Full wwPDB X-ray Structure Validation Report ⓘ

Feb 23, 2022 – 12:14 pm GMT

PDB ID	:	7OHL
Title	:	SaFtsZ complexed with GDP, BeF3- and Mn2+
Authors	:	Fernandez-Tornero, C.; Ruiz, F.M.; Andreu, J.M.
Deposited on	:	2021-05-11
Resolution	:	1.75 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 following versions of software and data (see references ⓘ) were used in the production of this report:

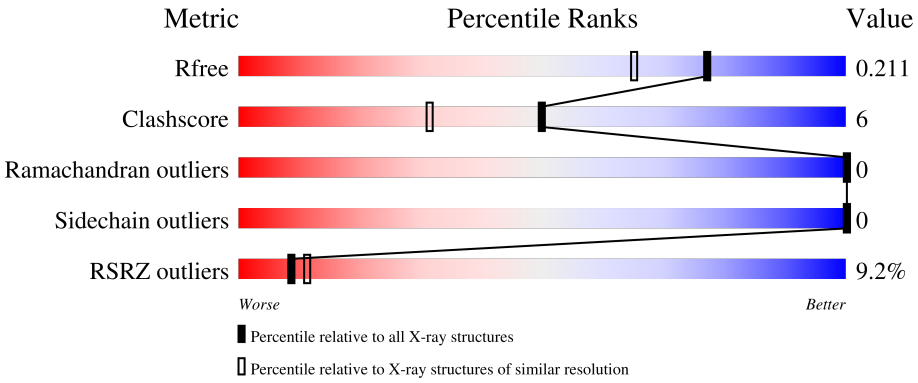
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	326	9% 79% 13% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4602 atoms, of which 2245 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.

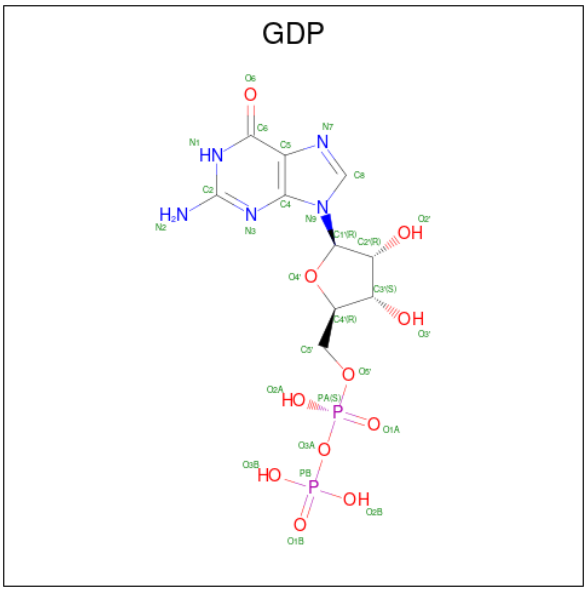
- Molecule 1 is a protein called Cell division protein FtsZ.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	305	4441	1366	2235	378	448	14	0	1	0

There are 21 discrepancies between the modelled and reference sequences:

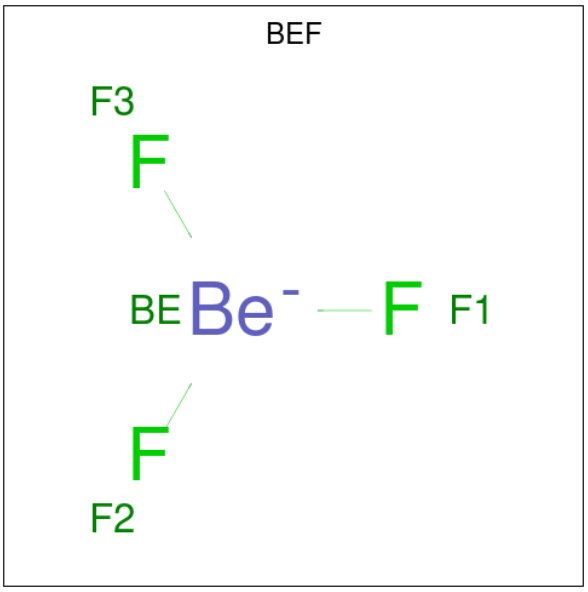
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP P0A031
A	-8	GLY	-	expression tag	UNP P0A031
A	-7	SER	-	expression tag	UNP P0A031
A	-6	SER	-	expression tag	UNP P0A031
A	-5	HIS	-	expression tag	UNP P0A031
A	-4	HIS	-	expression tag	UNP P0A031
A	-3	HIS	-	expression tag	UNP P0A031
A	-2	HIS	-	expression tag	UNP P0A031
A	-1	HIS	-	expression tag	UNP P0A031
A	0	HIS	-	expression tag	UNP P0A031
A	1	SER	-	expression tag	UNP P0A031
A	2	SER	-	expression tag	UNP P0A031
A	3	GLY	-	expression tag	UNP P0A031
A	4	LEU	-	expression tag	UNP P0A031
A	5	VAL	-	expression tag	UNP P0A031
A	6	PRO	-	expression tag	UNP P0A031
A	7	ARG	-	expression tag	UNP P0A031
A	8	GLY	-	expression tag	UNP P0A031
A	9	SER	-	expression tag	UNP P0A031
A	10	HIS	-	expression tag	UNP P0A031
A	11	MET	-	expression tag	UNP P0A031

