



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:41 am BST

PDB ID : 4BO0
Title : Crystal structure of 3-oxoacyl-(acyl-carrier-protein) reductase (FabG) from *Pseudomonas aeruginosa* in complex with 1-(4-methoxy-1-methylindazol-3-yl)-3-(2-methoxyphenyl)urea at 2.4Å resolution
Authors : Cukier, C.D.; Schnell, R.; Lindqvist, Y.; Schneider, G.
Deposited on : 2013-05-17
Resolution : 2.40 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

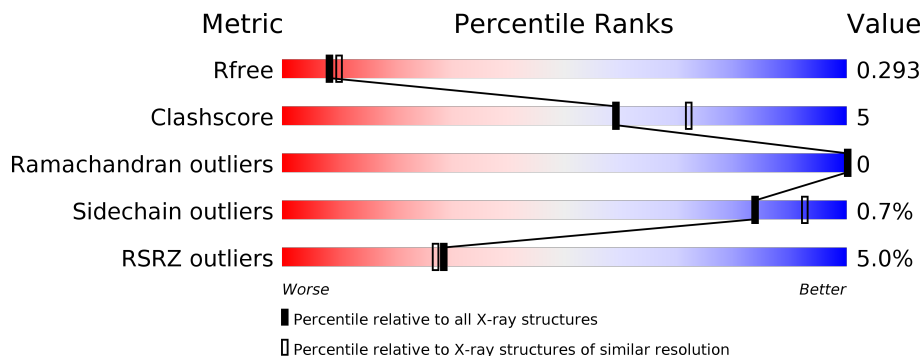
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 ≥ 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	269	 6% 81% 6% 13%
1	B	269	 4% 82% 6% 12%
1	C	269	 5% 81% 10% 9%
1	D	269	 3% 79% 11% 10%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7081 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 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	235	Total 1703	C 1061	N 306	O 330	S 6	0	2	0
1	B	237	Total 1718	C 1072	N 306	O 334	S 6	0	2	0
1	C	244	Total 1799	C 1125	N 326	O 343	S 5	0	1	0
1	D	241	Total 1763	C 1097	N 318	O 341	S 7	0	3	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP O54438
A	-20	HIS	-	expression tag	UNP O54438
A	-19	HIS	-	expression tag	UNP O54438
A	-18	HIS	-	expression tag	UNP O54438
A	-17	HIS	-	expression tag	UNP O54438
A	-16	HIS	-	expression tag	UNP O54438
A	-15	HIS	-	expression tag	UNP O54438
A	-14	SER	-	expression tag	UNP O54438
A	-13	SER	-	expression tag	UNP O54438
A	-12	GLY	-	expression tag	UNP O54438
A	-11	VAL	-	expression tag	UNP O54438
A	-10	ASP	-	expression tag	UNP O54438
A	-9	LEU	-	expression tag	UNP O54438
A	-8	GLY	-	expression tag	UNP O54438
A	-7	THR	-	expression tag	UNP O54438
A	-6	GLU	-	expression tag	UNP O54438
A	-5	ASN	-	expression tag	UNP O54438
A	-4	LEU	-	expression tag	UNP O54438
A	-3	TYR	-	expression tag	UNP O54438
A	-2	PHE	-	expression tag	UNP O54438

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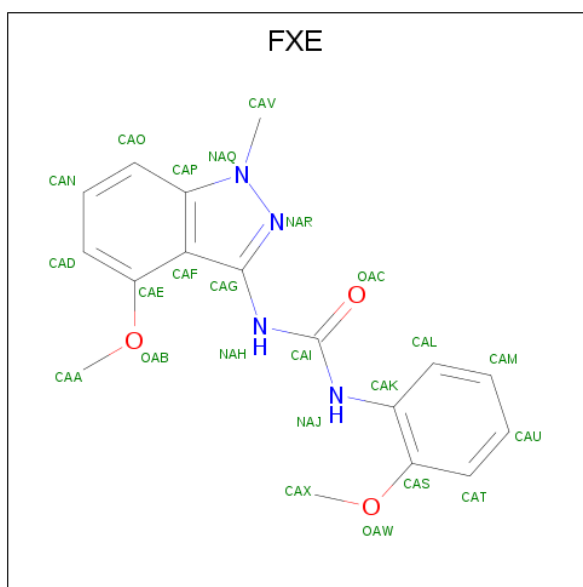
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP O54438
A	0	SER	-	expression tag	UNP O54438
B	-21	MET	-	expression tag	UNP O54438
B	-20	HIS	-	expression tag	UNP O54438
B	-19	HIS	-	expression tag	UNP O54438
B	-18	HIS	-	expression tag	UNP O54438
B	-17	HIS	-	expression tag	UNP O54438
B	-16	HIS	-	expression tag	UNP O54438
B	-15	HIS	-	expression tag	UNP O54438
B	-14	SER	-	expression tag	UNP O54438
B	-13	SER	-	expression tag	UNP O54438
B	-12	GLY	-	expression tag	UNP O54438
B	-11	VAL	-	expression tag	UNP O54438
B	-10	ASP	-	expression tag	UNP O54438
B	-9	LEU	-	expression tag	UNP O54438
B	-8	GLY	-	expression tag	UNP O54438
B	-7	THR	-	expression tag	UNP O54438
B	-6	GLU	-	expression tag	UNP O54438
B	-5	ASN	-	expression tag	UNP O54438
B	-4	LEU	-	expression tag	UNP O54438
B	-3	TYR	-	expression tag	UNP O54438
B	-2	PHE	-	expression tag	UNP O54438
B	-1	GLN	-	expression tag	UNP O54438
B	0	SER	-	expression tag	UNP O54438
C	-21	MET	-	expression tag	UNP O54438
C	-20	HIS	-	expression tag	UNP O54438
C	-19	HIS	-	expression tag	UNP O54438
C	-18	HIS	-	expression tag	UNP O54438
C	-17	HIS	-	expression tag	UNP O54438
C	-16	HIS	-	expression tag	UNP O54438
C	-15	HIS	-	expression tag	UNP O54438
C	-14	SER	-	expression tag	UNP O54438
C	-13	SER	-	expression tag	UNP O54438
C	-12	GLY	-	expression tag	UNP O54438
C	-11	VAL	-	expression tag	UNP O54438
C	-10	ASP	-	expression tag	UNP O54438
C	-9	LEU	-	expression tag	UNP O54438
C	-8	GLY	-	expression tag	UNP O54438
C	-7	THR	-	expression tag	UNP O54438
C	-6	GLU	-	expression tag	UNP O54438
C	-5	ASN	-	expression tag	UNP O54438
C	-4	LEU	-	expression tag	UNP O54438

