

### wwPDB X-ray Structure Validation Summary Report (i)

Dec 8, 2022 – 12:24 pm GMT

PDB ID : 7PVA

Title: 1.9 Angstrom crystal structure of dimeric PorX, co-crystallized in the presence

of zinc

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Deposited on : 2021-10-01

Resolution : 1.91 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.31.3 buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0267$ 

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

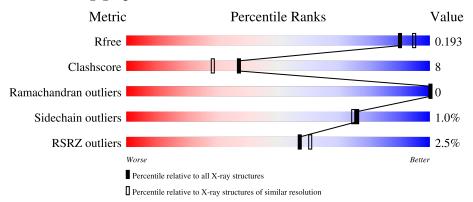
Validation Pipeline (wwPDB-VP) : 2.31.3

### 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 1.91 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
$R_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	523	80%	17%	
1	В	523	79%	17%	
1	С	523	2%	14% •	
1	D	523	80%	15% • •	

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
6	FMT	D	607	-	-	-	X



### 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 37158 atoms, of which 17552 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 Response regulator.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	Λ	513	Total	С	Н	N	О	Se	0	38	0
1	A	919	8933	2874	4440	751	847	21	0	36	
1	В	505	Total	С	Н	N	О	Se	0	20	0
1	D	303	8545	2749	4262	720	793	21	0		
1	С	513	Total	С	Н	N	О	Se	0	45	0
1		313	8981	2880	4469	759	851	22	0	40	
1	D	502	Total	С	Н	N	О	Se	0	29	0
1	D	302	8585	2772	4269	715	809	20	U	29	

There are 20 discrepancies between the modelled and reference sequences:

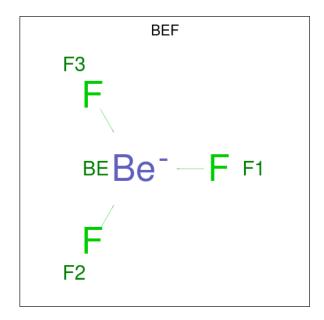
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q7MVV4
A	-3	PRO	-	expression tag	UNP Q7MVV4
A	-2	LEU	- expression tag		UNP Q7MVV4
A	-1	GLY	-	expression tag	UNP Q7MVV4
A	0	SER	-	expression tag	UNP Q7MVV4
В	-4	GLY	-	expression tag	UNP Q7MVV4
В	-3	PRO	-	expression tag	UNP Q7MVV4
В	-2	LEU	-	expression tag	UNP Q7MVV4
В	-1	GLY	-	expression tag	UNP Q7MVV4
В	0	SER	-	expression tag	UNP Q7MVV4
С	-4	GLY	-	expression tag	UNP Q7MVV4
С	-3	PRO	-	expression tag	UNP Q7MVV4
С	-2	LEU	-	expression tag	UNP Q7MVV4
С	-1	GLY	-	expression tag	UNP Q7MVV4
С	0	SER	-	expression tag	UNP Q7MVV4
D	-4	GLY	-	expression tag	UNP Q7MVV4
D	-3	PRO	-	expression tag	UNP Q7MVV4
D	-2	LEU	-	expression tag	UNP Q7MVV4
D	-1	GLY	-	expression tag	UNP Q7MVV4
D	0	SER	-	expression tag	UNP Q7MVV4



• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	В	3	Total Mg 3 3	0	0
2	С	3	Total Mg 3 3	0	0
2	D	3	Total Mg 3 3	0	0

• Molecule 3 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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



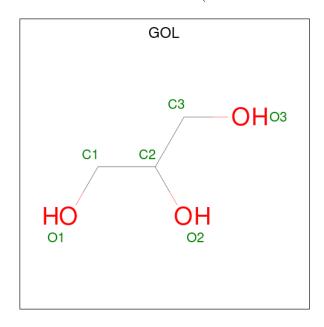
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Be F 4 1 3	0	0
3	D	1	Total Be F 4 1 3	0	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	$\begin{array}{cc} \text{Total} & \text{Zn} \\ 2 & 2 \end{array}$	0	0
4	В	1	Total Zn 1 1	0	0
4	С	2	$\begin{array}{cc} \text{Total} & \text{Zn} \\ 2 & 2 \end{array}$	0	0
4	D	1	Total Zn 1 1	0	0

• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



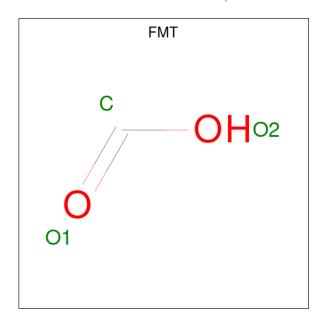
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 14 3 8 3	0	0
5	A	1	Total C H O 14 3 8 3	0	0
5	A	1	Total C H O 14 3 8 3	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total C H O	0	0
9	Б	1	14 3 8 3	0	0
5	В	1	Total C H O	0	0
9	Б	1	14 3 8 3	U	0
5	В	1	Total C H O	0	0
9	Б	1	14 3 8 3	U	U
5	В	1	Total C H O	0	0
9	Б	1	14 3 8 3		
5	В	1	Total C H O	0	0
9	Б	1	14 3 8 3		
5	С	1	Total C H O	0	0
9		1	14 3 8 3		0
5	С	1	Total C H O	0	0
		1	14 3 8 3	0	U
5	С	1	Total C H O	0	0
		1	14 3 8 3		
5	D	1	Total C H O	0	0
	D	1	14 3 8 3		U

 $\bullet$  Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula:  $\mathrm{CH_2O_2}).$ 



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 4	C 1	H 1	O 2	0	0
6	A	1	Total 4	C 1	H 1	O 2	0	0



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Mol		Residues	A	ton	ns		ZeroOcc	AltConf
6	A	1	Total			О	0	0
	71	1	4	1	1	2	0	U
6	В	1	Total	С	Η	O	0	0
		_	4	1	1	2	,	
6	В	1	Total	С	H	0	0	0
			4	$\frac{1}{C}$	1	2		
6	В	1	Total	1	H 1	0	0	0
			4 Total	$\frac{1}{C}$	H	2 O		
6	В	1	4	1	1	2	0	0
			Total	$\frac{1}{C}$	<u> </u>	O		
6	В	1	4	1	1	2	0	0
	- D		Total	$\overline{\mathrm{C}}$	Н	O		0
6	В	1	4	1	1	2	0	0
6	C	1	Total	С	Н	О	0	0
6	С	1	4	1	1	2	0	0
6	С	1	Total	С	Н	О	0	0
	C	1	4	1	1	2	0	U
6	D	1	Total	С	Η	Ο	0	0
		1	4	1	1	2		
6	D	1	Total	С	Н	O	0	0
			4	1	1	2		
6	D	1	Total	$C_{1}$	H	0	0	0
			4 Total	$\frac{1}{C}$	1 H	2 O		
6	D	1	10tai 4	1	п 1	2	0	0
			Total	$\frac{1}{C}$	H	O		
6	D	1	4	1	1	2	0	0

• Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0
7	С	1	Total Cl 1 1	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	492	Total O 492 492	0	0



