



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 11:14 am BST

PDB ID : 1O7T  
Title : Metal nanoclusters bound to the Ferric Binding Protein from *Neisseria gonorrhoeae*.  
Authors : Alexeev, D.; Zu, H.; Guo, M.; Zhong, W.; Hunter, D.J.B.; Yang, W.; Campopiano, D.J.; Sadler, P.J.  
Deposited on : 2002-11-12  
Resolution : 1.65 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](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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

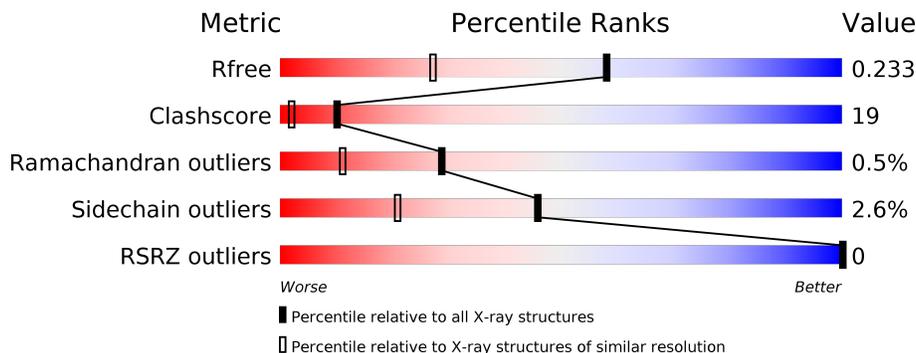
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	
1	B	309	
1	C	309	
1	D	309	
1	E	309	
1	F	309	

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Mol	Chain	Length	Quality of chain
1	G	309	 67% 32%
1	H	309	 61% 38%
1	I	309	 66% 32%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23605 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 IRON BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2377	1507	423	446	1	0	0	0
1	B	309	2377	1507	423	446	1	0	0	0
1	C	309	2377	1507	423	446	1	0	0	0
1	D	309	2377	1507	423	446	1	0	0	0
1	E	309	2377	1507	423	446	1	0	0	0
1	F	309	2377	1507	423	446	1	0	0	0
1	G	309	2377	1507	423	446	1	0	0	0
1	H	309	2377	1507	423	446	1	0	0	0
1	I	309	2377	1507	423	446	1	0	0	0

- Molecule 2 is HF OXO CLUSTER HF5 (three-letter code: HF5) (formula: H<sub>12</sub>Hf<sub>5</sub>O<sub>21</sub>).





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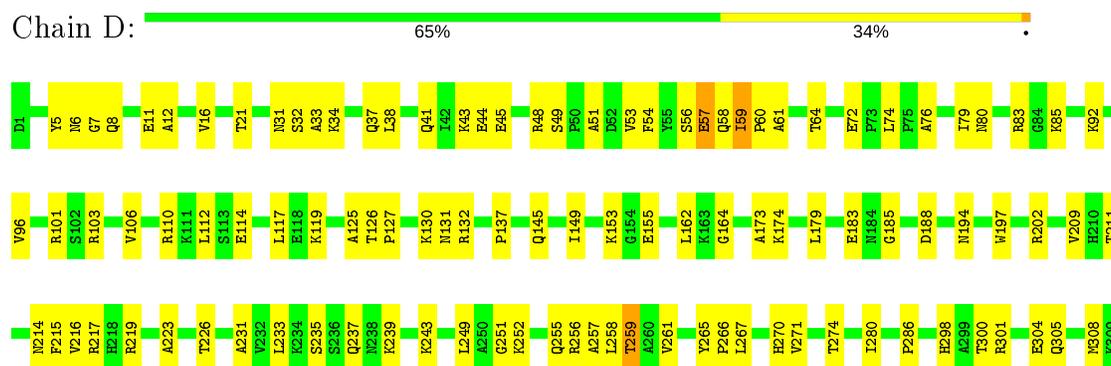
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Hf	O	P		
4	I	1	29	5	23	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	256	Total 256	O 256	0	0
5	B	220	Total 220	O 220	0	0
5	C	223	Total 223	O 223	0	0
5	D	210	Total 210	O 210	0	0
5	E	243	Total 243	O 243	0	0
5	F	227	Total 227	O 227	0	0
5	G	212	Total 212	O 212	0	0
5	H	188	Total 188	O 188	0	0
5	I	197	Total 197	O 197	0	0



