



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 10:16 AM EDT

PDB ID : 7YZR / pdb_00007yzr
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 ⓘ 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

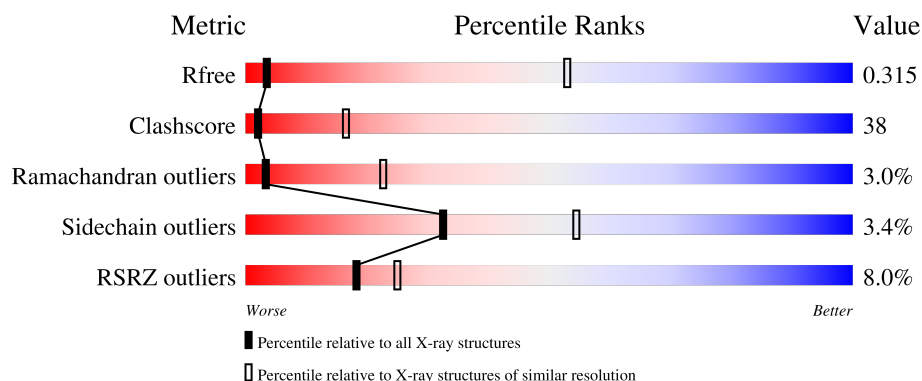
1 Overall quality at a glance

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}	180053	1166 (9.70-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1053 (9.70-4.00)
Sidechain outliers	187428	1016 (9.70-4.00)
RSRZ outliers	180081	1159 (9.70-4.00)

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	1020	
1	C	1020	
2	B	302	
2	D	302	

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Mol	Chain	Length	Quality of chain
3	E	64	
3	G	64	

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

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			

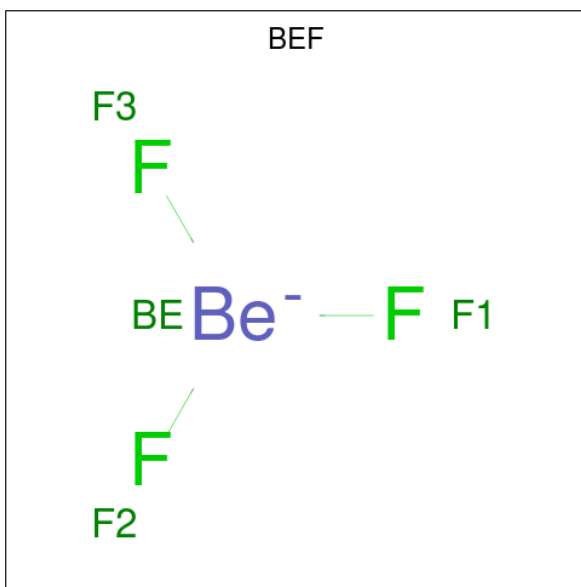
- Molecule 3 is a protein called FXYD domain-containing ion transport regulator.

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 (CCD ID: 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		

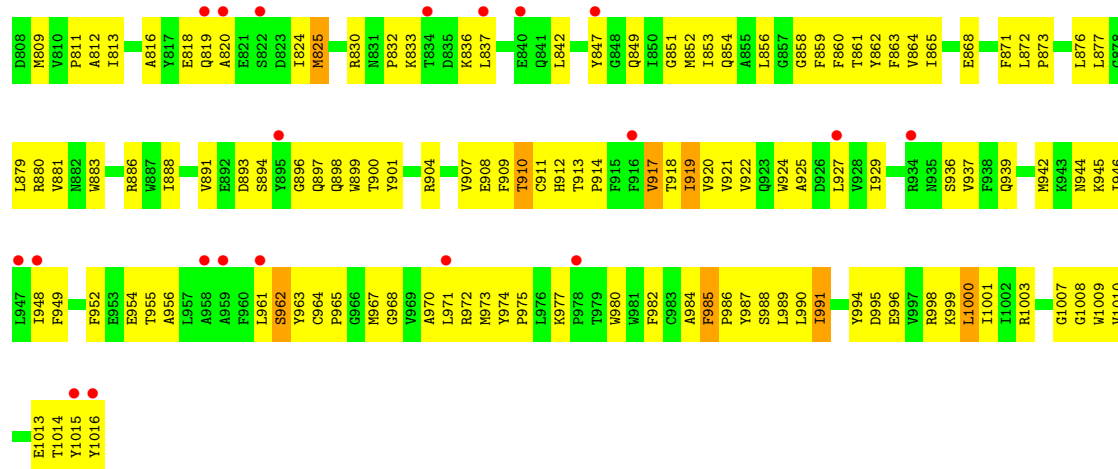
- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



