



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:15 PM UTC

PDB ID : 7FXQ / pdb_00007fxq
Title : Crystal Structure of human FABP4 in complex with 2-(5,6,7,8,9,10-hexahydrobenzo[8]annulen-3-yl)acetic acid, i.e. SMILES c12c(ccc(c1)CC(=O)O)CCC2 with IC50=0.725 microM
Authors : Ehler, A.; Benz, J.; Obst, U.; Unknown, N.; Rudolph, M.G.
Deposited on : 2023-04-27
Resolution : 1.12 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

i

X-RAY DIFFRACTION

A.

Metric	Percentile Rank	Value
Mean	50	1.00
Median	50	1.00
Mode	50	1.00
Standard Deviation	50	1.00
Skewness	50	1.00
Kurtosis	50	1.00
Minimum	50	1.00
Maximum	50	1.00
Range	50	1.00
Interquartile Range	50	1.00
Five-Number Summary	50	1.00
Normality Test	50	1.00
Shapiro-Wilk Test	50	1.00
Anderson-Darling Test	50	1.00
Kolmogorov-Smirnov Test	50	1.00
Lilliefors Test	50	1.00
Jarque-Bera Test	50	1.00
Portmanteau Test	50	1.00
Box-Cox Test	50	1.00
Robustness Test	50	1.00
Outlier Detection	50	1.00
Correlation Analysis	50	1.00
Regression Analysis	50	1.00
Time Series Analysis	50	1.00
Forecasting Accuracy	50	1.00
Model Fit	50	1.00
Model Selection	50	1.00
Model Validation	50	1.00
Model Interpretation	50	1.00
Model Deployment	50	1.00
Model Monitoring	50	1.00
Model Maintenance	50	1.00
Model Documentation	50	1.00
Model Communication	50	1.00
Model Evaluation	50	1.00
Model Improvement	50	1.00
Model Refinement	50	1.00
Model Optimization	50	1.00
Model Automation	50	1.00
Model Integration	50	1.00
Model Interoperability	50	1.00
Model Scalability	50	1.00
Model Flexibility	50	1.00
Model Reliability	50	1.00
Model Security	50	1.00
Model Privacy	50	1.00
Model Transparency	50	1.00
Model Accountability	50	1.00
Model Explainability	50	1.00
Model Auditability	50	1.00
Model Governance	50	1.00
Model Compliance	50	1.00
Model Ethics	50	1.00
Model Social Impact	50	1.00
Model Environmental Impact	50	1.00
Model Economic Impact	50	1.00
Model Cultural Impact	50	1.00
Model Political Impact	50	1.00
Model Legal Impact	50	1.00
Model Religious Impact	50	1.00
Model Philosophical Impact	50	1.00
Model Historical Impact	50	1.00
Model Future Impact	50	1.00
Model Global Impact	50	1.00
Model Local Impact	50	1.00
Model Regional Impact	50	1.00
Model National Impact	50	1.00
Model International Impact	50	1.00
Model Transnational Impact	50	1.00
Model Multinational Impact	50	1.00
Model Globalized Impact	50	1.00
Model Globalization Impact	50	1.00
Model Globalization Process	50	1.00
Model Globalization Outcome	50	1.00
Model Globalization Challenge	50	1.00
Model Globalization Opportunity	50	1.00
Model Globalization Risk	50	1.00
Model Globalization Benefit	50	1.00
Model Globalization Cost	50	1.00
Model Globalization Impact Assessment	50	1.00
Model Globalization Impact Study	50	1.00
Model Globalization Impact Report	50	1.00
Model Globalization Impact Review	50	1.00
Model Globalization Impact Analysis	50	1.00
Model Globalization Impact Evaluation	50	1.00
Model Globalization Impact Measurement	50	1.00
Model Globalization Impact Monitoring	50	1.00
Model Globalization Impact Tracking	50	1.00
Model Globalization Impact Reporting	50	1.00
Model Globalization Impact Communication	50	1.00
Model Globalization Impact Documentation	50	1.00
Model Globalization Impact Maintenance	50	1.00
Model Globalization Impact Improvement	50	1.00
Model Globalization Impact Refinement	50	1.00
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Model Globalization Impact Flexibility	50	1.00
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Model Globalization Impact Security	50	1.00
Model Globalization Impact Privacy	50	1.00
Model Globalization Impact Transparency	50	1.00
Model Globalization Impact Accountability	50	1.00
Model Globalization Impact Explainability	50	1.00
Model Globalization Impact Auditability	50	1.00
Model Globalization Impact Governance	50	1.00
Model Globalization Impact Compliance	50	1.00
Model Globalization Impact Ethics	50	1.00
Model Globalization Impact Social Impact	50	1.00
Model Globalization Impact Environmental Impact	50	1.00
Model Globalization Impact Economic Impact	50	1.00
Model Globalization Impact Cultural Impact	50	1.00
Model Globalization Impact Political Impact	50	1.00
Model Globalization Impact Legal Impact	50	1.00
Model Globalization Impact Religious Impact	50	



