wwPDB X-ray Structure Validation Summary Report (i)

Dec 2, 2023 – 03:51 pm GMT

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)

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

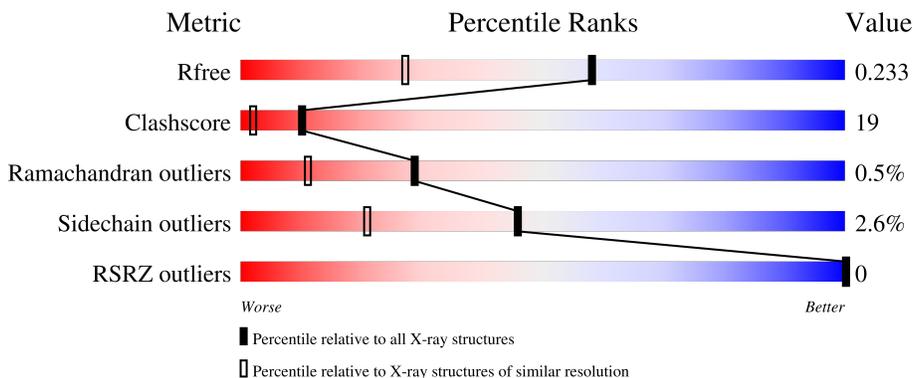|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.233
Clashscore		19
Ramachandran outliers		0.5%
Sidechain outliers		2.6%
RSRZ outliers		0

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 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	309	76% ... 22% ·
1	B	309	74% ... 24% ·
1	C	309	73% ... 26% ·
1	D	309	65% ... 34% ·

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| Mol	Chain	Length	Quality of chain
1	E	309	71% 27%
1	F	309	72% 28%
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
1	A	309	Total	C	N	O	S	0	0	0
			2377	1507	423	446	1			
1	B	309	Total	C	N	O	S	0	0	0
			2377	1507	423	446	1			
1	C	309	Total	C	N	O	S	0	0	0
			2377	1507	423	446	1			
1	D	309	Total	C	N	O	S	0	0	0
			2377	1507	423	446	1			
1	E	309	Total	C	N	O	S	0	0	0
			2377	1507	423	446	1			
1	F	309	Total	C	N	O	S	0	0	0
			2377	1507	423	446	1			
1	G	309	Total	C	N	O	S	0	0	0
			2377	1507	423	446	1			
1	H	309	Total	C	N	O	S	0	0	0
			2377	1507	423	446	1			
1	I	309	Total	C	N	O	S	0	0	0
			2377	1507	423	446	1			

- Molecule 2 is HF OXO CLUSTER HF5 (three-letter code: HF5) (formula: $H_{12}Hf_5O_{21}$).
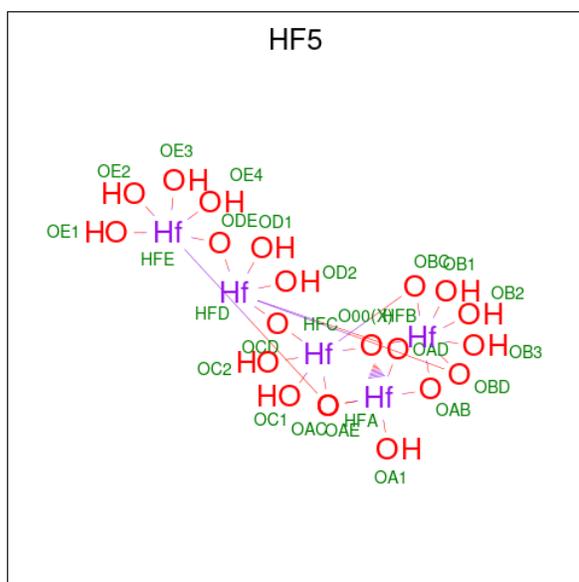
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Hf	O	0	0
			26	5	21		
2	B	1	Total	Hf	O	0	0
			26	5	21		
2	C	1	Total	Hf	O	0	0
			26	5	21		
2	E	1	Total	Hf	O	0	0
			26	5	21		
2	F	1	Total	Hf	O	0	0
			26	5	21		

- Molecule 3 is SMALLEST HF-OXO-PHOSPHATE CLUSTER HF3 (three-letter code: HF3) (formula: $H_7Hf_3O_{15}P$).

