94.13° 90.00°	Depositor
Resolution (Å)	89.74 – 1.70 89.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	65.5 (89.74-1.70) 65.9 (89.74-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.195 , 0.225 0.200 , 0.229	Depositor DCC
R_{free} test set	5509 reflections (3.28%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12192	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, MG, BEF, CL, GOL, MES, NA, PEG, ADP, EDO, CA

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	1.06	0/2769	1.39	0/3744
1	B	1.07	0/2718	1.41	0/3676
1	C	1.06	0/2734	1.41	0/3696
1	D	1.06	0/2760	1.41	0/3733
All	All	1.06	0/10981	1.41	0/14849

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	2726	0	2773	6	0
1	B	2675	0	2718	5	0
1	C	2691	0	2723	4	0
1	D	2717	0	2736	9	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	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
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
7	A	12	0	13	0	0
7	B	12	0	13	0	0
8	A	12	0	18	0	0
8	B	8	0	12	0	0
8	C	8	0	12	0	0
8	D	4	0	6	0	0
9	A	12	0	9	0	0
9	B	4	0	3	0	0
9	C	4	0	3	0	0
9	D	8	0	6	0	0
10	A	7	0	10	0	0
11	A	12	0	16	0	0
11	C	6	0	8	0	0
11	D	6	0	8	0	0
12	B	2	0	0	0	0
13	A	324	0	0	1	0
13	B	281	0	0	0	0
13	C	252	0	0	1	0
13	D	271	0	0	0	0
All	All	12192	0	11135	24	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 (24) 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:250[B]:ASN:O	1:D:250[B]:ASN:OD1	1.99	0.80
1:D:250[B]:ASN:OD1	1:D:250[B]:ASN:C	2.37	0.66
1:C:168[A]:ASN:ND2	1:C:170[A]:SER:OG	2.28	0.65
1:B:114:THR:HB	1:B:151[B]:THR:CG2	2.37	0.54
1:C:222:ASN:ND2	13:C:501:HOH:O	2.44	0.51
1:D:61[B]:ILE:HG23	1:D:61[B]:ILE:O	2.11	0.51
1:A:61[A]:ILE:HG23	1:A:61[A]:ILE:O	2.12	0.48
1:B:305[A]:VAL:HG12	1:B:305[A]:VAL:O	2.15	0.46
1:D:36[B]:ILE:HG22	1:D:61[B]:ILE:HD11	1.97	0.46
1:A:36[A]:ILE:HD11	1:A:180:VAL:HG22	1.98	0.46
1:D:36[A]:ILE:CD1	1:D:47:ILE:HG21	2.48	0.43
1:B:256:CYS:SG	1:B:273:ARG:HD2	2.59	0.43
1:A:256:CYS:SG	1:A:273:ARG:HD2	2.58	0.43
1:C:61[B]:ILE:HG23	1:C:61[B]:ILE:O	2.19	0.42
1:A:301:GLN:HG3	13:A:685:HOH:O	2.19	0.42
1:A:68:ILE:HB	1:A:117:THR:HG21	2.02	0.42
1:C:68:ILE:HB	1:C:117:THR:HG21	2.02	0.41
1:B:114:THR:HB	1:B:151[B]:THR:HG22	2.02	0.41
1:B:91[A]:LEU:HA	1:B:91[A]:LEU:HD23	1.80	0.41
1:D:51[B]:VAL:HG21	1:D:173:TYR:CD1	2.55	0.41
1:D:231:ILE:HD11	1:D:294:LEU:CD2	2.51	0.41
1:D:279:VAL:HG13	1:D:331:GLU:HG2	2.02	0.40
1:A:49:VAL:HG22	1:A:61[B]:ILE:HG12	2.04	0.40
1:D:51[A]:VAL:HG13	1:D:55:GLY:N	2.37	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	347/341 (102%)	340 (98%)	6 (2%)	1 (0%)	36 22
1	B	341/341 (100%)	332 (97%)	8 (2%)	1 (0%)	36 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	343/341 (101%)	335 (98%)	7 (2%)	1 (0%)	36	22
1	D	347/341 (102%)	338 (97%)	8 (2%)	1 (0%)	36	22
All	All	1378/1364 (101%)	1345 (98%)	29 (2%)	4 (0%)	36	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	PHE
1	B	99	PHE
1	C	99	PHE
1	D	99	PHE

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	303/294 (103%)	302 (100%)	1 (0%)	86	83
1	B	297/294 (101%)	297 (100%)	0	100	100
1	C	299/294 (102%)	299 (100%)	0	100	100
1	D	303/294 (103%)	300 (99%)	3 (1%)	68	58
All	All	1202/1176 (102%)	1198 (100%)	4 (0%)	86	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	D	85	LEU
1	D	286	LYS
1	D	335	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	145	ASN
1	A	149	GLN
1	A	209	ASN
1	A	243	ASN
1	A	318	HIS
1	B	48	GLN
1	B	62	GLN
1	B	209	ASN
1	C	197	GLN
1	C	306	ASN
1	D	306	ASN
1	D	338	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 46 ligands modelled in this entry, 16 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
11	GOL	A	414	-	5,5,5	0.11	0	5,5,5	0.33	0
9	ACT	A	411	-	3,3,3	0.94	0	3,3,3	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	MES	A	407	-	12,12,12	0.75	0	14,16,16	0.65	0
8	EDO	C	409	-	3,3,3	0.07	0	2,2,2	0.22	0
8	EDO	D	407	-	3,3,3	0.09	0	2,2,2	0.26	0
8	EDO	C	410	-	3,3,3	0.09	0	2,2,2	0.15	0
4	BEF	C	403	2	0,3,3	-	-	-		
4	BEF	B	403	2	0,3,3	-	-	-		
2	ADP	D	401	4,3	27,29,29	0.39	0	42,45,45	0.51	0
8	EDO	B	410	-	3,3,3	0.11	0	2,2,2	0.29	0
9	ACT	A	409	-	3,3,3	1.04	0	3,3,3	0.76	0
11	GOL	D	408	-	5,5,5	0.10	0	5,5,5	0.31	0
2	ADP	A	401	4,3	27,29,29	0.46	0	42,45,45	0.45	0
8	EDO	A	412	-	3,3,3	0.12	0	2,2,2	0.42	0
4	BEF	D	403	2	0,3,3	-	-	-		
10	PEG	A	413	-	6,6,6	0.14	0	5,5,5	0.21	0
9	ACT	D	409	-	3,3,3	0.99	0	3,3,3	0.81	0
4	BEF	A	403	2	0,3,3	-	-	-		
8	EDO	A	410	-	3,3,3	0.11	0	2,2,2	0.28	0
2	ADP	B	401	4,3	27,29,29	0.44	0	42,45,45	0.49	0
11	GOL	A	415	-	5,5,5	0.12	0	5,5,5	0.36	0
9	ACT	D	406	-	3,3,3	0.88	0	3,3,3	0.84	0
8	EDO	B	409	-	3,3,3	0.07	0	2,2,2	0.50	0
7	MES	B	406	-	12,12,12	0.76	0	14,16,16	0.59	0
9	ACT	B	411	-	3,3,3	0.95	0	3,3,3	0.76	0
11	GOL	C	408	-	5,5,5	0.13	0	5,5,5	0.44	0
9	ACT	A	416	-	3,3,3	0.96	0	3,3,3	0.88	0
8	EDO	A	408	-	3,3,3	0.11	0	2,2,2	0.34	0
9	ACT	C	407	-	3,3,3	0.98	0	3,3,3	0.79	0
2	ADP	C	401	4,3	27,29,29	0.45	0	42,45,45	0.48	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
11	GOL	A	414	-	-	0/4/4/4	-
7	MES	A	407	-	-	0/6/14/14	0/1/1/1
8	EDO	C	409	-	-	0/1/1/1	-
8	EDO	D	407	-	-	0/1/1/1	-
8	EDO	C	410	-	-	0/1/1/1	-
2	ADP	D	401	4,3	-	1/16/32/32	0/3/3/3
8	EDO	B	410	-	-	1/1/1/1	-
11	GOL	D	408	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	401	4,3	-	3/16/32/32	0/3/3/3
8	EDO	A	412	-	-	1/1/1/1	-
10	PEG	A	413	-	-	1/4/4/4	-
8	EDO	A	410	-	-	0/1/1/1	-
2	ADP	B	401	4,3	-	2/16/32/32	0/3/3/3
11	GOL	A	415	-	-	0/4/4/4	-
8	EDO	B	409	-	-	0/1/1/1	-
7	MES	B	406	-	-	0/6/14/14	0/1/1/1
11	GOL	C	408	-	-	3/4/4/4	-
8	EDO	A	408	-	-	0/1/1/1	-
2	ADP	C	401	4,3	-	3/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	ADP	PA-O3A-PB-O3B
11	C	408	GOL	C1-C2-C3-O3
2	C	401	ADP	PA-O3A-PB-O1B
2	A	401	ADP	PA-O3A-PB-O3B
2	B	401	ADP	PA-O3A-PB-O3B
8	A	412	EDO	O1-C1-C2-O2
11	C	408	GOL	O1-C1-C2-C3
10	A	413	PEG	O2-C3-C4-O4
2	A	401	ADP	PA-O3A-PB-O1B
2	B	401	ADP	PA-O3A-PB-O1B
8	B	410	EDO	O1-C1-C2-O2
2	A	401	ADP	PA-O3A-PB-O2B
2	C	401	ADP	PA-O3A-PB-O2B
2	C	401	ADP	PA-O3A-PB-O3B
11	C	408	GOL	O1-C1-C2-O2

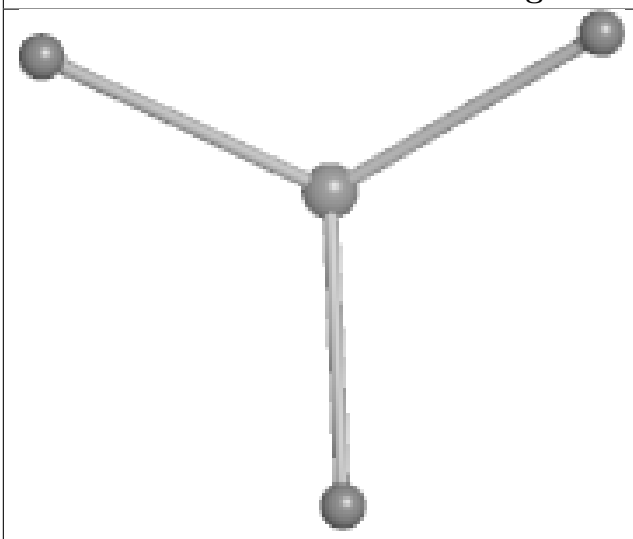
There are no ring outliers.

