



# Full wwPDB X-ray Structure Validation Report i

Oct 31, 2024 – 12:42 pm GMT

PDB ID : 9GKU  
Title : Crystal Structure of Propanil hydrolase (PrpH) from Sphingomonas sp. Y57  
Authors : Graf, L.G.; Lammers, L.; Palm, G.J.; Schulze, S.  
Deposited on : 2024-08-26  
Resolution : 1.48 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](mailto: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>.

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The following versions of software and data (see [references](#) i) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

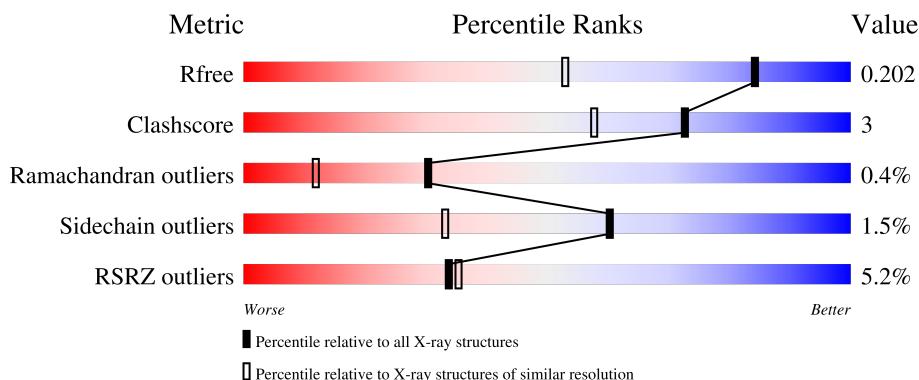
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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))
$R_{free}$	164625	6131 (1.50-1.46)
Clashscore	180529	6623 (1.50-1.46)
Ramachandran outliers	177936	6521 (1.50-1.46)
Sidechain outliers	177891	6518 (1.50-1.46)
RSRZ outliers	164620	6132 (1.50-1.46)

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.



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Mol	Chain	Length	Quality of chain		
1	F	380	3%	90%	8% •
1	G	380	4%	90%	7% •
1	H	380	8%	90%	7% •

## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25009 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 Propanil hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total 2861	C 1806	N 501	O 533	S 21	0	6	0
1	B	371	Total 2856	C 1801	N 506	O 529	S 20	0	3	0
1	C	371	Total 2829	C 1785	N 499	O 526	S 19	0	0	0
1	D	371	Total 2842	C 1794	N 499	O 528	S 21	0	2	0
1	E	369	Total 2839	C 1792	N 500	O 527	S 20	0	3	0
1	F	371	Total 2845	C 1795	N 502	O 528	S 20	0	2	0
1	G	369	Total 2850	C 1800	N 503	O 526	S 21	0	4	0
1	H	368	Total 2817	C 1778	N 496	O 524	S 19	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP G3JWW8
A	1	ALA	-	expression tag	UNP G3JWW8
A	2	HIS	-	expression tag	UNP G3JWW8
A	3	HIS	-	expression tag	UNP G3JWW8
A	4	HIS	-	expression tag	UNP G3JWW8
A	5	HIS	-	expression tag	UNP G3JWW8
A	6	HIS	-	expression tag	UNP G3JWW8
A	7	HIS	-	expression tag	UNP G3JWW8
A	8	VAL	-	expression tag	UNP G3JWW8
A	9	GLY	-	expression tag	UNP G3JWW8
A	10	THR	-	expression tag	UNP G3JWW8
B	0	MET	-	initiating methionine	UNP G3JWW8
B	1	ALA	-	expression tag	UNP G3JWW8

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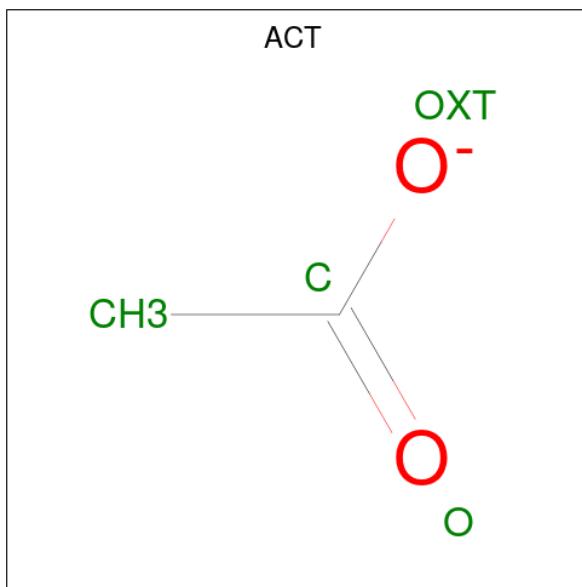
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	HIS	-	expression tag	UNP G3JWW8
B	3	HIS	-	expression tag	UNP G3JWW8
B	4	HIS	-	expression tag	UNP G3JWW8
B	5	HIS	-	expression tag	UNP G3JWW8
B	6	HIS	-	expression tag	UNP G3JWW8
B	7	HIS	-	expression tag	UNP G3JWW8
B	8	VAL	-	expression tag	UNP G3JWW8
B	9	GLY	-	expression tag	UNP G3JWW8
B	10	THR	-	expression tag	UNP G3JWW8
C	0	MET	-	initiating methionine	UNP G3JWW8
C	1	ALA	-	expression tag	UNP G3JWW8
C	2	HIS	-	expression tag	UNP G3JWW8
C	3	HIS	-	expression tag	UNP G3JWW8
C	4	HIS	-	expression tag	UNP G3JWW8
C	5	HIS	-	expression tag	UNP G3JWW8
C	6	HIS	-	expression tag	UNP G3JWW8
C	7	HIS	-	expression tag	UNP G3JWW8
C	8	VAL	-	expression tag	UNP G3JWW8
C	9	GLY	-	expression tag	UNP G3JWW8
C	10	THR	-	expression tag	UNP G3JWW8
D	0	MET	-	initiating methionine	UNP G3JWW8
D	1	ALA	-	expression tag	UNP G3JWW8
D	2	HIS	-	expression tag	UNP G3JWW8
D	3	HIS	-	expression tag	UNP G3JWW8
D	4	HIS	-	expression tag	UNP G3JWW8
D	5	HIS	-	expression tag	UNP G3JWW8
D	6	HIS	-	expression tag	UNP G3JWW8
D	7	HIS	-	expression tag	UNP G3JWW8
D	8	VAL	-	expression tag	UNP G3JWW8
D	9	GLY	-	expression tag	UNP G3JWW8
D	10	THR	-	expression tag	UNP G3JWW8
E	0	MET	-	initiating methionine	UNP G3JWW8
E	1	ALA	-	expression tag	UNP G3JWW8
E	2	HIS	-	expression tag	UNP G3JWW8
E	3	HIS	-	expression tag	UNP G3JWW8
E	4	HIS	-	expression tag	UNP G3JWW8
E	5	HIS	-	expression tag	UNP G3JWW8
E	6	HIS	-	expression tag	UNP G3JWW8
E	7	HIS	-	expression tag	UNP G3JWW8
E	8	VAL	-	expression tag	UNP G3JWW8
E	9	GLY	-	expression tag	UNP G3JWW8
E	10	THR	-	expression tag	UNP G3JWW8

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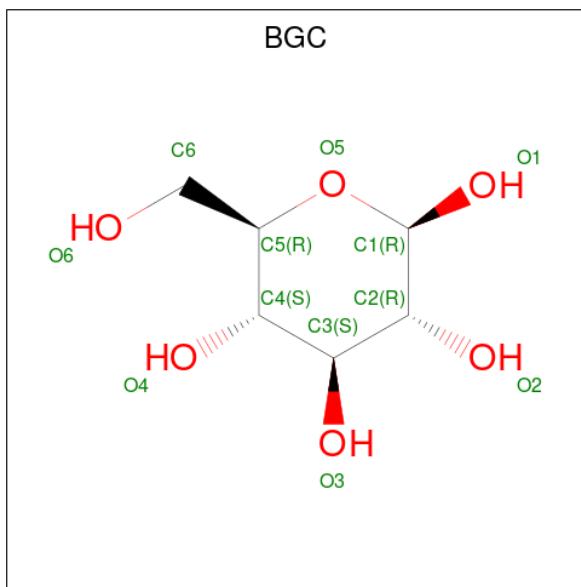
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	MET	-	initiating methionine	UNP G3JWV8
F	1	ALA	-	expression tag	UNP G3JWV8
F	2	HIS	-	expression tag	UNP G3JWV8
F	3	HIS	-	expression tag	UNP G3JWV8
F	4	HIS	-	expression tag	UNP G3JWV8
F	5	HIS	-	expression tag	UNP G3JWV8
F	6	HIS	-	expression tag	UNP G3JWV8
F	7	HIS	-	expression tag	UNP G3JWV8
F	8	VAL	-	expression tag	UNP G3JWV8
F	9	GLY	-	expression tag	UNP G3JWV8
F	10	THR	-	expression tag	UNP G3JWV8
G	0	MET	-	initiating methionine	UNP G3JWV8
G	1	ALA	-	expression tag	UNP G3JWV8
G	2	HIS	-	expression tag	UNP G3JWV8
G	3	HIS	-	expression tag	UNP G3JWV8
G	4	HIS	-	expression tag	UNP G3JWV8
G	5	HIS	-	expression tag	UNP G3JWV8
G	6	HIS	-	expression tag	UNP G3JWV8
G	7	HIS	-	expression tag	UNP G3JWV8
G	8	VAL	-	expression tag	UNP G3JWV8
G	9	GLY	-	expression tag	UNP G3JWV8
G	10	THR	-	expression tag	UNP G3JWV8
H	0	MET	-	initiating methionine	UNP G3JWV8
H	1	ALA	-	expression tag	UNP G3JWV8
H	2	HIS	-	expression tag	UNP G3JWV8
H	3	HIS	-	expression tag	UNP G3JWV8
H	4	HIS	-	expression tag	UNP G3JWV8
H	5	HIS	-	expression tag	UNP G3JWV8
H	6	HIS	-	expression tag	UNP G3JWV8
H	7	HIS	-	expression tag	UNP G3JWV8
H	8	VAL	-	expression tag	UNP G3JWV8
H	9	GLY	-	expression tag	UNP G3JWV8
H	10	THR	-	expression tag	UNP G3JWV8

