



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:50 PM UTC

PDB ID : 4IU6 / pdb_00004iu6
Title : Human Methionine Aminopeptidase in complex with FZ1: Pyridinylquinazoli
nes Selectively Inhibit Human Methionine Aminopeptidase-1
Authors : Gabelli, S.B.; Zhang, F.; Miller, M.; Liu, J.; Amzel, L.M.
Deposited on : 2013-01-19
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

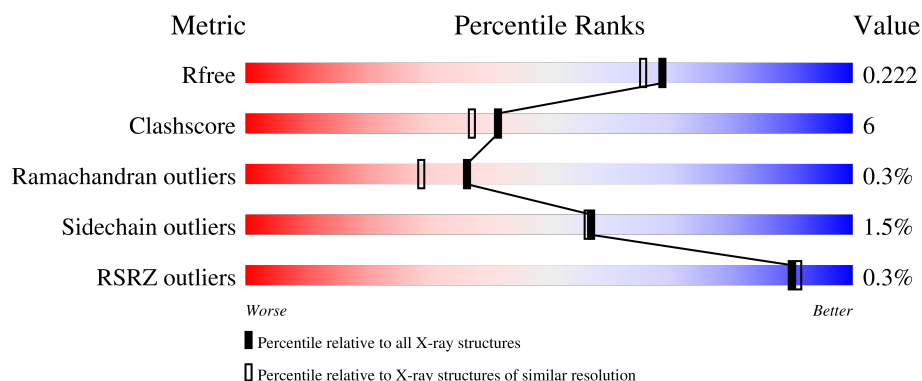
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	384	 69% 10% 21%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2731 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 Methionine aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	3	0
			2411	1517	430	445	19			

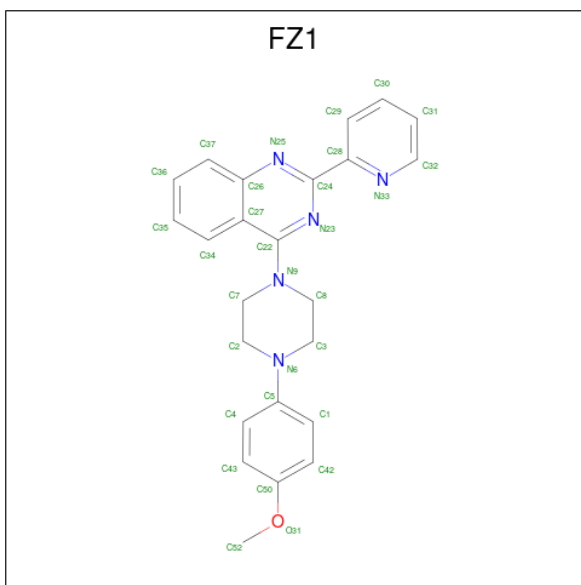
- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Co	0	0
			3	3		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		

- Molecule 4 is 4-[4-(4-methoxyphenyl)piperazin-1-yl]-2-(pyridin-2-yl)quinazoline (CCD ID: FZ1) (formula: C₂₄H₂₃N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			30	24	5	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	276	Total 276	O 276	0	0

i

- Molecule 1: Methionine aminopeptidase 1

Chain A:

69% 10% 21%

Met Ala Val Thr Arg Cys Asp Gly Cys Ser Ser Glu Lys Leu Gln Pro Thr Cys Ile Lys Leu Gly Ile Glu Gly Trp Phe Ser Glu Cys Phe Lys Gly Ser Trp Ala His Lys Leu His Lys Ala Lys Asp Glu Lys

Lys Arg Glu Val Ser Ser Trp Thr Val Glu Gly Asp Ile Asn Thr Asp Pro Trp Ala Gly Y90 K95 Y100 P101 E126 L131 T134 S135 K138 M148 D160 M187 C211 E222 D229 N235 N242 R255 K256 L257 L265 L269

K273 Q290 R298 H306 K307 L308 H317 S329 V332 I335 E336 F337 M338 E341 W344 Q365 L370 H390 S393

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.30Å 77.34Å 47.82Å 90.00° 91.49° 90.00°	Depositor
Resolution (Å)	47.80 – 1.90 47.80 – 1.90	Depositor EDS
% Data completeness (in resolution range)	91.5 (47.80-1.90) 91.8 (47.80-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.172 , 0.223 0.170 , 0.222	Depositor DCC
R_{free} test set	1259 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.043 for h,-k,-l 0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2731	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.69% 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: FZ1, SO4, K, CO

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	0.82	0/2480	0.88	1/3365 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	95	LYS	N-CA-C	5.29	117.13	111.36

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	2411	0	2368	28	0
2	A	3	0	0	0	0
3	A	1	0	0	0	0
4	A	30	0	23	3	0
5	A	10	0	0	0	0
6	A	276	0	0	9	0
All	All	2731	0	2391	31	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 6.