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 3 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0

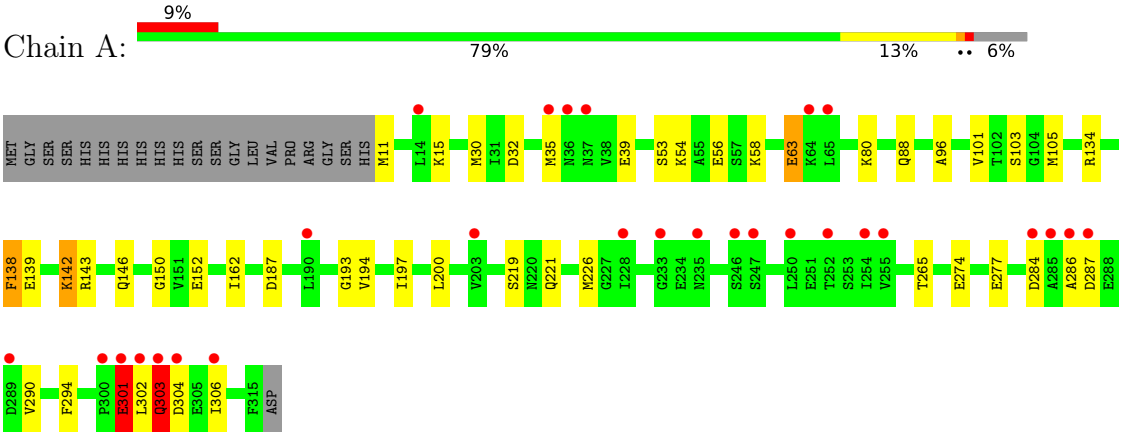
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	117	Total O 117 117	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: Cell division protein FtsZ



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	72.02Å 51.49Å 88.02Å 90.00° 110.82° 90.00°	Depositor
Resolution (Å)	41.14 – 1.75 41.14 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.4 (41.14-1.75) 98.4 (41.14-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.170 , 0.211 0.170 , 0.211	Depositor DCC
R_{free} test set	1505 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4602	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.82% 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: BEF, MN, K, GDP

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	1.40	23/2225 (1.0%)	2.55	36/3002 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	PHE	CG-CD2	15.06	1.61	1.38
1	A	138	PHE	CE1-CZ	-13.39	1.11	1.37
1	A	142	LYS	CD-CE	10.27	1.76	1.51
1	A	139	GLU	CD-OE2	9.73	1.36	1.25
1	A	303	GLN	CG-CD	9.32	1.72	1.51
1	A	138	PHE	CD2-CE2	8.59	1.56	1.39
1	A	304	ASP	CA-CB	7.90	1.71	1.53
1	A	304	ASP	CB-CG	7.61	1.67	1.51
1	A	103	SER	CB-OG	-7.44	1.32	1.42
1	A	56	GLU	CB-CG	6.64	1.64	1.52
1	A	39	GLU	CB-CG	5.89	1.63	1.52
1	A	63	GLU	CG-CD	5.81	1.60	1.51
1	A	303	GLN	CD-OE1	-5.79	1.11	1.24
1	A	56	GLU	CG-CD	5.75	1.60	1.51
1	A	101	VAL	CB-CG1	5.71	1.64	1.52
1	A	138	PHE	CB-CG	-5.61	1.41	1.51
1	A	294	PHE	CB-CG	-5.52	1.42	1.51
1	A	138	PHE	CD1-CE1	-5.48	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	GLU	CG-CD	5.33	1.59	1.51
1	A	152	GLU	CG-CD	5.24	1.59	1.51
1	A	277	GLU	CG-CD	5.20	1.59	1.51
1	A	303	GLN	CD-NE2	5.17	1.45	1.32
1	A	284	ASP	CB-CG	5.05	1.62	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	PHE	CB-CG-CD1	74.56	173.00	120.80
1	A	304	ASP	CB-CG-OD1	59.59	171.93	118.30
1	A	138	PHE	CB-CG-CD2	-50.00	85.80	120.80
1	A	301	GLU	OE1-CD-OE2	-24.59	93.80	123.30
1	A	138	PHE	CD1-CG-CD2	-21.96	89.76	118.30
1	A	304	ASP	OD1-CG-OD2	-21.71	82.06	123.30
1	A	304	ASP	CB-CG-OD2	-20.09	100.22	118.30
1	A	138	PHE	CG-CD1-CE1	16.45	138.89	120.80
1	A	63	GLU	OE1-CD-OE2	-16.01	104.09	123.30
1	A	301	GLU	CG-CD-OE1	14.25	146.80	118.30
1	A	303	GLN	N-CA-CB	12.83	133.69	110.60
1	A	142	LYS	CA-CB-CG	-9.69	92.08	113.40
1	A	11	MET	CG-SD-CE	9.09	114.75	100.20
1	A	200	LEU	CB-CG-CD1	-8.54	96.49	111.00
1	A	303	GLN	CG-CD-NE2	-8.04	97.39	116.70
1	A	142	LYS	CB-CG-CD	-8.03	90.71	111.60
1	A	301	GLU	CG-CD-OE2	-8.00	102.31	118.30
1	A	303	GLN	N-CA-C	-7.67	90.28	111.00
1	A	63	GLU	CG-CD-OE1	7.35	133.00	118.30
1	A	200	LEU	CB-CA-C	7.01	123.53	110.20
1	A	303	GLN	CG-CD-OE1	6.76	135.11	121.60
1	A	143	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	142	LYS	CG-CD-CE	-6.19	93.33	111.90
1	A	63	GLU	CA-CB-CG	6.12	126.86	113.40
1	A	187	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	143	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	187	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	197	ILE	CA-CB-CG1	-5.81	99.97	111.00
1	A	302	LEU	C-N-CA	-5.36	108.30	121.70
1	A	303	GLN	CA-CB-CG	-5.31	101.72	113.40
1	A	138	PHE	CE1-CZ-CE2	-5.26	110.53	120.00
1	A	303	GLN	CB-CG-CD	-5.18	98.14	111.60
1	A	134	ARG	NE-CZ-NH1	5.17	122.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	290	VAL	CA-CB-CG1	-5.17	103.15	110.90
1	A	143	ARG	CG-CD-NE	-5.14	101.01	111.80
1	A	304	ASP	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	PHE	Sidechain
1	A	301	GLU	Sidechain
1	A	303	GLN	Sidechain
1	A	63	GLU	Sidechain