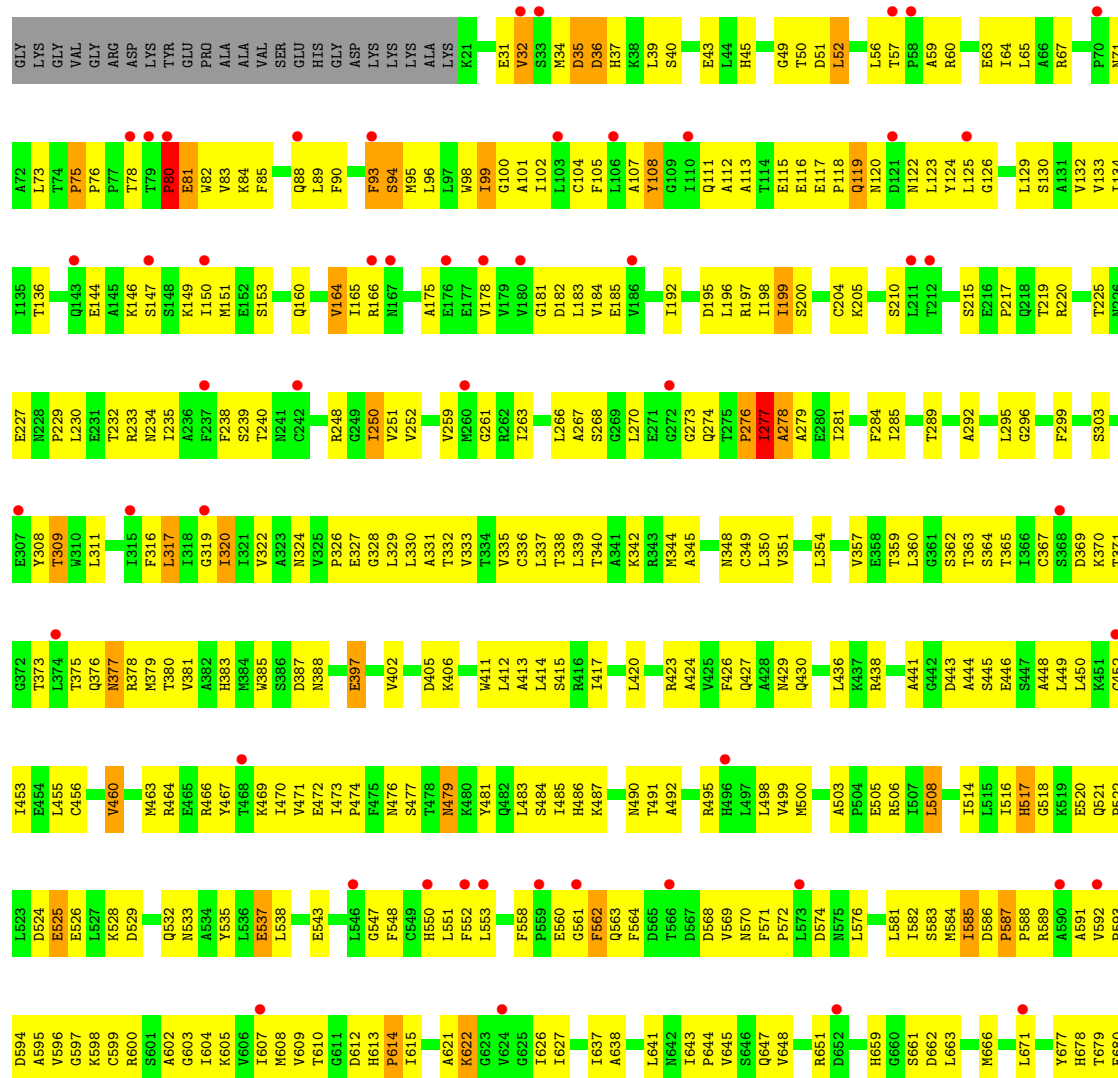
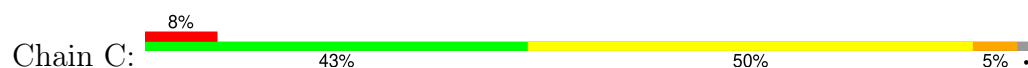
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Be	F	0	0
			4	1	3		
5	C	1	Total	Be	F	0	0
			4	1	3		

