wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 01:36 AM EDT

PDB ID	:	2FHJ
Title	:	Crystal structure of formylmethanofuran: tetrahydromethanopterin formyltransferase in complex with its coenzymes
Authors	:	Acharya, P.; Warkentin, E.; Thauer, R.K.; Shima, S.; Ermler, U.
Deposited on	:	2005-12-25
Resolution	:	2.00 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:

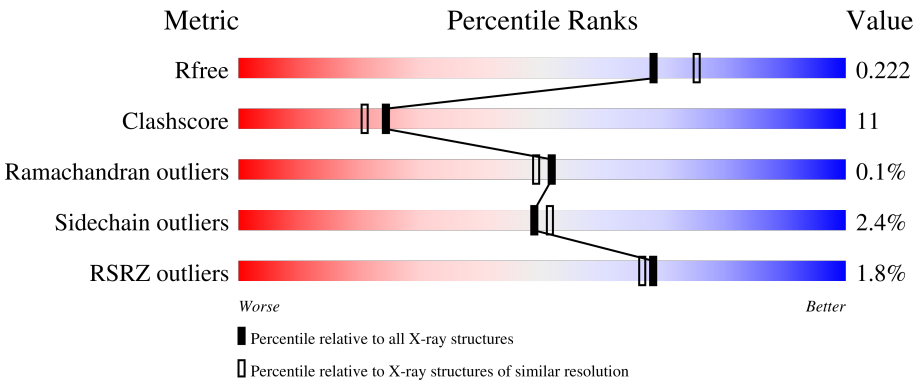
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	296	2% 83% 16% •
1	B	296	3% 84% 14% •
1	C	296	% 83% 16%
2	D	296	% 80% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MFN	A	900[A]	X	-	-	-
4	MFN	A	900[B]	X	-	-	-
4	MFN	A	902[A]	-	X	-	-
4	MFN	A	902[B]	-	X	-	-
4	MFN	C	901[A]	X	-	-	-
4	MFN	C	901[B]	X	-	-	-
4	MFN	D	903	X	-	-	-
5	H4Z	A	905[A]	-	-	-	X
5	H4Z	A	905[B]	-	-	-	X
6	PE4	A	922	-	-	X	-
6	PE4	D	921	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9818 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 Formylmethanofuran--tetrahydromethanopterin formyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2255	1423	362	453	17	0	9	0
1	B	296	2218	1398	358	446	16	0	6	0
1	C	296	2216	1398	357	446	15	0	2	0

- Molecule 2 is a protein called Formylmethanofuran--tetrahydromethanopterin formyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	296	2261	1426	364	455	16	0	14	0

There is a discrepancy between the modelled and reference sequences:

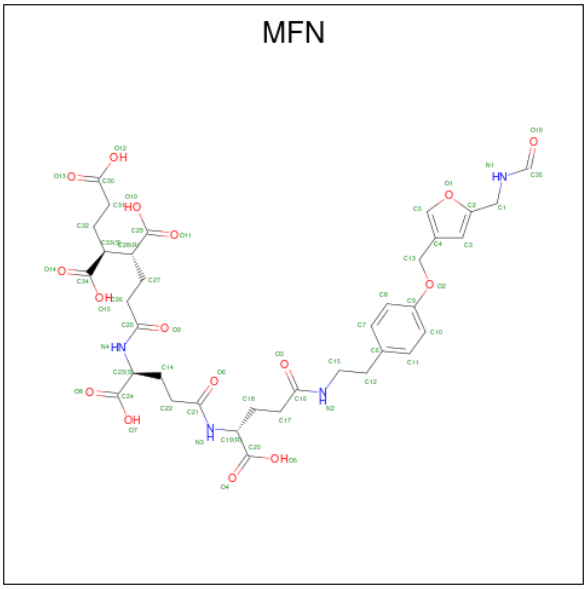
Chain	Residue	Modelled	Actual	Comment	Reference
D	58	CSO	CYS	modified residue	UNP Q49610

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
3	A	4	4	4	0	0
3	B	5	5	5	0	0
3	C	4	4	4	0	0
3	D	4	4	4	0	0

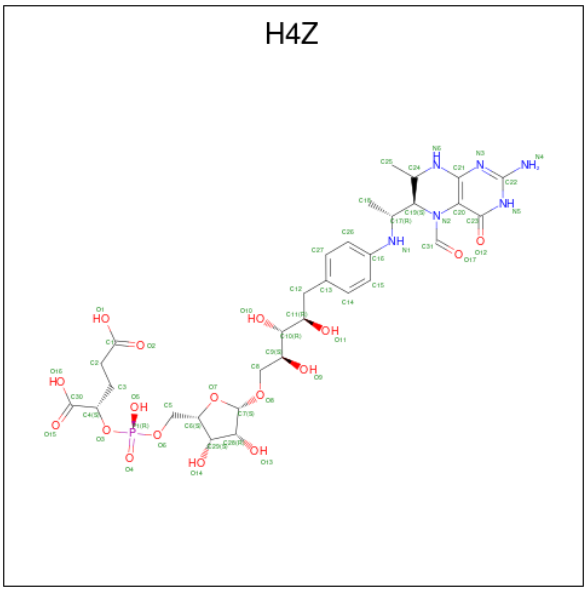
- Molecule 4 is N-[4,5,7-TRICARBOXYHEPTANOYL]-L-GAMMA-GLUTAMYL-N-{2-[4-({

5-[(FORMYLAMINO)METHYL]-3-FURYL}METHOXY)PHENYL]ETHYL}-D-GLUTAMINE (three-letter code: MFN) (formula: $C_{35}H_{44}N_4O_{16}$).



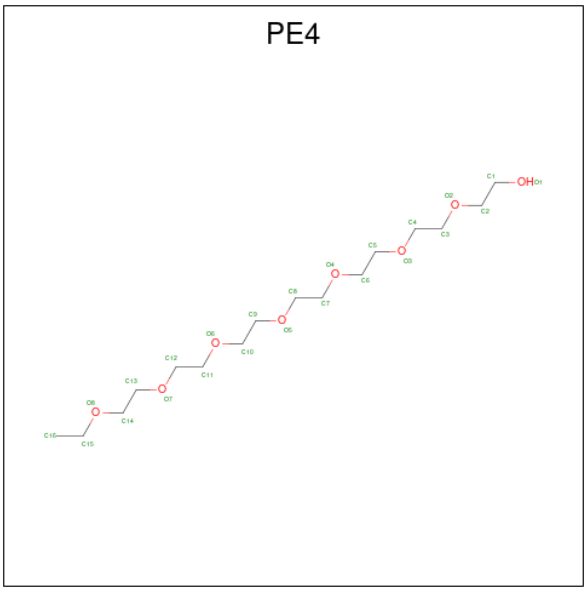
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	80	53	8	19	0	1
			Total	C	N	O		
4	A	1	90	59	8	23	0	1
			Total	C	N	O		
4	C	1	64	44	6	14	0	1
			Total	C	N	O		
4	D	1	32	22	3	7	0	0

- Molecule 5 is 5-(4-{[1-(2-AMINO-5-FORMYL-7-METHYL-4-OXO-3,4,5,6,7,8-HEXAHYDROPTERIDIN-6-YL)ETHYL]AMINO}PHENYL)-5-DEOXY-1-O-{5-O-[(1,3-DICARBOXYPROPOXY)(HYDROXY)PHOSPHORYL]PENTOFURANOSYL}PENTITOL (three-letter code: H4Z) (formula: $C_{31}H_{45}N_6O_{17}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	47	32	12	3	0	1
			Total	C	N	O		
5	C	1	18	10	6	2	0	0

- Molecule 6 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	18	12	6	0	0

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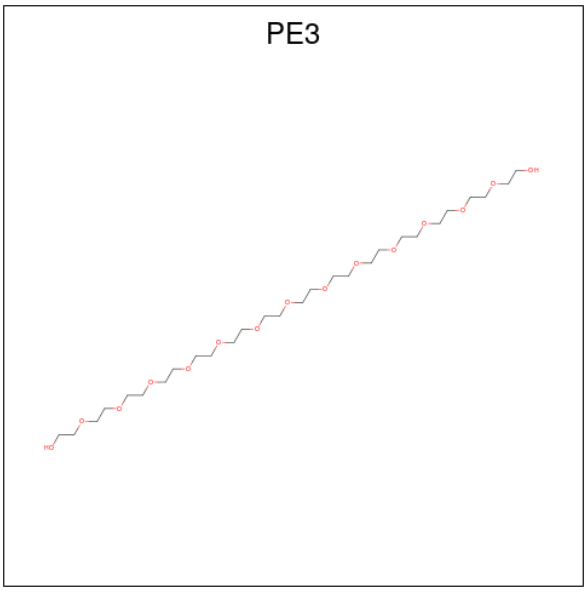
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	D	1	24	16	8	0	0
			Total	C	O		
6	D	1	18	12	6	0	0

- Molecule 7 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1,41-DIOL (three-letter code: PE3) (formula: $C_{28}H_{58}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	C	1	9	6	3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	123	123	123	0	0
			Total	O		
8	B	79	79	79	0	0
			Total	O		
8	C	125	125	125	0	0
			Total	O		
8	D	124	124	124	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: Formylmethanofuran--tetrahydromethanopterin formyltransferase

Chain A: 2% 83% 16%

M1 I8 F12 F16 H30 A33 V37 S46 V47 I48 M49 I56 V73 I77 G78 H79 N80 D81 R92 E113 E117 D118 R119 Y122 F127 G128 D129 E136 R140 V148 S157 V164 P177 Q181 E184 F200

V205 S209 K210 D217 F218 L219 P220 D225 V231 E232 D233 N234 E238 K241 C242 V243 V247 I248 N249 N252 E253 E254 R261 F281 G282 L285 E289 H293 D294 L295 F296

