wwPDB X-ray Structure Validation Summary Report (i)

Apr 23, 2024 – 12:50 PM JST

PDB ID	:	8J9D
Title	:	Crystal structure of M61 peptidase (bestatin-bound) from Xanthomonas campestris
Authors	:	Yadav, P.; Kumar, A.; Kulkarni, B.S.; Jamdar, S.N.; Makde, R.D.
Deposited on	:	2023-05-03
Resolution	:	1.90 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:

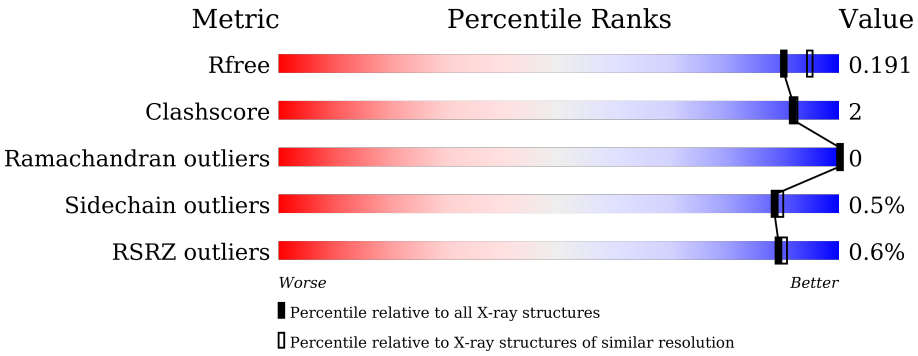
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	647	90% · 6%
1	B	647	% 89% · 6%
1	C	647	% 89% 5% 6%
1	D	647	88% 5% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21434 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative glycyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	0	2	0
			4783	3036	823	904	20			
1	B	605	Total	C	N	O	S	0	1	0
			4777	3033	822	902	20			
1	C	605	Total	C	N	O	S	0	3	0
			4787	3039	822	906	20			
1	D	605	Total	C	N	O	S	0	4	0
			4801	3046	826	909	20			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP B0RY21
A	-19	GLY	-	expression tag	UNP B0RY21
A	-18	SER	-	expression tag	UNP B0RY21
A	-17	SER	-	expression tag	UNP B0RY21
A	-16	HIS	-	expression tag	UNP B0RY21
A	-15	HIS	-	expression tag	UNP B0RY21
A	-14	HIS	-	expression tag	UNP B0RY21
A	-13	HIS	-	expression tag	UNP B0RY21
A	-12	HIS	-	expression tag	UNP B0RY21
A	-11	HIS	-	expression tag	UNP B0RY21
A	-10	SER	-	expression tag	UNP B0RY21
A	-9	SER	-	expression tag	UNP B0RY21
A	-8	GLY	-	expression tag	UNP B0RY21
A	-7	LEU	-	expression tag	UNP B0RY21
A	-6	VAL	-	expression tag	UNP B0RY21
A	-5	PRO	-	expression tag	UNP B0RY21
A	-4	ARG	-	expression tag	UNP B0RY21
A	-3	GLY	-	expression tag	UNP B0RY21
A	-2	SER	-	expression tag	UNP B0RY21
A	-1	HIS	-	expression tag	UNP B0RY21
A	0	MET	-	expression tag	UNP B0RY21

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	GLN	engineered mutation	UNP B0RY21
B	-20	MET	-	initiating methionine	UNP B0RY21
B	-19	GLY	-	expression tag	UNP B0RY21
B	-18	SER	-	expression tag	UNP B0RY21
B	-17	SER	-	expression tag	UNP B0RY21
B	-16	HIS	-	expression tag	UNP B0RY21
B	-15	HIS	-	expression tag	UNP B0RY21
B	-14	HIS	-	expression tag	UNP B0RY21
B	-13	HIS	-	expression tag	UNP B0RY21
B	-12	HIS	-	expression tag	UNP B0RY21
B	-11	HIS	-	expression tag	UNP B0RY21
B	-10	SER	-	expression tag	UNP B0RY21
B	-9	SER	-	expression tag	UNP B0RY21
B	-8	GLY	-	expression tag	UNP B0RY21
B	-7	LEU	-	expression tag	UNP B0RY21
B	-6	VAL	-	expression tag	UNP B0RY21
B	-5	PRO	-	expression tag	UNP B0RY21
B	-4	ARG	-	expression tag	UNP B0RY21
B	-3	GLY	-	expression tag	UNP B0RY21
B	-2	SER	-	expression tag	UNP B0RY21
B	-1	HIS	-	expression tag	UNP B0RY21
B	0	MET	-	expression tag	UNP B0RY21
B	22	ALA	GLN	engineered mutation	UNP B0RY21
C	-20	MET	-	initiating methionine	UNP B0RY21
C	-19	GLY	-	expression tag	UNP B0RY21
C	-18	SER	-	expression tag	UNP B0RY21
C	-17	SER	-	expression tag	UNP B0RY21
C	-16	HIS	-	expression tag	UNP B0RY21
C	-15	HIS	-	expression tag	UNP B0RY21
C	-14	HIS	-	expression tag	UNP B0RY21
C	-13	HIS	-	expression tag	UNP B0RY21
C	-12	HIS	-	expression tag	UNP B0RY21
C	-11	HIS	-	expression tag	UNP B0RY21
C	-10	SER	-	expression tag	UNP B0RY21
C	-9	SER	-	expression tag	UNP B0RY21
C	-8	GLY	-	expression tag	UNP B0RY21
C	-7	LEU	-	expression tag	UNP B0RY21
C	-6	VAL	-	expression tag	UNP B0RY21
C	-5	PRO	-	expression tag	UNP B0RY21
C	-4	ARG	-	expression tag	UNP B0RY21
C	-3	GLY	-	expression tag	UNP B0RY21
C	-2	SER	-	expression tag	UNP B0RY21

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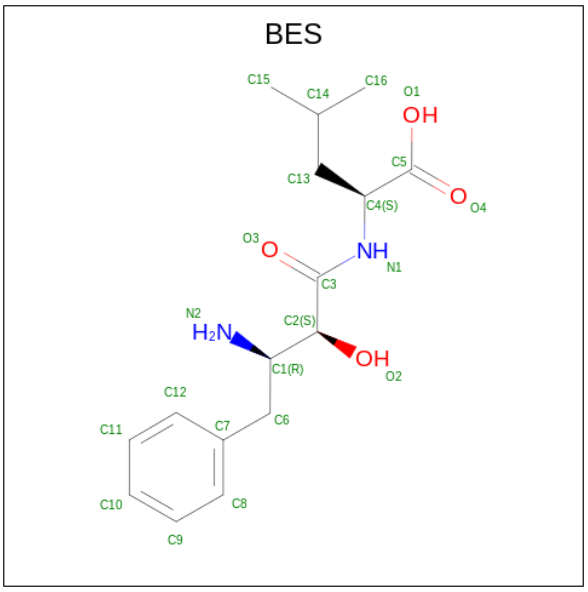
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	expression tag	UNP B0RY21
C	0	MET	-	expression tag	UNP B0RY21
C	22	ALA	GLN	engineered mutation	UNP B0RY21
D	-20	MET	-	initiating methionine	UNP B0RY21
D	-19	GLY	-	expression tag	UNP B0RY21
D	-18	SER	-	expression tag	UNP B0RY21
D	-17	SER	-	expression tag	UNP B0RY21
D	-16	HIS	-	expression tag	UNP B0RY21
D	-15	HIS	-	expression tag	UNP B0RY21
D	-14	HIS	-	expression tag	UNP B0RY21
D	-13	HIS	-	expression tag	UNP B0RY21
D	-12	HIS	-	expression tag	UNP B0RY21
D	-11	HIS	-	expression tag	UNP B0RY21
D	-10	SER	-	expression tag	UNP B0RY21
D	-9	SER	-	expression tag	UNP B0RY21
D	-8	GLY	-	expression tag	UNP B0RY21
D	-7	LEU	-	expression tag	UNP B0RY21
D	-6	VAL	-	expression tag	UNP B0RY21
D	-5	PRO	-	expression tag	UNP B0RY21
D	-4	ARG	-	expression tag	UNP B0RY21
D	-3	GLY	-	expression tag	UNP B0RY21
D	-2	SER	-	expression tag	UNP B0RY21
D	-1	HIS	-	expression tag	UNP B0RY21
D	0	MET	-	expression tag	UNP B0RY21
D	22	ALA	GLN	engineered mutation	UNP B0RY21