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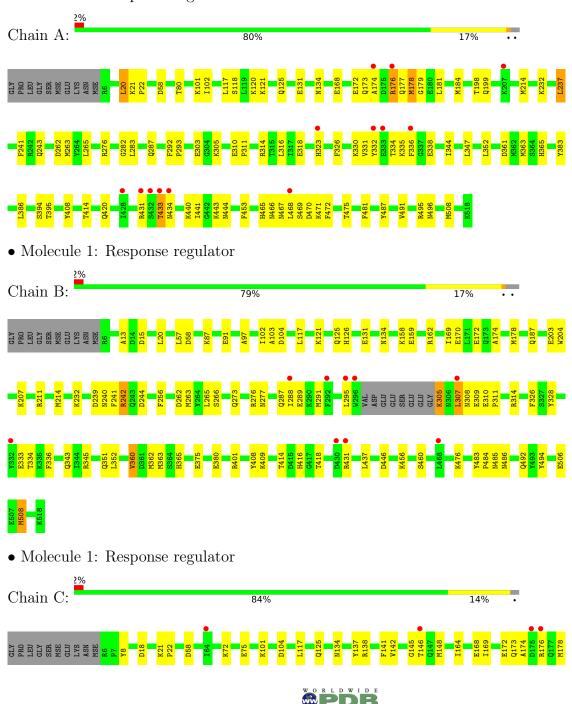
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	566	Total O 566 566	0	0
8	С	372	Total O 372 372	0	0
8	D	401	Total O 401 401	0	0

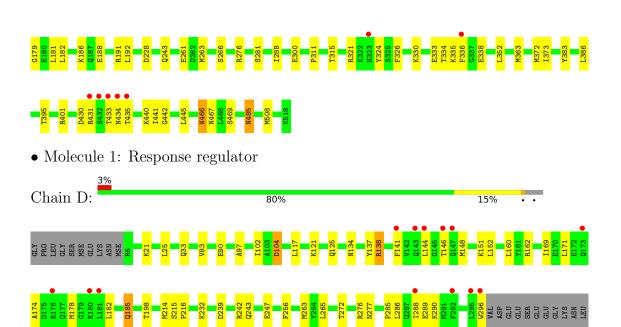


### 3 Residue-property plots (i)

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: Response regulator









### 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	61.48Å 77.29Å 138.83Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$82.42^{\circ}$ $81.61^{\circ}$ $76.51^{\circ}$	Depositor
Resolution (Å)	68.59 - 1.91	Depositor
Resolution (A)	68.59 - 1.91	EDS
% Data completeness	98.2 (68.59-1.91)	Depositor
(in resolution range)	98.3 (68.59-1.91)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.72 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
D.D.	0.159 , 0.192	Depositor
$R, R_{free}$	0.160 , $0.193$	DCC
$R_{free}$ test set	1877 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	37158	wwPDB-VP
Average B, all atoms $(Å^2)$	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

### 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: GOL, MG, BEF, ZN, CL, FMT

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).

Mal	Mol Chain	Bo	nd lengths	Bond angles		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	0.74	0/4641	0.76	5/6242 (0.1%)	
1	В	0.84	3/4448 (0.1%)	0.85	10/5978 (0.2%)	
1	С	0.68	0/4677	0.69	$2/6282 \ (0.0\%)$	
1	D	0.73	$2/4468 \; (0.0\%)$	0.70	0/6010	
All	All	0.75	5/18234 (0.0%)	0.75	17/24512 (0.1%)	

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}( ext{\AA})$
1	D	506	GLU	CD-OE1	5.96	1.32	1.25
1	В	242	ARG	CB-CG	-5.58	1.37	1.52
1	В	508	MSE	CB-CG	-5.55	1.35	1.52
1	В	506	GLU	CD-OE1	5.40	1.31	1.25
1	D	185	GLN	CB-CG	-5.14	1.38	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	20[A]	LEU	CB-CG-CD1	11.18	130.01	111.00
1	A	20[B]	LEU	CB-CG-CD1	11.18	130.01	111.00
1	В	360	VAL	CG1-CB-CG2	10.21	127.23	110.90
1	В	360	VAL	N-CA-CB	-7.35	95.33	111.50
1	В	15	ASP	CB-CG-OD1	6.68	124.31	118.30

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	4493	4440	4370	81	0
1	В	4283	4262	4185	76	0
1	С	4512	4469	4364	67	0
1	D	4316	4269	4197	62	0
2	A	2	0	0	0	0
2	В	3	0	0	0	0
2	С	3	0	0	0	0
2	D	3	0	0	0	0
3	A	8	0	0	0	0
3	В	8	0	0	0	0
3	С	8	0	0	0	0
3	D	8	0	0	0	0
4	A	2	0	0	0	0
4	В	1	0	0	0	0
4	С	2	0	0	0	0
4	D	1	0	0	1	0
5	A	18	24	23	0	0
5	В	30	40	39	7	0
5	С	18	24	24	1	0
5	D	6	8	8	0	0
6	A	9	3	3	0	0
6	В	18	6	6	1	0
6	С	6	2	2	0	0
6	D	15	5	5	0	0
7	A	1	0	0	0	0
7	С	1	0	0	0	0
8	A	492	0	0	10	2
8	В	566	0	0	22	1
8	С	372	0	0	17	1
8	D	401	0	0	11	1
All	All	19606	17552	17226	274	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 8.

The worst 5 of 274 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$egin{aligned} & & & & & & & & & \\ & & & & & & & & & $	Clash overlap (Å)
		distance (A)	overiap (A)
1:A:363[B]:MSE:HE2	1:A:386:LEU:HD23	1.40	1.04
1:A:363[B]:MSE:CE	1:A:386:LEU:HD23	1.96	0.94
1:B:91:GLU:OE1	8:B:701:HOH:O	1.89	0.91
1:C:138:ARG:NH2	8:C:702:HOH:O	2.05	0.90
1:B:240:ASN:OD1	1:B:418:THR:HG23	1.72	0.90

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	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	Clash overlap (Å)
8:A:916:HOH:O	8:B:1130:HOH:O[1_455]	1.99	0.21
8:D:1054:HOH:O	8:D:1100:HOH:O[1_545]	2.15	0.05
8:A:847:HOH:O	8:C:1042:HOH:O[1_564]	2.18	0.02

### 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	550/523~(105%)	541 (98%)	9 (2%)	0	100 100
1	В	523/523 (100%)	513 (98%)	10 (2%)	0	100 100
1	С	556/523~(106%)	541 (97%)	15 (3%)	0	100 100
1	D	527/523 (101%)	516 (98%)	11 (2%)	0	100 100
All	All	$2156/2092\ (103\%)$	2111 (98%)	45 (2%)	0	100 100

There are no Ramachandran outliers to report.

### 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 o	of residues	for	which	the	${\rm sidechain}$	conformation	was
analysed, and the total number of	residues.							

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	A	507/459~(110%)	498 (98%)	9 (2%)	59	53
1	В	484/459 (105%)	479 (99%)	5 (1%)	76	75
1	$\mathbf{C}$	511/459 (111%)	507 (99%)	4 (1%)	81	81
1	D	488/459 (106%)	484 (99%)	4 (1%)	81	81
All	All	1990/1836 (108%)	1968 (99%)	22 (1%)	76	72

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	104	ASP
1	С	485	ASN
1	С	467	ASN
1	D	104	ASP
1	A	323	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	В	465	HIS

### 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 55 ligands modelled in this entry, 19 are monoatomic - leaving 36 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).