• Molecule 1: Formylmethanofuran--tetrahydromethanopterin formyltransferase

Chain B: 3% 84% 14%

M1 I8 F12 H30 K31 W32 V37 G42 S46 I56 Y60 E64 E65 V73 H79 N80 D81 R92 M98 A112 E113 R119 F127 E136 L137 D138 G139 R140 V148 S157 Q176 F200 V205 G212 S213 D225

V231 E232 D233 N234 E238 K241 C242 V243 N252 R261 A266 Q269 F281 K284 L285 G286 Q287 Y288 E289 H293 D294 L295 F296

• Molecule 1: Formylmethanofuran--tetrahydromethanopterin formyltransferase

Chain C: % 83% 16%

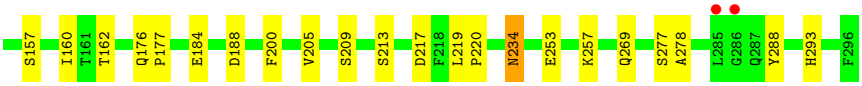
M1 D10 R22 T26 I35 A36 V37 K38 E39 S46 V47 I48 M49 C50 E53 I56 G69 H79 N80 D81 R92 I93 G94 Q95 C96 V97 M98 T99 A100 A103 E115 R119 V120 F127 G128 D129 D138 S157 T162 Q176 P177

L180 Q181 E184 D188 K191 F200 V205 K210 F218 D233 N234 E245 R261 E265 K284 H293 F296

• Molecule 2: Formylmethanofuran--tetrahydromethanopterin formyltransferase

Chain D: % 80% 20%

M1 E7 D10 A21 R22 V23 L24 I25 T26 H30 K31 W32 A33 M34 V37 K38 S46 V47 I48 M49 C50 E53 I56 G59 Y60 V73 H79 N80 D81 R92 I93 G94 Q95 C96 V97 M98 A103 E115 R119 V120 K123 K144 I145


S157
I160
T161
T162
Q176
P177
E184
D188
F200
V205
S209
S213
D217
F218
L219
P220
N234
E253
K257
Q269
S277
A278
L285
G286
Q287
Y288
H293
F296

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.00Å 74.15Å 103.87Å 90.00° 113.54° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.53 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-2.00) 96.4 (19.53-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.219 , 0.256 0.229 , 0.222	Depositor DCC
R_{free} test set	3856 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.785	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 65.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9818	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.02% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: H4Z, MFN, PE3, PE4, CSO, K

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	0.51	0/2321	0.88	8/3143 (0.3%)
1	B	0.51	0/2273	0.97	7/3084 (0.2%)
1	C	0.56	0/2267	0.74	3/3072 (0.1%)
2	D	0.59	1/2349 (0.0%)	0.80	3/3178 (0.1%)
All	All	0.54	1/9210 (0.0%)	0.85	21/12477 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
2	D	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	23	VAL	CB-CG2	5.11	1.63	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	22	ARG	NE-CZ-NH2	-22.31	109.15	120.30
1	B	261	ARG	NE-CZ-NH2	-21.73	109.44	120.30
1	B	92	ARG	NE-CZ-NH2	-21.20	109.70	120.30
1	B	92	ARG	NE-CZ-NH1	17.76	129.18	120.30
1	A	261	ARG	NE-CZ-NH1	-17.55	111.53	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	ARG	Sidechain
1	B	119	ARG	Sidechain
1	B	261	ARG	Sidechain
1	B	92	ARG	Sidechain
2	D	22	ARG	Sidechain

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	2255	0	2154	53	0
1	B	2218	0	2085	43	0
1	C	2216	0	2114	45	0
2	D	2261	0	2128	51	0
3	A	4	0	0	0	0
3	B	5	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	170	0	121	25	0
4	C	64	0	46	11	0
4	D	32	0	23	3	0
5	A	47	0	32	9	0
5	C	18	0	12	5	0
6	A	18	0	23	25	0
6	D	42	0	59	6	0
7	C	9	0	11	4	0
8	A	123	0	0	7	0
8	B	79	0	0	4	0
8	C	125	0	0	3	0
8	D	124	0	0	3	0
All	All	9818	0	8808	201	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 11.

The worst 5 of 201 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:A:49:MET:SD	4:A:902[A]:MFN:O5	2.16	1.03
1:A:49:MET:SD	4:A:902[B]:MFN:O5	2.20	0.98
5:A:905[B]:H4Z:H251	8:A:8000:HOH:O	1.70	0.92
1:B:269[A]:GLN:NE2	1:C:69:GLY:O	2.07	0.87
6:A:922:PE4:H12	1:C:184:GLU:OE1	1.79	0.83

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	302/296 (102%)	290 (96%)	12 (4%)	0	100	100
1	B	300/296 (101%)	284 (95%)	16 (5%)	0	100	100
1	C	296/296 (100%)	287 (97%)	8 (3%)	1 (0%)	41	37
2	D	307/296 (104%)	296 (96%)	11 (4%)	0	100	100
All	All	1205/1184 (102%)	1157 (96%)	47 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	138	ASP

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	233/229 (102%)	225 (97%)	8 (3%)	37	36
1	B	222/229 (97%)	211 (95%)	11 (5%)	24	20
1	C	226/229 (99%)	223 (99%)	3 (1%)	69	74
2	D	231/228 (101%)	229 (99%)	2 (1%)	78	83
All	All	912/915 (100%)	888 (97%)	24 (3%)	49	48

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	241	LYS
1	B	293	HIS
1	B	269[B]	GLN
1	B	294	ASP
1	A	293	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	234	ASN
2	D	293	HIS
1	C	79	HIS
1	C	95	GLN
1	C	215	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
2	CSO	D	58	2	3,6,7	0.39	0	0,6,8	-	-

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
2	CSO	D	58	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 17 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
5	H4Z	A	905[A]	-	23,24,58	2.48	5 (21%)	27,34,84	3.89	11 (40%)
7	PE3	C	3792	-	8,8,42	0.56	0	7,7,41	0.25	0
4	MFN	C	901[A]	-	29,33,56	1.86	6 (20%)	34,42,73	2.45	17 (50%)
6	PE4	D	920	-	23,23,23	0.57	0	22,22,22	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	H4Z	C	904	-	18,19,58	3.56	6 (33%)	13,28,84	3.57	9 (69%)
4	MFN	A	902[A]	-	41,45,56	1.94	13 (31%)	52,58,73	2.86	19 (36%)
5	H4Z	A	905[B]	-	26,27,58	2.94	7 (26%)	24,39,84	2.20	9 (37%)
6	PE4	D	921	-	17,17,23	0.54	0	16,16,22	0.66	0
4	MFN	C	901[B]	-	29,33,56	1.99	8 (27%)	34,42,73	2.77	13 (38%)
4	MFN	A	900[A]	-	36,40,56	1.75	8 (22%)	46,52,73	2.13	15 (32%)
4	MFN	A	902[B]	-	43,47,56	1.94	13 (30%)	52,60,73	2.70	23 (44%)
4	MFN	D	903	-	29,33,56	1.91	8 (27%)	34,42,73	1.78	10 (29%)
6	PE4	A	922	-	17,17,23	0.38	0	16,16,22	0.88	0
4	MFN	A	900[B]	-	38,42,56	1.80	9 (23%)	46,54,73	2.06	16 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	H4Z	A	905[A]	-	-	4/5/17/79	0/3/3/4
7	PE3	C	3792	-	-	3/6/6/40	-
4	MFN	C	901[A]	-	1/1/4/17	12/24/28/63	0/2/2/2
6	PE4	D	920	-	-	13/21/21/21	-
5	H4Z	C	904	-	-	3/4/22/79	0/1/2/4
4	MFN	A	902[A]	-	-	29/41/45/63	0/2/2/2
5	H4Z	A	905[B]	-	-	7/10/26/79	0/2/3/4
6	PE4	D	921	-	-	13/15/15/21	-
4	MFN	C	901[B]	-	1/1/4/17	12/24/28/63	0/2/2/2
4	MFN	A	900[A]	-	1/1/7/17	16/35/39/63	0/2/2/2
4	MFN	A	902[B]	-	-	28/43/47/63	0/2/2/2
4	MFN	D	903	-	1/1/4/17	9/24/28/63	0/2/2/2
6	PE4	A	922	-	-	12/15/15/21	-
4	MFN	A	900[B]	-	1/1/7/17	14/37/41/63	0/2/2/2

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	904	H4Z	C31-N2	9.89	1.49	1.35
5	A	905[B]	H4Z	C31-N2	9.81	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	904	H4Z	C20-C23	7.67	1.51	1.41
5	A	905[A]	H4Z	C20-C23	7.55	1.51	1.41
5	A	905[B]	H4Z	C20-C23	6.74	1.50	1.41

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	905[A]	H4Z	C25-C24-C19	11.09	131.06	113.31
5	A	905[A]	H4Z	C24-C19-N2	9.77	117.83	108.62
4	A	902[A]	MFN	C22-C21-N3	9.76	132.77	115.83
5	A	905[A]	H4Z	C19-C24-N6	9.37	117.45	108.62
4	A	902[B]	MFN	C22-C21-N3	9.03	131.50	115.83

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	900[A]	MFN	C23
4	A	900[B]	MFN	C23
4	C	901[A]	MFN	C19
4	C	901[B]	MFN	C19
4	D	903	MFN	C19

5 of 175 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	900[A]	MFN	O6-C21-N3-C19
4	A	900[A]	MFN	C22-C21-N3-C19
4	A	900[A]	MFN	O9-C25-N4-C23
4	A	900[A]	MFN	C26-C25-N4-C23
4	A	900[A]	MFN	C17-C18-C19-N3

There are no ring outliers.