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}

Clashscore

Ramachandran outliers

Sidechain outliers

RSRZ outliers

180053

190562

187476

187428

180081

similar resolution

 $(\# \text{Entries}, \text{resolution range}(\text{\AA}))$

1985 (1.14-1.10)

2021 (1.14-1.10)

1978 (1.14-1.10)

1974 (1.14-1.10)

1984 (1.14-1.10)

Mol

Chain

Length

Quality of chain

1

A

135

0.

86%

12%

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	FMT	A	203	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2498 atoms, of which 1145 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.

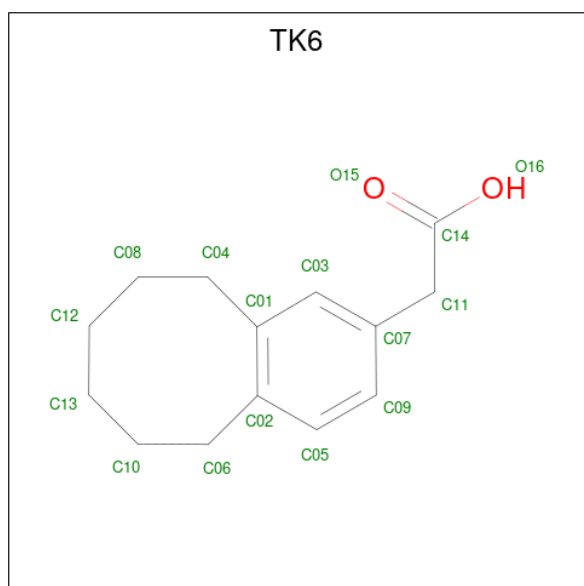
- Molecule 1 is a protein called Fatty acid-binding protein, adipocyte.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	133	2233	699	1128	183	216	7	0	11	0

There are 3 discrepancies between the modelled and reference sequences:

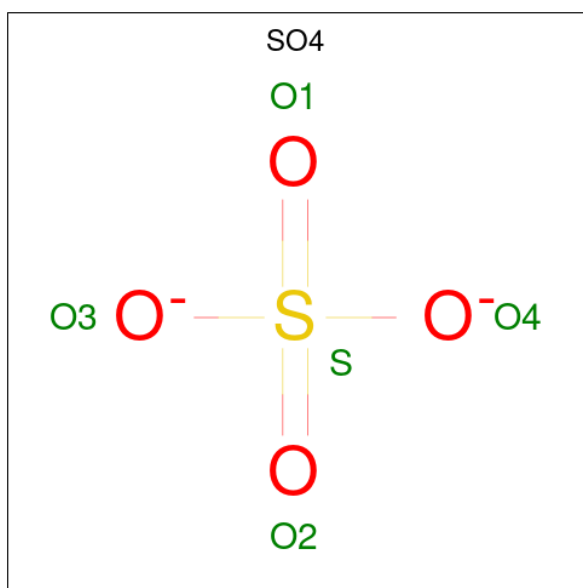
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P15090
A	-2	SER	-	expression tag	UNP P15090
A	-1	HIS	-	expression tag	UNP P15090

- Molecule 2 is (5,6,7,8,9,10-hexahydrobenzo[8]annulen-2-yl)acetic acid (CCD ID: TK6) (formula: C₁₄H₁₈O₂) (labeled as "Ligand of Interest" by depositor).