No monomer is involved in short contacts.

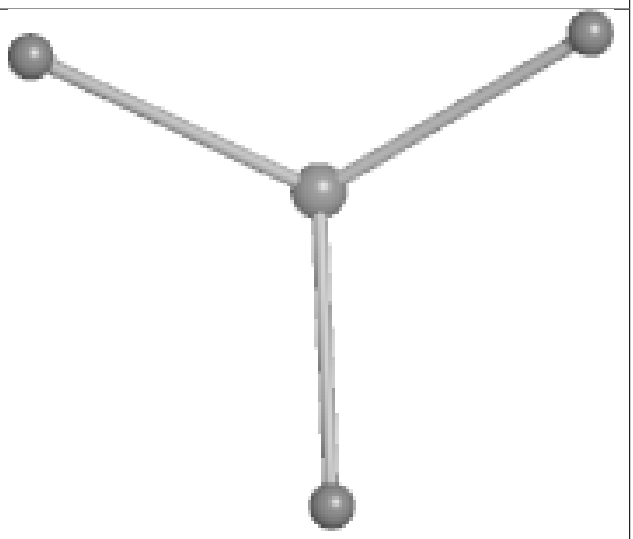
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

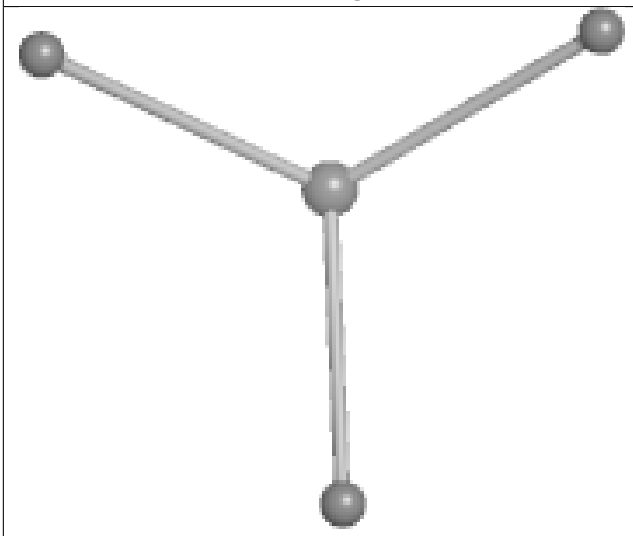
Ligand BEF C 403



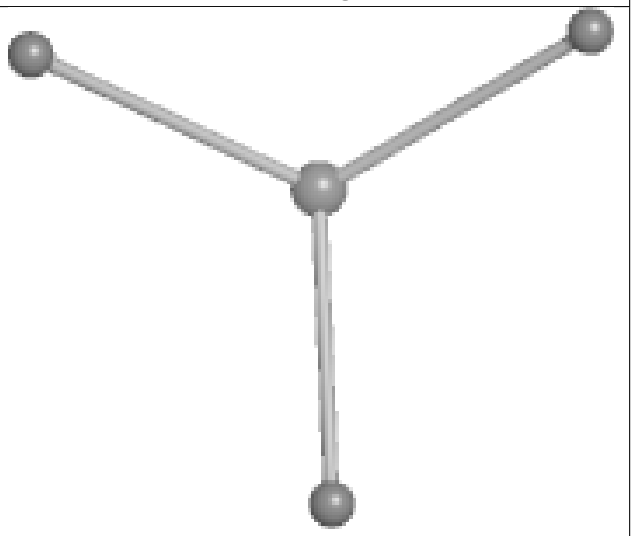
Bond lengths



Bond angles

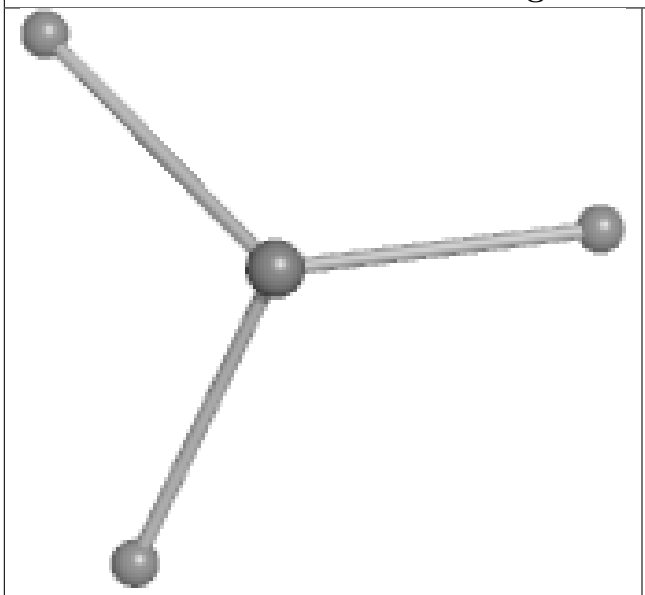


Torsions

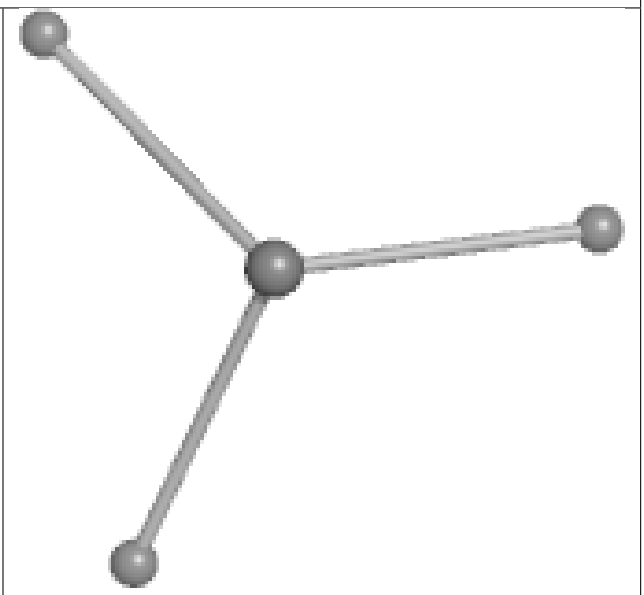


Rings

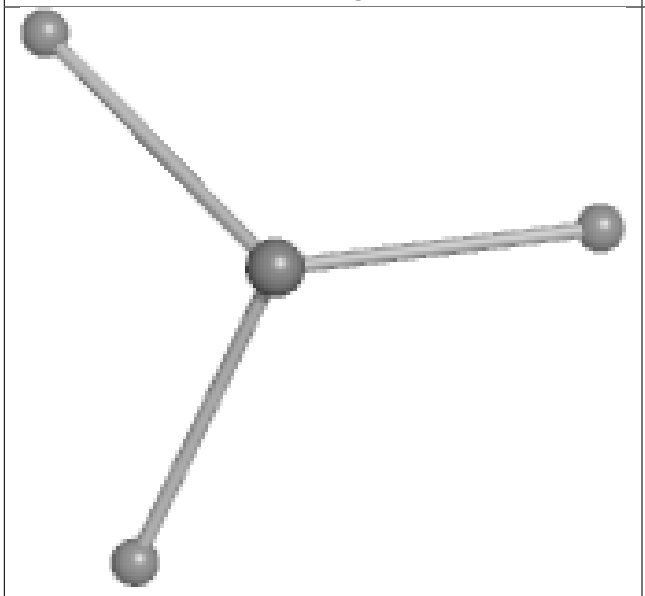
Ligand BEF B 403



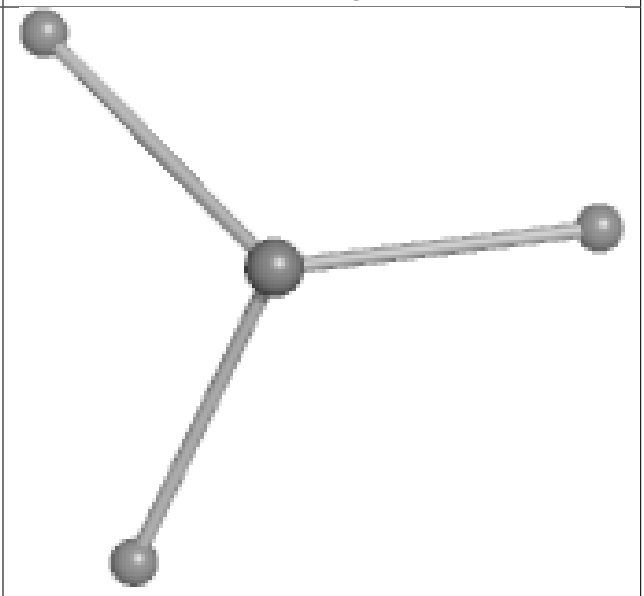
Bond lengths



Bond angles

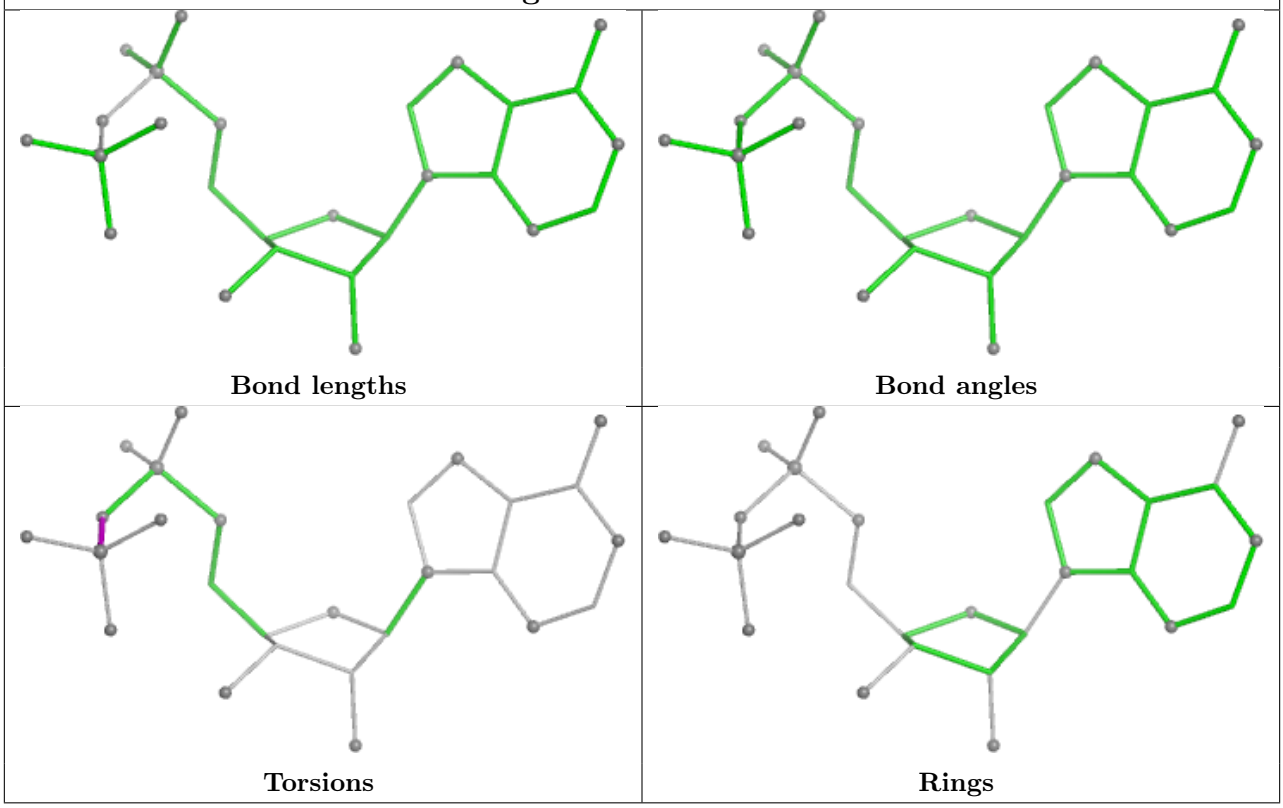


Torsions

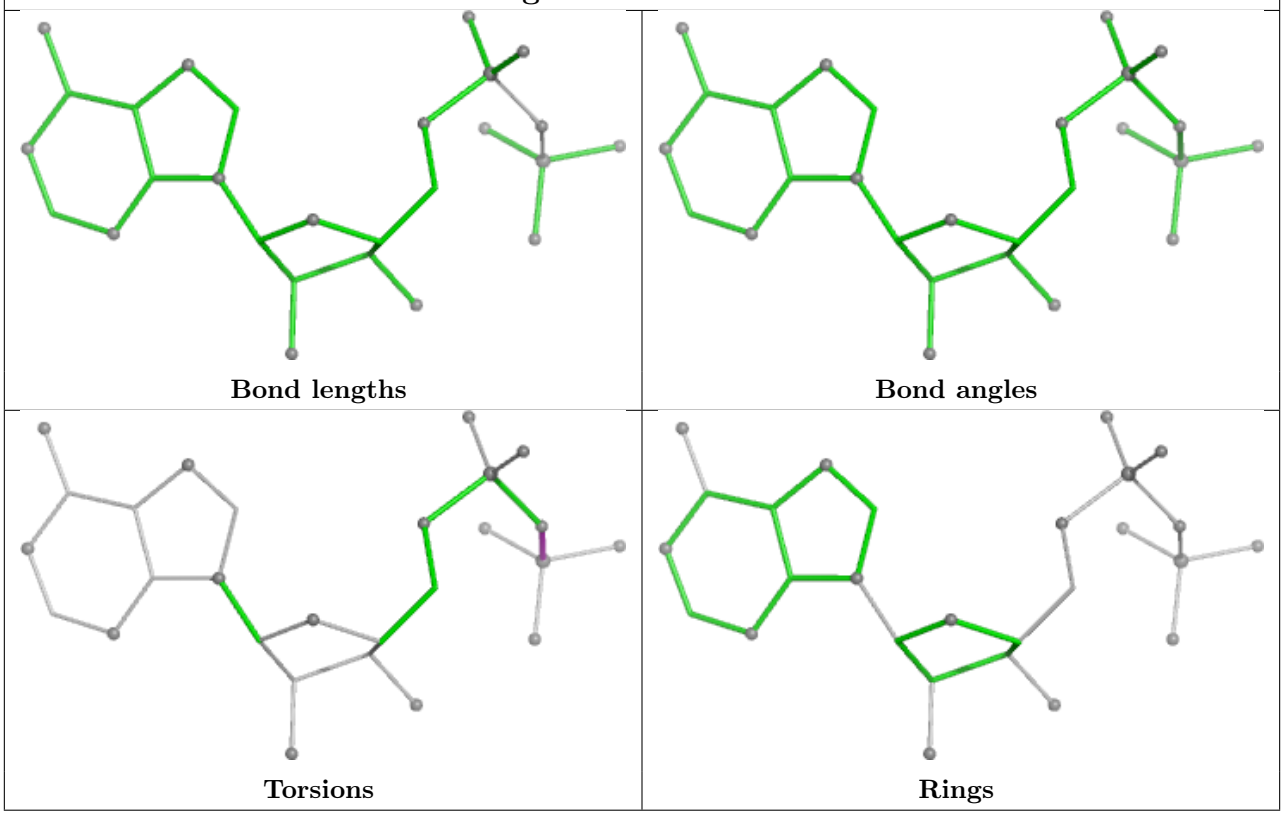


Rings

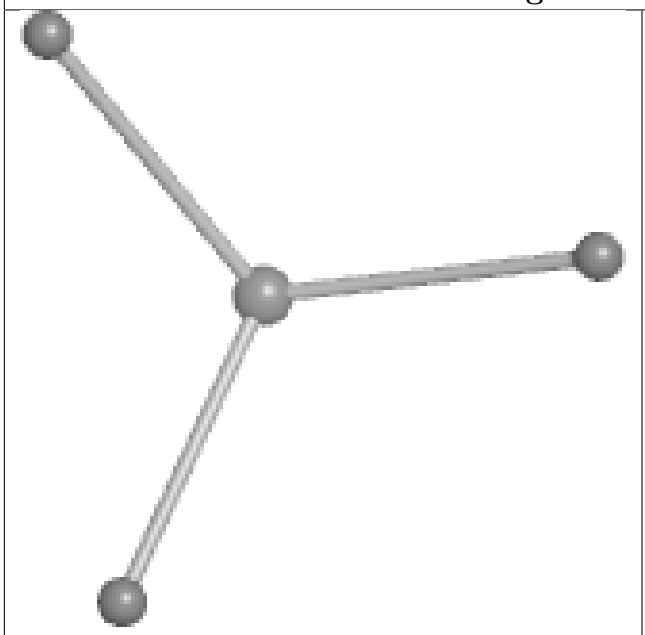
Ligand ADP D 401



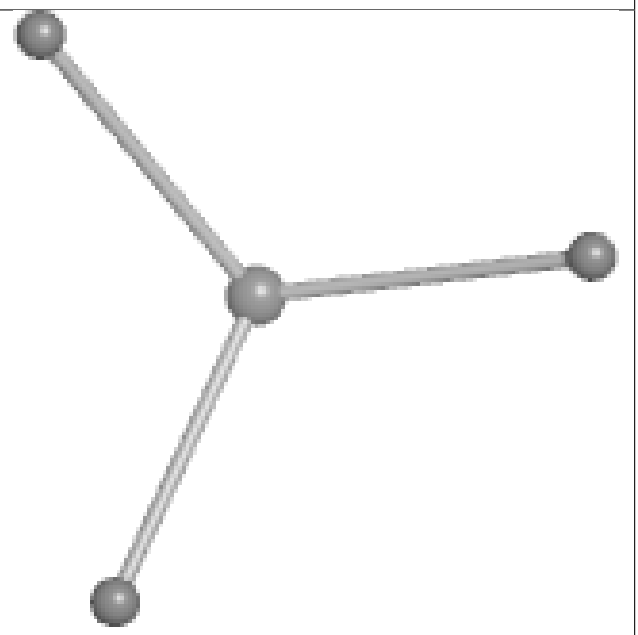
Ligand ADP A 401



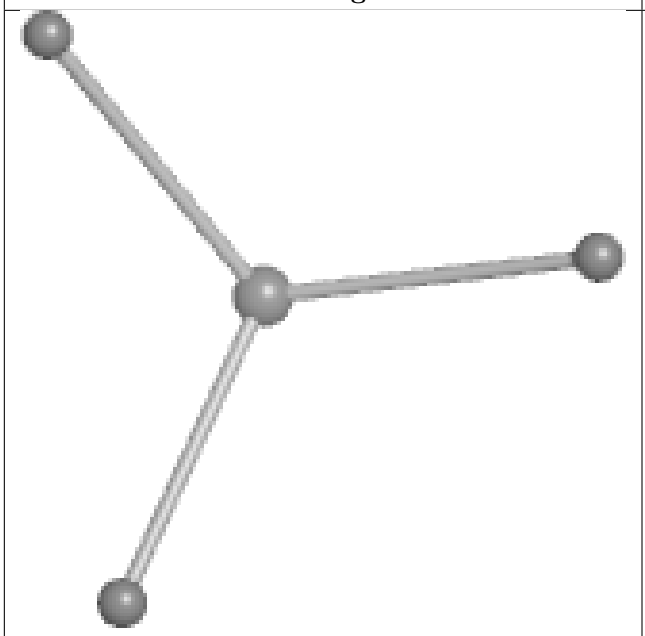
Ligand BEF D 403



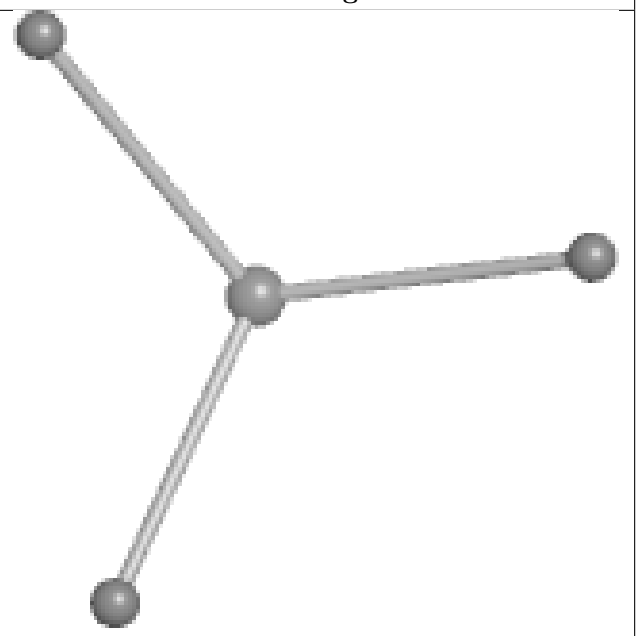
Bond lengths



Bond angles

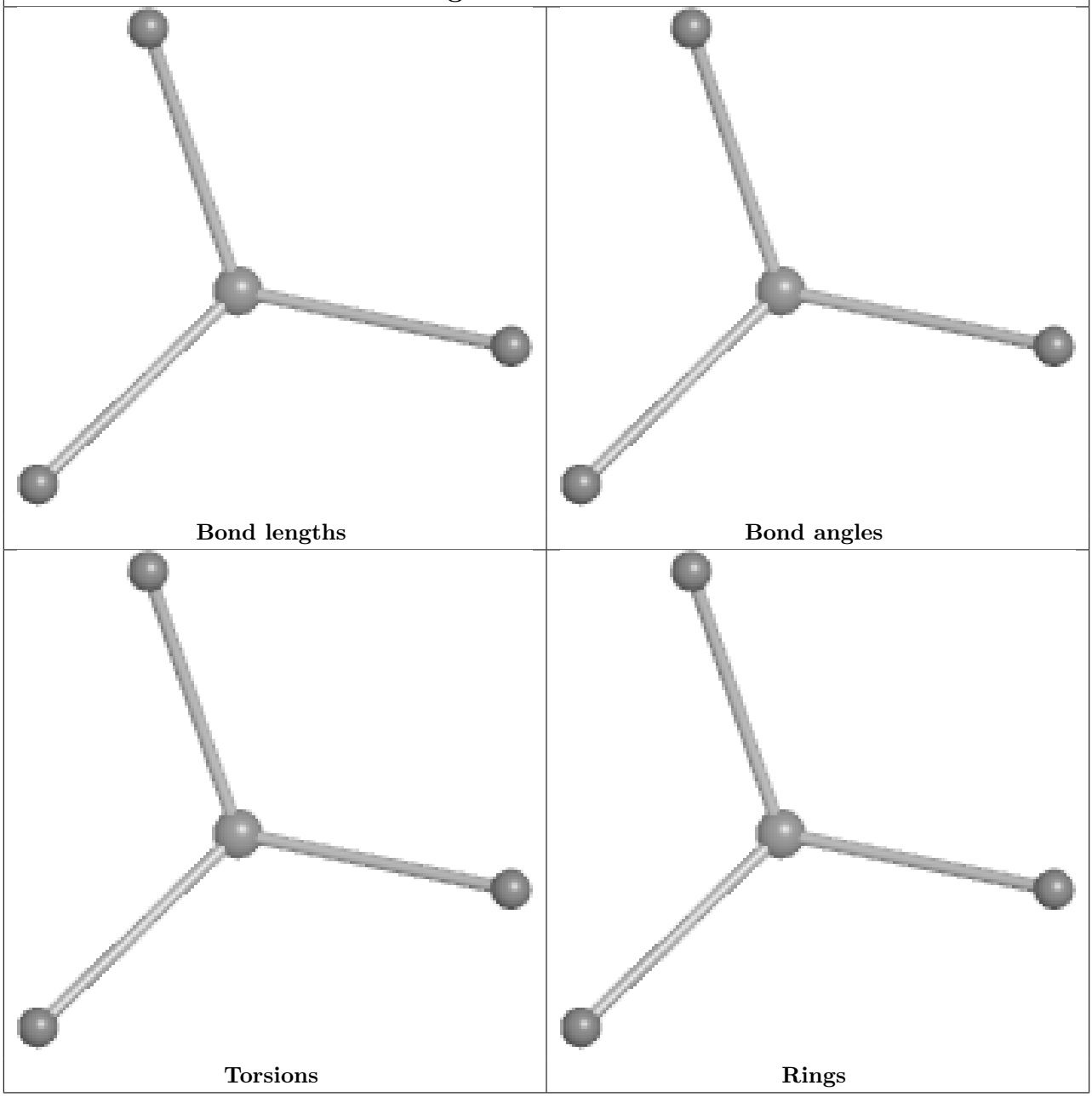


Torsions

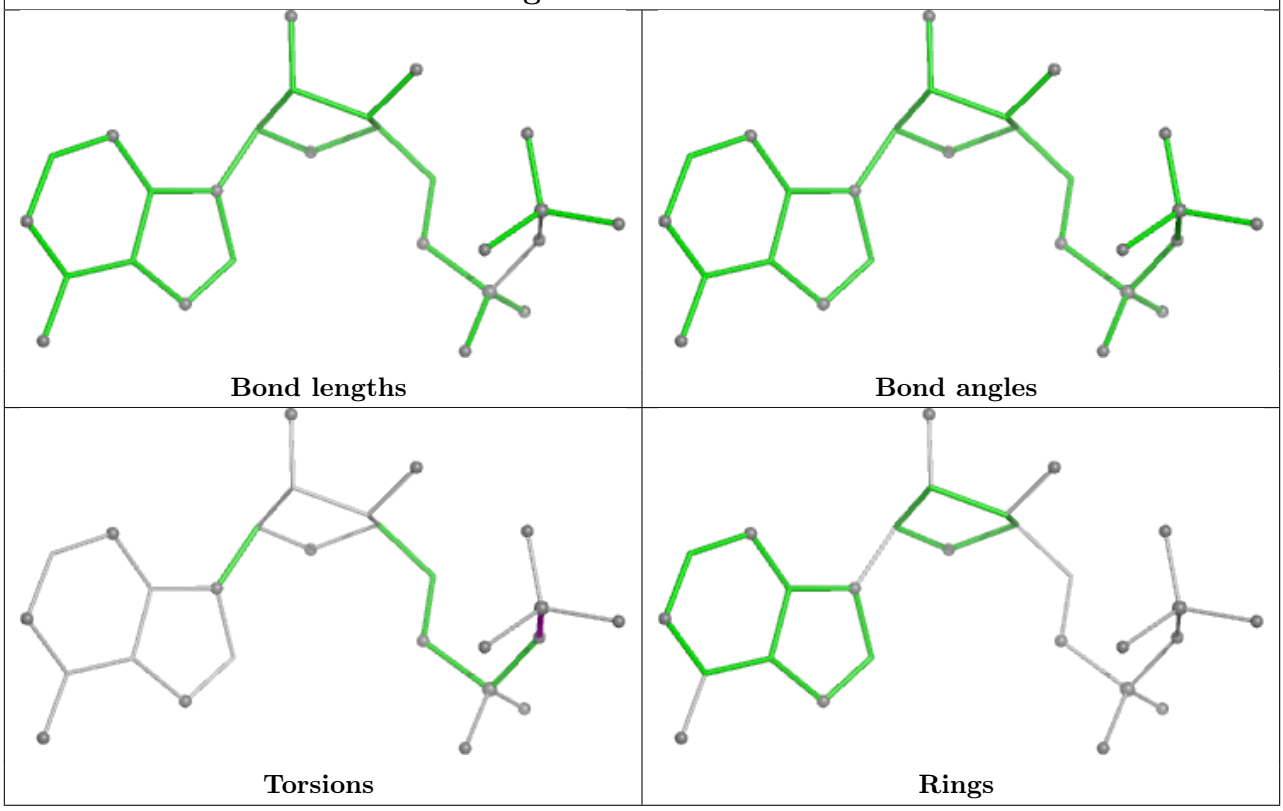


Rings