14 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	905[A]	H4Z	2	0
7	C	3792	PE3	4	0
4	C	901[A]	MFN	5	0
6	D	920	PE4	1	0
5	C	904	H4Z	5	0
4	A	902[A]	MFN	10	0

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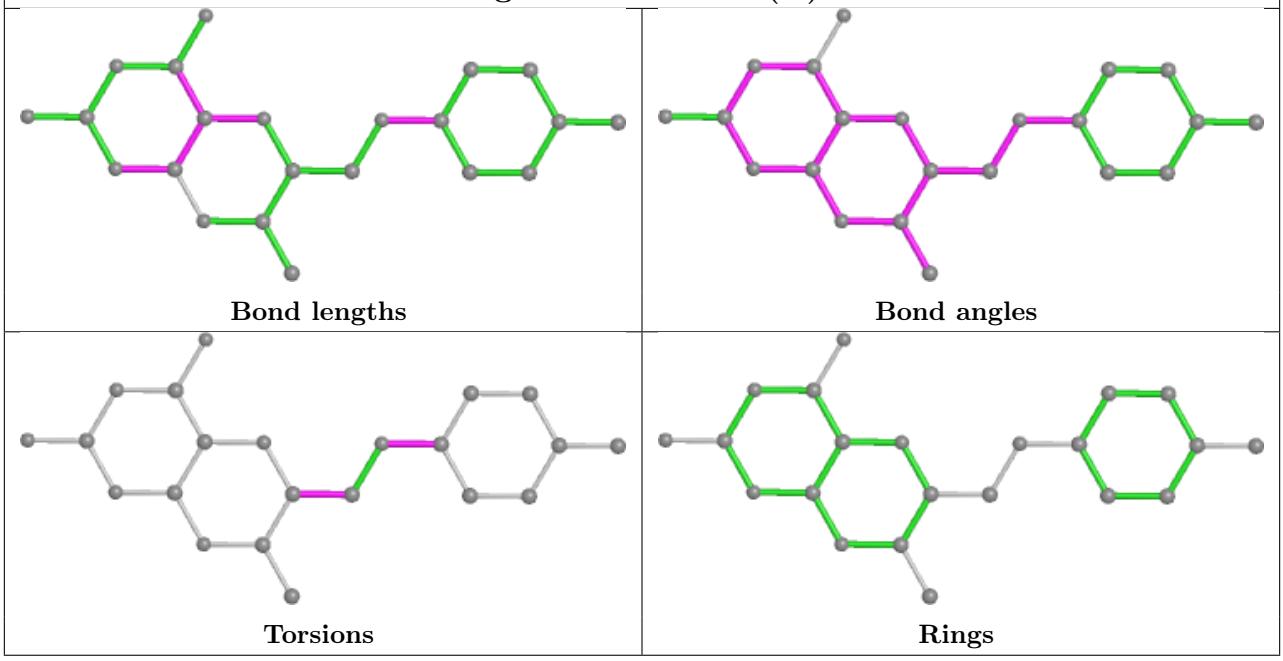
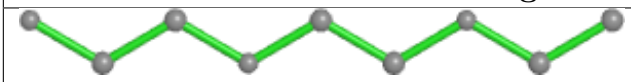
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	905[B]	H4Z	7	0
6	D	921	PE4	5	0
4	C	901[B]	MFN	6	0
4	A	900[A]	MFN	2	0
4	A	902[B]	MFN	11	0
4	D	903	MFN	3	0
6	A	922	PE4	25	0
4	A	900[B]	MFN	2	0

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.

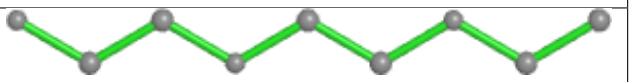
Ligand H4Z A 905 (A)



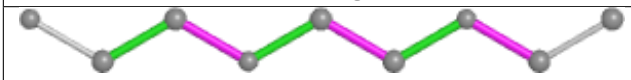
Ligand PE3 C 3792



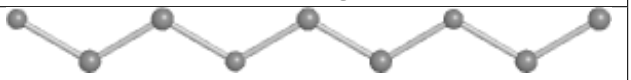
Bond lengths



Bond angles

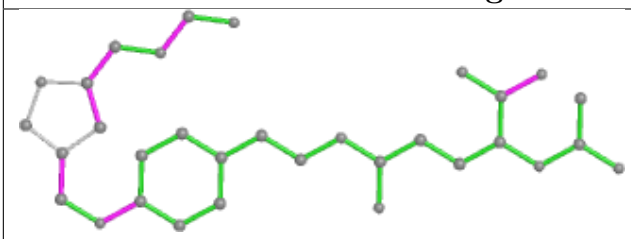


Torsions

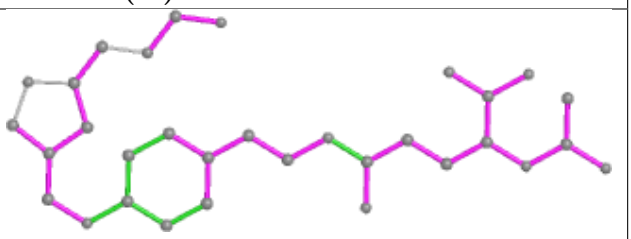


Rings

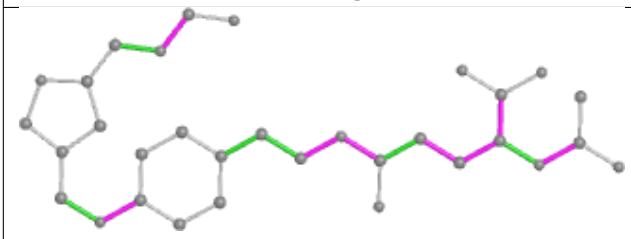
Ligand MFN C 901 (A)