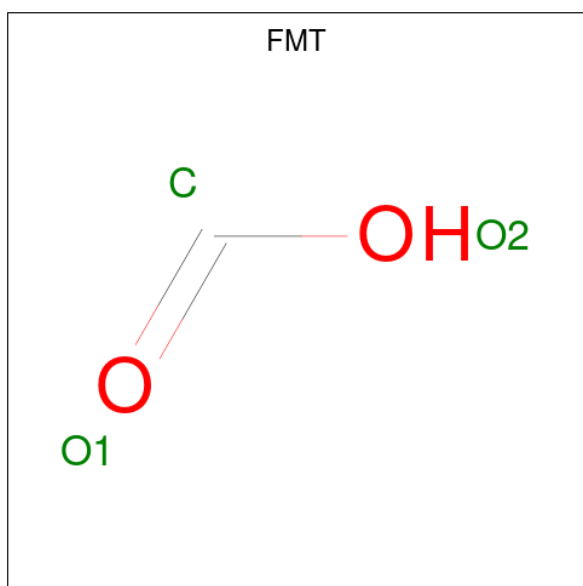
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	33	14	17	2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	216	Total 219	O 219	0	3

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: Fatty acid-binding protein, adipocyte

Chain A:  % 86% 12% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	32.34Å 53.94Å 75.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.53 – 1.12 37.53 – 1.12	Depositor EDS
% Data completeness (in resolution range)	97.7 (37.53-1.12) 97.7 (37.53-1.12)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 1.12Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.130 , 0.157 0.129 , 0.157	Depositor DCC
R_{free} test set	2573 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	10.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2498	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.06% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FMT, TK6

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	1.20	3/1146 (0.3%)	0.98	4/1538 (0.3%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	HIS	ND1-CE1	-6.38	1.26	1.32
1	A	0	MET	N-CA	-5.70	1.38	1.46
1	A	55	SER	N-CA	-5.51	1.39	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	0	MET	CA-C-O	7.54	129.37	120.70
1	A	0	MET	CG-SD-CE	-6.52	86.55	100.90
1	A	0	MET	CB-CG-SD	-5.47	96.30	112.70
1	A	79	LYS	CB-CG-CD	5.05	122.92	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1105	1128	1141	10	0
2	A	16	17	0	0	0
3	A	10	0	0	0	0
4	A	3	0	2	0	0
5	A	219	0	0	6	0
All	All	1353	1145	1143	10	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 4.

All (10) 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:55:SER:HB3	1:A:58[A]:LYS:O	1.62	0.97
1:A:14[B]:GLU:CG	5:A:306:HOH:O	2.34	0.76
1:A:32[A]:VAL:HG11	5:A:505:HOH:O	1.87	0.74
1:A:14[B]:GLU:HG3	5:A:306:HOH:O	1.88	0.73
1:A:107:LYS:HD2	1:A:109[A]:GLU:OE2	2.06	0.55
1:A:58[A]:LYS:HG2	5:A:468:HOH:O	2.10	0.50
1:A:107:LYS:HE3	5:A:452:HOH:O	2.14	0.47
1:A:40:MET:HE1	1:A:113:LEU:HD22	1.99	0.44
1:A:123[B]:THR:HG22	5:A:315:HOH:O	2.17	0.43
1:A:80:VAL:HG12	1:A:97:TRP:HB3	2.02	0.42

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	142/135 (105%)	138 (97%)	4 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	128/118 (108%)	125 (98%)	3 (2%)	44	8