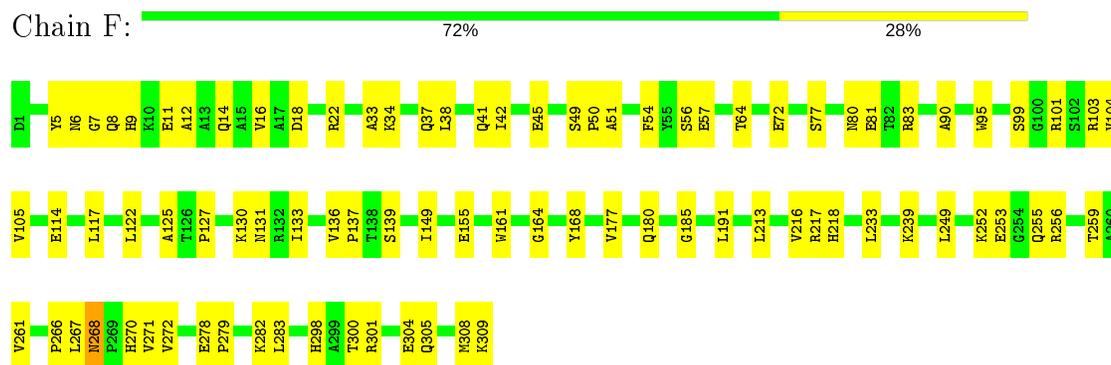
- Molecule 1: IRON BINDING PROTEIN



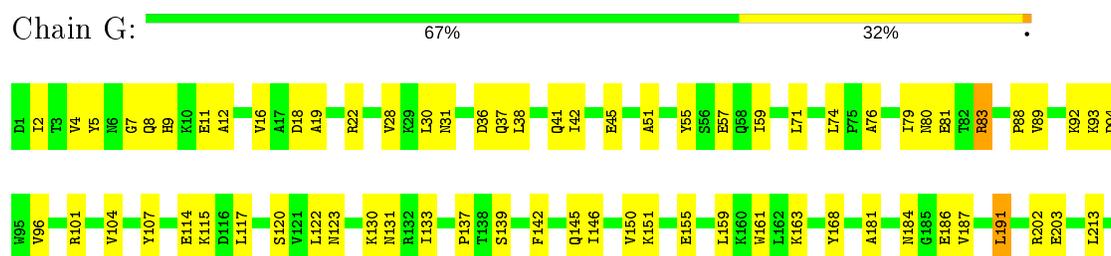
- Molecule 1: IRON BINDING PROTEIN



- Molecule 1: IRON BINDING PROTEIN



- Molecule 1: IRON BINDING PROTEIN





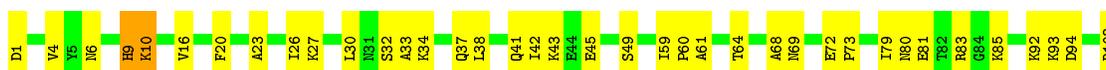
• Molecule 1: IRON BINDING PROTEIN

Chain H: 61% 38%



• Molecule 1: IRON BINDING PROTEIN

Chain I: 66% 32%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.13Å 148.13Å 115.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.65 29.43 – 1.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-1.65) 98.5 (29.43-1.55)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 1.55Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.164 , 0.262 0.168 , 0.233	Depositor DCC
$R_{free}$ test set	27813 reflections (6.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.090 for -h,-k,l 0.089 for h,-h-k,-l 0.427 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	23605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.82% 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  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HF3, HF5, PHF

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	0.37	0/2422	0.63	0/3279
1	B	0.36	0/2422	0.59	0/3279
1	C	0.37	0/2422	0.60	0/3279
1	D	0.36	0/2422	0.58	0/3279
1	E	0.37	0/2422	0.60	0/3279
1	F	0.35	0/2422	0.61	0/3279
1	G	0.36	0/2422	0.59	0/3279
1	H	0.34	0/2422	0.60	0/3279
1	I	0.35	0/2422	0.58	0/3279
All	All	0.36	0/21798	0.60	0/29511

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	2377	0	2422	59	0
1	B	2377	0	2422	74	0
1	C	2377	0	2422	84	0
1	D	2377	0	2422	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2377	0	2422	79	0
1	F	2377	0	2422	78	0
1	G	2377	0	2422	97	0
1	H	2377	0	2422	135	0
1	I	2377	0	2422	98	0
2	A	26	0	0	3	0
2	B	26	0	0	1	0
2	C	26	0	0	2	0
2	E	26	0	0	3	0
2	F	26	0	0	0	0
3	D	19	0	0	2	0
4	G	29	0	0	2	0
4	H	29	0	0	2	0
4	I	29	0	0	3	0
5	A	256	0	0	8	0
5	B	220	0	0	12	0
5	C	223	0	0	7	0
5	D	210	0	0	12	0
5	E	243	0	0	10	0
5	F	227	0	0	5	0
5	G	212	0	0	13	0
5	H	188	0	0	19	0
5	I	197	0	0	7	0
All	All	23605	0	21798	821	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 19.

The worst 5 of 821 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:F:259:THR:HG21	1:F:266:PRO:HG3	1.29	1.12
1:D:202:ARG:HH22	1:D:274:THR:HG22	1.08	1.08
1:H:288:VAL:HG12	1:H:289:SER:H	1.17	1.05
1:A:259:THR:HG21	1:A:266:PRO:HG3	1.37	1.03
1:D:101:ARG:HH12	1:D:226:THR:HB	1.18	1.03

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	307/309 (99%)	298 (97%)	9 (3%)	0	100	100
1	B	307/309 (99%)	298 (97%)	8 (3%)	1 (0%)	41	22
1	C	307/309 (99%)	296 (96%)	11 (4%)	0	100	100
1	D	307/309 (99%)	290 (94%)	15 (5%)	2 (1%)	22	6
1	E	307/309 (99%)	295 (96%)	11 (4%)	1 (0%)	41	22
1	F	307/309 (99%)	293 (95%)	14 (5%)	0	100	100
1	G	307/309 (99%)	294 (96%)	13 (4%)	0	100	100
1	H	307/309 (99%)	281 (92%)	20 (6%)	6 (2%)	7	0
1	I	307/309 (99%)	285 (93%)	18 (6%)	4 (1%)	12	1
All	All	2763/2781 (99%)	2630 (95%)	119 (4%)	14 (0%)	29	11

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	239	LYS
1	H	34	LYS
1	H	93	LYS
1	H	280	ILE
1	I	9	HIS