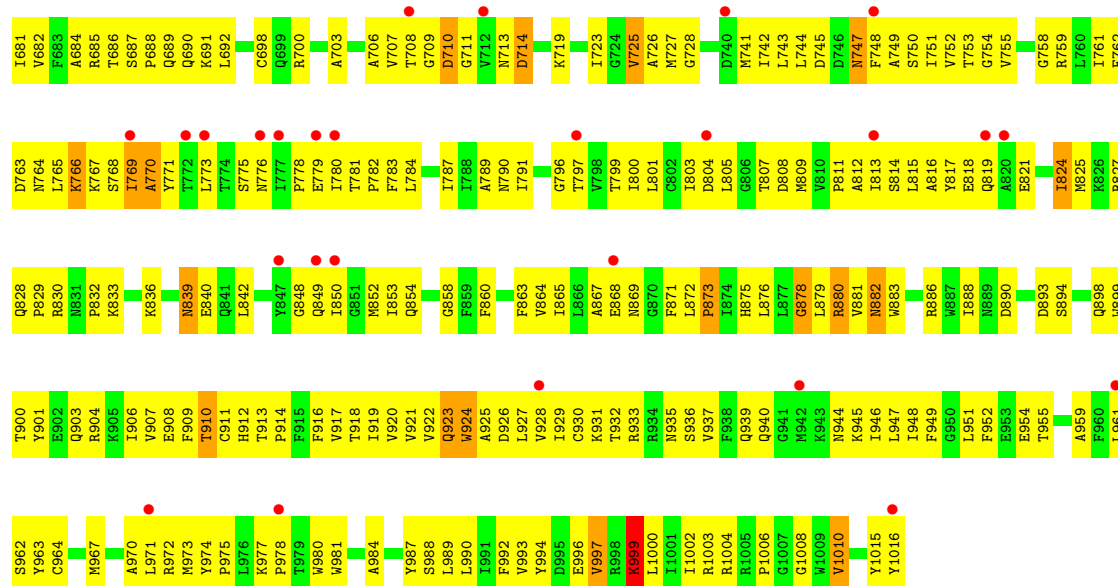
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1



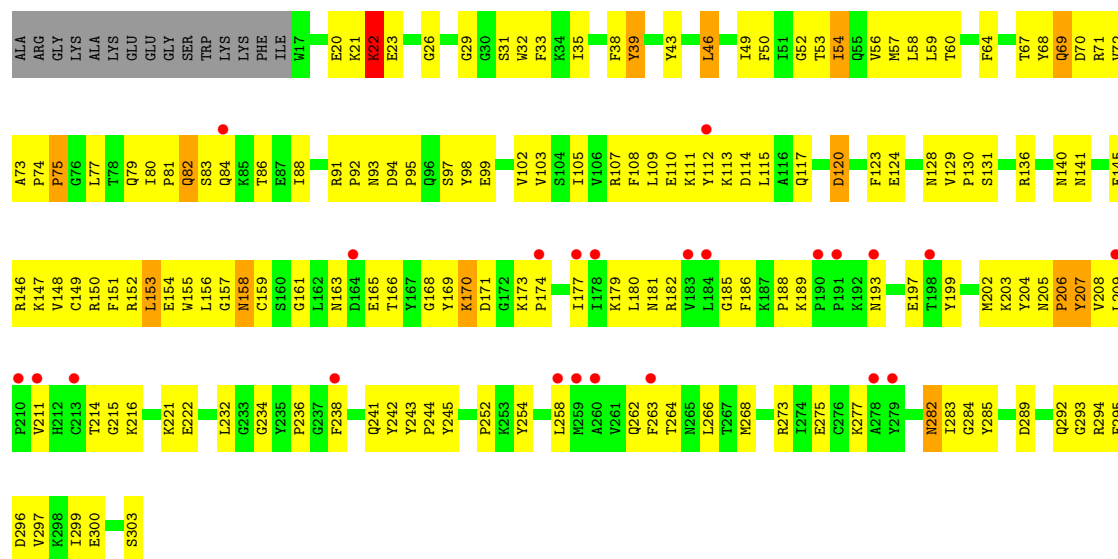
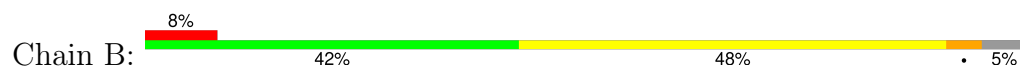


• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

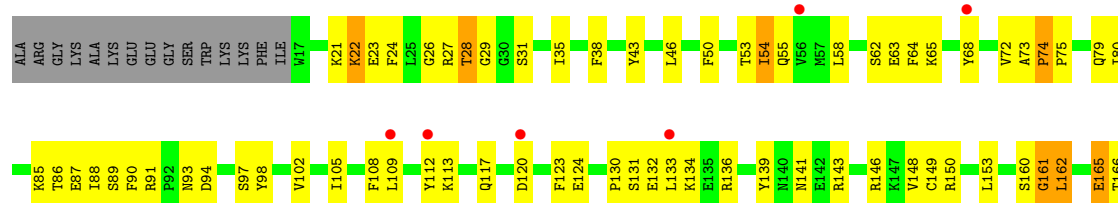


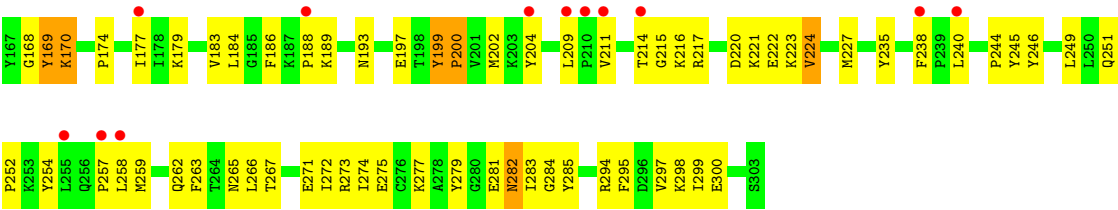


• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



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

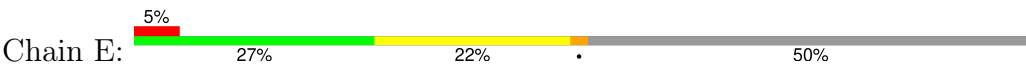




● Molecule 3: FXYP domain-containing ion transport regulator



● Molecule 3: FXYP domain-containing ion transport regulator



4 Data and refinement statistics

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 24.99 – 6.92	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.99-6.92) 97.4 (24.99-6.92)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 6.68Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.289 , 0.309 0.316 , 0.315	Depositor DCC
R_{free} test set	1180 reflections (9.68%)	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)	0.20 , 244.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.030 for k,h,-l	Xtriage
F_o, F_c correlation	0.83	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.75	2/7876 (0.0%)	0.91	16/10688 (0.1%)
1	C	0.83	4/7876 (0.1%)	0.95	30/10688 (0.3%)
2	B	0.83	1/2411 (0.0%)	0.94	8/3252 (0.2%)
2	D	0.75	2/2411 (0.1%)	0.95	7/3252 (0.2%)
3	E	0.86	0/261	0.90	0/354
3	G	0.76	0/261	0.78	0/354
All	All	0.79	9/21096 (0.0%)	0.93	61/28588 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	PRO	CA-C	-14.79	1.43	1.51
2	B	207	TYR	C-N	-10.07	1.27	1.33
1	C	279	ALA	CA-C	-8.82	1.40	1.52
1	C	35	ASP	CA-C	7.47	1.62	1.52
1	A	756	GLU	CA-C	-6.45	1.44	1.52

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	PRO	O-C-N	-11.28	116.12	121.31
1	C	94	SER	N-CA-C	9.48	123.94	112.38
1	A	1008	GLY	N-CA-C	9.10	124.15	112.68
2	B	33	PHE	N-CA-C	8.68	122.85	111.75
1	C	324	ASN	N-CA-C	8.64	120.69	111.28

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	7726	7777	7778	603	0
1	C	7726	7773	7777	665	3
2	B	2349	2317	2318	190	3
2	D	2349	2318	2318	166	0
3	E	255	259	259	37	0
3	G	255	259	259	32	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	4	0	0	4	0
5	C	4	0	0	1	0
All	All	20670	20703	20709	1566	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 38.

The worst 5 of 1566 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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	994/1020 (98%)	865 (87%)	106 (11%)	23 (2%)	5	28
1	C	994/1020 (98%)	837 (84%)	123 (12%)	34 (3%)	3	21
2	B	285/302 (94%)	230 (81%)	44 (15%)	11 (4%)	2	19
2	D	285/302 (94%)	239 (84%)	36 (13%)	10 (4%)	3	20
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%)	3	23

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

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%)	816 (96%)	31 (4%)	30	51
1	C	847/864 (98%)	818 (97%)	29 (3%)	32	54
2	B	257/268 (96%)	246 (96%)	11 (4%)	26	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	257/268 (96%)	253 (98%)	4 (2%)	55	70
3	E	26/51 (51%)	25 (96%)	1 (4%)	29	50
3	G	26/51 (51%)	25 (96%)	1 (4%)	29	50
All	All	2260/2366 (96%)	2183 (97%)	77 (3%)	32	54

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	537	GLU
1	C	1010	VAL
1	C	725	VAL
1	C	890	ASP
2	D	282	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	944	ASN
2	D	84	GLN
1	C	71	ASN
1	C	156	ASN
1	C	234	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	A	1102	-	0,3,3	-	-	-		
5	BEF	C	1102	1	0,3,3	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