HF3
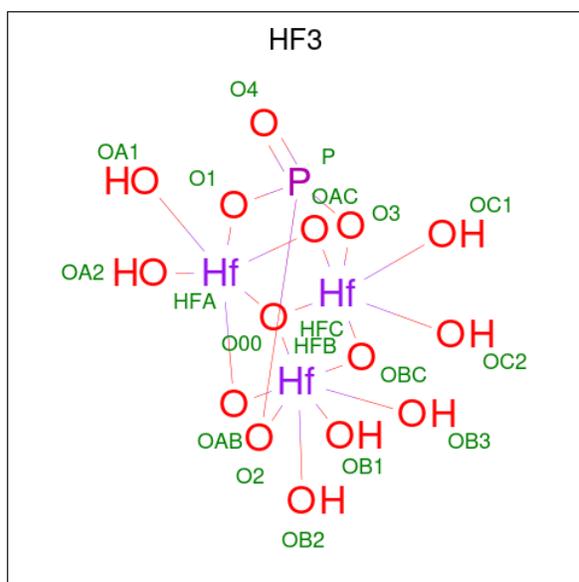
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	Hf	O	P	0	0
			19	3	15	1		

- Molecule 4 is HF-OXO-PHOSPHATE CLUSTER PHF (three-letter code: PHF) (formula: $H_{11}Hf_5O_{23}P$).
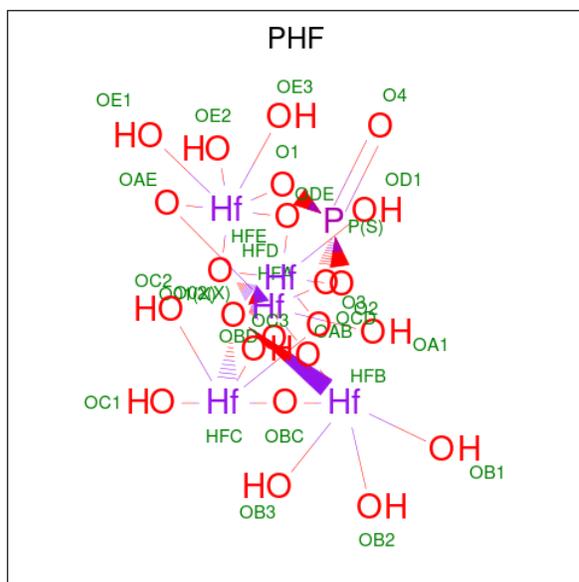
PHF

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

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

3 Residue-property plots ⓘ

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: IRON BINDING PROTEIN

Chain A:

- Molecule 1: IRON BINDING PROTEIN

Chain B:

- Molecule 1: IRON BINDING PROTEIN

Chain C:

• Molecule 1: IRON BINDING PROTEIN

Chain D:

• Molecule 1: IRON BINDING PROTEIN

Chain E:

• Molecule 1: IRON BINDING PROTEIN

Chain F:

• Molecule 1: IRON BINDING PROTEIN

Chain G:

V216 R217 L224 V225 T226 Y227 L233 K234 N238 K239 D240 E241 K244 K252 Q255 R256 T259 Y265 P266 H270 T274 E278 K282 V288 S289 T292 E295 K296 E297 H298 R301 L302 L303 A306 G307 M308 K309

• Molecule 1: IRON BINDING PROTEIN

Chain H:

61% 38%

D1 I2 T3 V4 Y5 N6 G7 Q8 H9 K10 E11 A12 V16 A17 D18 A19 F20 T21 I26 K27 V28 K29 L30 N31 S32 A33 K34 G35 D36 Q37 L38 Q41 I42 E45 R48 S49 P50 A51 D52 V53 F54 Y55 I59 P60 T64 N69 L70 L71 E72 S77 T78

I79 N80 E81 T82 R83 G84 K93 D94 S99 G100 R101 S102 R103 V104 V105 V106 Y107 L112 S113 E114 K115 D116 P127 I133 P137 F142 K151 E155 Y168 S176 N184 L191 T211 R212 L213 N214 F215 V216 R217 A231 V232 L233 K234 S235 S236

Q237 N238 K239 D240 E241 A242 K243 K244 F245 V246 A247 F248 L249 A250 G251 K252 E253 G254 Q255 R256 A257 L258 T259 A260 V261 R262 P266 L267 N268 P269 H270 V271 V272 S273 E278 P279 I280 A281 K282 V288 S289 T292 V293 S294 E295 K296 E297 H298 A299 T300 R301 K309

• Molecule 1: IRON BINDING PROTEIN

Chain I:

66% 32%

D1 V4 Y5 N6 H9 K10 V16 F20 A23 I26 K27 L30 N31 S32 A33 K34 Q37 L38 Q41 I42 K43 E44 E45 S49 I59 P60 A61 T64 A68 N69 E72 P73 I79 N80 E81 T82 R83 G84 K85 K92 K93 D94 R103

V104 V105 V106 R110 S120 V121 L122 N123 I133 V136 P137 T138 S139 F142 L159 K160 W161 L162 K163 G164 L165 K166 E167 Y168 Y172 A173 K174 N175 S176 V177 A181 V182 E183 E186 V187 L191 N194 Y195 Y196 W197 F200 A201 R202 E203 K204 G205 N208

V209 H210 T211 R212 V216 R217 A223 S236 K239 F245 F248 L249 A250 G251 K252 E253 G254 Q255 R256 T259 Y265 P266 L267 N268 P279 K282 L283 Q287 V293 K296 R301 E304 M308 K309

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	28.0	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 51.3	EDS
L-test for twinning[2]	$< |L| > = 0.41, < L^2 > = 0.23$	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^2)	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.*

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[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 (i)