### 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	245/245 (100%)	237 (97%)	8 (3%)	38	12
1	B	245/245 (100%)	239 (98%)	6 (2%)	49	23
1	C	245/245 (100%)	238 (97%)	7 (3%)	42	16
1	D	245/245 (100%)	239 (98%)	6 (2%)	49	23
1	E	245/245 (100%)	237 (97%)	8 (3%)	38	12
1	F	245/245 (100%)	241 (98%)	4 (2%)	62	41
1	G	245/245 (100%)	239 (98%)	6 (2%)	49	23
1	H	245/245 (100%)	239 (98%)	6 (2%)	49	23
1	I	245/245 (100%)	239 (98%)	6 (2%)	49	23
All	All	2205/2205 (100%)	2148 (97%)	57 (3%)	46	21

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	214	ASN
1	E	191	LEU
1	I	174	LYS
1	D	259	THR
1	E	101	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	131	ASN
1	E	255	GLN
1	H	255	GLN
1	D	208	ASN
1	D	305	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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	HF3	D	1310	1	4,23,23	3.34	3 (75%)	3,66,66	0.24	0
2	HF5	C	1310	1	0,31,31	0.00	-	-		
4	PHF	G	1310	1	6,37,37	3.79	5 (83%)	3,117,117	2.27	1 (33%)
2	HF5	F	1310	1	0,31,31	0.00	-	-		
2	HF5	B	1310	1	0,31,31	0.00	-	-		
4	PHF	H	1310	1	6,37,37	3.61	4 (66%)	3,117,117	1.55	1 (33%)
2	HF5	E	1310	1	0,31,31	0.00	-	-		
2	HF5	A	1310	1	0,31,31	0.00	-	-		
4	PHF	I	1310	1	6,37,37	4.80	4 (66%)	3,117,117	1.47	0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1310	PHF	P-O3	8.76	1.73	1.54
4	H	1310	PHF	P-O3	6.66	1.68	1.54
4	G	1310	PHF	P-O2	5.95	1.67	1.54
4	I	1310	PHF	O02-HFC	5.27	2.57	2.27
4	G	1310	PHF	P-O3	-4.91	1.43	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1310	PHF	O1-P-O4	3.16	124.76	110.67
4	H	1310	PHF	O1-P-O4	2.25	120.70	110.67

There are no chirality outliers.

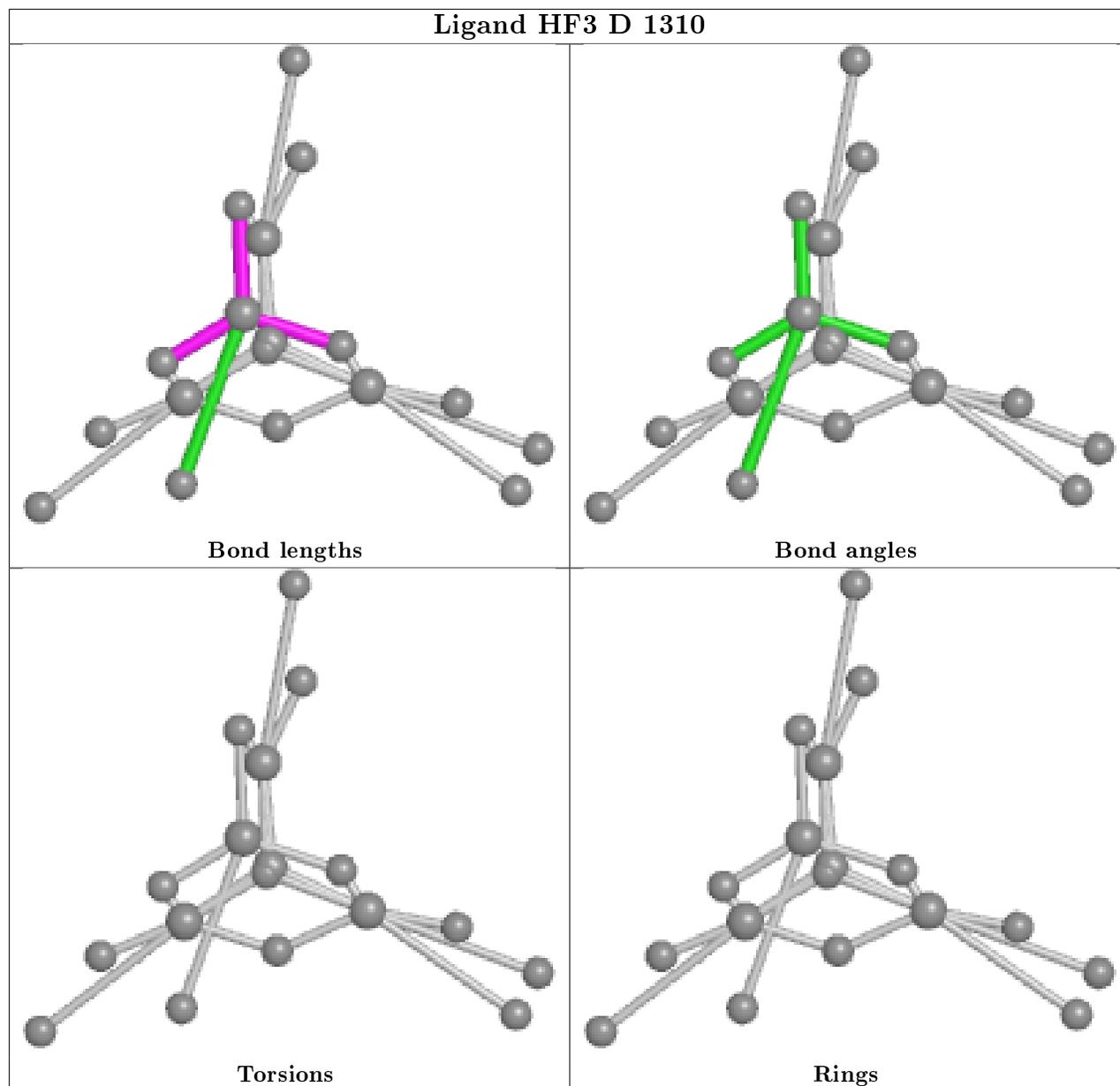
There are no torsion outliers.