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	TYR	-	expression tag	UNP O54438
C	-2	PHE	-	expression tag	UNP O54438
C	-1	GLN	-	expression tag	UNP O54438
C	0	SER	-	expression tag	UNP O54438
D	-21	MET	-	expression tag	UNP O54438
D	-20	HIS	-	expression tag	UNP O54438
D	-19	HIS	-	expression tag	UNP O54438
D	-18	HIS	-	expression tag	UNP O54438
D	-17	HIS	-	expression tag	UNP O54438
D	-16	HIS	-	expression tag	UNP O54438
D	-15	HIS	-	expression tag	UNP O54438
D	-14	SER	-	expression tag	UNP O54438
D	-13	SER	-	expression tag	UNP O54438
D	-12	GLY	-	expression tag	UNP O54438
D	-11	VAL	-	expression tag	UNP O54438
D	-10	ASP	-	expression tag	UNP O54438
D	-9	LEU	-	expression tag	UNP O54438
D	-8	GLY	-	expression tag	UNP O54438
D	-7	THR	-	expression tag	UNP O54438
D	-6	GLU	-	expression tag	UNP O54438
D	-5	ASN	-	expression tag	UNP O54438
D	-4	LEU	-	expression tag	UNP O54438
D	-3	TYR	-	expression tag	UNP O54438
D	-2	PHE	-	expression tag	UNP O54438
D	-1	GLN	-	expression tag	UNP O54438
D	0	SER	-	expression tag	UNP O54438

- Molecule 2 is 1-(4-methoxy-1-methyl-indazol-3-yl)-3-(2-methoxyphenyl)urea (three-letter code: FXE) (formula: C₁₇H₁₈N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	17	4	3		
2	C	1	Total	C	N	O	0	0
			24	17	4	3		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ni	0	0
			1	1		

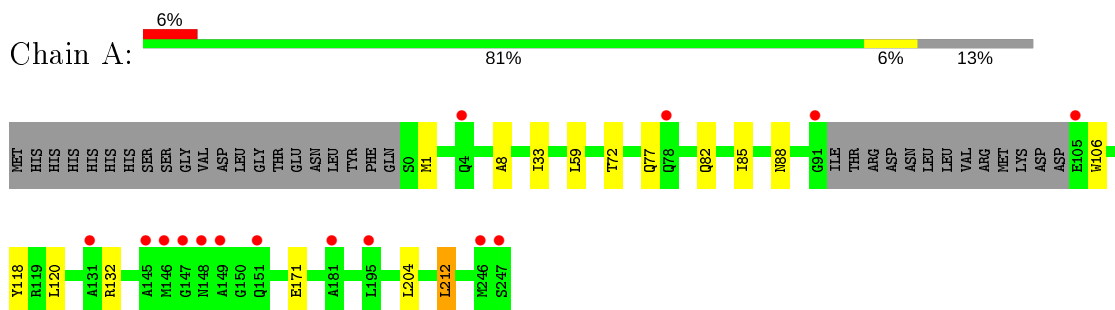
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	15	Total	O	0	0
			15	15		
4	C	5	Total	O	0	0
			5	5		
4	D	16	Total	O	0	0
			16	16		