N # 1	TD.	GI :	Ъ	т. 1	В	ond leng	$_{ m gths}$	Е	Bond ang	gles
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BEF	В	615	-	0,3,3	-	-	-		
3	BEF	A	611	1	0,3,3	-	-	-		
3	BEF	A	602	1	0,3,3	-	-	-		
6	FMT	A	610	-	2,2,2	0.64	0	1,1,1	0.50	0
6	FMT	В	611	-	2,2,2	0.65	0	1,1,1	0.56	0
6	FMT	С	609	-	2,2,2	0.67	0	1,1,1	0.53	0
3	BEF	D	610	-	0,3,3	-	-	-		
3	BEF	В	602	1	0,3,3	-	-	-		
5	GOL	С	606	-	5,5,5	0.75	0	5,5,5	0.80	0
5	GOL	С	607	_	5,5,5	0.84	0	5,5,5	0.84	0
5	GOL	В	607	_	5,5,5	1.33	1 (20%)	5,5,5	0.61	0
3	BEF	D	602	1	0,3,3	-	-	-		
5	GOL	A	605	-	5,5,5	1.01	0	5,5,5	0.86	0
6	FMT	D	607	-	2,2,2	0.61	0	1,1,1	0.43	0
6	FMT	В	614	-	2,2,2	0.72	0	1,1,1	0.48	0
6	FMT	A	608	-	2,2,2	0.67	0	1,1,1	0.36	0
3	BEF	С	602	1	0,3,3	-	-	-		
6	FMT	С	608	-	2,2,2	0.75	0	1,1,1	0.51	0
5	GOL	D	604	-	5,5,5	0.52	0	5,5,5	1.05	0
6	FMT	D	605	-	2,2,2	0.62	0	1,1,1	0.29	0
6	FMT	D	606	-	2,2,2	0.68	0	1,1,1	0.54	0
6	FMT	В	610	-	2,2,2	0.59	0	1,1,1	0.50	0
5	GOL	С	605	_	5,5,5	1.04	0	5,5,5	1.00	0
6	FMT	В	612	-	2,2,2	0.80	0	1,1,1	0.18	0
5	GOL	В	608	_	5,5,5	0.94	0	5,5,5	0.97	0
3	BEF	С	610	1	0,3,3	-	-	-		
5	GOL	A	607	-	5,5,5	0.25	0	5,5,5	0.60	0
5	GOL	В	605	-	5,5,5	0.58	0	5,5,5	0.78	0
6	FMT	В	613	-	2,2,2	0.59	0	1,1,1	0.42	0
6	FMT	В	609	-	2,2,2	0.71	0	1,1,1	0.36	0
5	GOL	В	606	-	5,5,5	0.93	0	5,5,5	0.84	0
5	GOL	В	604	_	5,5,5	1.14	0	5,5,5	0.68	0
6	FMT	D	608	-	2,2,2	0.47	0	1,1,1	0.50	0
6	FMT	A	609	-	2,2,2	0.61	0	1,1,1	0.54	0
5	GOL	A	606	-	5,5,5	0.63	0	5,5,5	1.04	0



Mol	Type	Chain	Res	Link	$\mathbf{B}_{0}$	ond leng	$\operatorname{gths}$	В	ond ang	gles
Moi Typ	Туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
6	FMT	D	609	-	2,2,2	0.64	0	1,1,1	0.52	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
5	GOL	D	604	-	-	0/4/4/4	-
5	GOL	A	607	-	-	4/4/4/4	-
5	GOL	В	605	-	-	2/4/4/4	-
5	GOL	С	605	-	-	2/4/4/4	-
5	GOL	A	605	-	-	0/4/4/4	-
5	GOL	В	606	-	-	0/4/4/4	-
5	GOL	В	604	-	-	1/4/4/4	-
5	GOL	С	607	-	-	2/4/4/4	-
5	GOL	С	606	-	-	2/4/4/4	-
5	GOL	В	608	-	-	2/4/4/4	-
5	GOL	A	606	-	-	0/4/4/4	-
5	GOL	В	607	-	-	2/4/4/4	-

### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
5	В	607	GOL	O2-C2	-2.78	1.35	1.43

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	607	GOL	O1-C1-C2-C3
5	С	606	GOL	O2-C2-C3-O3
5	A	607	GOL	O2-C2-C3-O3
5	С	607	GOL	O2-C2-C3-O3
5	A	607	GOL	C1-C2-C3-O3

There are no ring outliers.

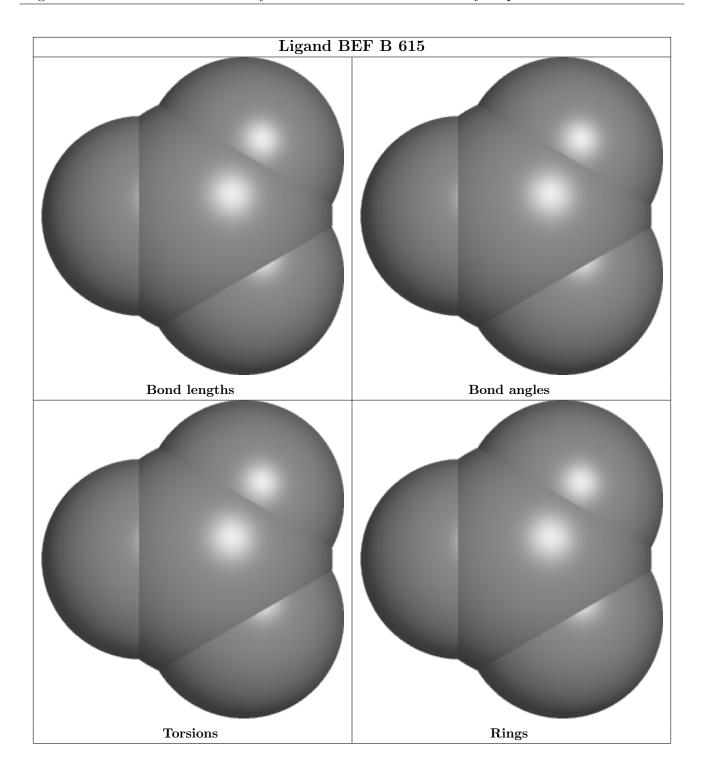
7 monomers are involved in 9 short contacts:



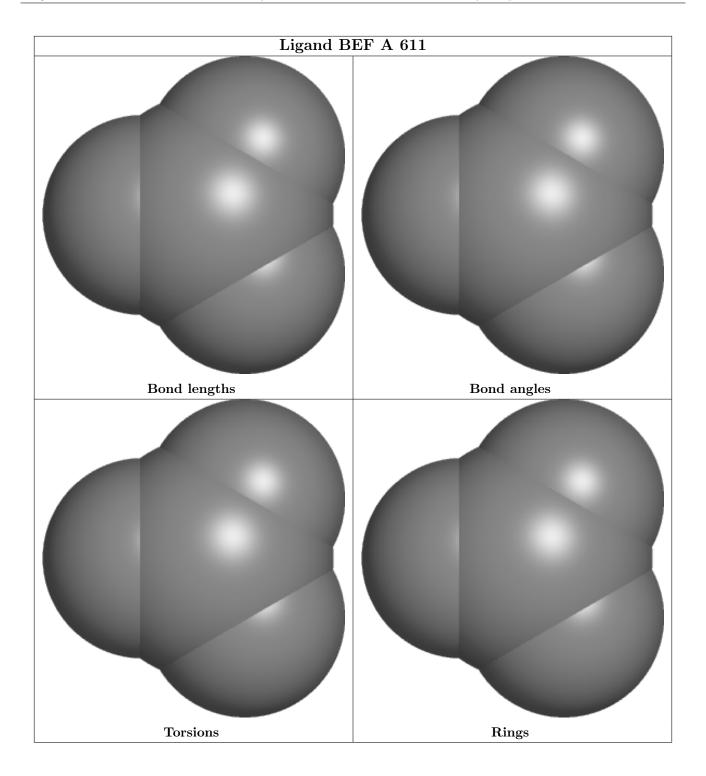
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	С	607	GOL	1	0
5	В	607	GOL	2	0
5	В	608	GOL	1	0
5	В	605	GOL	1	0
6	В	613	FMT	1	0
5	В	606	GOL	2	0
5	В	604	GOL	1	0

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 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.