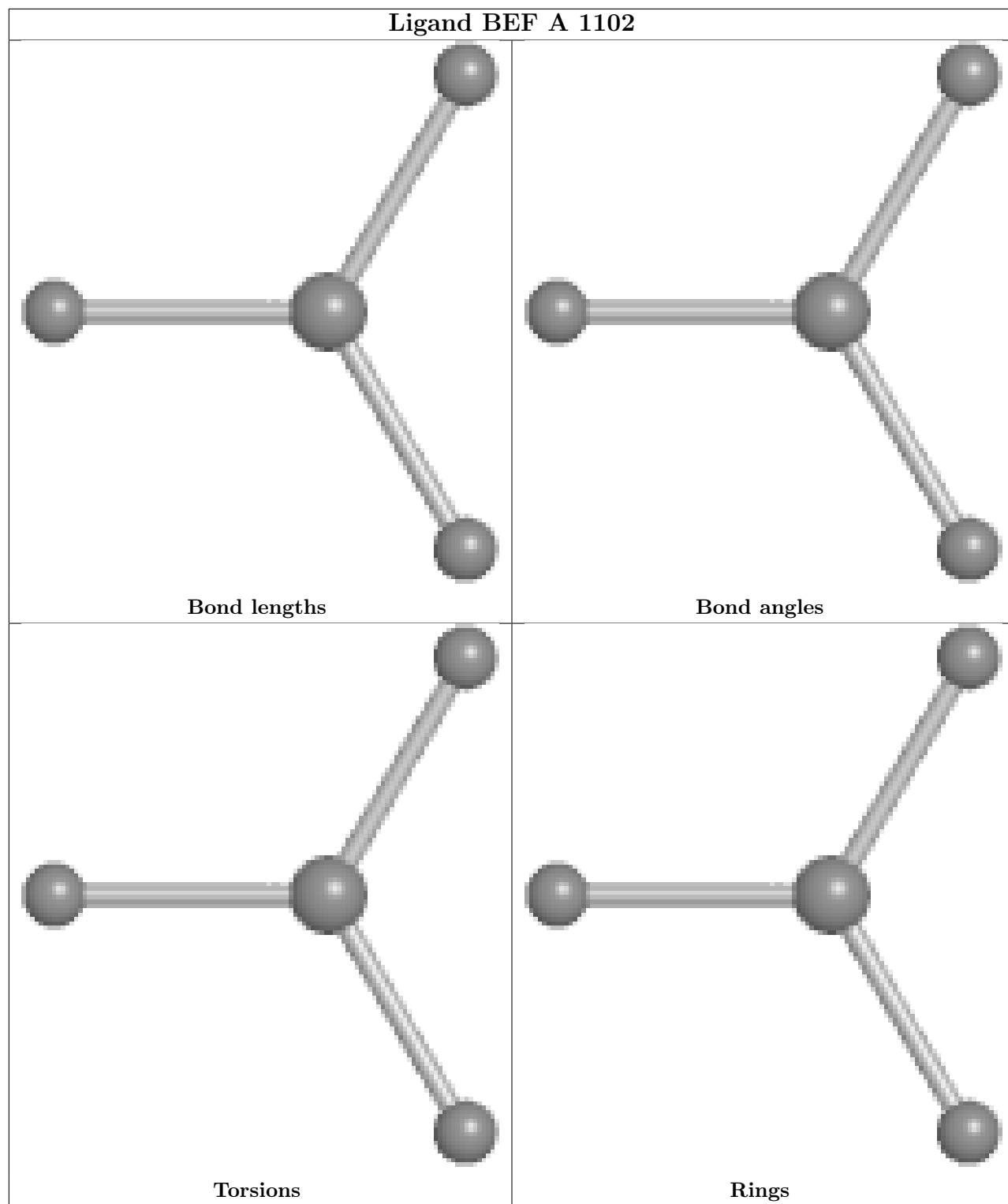
There are no torsion outliers.