5.1 Standard geometry (i)

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

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 (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	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:C:202:ARG:HH22	1:C:274:THR:HG23	1.21	1.03

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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	E	101	ARG
1	I	282	LYS
1	F	103	ARG
1	I	202	ARG
1	H	259	THR

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

Mol	Chain	Res	Type
1	G	184	ASN
1	I	9	HIS
1	G	255	GLN
1	H	80	ASN
1	C	208	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

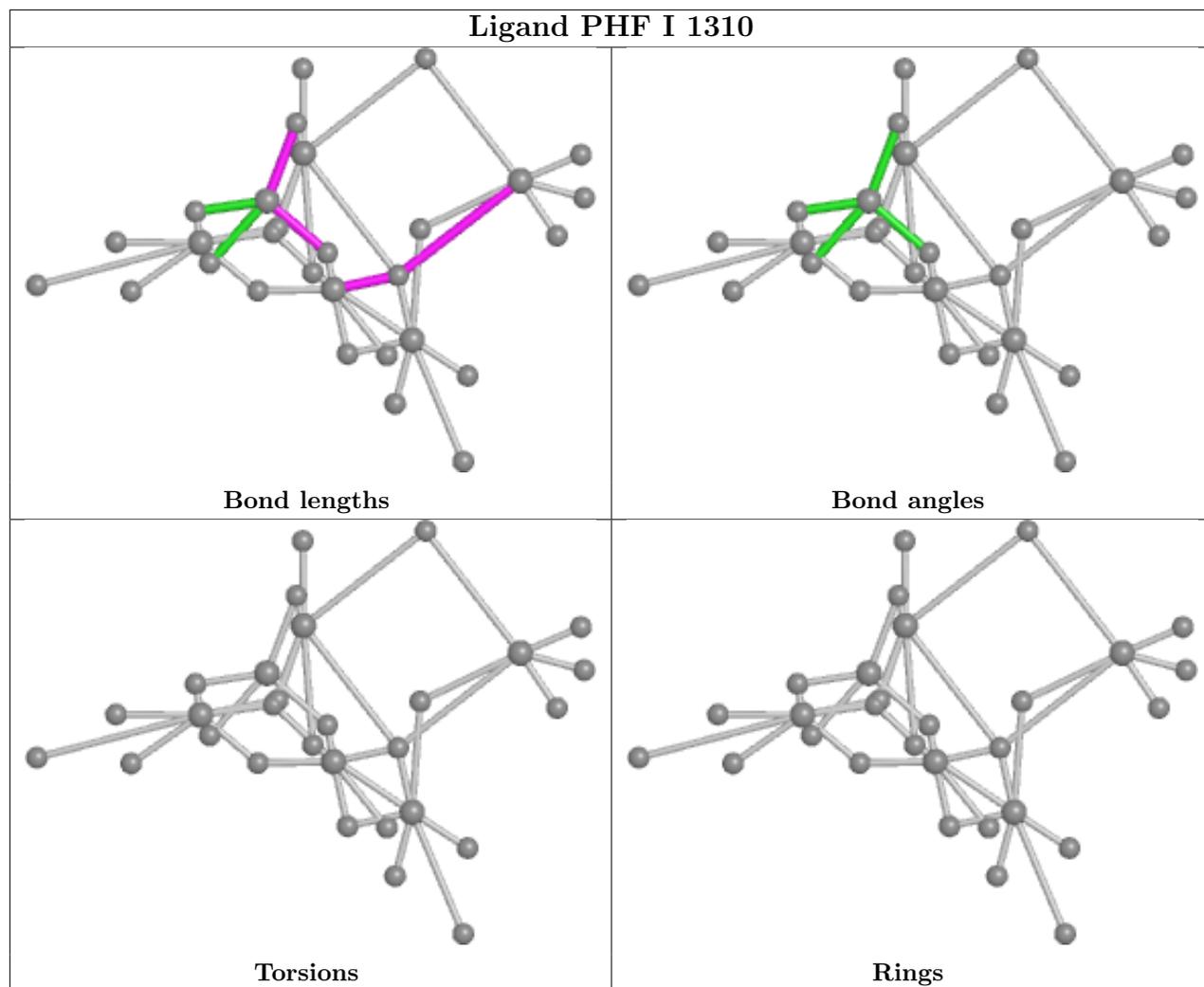There are no chirality outliers.