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	86[A]	LEU
1	A	86[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	204	-	4,4,4	0.70	0	6,6,6	0.76	0
2	TK6	A	201	-	17,17,17	1.13	2 (11%)	22,22,22	1.18	2 (9%)
4	FMT	A	203	-	2,2,2	2.68	2 (100%)	1,1,1	1.48	0
3	SO4	A	202	-	4,4,4	0.29	0	6,6,6	0.80	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
2	TK6	A	201	-	-	4/4/13/13	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	FMT	O2-C	2.87	1.43	1.28
2	A	201	TK6	C11-C07	-2.77	1.47	1.51
4	A	203	FMT	O1-C	2.48	1.35	1.22
2	A	201	TK6	C10-C06	-2.16	1.50	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	TK6	C01-C03-C07	2.26	125.28	121.76
2	A	201	TK6	C03-C01-C02	-2.00	116.28	118.86

There are no chirality outliers.

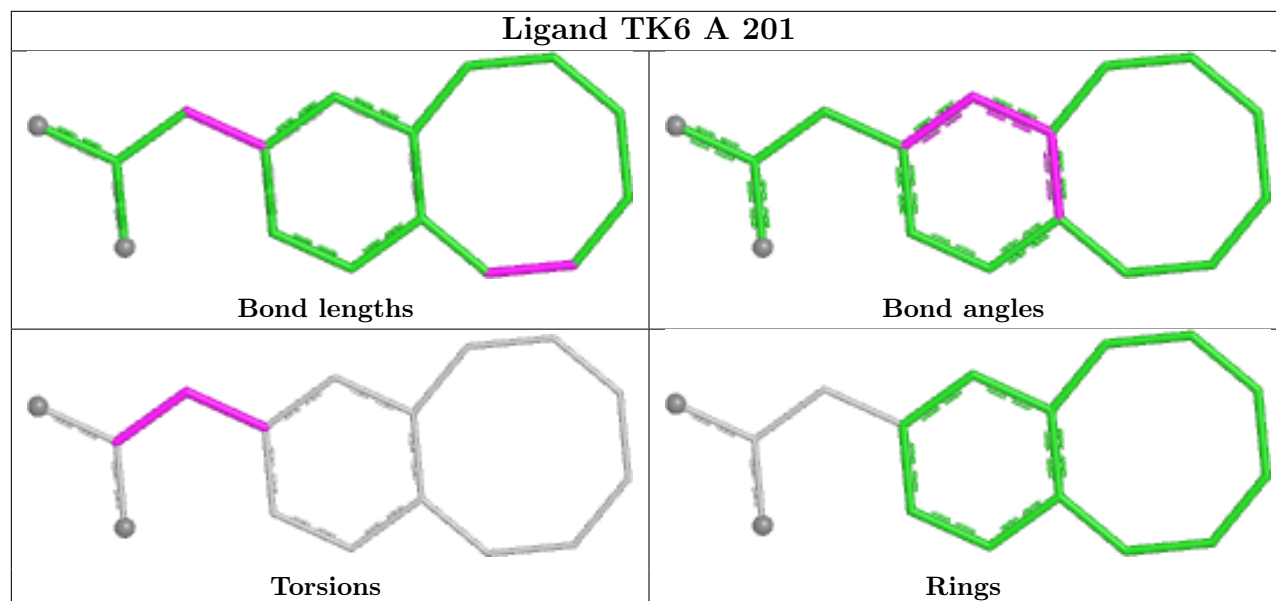
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	TK6	C09-C07-C11-C14
2	A	201	TK6	C03-C07-C11-C14
2	A	201	TK6	C07-C11-C14-O16
2	A	201	TK6	C07-C11-C14-O15

There are no ring outliers.

No monomer is involved in short contacts.

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	133/135 (98%)	-0.26	2 (1%) 72 77	6, 12, 23, 32	11 (8%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	CYS	3.1
1	A	0	MET	2.6

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.