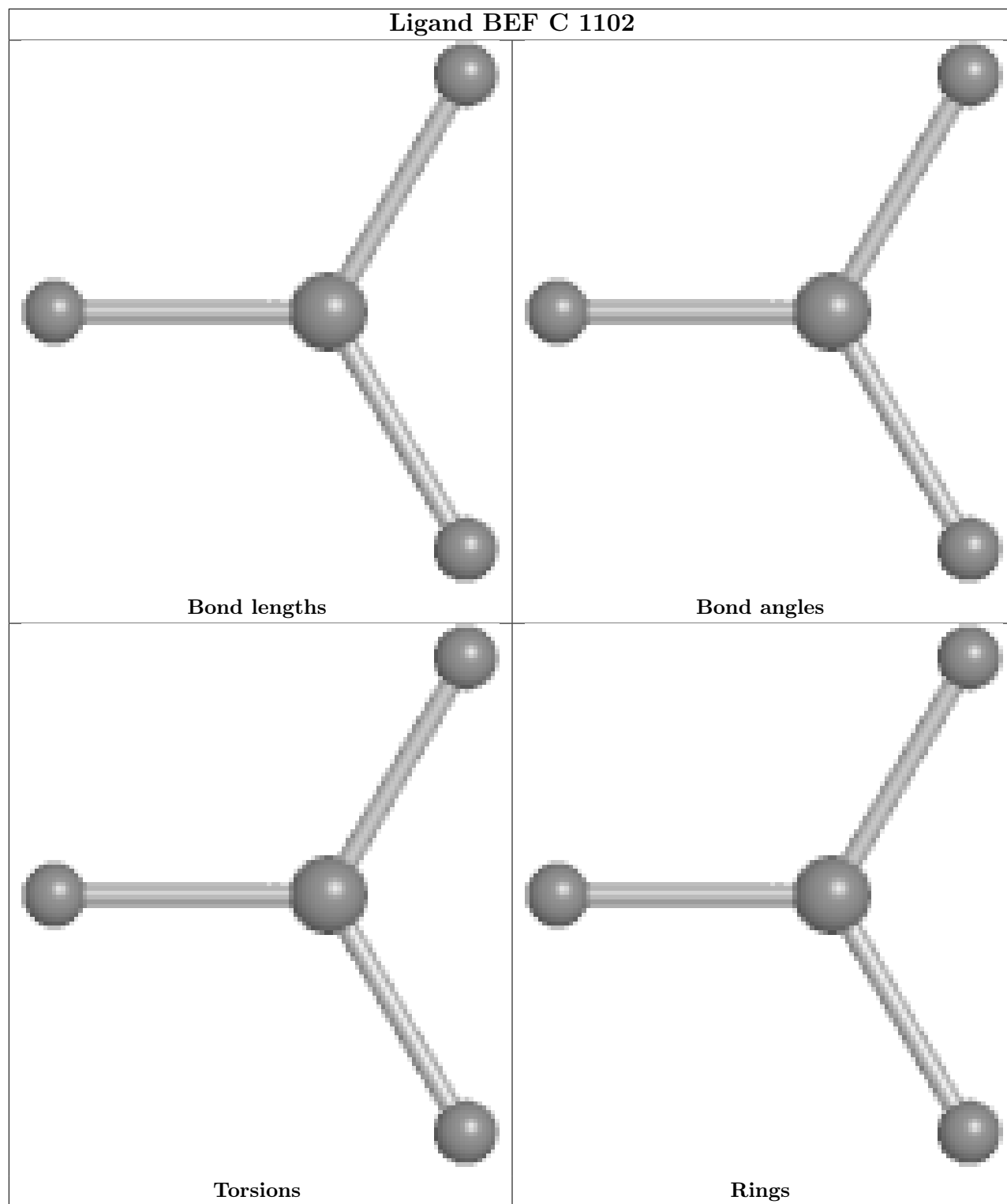
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1102	BEF	4	0
5	C	1102	BEF	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	996/1020 (97%)	0.43	86 (8%)	16 23	311, 372, 503, 566	0
1	C	996/1020 (97%)	0.39	78 (7%)	19 25	320, 402, 569, 691	0
2	B	287/302 (95%)	0.47	23 (8%)	18 25	334, 431, 524, 604	0
2	D	287/302 (95%)	0.34	18 (6%)	26 31	328, 416, 518, 620	0
3	E	32/64 (50%)	0.35	3 (9%)	14 21	326, 357, 412, 457	0
3	G	32/64 (50%)	0.20	3 (9%)	14 21	324, 350, 442, 451	0
All	All	2630/2772 (94%)	0.40	211 (8%)	18 25	311, 396, 530, 691	0

The worst 5 of 211 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	258	LEU	12.4
2	B	259	MET	10.3
1	C	773	LEU	7.5
2	D	210	PRO	6.3
1	C	740	ASP	6.0

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](#)