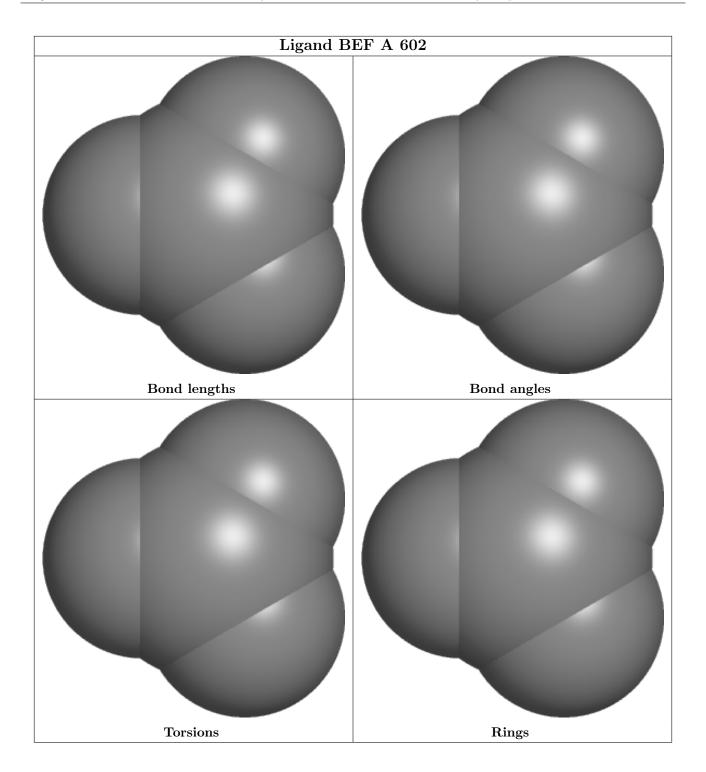




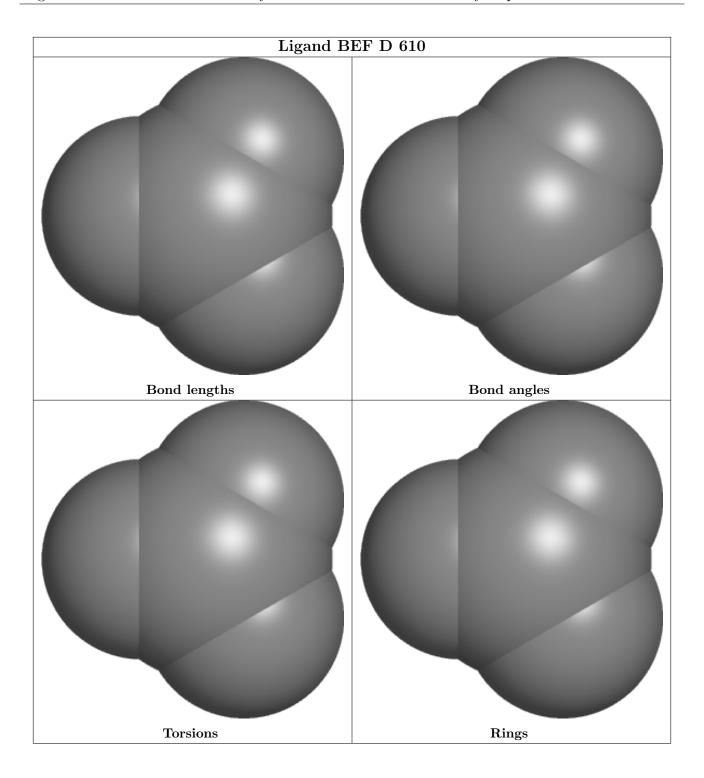




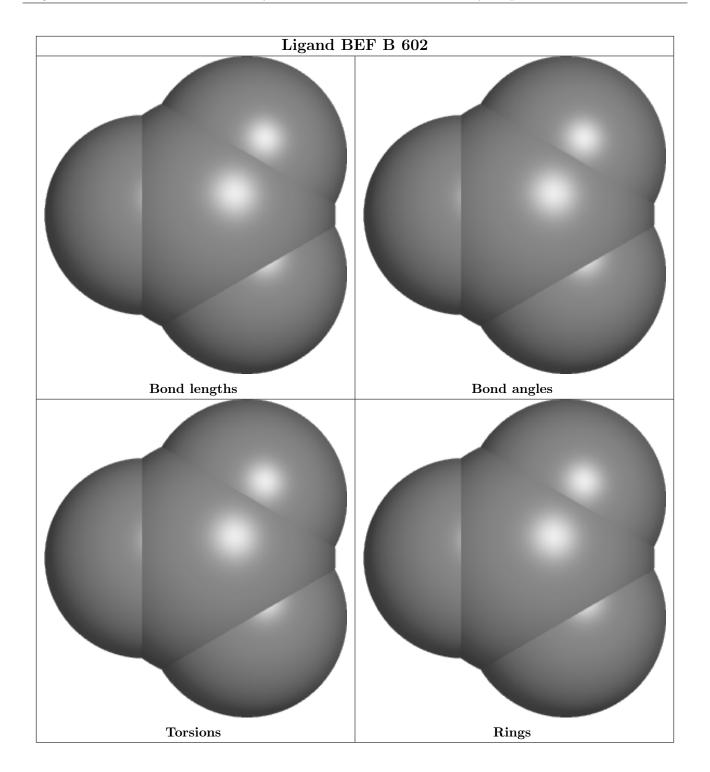




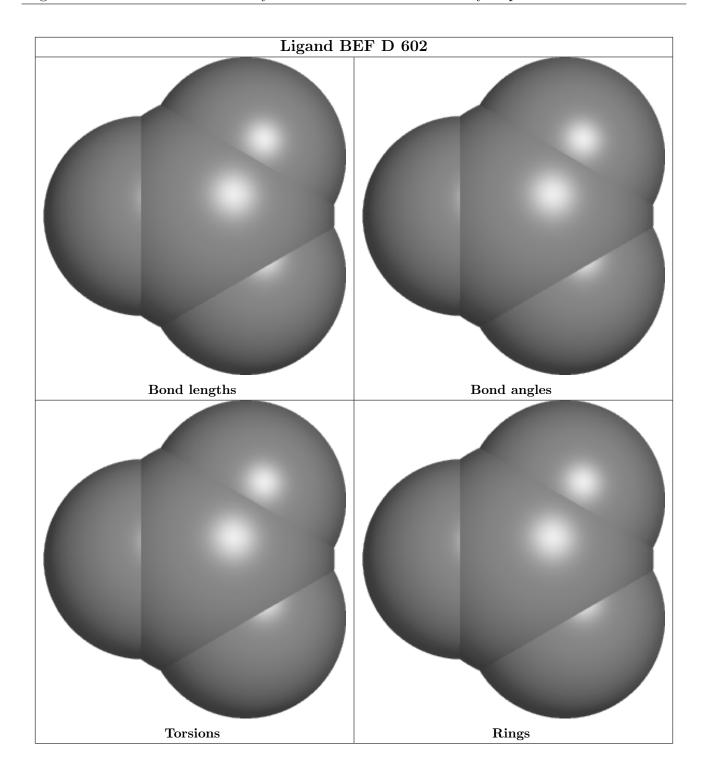




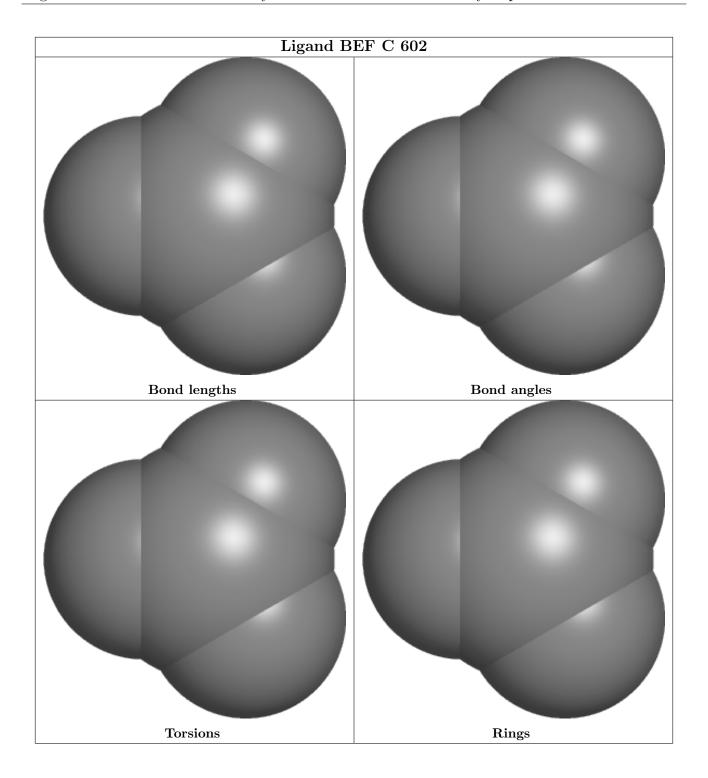




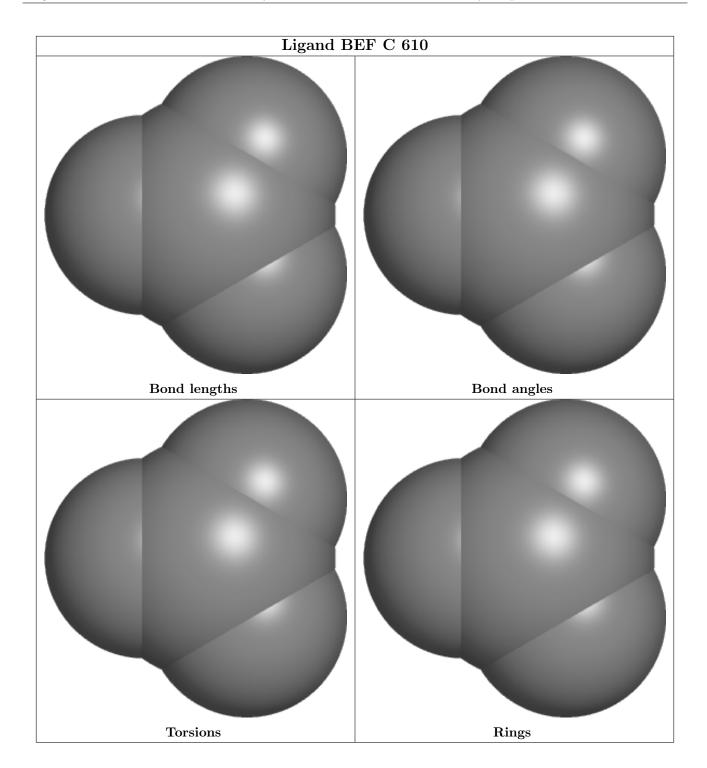












### 5.7 Other polymers (i)

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,  $95^{th}$  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>	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
1	A	495/523 (94%)	0.03	13 (2%) 56 59	32, 52, 88, 118	0
1	В	487/523 (93%)	-0.06	9 (1%) 68 71	27, 44, 91, 132	0
1	С	495/523 (94%)	0.04	11 (2%) 62 65	38, 56, 90, 128	0
1	D	484/523 (92%)	0.08	17 (3%) 44 47	34, 53, 103, 140	0
All	All	1961/2092 (93%)	0.03	50 (2%) 57 60	27, 52, 93, 140	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	295	LEU	5.3
1	D	295	LEU	4.9
1	С	64	ILE	4.3
1	С	433[A]	THR	4.2
1	С	176[A]	ARG	3.9

### 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	$\operatorname{B-factors}(\mathrm{\AA}^2)$	Q<0.9
3	BEF	D	610	4/4	0.26	0.29	94,95,97,102	0
3	BEF	В	615	4/4	0.69	0.21	84,88,89,92	0
6	FMT	D	607	3/3	0.72	0.48	102,102,103,123	0
6	FMT	A	610	3/3	0.73	0.25	98,99,99,119	0
5	GOL	В	607	6/6	0.74	0.24	79,95,114,114	0
6	FMT	D	608	3/3	0.74	0.19	105,106,106,126	0
2	MG	С	612	1/1	0.75	0.17	117,117,117,117	0
6	FMT	С	608	3/3	0.77	0.18	98,99,100,118	0
5	GOL	В	608	6/6	0.78	0.24	105,126,132,132	0