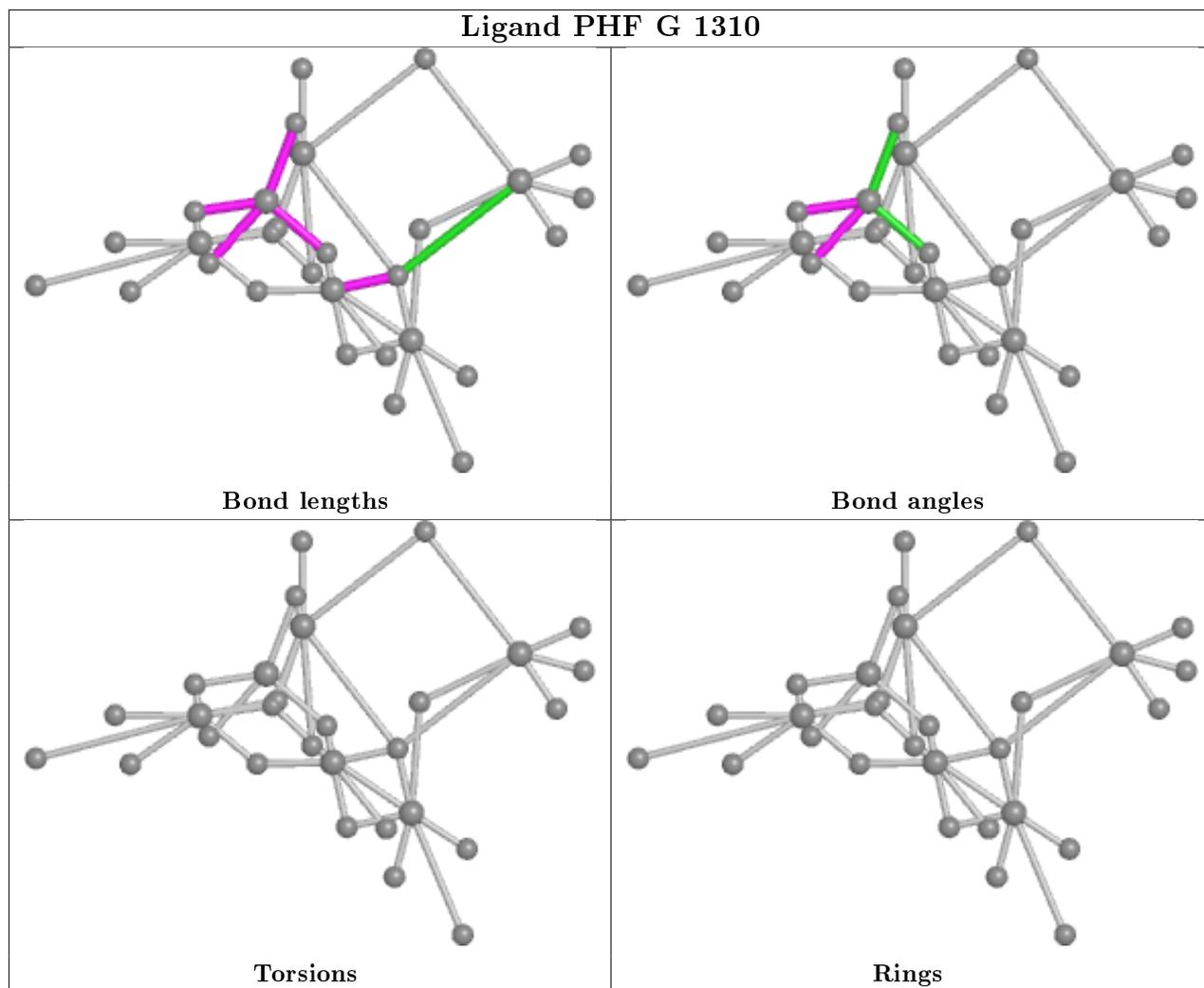
There are no ring outliers.