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

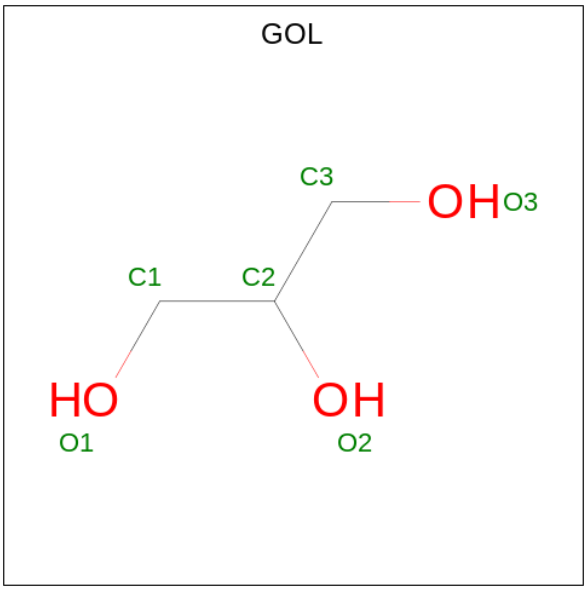
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (three-letter code: BES) (formula: $C_{16}H_{24}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



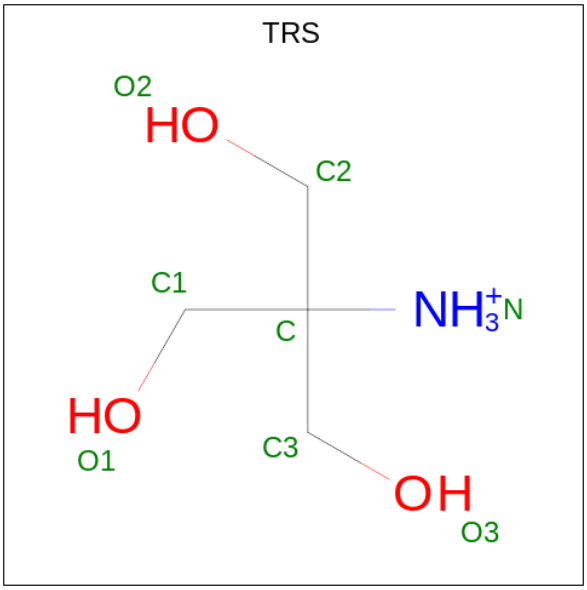
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	16	2	4		
3	B	1	Total	C	N	O	0	0
			22	16	2	4		
3	C	1	Total	C	N	O	0	0
			22	16	2	4		
3	D	1	Total	C	N	O	0	0
			22	16	2	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 8 4 1 3	0	0
5	D	1	Total C N O 8 4 1 3	0	0

- Molecule 6 is water.

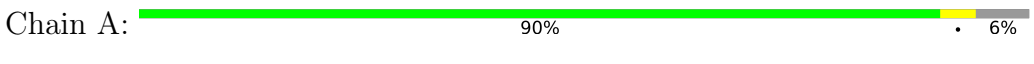
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	573	Total O 573 573	0	0
6	B	576	Total O 576 576	0	0
6	C	477	Total O 477 477	0	0
6	D	546	Total O 546 546	0	0

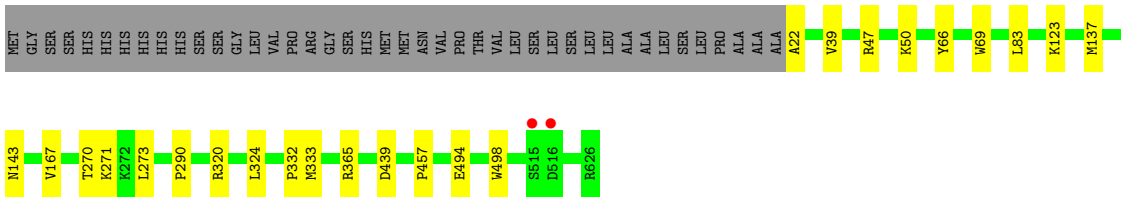
3 Residue-property plots (i)

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: Putative glycyl aminopeptidase

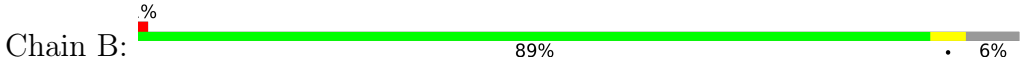
Chain A:

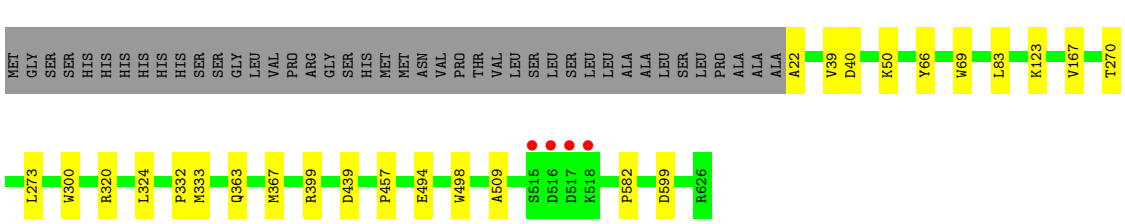




• Molecule 1: Putative glycyl aminopeptidase

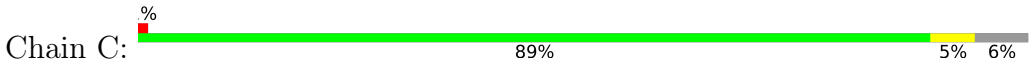
Chain B:

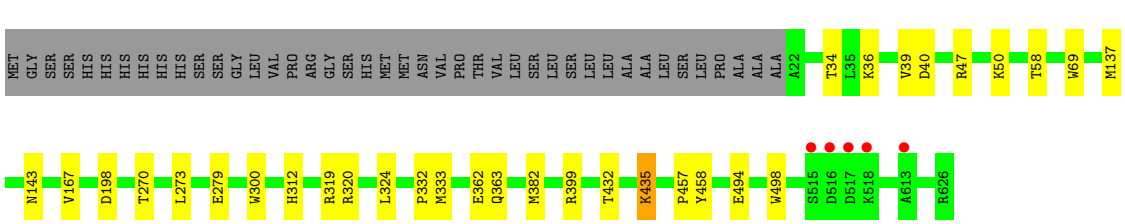




• Molecule 1: Putative glycyl aminopeptidase

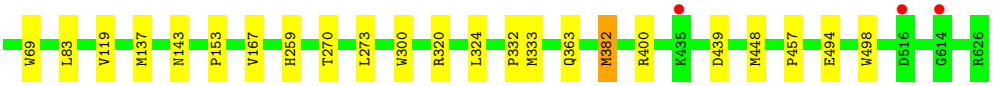
Chain C:





• Molecule 1: Putative glycyl aminopeptidase

Chain D:


W69
L83
V119
M137
N143
P153
V167
H259
T270
L273
W300
R320
L324
P332
M333
Q363
M382
R400
K435
D439
M448
P457
E494
W498
D516
G614
R626

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.01Å 95.20Å 144.49Å 90.00° 104.47° 90.00°	Depositor
Resolution (Å)	44.36 – 1.90 47.08 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.36-1.90) 99.4 (47.08-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.171 , 0.191 0.171 , 0.191	Depositor DCC
R_{free} test set	10806 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	20.5	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21434	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: GOL, ZN, TRS, BES

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	0.30	0/4907	0.51	0/6660
1	B	0.30	0/4901	0.51	0/6652
1	C	0.29	0/4911	0.49	0/6665
1	D	0.29	0/4925	0.51	0/6684
All	All	0.29	0/19644	0.51	0/26661

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4783	0	4640	12	0
1	B	4777	0	4636	14	0
1	C	4787	0	4644	17	0
1	D	4801	0	4652	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	22	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	22	0	22	1	0
3	C	22	0	22	1	0
3	D	22	0	22	0	0
4	B	6	0	8	0	0
5	C	8	0	12	1	0
5	D	8	0	12	0	0
6	A	573	0	0	1	0
6	B	576	0	0	1	0
6	C	477	0	0	2	0
6	D	546	0	0	2	0
All	All	21434	0	18692	60	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 2.

The worst 5 of 60 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:C:432:THR:O	1:C:435:LYS:HE3	2.06	0.55
1:B:399:ARG:NH1	3:B:702:BES:O1	2.31	0.55
1:A:271:LYS:HE2	1:A:290:PRO:HD2	1.90	0.53
1:C:399:ARG:NH1	3:C:702:BES:O1	2.39	0.52
1:A:69:TRP:CE2	1:A:332:PRO:HA	2.46	0.51

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	605/647 (94%)	590 (98%)	15 (2%)	0	100	100
1	B	604/647 (93%)	592 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	606/647 (94%)	593 (98%)	13 (2%)	0	100	100
1	D	607/647 (94%)	593 (98%)	14 (2%)	0	100	100
All	All	2422/2588 (94%)	2368 (98%)	54 (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 of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	501/533 (94%)	499 (100%)	2 (0%)	91	91
1	B	500/533 (94%)	499 (100%)	1 (0%)	93	94
1	C	502/533 (94%)	498 (99%)	4 (1%)	81	82
1	D	503/533 (94%)	500 (99%)	3 (1%)	86	87
All	All	2006/2132 (94%)	1996 (100%)	10 (0%)	88	89

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	143	ASN
1	D	382	MET
1	D	439	ASP
1	C	58	THR
1	C	143	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	BES	D	702	2	22,22,22	1.58	2 (9%)	27,29,29	1.00	1 (3%)
5	TRS	D	703	-	7,7,7	0.31	0	9,9,9	0.42	0
4	GOL	B	703	-	5,5,5	0.93	0	5,5,5	1.13	0
3	BES	A	702	2	22,22,22	1.61	2 (9%)	27,29,29	0.97	1 (3%)
3	BES	C	702	2	22,22,22	1.64	2 (9%)	27,29,29	1.04	1 (3%)
5	TRS	C	703	-	7,7,7	0.32	0	9,9,9	0.56	0
3	BES	B	702	2	22,22,22	1.61	2 (9%)	27,29,29	0.98	2 (7%)

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
3	BES	D	702	2	-	6/24/24/24	0/1/1/1
5	TRS	D	703	-	-	6/9/9/9	-
4	GOL	B	703	-	-	2/4/4/4	-
3	BES	A	702	2	-	9/24/24/24	0/1/1/1
3	BES	C	702	2	-	7/24/24/24	0/1/1/1
5	TRS	C	703	-	-	1/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BES	B	702	2	-	7/24/24/24	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	702	BES	C3-N1	6.06	1.47	1.34
3	B	702	BES	C3-N1	5.94	1.47	1.34
3	A	702	BES	C3-N1	5.85	1.46	1.34
3	D	702	BES	C3-N1	5.58	1.46	1.34
3	D	702	BES	C6-C7	2.92	1.58	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	702	BES	C5-C4-N1	-2.64	104.29	110.55
3	C	702	BES	C6-C1-C2	-2.57	104.41	111.38
3	A	702	BES	C5-C4-N1	-2.30	105.10	110.55
3	B	702	BES	C5-C4-N1	-2.15	105.45	110.55
3	B	702	BES	C6-C1-C2	-2.14	105.56	111.38

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	703	GOL	C1-C2-C3-O3
4	B	703	GOL	O2-C2-C3-O3
5	D	703	TRS	N-C-C1-O1
5	D	703	TRS	N-C-C2-O2
5	D	703	TRS	N-C-C3-O3

There are no ring outliers.

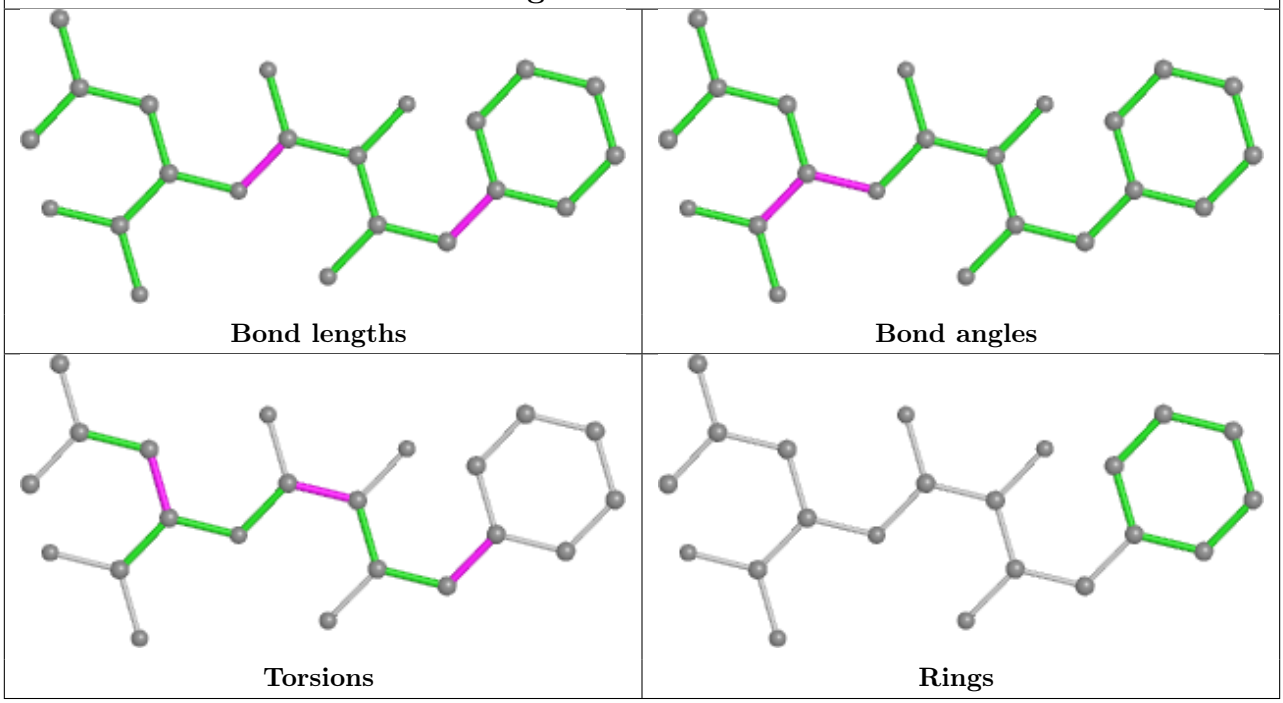
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	BES	1	0
5	C	703	TRS	1	0
3	B	702	BES	1	0

