wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2022 – 03:16 pm GMT

PDB ID	:	7YZR
Title	:	50 mM Rb+ soak of beryllium fluoride inhibited Na+,K+-ATPase, E2-BeFx (rigid body model)
Authors	:	Fruergaard, M.U.; Dach, I.; Andersen, J.L.; Ozol, M.; Shasavar, A.; Quistgaard, E.M.; Poulsen, H.; Fedosova, N.U.; Nissen, P.
Deposited on	:	2022-02-21
Resolution	:	6.92 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

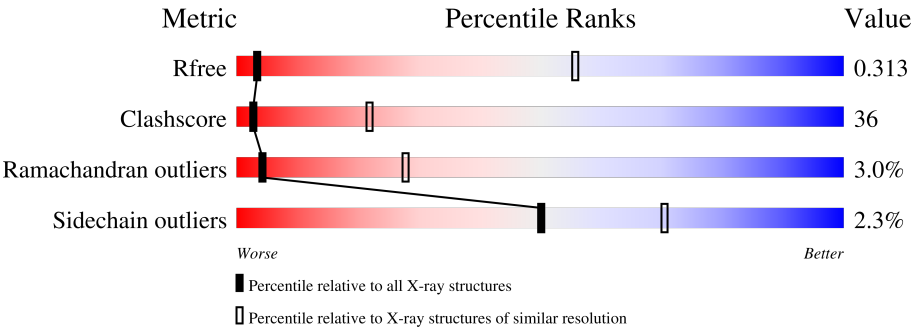
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 6.92 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1003 (9.70-3.90)
Clashscore	141614	1067 (9.70-3.90)
Ramachandran outliers	138981	1001 (9.70-3.90)
Sidechain outliers	138945	1001 (9.70-3.86)

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%

Mol	Chain	Length	Quality of chain
1	A	1020	52% 43%
1	C	1020	45% 49%
2	B	302	46% 44% 5%
2	D	302	53% 39% 5%
3	E	64	27% 23% 50%
3	G	64	28% 22% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BEF	A	1102	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 41373 atoms, of which 20703 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	996	Total	C	H	N	O	S	0	0	0
			15503	4922	7777	1301	1456	47			
1	C	996	Total	C	H	N	O	S	0	0	0
			15499	4922	7773	1301	1456	47			

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	287	Total	C	H	N	O	S	0	0	0
			4666	1519	2317	384	433	13			
2	D	287	Total	C	H	N	O	S	0	0	0
			4667	1519	2318	384	433	13			

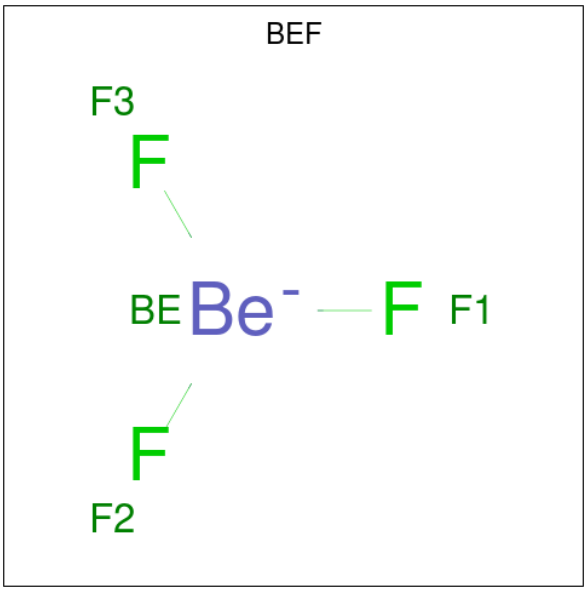
- Molecule 3 is a protein called FXYD domain-containing ion transport regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	32	Total	C	H	N	O	0	0	0
			514	174	259	37	44			
3	E	32	Total	C	H	N	O	0	0	0
			514	174	259	37	44			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