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0

- Molecule 3 is beta-D-glucopyranose (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0
3	B	1	Total C O 12 6 6	0	0
3	C	1	Total C O 12 6 6	0	0
3	C	1	Total C O 12 6 6	0	0
3	E	1	Total C O 12 6 6	0	0
3	E	1	Total C O 12 6 6	0	0
3	F	1	Total C O 12 6 6	0	0
3	G	1	Total C O 12 6 6	0	0
3	H	1	Total C O 12 6 6	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	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	E	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0
4	G	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0
5	E	1	Total K 1 1	0	0
5	F	1	Total K 1 1	0	0
5	G	1	Total K 1 1	0	0
5	H	1	Total K 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	267	Total O 267 267	0	0
6	B	215	Total O 215 215	0	0
6	C	253	Total O 253 253	0	0

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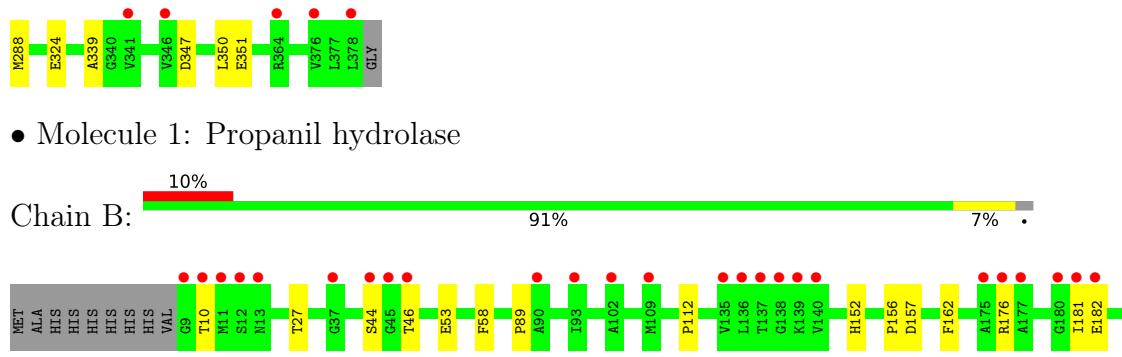
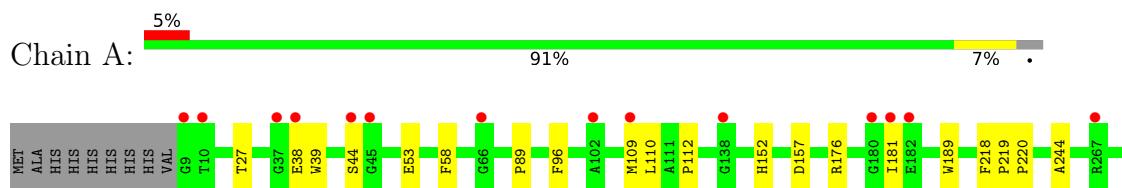
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	264	Total O 264 264	0	0
6	E	308	Total O 308 308	0	0
6	F	327	Total O 327 327	0	0
6	G	252	Total O 252 252	0	0
6	H	228	Total O 228 228	0	0

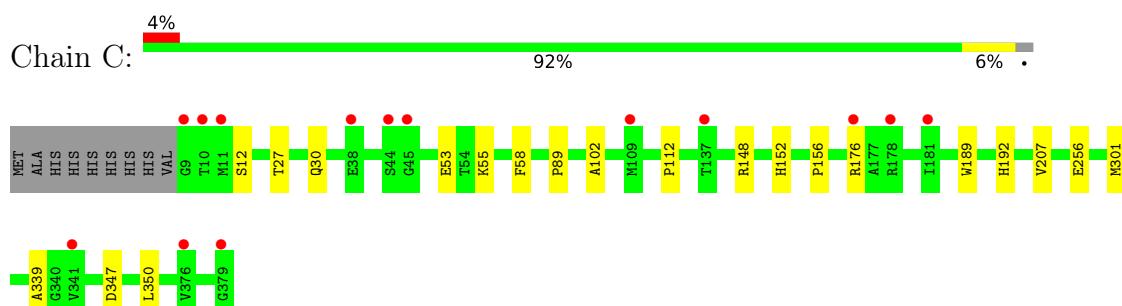
### 3 Residue-property plots (i)

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: Propanil hydrolase



- Molecule 1: Propanil hydrolase

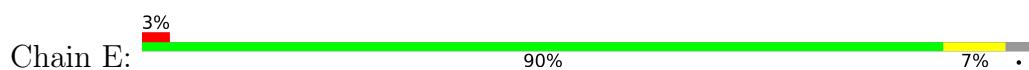


- Molecule 1: Propanil hydrolase

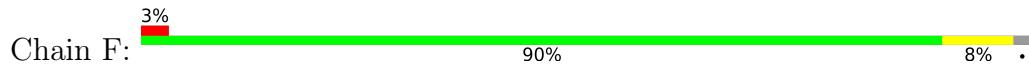




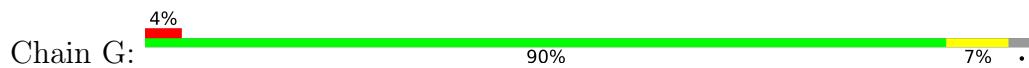
- Molecule 1: Propanil hydrolase



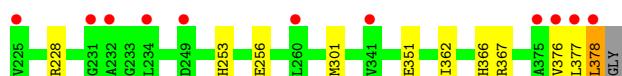
- Molecule 1: Propanil hydrolase



- Molecule 1: Propanil hydrolase



- Molecule 1: Propanil hydrolase



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.86 Å    103.70 Å    104.50 Å 113.60°    93.00°    120.61°	Depositor
Resolution (Å)	44.56 – 1.48 44.56 – 1.48	Depositor EDS
% Data completeness (in resolution range)	91.1 (44.56-1.48) 91.1 (44.56-1.48)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.05 (at 1.48 Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
$R$ , $R_{free}$	0.173 , 0.199 0.176 , 0.202	Depositor DCC
$R_{free}$ test set	27259 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 33.1	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50$ , $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for k,h,-h-k-l 0.005 for -h-k-l,l,k 0.064 for l,-h-k-l,h	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	25009	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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: K, BGC, ZN, ACT

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	0.33	0/2948	0.63	0/4009
1	B	0.31	0/2931	0.60	0/3984
1	C	0.32	0/2898	0.62	0/3942
1	D	0.31	0/2917	0.61	1/3966 (0.0%)
1	E	0.34	0/2917	0.64	0/3966
1	F	0.33	0/2920	0.64	0/3970
1	G	0.34	0/2931	0.64	0/3984
1	H	0.32	0/2886	0.61	0/3926
All	All	0.33	0/23348	0.62	1/31747 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	PHE	CB-CG-CD1	5.08	124.36	120.80

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	2861	0	2789	17	0
1	B	2856	0	2783	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2829	0	2747	13	0
1	D	2842	0	2767	13	0
1	E	2839	0	2765	18	0
1	F	2845	0	2771	27	0
1	G	2850	0	2787	19	0
1	H	2817	0	2736	17	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
2	F	4	0	3	0	0
2	G	4	0	3	0	0
2	H	4	0	3	0	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
3	C	24	0	24	2	0
3	E	24	0	24	0	0
3	F	12	0	12	3	0
3	G	12	0	12	2	0
3	H	12	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	267	0	0	7	3
6	B	215	0	0	5	0
6	C	253	0	0	4	1
6	D	264	0	0	6	5
6	E	308	0	0	10	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	327	0	0	17	4
6	G	252	0	0	10	3
6	H	228	0	0	9	6
All	All	25009	0	22277	139	12

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 3.