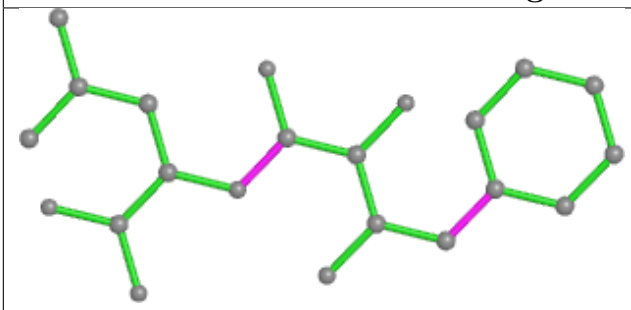
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

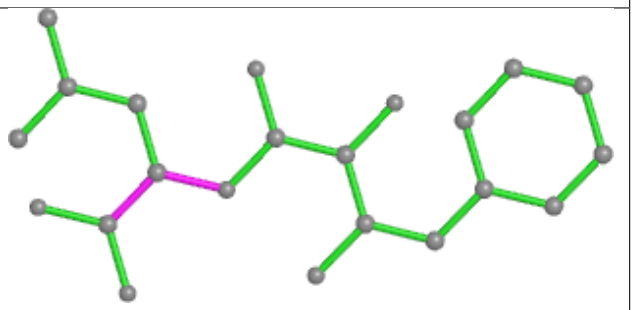
Ligand BES D 702



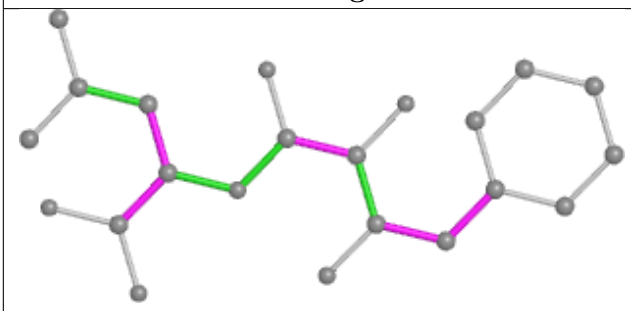
Ligand BES A 702



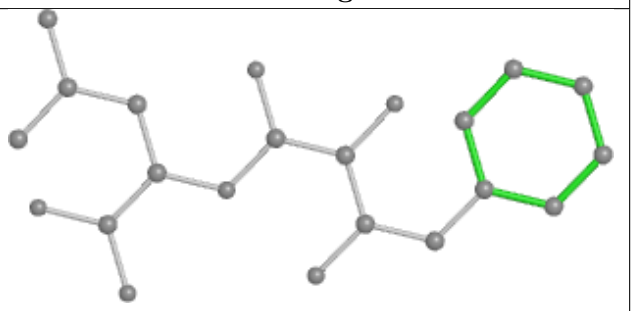
Bond lengths



Bond angles

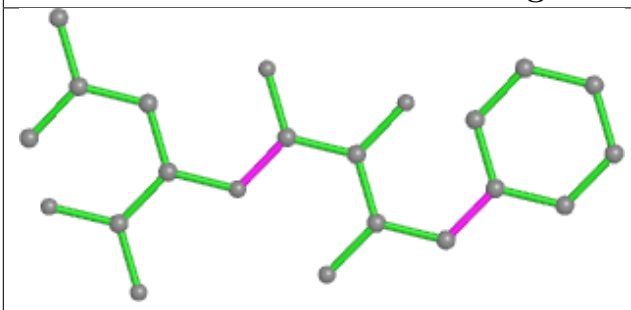


Torsions

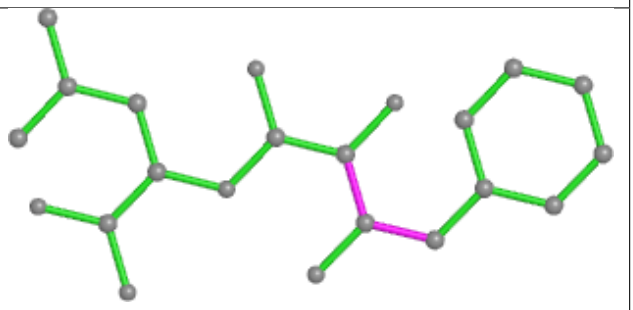


Rings

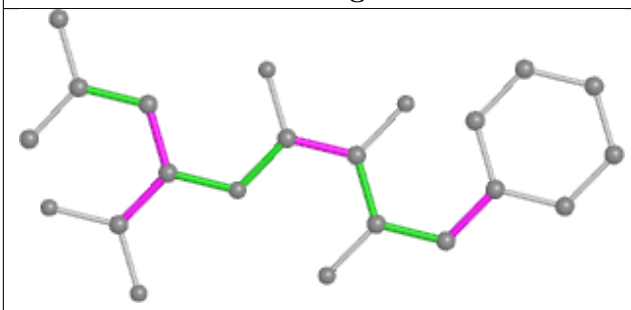
Ligand BES C 702



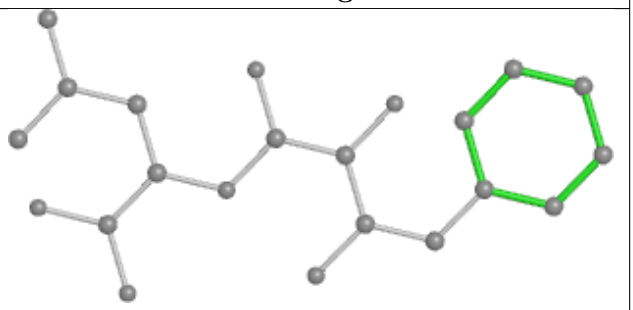
Bond lengths



Bond angles

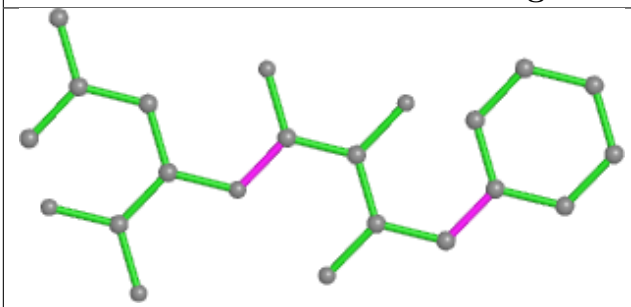


Torsions

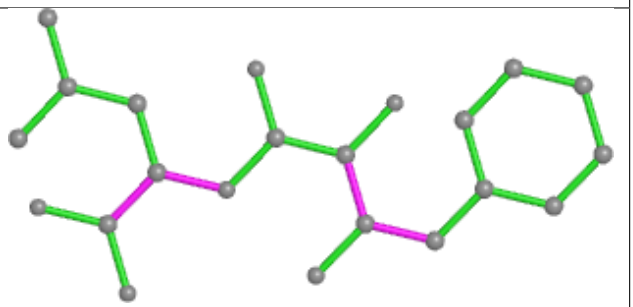


Rings

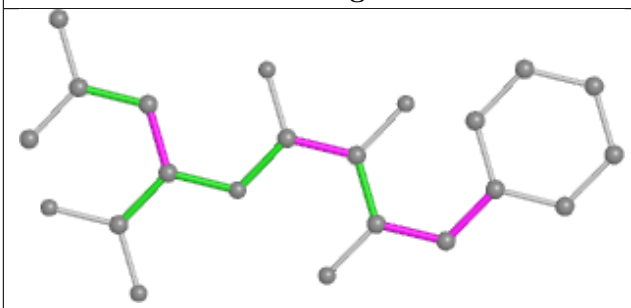
Ligand BES B 702



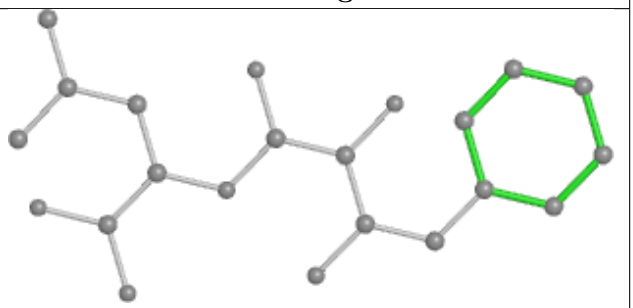
Bond lengths



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	605/647 (93%)	-0.44	2 (0%)	94	94	14, 19, 30, 65	0
1	B	605/647 (93%)	-0.37	4 (0%)	87	88	14, 20, 32, 78	0