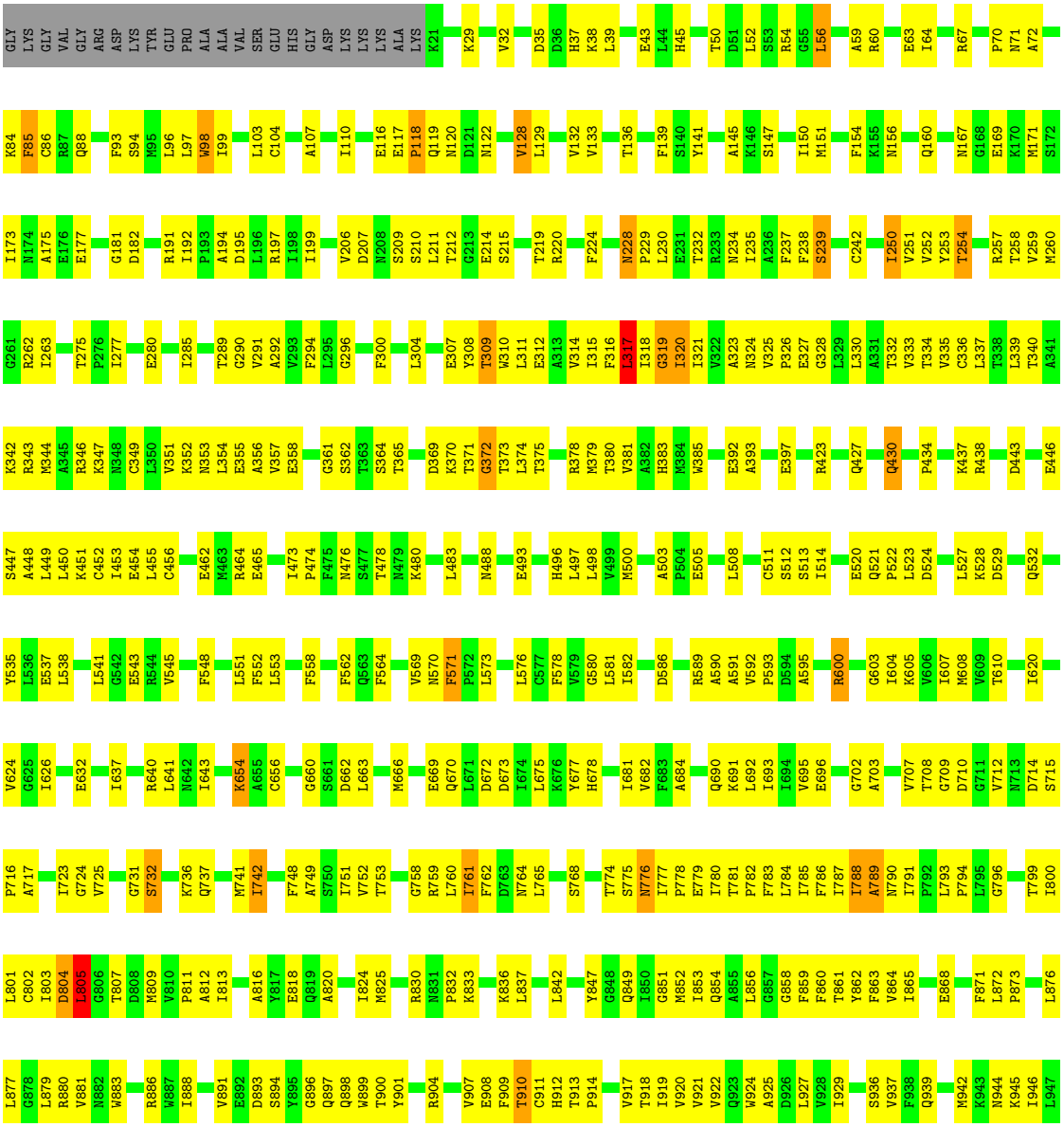
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Be F 4 1 3	0	0
5	C	1	Total Be F 4 1 3	0	0

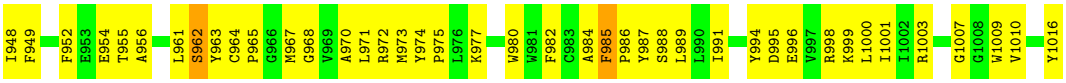
3 Residue-property plots (i)

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. 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. 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: Sodium/potassium-transporting ATPase subunit alpha-1