5	GOL	В	606	6/6	0.79	0.18	85,102,117,117	0
6	FMT	A	609	3/3	0.79	0.22	98,99,101,119	0
5	GOL	В	604	6/6	0.79	0.22	49,71,82,85	0
3	BEF	A	611	4/4	0.82	0.11	53,53,56,58	0
2	MG	С	611	1/1	0.82	0.10	89,89,89,89	0
7	CL	A	613	1/1	0.82	0.21	116,116,116,116	0
5	GOL	D	604	6/6	0.83	0.15	71,88,105,105	0
6	FMT	В	611	3/3	0.83	0.22	109,109,112,131	0
6	FMT	D	609	3/3	0.83	0.14	99,100,101,119	0
5	GOL	С	606	6/6	0.83	0.19	79,95,100,106	0
6	FMT	В	612	3/3	0.84	0.16	67,68,72,87	0
6	FMT	A	608	3/3	0.84	0.09	53,56,59,71	0
6	FMT	В	609	3/3	0.85	0.14	57,65,66,79	0
5	GOL	С	607	6/6	0.85	0.15	91,109,124,124	0
7	CL	С	613	1/1	0.85	0.21	110,110,110,110	0
6	FMT	С	609	3/3	0.86	0.12	78,79,79,95	0
2	MG	В	617	1/1	0.87	0.28	63,63,63,63	0
5	GOL	A	605	6/6	0.88	0.14	64,77,86,89	0
2	MG	A	612	1/1	0.88	0.07	101,101,101,101	0
4	ZN	С	604	1/1	0.88	0.11	55,55,55,55	1
6	FMT	В	613	3/3	0.90	0.23	97,99,102,119	0
3	BEF	С	602	4/4	0.90	0.08	48,50,51,51	0
5	GOL	A	607	6/6	0.90	0.19	72,86,94,101	0
3	BEF	С	610	4/4	0.90	0.12	53,56,56,59	0
6	FMT	D	606	3/3	0.91	0.18	65,67,67,81	0
6	FMT	В	610	3/3	0.91	0.13	98,99,101,118	0
5	GOL	В	605	6/6	0.91	0.23	82,98,105,107	0
2	MG	В	616	1/1	0.92	0.06	66,66,66,66	0
2	MG	С	601	1/1	0.92	0.06	52,52,52,52	0
6	FMT	D	605	3/3	0.92	0.09	66,66,66,79	0
3	BEF	D	602	4/4	0.93	0.08	33,37,38,40	0
2	MG	D	611	1/1	0.93	0.10	64,64,64	0
6	FMT	В	614	3/3	0.94	0.24	100,101,101,121	0
3	BEF	A	602	4/4	0.94	0.10	34,36,37,39 Continued on nex	0