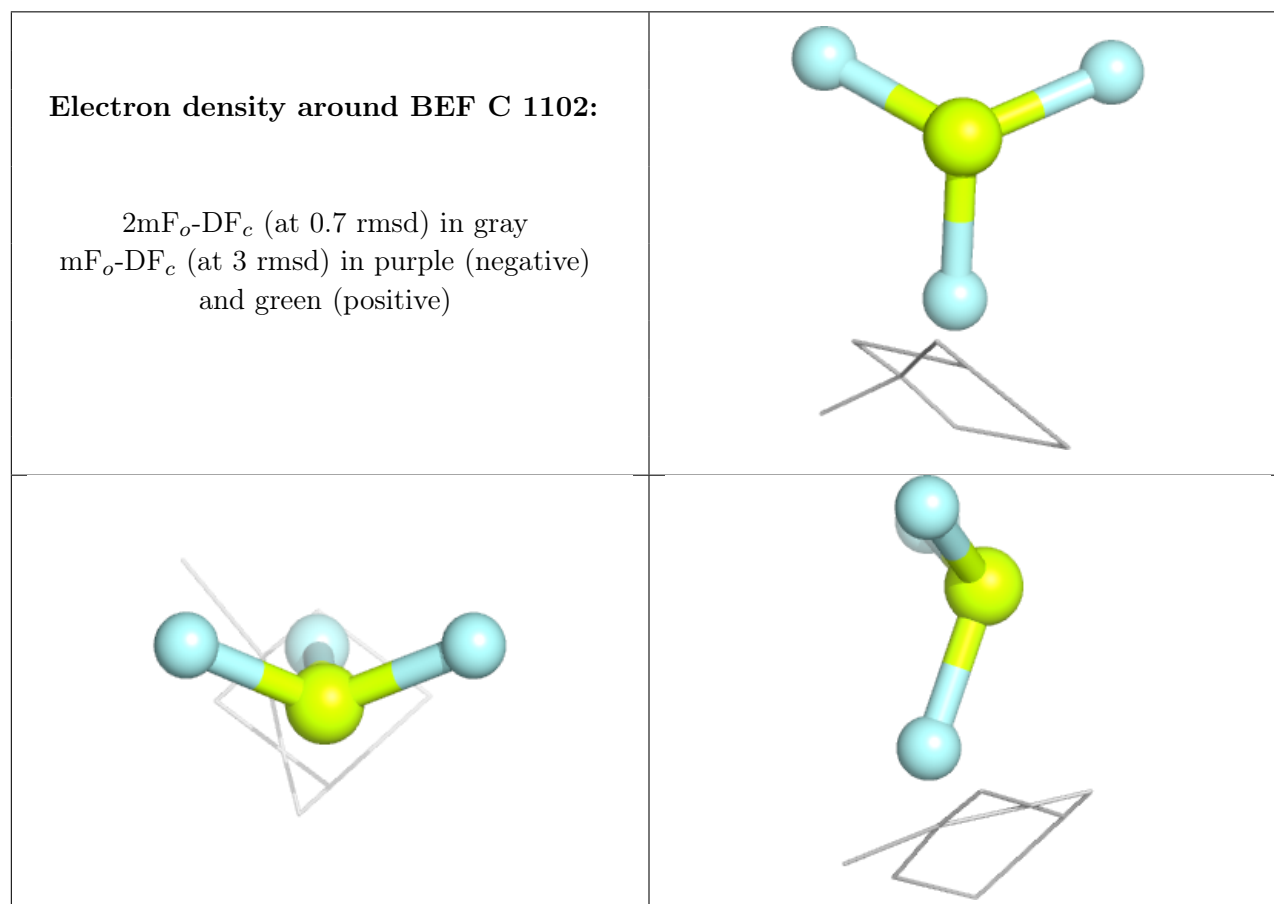
There are no oligosaccharides in this entry.

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.

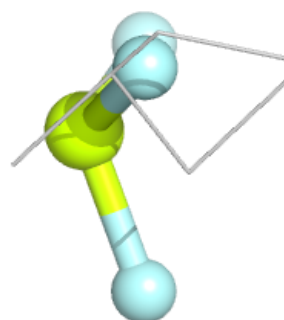
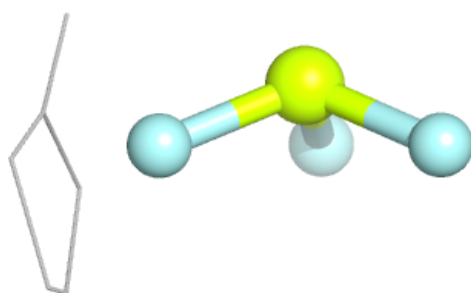
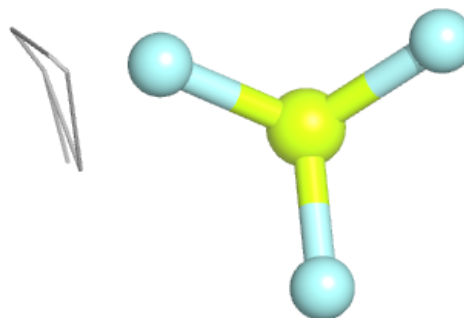
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BEF	C	1102	4/4	0.92	0.05	403,440,459,474	0
5	BEF	A	1102	4/4	0.93	0.09	461,463,467,478	0
4	MG	A	1101	1/1	0.94	0.11	393,393,393,393	0
4	MG	C	1101	1/1	0.97	0.03	357,357,357,357	0

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.