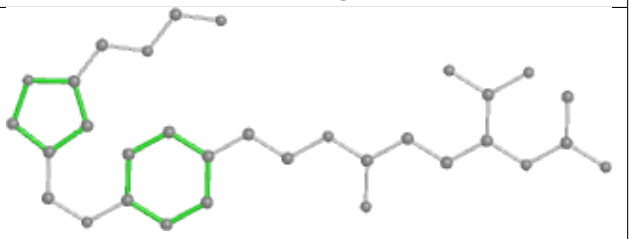
Bond lengths



Bond angles



Torsions

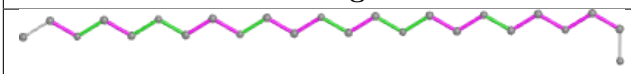


Rings

Ligand PE4 D 920

Bond lengths

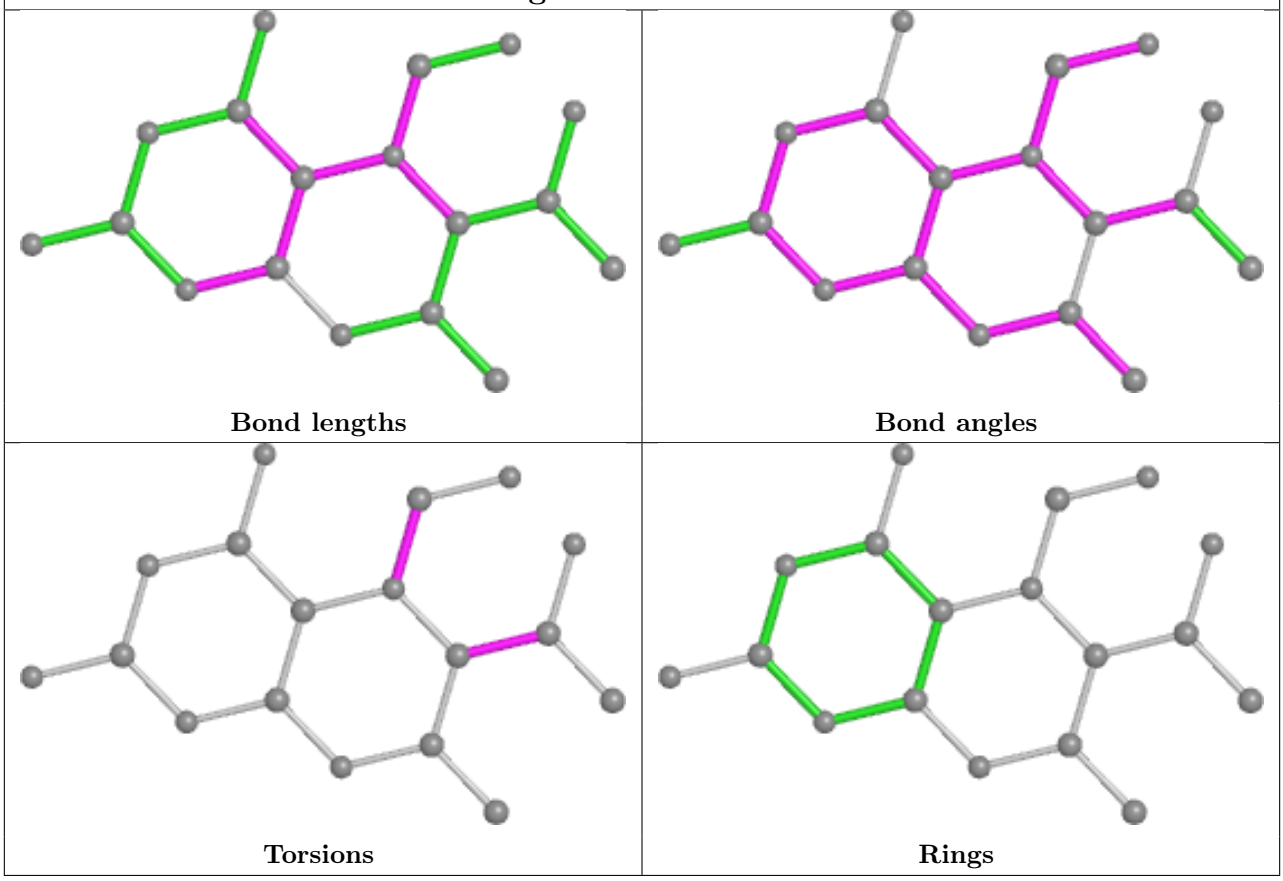
Bond angles



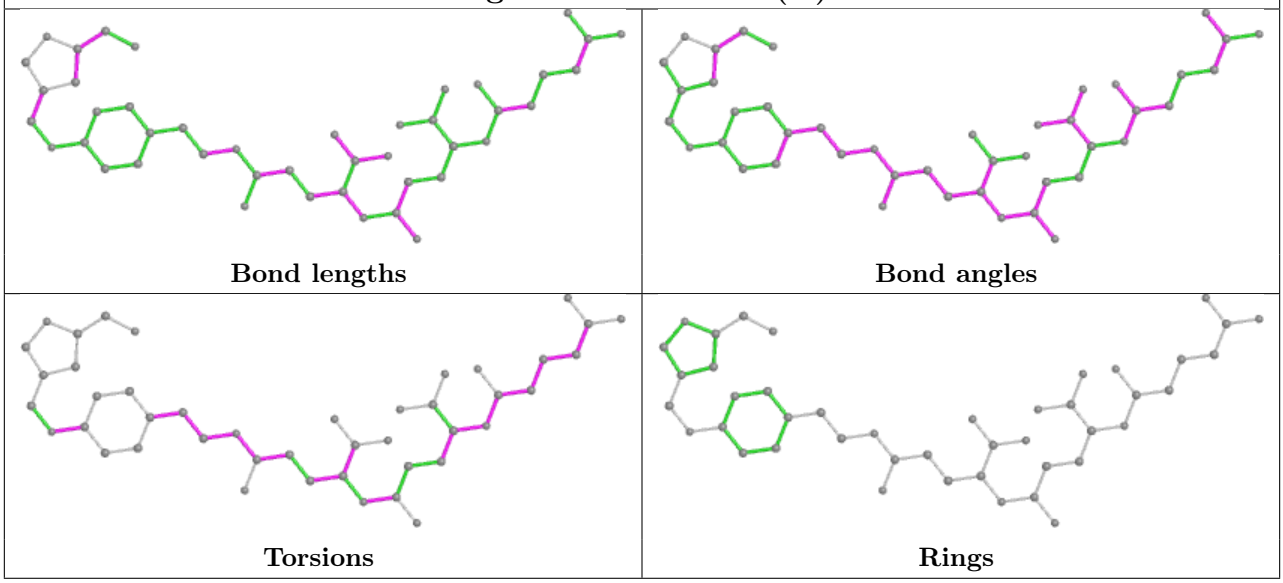
Torsions

Rings

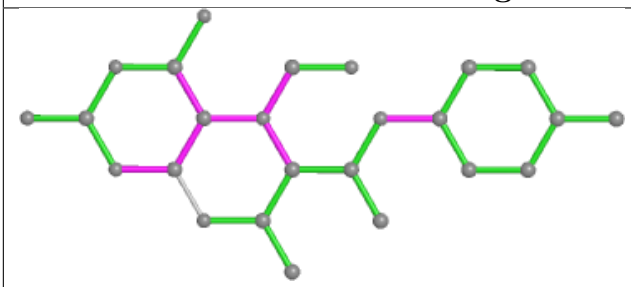
Ligand H4Z C 904



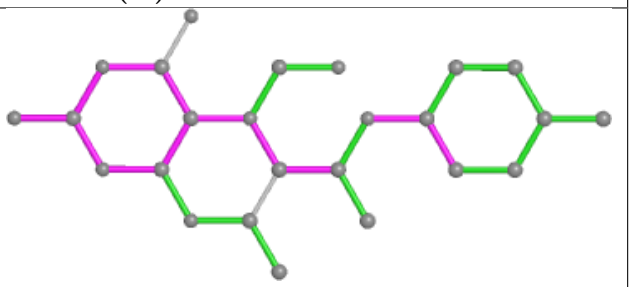
Ligand MFN A 902 (A)



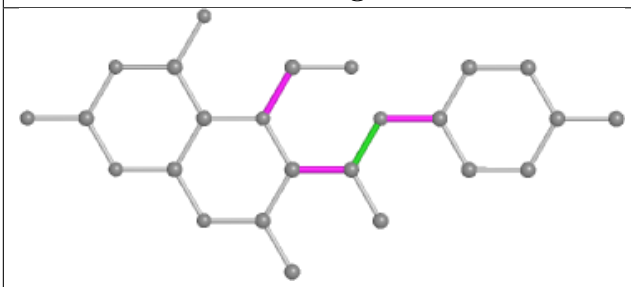
Ligand H4Z A 905 (B)



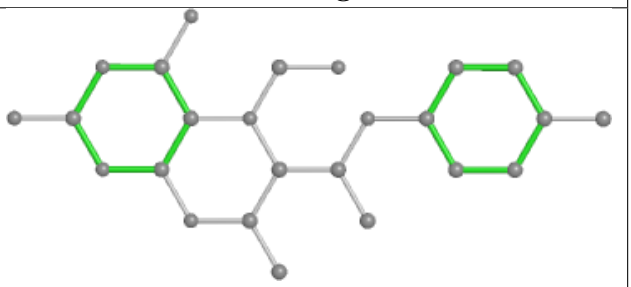
Bond lengths



Bond angles



Torsions



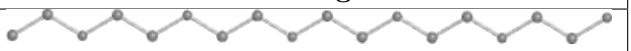
Rings

Ligand PE4 D 921

Bond lengths

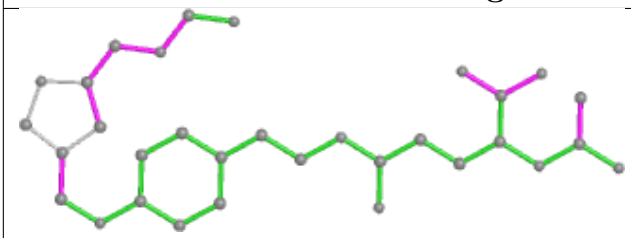
Bond angles

Torsions

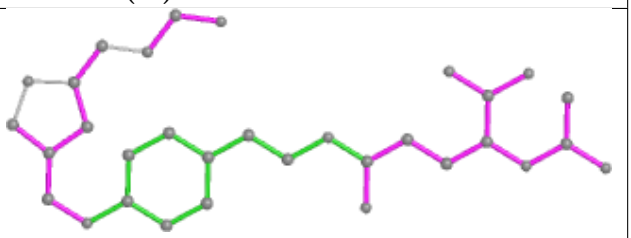


Rings

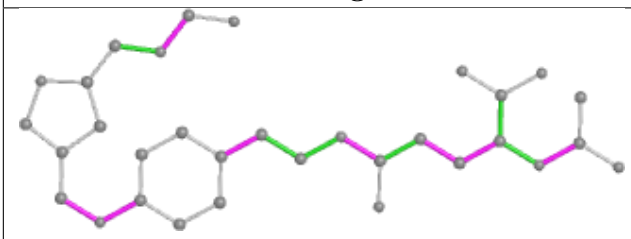
Ligand MFN C 901 (B)