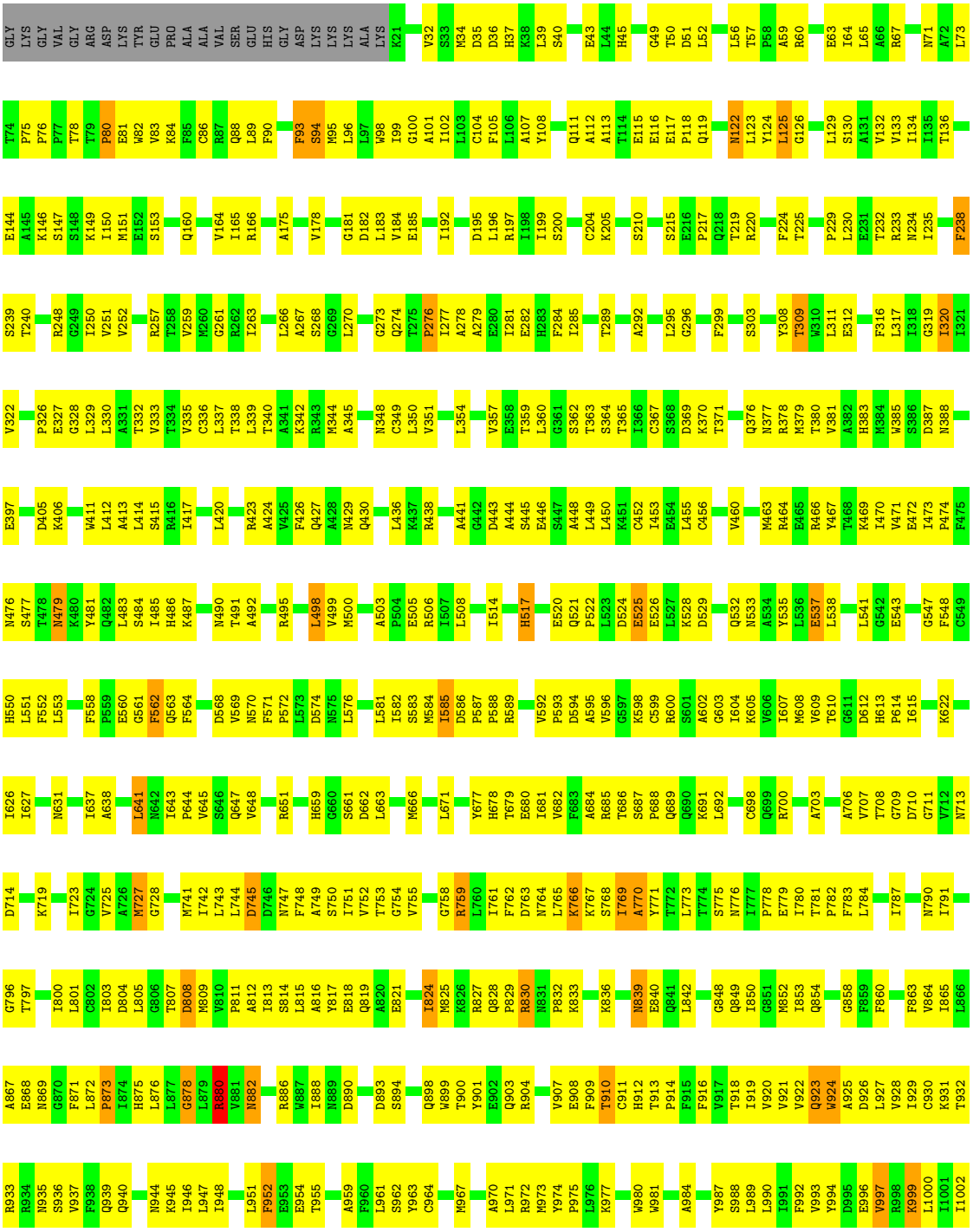
Chain A:

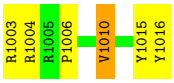




• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

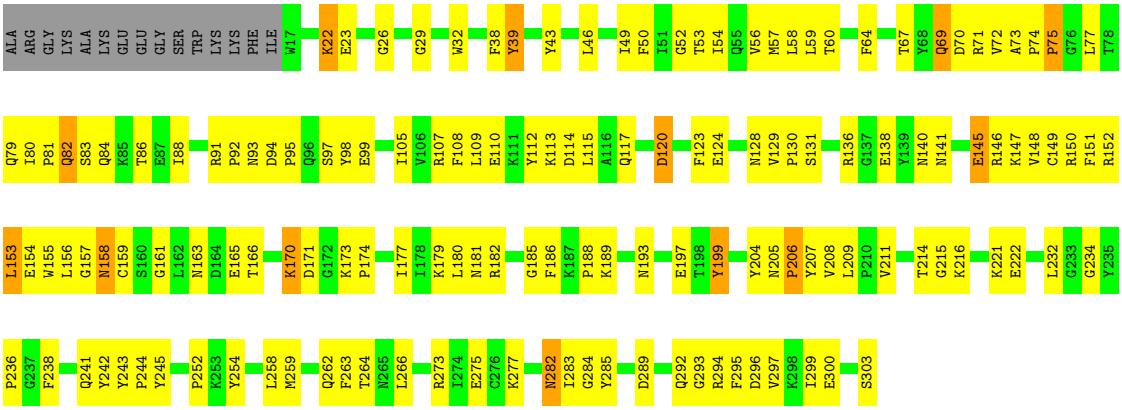
Chain C:





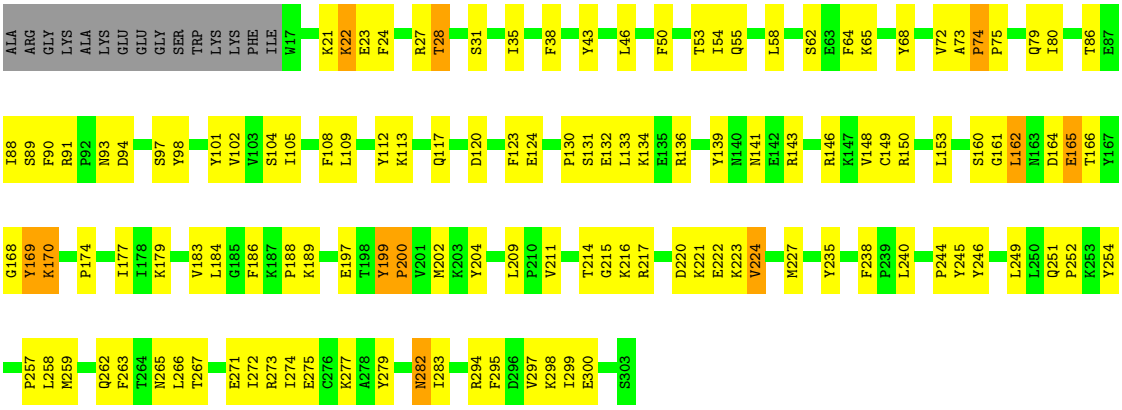
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain B:



• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain D:

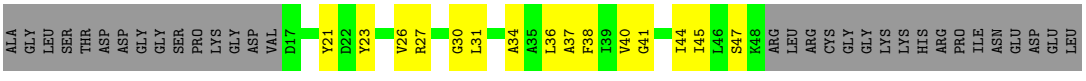


• Molecule 3: FXYD domain-containing ion transport regulator

Chain G:

• Molecule 3: FXYD domain-containing ion transport regulator

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.94Å 118.92Å 496.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.99 – 6.92 49.96 – 6.92	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.99-6.92) 99.9 (49.96-6.92)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 6.68Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.289 , 0.309 0.308 , 0.313	Depositor DCC
R_{free} test set	1180 reflections (9.74%)	wwPDB-VP
Wilson B-factor (Å^2)	283.1	Xtriage
Anisotropy	1.153	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.030 for k,h,-l	Xtriage
F_o,F_c correlation	0.30	EDS
Total number of atoms	41373	wwPDB-VP
Average B, all atoms (Å^2)	407.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF

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	0.72	2/7876 (0.0%)	0.81	6/10688 (0.1%)
1	C	0.77	4/7876 (0.1%)	0.84	13/10688 (0.1%)
2	B	0.84	3/2411 (0.1%)	0.84	1/3252 (0.0%)
2	D	0.76	0/2411	0.81	2/3252 (0.1%)
3	E	0.93	0/261	0.81	0/354
3	G	0.86	0/261	0.74	0/354
All	All	0.76	9/21096 (0.0%)	0.83	22/28588 (0.1%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	312	GLU	CB-CG	-6.22	1.40	1.52
1	C	282	GLU	CB-CG	5.60	1.62	1.52
1	A	86	CYS	CB-SG	5.30	1.91	1.82
2	B	138	GLU	CG-CD	5.29	1.59	1.51
2	B	138	GLU	CB-CG	5.26	1.62	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	317	LEU	CA-CB-CG	7.75	133.12	115.30
1	C	880	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	A	805	LEU	CA-CB-CG	6.74	130.79	115.30
1	A	804	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	802	CYS	CA-CB-SG	-6.20	102.85	114.00

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	7726	7777	7778	566	0
1	C	7726	7773	7777	620	3
2	B	2349	2317	2318	180	3
2	D	2349	2318	2318	160	0
3	E	255	259	259	37	0
3	G	255	259	259	31	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	4	0	0	3	0
5	C	4	0	0	1	0
All	All	20670	20703	20709	1471	3

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 36.

The worst 5 of 1471 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:PHE:CE2	1:A:830:ARG:CD	2.05	1.37
1:C:963:TYR:CE1	3:E:26:VAL:HG12	1.68	1.28
1:C:108:TYR:CD2	1:C:123:LEU:HG	1.75	1.22
1:A:732:SER:O	1:A:736:LYS:HD3	1.40	1.20
1:A:762:PHE:CD2	1:A:830:ARG:NE	2.12	1.17

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ASN:ND2	1:C:647:GLN:OE1[3_554]	1.95	0.25
2:B:163:ASN:OD1	1:C:63:GLU:OE2[1_565]	1.96	0.24
2:B:163:ASN:HD21	1:C:647:GLN:OE1[3_554]	1.56	0.04

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	994/1020 (98%)	865 (87%)	106 (11%)	23 (2%)	6 34
1	C	994/1020 (98%)	837 (84%)	123 (12%)	34 (3%)	3 26
2	B	285/302 (94%)	230 (81%)	44 (15%)	11 (4%)	3 23
2	D	285/302 (94%)	239 (84%)	36 (13%)	10 (4%)	3 25
3	E	30/64 (47%)	26 (87%)	4 (13%)	0	100 100
3	G	30/64 (47%)	23 (77%)	7 (23%)	0	100 100
All	All	2618/2772 (94%)	2220 (85%)	320 (12%)	78 (3%)	4 28

5 of 78 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	277	ILE
2	B	158	ASN
1	C	32	VAL
1	C	113	ALA

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	847/864 (98%)	828 (98%)	19 (2%)	52 71
1	C	847/864 (98%)	825 (97%)	22 (3%)	46 66
2	B	257/268 (96%)	251 (98%)	6 (2%)	50 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	257/268 (96%)	252 (98%)	5 (2%)	57 75
3	E	26/51 (51%)	26 (100%)	0	100 100
3	G	26/51 (51%)	26 (100%)	0	100 100
All	All	2260/2366 (96%)	2208 (98%)	52 (2%)	50 70

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	238	PHE
1	C	727	MET
2	D	164	ASP
1	C	257	ARG
1	C	537	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	234	ASN
1	C	849	GLN
1	C	882	ASN
1	A	898	GLN
1	A	234	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	BEF	C	1102	1	0,3,3	-	-	-		
5	BEF	A	1102	-	0,3,3	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