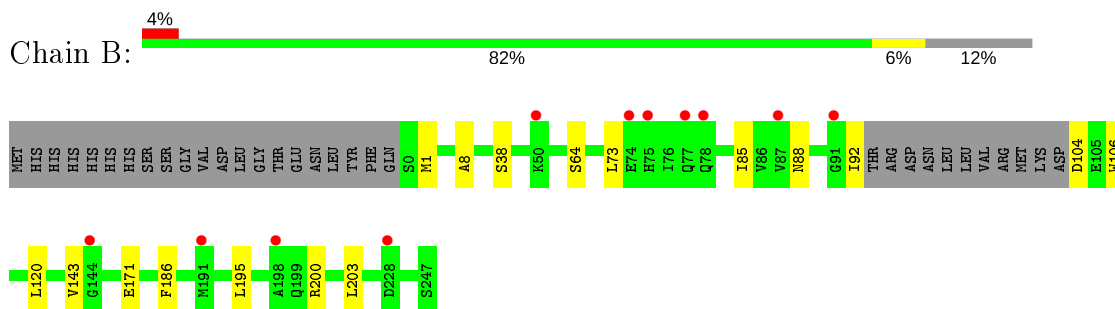
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

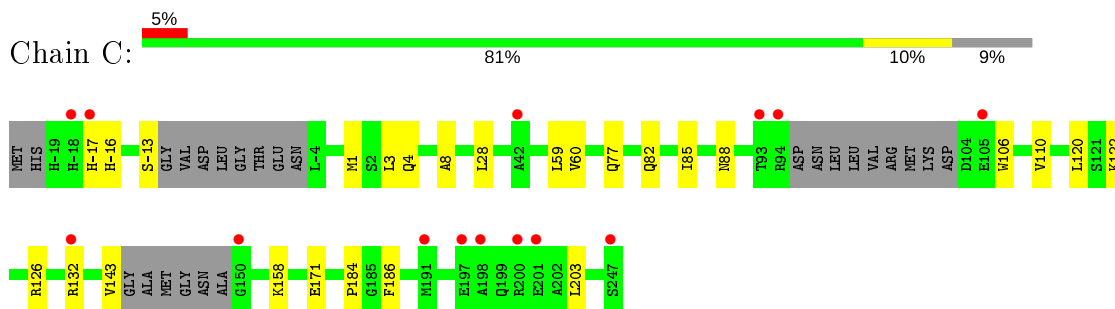
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG



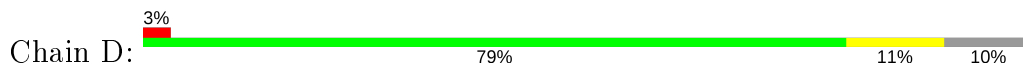
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG

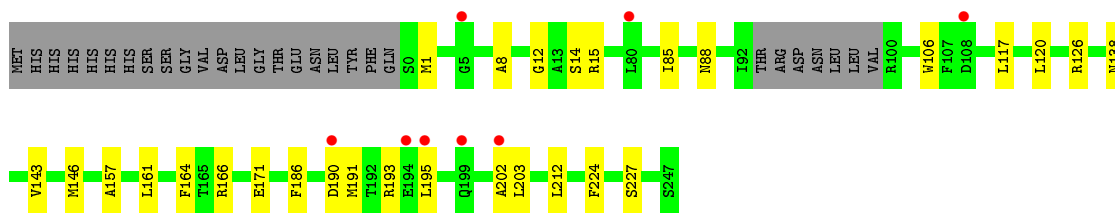


- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG



- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.32Å 108.73Å 148.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 2.40 29.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.72-2.40) 98.4 (29.71-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.255 , 0.297 0.253 , 0.293	Depositor DCC
R_{free} test set	1763 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtrriage
Anisotropy	0.447	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7081	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FXE, NI

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	0.53	0/1726	0.70	0/2335
1	B	0.53	0/1741	0.72	0/2356
1	C	0.54	0/1824	0.74	3/2466 (0.1%)
1	D	0.52	0/1789	0.67	0/2417
All	All	0.53	0/7080	0.71	3/9574 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	LEU	CB-CA-C	5.31	120.29	110.20
1	C	126	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	C	158	LYS	CD-CE-NZ	5.06	123.34	111.70

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	1703	0	1742	12	0
1	B	1718	0	1758	12	0
1	C	1799	0	1826	18	0
1	D	1763	0	1807	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	24	0	18	5	0
2	C	24	0	18	4	0
3	B	1	0	0	0	0
4	A	13	0	0	0	0
4	B	15	0	0	1	0
4	C	5	0	0	0	0
4	D	16	0	0	4	0
All	All	7081	0	7169	66	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 5.