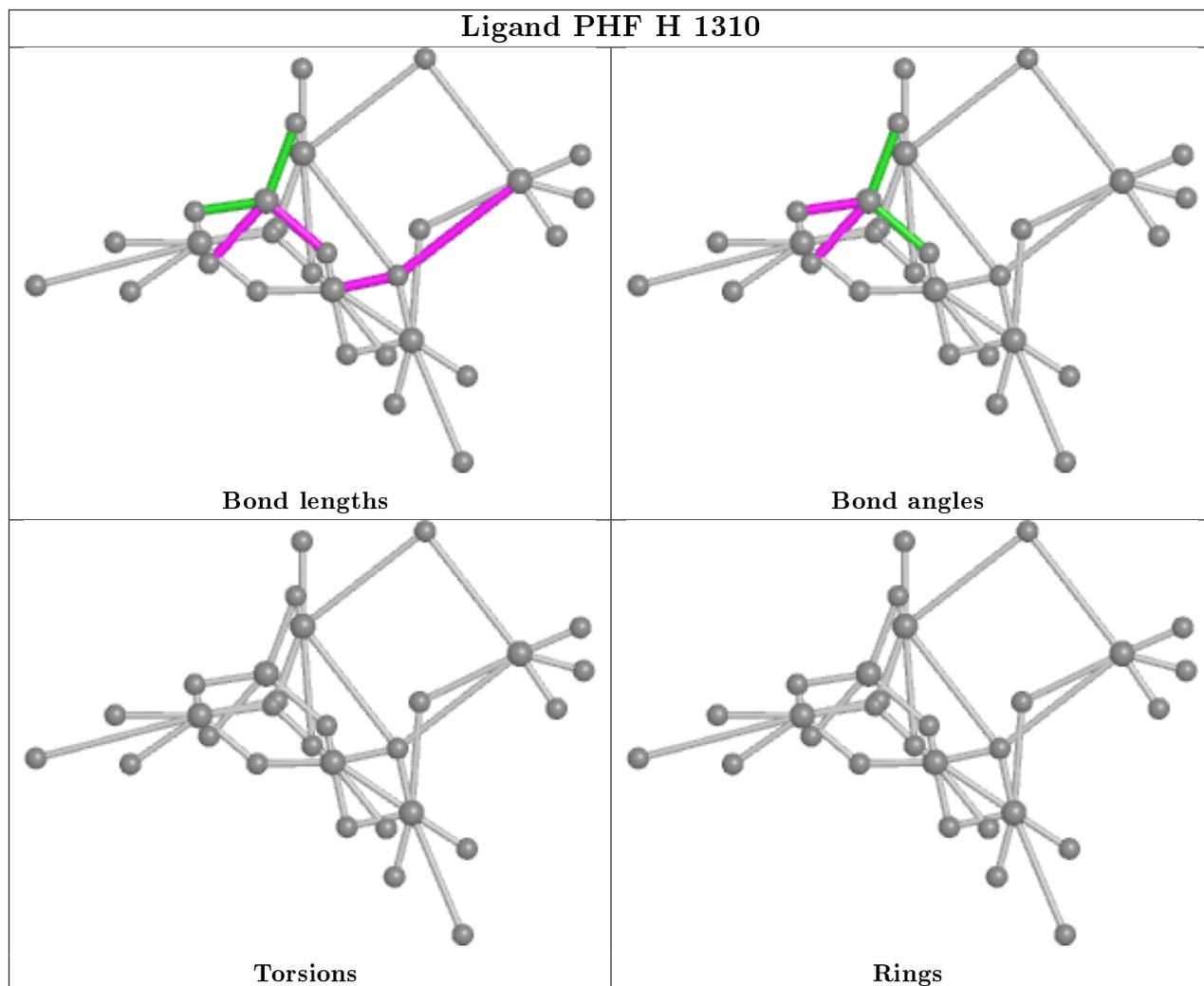
8 monomers are involved in 18 short contacts:

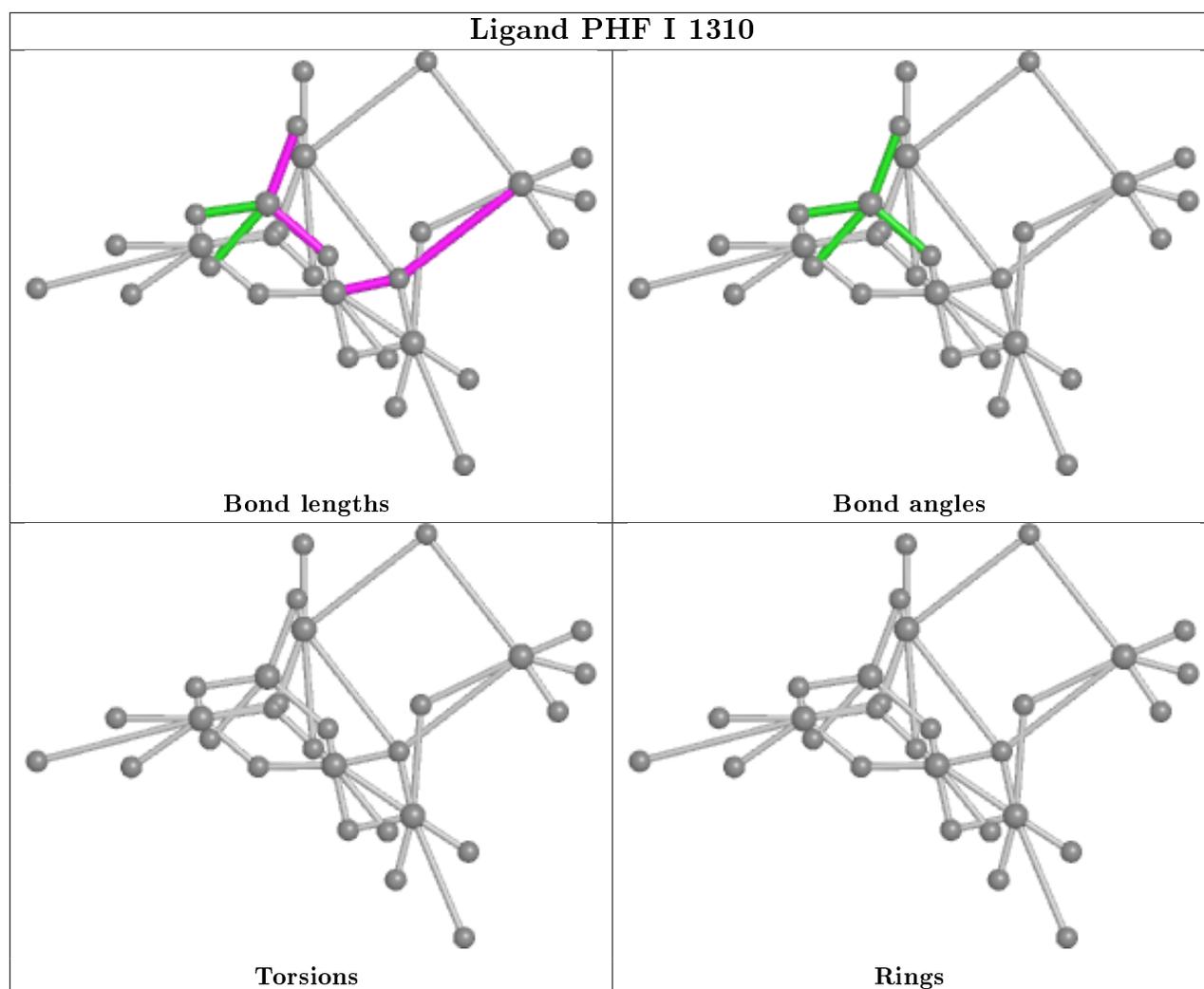
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1310	HF3	2	0
2	C	1310	HF5	2	0
4	G	1310	PHF	2	0
2	B	1310	HF5	1	0
4	H	1310	PHF	2	0
2	E	1310	HF5	3	0
2	A	1310	HF5	3	0
4	I	1310	PHF	3	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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	309/309 (100%)	-0.81	0 100 100	18, 26, 38, 49	0
1	B	309/309 (100%)	-0.74	0 100 100	16, 29, 45, 61	0
1	C	309/309 (100%)	-0.74	0 100 100	18, 29, 44, 52	0
1	D	309/309 (100%)	-0.74	0 100 100	20, 30, 45, 61	0
1	E	309/309 (100%)	-0.82	0 100 100	18, 27, 38, 47	0
1	F	309/309 (100%)	-0.81	0 100 100	18, 27, 39, 52	0
1	G	309/309 (100%)	-0.76	0 100 100	21, 31, 41, 48	0
1	H	309/309 (100%)	-0.49	0 100 100	20, 34, 59, 65	0
1	I	309/309 (100%)	-0.71	0 100 100	21, 33, 45, 59	0
All	All	2781/2781 (100%)	-0.74	0 100 100	16, 30, 46, 65	0