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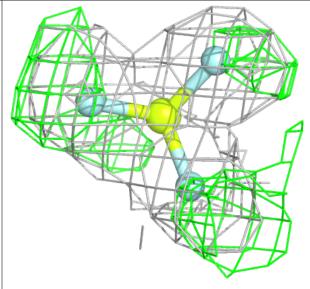
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	MG	D	601	1/1	0.95	0.05	44,44,44,44	0
2	MG	В	601	1/1	0.95	0.10	40,40,40,40	0
5	GOL	С	605	6/6	0.96	0.21	64,77,86,87	0
2	MG	D	612	1/1	0.96	0.22	83,83,83,83	0
4	ZN	D	603	1/1	0.97	0.10	41,41,41,41	1
3	BEF	В	602	4/4	0.97	0.07	28,30,32,32	0
2	MG	A	601	1/1	0.98	0.09	43,43,43,43	0
5	GOL	A	606	6/6	0.98	0.16	55,66,72,73	0
4	ZN	A	604	1/1	0.98	0.11	46,46,46,46	1
4	ZN	В	603	1/1	0.99	0.12	36,36,36,36	1
4	ZN	С	603	1/1	0.99	0.12	45,45,45,45	1
4	ZN	A	603	1/1	1.00	0.14	47,47,47,47	1

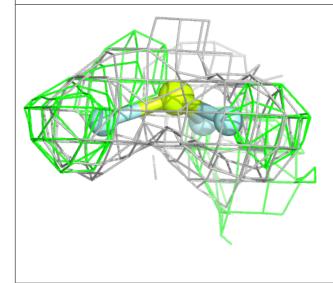
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

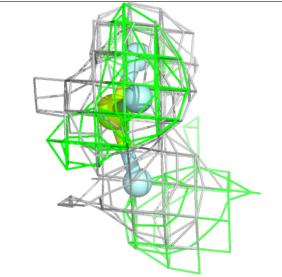


### Electron density around BEF D 610:

 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)







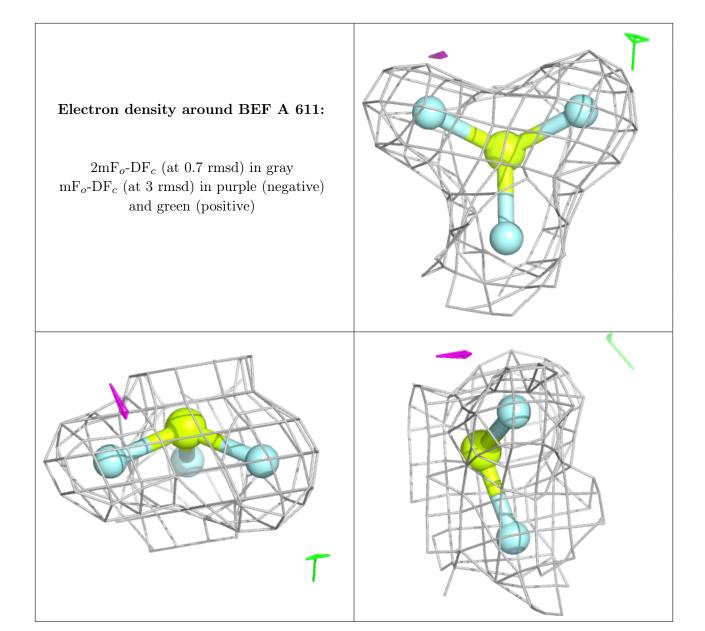






### Electron density around MG C 612: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)







## Electron density around MG C 611: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_{o}\text{-}\mathrm{DF}_{c}$ (at 3 rmsd) in purple (negative) and green (positive)