All (31) 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)
4:A:405:FZ1:H11	4:A:405:FZ1:H23	1.41	0.99
1:A:338:MET:SD	6:A:681:HOH:O	2.26	0.92
4:A:405:FZ1:H11	4:A:405:FZ1:C34	2.11	0.80
4:A:405:FZ1:H23	4:A:405:FZ1:C7	2.12	0.79
1:A:338:MET:HE3	1:A:365:GLN:NE2	1.98	0.78
1:A:338:MET:HE3	1:A:365:GLN:HE22	1.49	0.77
1:A:131:LEU:O	1:A:134:THR:HG22	1.90	0.71
1:A:255:ARG:NH2	6:A:684:HOH:O	2.19	0.67
1:A:269:ILE:HD12	1:A:370:LEU:HD21	1.77	0.67
1:A:90:TYR:N	6:A:578:HOH:O	2.28	0.66
1:A:187[A]:ASN:ND2	6:A:762:HOH:O	2.31	0.64
1:A:265:LEU:O	1:A:269:ILE:HG12	2.02	0.60
1:A:211:CYS:HB3	1:A:338:MET:HE2	1.84	0.60
1:A:317:HIS:CE1	1:A:336:GLU:H	2.21	0.59
1:A:235:ASN:ND2	6:A:707:HOH:O	2.40	0.54
1:A:100:TYR:HB3	1:A:101:PRO:HA	1.90	0.54
1:A:298:ARG:HD3	1:A:344:TRP:CE3	2.42	0.54
1:A:317:HIS:HE1	1:A:336:GLU:H	1.56	0.54
1:A:160:ASP:OD1	1:A:390:HIS:HE1	1.93	0.52
1:A:148:MET:HE2	1:A:332:VAL:HG11	1.94	0.50
1:A:269:ILE:HD13	1:A:370:LEU:HD11	1.95	0.49
1:A:138:LYS:HE2	6:A:683:HOH:O	2.13	0.47
1:A:222:GLU:HG2	6:A:661:HOH:O	2.14	0.47
1:A:257:LEU:HD22	1:A:341:GLU:HG3	1.96	0.47
1:A:131:LEU:HD12	1:A:308:LEU:HD11	1.96	0.46
1:A:298:ARG:HD3	1:A:344:TRP:CZ3	2.50	0.46
1:A:126:GLU:HG2	6:A:617:HOH:O	2.16	0.46
1:A:269:ILE:HD13	1:A:335:ILE:HD12	1.98	0.45
1:A:273:LYS:NZ	6:A:568:HOH:O	2.46	0.43
1:A:229:ASP:HA	1:A:242:ASN:HB3	2.02	0.41
1:A:160:ASP:OD1	1:A:390:HIS:CE1	2.74	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	305/384 (79%)	298 (98%)	6 (2%)	1 (0%)	36	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	HIS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	264/328 (80%)	260 (98%)	4 (2%)	57	56

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	SER
1	A	290	GLN
1	A	329	SER
1	A	393	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN

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Mol	Chain	Res	Type
1	A	259	GLN
1	A	317	HIS
1	A	365	GLN
1	A	390	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	SO4	A	407	-	4,4,4	0.31	0	6,6,6	0.17	0
4	FZ1	A	405	2	34,34,34	1.48	3 (8%)	47,47,47	2.44	20 (42%)
5	SO4	A	406	-	4,4,4	0.33	0	6,6,6	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FZ1	A	405	2	-	8/14/24/24	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	FZ1	C27-C26	5.90	1.51	1.42
4	A	405	FZ1	C22-C27	3.10	1.49	1.43
4	A	405	FZ1	C22-N23	2.19	1.34	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	FZ1	C24-N25-C26	-6.83	111.89	116.56
4	A	405	FZ1	C31-C30-C29	-4.85	114.25	120.24
4	A	405	FZ1	C22-C27-C26	4.53	118.48	115.47
4	A	405	FZ1	C8-C3-N6	-4.12	102.11	110.78
4	A	405	FZ1	C8-N9-C7	3.99	120.55	111.57
4	A	405	FZ1	C27-C22-N23	-3.94	114.81	122.44
4	A	405	FZ1	N23-C22-N9	3.75	119.85	117.17
4	A	405	FZ1	C32-N33-C28	-3.44	112.42	117.24
4	A	405	FZ1	C7-C2-N6	-3.35	103.73	110.78
4	A	405	FZ1	C3-N6-C2	3.34	119.08	111.57
4	A	405	FZ1	C29-C28-N33	3.29	127.14	122.24
4	A	405	FZ1	C37-C26-C27	-3.20	115.69	119.13
4	A	405	FZ1	N25-C24-N23	2.88	130.32	126.49
4	A	405	FZ1	C24-C28-N33	-2.51	113.84	116.75
4	A	405	FZ1	C22-N23-C24	2.51	121.92	115.84
4	A	405	FZ1	C27-C22-N9	2.42	125.33	121.18
4	A	405	FZ1	C28-C24-N25	-2.14	114.53	117.47
4	A	405	FZ1	C37-C26-N25	2.10	121.76	118.69
4	A	405	FZ1	C30-C31-C32	2.07	122.41	118.62
4	A	405	FZ1	C34-C27-C22	-2.00	121.20	124.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	FZ1	C27-C22-N9-C7
4	A	405	FZ1	C42-C50-O31-C52
4	A	405	FZ1	C43-C50-O31-C52
4	A	405	FZ1	C4-C5-N6-C3
4	A	405	FZ1	N23-C22-N9-C7

