wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2023 – 10:30 AM EDT

PDB ID	:	8FEC
Title	:	Structure of J-PKAc chimera complexed with Aplithianine derivative
Authors	:	Du, L.; Wilson, B.A.P.; Li, N.; Martinez Fiesco, J.A.; Dalilian, M.; Wang, D.; Smith, E.A.; Wamiru, A.; Goncharova, E.I.; Zhang, P.; O'Keefe, B.R.
Deposited on	:	2022-12-06
Resolution	:	2.70 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:

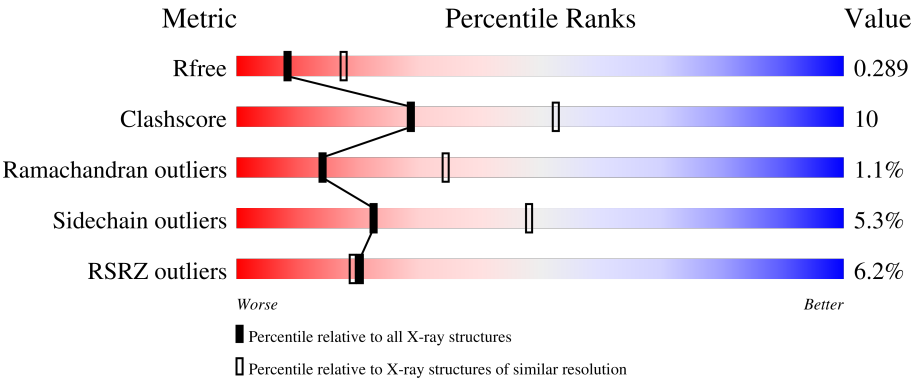
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	405	8% 75% 24% .
2	I	20	85% 15%
2	J	20	5% 55% 40% 5%
3	B	405	5% 68% 29% .

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7064 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 DnaJ homolog subfamily B member 1,cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	404	3356	2160	570	615	3	8	0	0	0

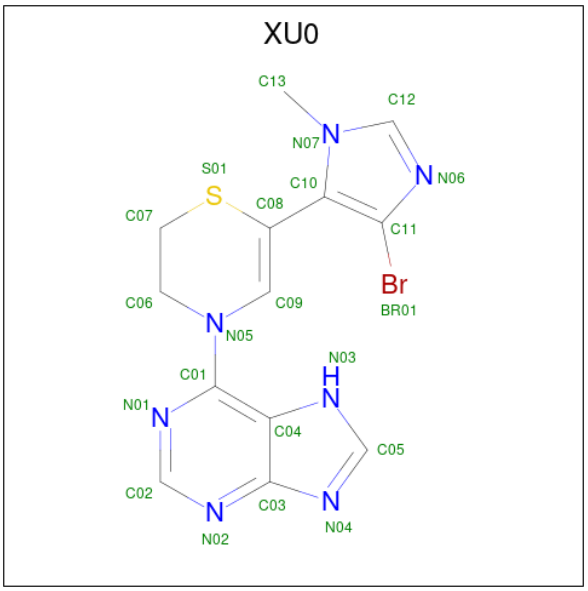
- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	20	156	94	32	30	0	0	0
2	J	20	156	94	32	30	0	0	0

- Molecule 3 is a protein called DnaJ homolog subfamily B member 1,cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
3	B	404	3352	2160	570	612	2	8	0	0	0

- Molecule 4 is 6-[(6P)-6-(4-bromo-1-methyl-1H-imidazol-5-yl)-2,3-dihydro-4H-1,4-thiazin-4-yl]-7H-purine (three-letter code: XU0) (formula: $C_{13}H_{12}BrN_7S$) (labeled as "Ligand of Interest" by depositor).