All (66) 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)
2:A:1248:FXE:HAX1	2:A:1248:FXE:HAV1	1.48	0.95
2:C:1248:FXE:HAL	2:C:1248:FXE:OAC	1.80	0.80
2:A:1248:FXE:NAR	2:A:1248:FXE:NAJ	2.24	0.75
1:B:64:SER:HB3	1:B:92:ILE:HG21	1.70	0.72
1:A:118:TYR:OH	1:B:104:ASP:HB2	1.90	0.71
2:A:1248:FXE:CAX	2:A:1248:FXE:HAV1	2.23	0.67
1:C:106:TRP:NE1	1:D:171:GLU:HG3	2.09	0.67
1:A:204:LEU:HD21	1:A:212:LEU:CD1	2.27	0.65
1:C:16:HIS:ND1	1:C:59:LEU:HD21	2.13	0.64
1:D:117:LEU:HD23	1:D:164:PHE:CD2	2.38	0.59
1:C:110:VAL:HB	2:C:1248:FXE:HAX3	1.84	0.59
1:D:126:ARG:NH1	4:D:2009:HOH:O	2.36	0.58
1:D:191:MET:HE2	1:D:195:LEU:HD21	1.85	0.58
1:A:59:LEU:HD13	1:A:72:THR:HG23	1.87	0.56
1:B:64:SER:HB3	1:B:92:ILE:CG2	2.34	0.56
1:C:186:PHE:CE1	1:C:203:LEU:HD11	2.41	0.56
1:D:202:ALA:HB3	4:D:2014:HOH:O	2.05	0.56
1:D:117:LEU:HD23	1:D:164:PHE:CE2	2.40	0.56
2:C:1248:FXE:NAR	2:C:1248:FXE:NAJ	2.51	0.54
1:C:132:ARG:O	1:C:132:ARG:HG3	2.11	0.51
1:D:157:ALA:HB3	4:D:2012:HOH:O	2.10	0.51
1:D:1:MET:HE1	1:D:224:PHE:HD1	1.75	0.50
1:D:146:MET:SD	1:D:203:LEU:HD13	2.52	0.49
1:B:186:PHE:CZ	1:B:203:LEU:HD11	2.47	0.49
1:D:143:VAL:HG11	1:D:186:PHE:CZ	2.48	0.49
1:D:186:PHE:CZ	1:D:203:LEU:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-17:HIS:CD2	1:C:60:VAL:HG21	2.48	0.48
1:A:77:GLN:HG2	1:A:82:GLN:HG2	1.96	0.47
1:D:88:ASN:OD1	1:D:120:LEU:HD23	2.15	0.47
1:B:143:VAL:HG11	1:B:186:PHE:CZ	2.51	0.46
2:A:1248:FXE:HAL	2:A:1248:FXE:OAC	2.16	0.46
1:A:204:LEU:HD21	1:A:212:LEU:HD12	1.97	0.46
1:A:33:ILE:HG21	1:A:59:LEU:HD21	1.97	0.46
1:B:88:ASN:OD1	1:B:120:LEU:HD23	2.16	0.46
1:C:106:TRP:CD1	1:D:171:GLU:HG3	2.51	0.46
1:C:1:MET:HB2	1:C:28:LEU:O	2.16	0.45
1:A:88:ASN:OD1	1:A:120:LEU:HD23	2.16	0.45
1:C:171:GLU:OE1	1:D:106:TRP:NE1	2.48	0.45
1:A:106:TRP:NE1	1:B:171:GLU:HG3	2.32	0.45
1:C:122:LYS:NZ	1:C:171:GLU:OE2	2.50	0.44
1:C:143:VAL:HG11	1:C:186:PHE:CZ	2.52	0.44
1:C:88:ASN:OD1	1:C:120:LEU:HD23	2.16	0.44
1:D:146:MET:HG2	1:D:191:MET:HE1	2.00	0.44
1:D:138:ASN:HB3	1:D:161:LEU:HD11	2.00	0.43
1:A:8:ALA:HA	1:A:85:ILE:O	2.20	0.42
1:B:8:ALA:HA	1:B:85:ILE:O	2.19	0.42
1:D:8:ALA:HA	1:D:85:ILE:O	2.19	0.42
1:A:132:ARG:O	1:A:132:ARG:HD3	2.19	0.42
1:C:4:GLN:O	1:C:4:GLN:CG	2.68	0.42
1:A:1:MET:O	1:A:1:MET:HG3	2.20	0.42
1:D:14:SER:C	1:D:15:ARG:HG3	2.40	0.42
1:A:171:GLU:OE1	1:B:106:TRP:NE1	2.30	0.42
1:C:8:ALA:HA	1:C:85:ILE:O	2.20	0.41
1:B:195:LEU:HD12	1:B:200:ARG:HG3	2.02	0.41
1:B:1:MET:HA	4:B:2001:HOH:O	2.19	0.41
1:C:110:VAL:HG12	2:C:1248:FXE:HAX2	2.01	0.41
2:A:1248:FXE:CAL	2:A:1248:FXE:OAC	2.68	0.41
1:C:4:GLN:O	1:C:4:GLN:HG2	2.21	0.41
1:D:190:ASP:OD1	1:D:193:ARG:NH1	2.54	0.41
1:D:1:MET:HG3	1:D:227:SER:CB	2.51	0.41
1:B:73[B]:LEU:HD12	1:B:73[B]:LEU:HA	1.91	0.41
1:C:-16:HIS:ND1	1:C:59:LEU:CD2	2.83	0.41
1:C:77:GLN:NE2	1:C:82:GLN:OE1	2.49	0.40
1:D:12:GLY:HA2	4:D:2003:HOH:O	2.22	0.40
1:D:186:PHE:CE1	1:D:203:LEU:HD11	2.56	0.40
1:D:186:PHE:HB3	1:D:212:LEU:HD23	2.02	0.40

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	233/269 (87%)	231 (99%)	2 (1%)	0	100	100
1	B	235/269 (87%)	231 (98%)	4 (2%)	0	100	100
1	C	237/269 (88%)	230 (97%)	7 (3%)	0	100	100
1	D	240/269 (89%)	238 (99%)	2 (1%)	0	100	100
All	All	945/1076 (88%)	930 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/201 (85%)	170 (99%)	1 (1%)	86	94
1	B	173/201 (86%)	172 (99%)	1 (1%)	86	94
1	C	183/201 (91%)	181 (99%)	2 (1%)	73	87
1	D	178/201 (89%)	177 (99%)	1 (1%)	86	94
All	All	705/804 (88%)	700 (99%)	5 (1%)	84	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	LEU
1	B	38	SER