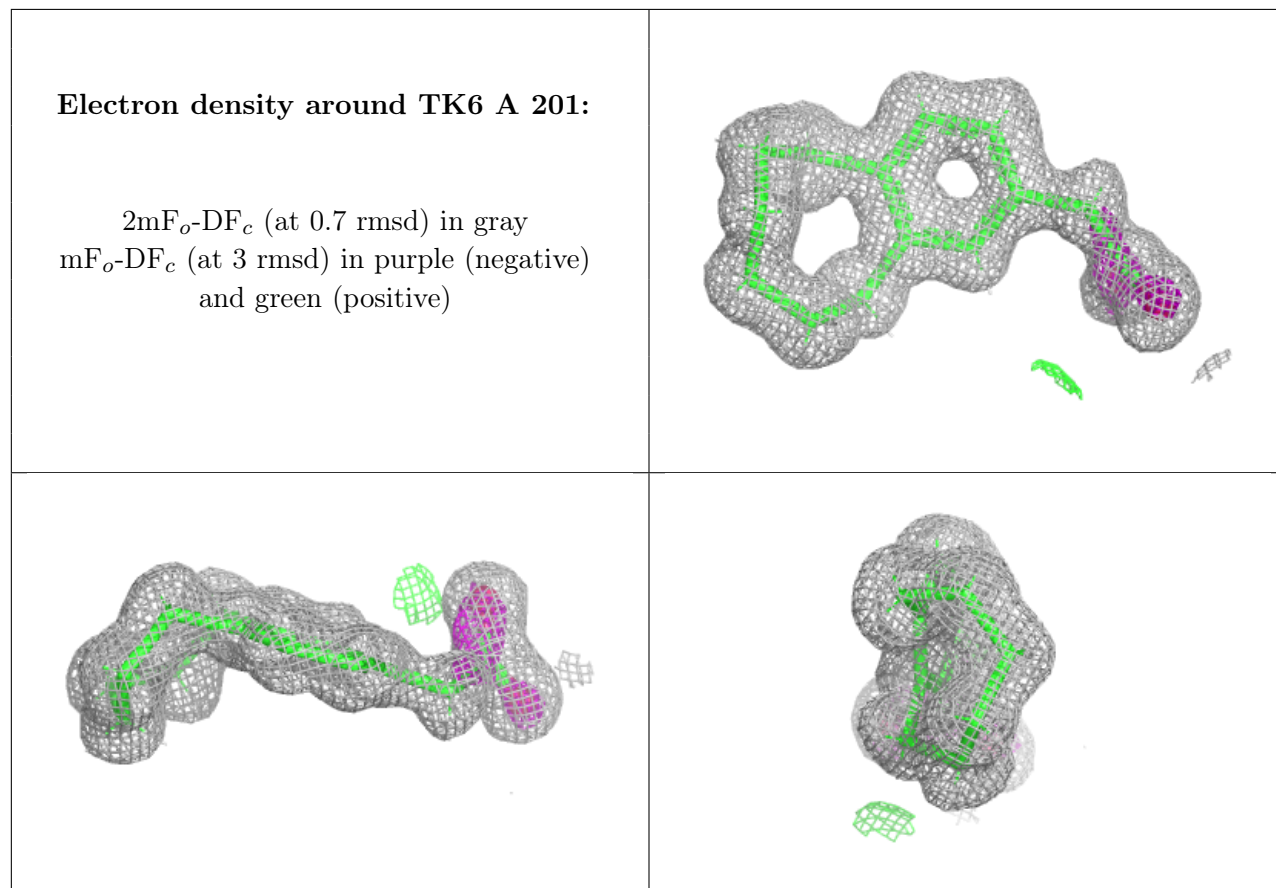
6.4 Ligands [i](#)

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
4	FMT	A	203	3/3	0.92	0.11	15,15,17,26	0
3	SO4	A	204	5/5	0.93	0.11	12,18,21,29	0
3	SO4	A	202	5/5	0.94	0.10	23,23,28,34	0
2	TK6	A	201	16/16	0.97	0.05	10,12,14,15	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.