All (139) 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:D:267:ARG:NH2	6:D:501:HOH:O	1.96	0.98
1:F:364:ARG:NH2	6:F:501:HOH:O	2.07	0.88
1:F:361:ARG:O	6:F:501:HOH:O	1.90	0.87
1:F:53:GLU:OE2	6:F:502:HOH:O	1.95	0.85
1:B:176:ARG:NH1	1:B:181:ILE:O	2.11	0.84
1:E:267:ARG:NH1	6:E:502:HOH:O	2.10	0.83
1:G:228:ARG:NH1	6:G:502:HOH:O	2.12	0.82
1:H:351:GLU:OE1	6:H:501:HOH:O	1.98	0.82
1:D:30:GLN:NE2	6:D:502:HOH:O	2.09	0.82
1:B:44:SER:OG	6:B:501:HOH:O	2.00	0.79
1:B:181:ILE:HD11	1:B:269:ASP:HB2	1.65	0.79
1:D:228:ARG:NH2	6:D:505:HOH:O	2.15	0.79
1:E:267:ARG:NH2	6:E:504:HOH:O	2.17	0.77
1:E:30:GLN:NE2	6:E:503:HOH:O	2.16	0.76
1:C:30:GLN:NE2	6:C:501:HOH:O	2.05	0.76
1:G:183:ARG:NH1	6:G:504:HOH:O	2.17	0.76
1:F:63[A]:ARG:NH1	6:F:506:HOH:O	2.19	0.76
3:G:402:BGC:O1	6:G:501:HOH:O	2.04	0.75
1:B:46:THR:HG23	1:G:46:THR:H	1.52	0.75
1:F:355:LEU:HD22	6:F:763:HOH:O	1.87	0.75
1:C:339:ALA:O	6:C:502:HOH:O	2.07	0.72
1:H:366:HIS:NE2	6:H:503:HOH:O	2.24	0.70
1:B:293:GLU:OE1	6:B:502:HOH:O	2.09	0.69
1:H:77:GLU:O	6:H:502:HOH:O	2.11	0.69
3:C:402:BGC:O6	3:C:402:BGC:O4	2.08	0.68
1:A:351:GLU:OE2	6:A:502:HOH:O	2.10	0.68
1:A:44:SER:OG	6:A:501:HOH:O	2.09	0.68
1:F:267:ARG:NH2	6:F:511:HOH:O	2.29	0.66
1:D:293:GLU:OE2	6:D:503:HOH:O	2.13	0.65
1:F:44:SER:OG	6:F:504:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:MET:HG2	1:A:110:LEU:HD13	1.80	0.63
1:B:162:PHE:O	6:B:503:HOH:O	2.16	0.62
1:G:60:ASN:ND2	6:G:510:HOH:O	2.34	0.61
1:F:53:GLU:HG2	6:F:769:HOH:O	2.00	0.60
1:E:11:MET:HG3	1:E:70:ARG:HG2	1.84	0.60
1:E:309:LEU:HD23	6:E:504:HOH:O	2.03	0.59
1:E:53:GLU:HG2	6:E:745:HOH:O	2.03	0.58
1:A:244:ALA:HA	1:A:288[B]:MET:HE2	1.86	0.58
1:E:371:ASP:OD2	6:E:505:HOH:O	2.17	0.58
1:A:157[A]:ASP:OD1	6:A:503:HOH:O	2.17	0.57
1:G:351:GLU:CD	1:G:351:GLU:H	2.07	0.57
1:G:351:GLU:OE1	6:G:503:HOH:O	2.17	0.57
1:E:267:ARG:HB2	6:E:587:HOH:O	2.03	0.57
1:A:244:ALA:HA	1:A:288[B]:MET:CE	2.35	0.57
1:H:362:ILE:HG23	6:H:503:HOH:O	2.04	0.57
1:H:12:SER:O	1:H:13:ASN:HB2	2.04	0.56
1:D:27:THR:HB	1:D:112:PRO:HG2	1.88	0.56
1:A:339:ALA:O	6:A:504:HOH:O	2.18	0.56
1:C:256:GLU:HG3	1:C:301:MET:HE3	1.88	0.55
1:B:365:PHE:HE2	1:G:362:ILE:HD13	1.71	0.55
1:H:376:VAL:C	1:H:378:LEU:H	2.08	0.55
1:F:176:ARG:NH2	6:F:507:HOH:O	2.26	0.55
1:A:27:THR:HB	1:A:112:PRO:HG2	1.89	0.54
1:C:192:HIS:CE1	3:C:402:BGC:O4	2.60	0.54
1:H:215:ASP:HB3	6:H:695:HOH:O	2.06	0.54
1:G:198:GLN:HE21	3:G:402:BGC:C6	2.21	0.54
1:G:336:GLU:HB3	6:G:516:HOH:O	2.08	0.54
6:D:501:HOH:O	1:G:183:ARG:HB2	2.07	0.53
1:A:324:GLU:OE1	6:A:505:HOH:O	2.18	0.53
1:A:53:GLU:HG2	6:A:726:HOH:O	2.09	0.53
1:D:10:THR:HG22	1:D:11:MET:N	2.24	0.53
1:B:27:THR:HB	1:B:112:PRO:HG2	1.91	0.52
1:F:304:ASP:HB3	6:F:532:HOH:O	2.08	0.52
1:H:178:ARG:HD2	1:H:179:HIS:CE1	2.44	0.52
1:A:176:ARG:NH1	6:A:508:HOH:O	2.25	0.52
1:C:53:GLU:OE1	6:C:504:HOH:O	2.19	0.51
1:B:352:MET:HE1	6:G:750:HOH:O	2.10	0.51
6:B:556:HOH:O	1:G:216:ARG:HD3	2.09	0.51
1:F:198:GLN:NE2	3:F:402:BGC:O6	2.41	0.51
1:D:53:GLU:HG2	6:D:723:HOH:O	2.10	0.50
1:F:206:ASP:O	6:F:507:HOH:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:HG2	1:A:39:TRP:CE2	2.48	0.49
1:H:376:VAL:O	1:H:378:LEU:N	2.40	0.49
1:G:347:ASP:HB3	1:G:350:LEU:HG	1.94	0.49
1:E:26:SER:OG	6:E:501:HOH:O	2.10	0.49
1:F:48:GLY:N	6:F:508:HOH:O	2.45	0.49
1:E:27:THR:HB	1:E:112:PRO:HG2	1.96	0.48
1:G:10:THR:O	1:G:11:MET:HB2	2.14	0.48
1:G:361[A]:ARG:NH1	6:G:517:HOH:O	2.44	0.48
1:H:27:THR:HB	1:H:112:PRO:HG2	1.94	0.47
1:D:256:GLU:HG3	1:D:301:MET:HE3	1.96	0.47
1:F:261:PRO:HB2	1:F:378:LEU:HD13	1.97	0.47
1:H:253:HIS:CD2	1:H:367:ARG:HG2	2.50	0.47
1:G:27:THR:HB	1:G:112:PRO:HG2	1.97	0.47
1:G:253:HIS:CD2	1:G:367:ARG:HG2	2.50	0.46
1:C:27:THR:HB	1:C:112:PRO:HG2	1.96	0.46
1:E:176:ARG:NH1	6:E:506:HOH:O	2.18	0.46
1:F:176:ARG:NH1	6:F:507:HOH:O	2.43	0.45
1:F:198:GLN:HG2	3:F:402:BGC:H6C2	1.98	0.45
1:H:129:ARG:NH1	6:H:502:HOH:O	2.22	0.45
1:C:347:ASP:HB3	1:C:350:LEU:HG	1.99	0.45
1:F:27:THR:HB	1:F:112:PRO:HG2	1.98	0.45
1:F:198:GLN:HE21	3:F:402:BGC:C6	2.30	0.45
1:F:355:LEU:CD2	6:F:763:HOH:O	2.53	0.45
1:B:218:PHE:HA	1:B:219:PRO:C	2.36	0.44
1:C:176:ARG:HH22	1:C:207:VAL:HG23	1.82	0.44
1:D:182:GLU:HB3	1:D:269:ASP:OD2	2.17	0.44
1:F:243:PRO:HB2	6:F:509:HOH:O	2.17	0.44
1:E:261:PRO:HB2	1:E:378:LEU:HD13	1.99	0.44
1:G:53:GLU:HG2	6:G:713:HOH:O	2.17	0.44
1:D:55:LYS:HD3	1:D:148:ARG:HD2	2.00	0.43
1:F:184:VAL:HG23	6:F:541:HOH:O	2.17	0.43
1:H:256:GLU:HG3	1:H:301:MET:HE1	2.01	0.43
1:B:89:PRO:HD2	1:B:156:PRO:O	2.18	0.43
1:B:181:ILE:HD12	1:B:182:GLU:H	1.83	0.43
1:E:191:VAL:HG11	1:E:286:ALA:HB2	1.99	0.43
1:D:360:ASP:HB3	1:D:364:ARG:NH1	2.34	0.43
1:C:256:GLU:HG3	1:C:301:MET:CE	2.49	0.43
1:C:176:ARG:HH22	1:C:207:VAL:CG2	2.32	0.43
1:D:13:ASN:N	1:D:13:ASN:OD1	2.51	0.43
1:H:228:ARG:NE	6:H:514:HOH:O	2.45	0.43
1:B:53:GLU:HG2	6:B:691:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:GLU:HG3	1:E:39:TRP:CE2	2.54	0.42
1:F:191:VAL:HG11	1:F:286:ALA:HB2	2.00	0.42
1:F:361:ARG:HE	1:F:364:ARG:HH21	1.67	0.42
1:E:256:GLU:HG3	1:E:301:MET:HE3	2.01	0.42
1:A:218:PHE:HA	1:A:219:PRO:C	2.40	0.42
1:B:355:LEU:HD22	1:F:90:ALA:HB1	2.02	0.42
1:F:218:PHE:HA	1:F:219:PRO:C	2.41	0.42
1:F:361:ARG:HG3	6:F:501:HOH:O	2.20	0.42
1:B:257:THR:O	1:B:378:LEU:HD11	2.20	0.41
1:D:218:PHE:HA	1:D:219:PRO:C	2.39	0.41
1:H:228:ARG:HH22	1:H:378:LEU:HD22	1.84	0.41
1:H:362:ILE:HG12	6:H:674:HOH:O	2.20	0.41
1:G:375:ALA:O	1:G:378:LEU:HB2	2.20	0.41
1:A:89:PRO:HG3	1:A:157[B]:ASP:OD1	2.20	0.41
1:A:347:ASP:HB3	1:A:350:LEU:HG	2.02	0.41
1:C:12:SER:HB2	6:C:502:HOH:O	2.20	0.41
1:C:89:PRO:HD2	1:C:156:PRO:O	2.21	0.41
1:B:188:ASP:HA	1:B:274:ALA:HB3	2.03	0.41
1:A:219:PRO:HA	1:A:220:PRO:HD3	1.95	0.41
1:E:47:TYR:HE2	6:E:501:HOH:O	2.04	0.41
1:C:55:LYS:HD3	1:C:148:ARG:HD2	2.02	0.41
1:F:219:PRO:HA	1:F:220:PRO:HD3	1.92	0.41
1:H:53:GLU:HG2	6:H:690:HOH:O	2.21	0.41
1:G:342:ARG:HD2	6:G:516:HOH:O	2.21	0.41
1:E:188:ASP:HA	1:E:274:ALA:HB3	2.04	0.40
1:A:176:ARG:NH1	1:A:181:ILE:O	2.54	0.40
1:E:176:ARG:NH1	1:E:181:ILE:O	2.54	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:594:HOH:O	6:F:502:HOH:O[1_566]	1.79	0.41
6:D:722:HOH:O	6:H:586:HOH:O[1_454]	1.84	0.36
6:A:565:HOH:O	6:F:735:HOH:O[1_566]	1.85	0.35
6:E:529:HOH:O	6:G:547:HOH:O[1_665]	2.00	0.20
6:D:504:HOH:O	6:H:503:HOH:O[1_454]	2.01	0.19
6:D:726:HOH:O	6:H:633:HOH:O[1_454]	2.04	0.16
6:C:730:HOH:O	6:G:681:HOH:O[1_665]	2.07	0.13
6:A:505:HOH:O	6:F:572:HOH:O[1_566]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:733:HOH:O	6:H:503:HOH:O[1_454]	2.09	0.11
6:E:531:HOH:O	6:G:514:HOH:O[1_665]	2.12	0.08
6:D:528:HOH:O	6:H:574:HOH:O[1_454]	2.13	0.07
6:F:696:HOH:O	6:H:608:HOH:O[1_444]	2.17	0.03