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	2206	2235	2236	26	0
2	A	28	10	12	0	0
3	A	4	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	117	0	0	1	0
All	All	2357	2245	2248	26	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 6.

All (26) 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:142:LYS:CE	1:A:142:LYS:CD	1.76	1.63
1:A:142:LYS:CE	1:A:142:LYS:CG	2.44	0.95
1:A:142:LYS:O	1:A:142:LYS:HG2	1.78	0.83
1:A:193:GLY:HA3	1:A:226:MET:HE3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:SER:HB3	1:A:58:LYS:HE2	1.71	0.72
1:A:142:LYS:CG	1:A:142:LYS:NZ	2.56	0.69
1:A:142:LYS:CD	1:A:142:LYS:NZ	2.60	0.63
1:A:142:LYS:NZ	1:A:142:LYS:HG3	2.14	0.63
1:A:35:MET:HE1	1:A:194:VAL:HB	1.81	0.62
1:A:32:ASP:OD1	1:A:54:LYS:HE2	2.00	0.61
1:A:193:GLY:HA3	1:A:226:MET:CE	2.31	0.60
1:A:142:LYS:HE3	1:A:146:GLN:NE2	2.20	0.57
1:A:219:SER:O	1:A:221:GLN:HG2	2.07	0.55
1:A:105[A]:MET:HE3	1:A:150:GLY:HA3	1.92	0.51
1:A:15:LYS:HE3	1:A:96:ALA:HB2	1.93	0.51
1:A:265:THR:O	1:A:306:ILE:HG13	2.13	0.49
1:A:162:ILE:HD11	1:A:226:MET:HG3	1.97	0.47
1:A:32:ASP:OD1	1:A:54:LYS:CE	2.63	0.46
1:A:286:ALA:O	1:A:287:ASP:HB3	2.16	0.46
1:A:142:LYS:HG3	1:A:142:LYS:HZ2	1.80	0.45
1:A:80:LYS:NZ	6:A:502:HOH:O	2.31	0.41
1:A:30:MET:HE2	1:A:30:MET:HB3	1.73	0.41
1:A:35:MET:HE2	1:A:194:VAL:HG12	2.03	0.41
1:A:301:GLU:O	1:A:303:GLN:OE1	2.38	0.41
1:A:88:GLN:OE1	1:A:88:GLN:N	2.47	0.41
1:A:35:MET:CE	1:A:194:VAL:CG1	3.00	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	304/326 (93%)	298 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	232/249 (93%)	232 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	283	GLN

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 monosaccharides 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	$\#\|Z\|>2$
3	BEF	A	402	2,4	0,3,3	-	-	-		
2	GDP	A	401	4,3	24,30,30	2.53	5 (20%)	31,47,47	1.96	7 (22%)

