wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 11:54 am BST

PDB ID	:	1UK0
Title	:	Crystal structure of catalytic domain of human poly(ADP-ribose) polymerase with a novel inhibitor
Authors	:	Kinoshita, T.
Deposited on	:	2003-08-13
Resolution	:	3.00 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 following versions of software and data (see references (1)) were used in the production of this report:

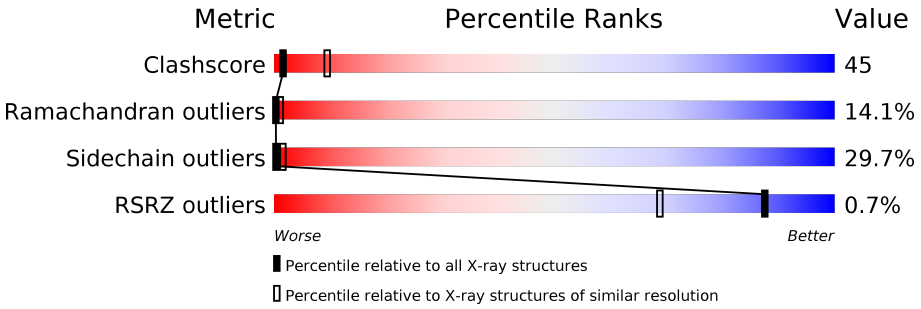
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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 <=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	350	% 15% 34% 29% 22%
1	B	350	% 8% 30% 37% 25%

2 Entry composition

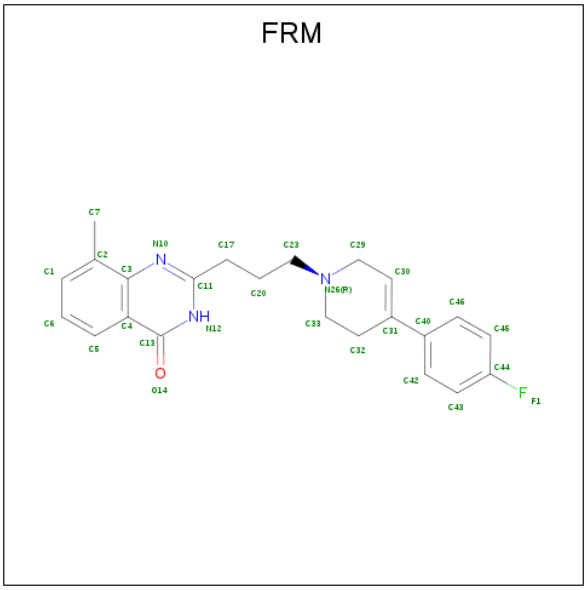
There are 3 unique types of molecules in this entry. The entry contains 5817 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Poly [ADP-ribose] polymerase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2754	1752	465	526	11			
1	B	350	Total	C	N	O	S	0	0	0
			2754	1752	465	526	11			

- Molecule 2 is 2-{3-[4-(4-FLUOROPHENYL)-3,6-DIHYDRO-1(2H)-PYRIDINYL]PROPYL} -8-METHYL-4(3H)-QUINAZOLINONE (three-letter code: FRM) (formula: $C_{23}H_{24}FN_3O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			28	23	1	3	1		
2	B	1	Total	C	F	N	O	0	0
			28	23	1	3	1		

- Molecule 3 is water.

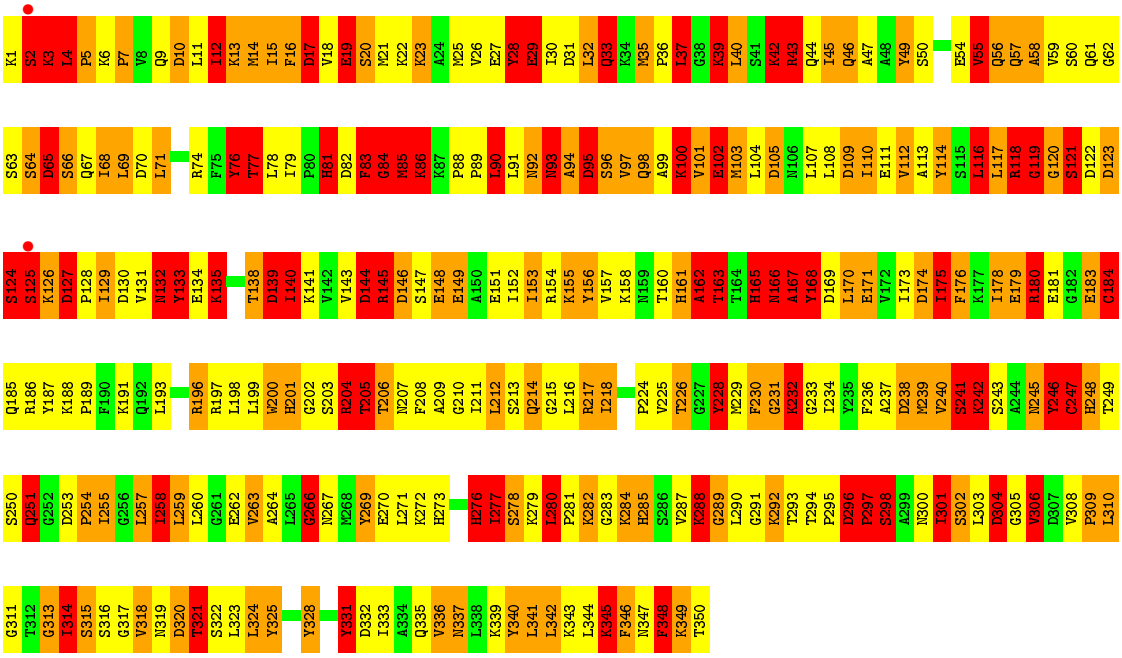
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	124	Total O 124 124	0	0
3	B	129	Total O 129 129	0	0