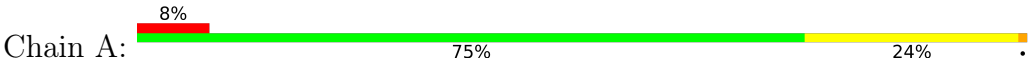
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	Br	C	N	S	0	0
			22	1	13	7	1		
4	B	1	Total	Br	C	N	S	0	0
			22	1	13	7	1		

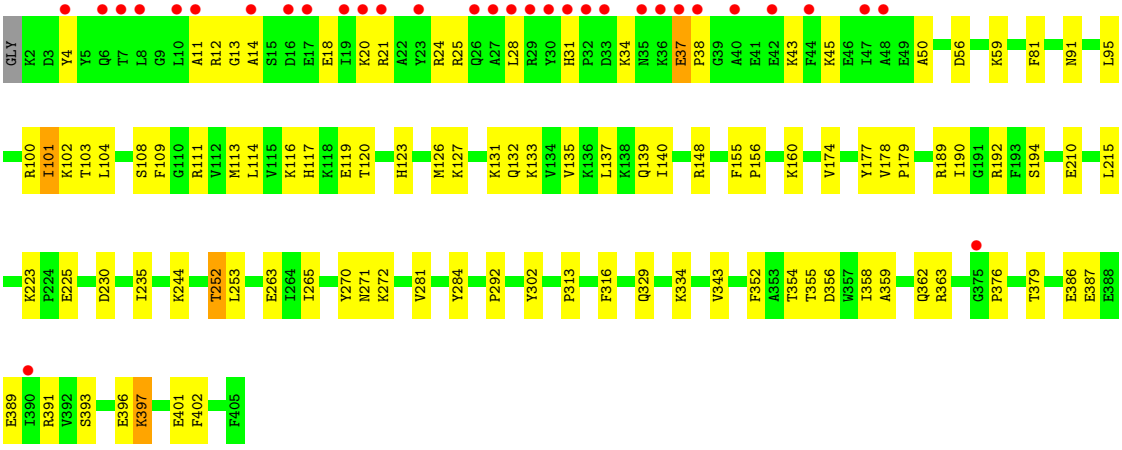
3 Residue-property plots (i)

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: DnaJ homolog subfamily B member 1,cAMP-dependent protein kinase catalytic subunit alpha

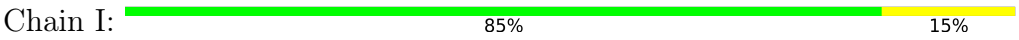
Chain A:

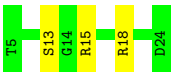




• Molecule 2: cAMP-dependent protein kinase inhibitor alpha

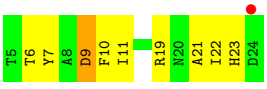
Chain I:





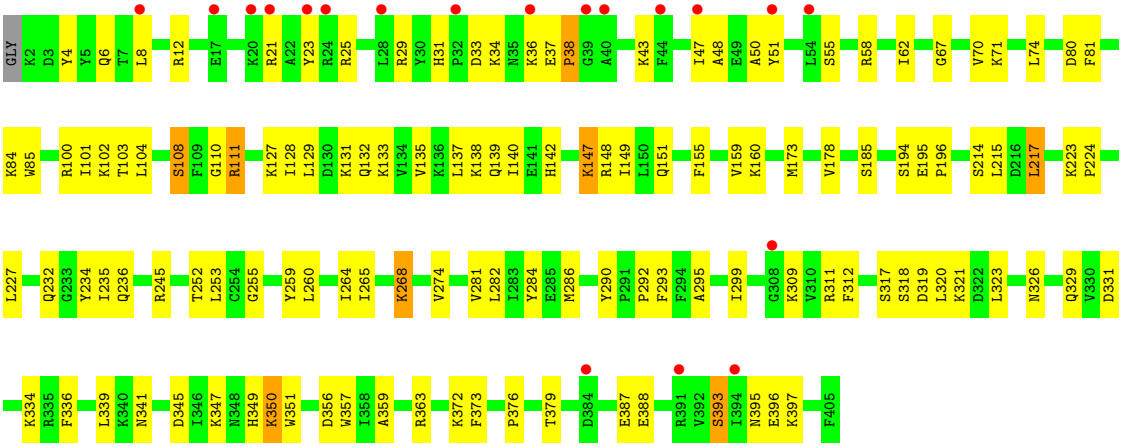
• Molecule 2: cAMP-dependent protein kinase inhibitor alpha