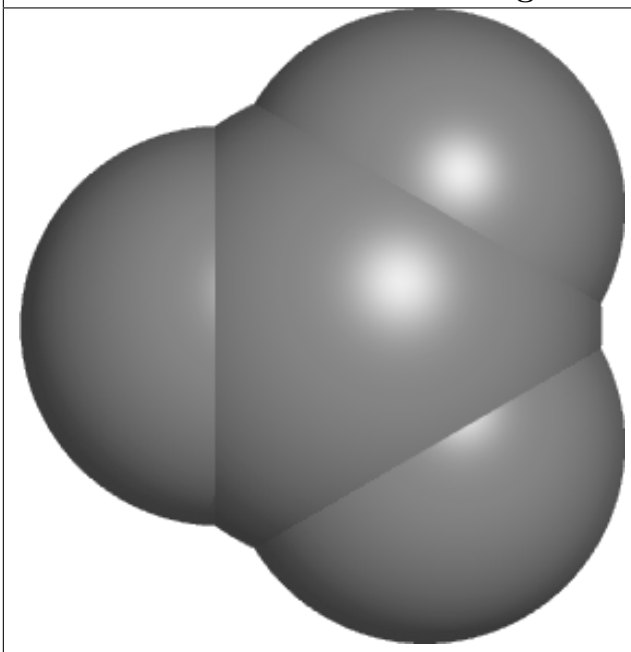
There are no ring outliers.

2 monomers are involved in 4 short contacts:

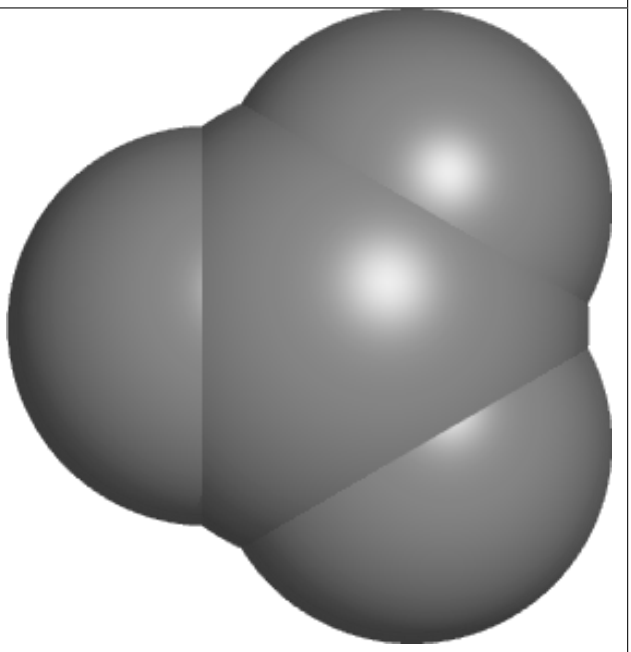
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1102	BEF	1	0
5	A	1102	BEF	3	0

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 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.