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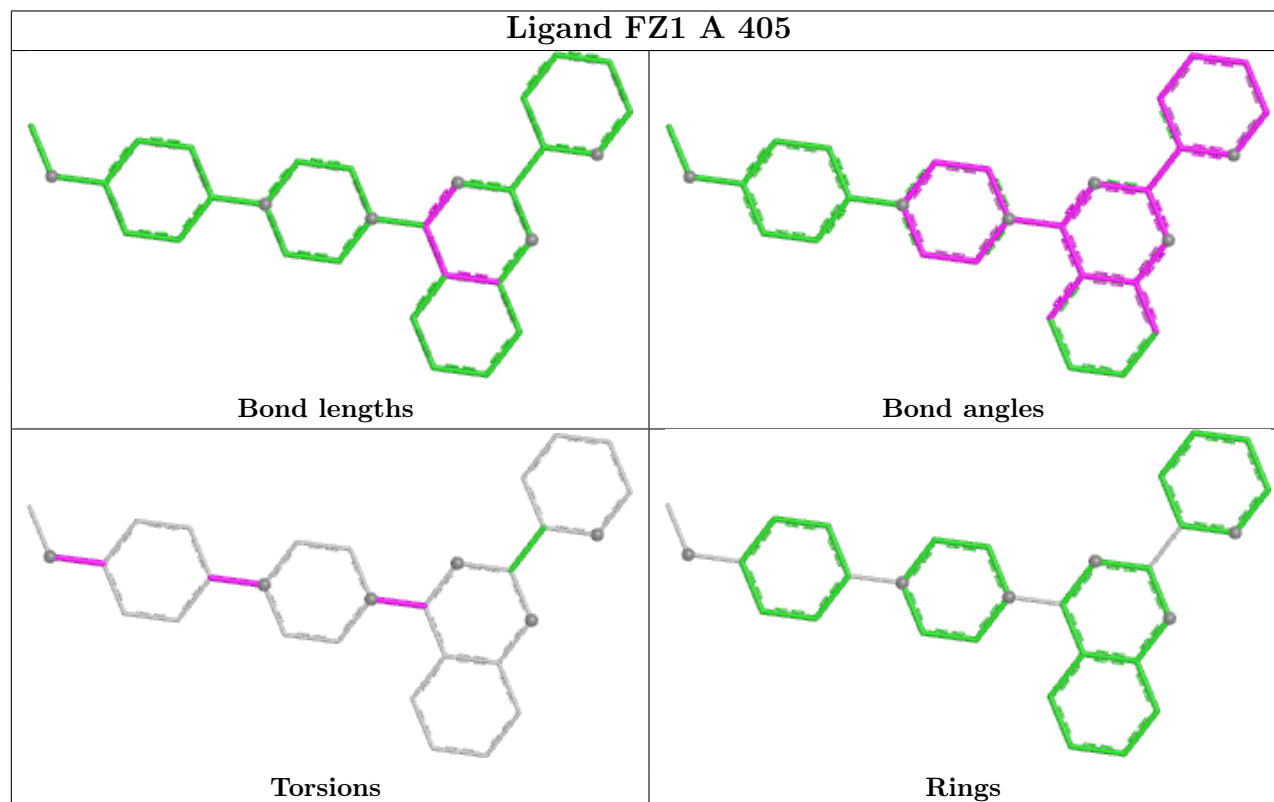
Mol	Chain	Res	Type	Atoms
4	A	405	FZ1	C1-C5-N6-C3
4	A	405	FZ1	C4-C5-N6-C2
4	A	405	FZ1	C1-C5-N6-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	FZ1	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	304/384 (79%)	-0.17	1 (0%) 90 91	14, 28, 44, 58	3 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	SER	3.0