## 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	374/380 (98%)	365 (98%)	9 (2%)	0	100 100
1	B	372/380 (98%)	359 (96%)	12 (3%)	1 (0%)	37 17
1	C	369/380 (97%)	360 (98%)	8 (2%)	1 (0%)	37 17
1	D	371/380 (98%)	358 (96%)	10 (3%)	3 (1%)	16 4
1	E	370/380 (97%)	361 (98%)	9 (2%)	0	100 100
1	F	371/380 (98%)	360 (97%)	10 (3%)	1 (0%)	37 17
1	G	371/380 (98%)	360 (97%)	9 (2%)	2 (0%)	25 8
1	H	366/380 (96%)	352 (96%)	11 (3%)	3 (1%)	16 4
All	All	2964/3040 (98%)	2875 (97%)	78 (3%)	11 (0%)	30 12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	THR
1	G	11	MET
1	H	377	LEU
1	D	180	GLY
1	F	102	ALA
1	H	180	GLY
1	D	10	THR
1	D	102	ALA

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Mol	Chain	Res	Type
1	G	102	ALA
1	C	102	ALA
1	H	102	ALA

### 5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	299/301 (99%)	295 (99%)	4 (1%)	65 39
1	B	296/301 (98%)	292 (99%)	4 (1%)	62 36
1	C	292/301 (97%)	289 (99%)	3 (1%)	73 50
1	D	295/301 (98%)	289 (98%)	6 (2%)	50 20
1	E	295/301 (98%)	292 (99%)	3 (1%)	73 50
1	F	295/301 (98%)	291 (99%)	4 (1%)	62 36
1	G	297/301 (99%)	292 (98%)	5 (2%)	56 27
1	H	292/301 (97%)	287 (98%)	5 (2%)	56 27
All	All	2361/2408 (98%)	2327 (99%)	34 (1%)	60 36

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	PHE
1	A	96	PHE
1	A	152	HIS
1	A	189	TRP
1	B	58	PHE
1	B	152	HIS
1	B	157	ASP
1	B	189	TRP
1	C	58	PHE
1	C	152	HIS
1	C	189	TRP
1	D	13	ASN

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Mol	Chain	Res	Type
1	D	44	SER
1	D	58	PHE
1	D	96	PHE
1	D	152	HIS
1	D	189	TRP
1	E	58	PHE
1	E	152	HIS
1	E	189	TRP
1	F	58	PHE
1	F	152	HIS
1	F	178	ARG
1	F	189	TRP
1	G	58	PHE
1	G	152	HIS
1	G	189	TRP
1	G	265	ARG
1	G	269	ASP
1	H	58	PHE
1	H	96	PHE
1	H	152	HIS
1	H	189	TRP
1	H	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	C	13	ASN
1	E	13	ASN
1	F	13	ASN