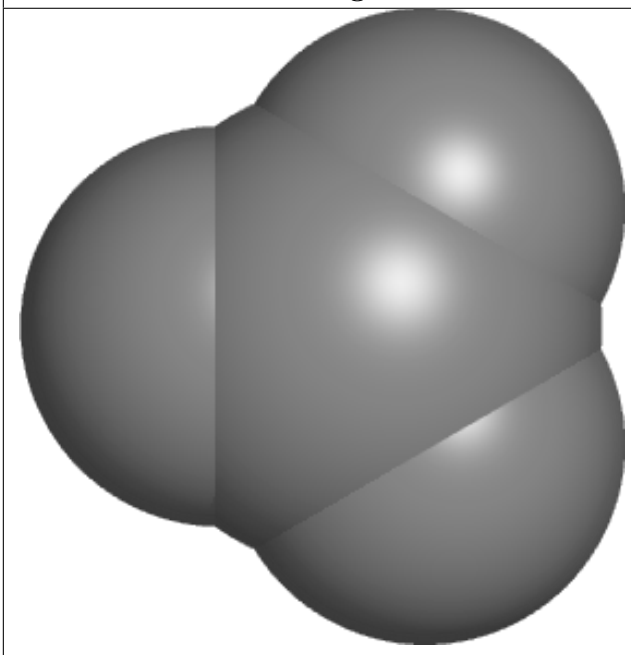
Ligand BEF C 1102



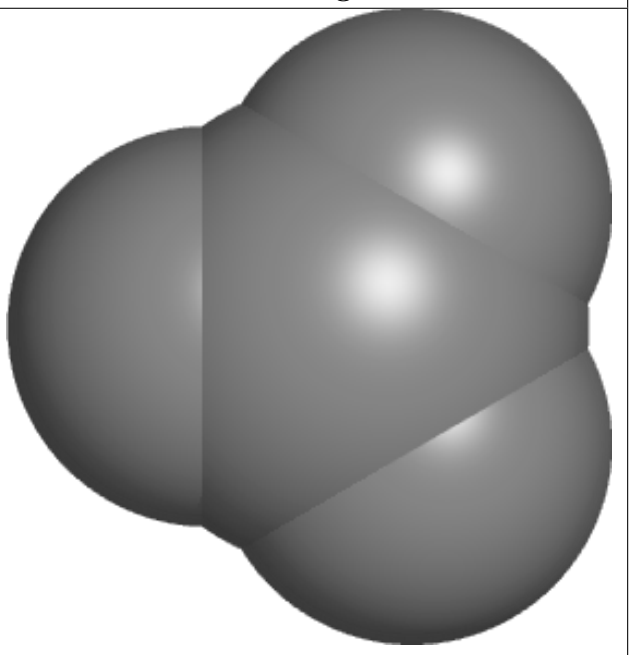
Bond lengths



Bond angles

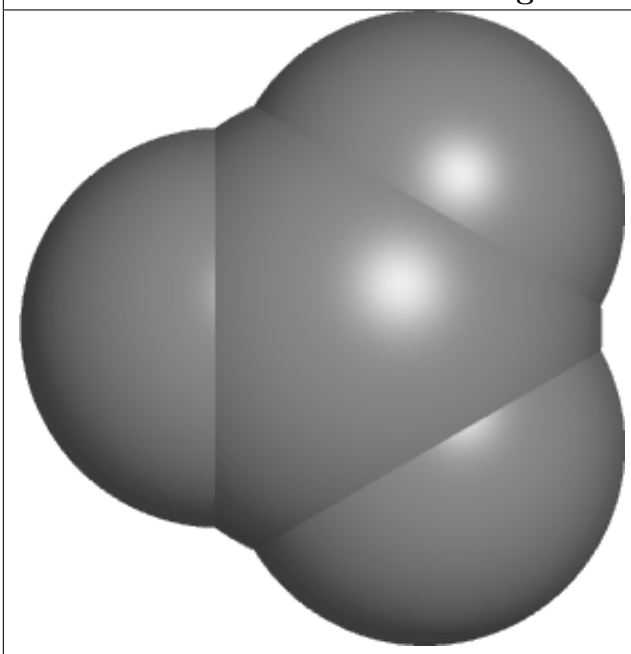


Torsions

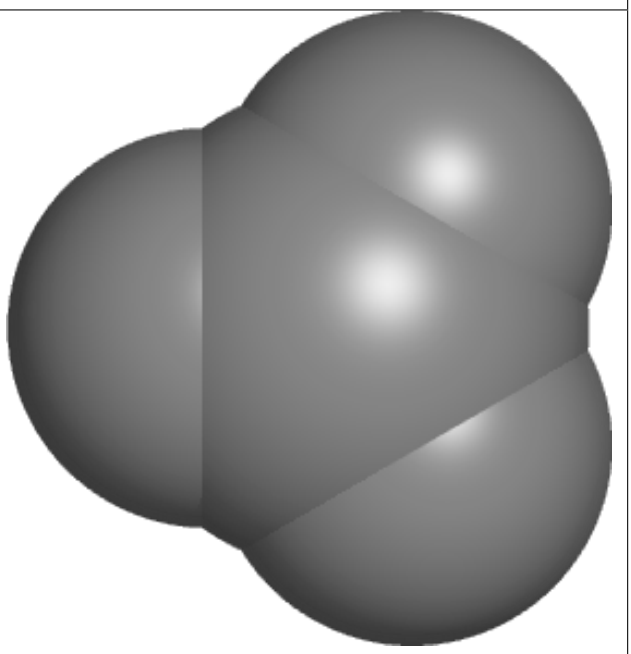


Rings

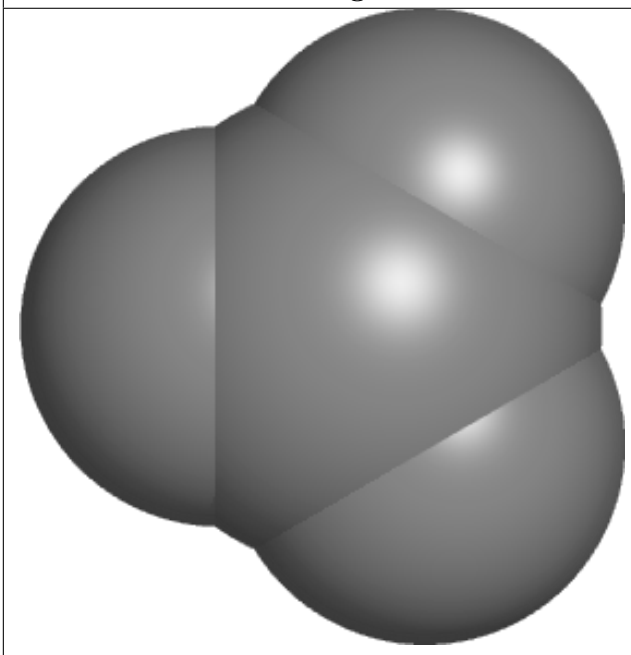
Ligand BEF A 1102



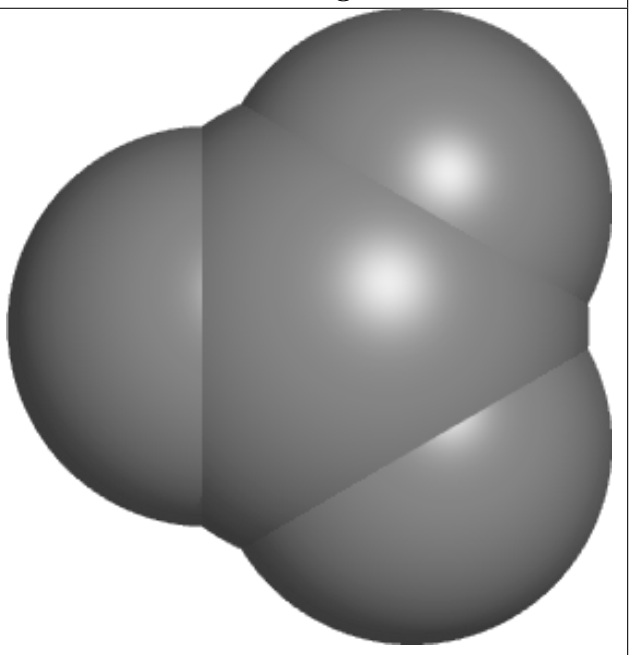
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

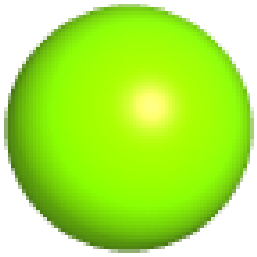
6.4 Ligands