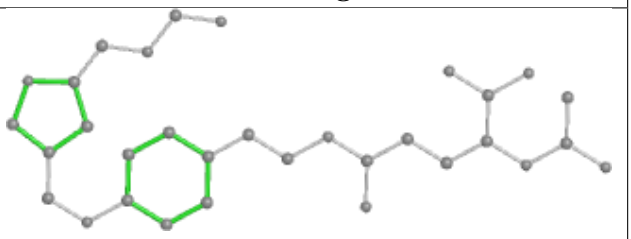
Bond lengths



Bond angles

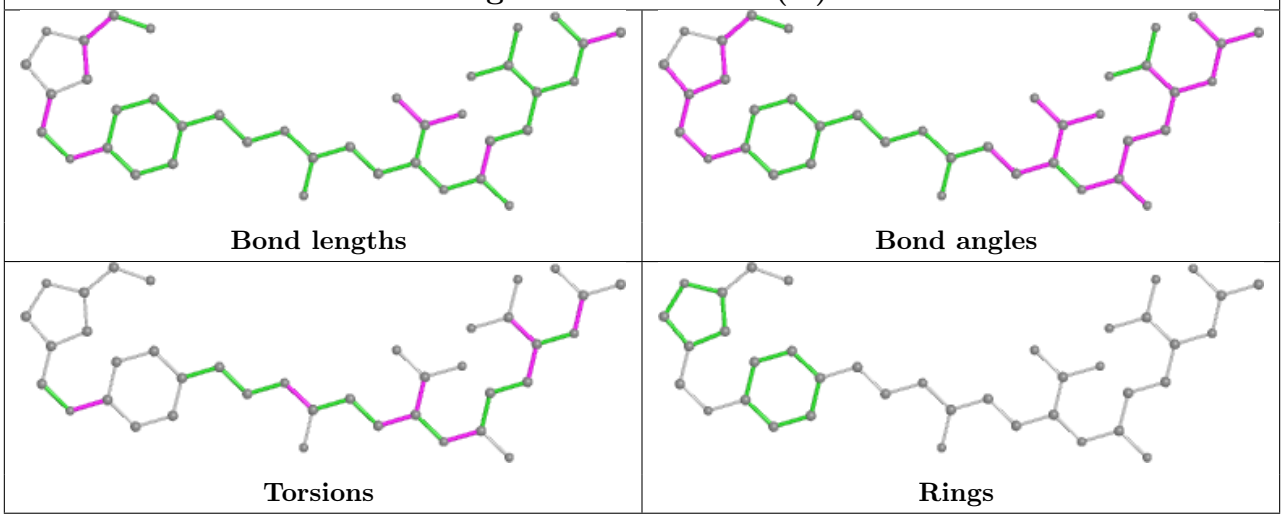


Torsions

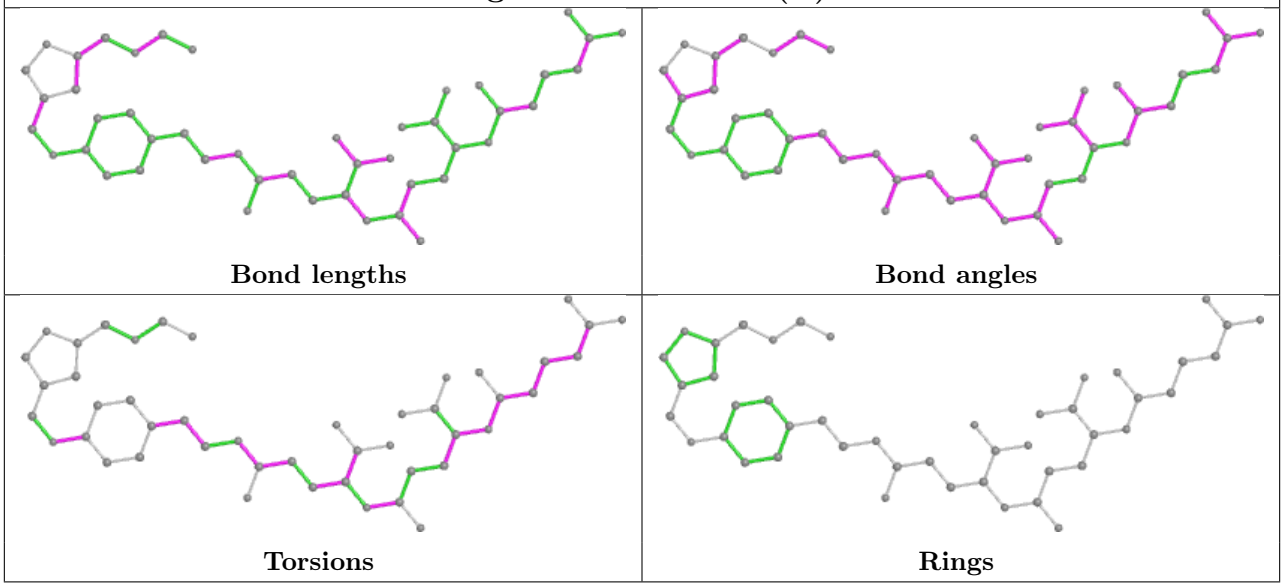


Rings

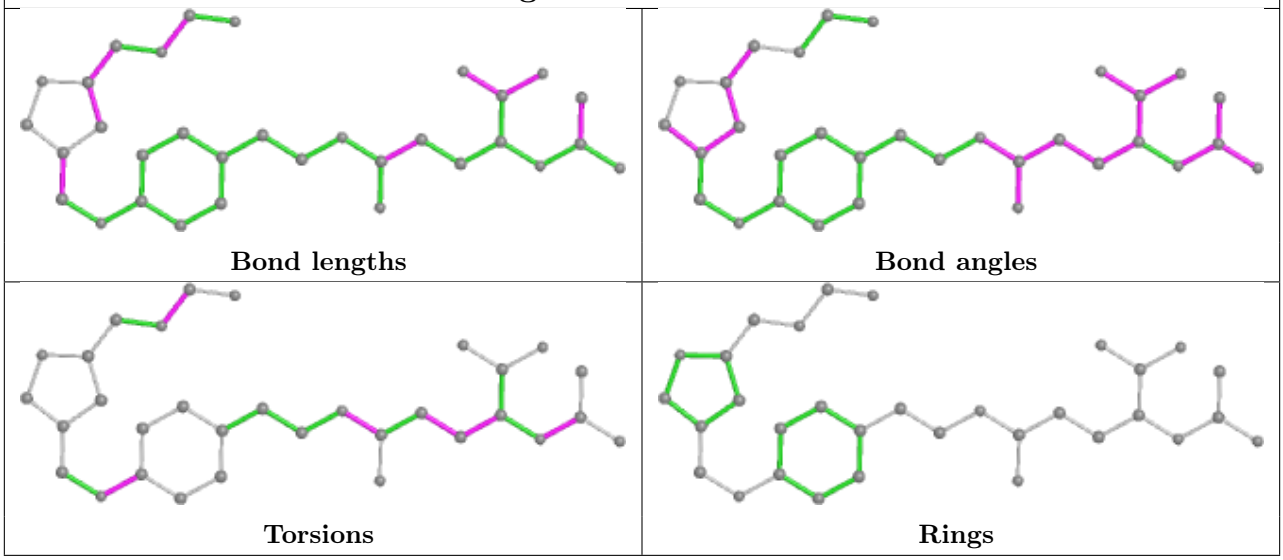
Ligand MFN A 900 (A)

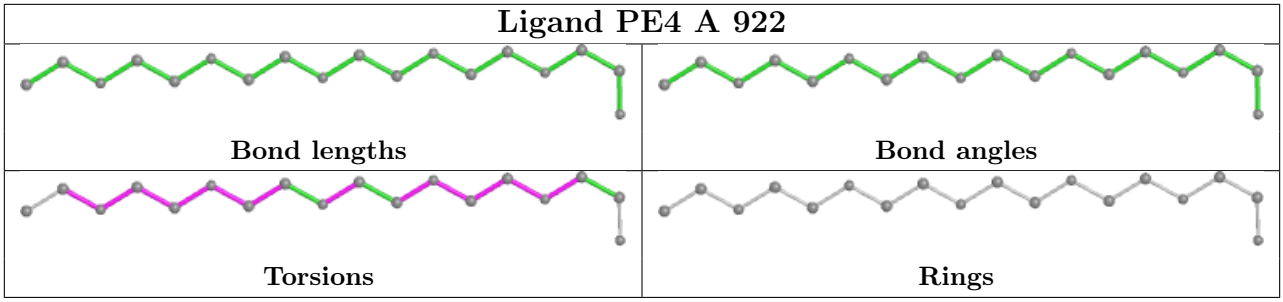


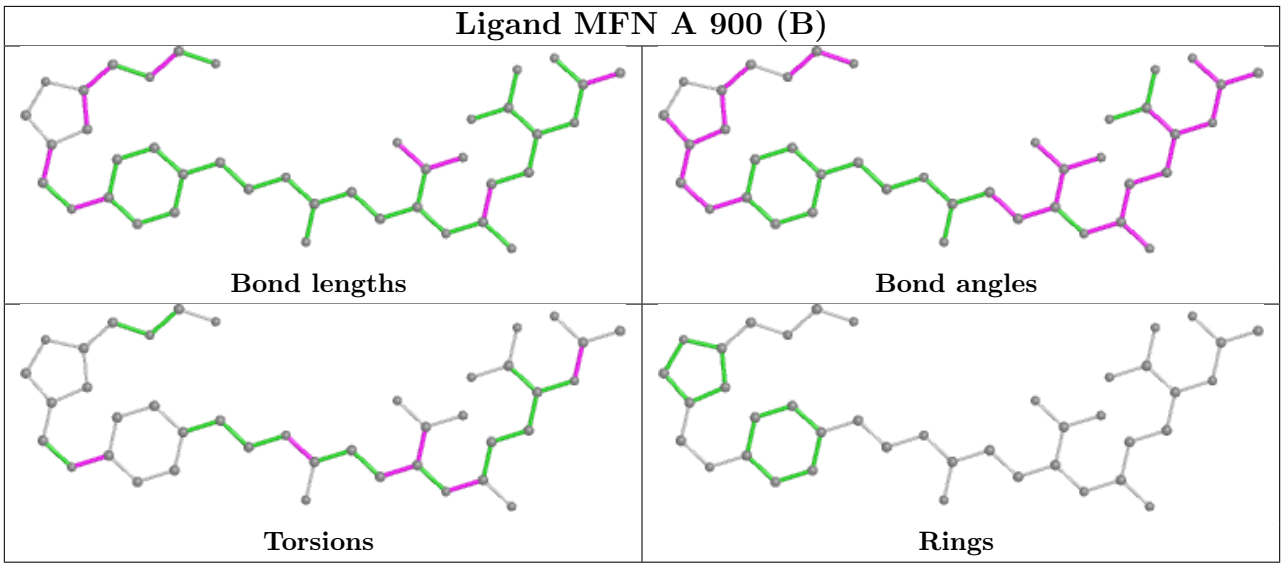
Ligand MFN A 902 (B)



Ligand MFN D 903







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, 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	296/296 (100%)	0.06	7 (2%)	59	57	19, 34, 48, 59	0
1	B	296/296 (100%)	0.16	10 (3%)	45	44	19, 34, 47, 58	0
1	C	296/296 (100%)	-0.21	2 (0%)	87	87	11, 27, 41, 49	0
2	D	295/296 (99%)	-0.14	2 (0%)	87	87	10, 27, 41, 49	0
All	All	1183/1184 (99%)	-0.03	21 (1%)	68	66	10, 30, 45, 59	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	LEU	6.1
1	B	232[A]	GLU	4.3
1	A	217[A]	ASP	3.8
1	A	238[A]	GLU	3.0
1	A	233	ASP	2.8

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	CSO	D	58	7/8	0.90	0.10	19,28,29,39	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