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](#)

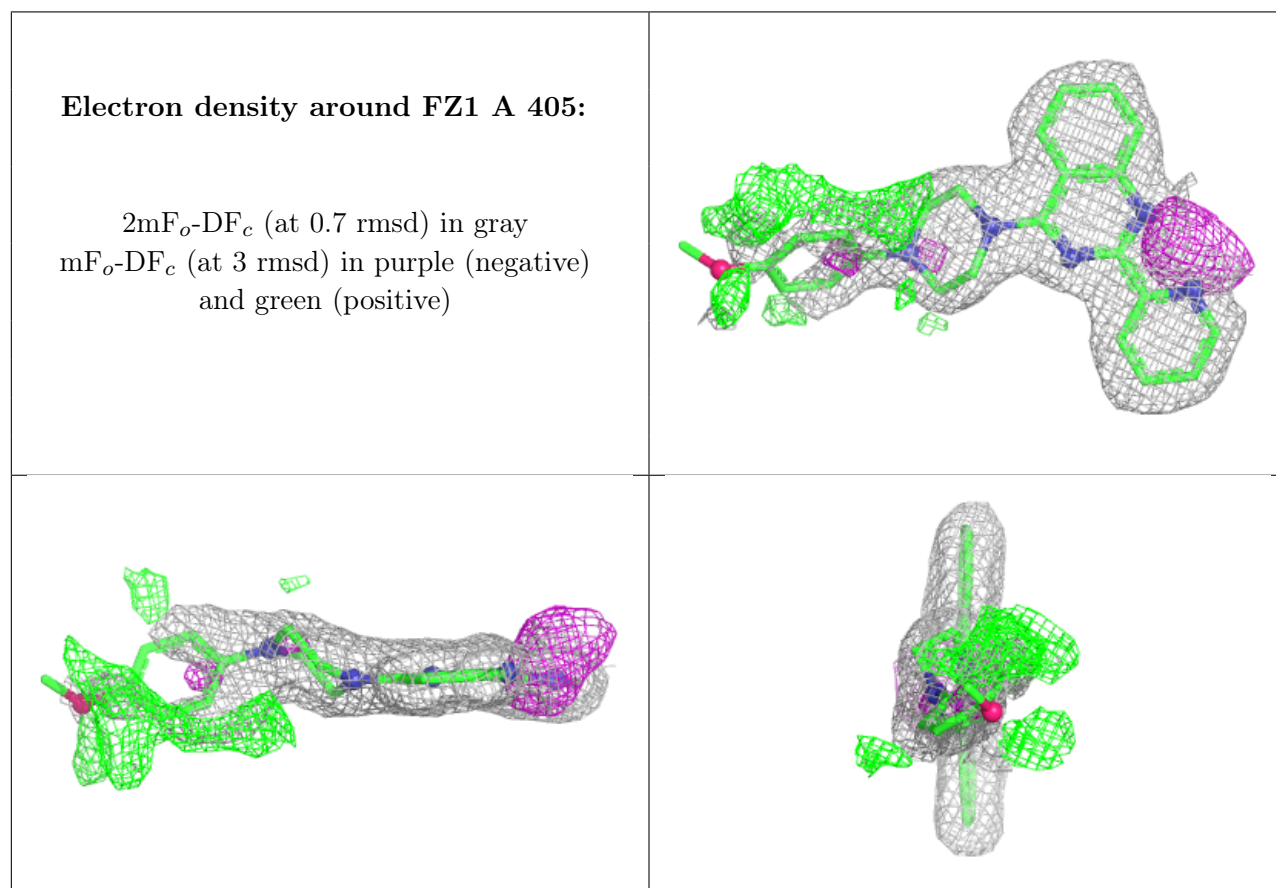
There are no oligosaccharides in this entry.

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
5	SO4	A	407	5/5	0.77	0.10	71,71,72,72	0
5	SO4	A	406	5/5	0.85	0.13	54,55,56,59	0
4	FZ1	A	405	30/30	0.88	0.14	24,29,45,46	5
2	CO	A	403	1/1	0.97	0.08	27,27,27,27	0
2	CO	A	402	1/1	0.98	0.03	21,21,21,21	0
3	K	A	404	1/1	0.99	0.03	21,21,21,21	0
2	CO	A	401	1/1	0.99	0.05	23,23,23,23	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 ⓘ

There are no such residues in this entry.