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Mol	Chain	Res	Type
1	C	-13	SER
1	C	184	PRO
1	D	166	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	77	GLN
1	C	82	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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	FXE	C	1248	-	23,26,26	2.44	5 (21%)	27,36,36	1.64	7 (25%)
2	FXE	A	1248	-	23,26,26	2.67	6 (26%)	27,36,36	1.87	10 (37%)

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	FXE	C	1248	-	-	2/10/12/12	0/3/3/3
2	FXE	A	1248	-	-	2/10/12/12	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1248	FXE	CAF-CAP	-7.76	1.33	1.42
2	C	1248	FXE	CAF-CAP	-7.43	1.33	1.42
2	A	1248	FXE	CAE-CAF	-5.86	1.30	1.42
2	A	1248	FXE	CAK-NAJ	-5.60	1.31	1.41
2	C	1248	FXE	CAK-NAJ	-4.40	1.33	1.41
2	C	1248	FXE	CAG-CAF	-4.03	1.32	1.45
2	C	1248	FXE	CAE-CAF	-3.92	1.34	1.42
2	A	1248	FXE	CAG-CAF	-3.79	1.32	1.45
2	C	1248	FXE	CAO-CAP	-3.44	1.34	1.41
2	A	1248	FXE	CAO-CAP	-3.42	1.34	1.41
2	A	1248	FXE	CAK-CAS	-2.03	1.36	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1248	FXE	CAS-CAK-NAJ	-4.20	109.14	116.66
2	C	1248	FXE	NAJ-CAI-NAH	4.09	119.63	112.49
2	A	1248	FXE	CAA-OAB-CAE	-3.83	112.38	117.75
2	C	1248	FXE	CAK-NAJ-CAI	-3.17	118.36	125.39
2	A	1248	FXE	CAL-CAK-NAJ	2.97	128.69	121.80
2	A	1248	FXE	OAB-CAE-CAF	-2.94	111.56	115.89
2	C	1248	FXE	OAW-CAS-CAK	2.89	118.35	114.80
2	C	1248	FXE	CAA-OAB-CAE	-2.69	113.99	117.75
2	C	1248	FXE	OAC-CAI-NAH	-2.50	119.39	123.62
2	A	1248	FXE	CAL-CAK-CAS	2.40	122.13	119.05
2	C	1248	FXE	CAX-OAW-CAS	-2.39	113.92	117.53
2	A	1248	FXE	NAJ-CAI-NAH	2.33	116.55	112.49
2	A	1248	FXE	OAW-CAS-CAK	-2.15	112.15	114.80
2	C	1248	FXE	OAW-CAS-CAT	-2.11	120.75	124.37
2	A	1248	FXE	CAF-CAP-NAQ	-2.10	106.25	109.17
2	A	1248	FXE	OAW-CAS-CAT	2.09	127.95	124.37
2	A	1248	FXE	CAN-CAD-CAE	-2.04	116.76	119.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