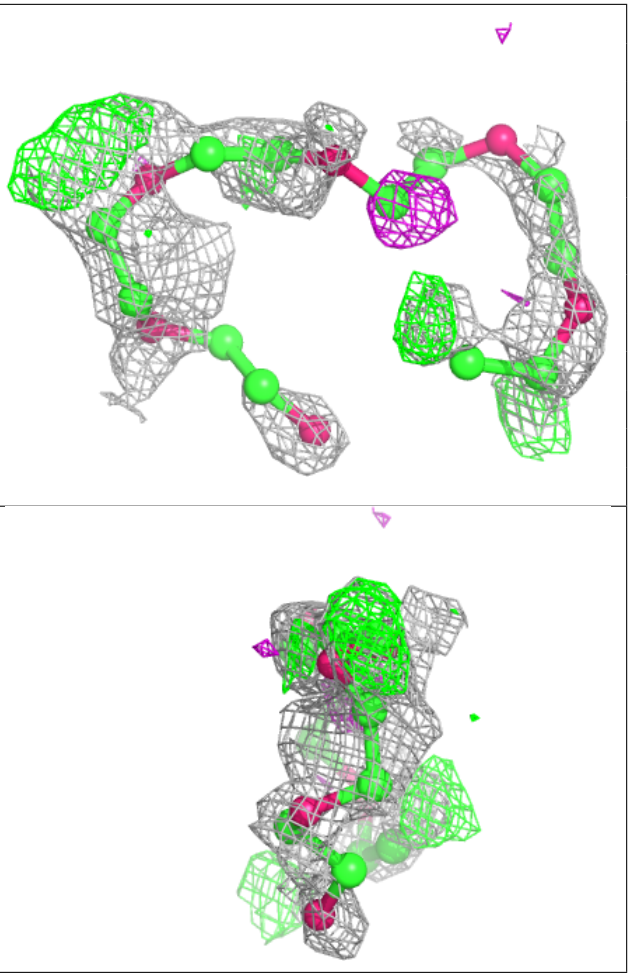
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

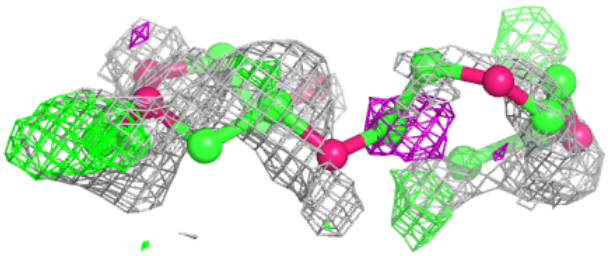
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PE4	D	921	18/24	0.42	0.45	85,95,102,102	0
5	H4Z	A	905[B]	25/55	0.60	0.42	46,52,64,65	25
5	H4Z	A	905[A]	22/55	0.60	0.42	23,43,57,59	22
6	PE4	D	920	24/24	0.69	0.25	36,78,88,90	0
5	H4Z	C	904	18/55	0.71	0.23	24,53,62,63	0
4	MFN	A	902[B]	46/55	0.72	0.33	51,77,102,104	46
4	MFN	A	902[A]	44/55	0.72	0.33	35,88,112,115	44
4	MFN	A	900[B]	41/55	0.76	0.22	25,53,81,82	41
4	MFN	A	900[A]	39/55	0.76	0.22	38,53,90,91	39
4	MFN	C	901[B]	32/55	0.79	0.26	65,83,87,88	32
4	MFN	C	901[A]	32/55	0.79	0.26	25,55,61,62	32
7	PE3	C	3792	9/43	0.79	0.35	57,63,71,77	0
6	PE4	A	922	18/24	0.85	0.27	13,51,62,64	0
4	MFN	D	903	32/55	0.87	0.13	29,38,59,63	0
3	K	B	504	1/1	0.88	0.09	58,58,58,58	0
3	K	B	319	1/1	0.97	0.04	38,38,38,38	0
3	K	B	505	1/1	0.97	0.14	38,38,38,38	0
3	K	C	506	1/1	0.98	0.08	24,24,24,24	0
3	K	B	322	1/1	0.98	0.04	27,27,27,27	0
3	K	C	306	1/1	0.98	0.05	28,28,28,28	0
3	K	C	309	1/1	0.99	0.03	24,24,24,24	0
3	K	A	312	1/1	0.99	0.03	29,29,29,29	0
3	K	D	500	1/1	0.99	0.02	18,18,18,18	0
3	K	D	501	1/1	0.99	0.03	18,18,18,18	0
3	K	D	502	1/1	0.99	0.03	28,28,28,28	0
3	K	D	503	1/1	0.99	0.04	29,29,29,29	0
3	K	A	313	1/1	0.99	0.04	27,27,27,27	0
3	K	A	315	1/1	0.99	0.04	25,25,25,25	0
3	K	A	316	1/1	0.99	0.06	27,27,27,27	0
3	K	B	317	1/1	0.99	0.03	30,30,30,30	0
3	K	C	303	1/1	1.00	0.02	24,24,24,24	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 PE4 D 921:

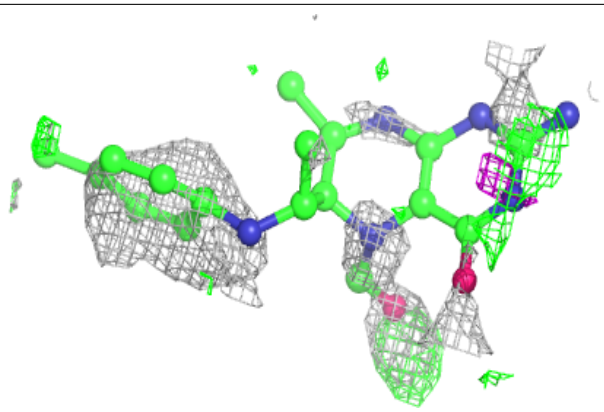
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

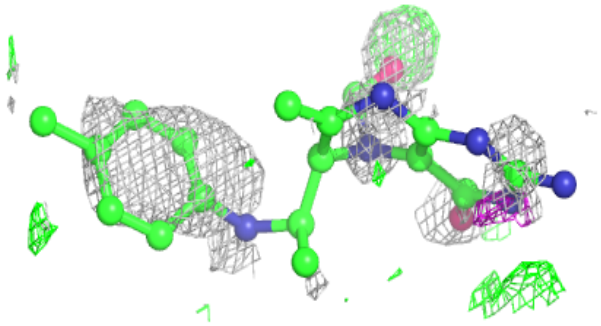


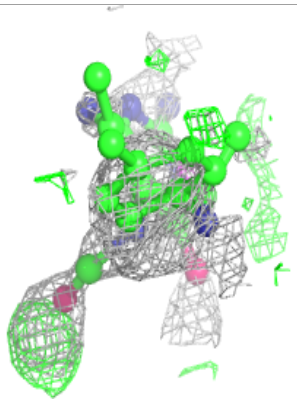


Electron density around H4Z A 905 (B):

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

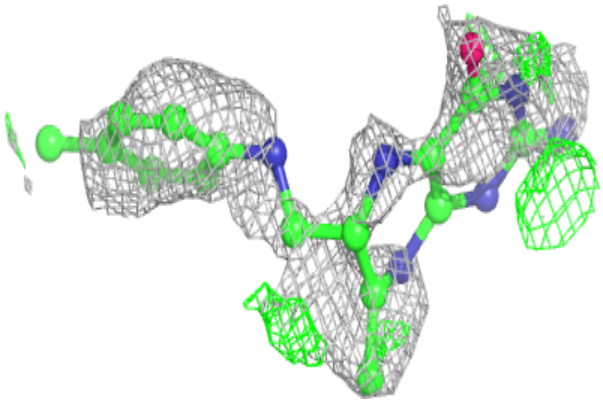


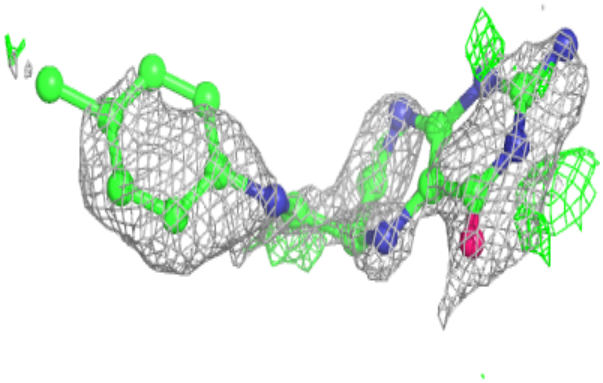


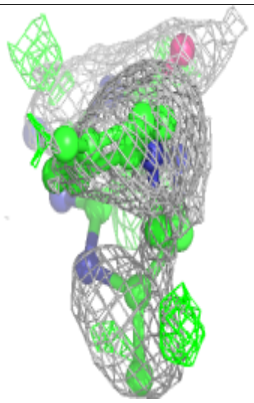


Electron density around H4Z A 905 (A):