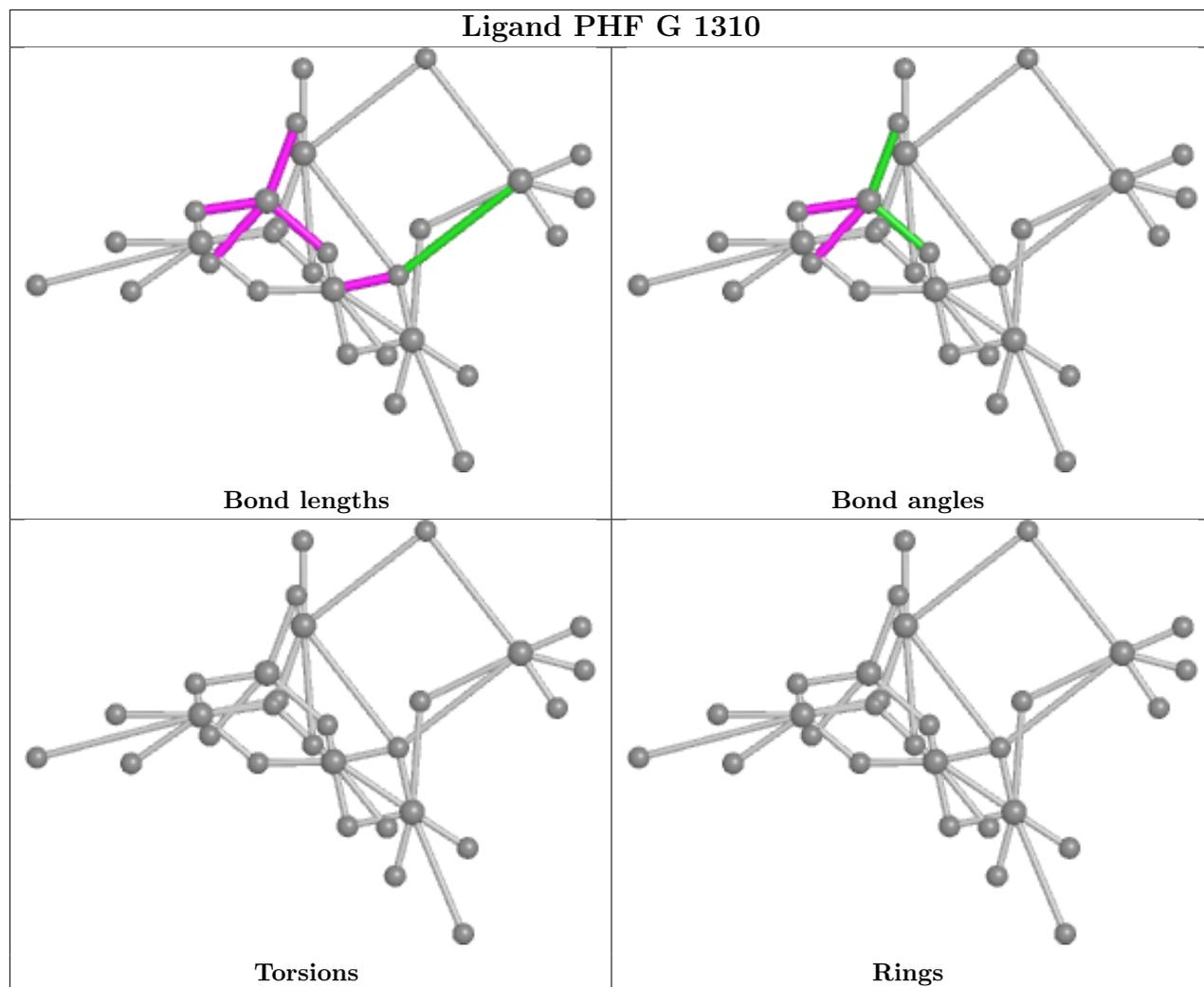There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