# Electron density around MG B 617: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

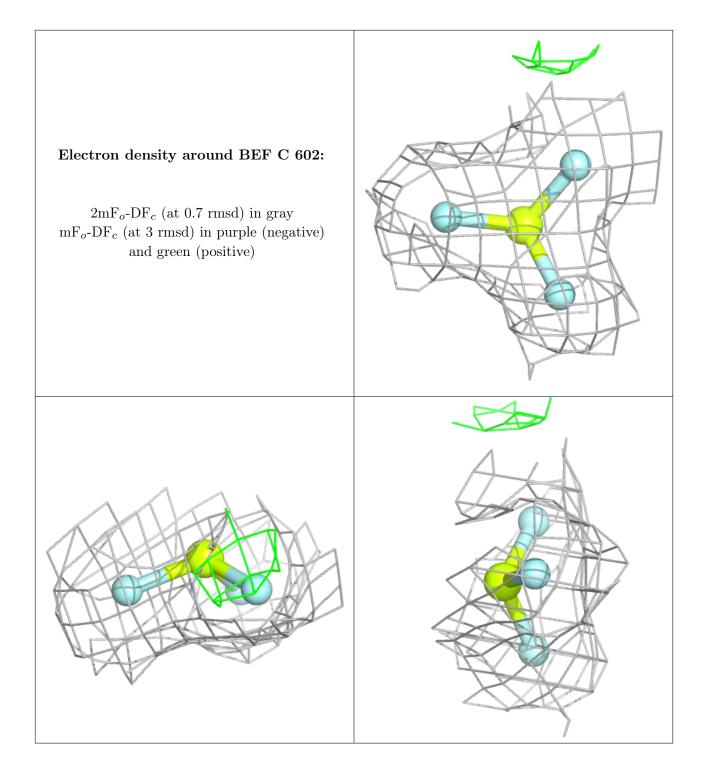


# Electron density around MG A 612: 2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)

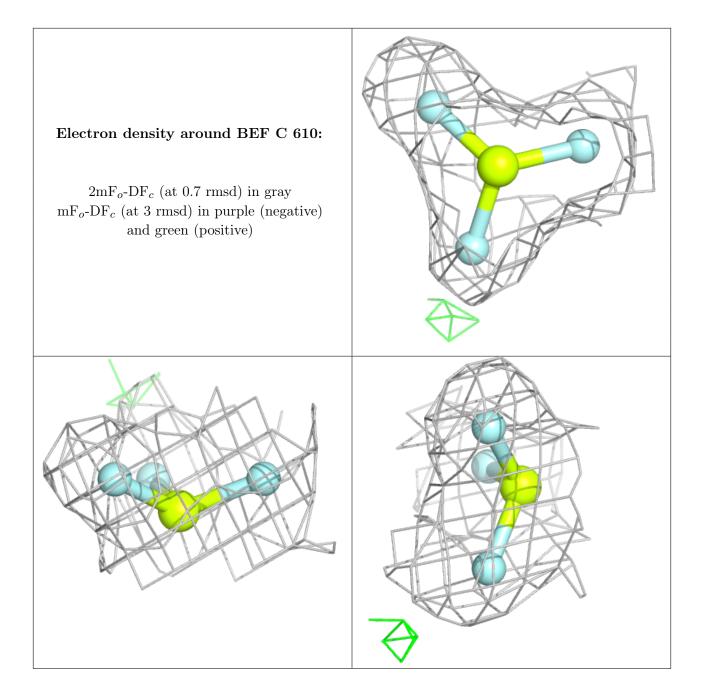


### 



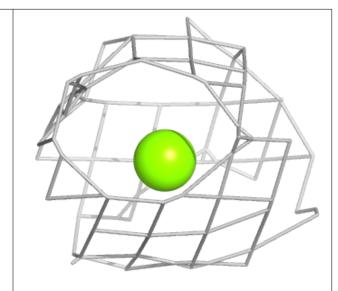


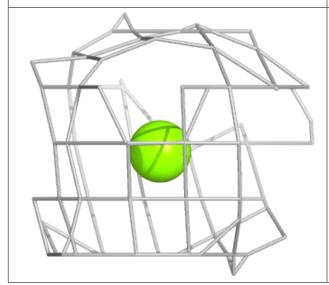


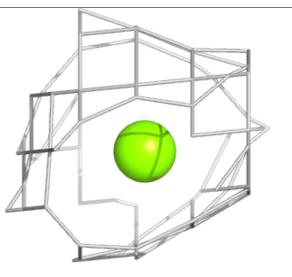


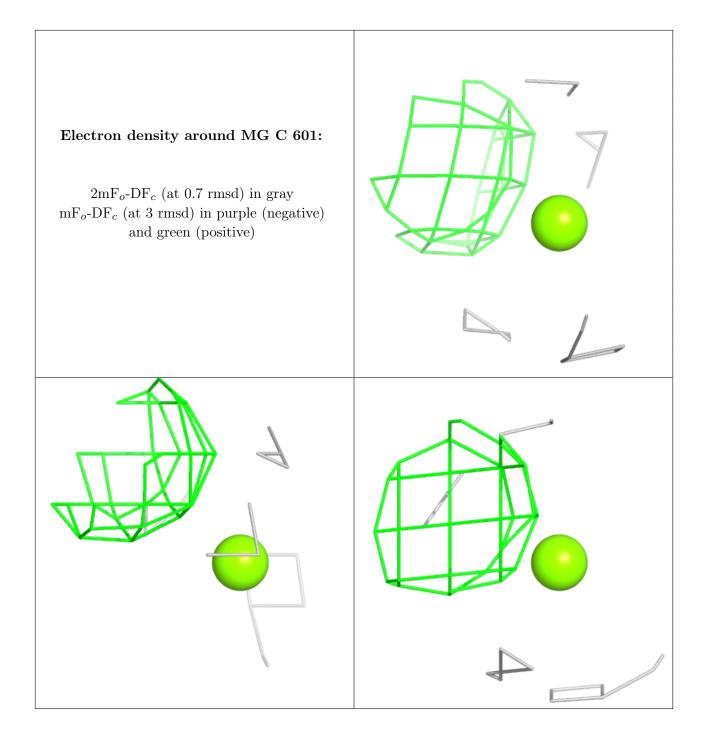


### Electron density around MG B 616:







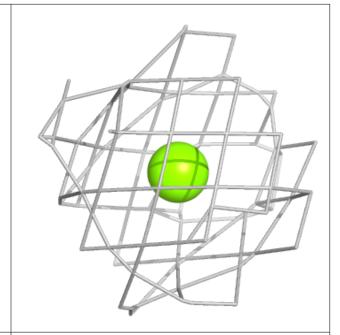


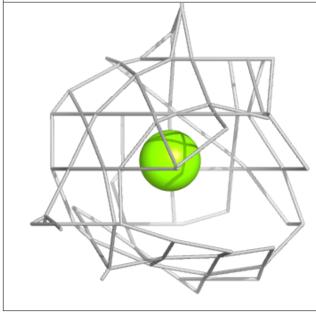


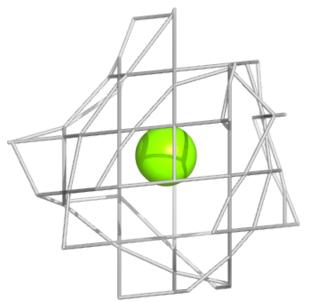
## Electron density around BEF D 602: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



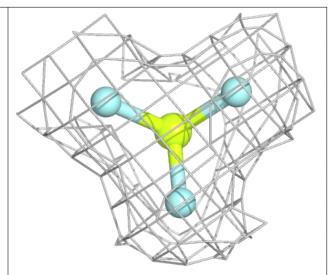
### Electron density around MG D 611:

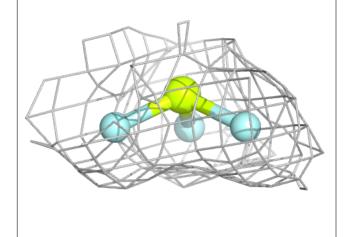


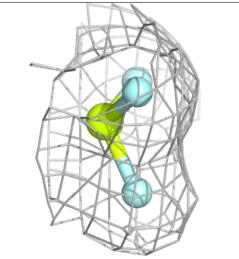




### Electron density around BEF A 602:









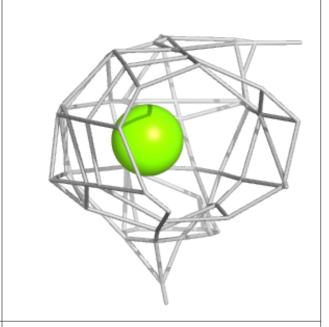
## Electron density around MG D 601: 2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)

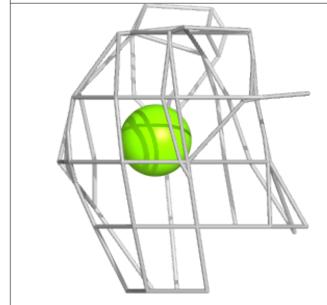


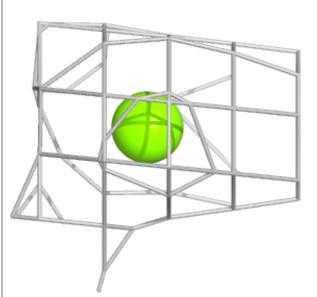
## Electron density around MG B 601: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