1	C	605/647 (93%)	-0.25	5 (0%)	86	87	15, 22, 35, 70	0
1	D	605/647 (93%)	-0.32	3 (0%)	91	92	14, 21, 33, 69	0
All	All	2420/2588 (93%)	-0.34	14 (0%)	89	90	14, 20, 34, 78	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	517	ASP	3.7
1	C	515	SER	3.6
1	C	613	ALA	3.1
1	B	516	ASP	3.1
1	B	518	LYS	2.9

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

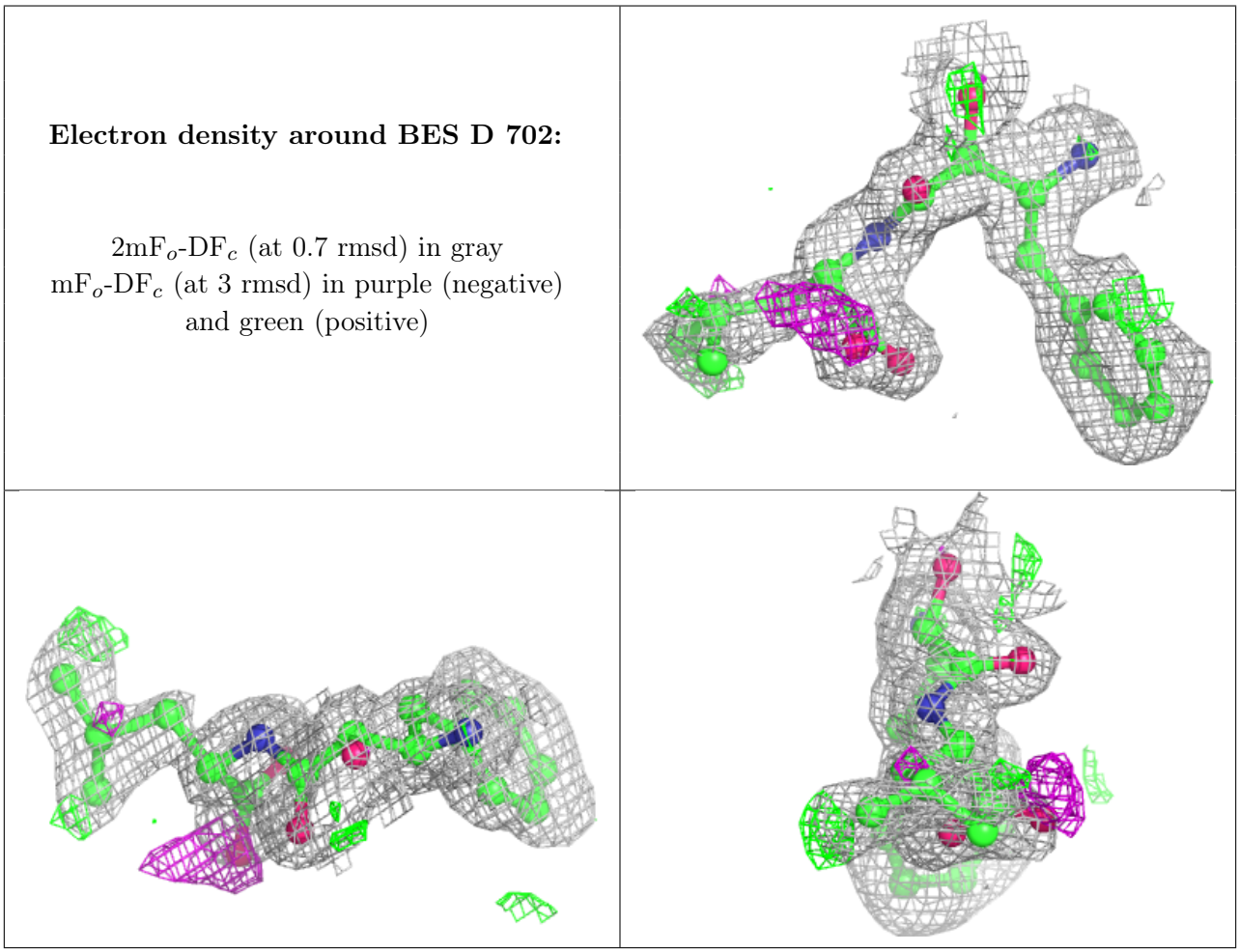
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	TRS	D	703	8/8	0.68	0.18	43,44,44,44	0
5	TRS	C	703	8/8	0.71	0.21	45,46,46,46	0
3	BES	D	702	22/22	0.84	0.18	22,25,36,36	0
4	GOL	B	703	6/6	0.84	0.14	29,30,31,31	0
3	BES	B	702	22/22	0.87	0.15	21,26,35,38	0
3	BES	A	702	22/22	0.88	0.15	20,27,35,37	0
3	BES	C	702	22/22	0.90	0.16	23,30,38,39	0
2	ZN	D	701	1/1	1.00	0.10	19,19,19,19	0
2	ZN	A	701	1/1	1.00	0.07	15,15,15,15	0
2	ZN	B	701	1/1	1.00	0.05	15,15,15,15	0
2	ZN	C	701	1/1	1.00	0.07	19,19,19,19	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.