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	GDP	A	401	4,3	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GDP	O4'-C1'	8.82	1.53	1.41
2	A	401	GDP	C2'-C1'	-5.31	1.45	1.53
2	A	401	GDP	C6-N1	3.49	1.39	1.33
2	A	401	GDP	O2'-C2'	2.37	1.48	1.43
2	A	401	GDP	C5'-C4'	2.35	1.58	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	GDP	C3'-C2'-C1'	6.26	110.41	100.98
2	A	401	GDP	C5-C6-N1	-5.36	116.10	123.43
2	A	401	GDP	O2'-C2'-C1'	-2.74	100.72	110.85
2	A	401	GDP	C2-N1-C6	2.56	120.00	115.93
2	A	401	GDP	C1'-N9-C4	-2.43	122.38	126.64
2	A	401	GDP	PA-O3A-PB	-2.39	124.61	132.83
2	A	401	GDP	O2A-PA-O5'	2.38	118.78	107.75

There are no chirality outliers.

There are no torsion outliers.

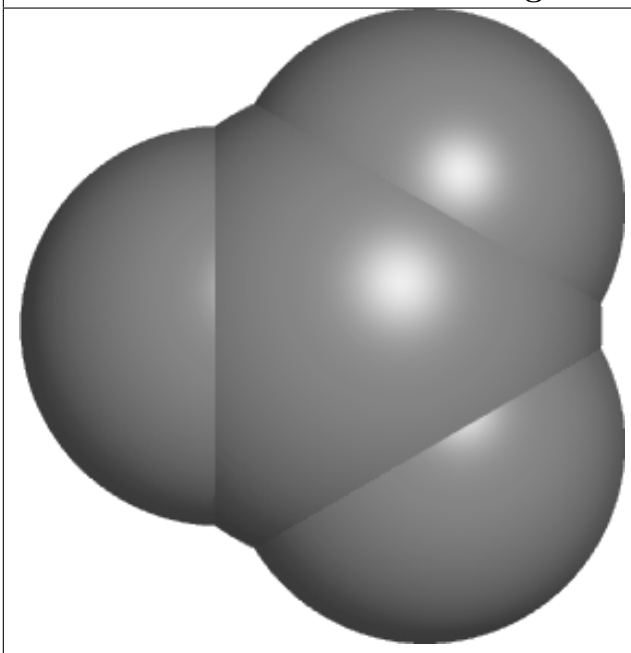
There are no ring outliers.

No monomer is involved in short contacts.

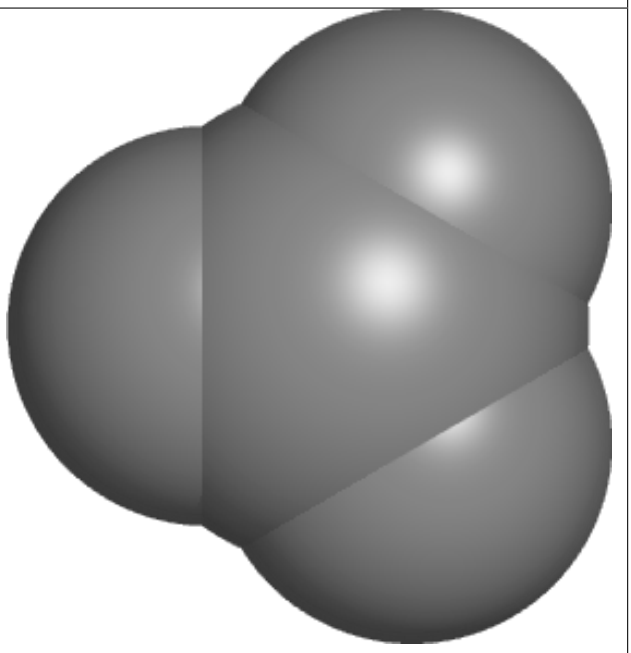
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