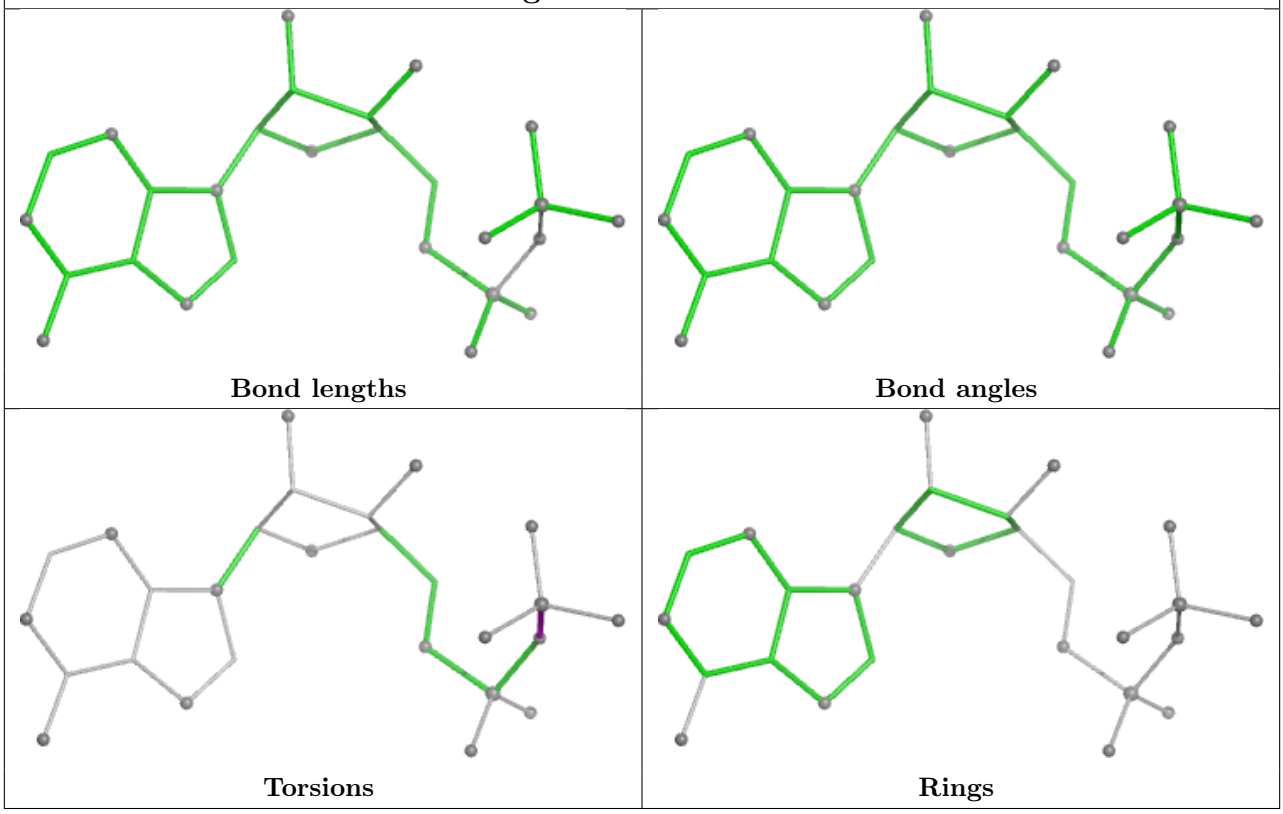
Ligand BEF A 403



Ligand ADP B 401



Ligand ADP C 401



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	334/341 (97%)	0.46	23 (6%)	23	25	9, 26, 47, 72	27 (8%)
1	B	334/341 (97%)	0.62	23 (6%)	23	25	10, 29, 49, 75	21 (6%)
1	C	335/341 (98%)	0.78	44 (13%)	7	7	10, 32, 56, 72	23 (6%)
1	D	337/341 (98%)	0.61	30 (8%)	15	16	10, 30, 51, 90	27 (8%)
All	All	1340/1364 (98%)	0.62	120 (8%)	15	16	9, 29, 52, 90	98 (7%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	PHE	5.6
1	A	335	LEU	5.4
1	A	91	LEU	4.9
1	C	335	LEU	4.9
1	A	166	LEU	4.8
1	A	88	PHE	4.7
1	C	249	ALA	4.5
1	C	3	PHE	4.3
1	B	336	GLY	4.2
1	A	165	ALA	4.2
1	A	3	PHE	4.2
1	C	88	PHE	4.2
1	D	250[A]	ASN	4.0
1	D	88	PHE	3.9
1	A	162	ARG	3.8
1	B	335	LEU	3.8
1	C	323	LEU	3.8
1	A	159	ILE	3.8
1	C	162	ARG	3.8
1	C	275	ALA	3.8
1	C	242	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	91[A]	LEU	3.6
1	D	282	ALA	3.5
1	D	166	LEU	3.3
1	A	161	THR	3.3
1	C	80	PHE	3.2
1	D	3	PHE	3.2