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.

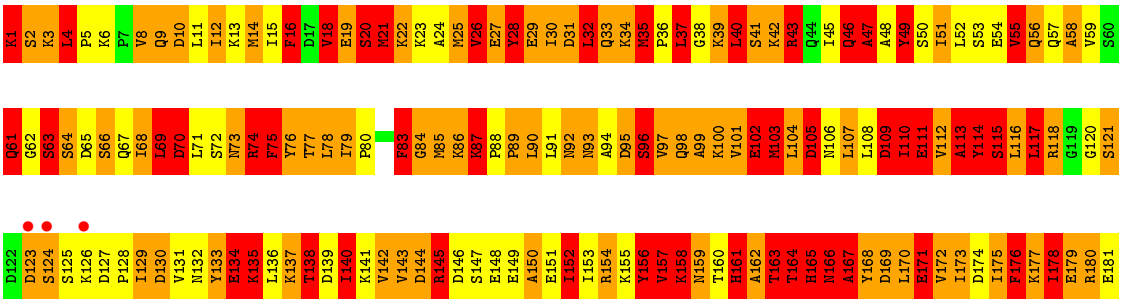
- Molecule 1: Poly [ADP-ribose] polymerase-1

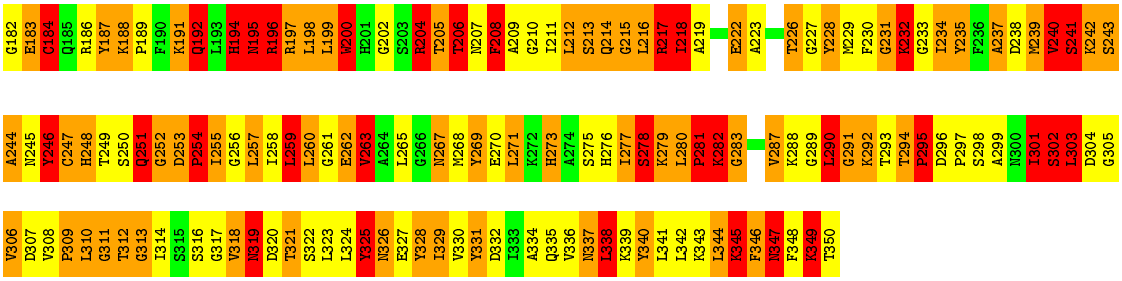
Chain A:



- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain B:




G182 E183 C184 Q185 R186 Y187 K188 P189 F190 K191 Q192 L193 H194 N195 R196 R197 L198 L199 W200 H201 G202 S203 R204 T205 T206 N207 F208 A209 G210 I211 L212 S213 Q214 G215 L216 R217 I218 A219 E222 A223 T226 G227 Y228 M229 F230 G231 K232 G233 I234 Y235 F236 A237 D238 M239 V240 S241 K242 S243
A244 N245 Y246 C247 H248 T249 S250 Q251 G252 D253 P254 I255 G256 L257 I258 L259 L260 G261 E262 V263 A264 L265 G266 N267 M268 Y269 E270 L271 K272 H273 A274 S275 H276 I277 S278 K279 L280 P281 K282 G283 V287 K288 G289 L290 G291 K292 T293 T294 P295 D296 P297 S298 A299 N300 I301 S302 L303 D304 G305
V306 D307 V308 P309 L310 G311 T312 G313 I314 S315 S316 G317 V318 N319 D320 T321 S322 L323 L324 Y325 N326 E327 Y328 I329 V330 Y331 D332 I333 A334 Q335 V336 N337 I338 K339 Y340 L341 L342 K343 L344 K345 F346 N347 F348 K349 T350