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

Bond lengths

Bond angles

Torsions

Rings

Ligand PHF H 1310

Bond lengths

Bond angles

Torsions

Rings

Ligand PHF G 1310

Bond lengths

Bond angles

Torsions

Rings

Ligand HF3 D 1310

Bond lengths

Bond angles

Torsions

Rings
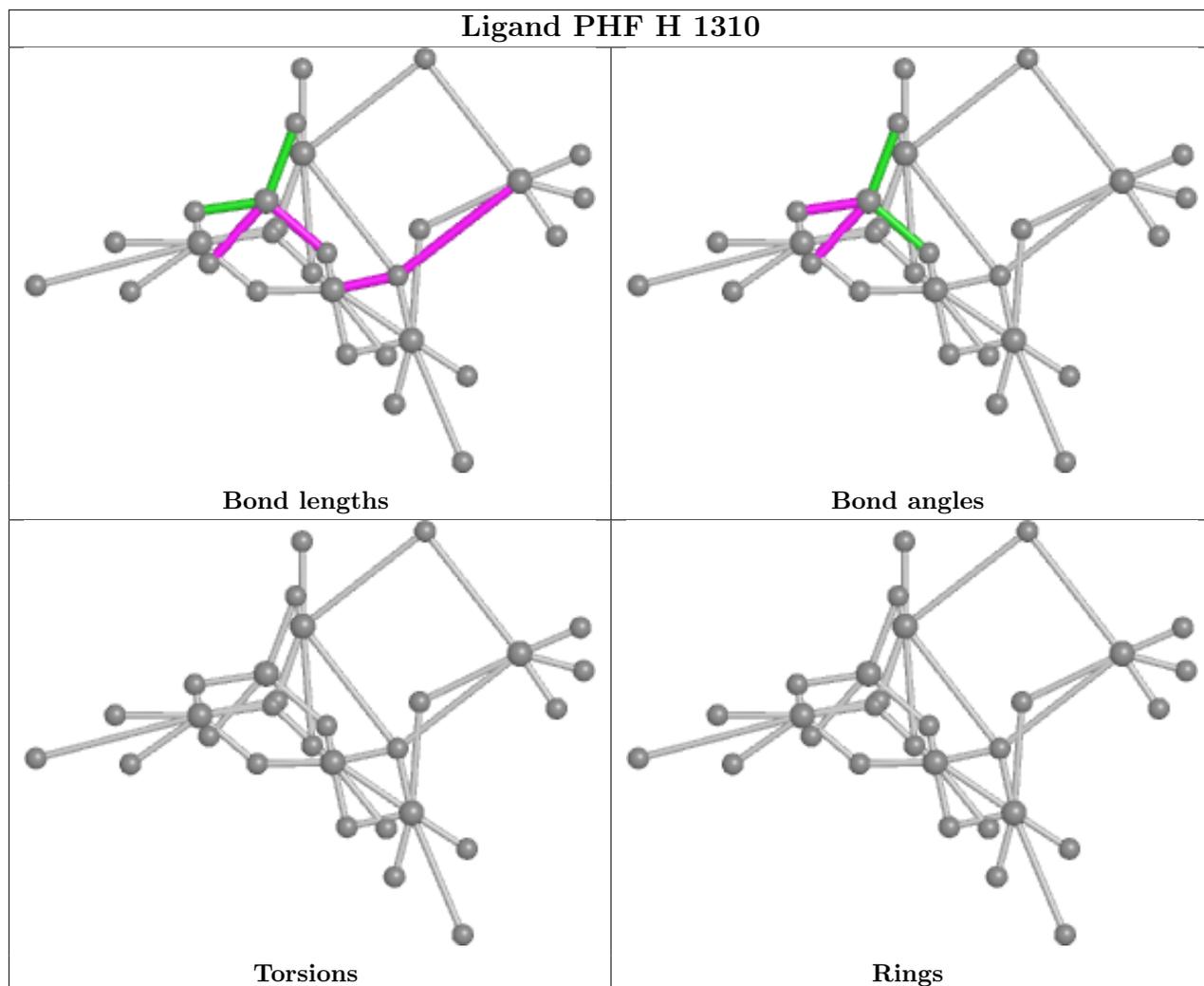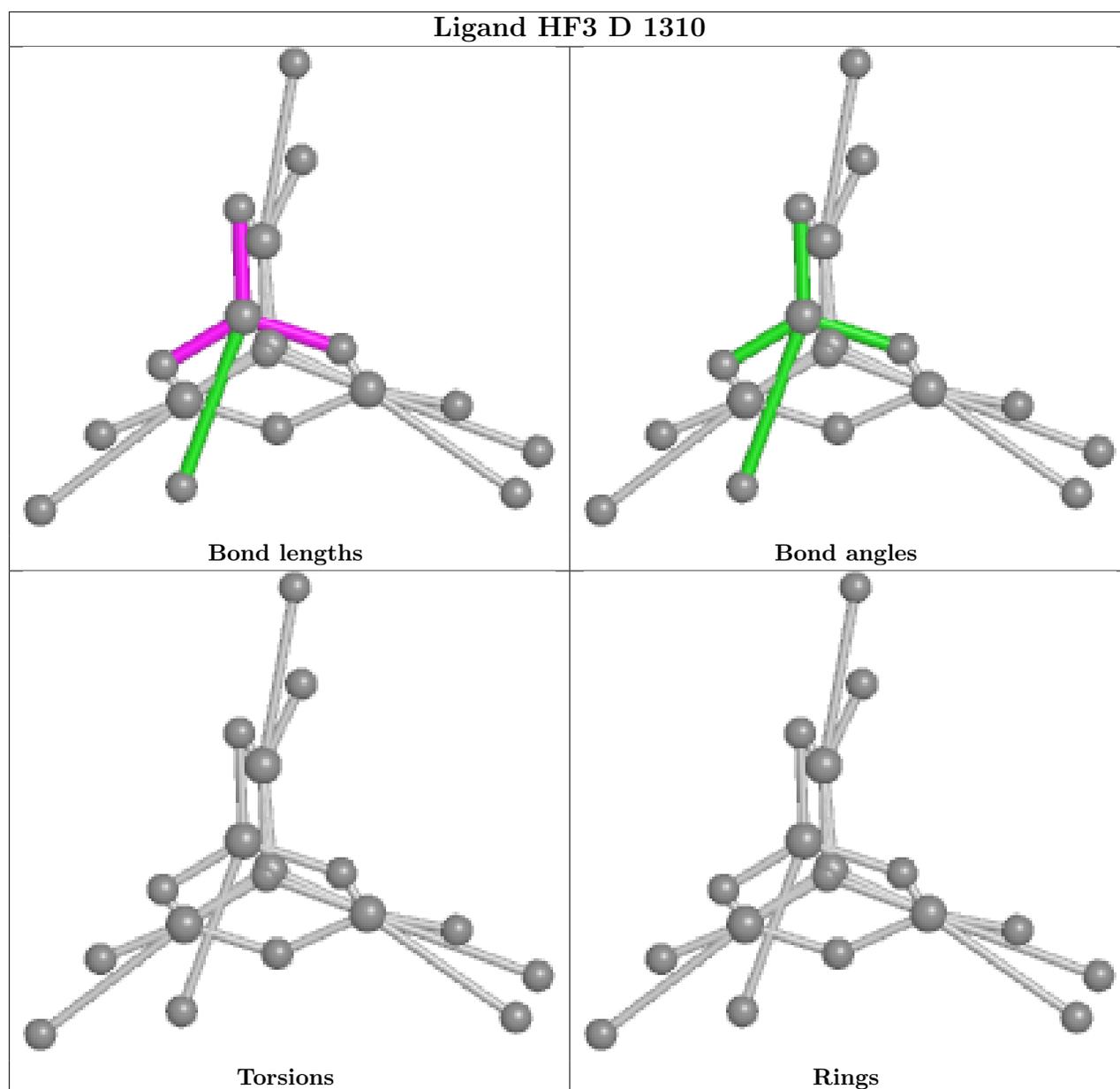
5.7 Other polymers ⓘ