1	B	161	THR	3.2
1	C	161	THR	3.2
1	C	284	LEU	3.1
1	A	80	PHE	3.1
1	D	337	SER	3.1
1	A	336	GLY	3.1
1	D	285	PRO	2.9
1	D	80	PHE	2.9
1	A	160	ALA	2.9
1	C	92	ALA	2.9
1	A	198	GLY	2.9
1	C	285	PRO	2.9
1	D	200[A]	THR	2.9
1	B	92	ALA	2.9
1	D	335	LEU	2.9
1	C	165	ALA	2.8
1	C	336	GLY	2.8
1	D	91	LEU	2.8
1	B	80	PHE	2.8
1	B	323	LEU	2.8
1	D	278[A]	THR	2.8
1	C	279	VAL	2.8
1	C	137	ALA	2.7
1	D	284	LEU	2.7
1	A	94	ILE	2.7
1	C	109[A]	HIS	2.7
1	D	336	GLY	2.7
1	B	88	PHE	2.7
1	D	4	VAL	2.7
1	B	334	LEU	2.7
1	C	334	LEU	2.7
1	A	92	ALA	2.7
1	B	166	LEU	2.7
1	C	272	LEU	2.7
1	A	167	LYS	2.7
1	C	281	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	286	LYS	2.6
1	D	286	LYS	2.6
1	D	198	GLY	2.6
1	D	270	THR	2.6
1	C	135	LEU	2.6
1	D	323	LEU	2.6
1	C	282	ALA	2.6
1	A	109	HIS	2.5
1	B	165	ALA	2.5
1	B	18	ARG	2.5
1	C	283	TYR	2.5
1	B	4	VAL	2.5
1	B	159	ILE	2.5
1	C	276	ILE	2.5
1	C	278	THR	2.5
1	A	163	ARG	2.4
1	C	170[A]	SER	2.4
1	D	94	ILE	2.4
1	C	250	ASN	2.4
1	B	167	LYS	2.4
1	D	279	VAL	2.4
1	B	132	ASP	2.4
1	D	165	ALA	2.4