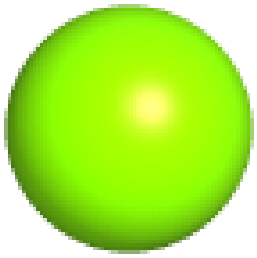
Unable to reproduce the depositors R factor - this section is therefore empty.

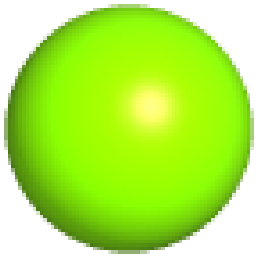
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MG A 1101:

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

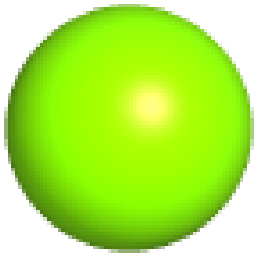


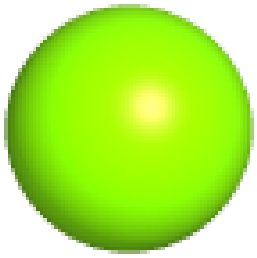


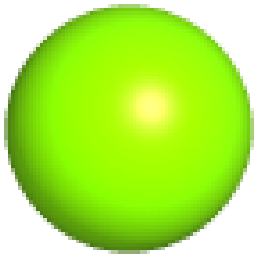


Electron density around MG C 1101:

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

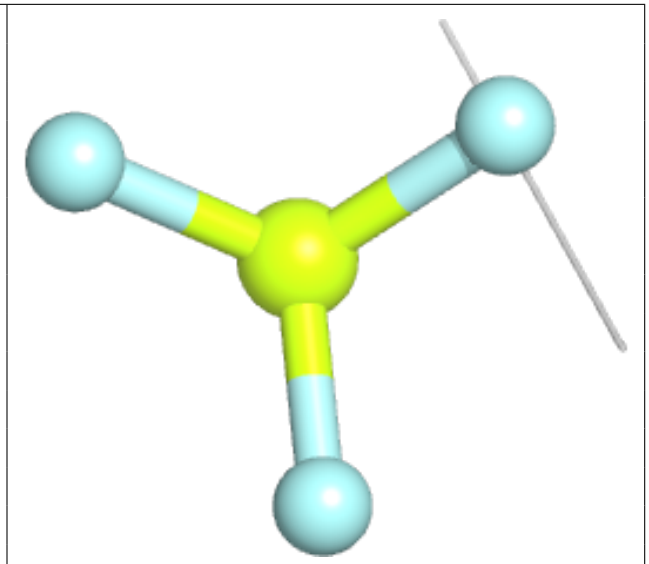


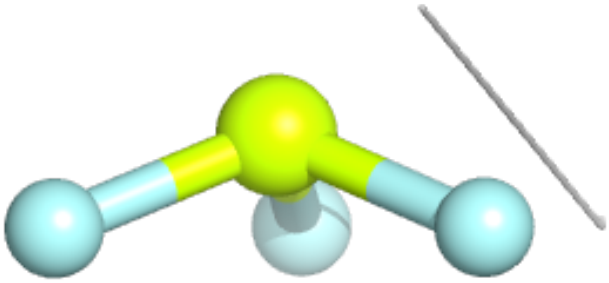


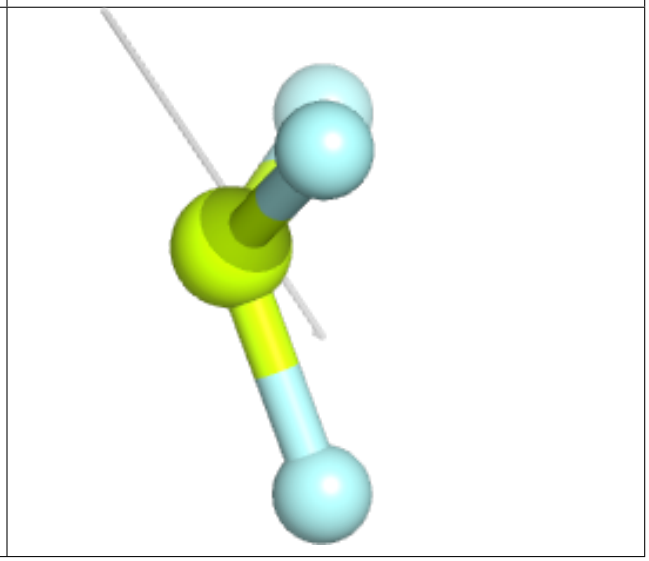


Electron density around BEF A 1102:

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

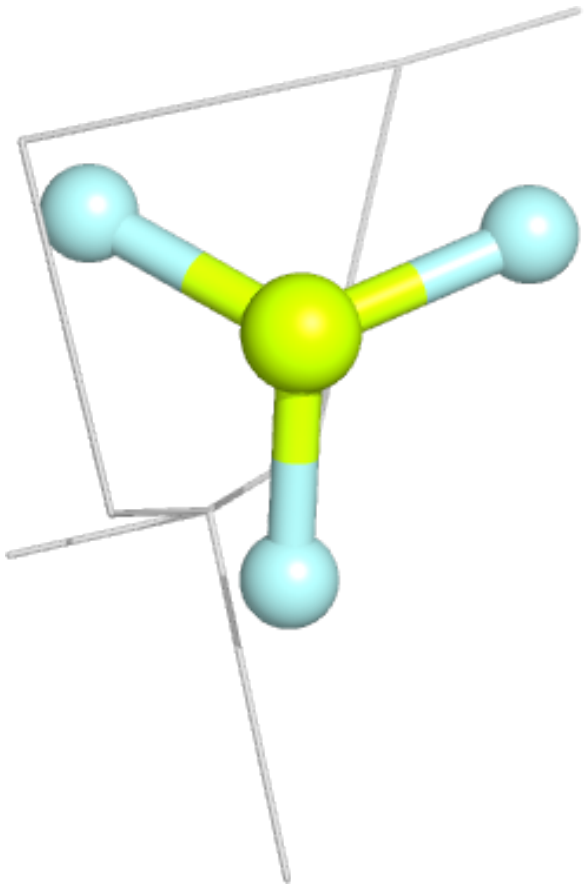


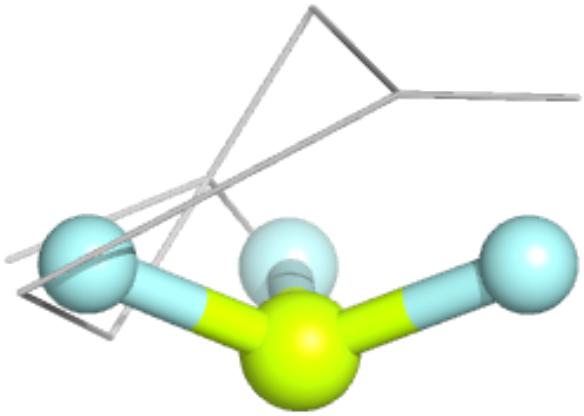


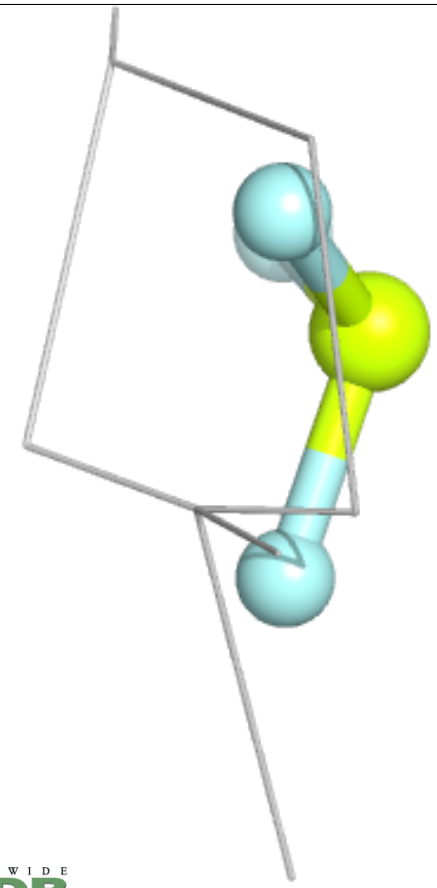


Electron density around BEF C 1102:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.