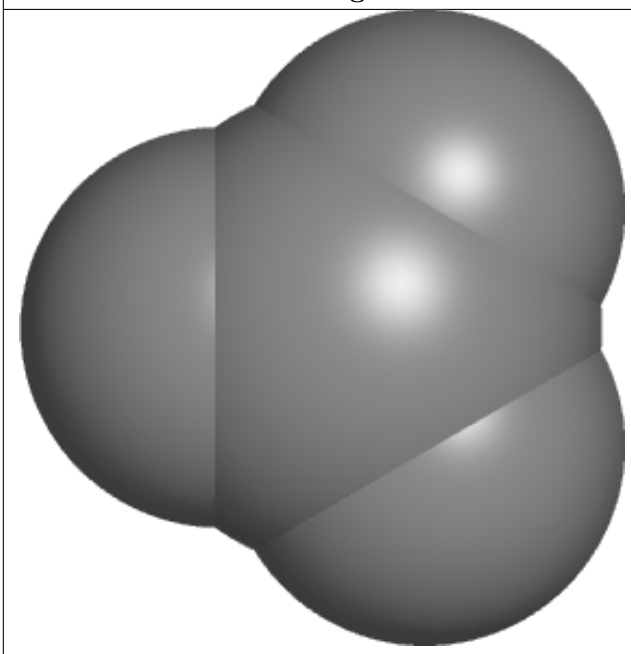
Ligand BEF A 402



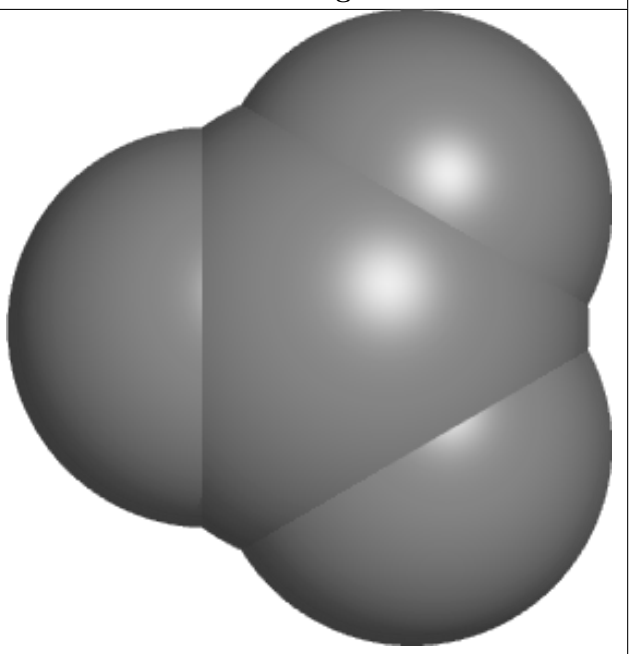
Bond lengths



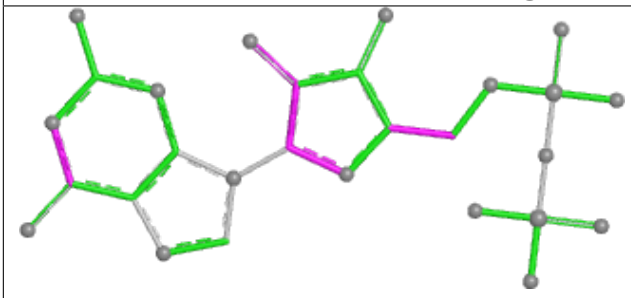
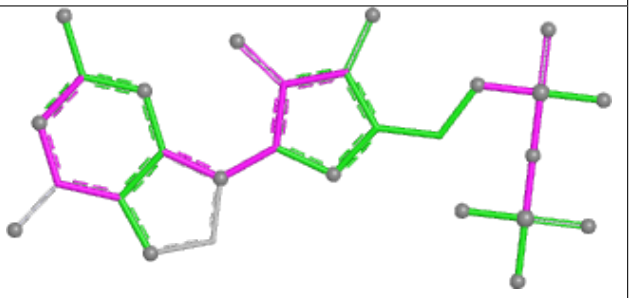
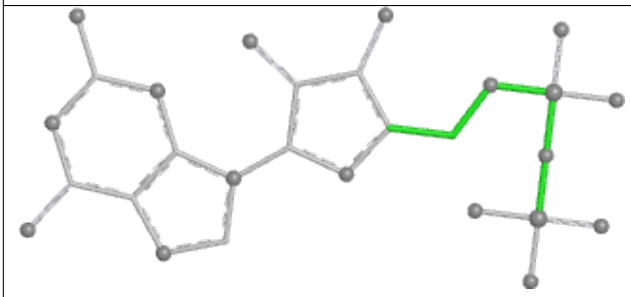
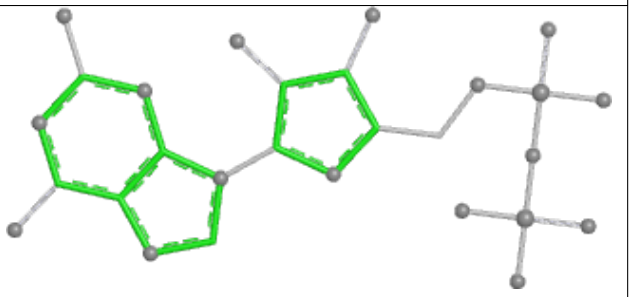
Bond angles



Torsions



Rings

Ligand GDP A 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

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, 95^{th} 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	305/326 (93%)	0.82	28 (9%)	9	11	28, 38, 67, 109	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	GLN	7.5
1	A	287	ASP	6.0
1	A	285	ALA	5.8
1	A	304	ASP	5.7
1	A	301	GLU	5.3
1	A	37	ASN	5.1
1	A	252	THR	5.0
1	A	246	SER	4.3
1	A	36	ASN	4.1
1	A	35	MET	3.9
1	A	203	VAL	3.6
1	A	306	ILE	3.6
1	A	289	ASP	3.5
1	A	254	ILE	3.5
1	A	247	SER	3.1
1	A	228	ILE	3.1
1	A	250	LEU	3.1
1	A	302	LEU	3.0
1	A	255	VAL	2.8
1	A	300	PRO	2.7
1	A	14	LEU	2.5
1	A	233	GLY	2.5
1	A	190	LEU	2.3
1	A	65	LEU	2.3
1	A	286	ALA	2.2
1	A	284	ASP	2.2
1	A	235	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	64	LYS	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