Chain J:



• Molecule 3: DnaJ homolog subfamily B member 1,cAMP-dependent protein kinase catalytic subunit alpha

Chain B:


GLY K2 D3 Y4 Y5 Q6 T7 L8 R12 E17 K20 R21 A22 Y23 R24 R25 L28 R29 Y30 H31 P32 D33 K34 N35 K36 E37 P38 G39 A40 K43 F44 I47 A48 E49 A50 Y51 L54 S55 R58 I62 G67 V70 K71 L74 D80 F81
K84 W85 R100 I101 K102 T103 L104 S108 F109 G110 R111 K127 I128 L129 D130 K131 Q132 K133 V134 V135 K136 L137 K138 Q139 I140 E141 H142 K147 R148 I149 L150 Q151 F155 V159 K160 M173 V178 S185 S194 E195 P196 S214 L215 D216 L217 K223 P224
L227 Q232 G233 Y234 I235 Q236 R245 T252 L253 C254 G255 Y259 L260 I264 I265 K268 V274 V281 L282 I283 Y284 E285 M286 Y290 P291 P292 F293 F294 A295 I299 G308 K309 V310 R311 F312 S317 S318 D319 L320 K321 D322 L323 N326 Q329 V330 D331
K334 R335 F336 L339 K340 N341 D345 I346 K347 N348 H349 K350 W351 D356 W357 I358 A359 R363 K372 F373 P376 T379 D384 E387 E388 R391 V392 S393 I394 N395 E396 K397 F405

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.64Å 59.10Å 91.01Å 88.95° 86.14° 89.86°	Depositor
Resolution (Å)	50.53 – 2.70 49.12 – 2.70	Depositor EDS
% Data completeness (in resolution range)	82.4 (50.53-2.70) 73.5 (49.12-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.287 0.210 , 0.289	Depositor DCC
R_{free} test set	1749 reflections (7.51%)	wwPDB-VP
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.023 for -h,k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7064	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.23% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, XU0, SEP

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	0.47	0/3407	0.63	1/4582 (0.0%)
2	I	0.44	0/158	0.70	0/212
2	J	0.45	0/158	0.66	0/212
3	B	0.47	0/3414	0.63	0/4593
All	All	0.47	0/7137	0.63	1/9599 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	253	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3356	0	3314	57	0
2	I	156	0	146	2	0
2	J	156	0	146	6	0
3	B	3352	0	3315	75	0
4	A	22	0	0	1	0
4	B	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7064	0	6921	136	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 10.

The worst 5 of 136 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)
3:B:101:ILE:HG22	3:B:102:LYS:HG3	1.50	0.93
1:A:4:TYR:HD1	1:A:50:ALA:HA	1.45	0.81
3:B:37:GLU:HB3	3:B:38:PRO:HD2	1.63	0.80
3:B:155:PHE:H	3:B:160:LYS:NZ	1.84	0.75
1:A:155:PHE:H	1:A:160:LYS:NZ	1.87	0.73

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	399/405 (98%)	368 (92%)	27 (7%)	4 (1%)	15 37
2	I	18/20 (90%)	16 (89%)	2 (11%)	0	100 100
2	J	18/20 (90%)	18 (100%)	0	0	100 100
3	B	400/405 (99%)	362 (90%)	33 (8%)	5 (1%)	12 30
All	All	835/850 (98%)	764 (92%)	62 (7%)	9 (1%)	14 34

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	12	ARG

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Mol	Chain	Res	Type
1	A	37	GLU
3	B	295	ALA
3	B	376	PRO