1	B	162	ARG	2.4
1	A	4	VAL	2.4
1	D	2	SER	2.3
1	B	198	GLY	2.3
1	B	160	ALA	2.3
1	B	12	ASP	2.3
1	A	14	THR	2.3
1	C	270	THR	2.3
1	C	332	SER	2.3
1	D	131	SER	2.3
1	D	281	ALA	2.2
1	C	237	THR	2.2
1	D	272	LEU	2.2
1	D	251	TYR	2.2
1	C	253	VAL	2.2
1	C	166	LEU	2.2
1	C	274	LYS	2.2
1	D	330	ILE	2.2
1	C	121	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	258	PHE	2.1
1	D	161	THR	2.1
1	C	297	GLU	2.1
1	B	143	ALA	2.1
1	C	4	VAL	2.1
1	A	170	SER	2.1
1	C	2	SER	2.1
1	C	200	THR	2.1
1	D	14	THR	2.1
1	A	168	ASN	2.0
1	A	164	LYS	2.0
1	C	331	GLU	2.0
1	C	287	ASN	2.0
1	B	61[A]	ILE	2.0
1	C	326	VAL	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(Å^2)	Q<0.9
11	GOL	D	408	6/6	0.57	0.22	84,85,86,86	0
8	EDO	C	409	4/4	0.59	0.21	73,74,75,75	0
9	ACT	A	409	4/4	0.61	0.23	57,57,58,61	0
10	PEG	A	413	7/7	0.63	0.25	59,63,70,71	0
8	EDO	B	410	4/4	0.66	0.21	66,66,66,66	0
8	EDO	C	410	4/4	0.74	0.18	63,64,65,65	0
11	GOL	C	408	6/6	0.75	0.19	65,67,67,68	0
8	EDO	B	409	4/4	0.76	0.23	54,54,55,56	0