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

Of 33 ligands modelled in this entry, 16 are monoatomic - leaving 17 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
2	ACT	H	401	4	3,3,3	1.05	0	3,3,3	1.20	0
3	BGC	A	402	-	12,12,12	0.60	0	17,17,17	0.85	0
3	BGC	H	402	-	12,12,12	0.55	0	17,17,17	1.21	2 (11%)
2	ACT	E	401	4	3,3,3	1.17	0	3,3,3	0.67	0
2	ACT	G	401	4	3,3,3	1.04	0	3,3,3	1.25	0
3	BGC	C	402	-	12,12,12	0.79	0	17,17,17	1.33	1 (5%)
3	BGC	E	402	-	12,12,12	0.59	0	17,17,17	1.16	1 (5%)
3	BGC	E	403	-	12,12,12	0.45	0	17,17,17	0.80	0
2	ACT	C	401	4	3,3,3	1.08	0	3,3,3	1.37	0
3	BGC	G	402	-	12,12,12	0.64	0	17,17,17	1.29	1 (5%)
2	ACT	A	401	4	3,3,3	1.09	0	3,3,3	1.11	0
3	BGC	B	402	-	12,12,12	0.55	0	17,17,17	0.81	0
3	BGC	F	402	-	12,12,12	0.50	0	17,17,17	1.44	2 (11%)
2	ACT	F	401	4	3,3,3	1.17	0	3,3,3	0.67	0
2	ACT	B	401	4	3,3,3	1.14	0	3,3,3	1.00	0
2	ACT	D	401	4	3,3,3	1.13	0	3,3,3	0.94	0
3	BGC	C	403	-	12,12,12	0.56	0	17,17,17	0.88	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
3	BGC	A	402	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	H	402	-	-	2/2/22/22	0/1/1/1
3	BGC	E	402	-	-	0/2/22/22	0/1/1/1
3	BGC	C	402	-	-	2/2/22/22	0/1/1/1
3	BGC	E	403	-	-	0/2/22/22	0/1/1/1
3	BGC	G	402	-	-	2/2/22/22	0/1/1/1
3	BGC	F	402	-	-	2/2/22/22	0/1/1/1
3	BGC	B	402	-	-	0/2/22/22	0/1/1/1
3	BGC	C	403	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	BGC	C3-C4-C5	-3.30	104.36	110.24
3	H	402	BGC	C1-C2-C3	-2.75	104.61	110.31
3	E	402	BGC	C3-C4-C5	-2.73	105.37	110.24
3	H	402	BGC	O3-C3-C2	2.31	115.69	110.35
3	F	402	BGC	C4-C3-C2	-2.30	106.80	110.82
3	G	402	BGC	O5-C5-C6	-2.08	101.26	106.44
3	C	402	BGC	C4-C3-C2	-2.01	107.32	110.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	402	BGC	O5-C5-C6-O6
3	G	402	BGC	O5-C5-C6-O6
3	G	402	BGC	C4-C5-C6-O6
3	C	402	BGC	O5-C5-C6-O6
3	F	402	BGC	C4-C5-C6-O6
3	H	402	BGC	O5-C5-C6-O6
3	C	402	BGC	C4-C5-C6-O6
3	H	402	BGC	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	BGC	2	0
3	G	402	BGC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	402	BGC	3	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	370/380 (97%)	0.46	19 (5%) 34 36	12, 27, 43, 79	6 (1%)
1	B	371/380 (97%)	0.82	37 (9%) 14 13	14, 30, 49, 78	3 (0%)
1	C	371/380 (97%)	0.45	14 (3%) 44 48	19, 27, 43, 85	0
1	D	371/380 (97%)	0.48	15 (4%) 43 46	15, 27, 44, 73	2 (0%)
1	E	369/380 (97%)	0.21	13 (3%) 47 51	14, 24, 38, 67	3 (0%)
1	F	371/380 (97%)	0.21	10 (2%) 56 59	15, 23, 39, 75	2 (0%)
1	G	369/380 (97%)	0.48	17 (4%) 38 40	14, 27, 43, 63	4 (1%)
1	H	368/380 (96%)	0.66	30 (8%) 19 19	19, 29, 46, 64	0
All	All	2960/3040 (97%)	0.47	155 (5%) 34 35	12, 27, 44, 85	20 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	THR	6.2
1	D	10	THR	5.2
1	D	9	GLY	5.1
1	G	10	THR	5.0
1	H	378	LEU	4.7
1	D	379	GLY	4.7
1	C	379	GLY	4.4
1	B	379	GLY	4.3
1	F	9	GLY	4.3
1	C	45	GLY	4.2
1	B	11	MET	4.1
1	B	378	LEU	4.0
1	G	378	LEU	3.9
1	B	37	GLY	3.9
1	B	45	GLY	3.8
1	A	45	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	376	VAL	3.5
1	E	11	MET	3.5
1	F	10	THR	3.4
1	B	177	ALA	3.4
1	F	37	GLY	3.3
1	G	11	MET	3.3
1	B	12	SER	3.3
1	C	10	THR	3.3
1	D	37	GLY	3.2
1	H	11	MET	3.2
1	B	376	VAL	3.2
1	E	109	MET	3.2
1	G	45	GLY	3.1
1	G	376	VAL	3.1
1	H	12	SER	3.0
1	B	9	GLY	3.0
1	H	179	HIS	3.0
1	H	218	PHE	3.0
1	B	232	ALA	3.0
1	B	136	LEU	3.0
1	A	37	GLY	3.0
1	H	375	ALA	3.0
1	B	137	THR	2.9
1	G	181	ILE	2.9
1	E	70	ARG	2.9
1	B	375	ALA	2.9
1	A	10	THR	2.9
1	D	341	VAL	2.9
1	H	180	GLY	2.9
1	C	9	GLY	2.9
1	H	377	LEU	2.9
1	E	12	SER	2.9
1	B	176	ARG	2.9
1	H	341	VAL	2.8
1	B	93	ILE	2.8
1	B	175	ALA	2.8
1	B	181	ILE	2.8
1	B	13	ASN	2.7
1	G	37	GLY	2.7
1	E	341	VAL	2.7
1	H	232	ALA	2.7
1	B	138	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	137	THR	2.7
1	D	12	SER	2.7
1	B	180	GLY	2.7
1	G	102	ALA	2.7
1	E	38	GLU	2.7
1	A	44	SER	2.6
1	H	102	ALA	2.6
1	G	377	LEU	2.6
1	G	375	ALA	2.6
1	A	181	ILE	2.6
1	B	109	MET	2.6
1	H	234	LEU	2.6
1	E	37	GLY	2.6
1	G	180	GLY	2.6
1	C	44	SER	2.6
1	G	341	VAL	2.5
1	A	9	GLY	2.5
1	B	377	LEU	2.5
1	E	360	ASP	2.5
1	H	219	PRO	2.5
1	E	13	ASN	2.5
1	F	102	ALA	2.5
1	C	137	THR	2.5
1	H	46	THR	2.5
1	C	181	ILE	2.5
1	F	364	ARG	2.5
1	H	249	ASP	2.5
1	C	38	GLU	2.5
1	A	378	LEU	2.4
1	D	11	MET	2.4
1	D	102	ALA	2.4
1	E	44	SER	2.4
1	G	351	GLU	2.4
1	H	136	LEU	2.4
1	H	37	GLY	2.4
1	H	231	GLY	2.4
1	A	109	MET	2.4
1	B	231	GLY	2.3
1	B	228	ARG	2.3
1	D	181	ILE	2.3
1	B	234	LEU	2.3
1	C	109	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	177	ALA	2.3
1	G	157	ASP	2.3
1	F	13	ASN	2.3
1	B	44	SER	2.3
1	A	180	GLY	2.3
1	A	364	ARG	2.3
1	A	376	VAL	2.3
1	D	376	VAL	2.3
1	A	267[A]	ARG	2.2
1	A	102	ALA	2.2
1	G	177	ALA	2.2
1	H	181	ILE	2.2
1	A	66	GLY	2.2
1	B	182	GLU	2.2
1	B	46	THR	2.2
1	B	139	LYS	2.2
1	B	307	ASP	2.2
1	H	260	LEU	2.2
1	A	341	VAL	2.2
1	C	341	VAL	2.2
1	H	225	VAL	2.2
1	D	177	ALA	2.2
1	A	138	GLY	2.2
1	E	45	GLY	2.2
1	H	45	GLY	2.2
1	C	11	MET	2.2
1	D	136	LEU	2.2
1	F	341	VAL	2.1
1	A	182	GLU	2.1
1	D	179	HIS	2.1
1	B	102	ALA	2.1
1	E	178	ARG	2.1
1	F	38	GLU	2.1
1	B	135	VAL	2.1
1	B	207	VAL	2.1
1	F	346	VAL	2.1
1	G	346	VAL	2.1
1	H	109	MET	2.1
1	G	232	ALA	2.1
1	H	90	ALA	2.1
1	A	346	VAL	2.1
1	E	72	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	44	SER	2.1
1	H	44	SER	2.1
1	C	178	ARG	2.0
1	B	90	ALA	2.0
1	B	140	VAL	2.0
1	C	376	VAL	2.0
1	D	352	MET	2.0
1	A	38	GLU	2.0
1	H	77	GLU	2.0
1	B	267	ARG	2.0
1	C	176	ARG	2.0
1	D	267	ARG	2.0
1	H	176	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

## 6.3 Carbohydrates [\(i\)](#)

There are no 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<sup>th</sup> 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.

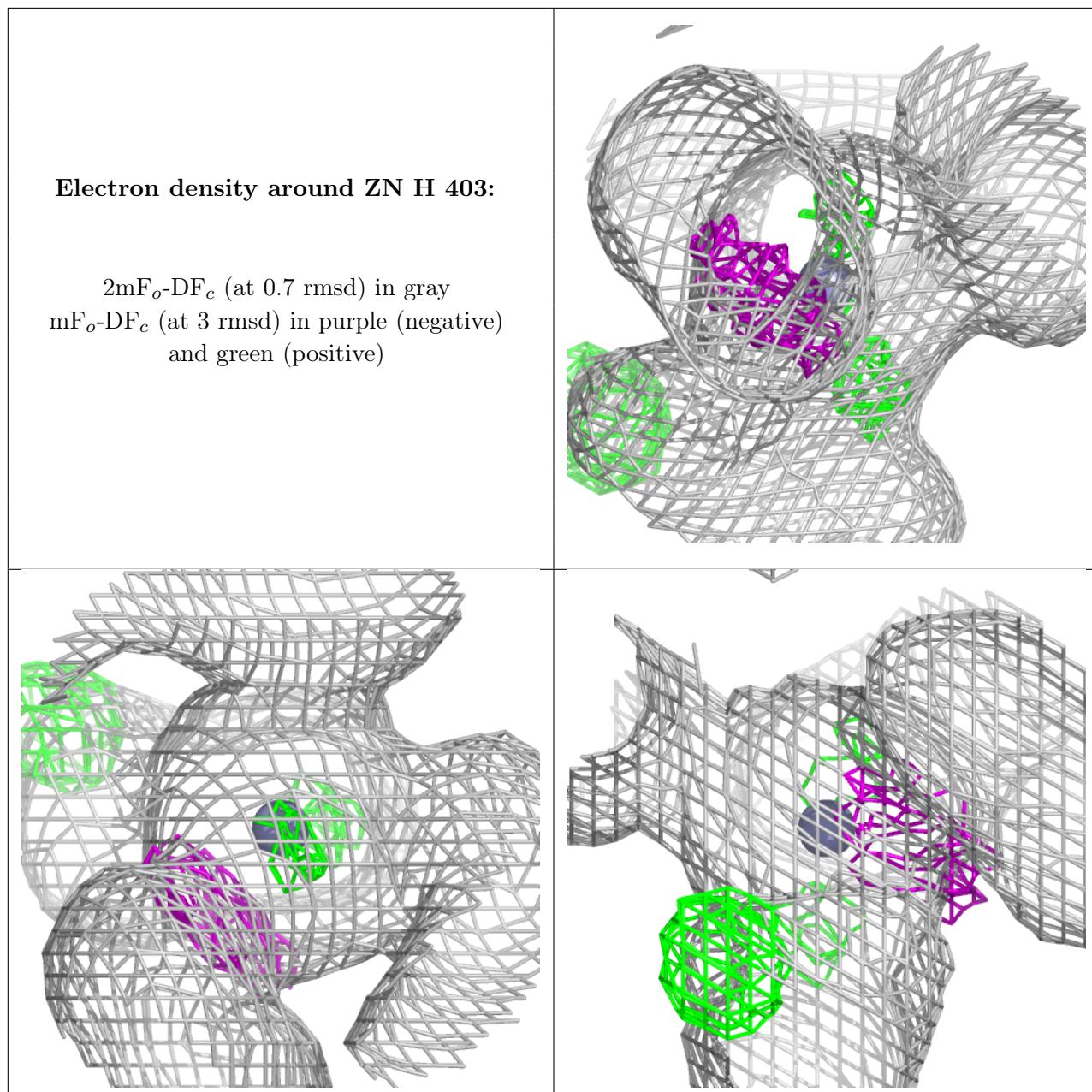
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BGC	G	402	12/12	0.74	0.15	33,50,62,63	0
3	BGC	B	402	12/12	0.76	0.27	26,31,41,42	12
3	BGC	F	402	12/12	0.77	0.14	26,46,56,61	0
3	BGC	E	402	12/12	0.78	0.30	24,32,39,39	12
3	BGC	C	402	12/12	0.79	0.29	27,31,46,47	12
3	BGC	A	402	12/12	0.82	0.29	24,30,36,41	12
3	BGC	C	403	12/12	0.84	0.15	31,37,44,49	12
3	BGC	H	402	12/12	0.84	0.12	38,47,54,54	0
3	BGC	E	403	12/12	0.87	0.13	28,45,58,72	0
2	ACT	H	401	4/4	0.95	0.07	26,26,27,28	0