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	351/351 (100%)	336 (96%)	15 (4%)	29 57
2	I	15/15 (100%)	15 (100%)	0	100 100
2	J	15/15 (100%)	13 (87%)	2 (13%)	4 9
3	B	352/352 (100%)	330 (94%)	22 (6%)	18 40
All	All	733/733 (100%)	694 (95%)	39 (5%)	22 48

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	232	GLN
3	B	373	PHE
3	B	245	ARG
3	B	318	SER
2	J	9	ASP

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

Mol	Chain	Res	Type
1	A	123	HIS
3	B	341	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	SEP	B	393	3	8,9,10	1.55	1 (12%)	8,12,14	1.74	2 (25%)
1	TPO	A	252	1	8,10,11	1.58	1 (12%)	10,14,16	1.80	2 (20%)
1	SEP	A	393	1	8,9,10	1.55	1 (12%)	8,12,14	1.89	2 (25%)
1	SEP	A	194	1	8,9,10	1.84	3 (37%)	8,12,14	1.67	2 (25%)
3	TPO	B	252	3	8,10,11	1.65	1 (12%)	10,14,16	1.57	1 (10%)

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
3	SEP	B	393	3	-	2/5/8/10	-
1	TPO	A	252	1	-	0/9/11/13	-
1	SEP	A	393	1	-	5/5/8/10	-
1	SEP	A	194	1	-	1/5/8/10	-
3	TPO	B	252	3	-	1/9/11/13	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	SEP	P-O1P	3.84	1.62	1.50
3	B	252	TPO	P-O1P	3.48	1.61	1.50
1	A	393	SEP	P-O1P	3.39	1.61	1.50
3	B	393	SEP	P-O1P	3.34	1.61	1.50
1	A	252	TPO	P-O1P	3.31	1.61	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	TPO	P-OG1-CB	-4.12	110.78	123.21
1	A	393	SEP	OG-CB-CA	3.57	111.61	108.14
1	A	194	SEP	OG-CB-CA	3.56	111.61	108.14
1	A	393	SEP	P-OG-CB	-3.43	108.86	118.30
3	B	393	SEP	OG-CB-CA	3.36	111.42	108.14

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	393	SEP	CA-CB-OG-P
1	A	393	SEP	CB-OG-P-O1P
1	A	393	SEP	CB-OG-P-O2P
1	A	393	SEP	CB-OG-P-O3P
3	B	393	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	393	SEP	1	0
1	A	252	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	XU0	A	501	-	19,25,25	2.89	9 (47%)	9,36,36	2.10	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	XU0	B	501	-	19,25,25	2.88	9 (47%)	9,36,36	2.17	3 (33%)

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	XU0	A	501	-	-	0/4/18/18	0/4/4/4
4	XU0	B	501	-	-	0/4/18/18	0/4/4/4

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	XU0	C09-N05	6.67	1.42	1.34
4	A	501	XU0	C09-N05	6.34	1.41	1.34
4	B	501	XU0	C09-C08	5.36	1.45	1.35
4	A	501	XU0	C09-C08	5.11	1.44	1.35
4	A	501	XU0	C10-C08	5.00	1.54	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	501	XU0	C03-C04-N03	-4.40	104.82	109.40
4	A	501	XU0	N02-C02-N01	-3.86	122.64	128.68
4	A	501	XU0	C03-C04-N03	-3.62	105.62	109.40
4	B	501	XU0	N02-C02-N01	-3.41	123.35	128.68
4	B	501	XU0	C02-N02-C03	2.91	120.27	113.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

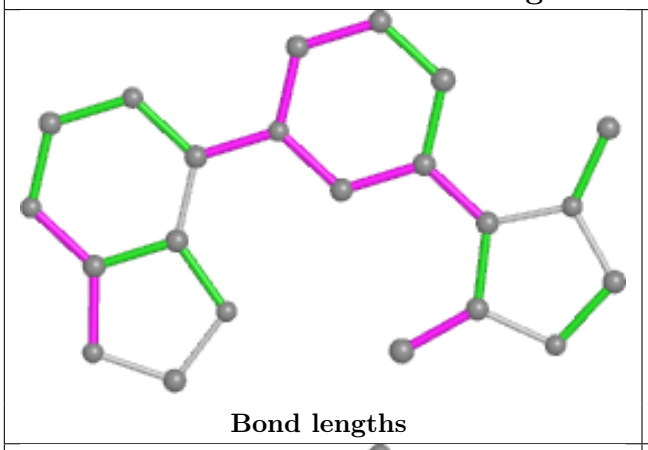
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	XU0	1	0
4	B	501	XU0	1	0