There are no RSRZ outliers to report.

### 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](#)

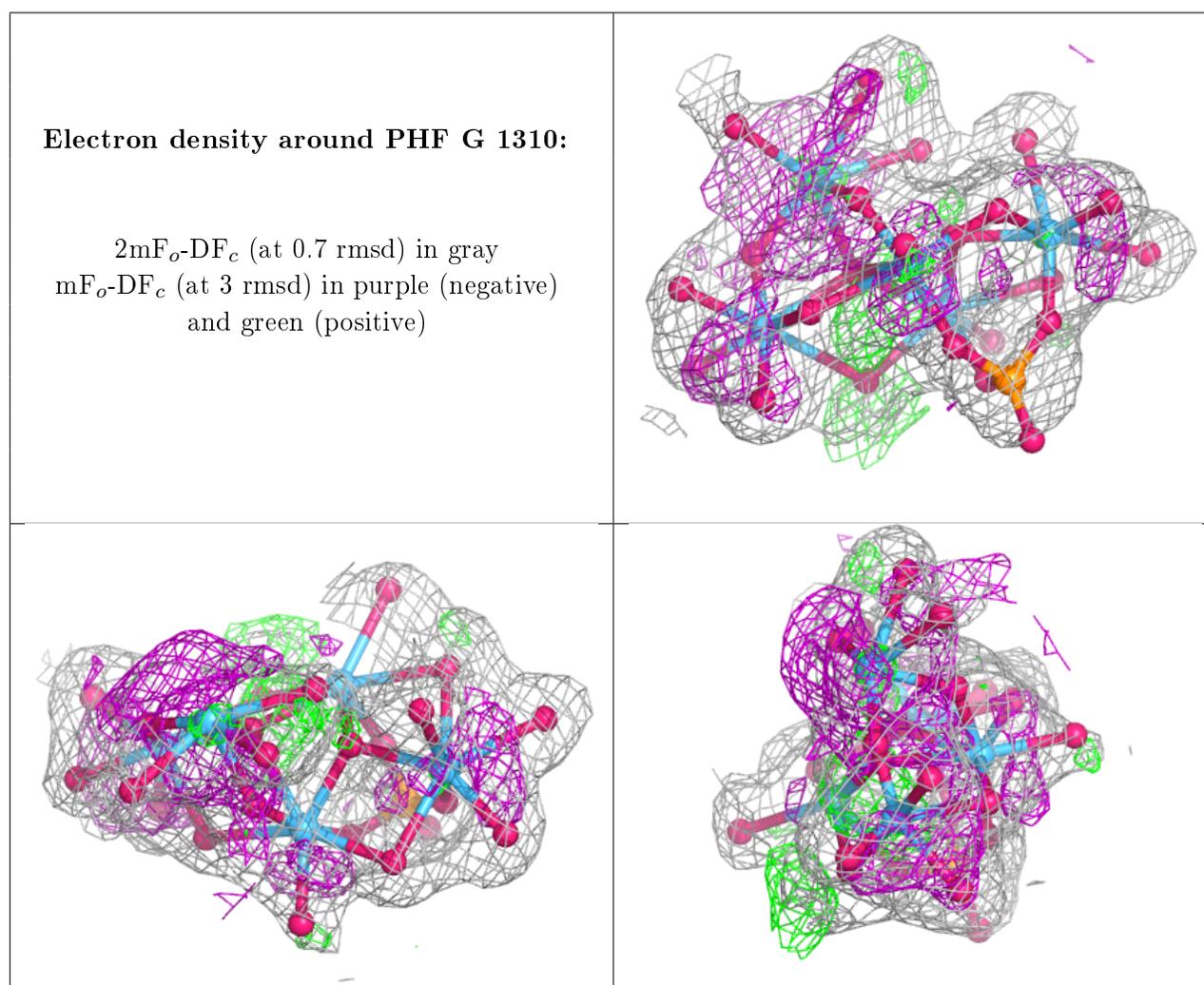
There are no carbohydrates in this entry.