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, 95th 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	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 ⓘ

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

6.3 Carbohydrates ⓘ
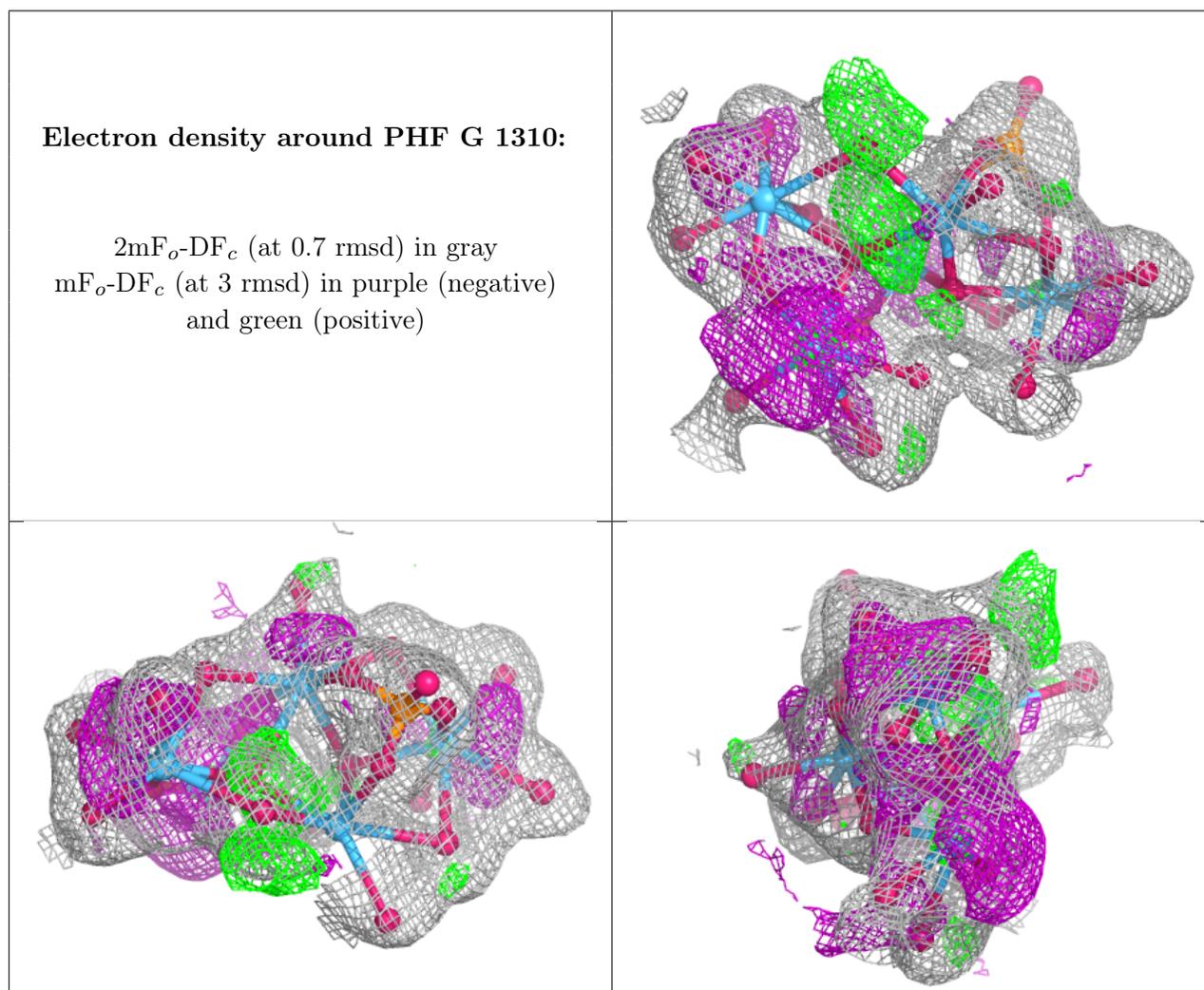
There are no monosaccharides in this entry.

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, 95th 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
2	HF5	E	1310	26/26	0.99	0.09	29,69,99,99	0
2	HF5	F	1310	26/26	0.99	0.09	34,73,99,99	0
4	PHF	G	1310	29/29	0.99	0.07	31,53,90,99	0
4	PHF	H	1310	29/29	0.99	0.07	34,65,83,89	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.
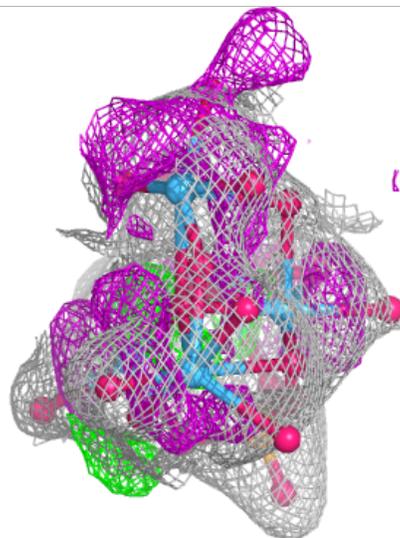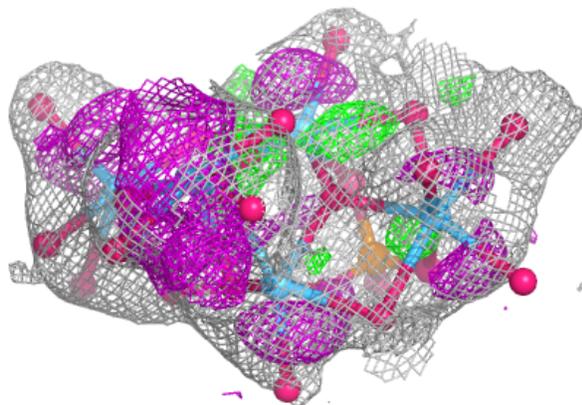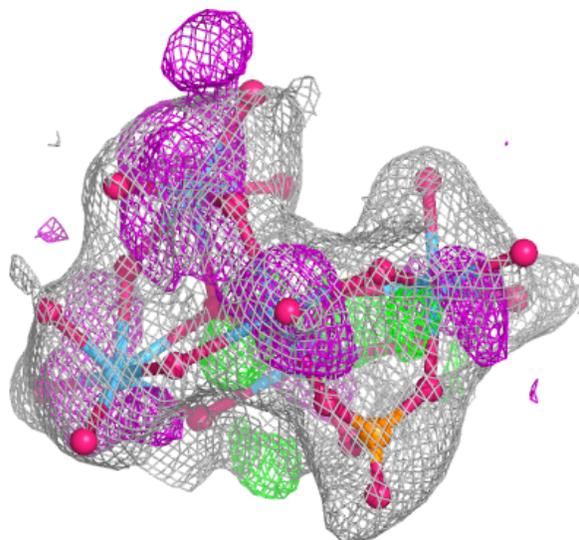
Electron density around PHF G 1310:

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

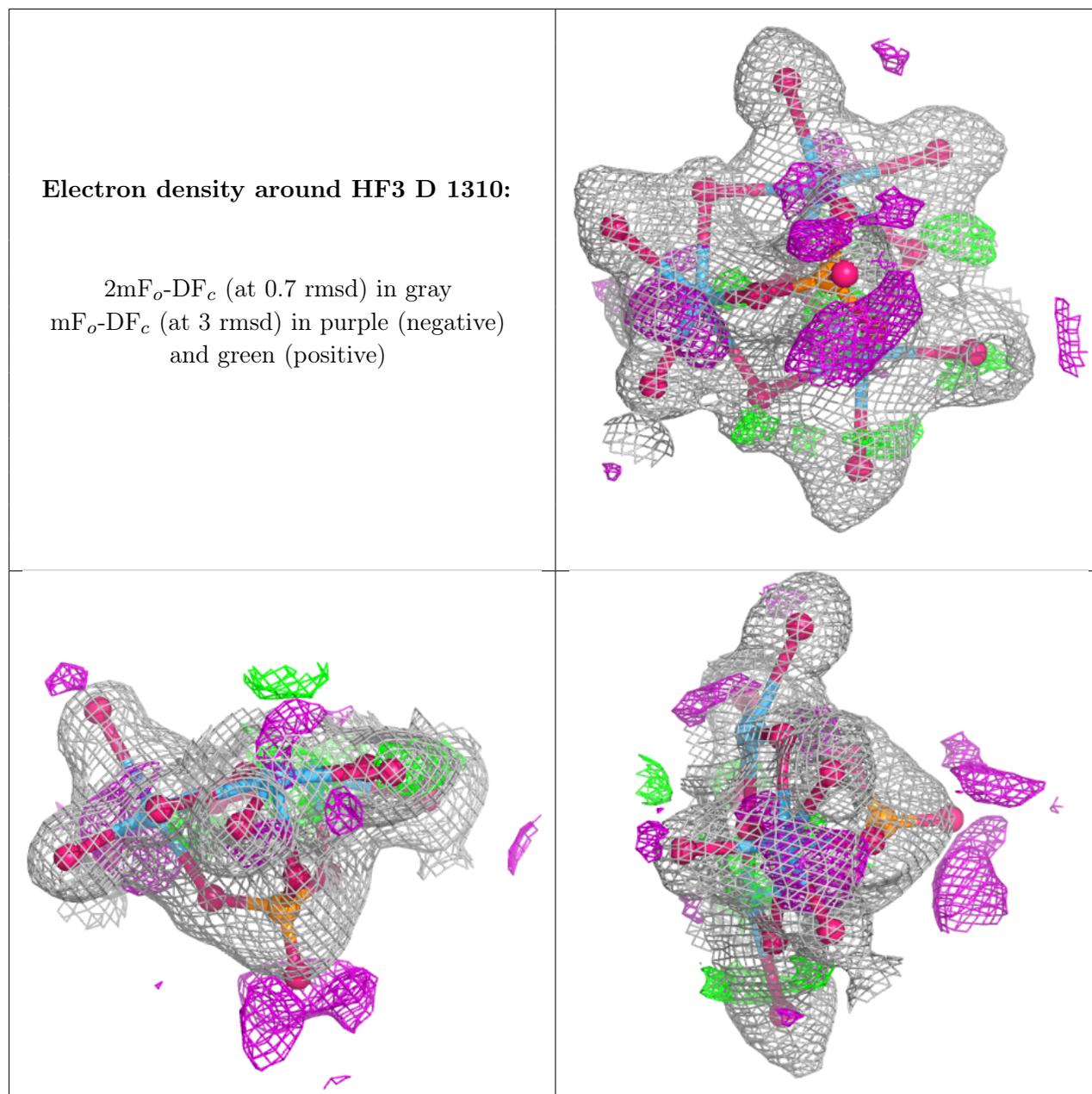**Electron density around PHF H 1310:**

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
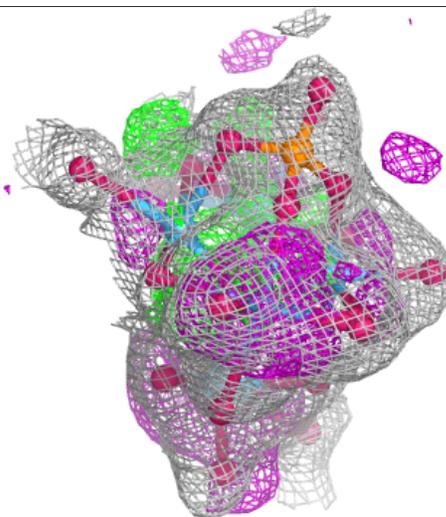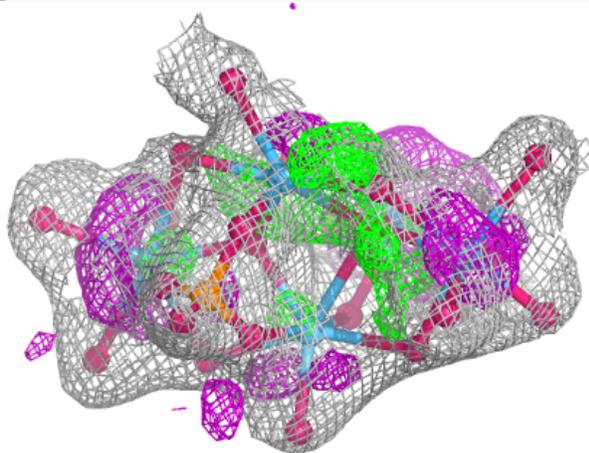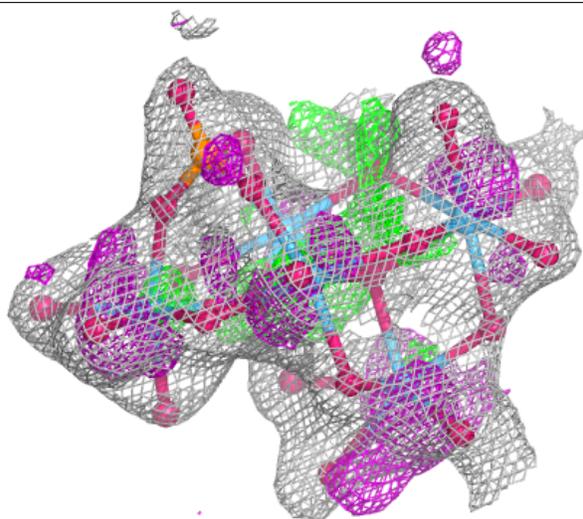
Electron density around PHF I 1310:

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

Electron density around HF3 D 1310:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.