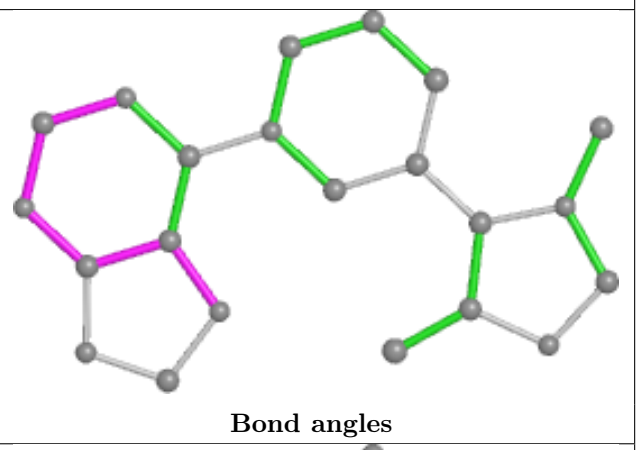
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

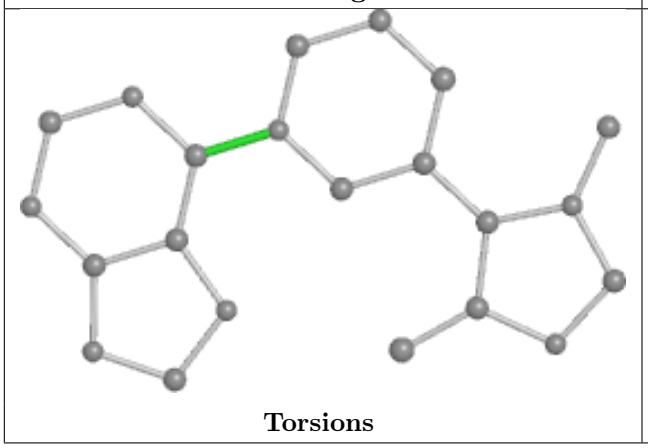
Ligand XU0 A 501



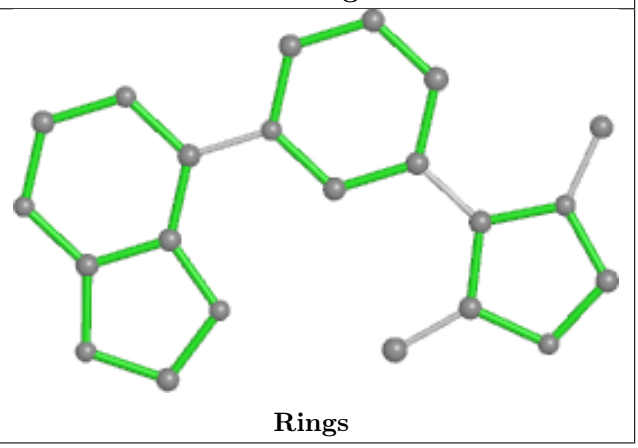
Bond lengths



Bond angles

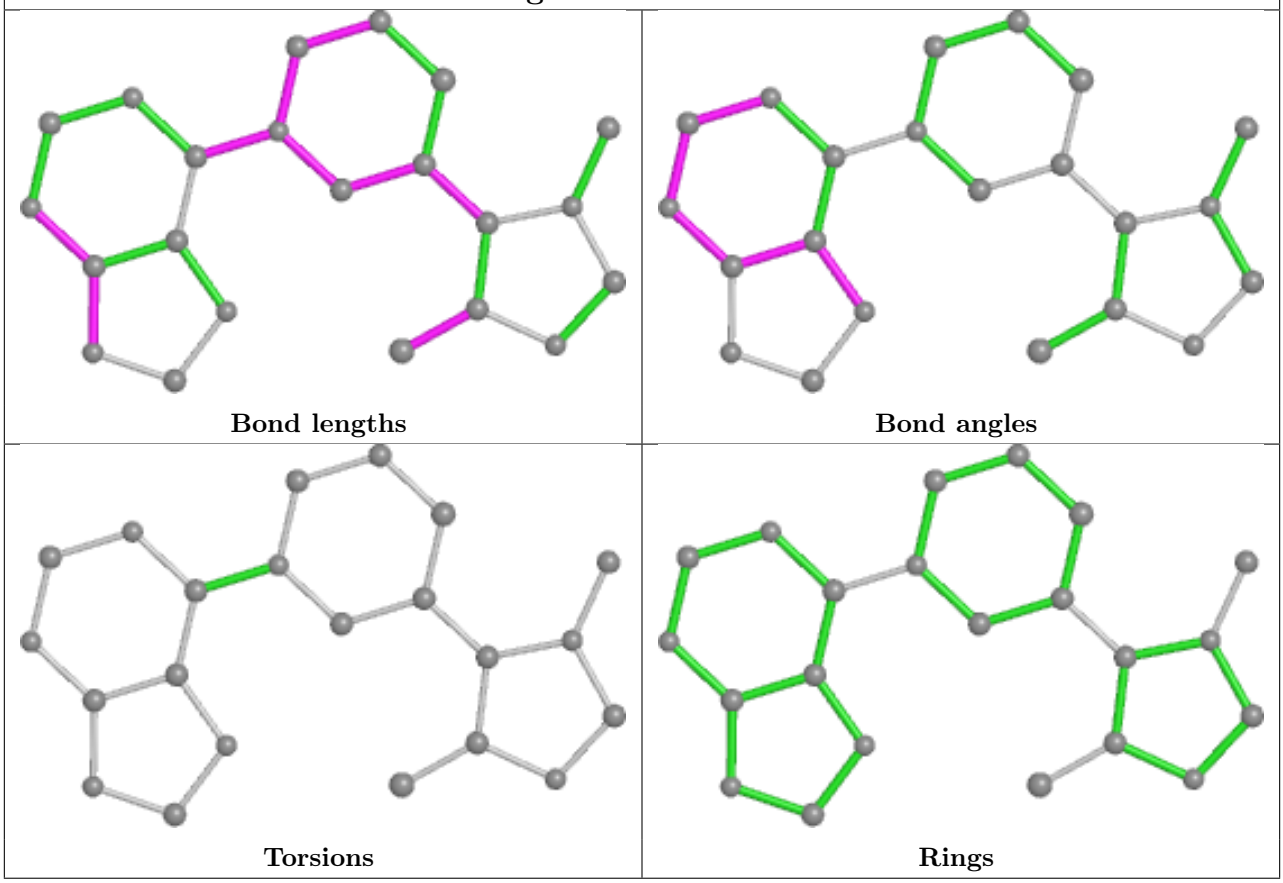


Torsions



Rings

Ligand XU0 B 501



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	401/405 (99%)	0.46	32 (7%) 12 10	47, 72, 123, 139	0
2	I	20/20 (100%)	-0.03	0 100 100	63, 75, 85, 87	0
2	J	20/20 (100%)	0.53	1 (5%) 28 27	77, 93, 103, 104	0
3	B	402/405 (99%)	0.34	19 (4%) 31 30	47, 76, 112, 129	0
All	All	843/850 (99%)	0.39	52 (6%) 20 19	47, 74, 117, 139	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	40	ALA	6.3
1	A	36	LYS	5.7
1	A	28	LEU	5.6
1	A	40	ALA	5.0
1	A	32	PRO	4.6