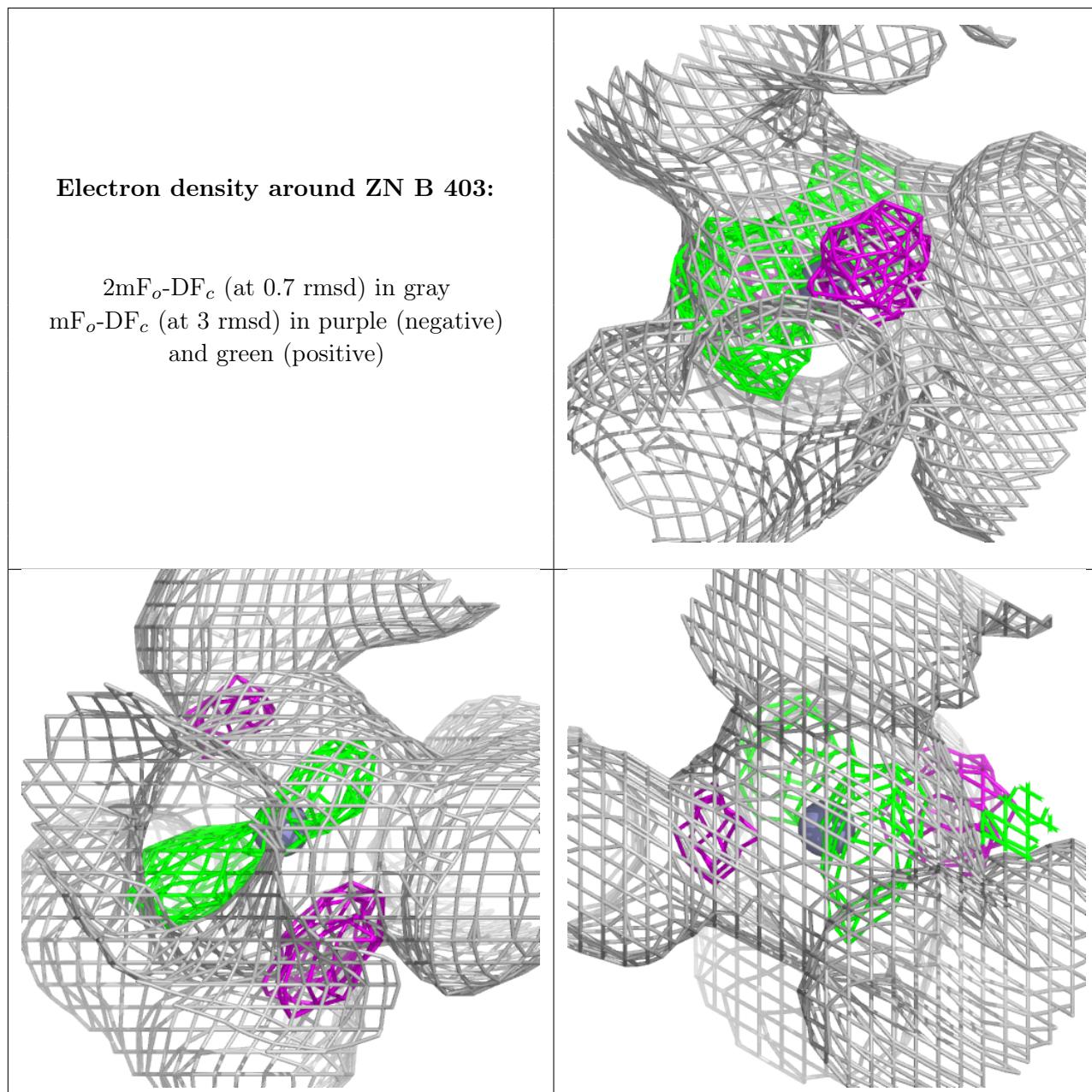
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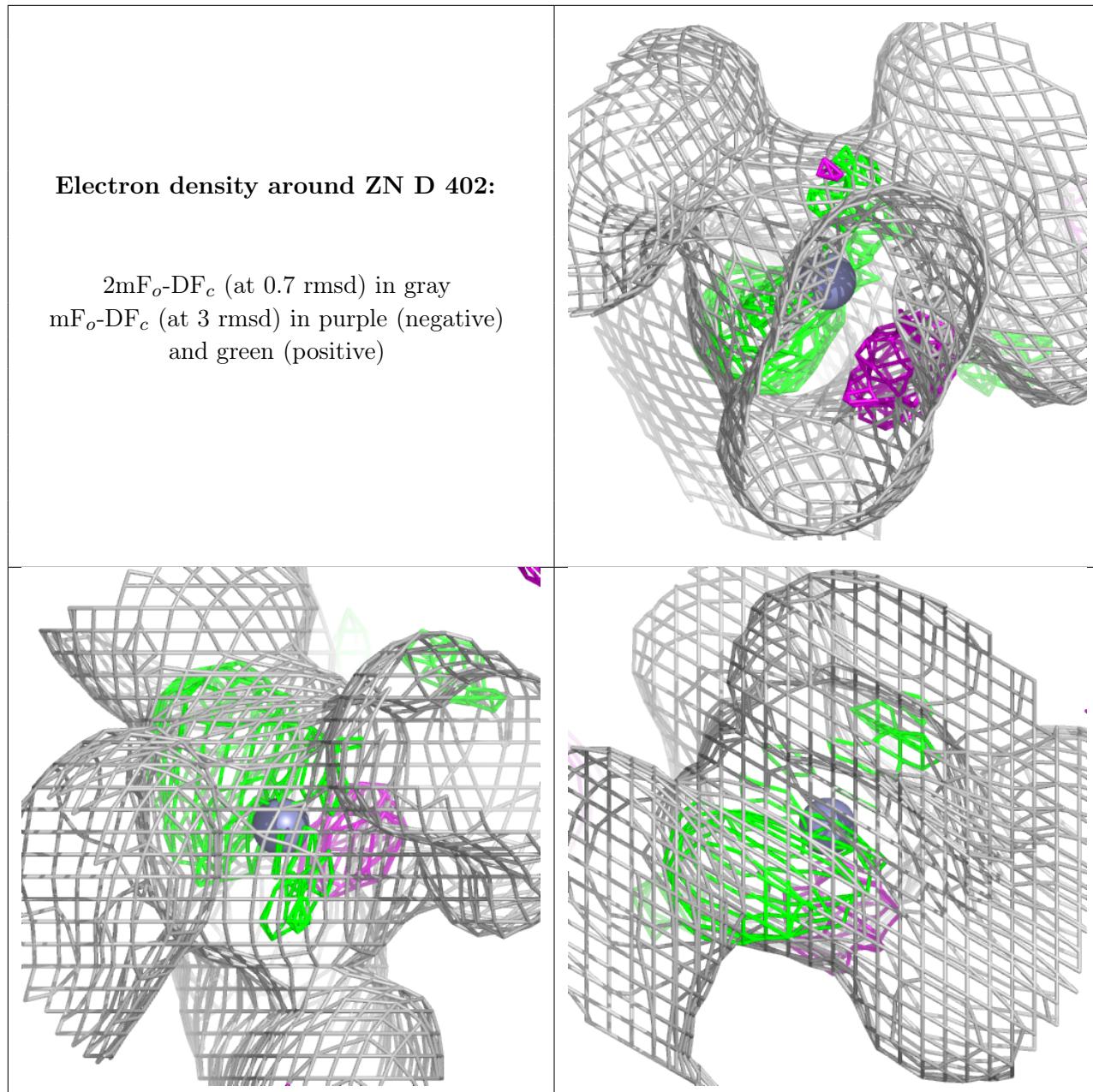
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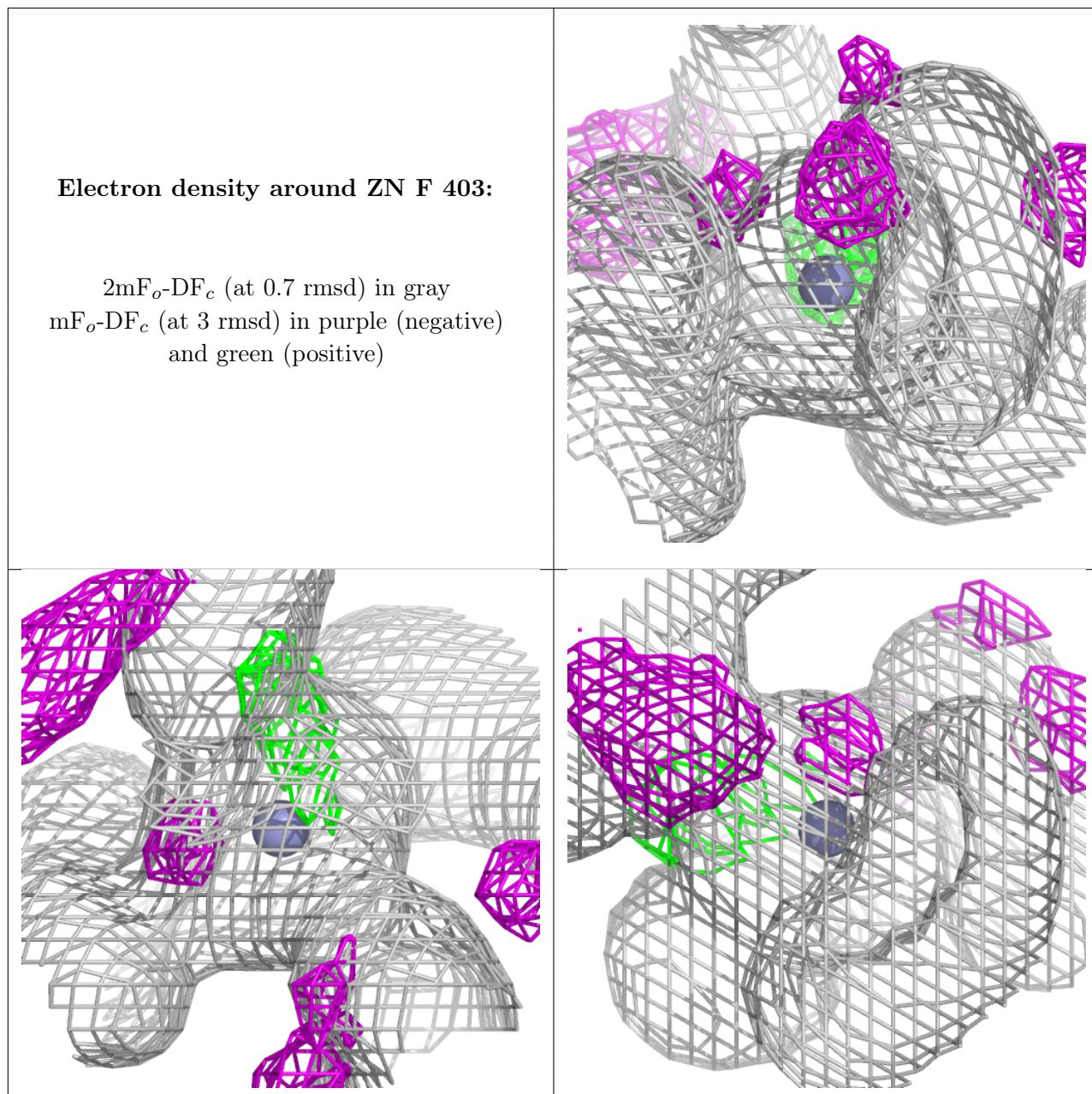
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACT	B	401	4/4	0.95	0.08	25,27,28,30	0
2	ACT	D	401	4/4	0.96	0.07	25,25,26,26	0
2	ACT	E	401	4/4	0.96	0.10	20,21,21,23	0
5	K	H	404	1/1	0.96	0.10	27,27,27,27	1
2	ACT	G	401	4/4	0.97	0.07	25,27,28,29	0
2	ACT	A	401	4/4	0.97	0.09	23,23,24,24	0
2	ACT	C	401	4/4	0.97	0.07	20,21,21,21	4
5	K	B	404	1/1	0.97	0.06	23,23,23,23	1
2	ACT	F	401	4/4	0.97	0.07	20,21,21,23	0
5	K	G	404	1/1	0.98	0.06	25,25,25,25	1
5	K	D	403	1/1	0.98	0.05	21,21,21,21	1
4	ZN	H	403	1/1	0.99	0.03	22,22,22,22	1
5	K	A	404	1/1	0.99	0.05	23,23,23,23	0
4	ZN	B	403	1/1	0.99	0.04	22,22,22,22	1
5	K	C	405	1/1	0.99	0.03	21,21,21,21	1
4	ZN	D	402	1/1	0.99	0.04	21,21,21,21	1
4	ZN	F	403	1/1	0.99	0.03	19,19,19,19	1
4	ZN	G	403	1/1	0.99	0.03	20,20,20,20	1
4	ZN	C	404	1/1	1.00	0.01	21,21,21,21	1
5	K	E	405	1/1	1.00	0.04	20,20,20,20	0
5	K	F	404	1/1	1.00	0.06	21,21,21,21	0
4	ZN	A	403	1/1	1.00	0.01	20,20,20,20	1
4	ZN	E	404	1/1	1.00	0.01	18,18,18,18	1