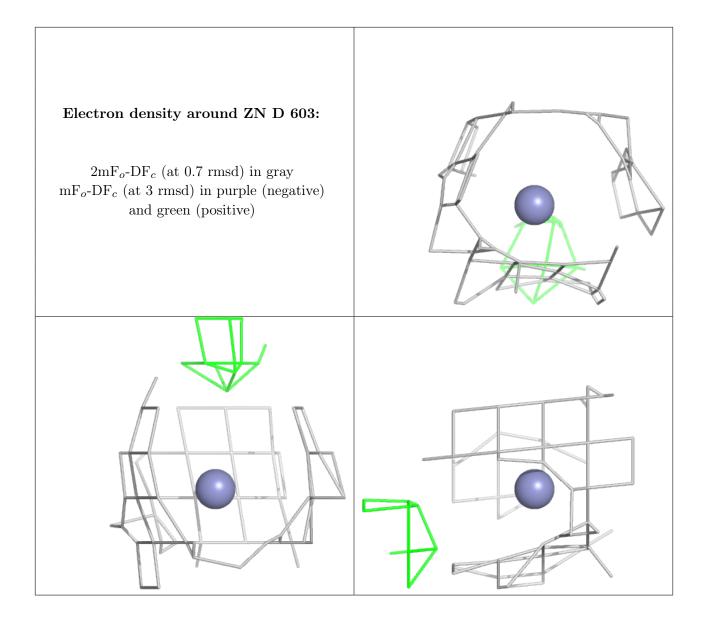


### Electron density around MG D 612:



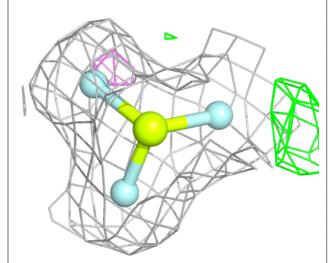


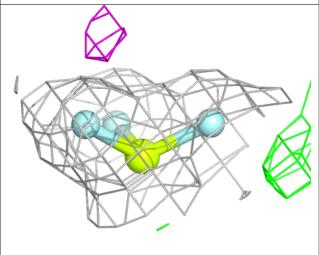


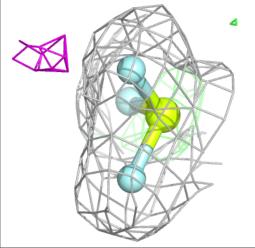




### Electron density around BEF B 602:



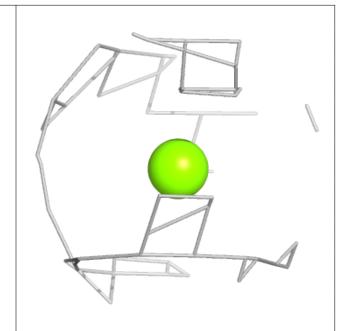


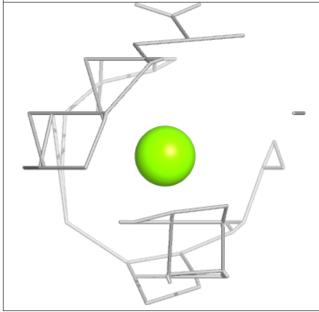


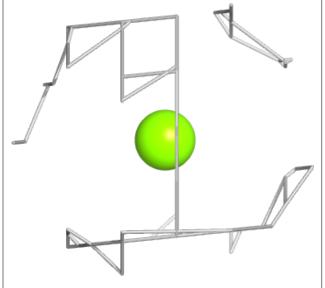


### Electron density around MG A 601:

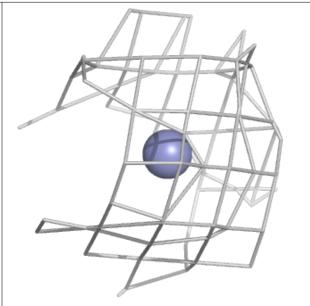
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

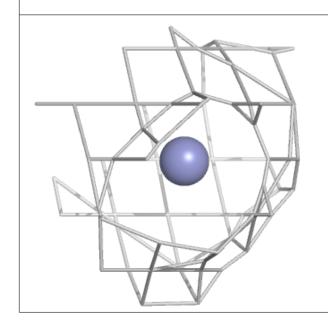


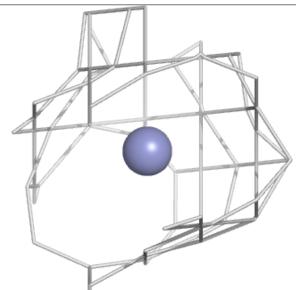




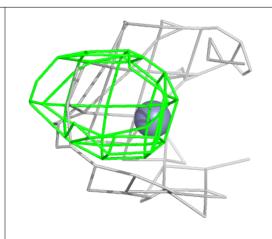
### Electron density around ZN A 604:

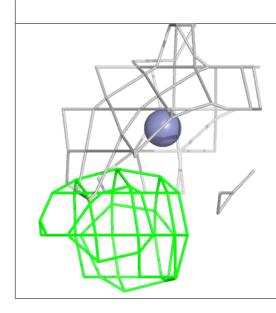


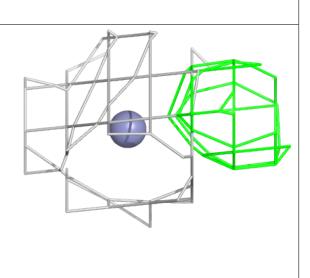




### Electron density around ZN B 603:



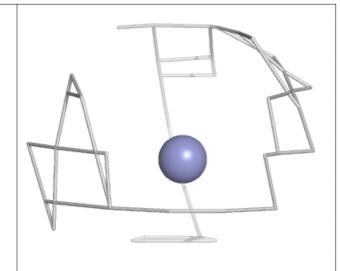


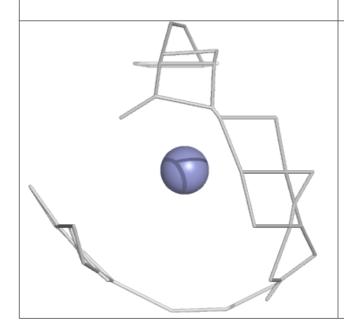


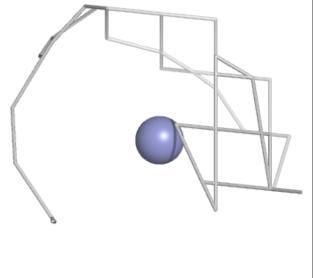


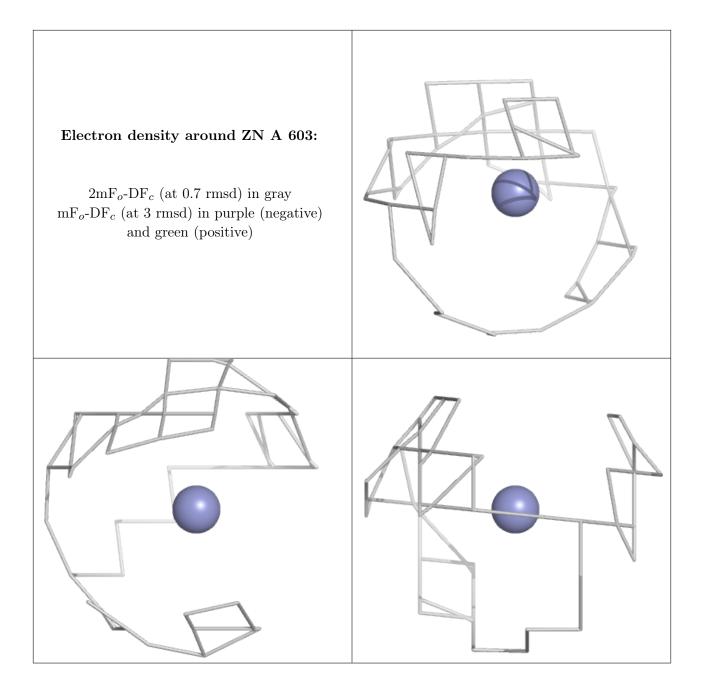
### Electron density around ZN C 603:

 $2 \text{mF}_o\text{-DF}_c$  (at 0.7 rmsd) in gray  $\text{mF}_o\text{-DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)









### 6.5 Other polymers (i)

There are no such residues in this entry.