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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
1	SEP	A	194	10/11	0.92	0.16	70,75,89,101	0
3	SEP	B	393	10/11	0.92	0.15	90,94,98,99	0
1	SEP	A	393	10/11	0.95	0.13	86,92,95,99	0
1	TPO	A	252	11/12	0.98	0.18	49,55,60,64	0
3	TPO	B	252	11/12	0.99	0.17	50,56,63,65	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

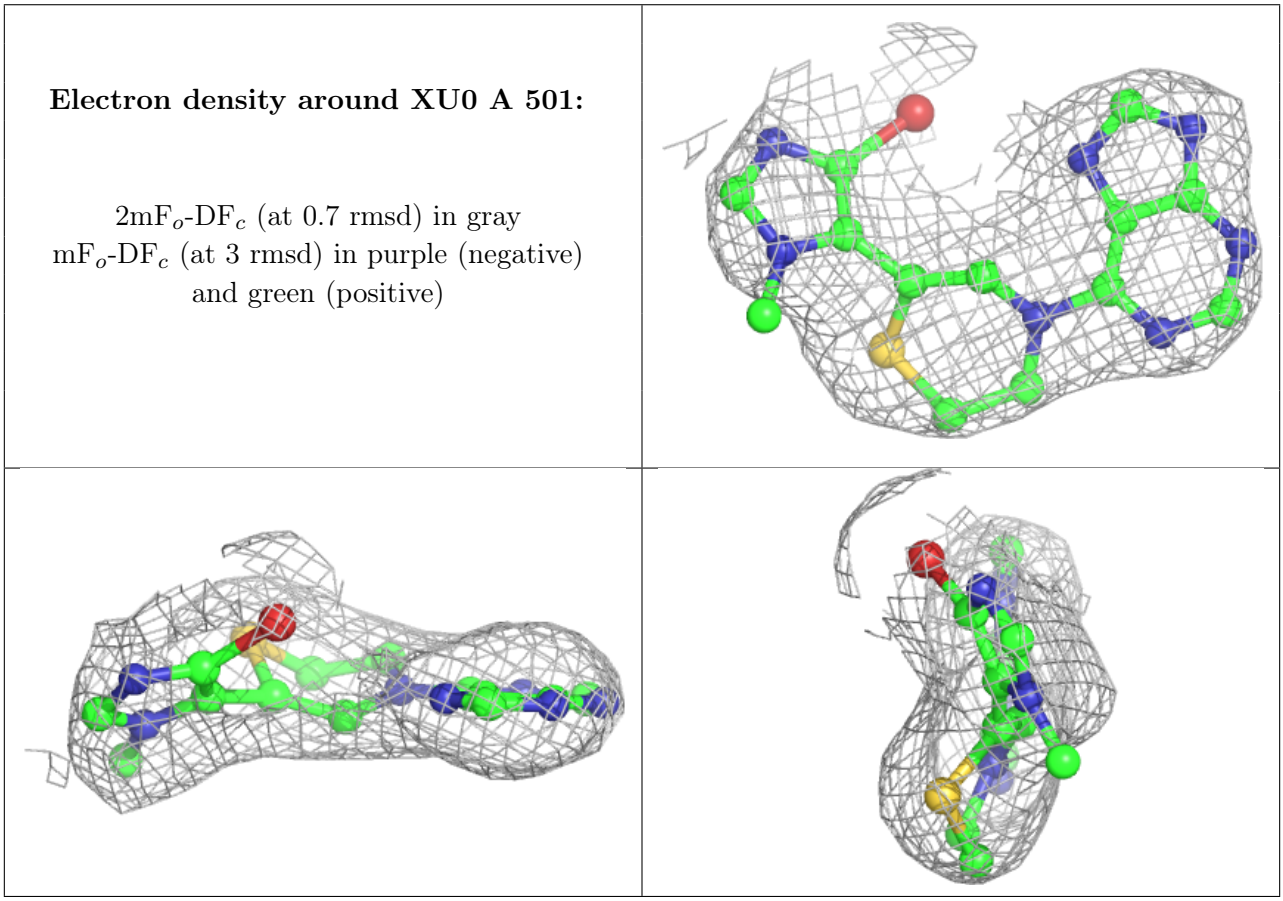
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	XU0	A	501	22/22	0.96	0.19	68,76,82,93	0
4	XU0	B	501	22/22	0.97	0.16	75,83,86,95	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.