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

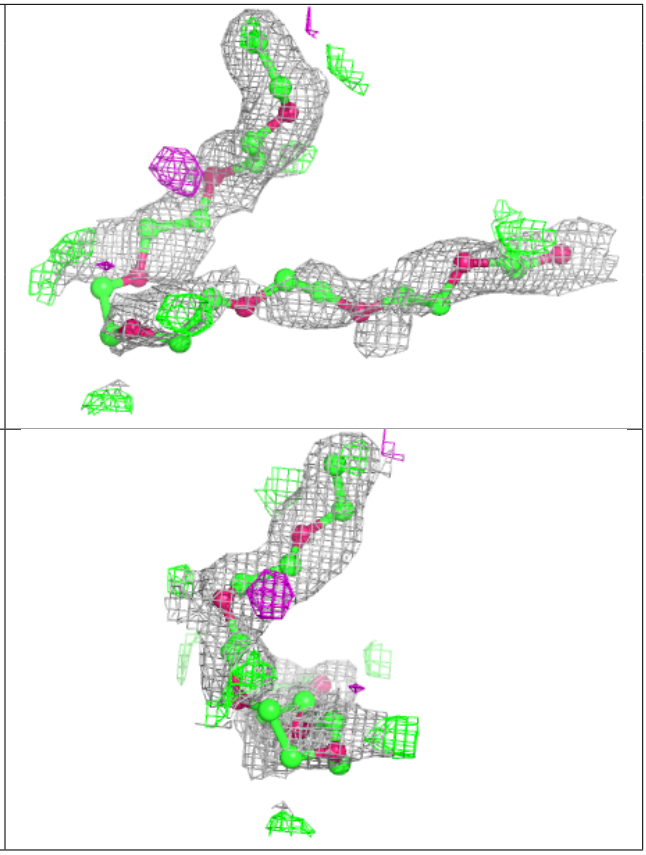






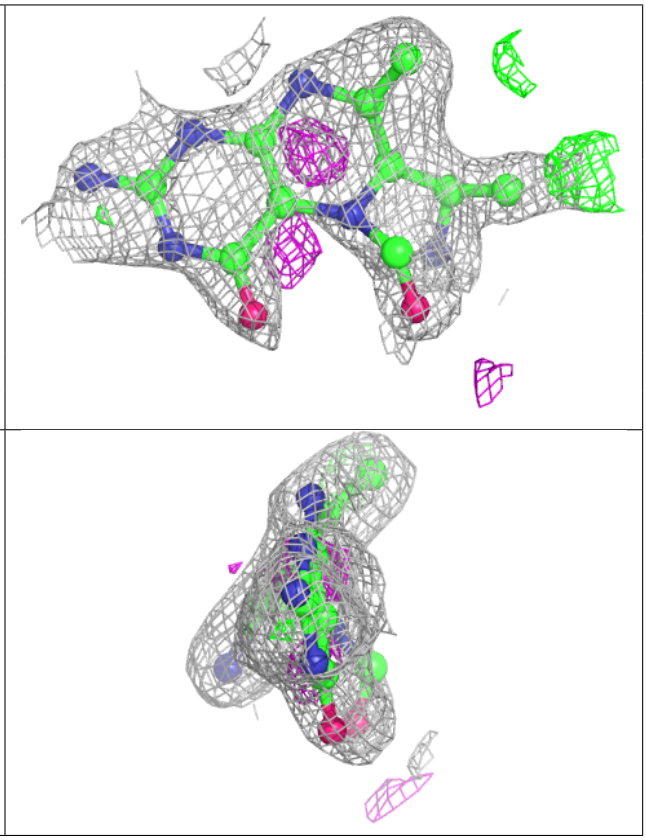
Electron density around PE4 D 920:

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



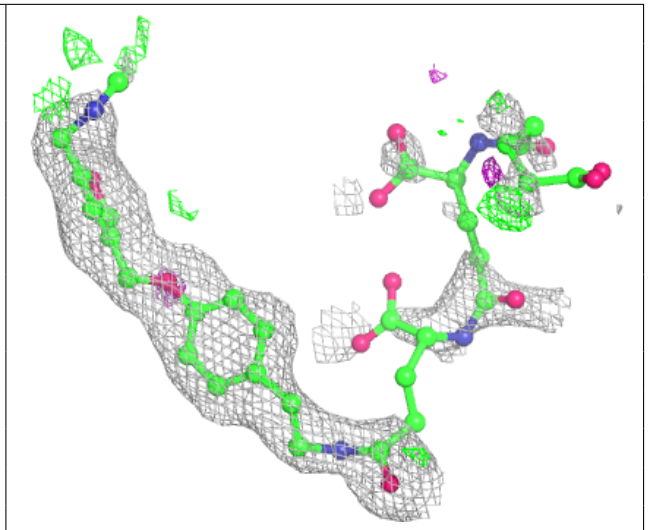
Electron density around H4Z C 904:

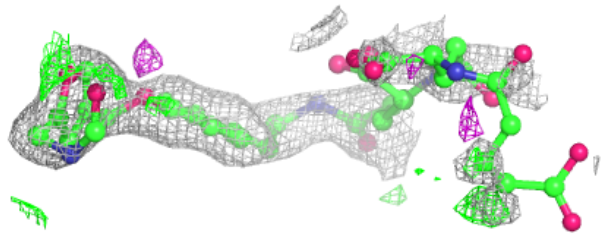
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

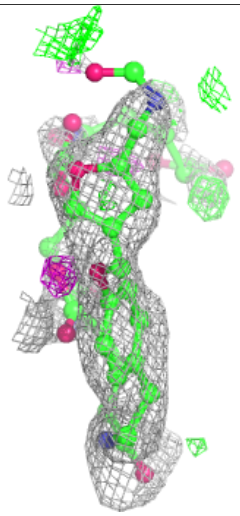


Electron density around MFN A 902 (B):

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

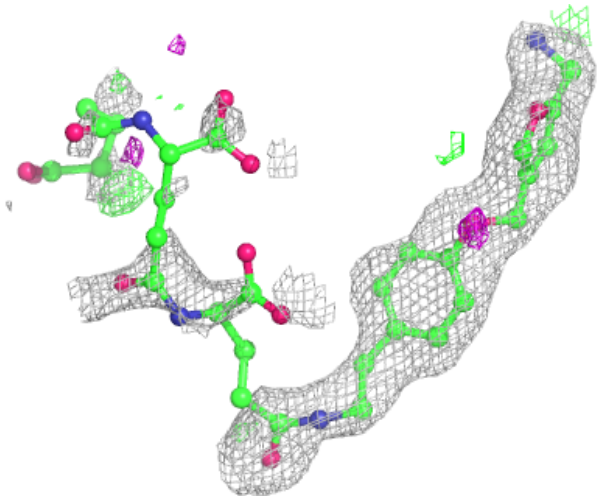


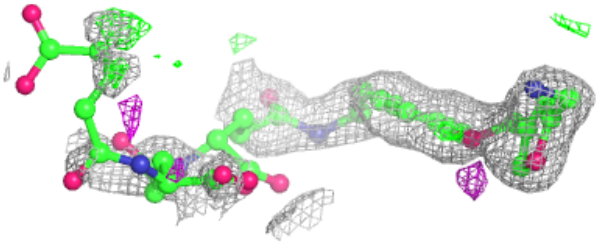


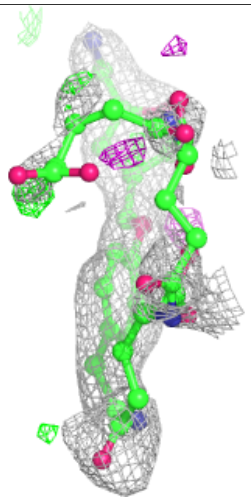


Electron density around MFN A 902 (A):

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

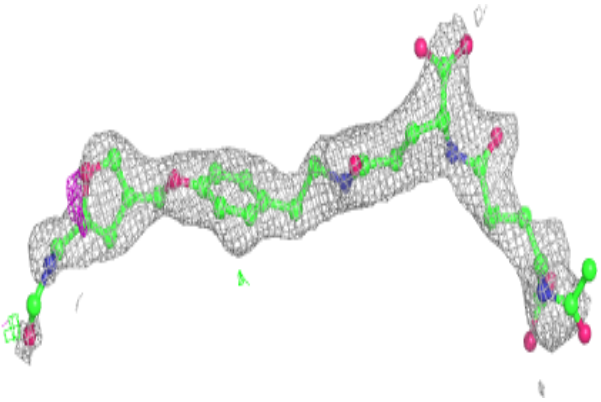


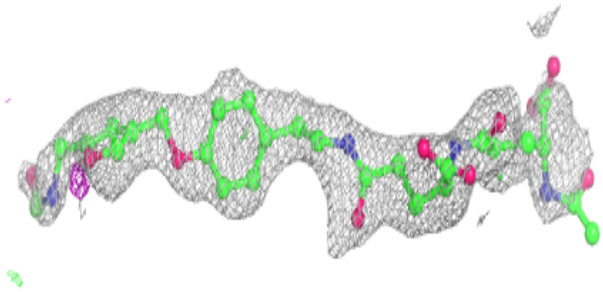


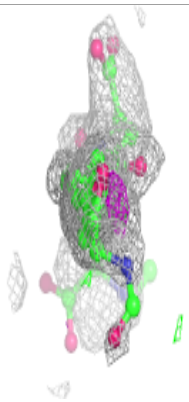


Electron density around MFN A 900 (B):

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

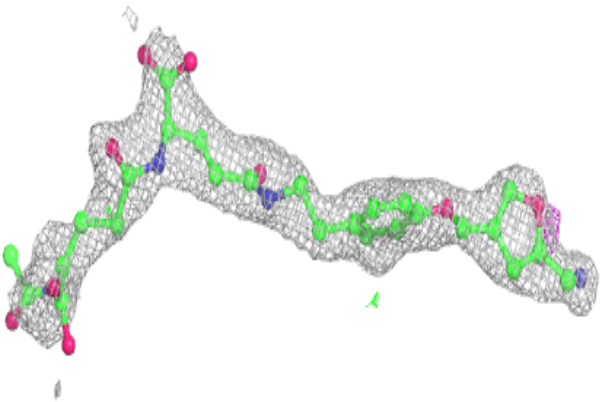


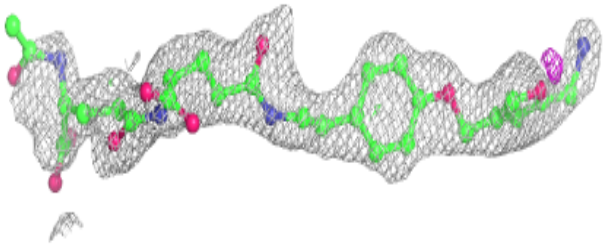


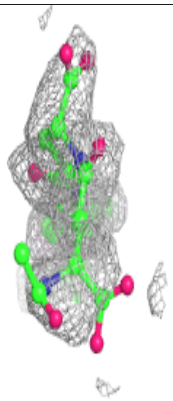


Electron density around MFN A 900 (A):