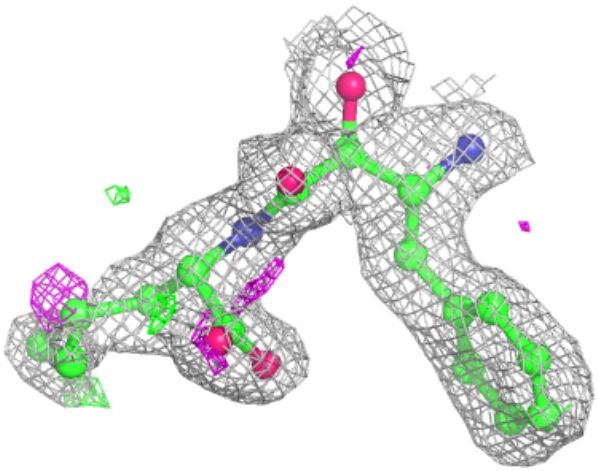
Electron density around BES D 702:

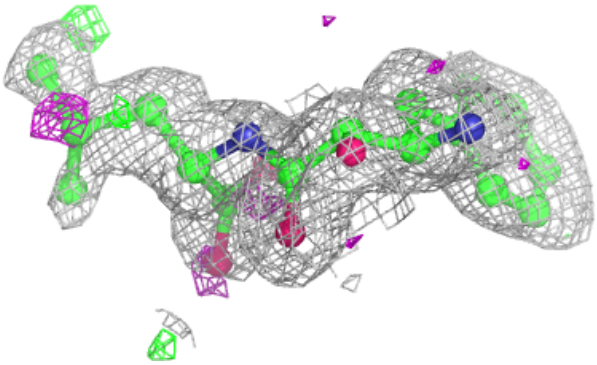
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

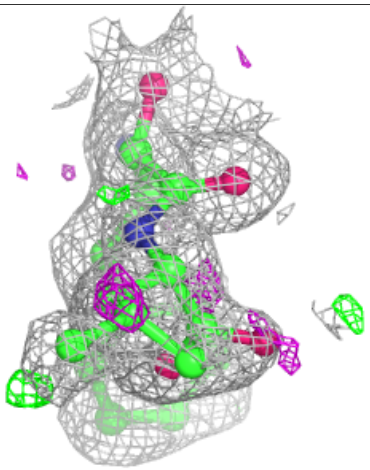


Electron density around BES B 702:

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

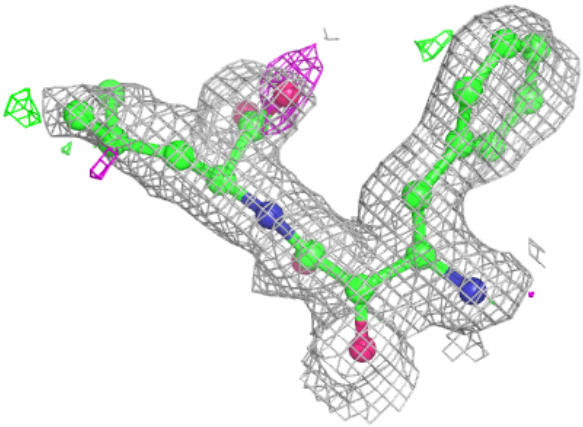


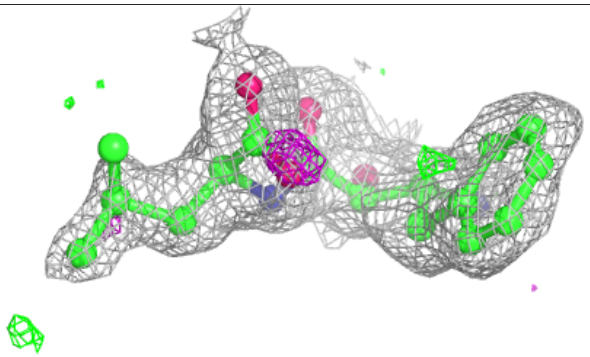




Electron density around BES A 702:

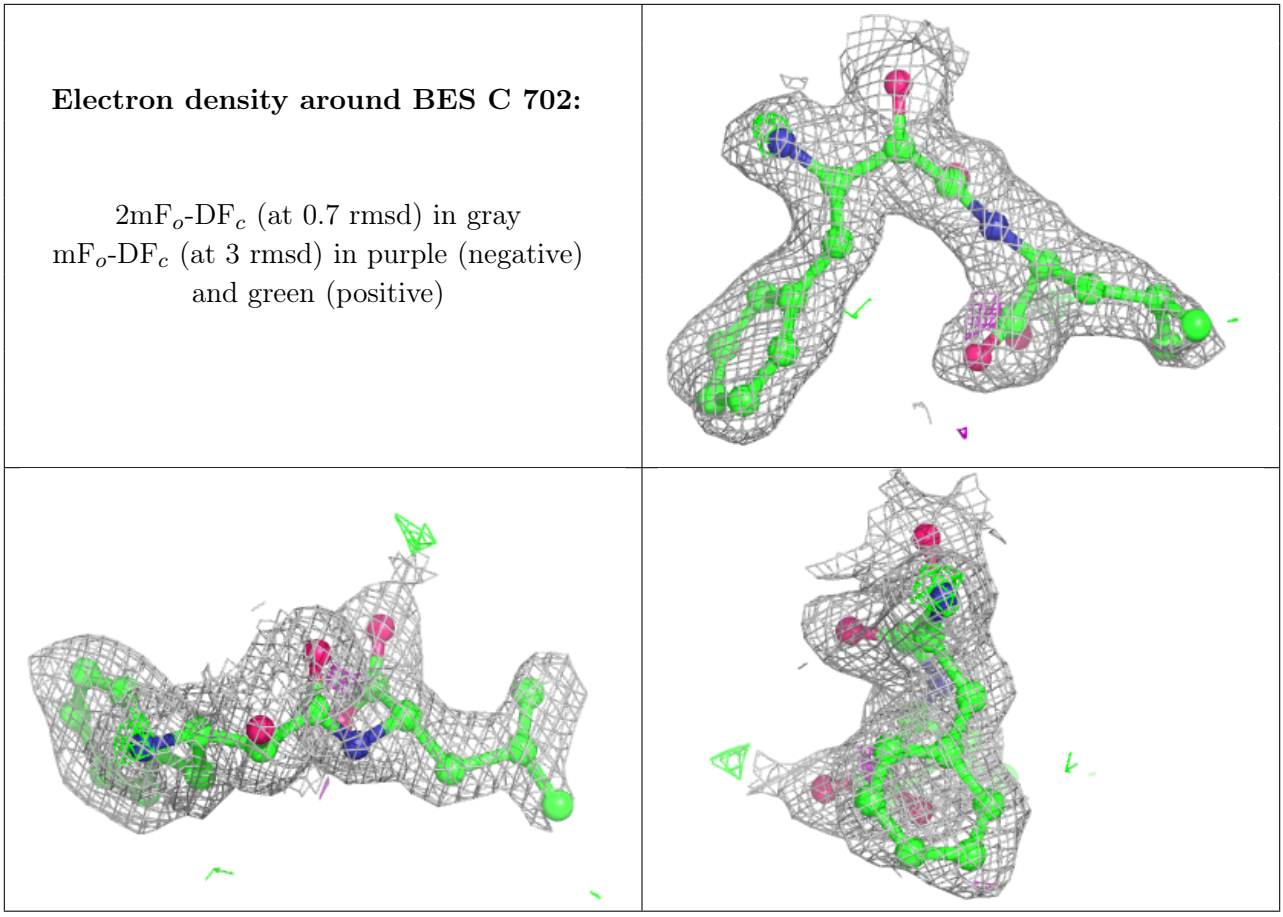
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