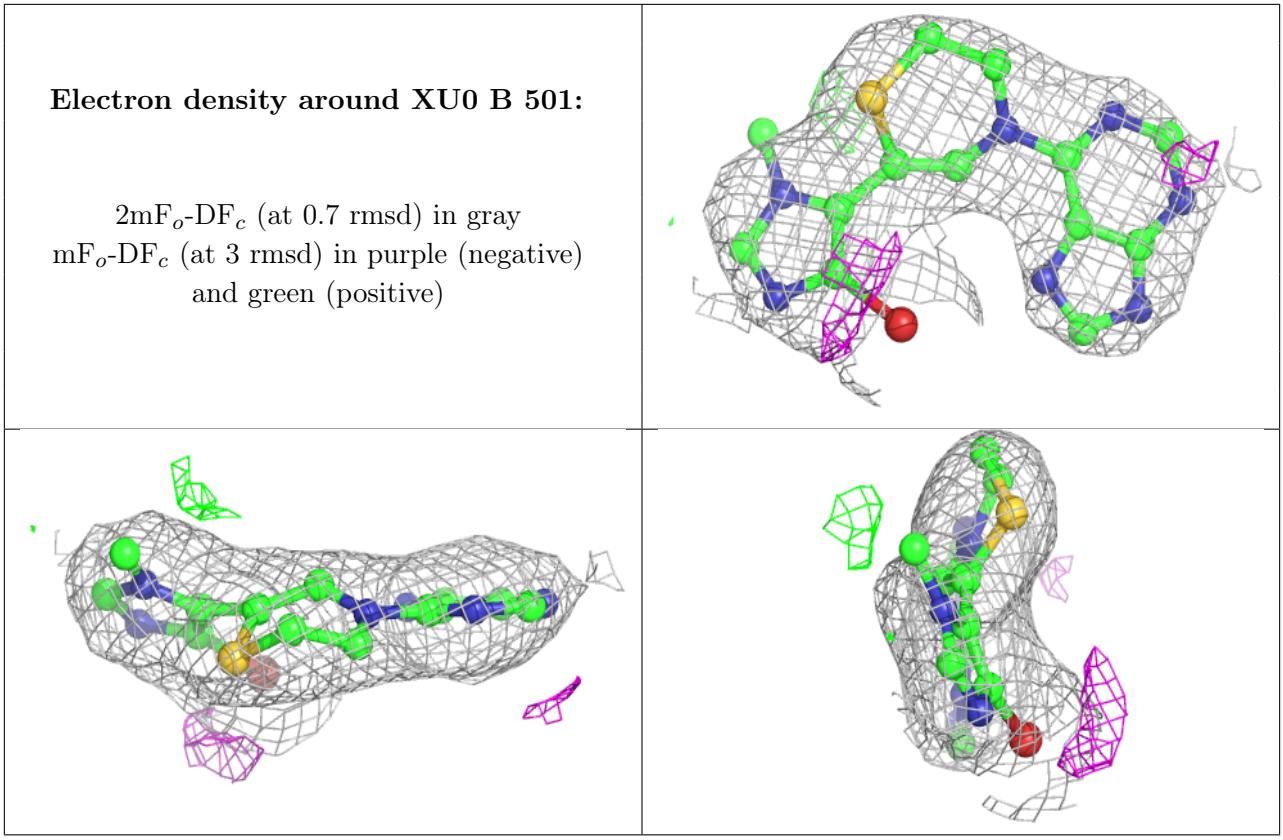
Electron density around XU0 A 501:

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



Electron density around XU0 B 501:

$2mF_o$-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.