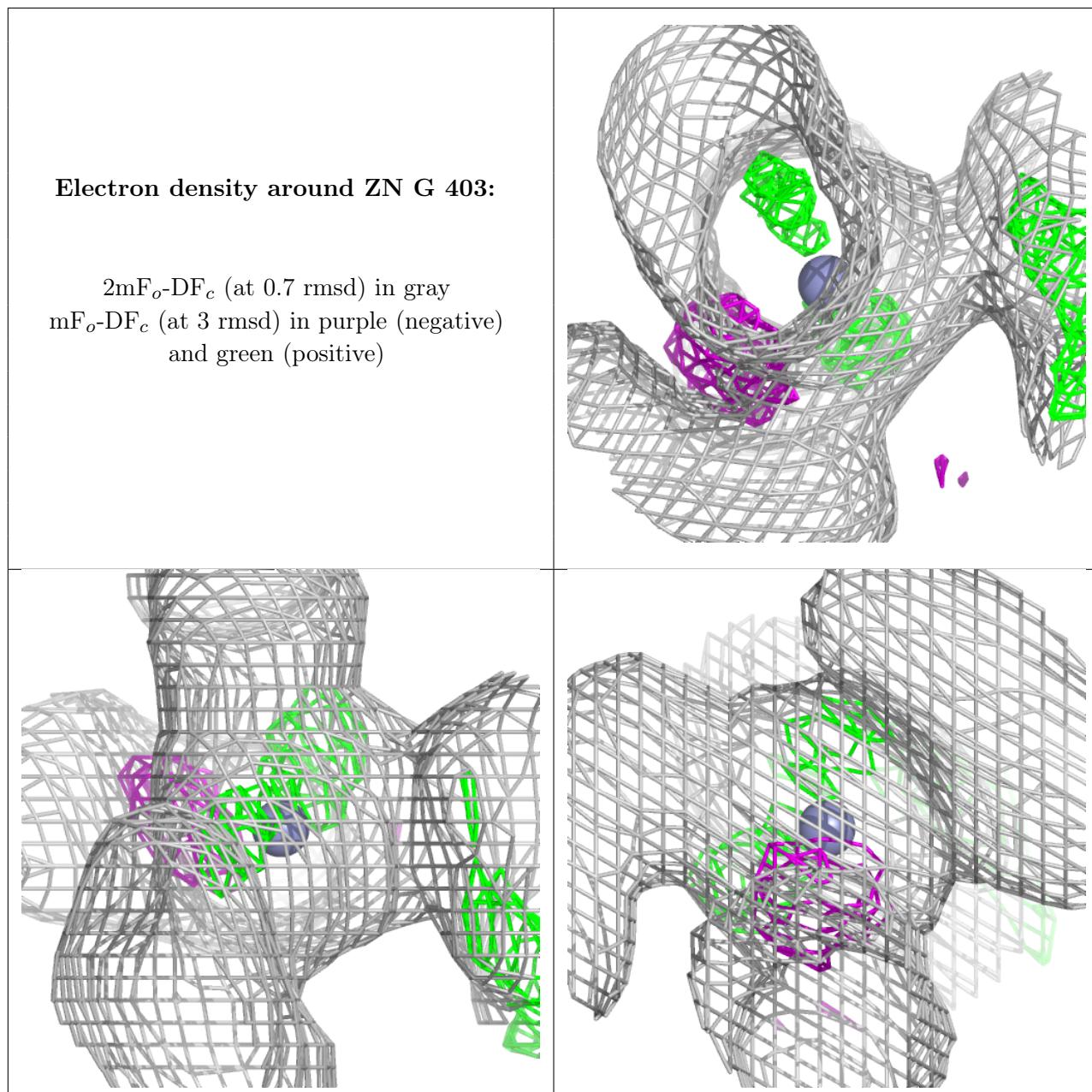
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