### 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.

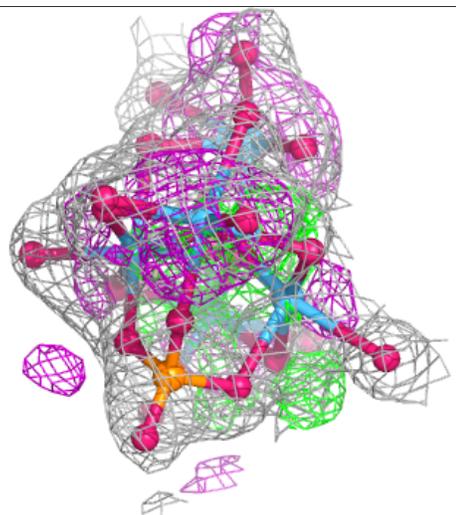
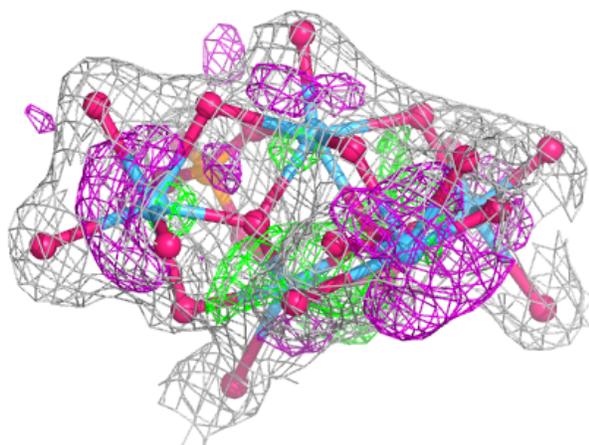
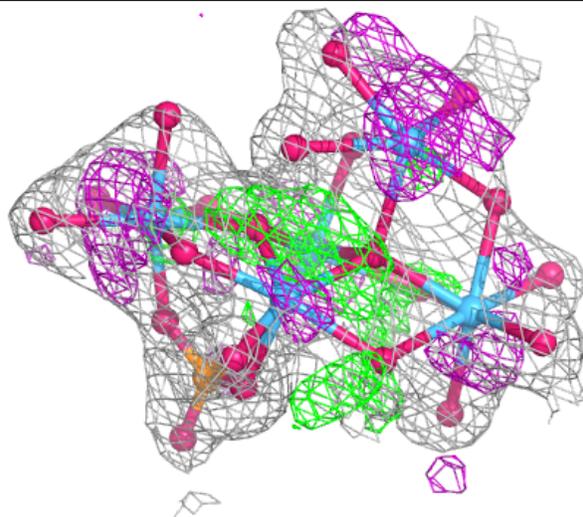
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PHF	G	1310	29/29	0.99	0.07	31,53,90,99	0
2	HF5	F	1310	26/26	0.99	0.09	34,73,99,99	0
4	PHF	H	1310	29/29	0.99	0.07	34,65,83,89	0
2	HF5	E	1310	26/26	0.99	0.09	29,69,99,99	0
4	PHF	I	1310	29/29	0.99	0.08	36,71,99,99	0
3	HF3	D	1310	19/19	1.00	0.07	25,34,66,74	0
2	HF5	C	1310	26/26	1.00	0.07	23,50,99,99	0
2	HF5	A	1310	26/26	1.00	0.08	25,56,99,99	0
2	HF5	B	1310	26/26	1.00	0.08	28,61,99,99	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.