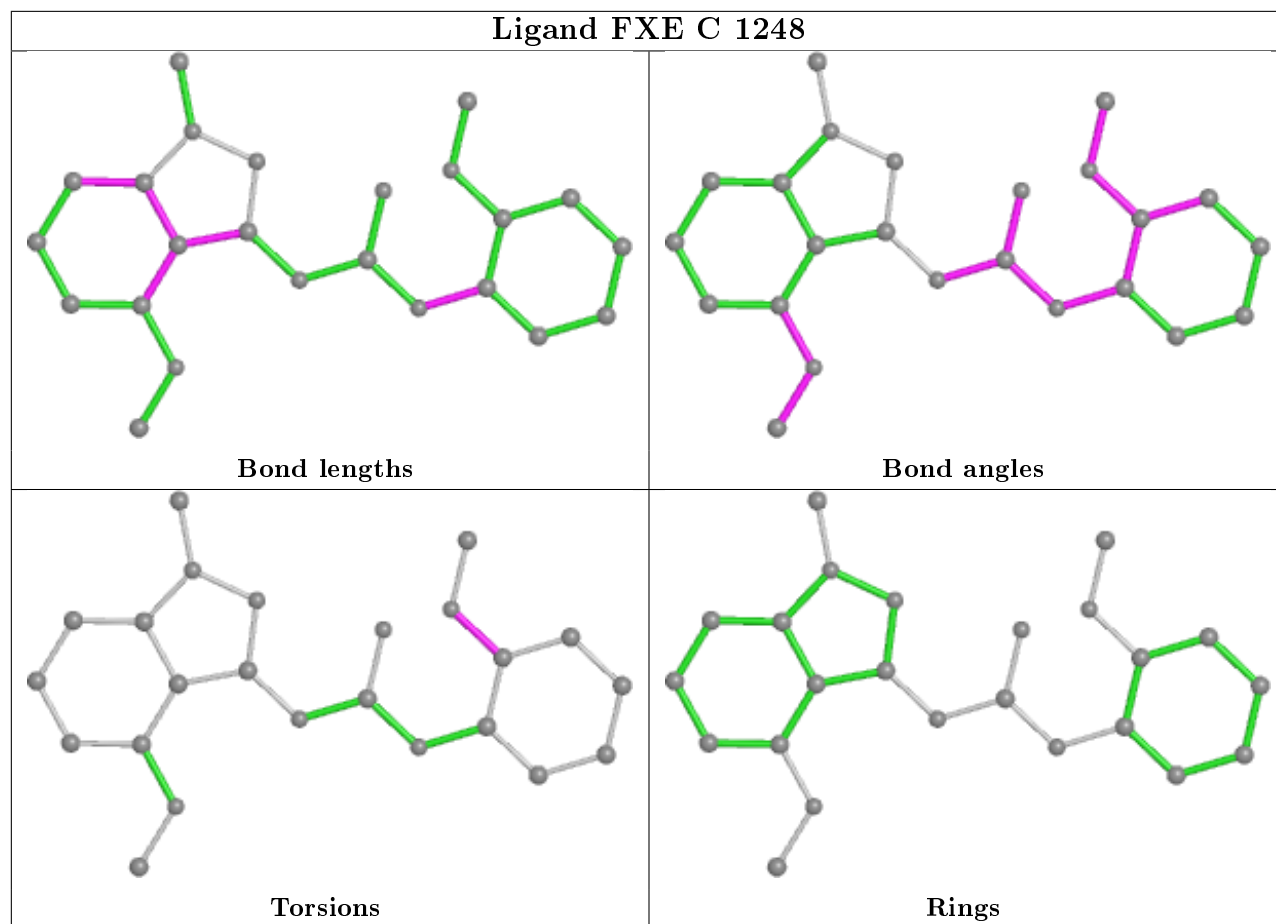
Mol	Chain	Res	Type	Atoms
2	A	1248	FXE	CAF-CAE-OAB-CAA
2	A	1248	FXE	CAD-CAE-OAB-CAA
2	C	1248	FXE	CAK-CAS-OAW-CAX
2	C	1248	FXE	CAT-CAS-OAW-CAX

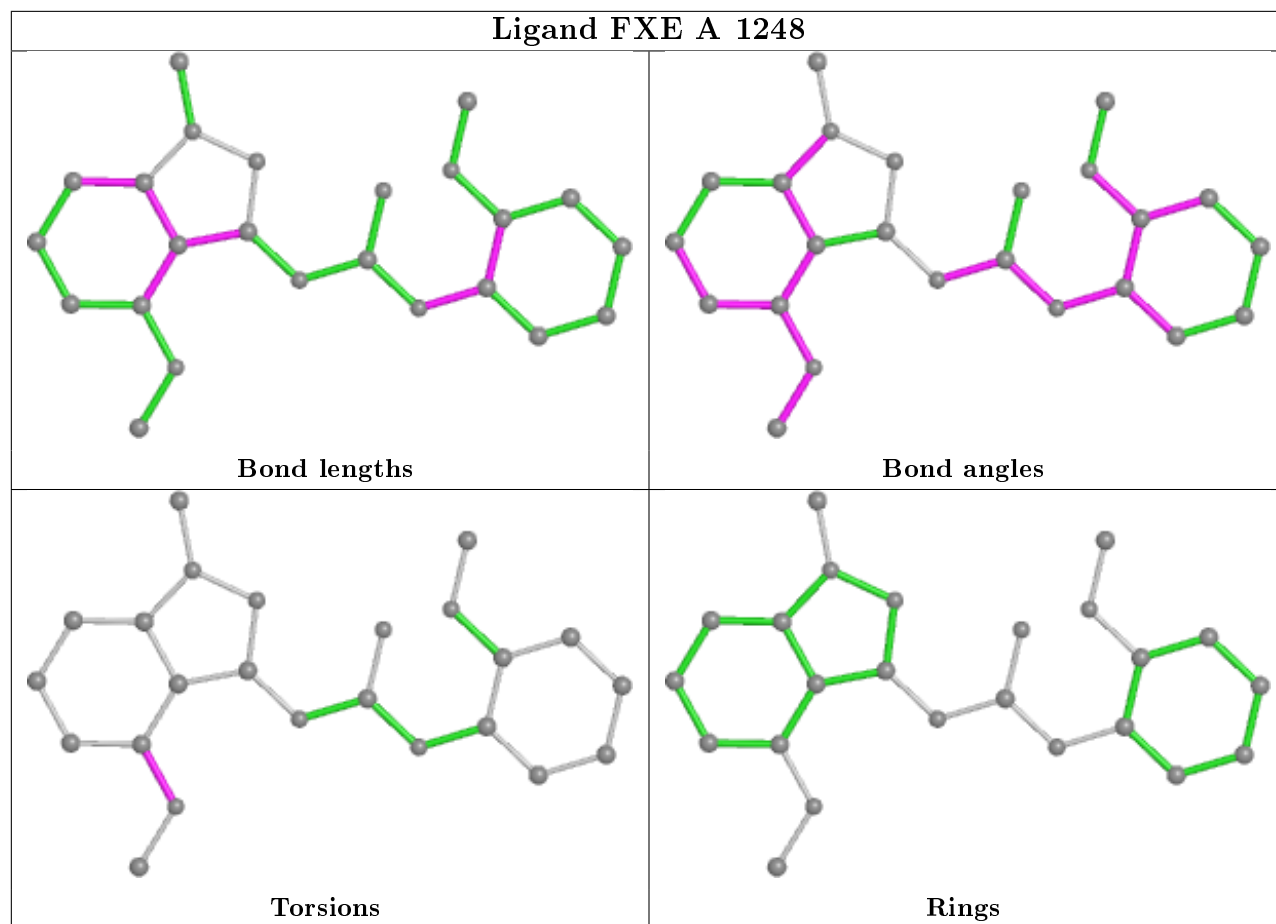
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1248	FXE	4	0
2	A	1248	FXE	5	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, 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	235/269 (87%)	0.31	15 (6%) 19 18	25, 39, 69, 91	0
1	B	237/269 (88%)	0.32	11 (4%) 32 31	21, 40, 68, 93	0
1	C	244/269 (90%)	0.38	14 (5%) 23 22	23, 39, 79, 103	0
1	D	241/269 (89%)	0.21	8 (3%) 46 45	23, 38, 75, 97	0
All	All	957/1076 (88%)	0.31	48 (5%) 28 27	21, 39, 73, 103	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	ASN	7.0
1	B	198	ALA	5.0
1	A	149	ALA	5.0
1	C	105	GLU	4.9
1	C	247	SER	4.6
1	D	195	LEU	4.3
1	B	78	GLN	4.2
1	A	78	GLN	4.0
1	B	74	GLU	4.0
1	D	190	ASP	3.9
1	A	246	MET	3.9
1	C	93	THR	3.7
1	C	200	ARG	3.6
1	A	105	GLU	3.5
1	C	198	ALA	3.4
1	A	147	GLY	3.4
1	A	146	MET	3.3
1	A	195	LEU	3.2
1	C	-18	HIS	3.1
1	A	145	ALA	3.1
1	A	151	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	108[A]	ASP	2.9
1	B	77	GLN	2.9
1	A	247	SER	2.8
1	B	191	MET	2.8
1	C	201	GLU	2.7
1	C	150	GLY	2.6
1	D	199	GLN	2.5
1	B	75	HIS	2.5
1	B	228[A]	ASP	2.5
1	D	194	GLU	2.5
1	D	80	LEU	2.5
1	C	-17	HIS	2.4
1	C	191	MET	2.4
1	A	131	ALA	2.4
1	D	202	ALA	2.4
1	B	50	LYS	2.4
1	A	91	GLY	2.3
1	B	144	GLY	2.3
1	C	94	ARG	2.3
1	C	42	ALA	2.3
1	D	5	GLY	2.2
1	A	4	GLN	2.2
1	C	197	GLU	2.2
1	B	87	VAL	2.2
1	C	132	ARG	2.1
1	B	91	GLY	2.0
1	A	181	ALA	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 carbohydrates in this entry.