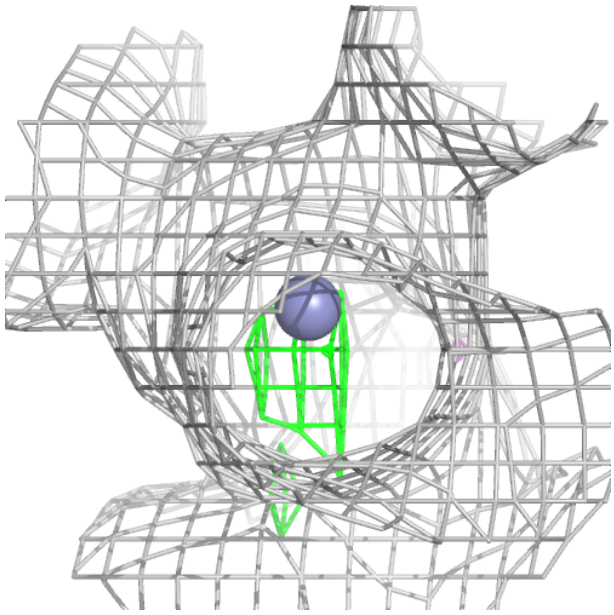
Electron density around BES C 702:

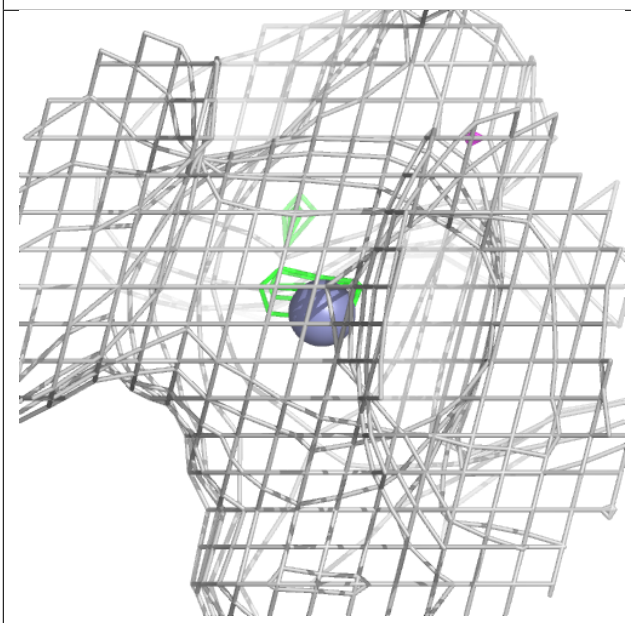
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

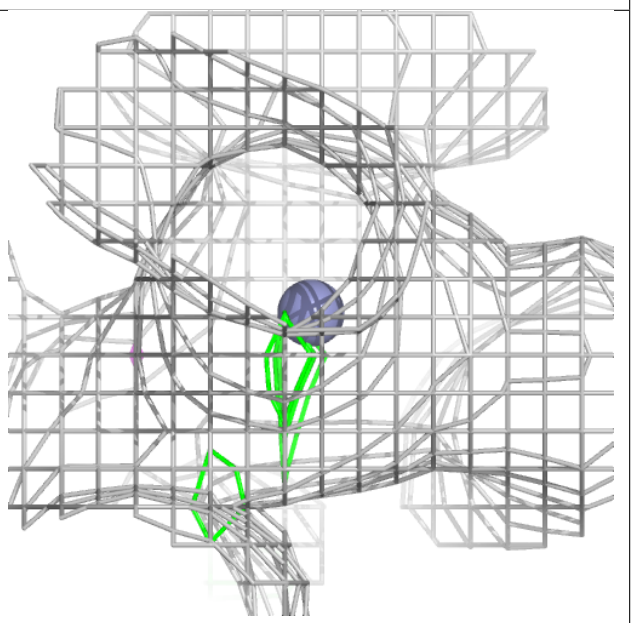


Electron density around ZN D 701:

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

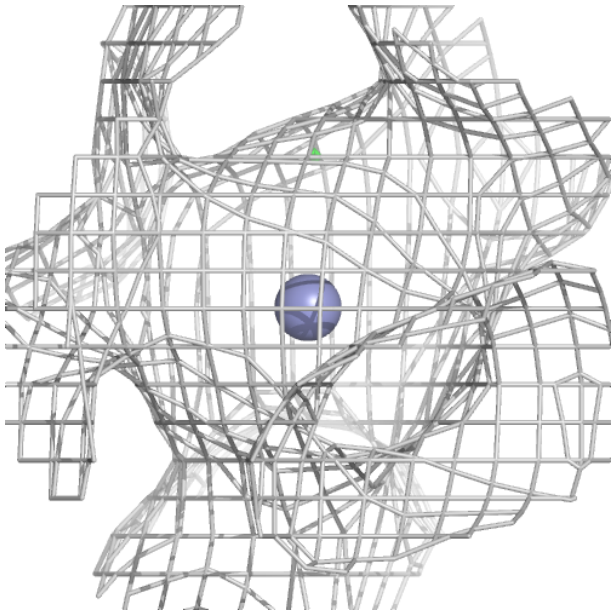


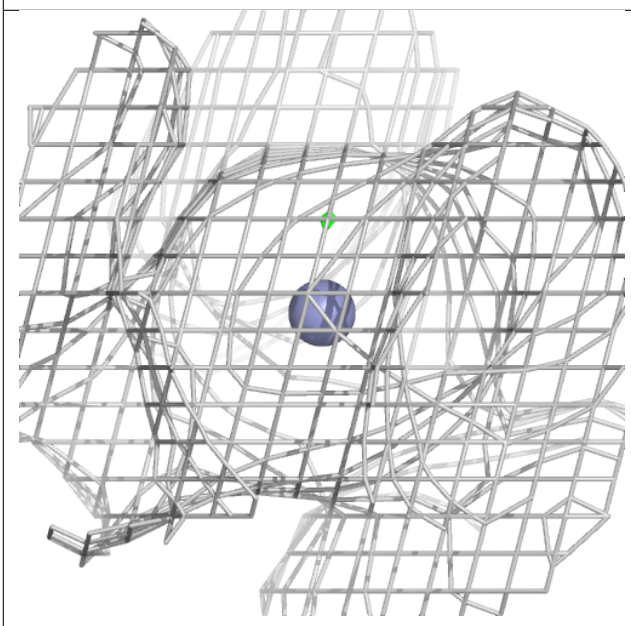




Electron density around ZN A 701:

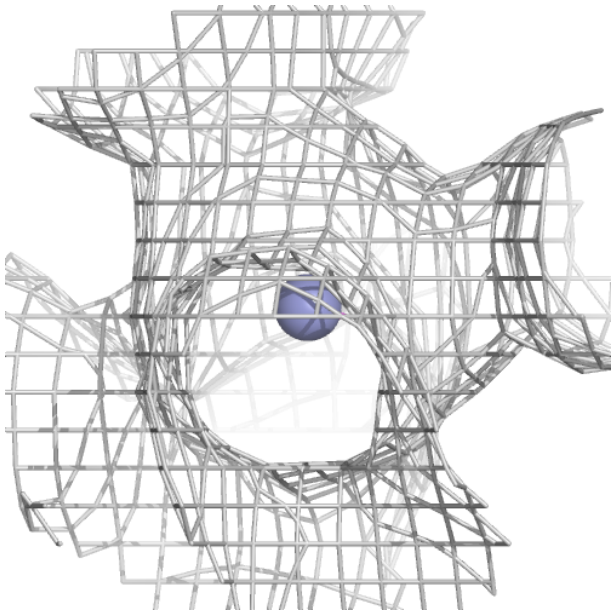
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

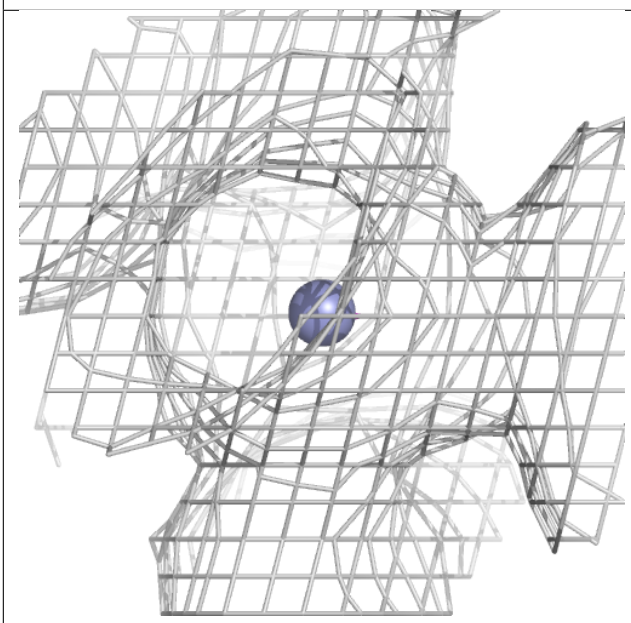


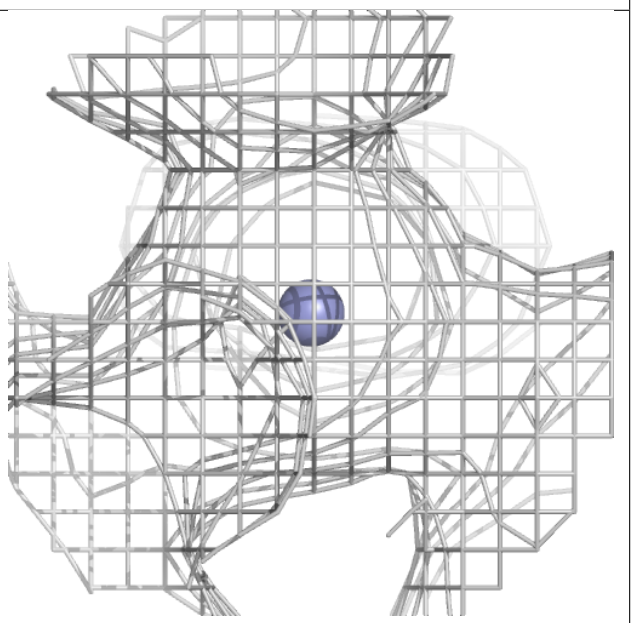


Electron density around ZN B 701:

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

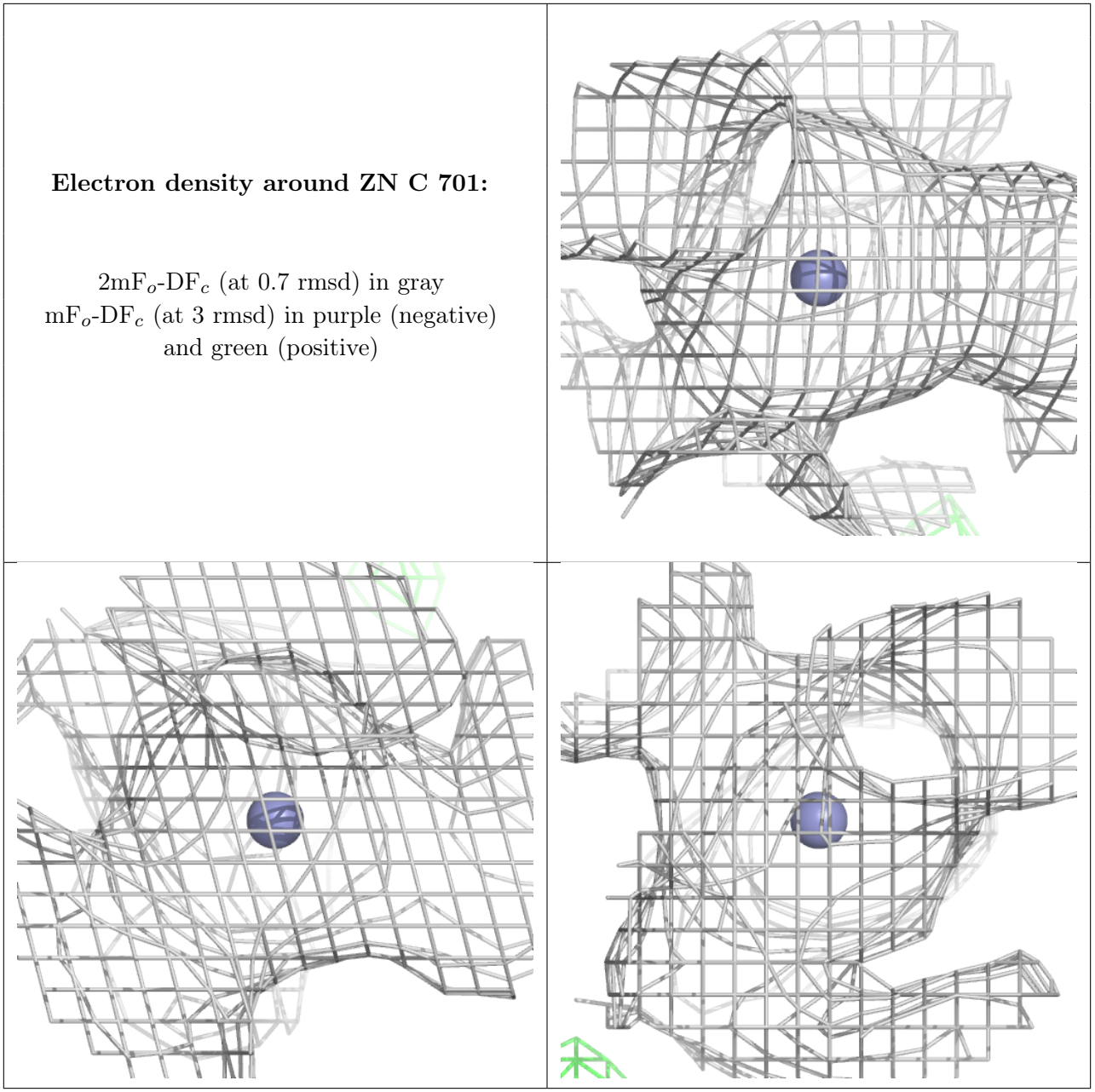






Electron density around ZN C 701:

$2mF_o$-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.