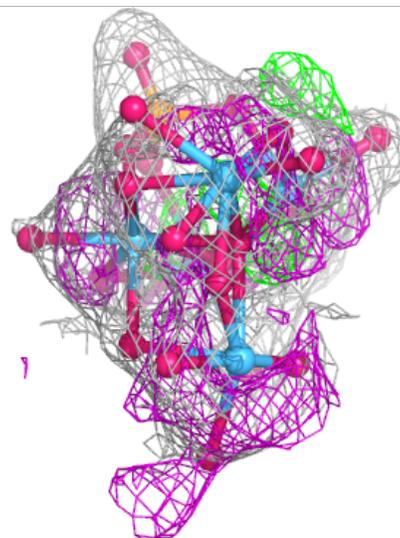
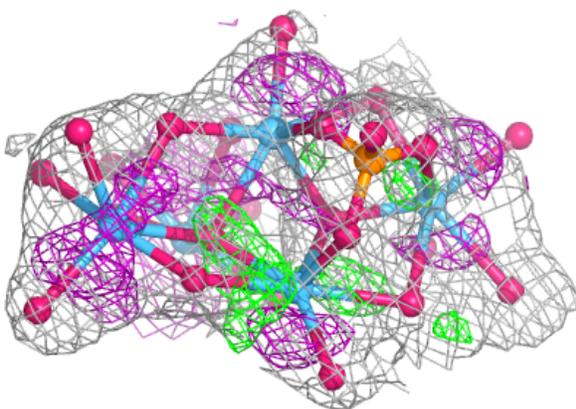
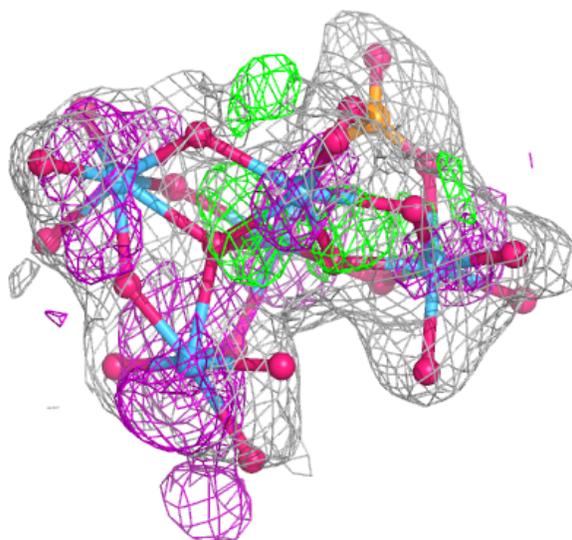
**Electron density around PHF H 1310:**

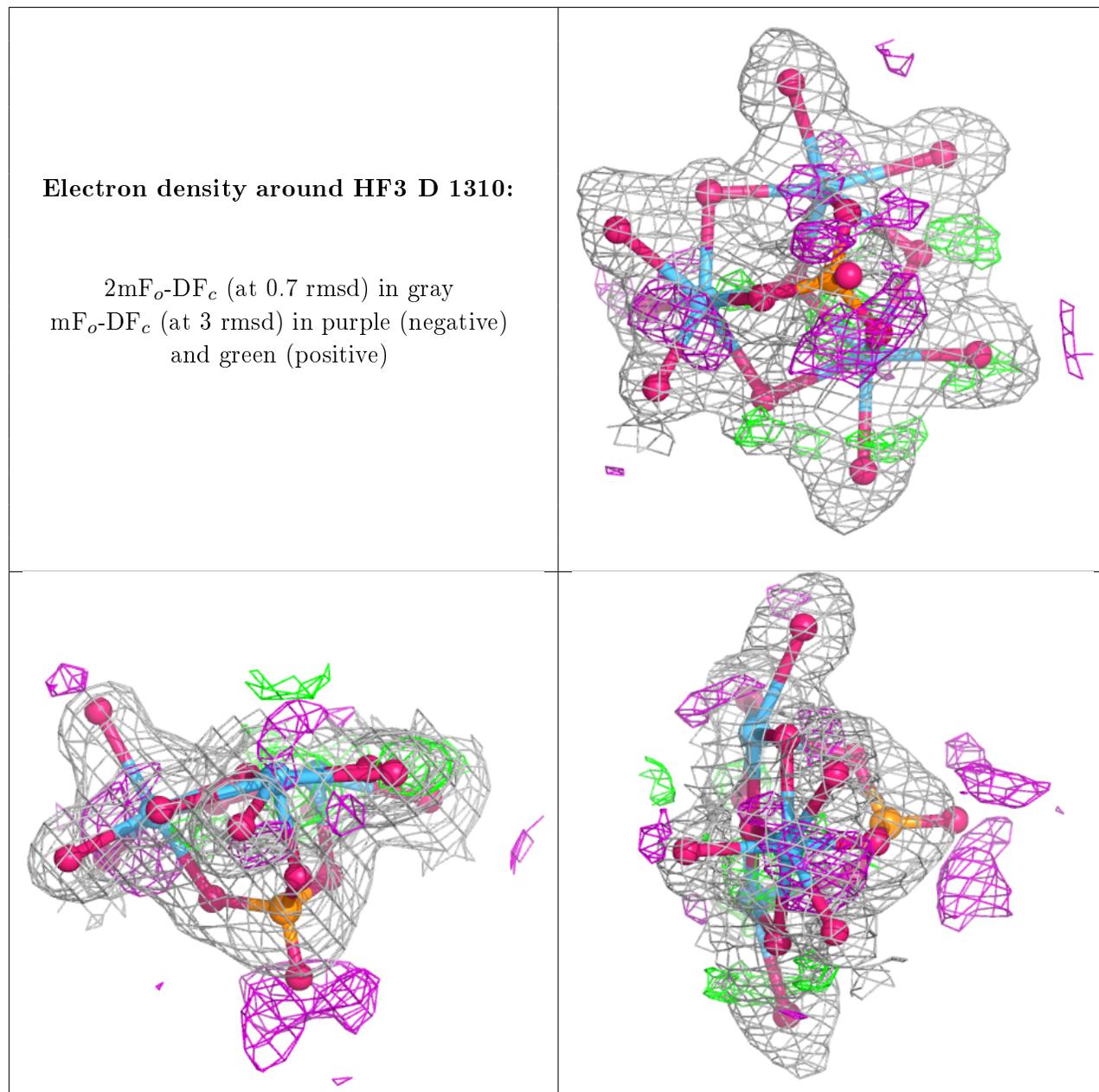
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PHF I 1310:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.