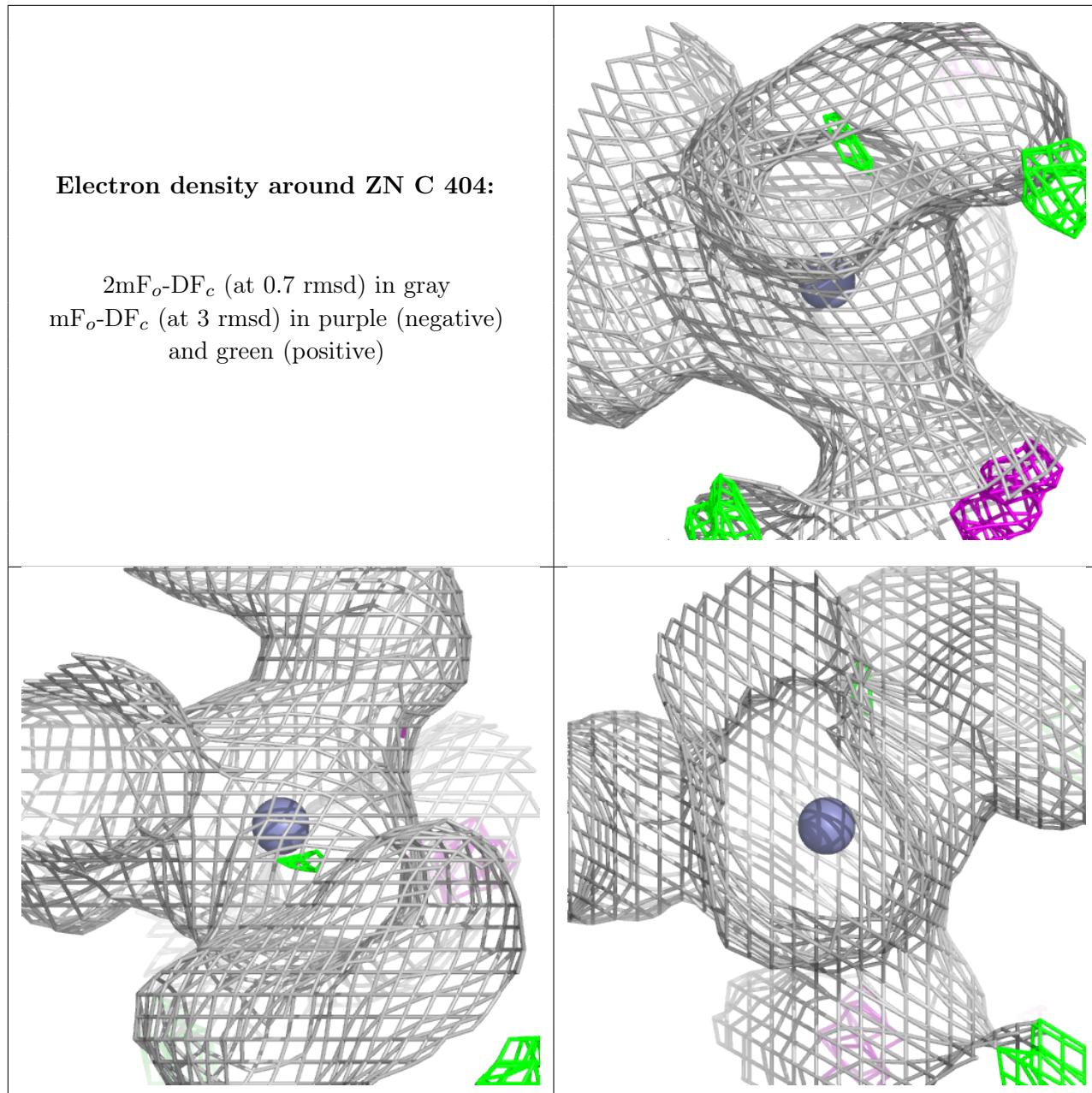


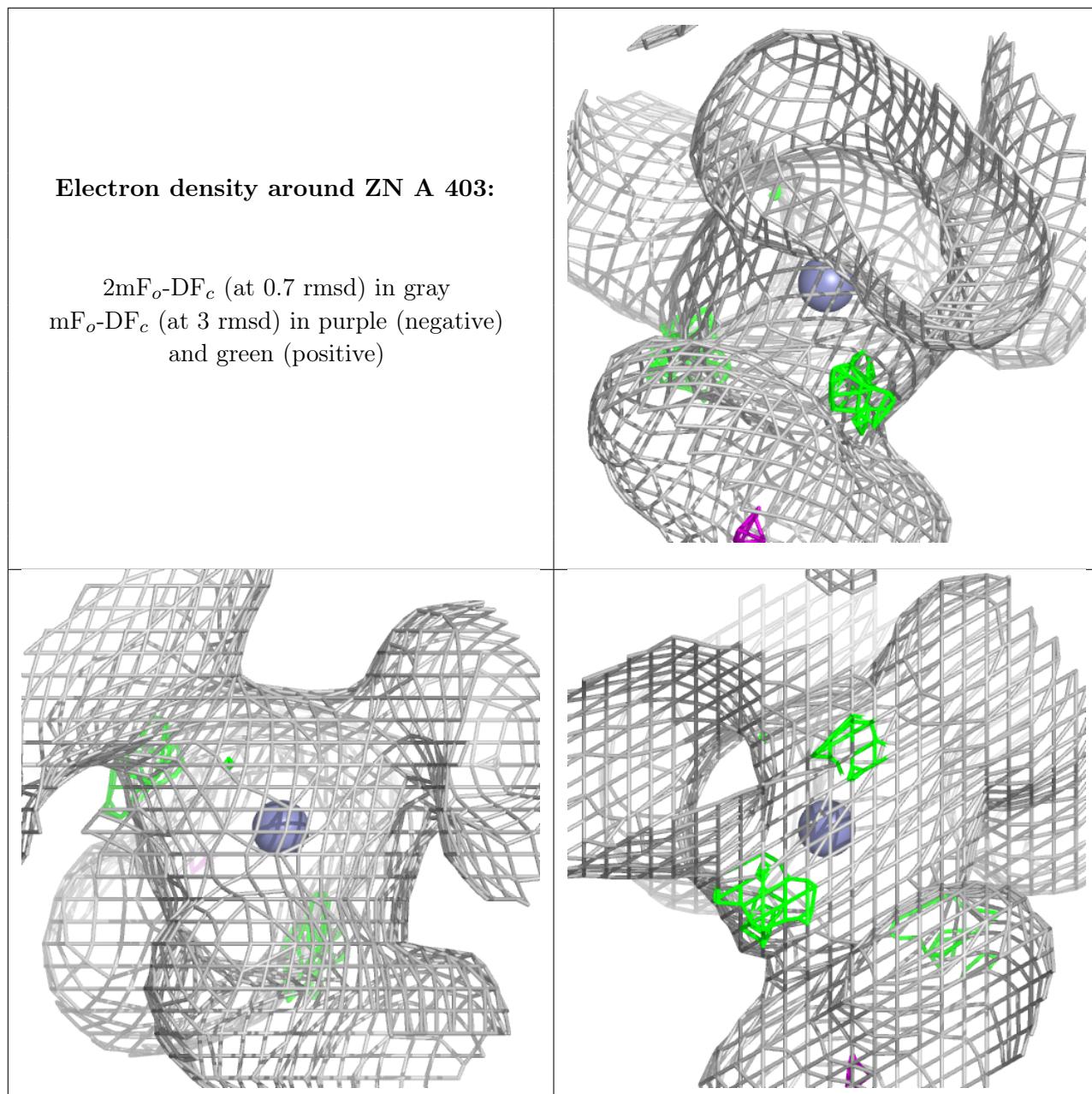


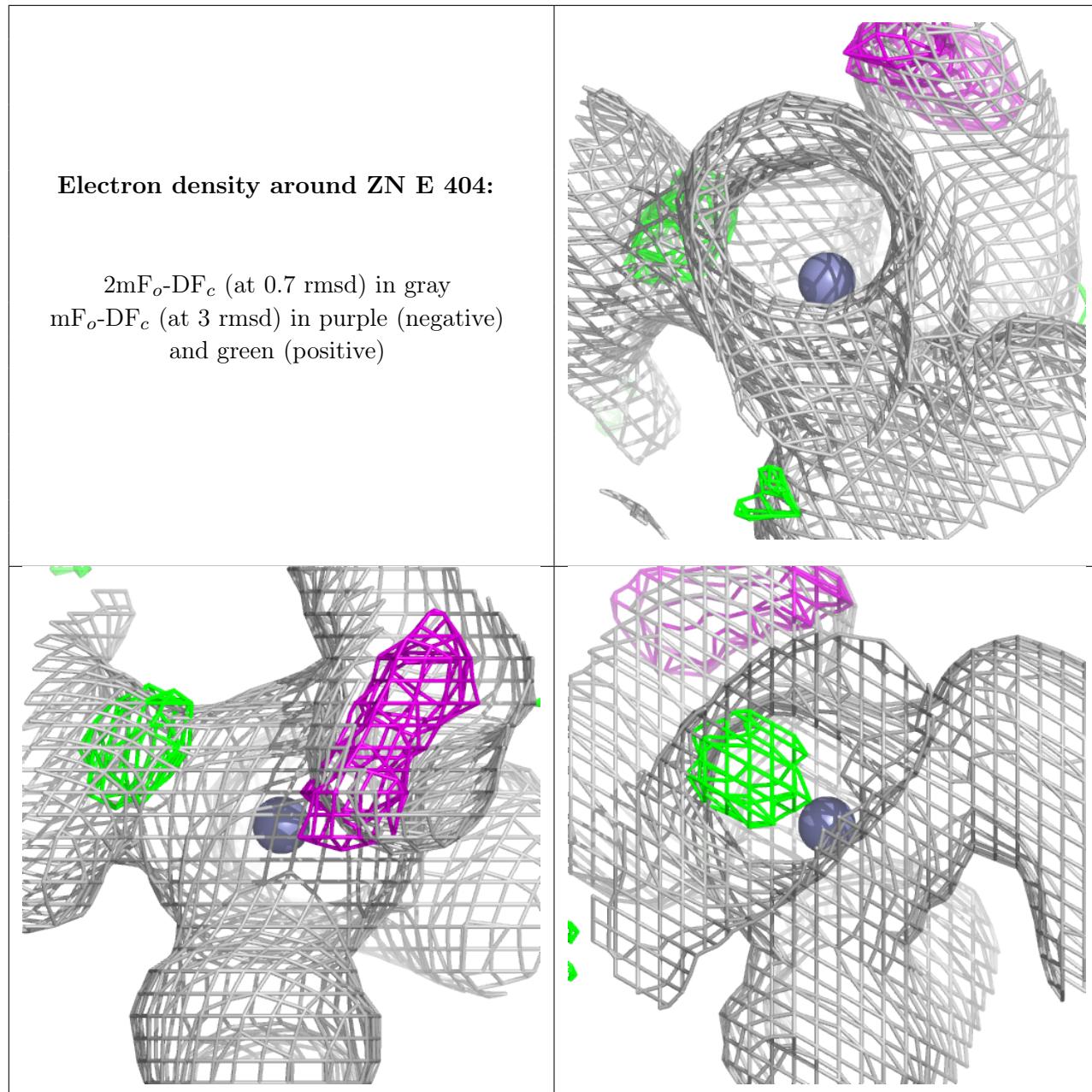












## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.