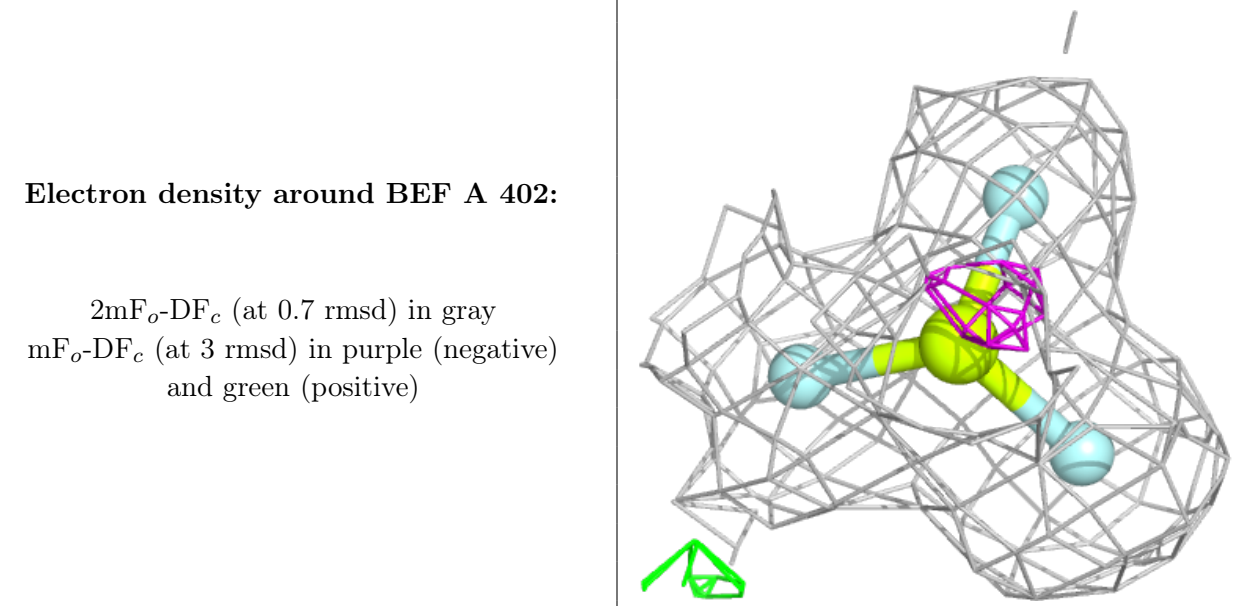
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

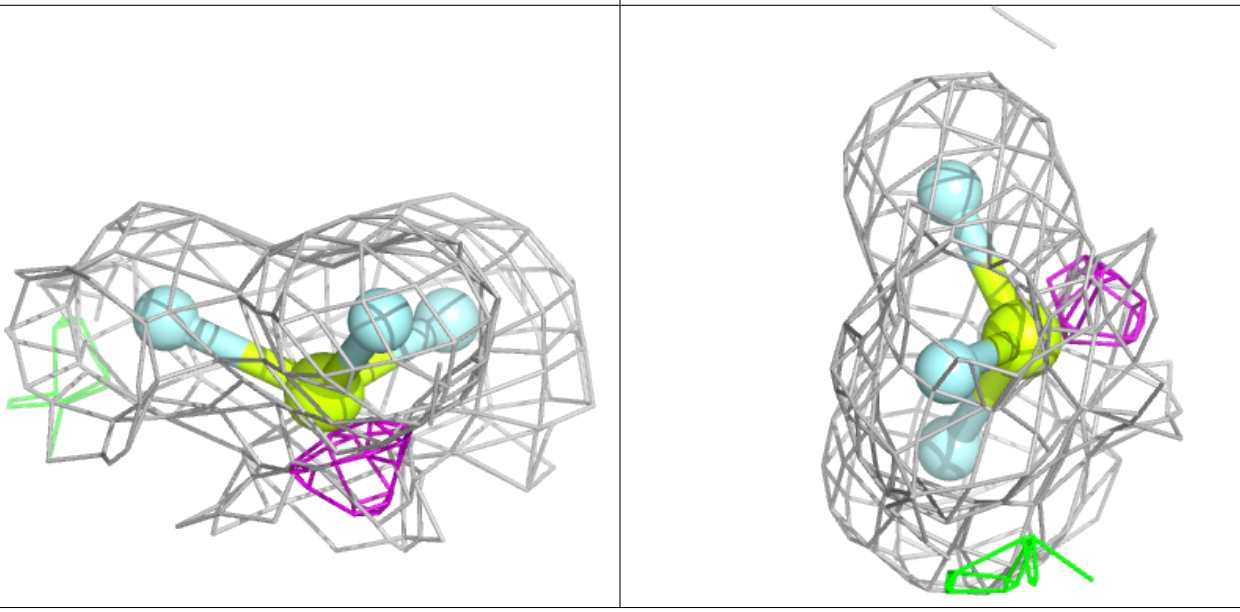
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BEF	A	402	4/4	0.71	0.16	28,28,30,31	0
2	GDP	A	401	28/28	0.95	0.11	25,31,39,40	0
5	K	A	404	1/1	0.98	0.12	36,36,36,36	0
4	MN	A	403	1/1	0.99	0.11	30,30,30,30	0