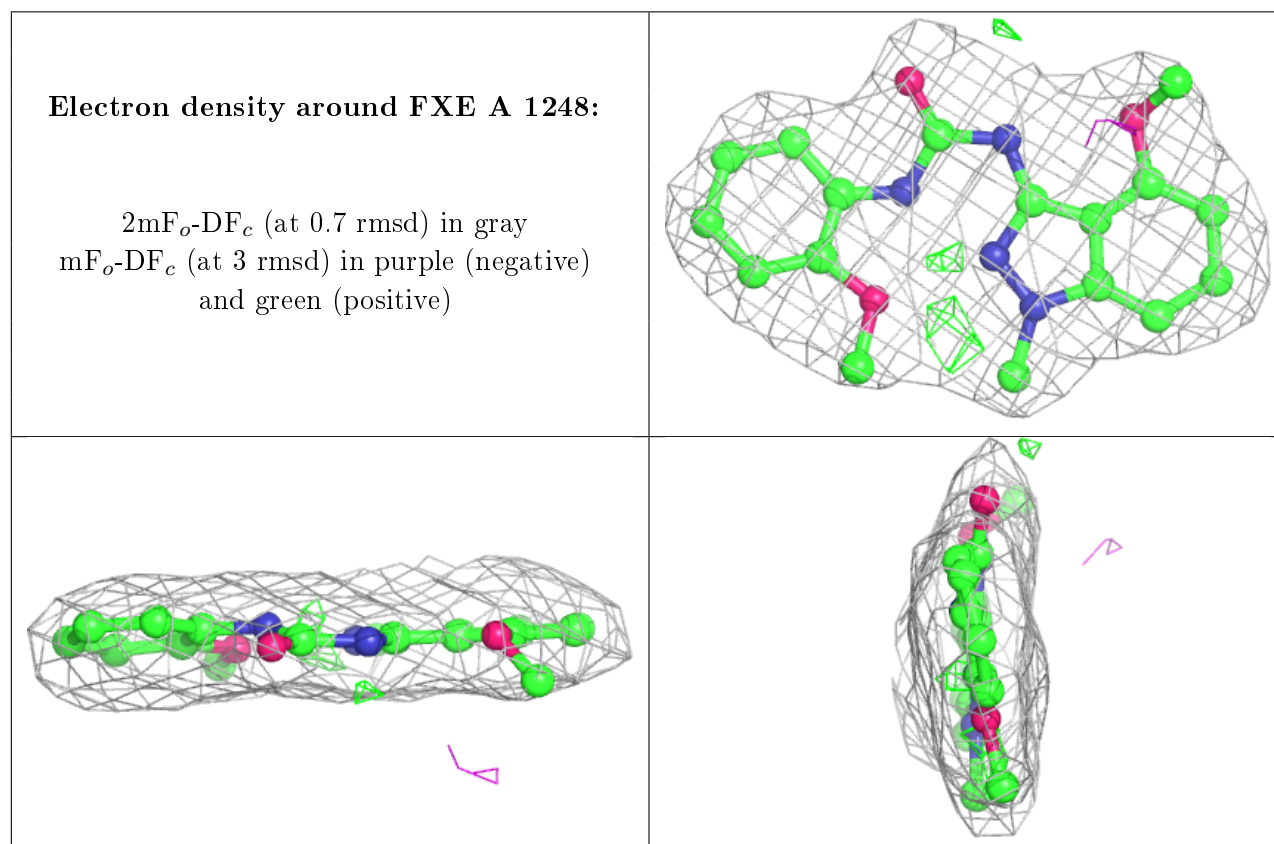
6.4 Ligands [i](#)