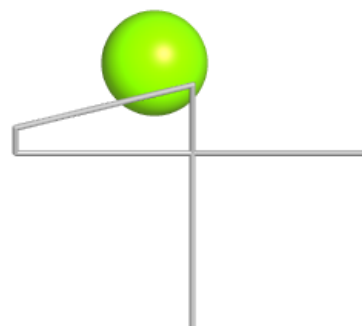
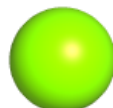
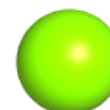


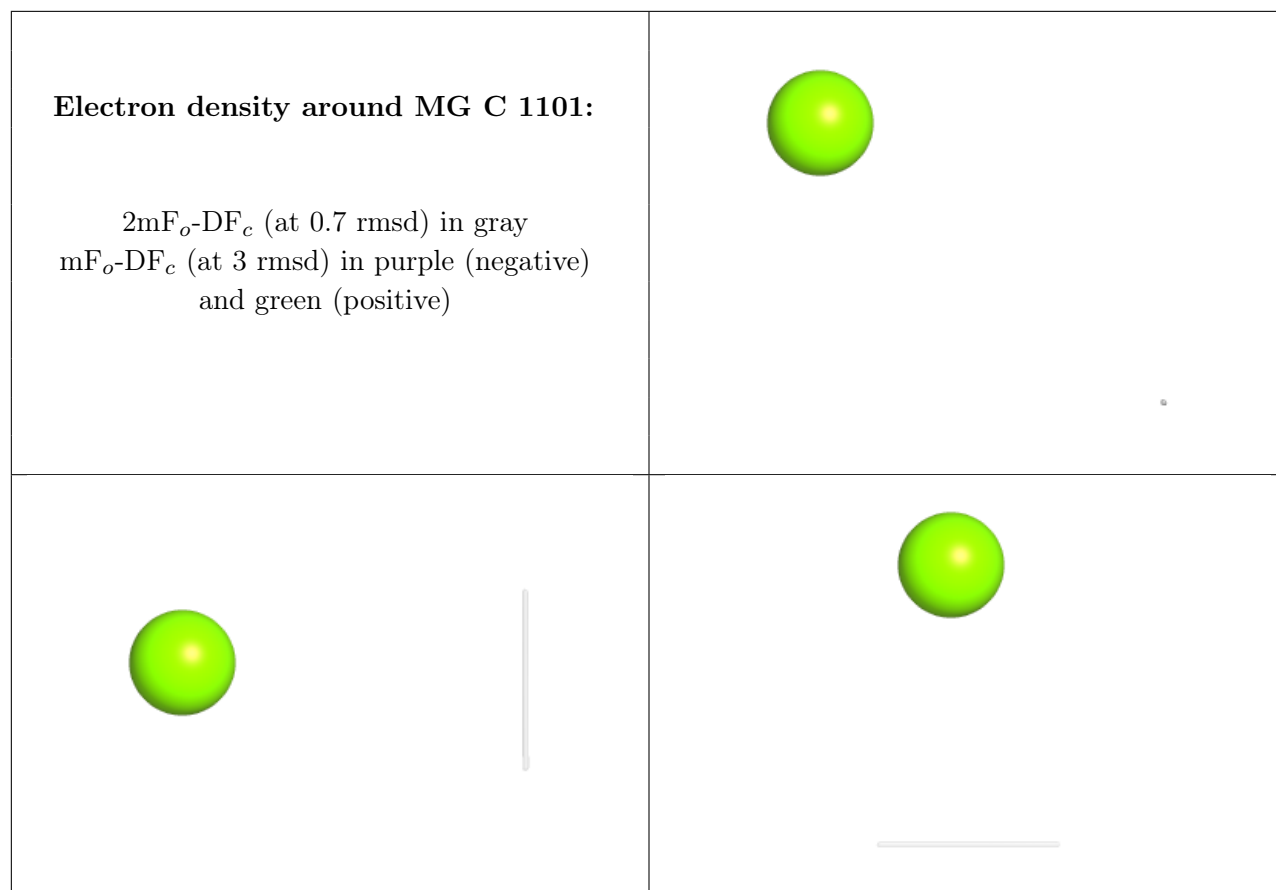
Electron density around BEF A 1102:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.