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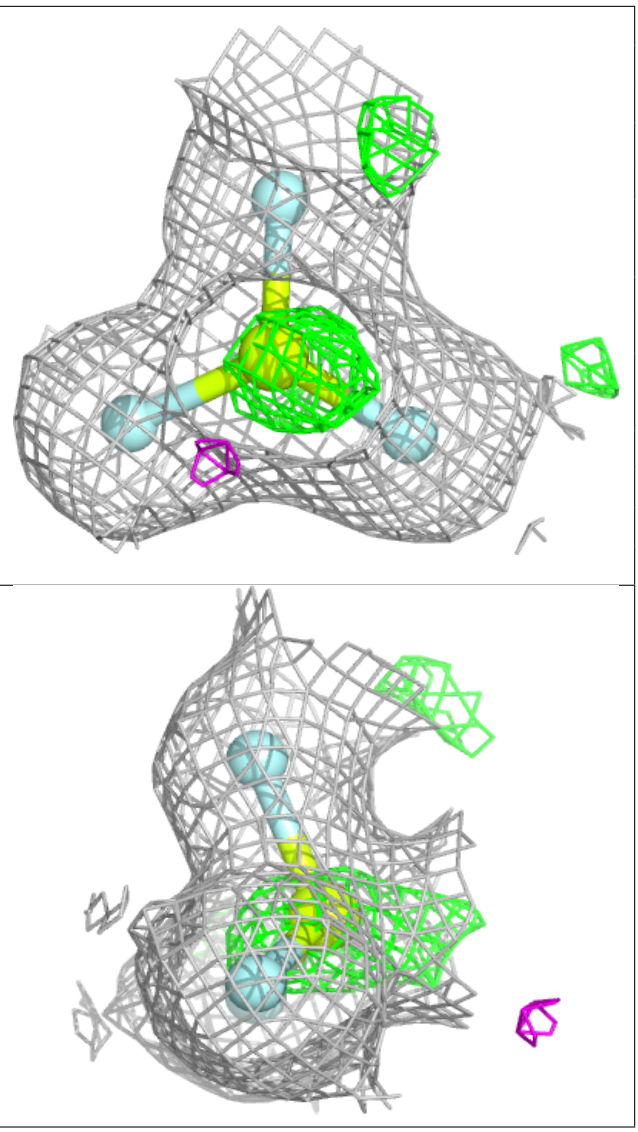
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	GOL	A	415	6/6	0.76	0.17	59,61,62,63	0
11	GOL	A	414	6/6	0.77	0.17	43,45,46,52	0
9	ACT	B	411	4/4	0.77	0.18	42,45,45,46	0
8	EDO	A	410	4/4	0.78	0.20	46,49,50,52	0
9	ACT	A	416	4/4	0.80	0.15	45,47,47,49	0
8	EDO	A	412	4/4	0.82	0.23	56,56,58,58	0
8	EDO	A	408	4/4	0.83	0.17	44,46,47,47	0
9	ACT	D	406	4/4	0.84	0.18	58,58,59,63	0
8	EDO	D	407	4/4	0.84	0.16	57,57,57,57	0
9	ACT	A	411	4/4	0.85	0.14	45,48,49,50	0
12	CL	B	408	1/1	0.85	0.14	77,77,77,77	0
9	ACT	C	407	4/4	0.88	0.16	53,55,55,55	0
9	ACT	D	409	4/4	0.88	0.13	50,50,52,53	0
12	CL	B	407	1/1	0.92	0.13	52,52,52,52	0
4	BEF	C	403	4/4	0.92	0.08	19,20,21,22	0
5	NA	B	404	1/1	0.94	0.06	23,23,23,23	0
5	NA	C	404	1/1	0.94	0.07	31,31,31,31	0
4	BEF	A	403	4/4	0.94	0.07	18,20,20,21	0
4	BEF	D	403	4/4	0.96	0.06	19,19,20,22	0
6	CA	C	405	1/1	0.96	0.08	45,45,45,45	0
4	BEF	B	403	4/4	0.96	0.06	15,18,19,19	0
5	NA	A	404	1/1	0.97	0.10	22,22,22,22	0
6	CA	C	406	1/1	0.97	0.05	54,54,54,54	0
6	CA	D	405	1/1	0.97	0.09	40,40,40,40	0
7	MES	A	407	12/12	0.97	0.06	22,24,25,26	0
7	MES	B	406	12/12	0.97	0.07	22,26,28,28	0
3	MG	B	402	1/1	0.97	0.05	17,17,17,17	0
3	MG	C	402	1/1	0.97	0.05	21,21,21,21	0
5	NA	D	404	1/1	0.97	0.07	26,26,26,26	0
6	CA	A	406	1/1	0.97	0.08	33,33,33,33	0
2	ADP	B	401	27/27	0.98	0.04	16,18,19,21	0
2	ADP	C	401	27/27	0.98	0.05	19,21,22,23	0
6	CA	B	405	1/1	0.98	0.03	23,23,23,23	0
2	ADP	D	401	27/27	0.98	0.04	16,19,20,21	0
2	ADP	A	401	27/27	0.98	0.04	16,17,19,19	0
6	CA	A	405	1/1	0.99	0.02	22,22,22,22	0
3	MG	A	402	1/1	0.99	0.04	16,16,16,16	0
3	MG	D	402	1/1	0.99	0.05	21,21,21,21	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.

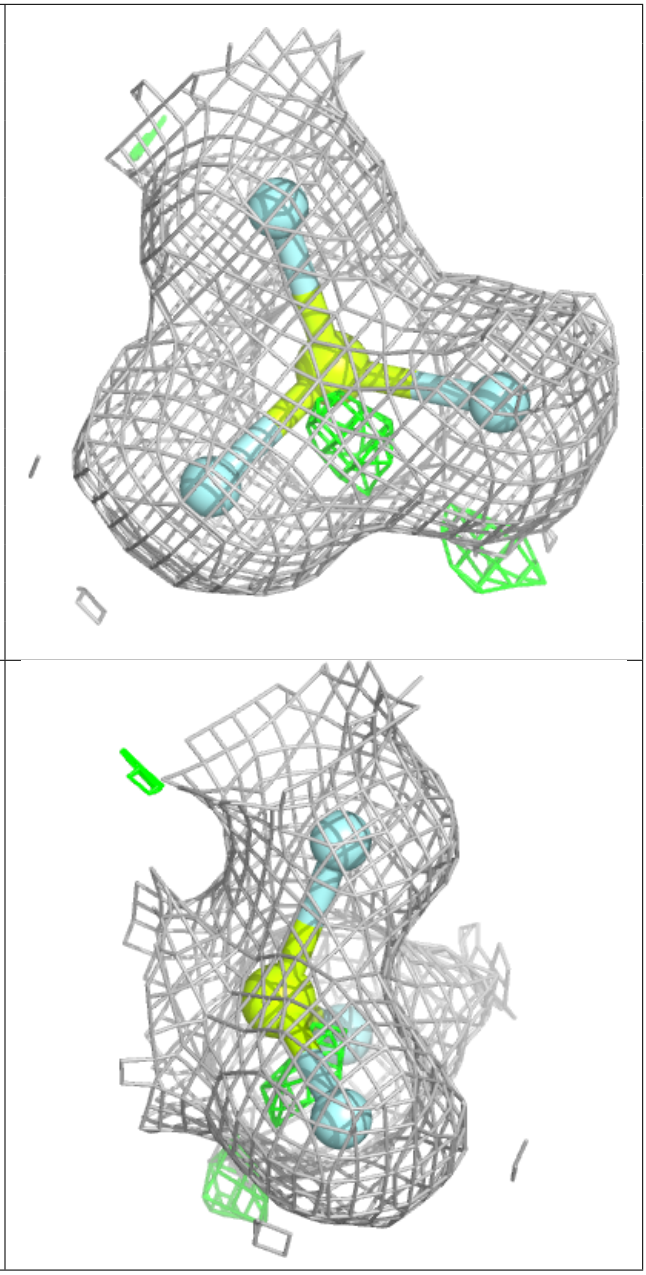
Electron density around BEF C 403:

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



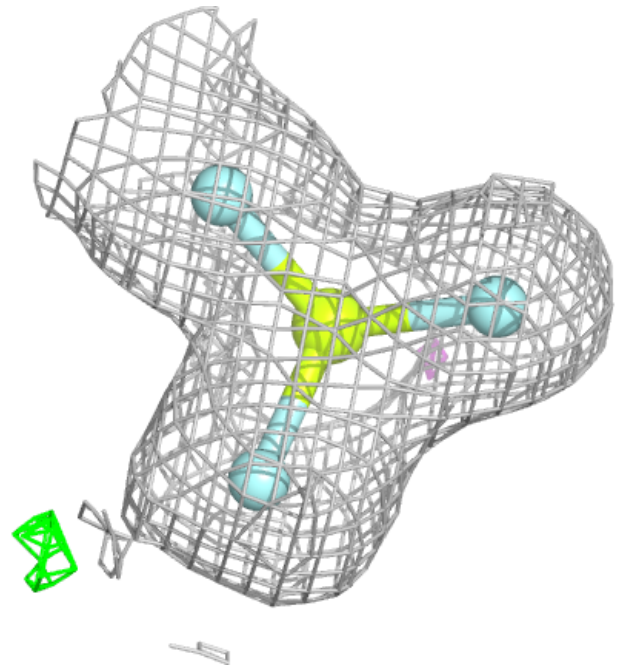
Electron density around BEF A 403:

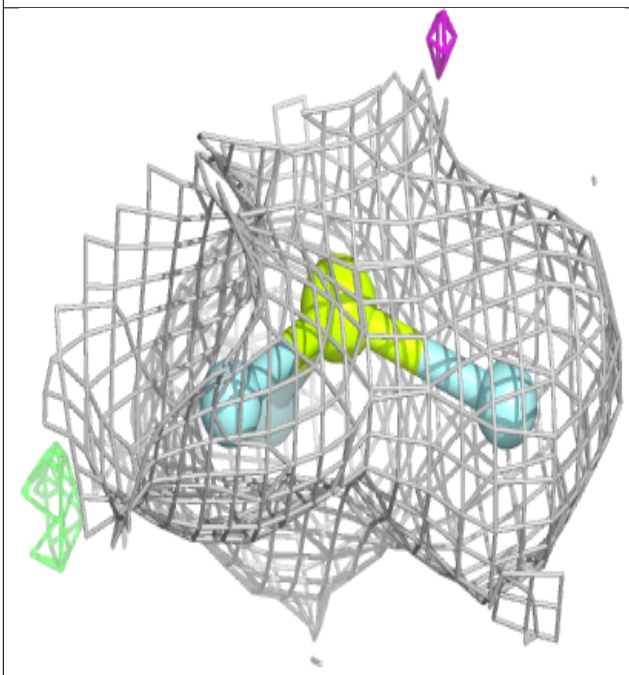
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

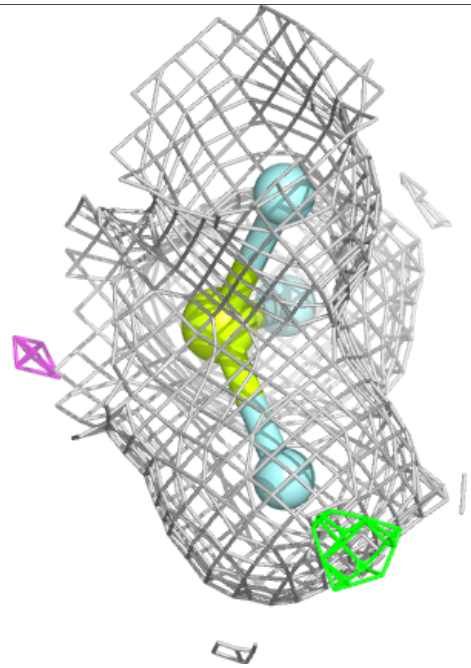


Electron density around BEF D 403:

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

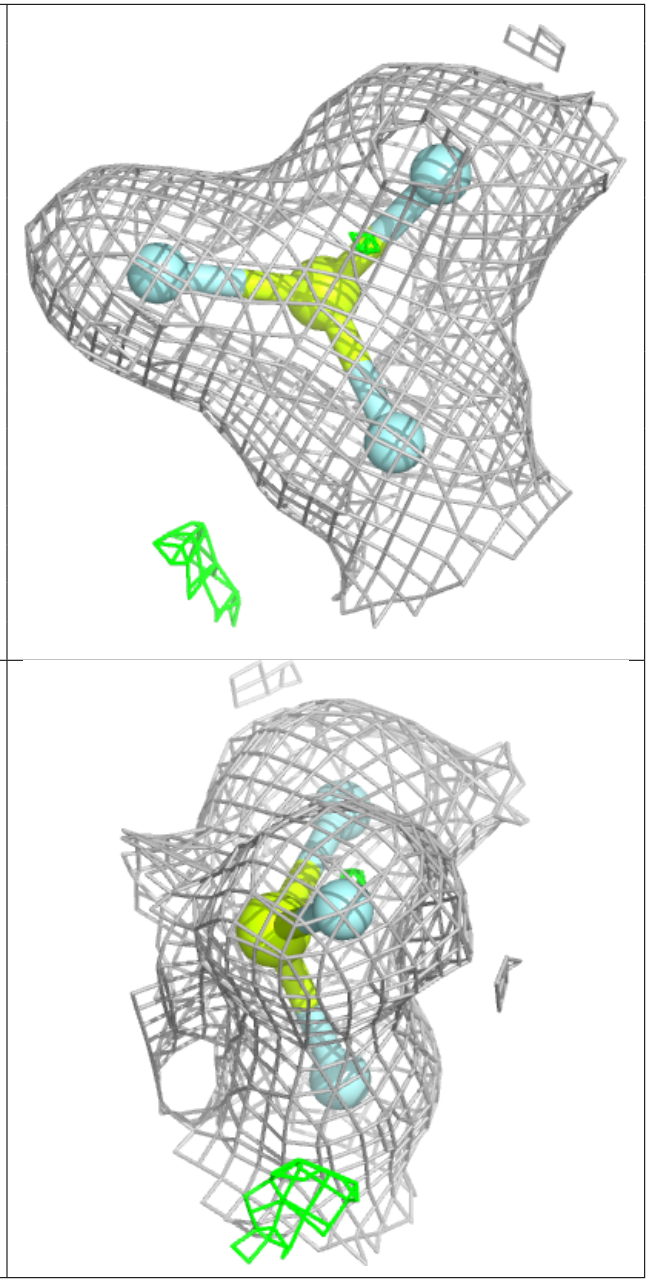






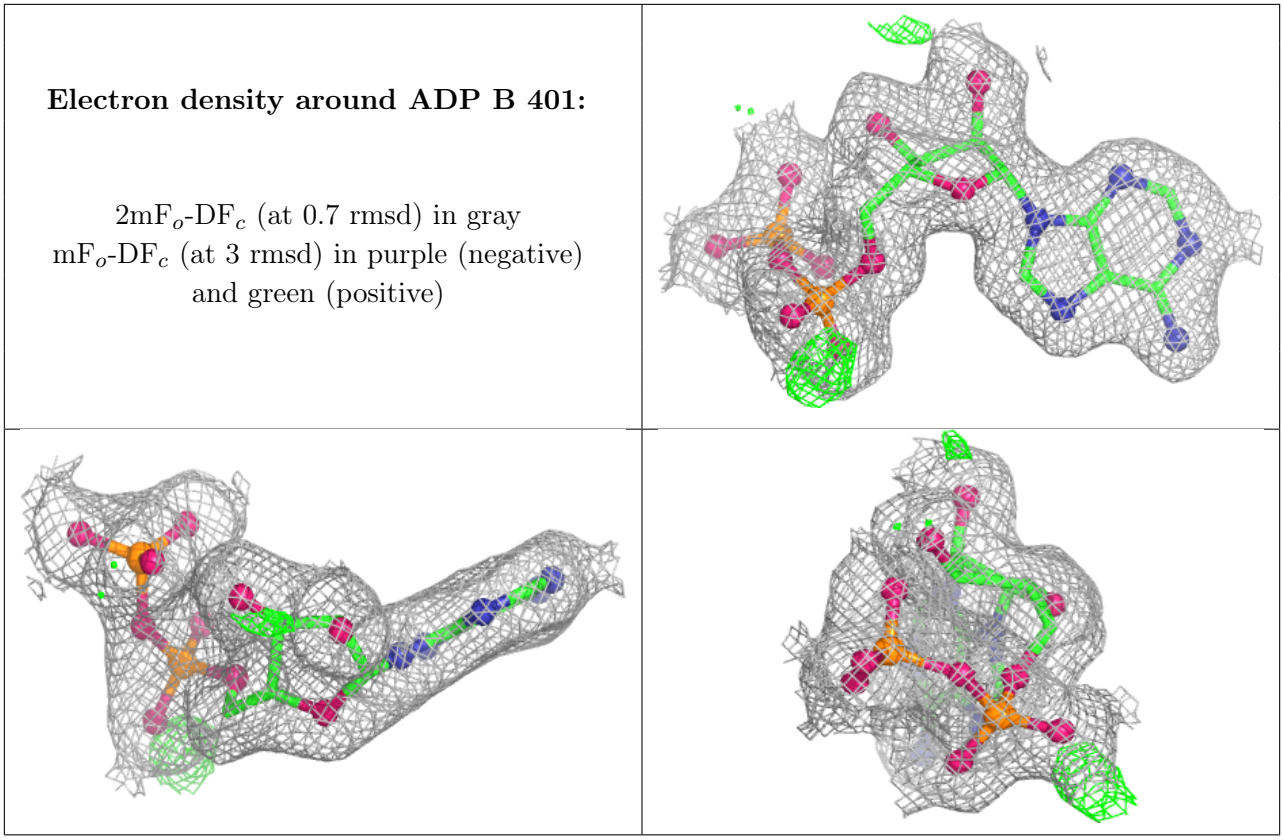
Electron density around BEF B 403:

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



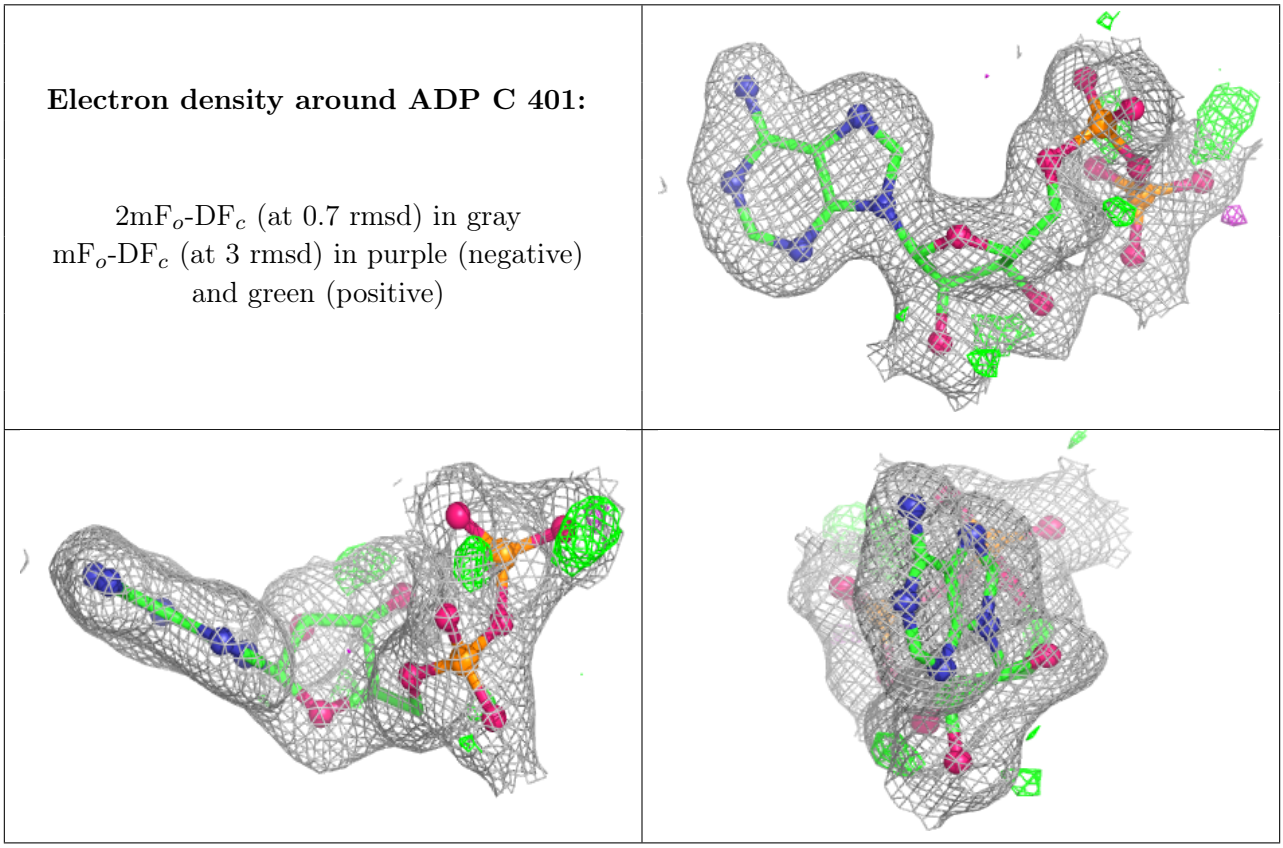
Electron density around ADP B 401:

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



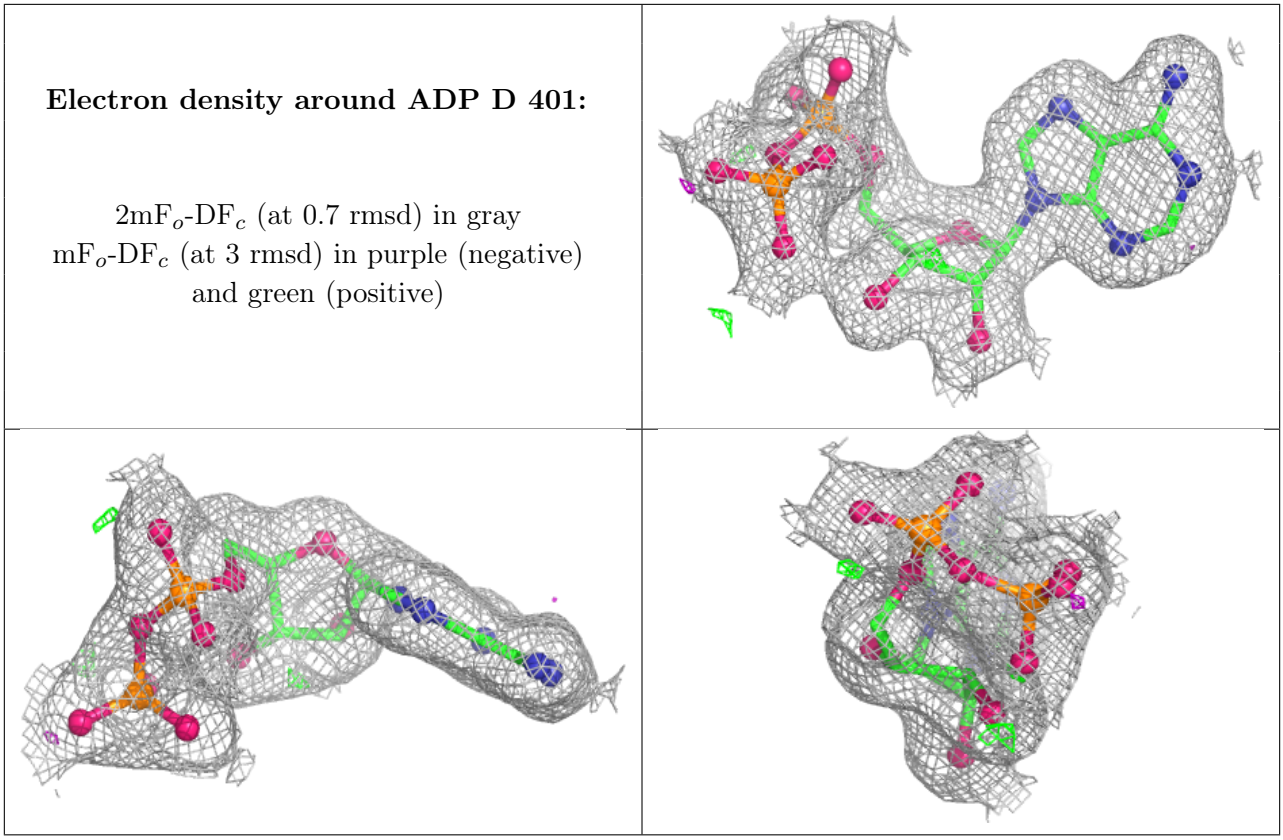
Electron density around ADP C 401:

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



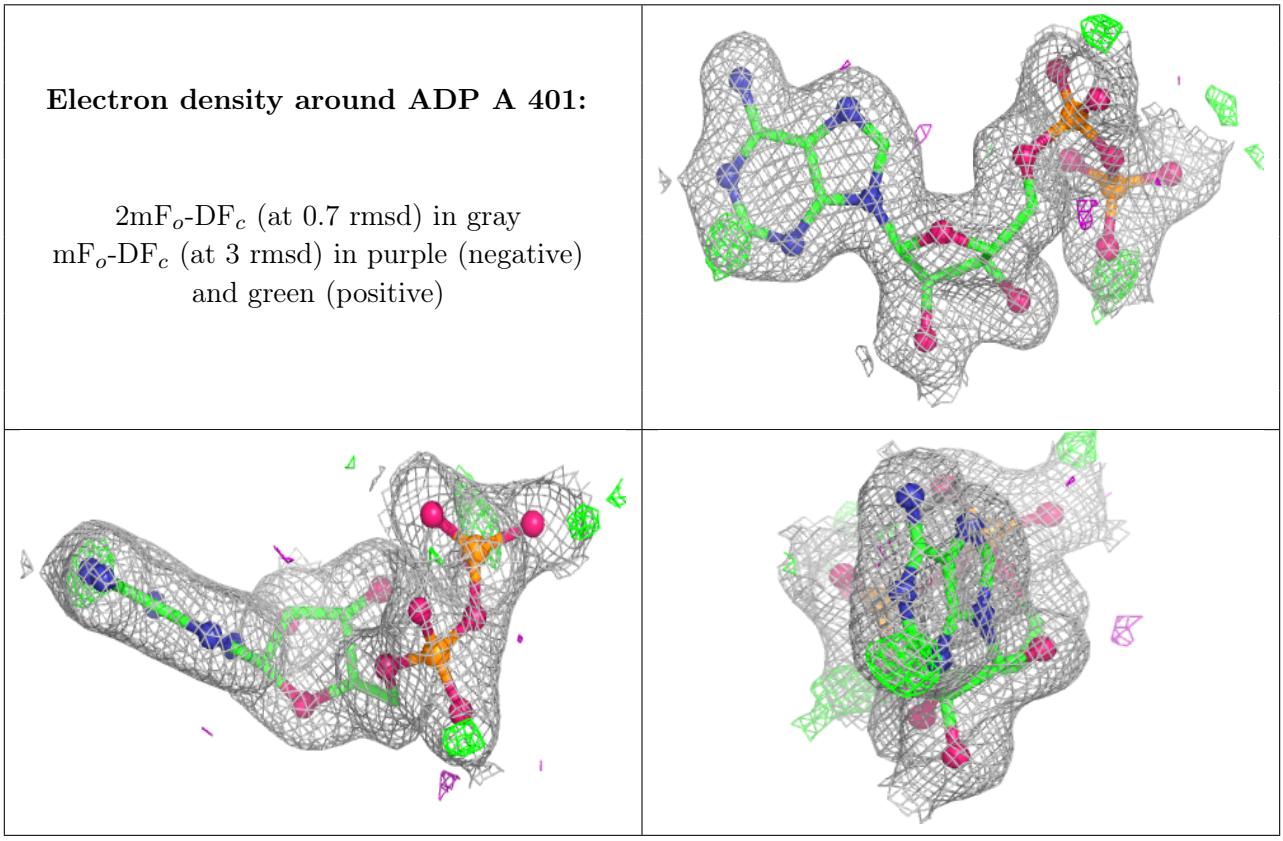
Electron density around ADP D 401:

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



Electron density around ADP 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)



6.5 Other polymers (i)

There are no such residues in this entry.