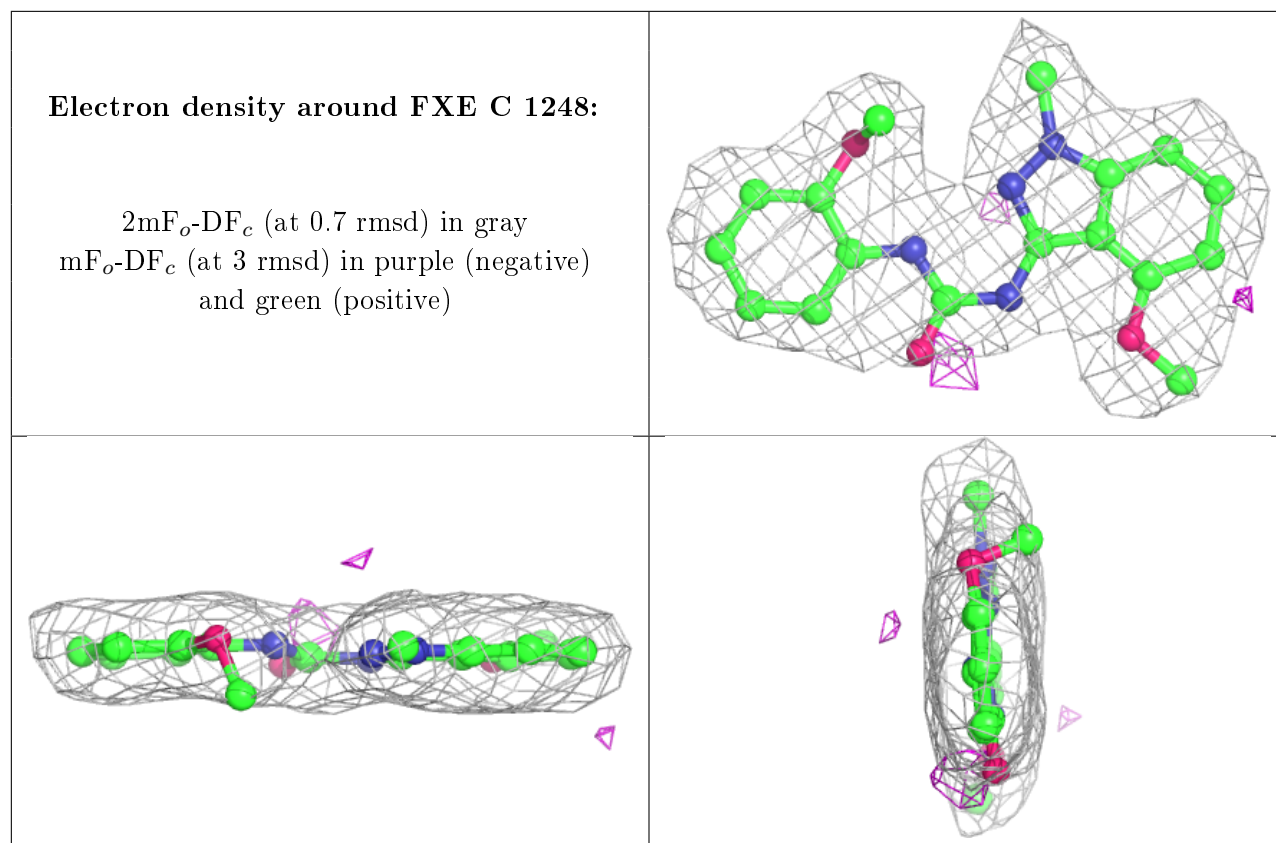
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
3	NI	B	1248	1/1	0.81	0.14	86,86,86,86	0
2	FXE	A	1248	24/24	0.92	0.12	31,37,41,43	0
2	FXE	C	1248	24/24	0.93	0.14	26,31,35,37	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.