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

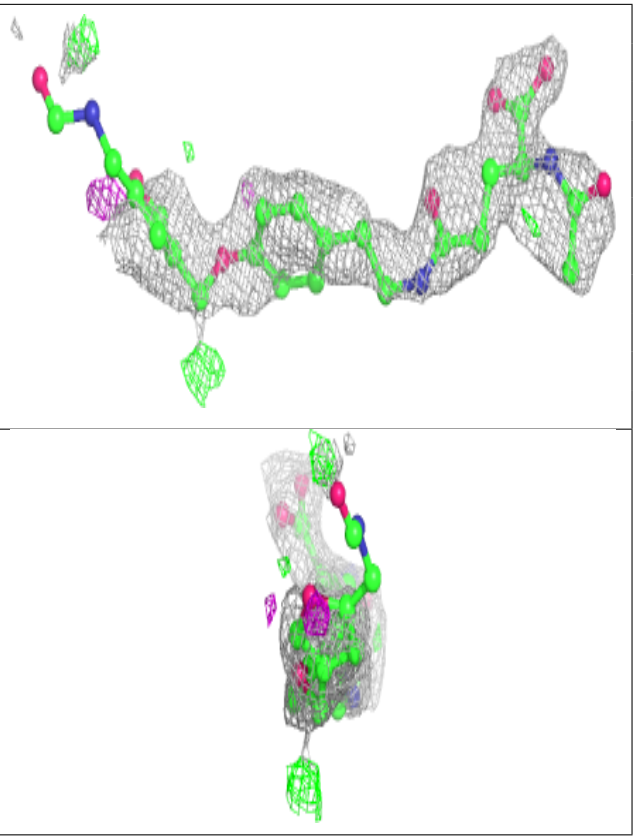






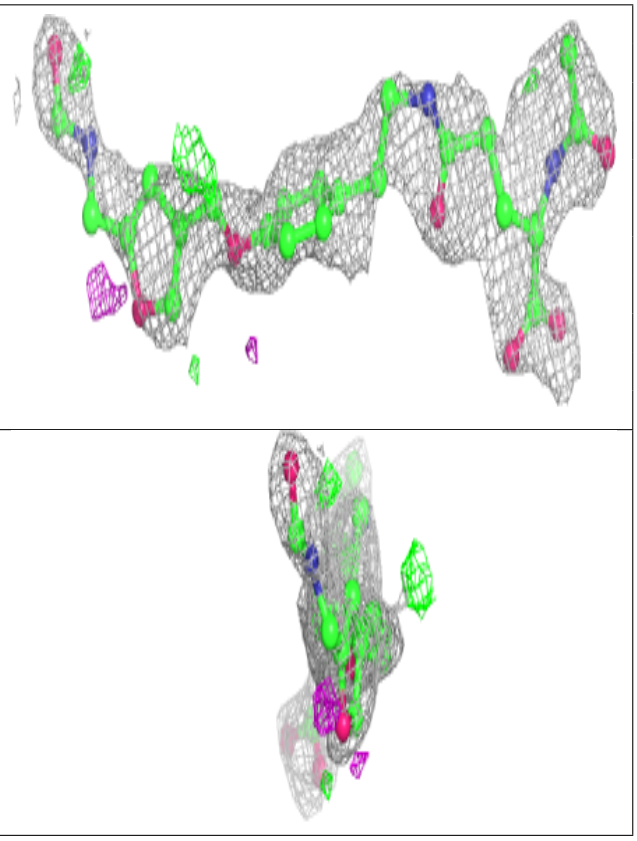
Electron density around MFN C 901 (B):

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



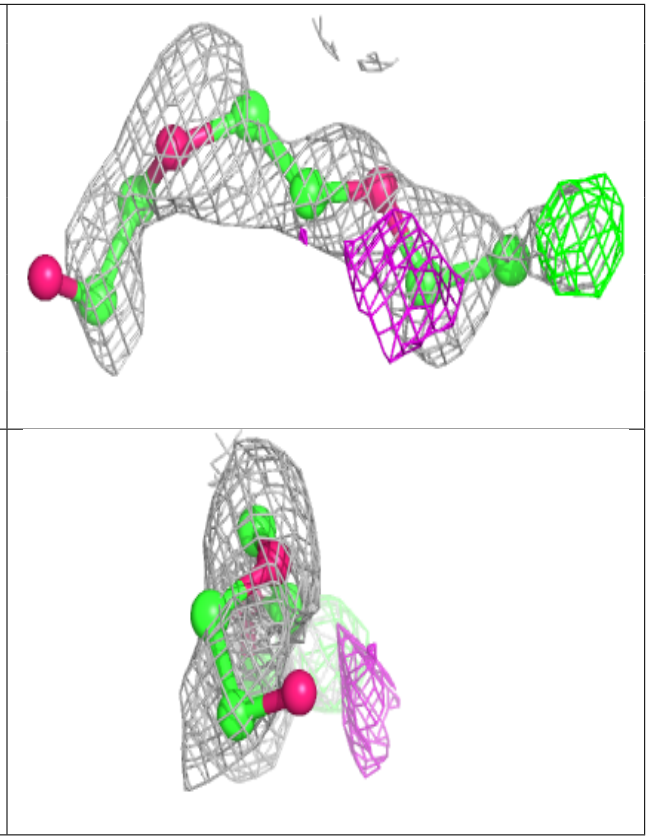
Electron density around MFN C 901 (A):

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



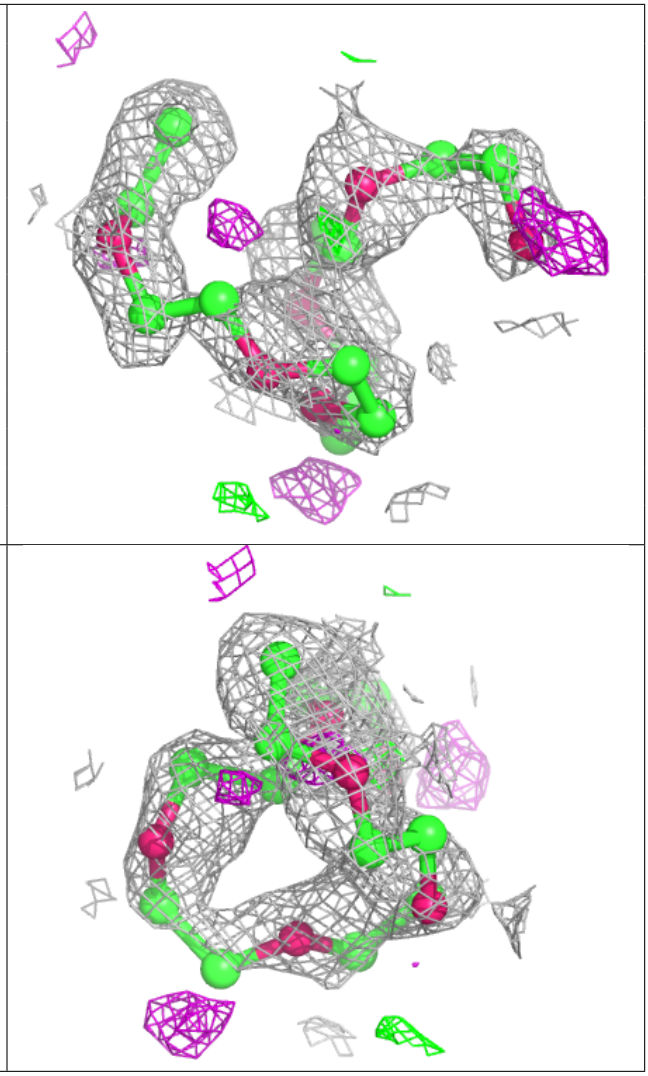
Electron density around PE3 C 3792:

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



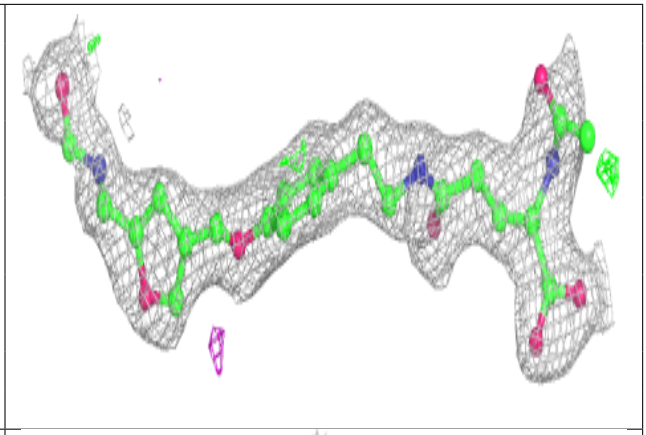
Electron density around PE4 A 922:

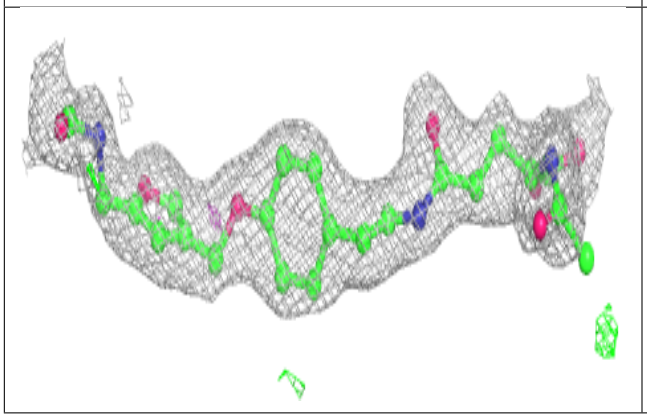
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

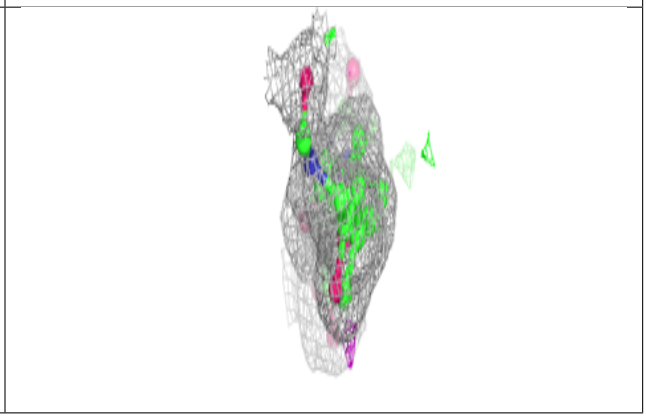


Electron density around MFN D 903:

$2mF_o$-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.