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 402:

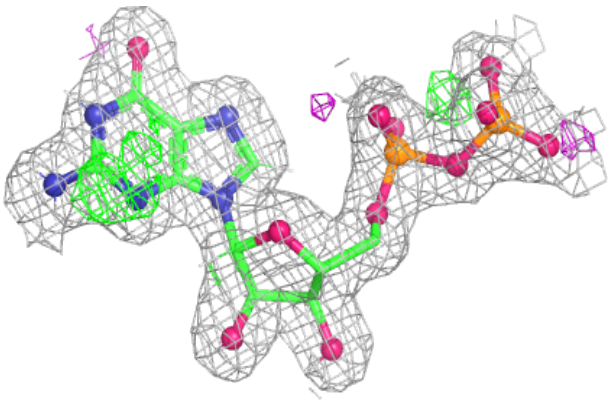
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

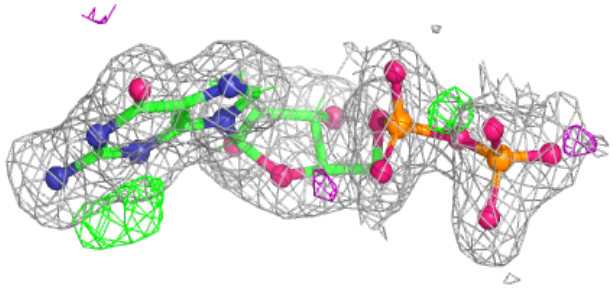


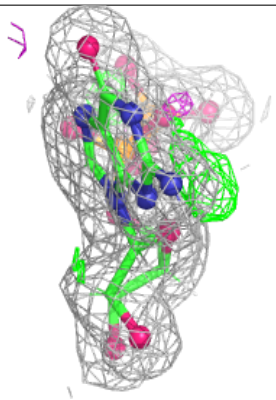


Electron density around GDP A 401:

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

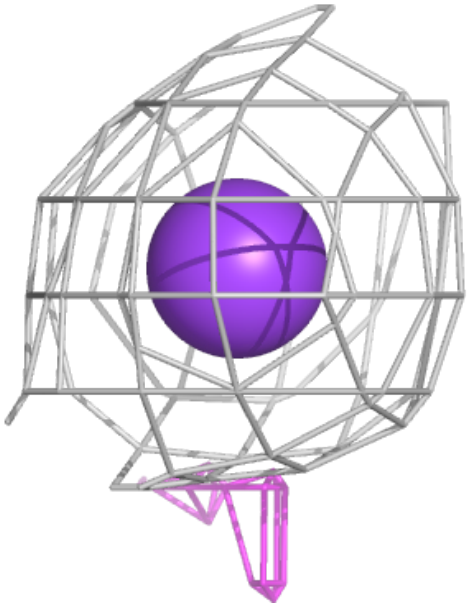


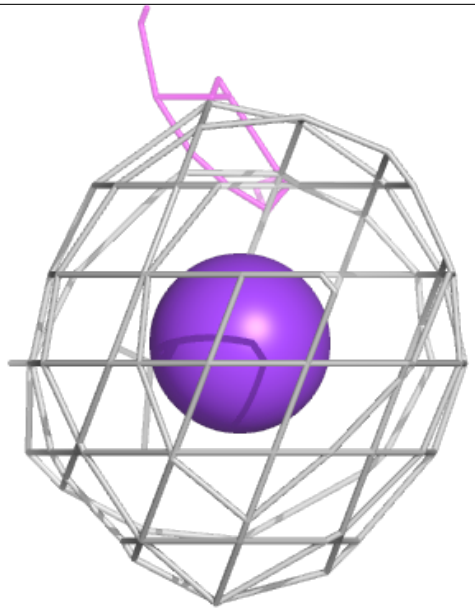


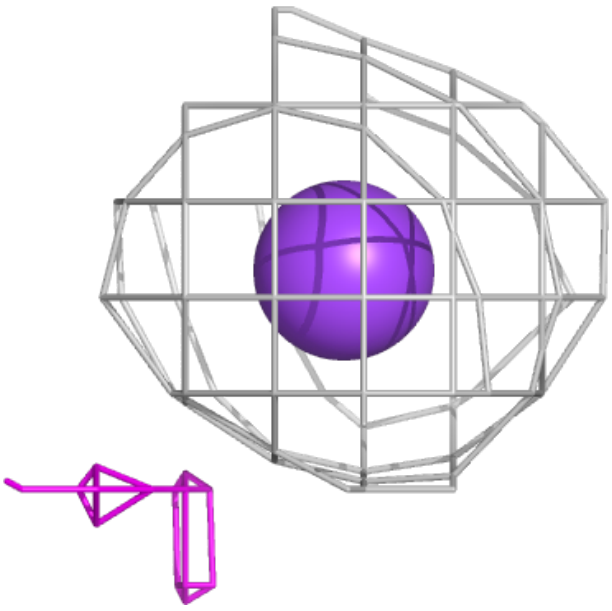


Electron density around K A 404:

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

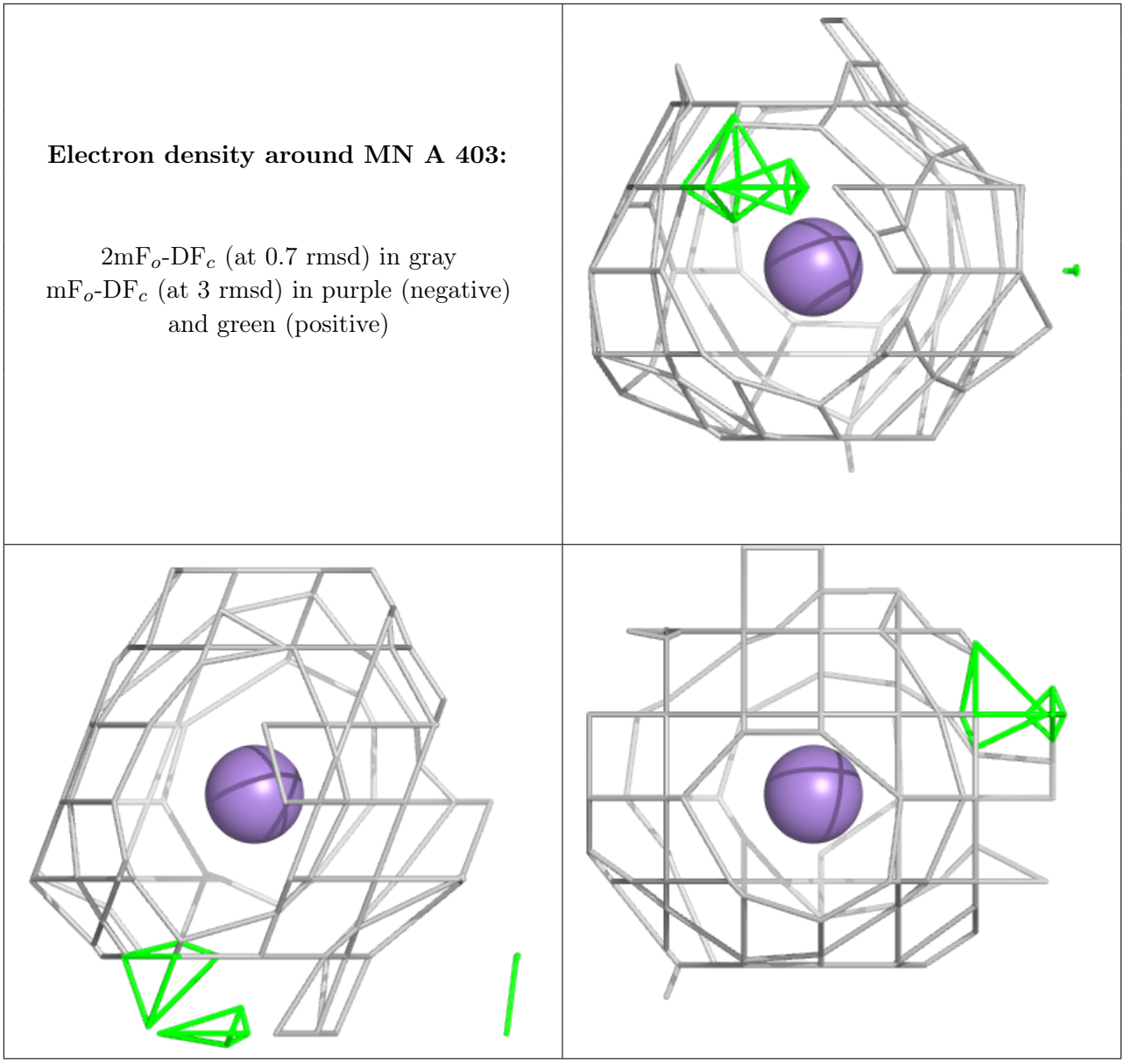






Electron density around MN A 403:

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



6.5 Other polymers

There are no such residues in this entry.