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	179.82Å 53.55Å 92.01Å 90.00° 114.40° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 95.8 (50.90-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.01Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.219 , 0.246 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 113.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5817	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: FRM

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	1.69	32/2806 (1.1%)	2.79	273/3786 (7.2%)
1	B	1.76	28/2806 (1.0%)	2.89	311/3786 (8.2%)
All	All	1.73	60/5612 (1.1%)	2.84	584/7572 (7.7%)

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	47
1	B	0	39
All	All	0	86

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	LYS	C-N	11.68	1.54	1.33
1	B	262	GLU	CD-OE2	11.28	1.38	1.25
1	B	304	ASP	CB-CG	10.02	1.72	1.51
1	B	282	LYS	C-O	-9.09	1.06	1.23
1	B	282	LYS	CA-C	8.97	1.76	1.52

The worst 5 of 584 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	ARG	NE-CZ-NH1	17.58	129.09	120.30
1	B	43	ARG	NE-CZ-NH1	-16.29	112.15	120.30
1	A	43	ARG	NE-CZ-NH1	15.72	128.16	120.30
1	A	118	ARG	NE-CZ-NH2	-14.63	112.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	204	ARG	NE-CZ-NH1	-14.05	113.27	120.30

There are no chirality outliers.

5 of 86 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	PHE	Sidechain
1	A	2	SER	Peptide
1	A	28	TYR	Sidechain
1	A	37	LEU	Peptide
1	A	39	LYS	Mainchain

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	2754	0	2798	212	0
1	B	2754	0	2798	294	0
2	A	28	0	24	2	0
2	B	28	0	24	0	0
3	A	124	0	0	11	0
3	B	129	0	0	23	0
All	All	5817	0	5644	506	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 45.

The worst 5 of 506 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:B:282:LYS:CA	1:B:282:LYS:C	1.76	1.51
1:A:138:THR:HG23	1:A:180:ARG:HB3	1.49	0.95
1:A:138:THR:HG21	1:A:212:LEU:HD23	1.52	0.90
1:B:202:GLY:HA3	1:B:243:SER:O	1.74	0.88
1:A:133:TYR:HE1	1:A:140:ILE:HG13	1.38	0.88

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	348/350 (99%)	241 (69%)	61 (18%)	46 (13%)	0 1
1	B	348/350 (99%)	235 (68%)	61 (18%)	52 (15%)	0 1
All	All	696/700 (99%)	476 (68%)	122 (18%)	98 (14%)	0 1

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	12	ILE
1	A	39	LYS
1	A	43	ARG
1	A	66	SER

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	308/308 (100%)	215 (70%)	93 (30%)	0 1
1	B	308/308 (100%)	218 (71%)	90 (29%)	0 2
All	All	616/616 (100%)	433 (70%)	183 (30%)	0 1

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ASP
1	B	27	GLU
1	B	278	SER
1	A	310	LEU
1	A	345	LYS

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

Mol	Chain	Res	Type
1	A	347	ASN
1	B	33	GLN
1	B	273	HIS
1	A	337	ASN
1	B	300	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\|>2$
2	FRM	B	502	-	30,31,31	1.63	7 (23%)	37,43,43	3.70	15 (40%)
2	FRM	A	501	-	30,31,31	1.27	2 (6%)	37,43,43	3.72	21 (56%)

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	FRM	B	502	-	-	3/10/20/20	0/4/4/4
2	FRM	A	501	-	-	4/10/20/20	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	FRM	C2-C3	-4.21	1.35	1.42
2	B	502	FRM	C29-N26	-3.86	1.42	1.46
2	A	501	FRM	C2-C3	-3.29	1.37	1.42
2	B	502	FRM	C40-C31	-3.22	1.43	1.48
2	B	502	FRM	C7-C2	-2.80	1.45	1.51

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	FRM	C4-C13-N12	-12.89	115.41	124.40
2	A	501	FRM	C11-N10-C3	10.75	124.06	115.45
2	B	502	FRM	C32-C33-N26	10.29	120.58	111.23
2	A	501	FRM	C13-C4-C3	-7.08	114.65	119.98
2	B	502	FRM	C13-C4-C3	-6.99	114.72	119.98

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FRM	C11-C17-C20-C23
2	A	501	FRM	C20-C23-N26-C29
2	B	502	FRM	C20-C23-N26-C29
2	A	501	FRM	C20-C23-N26-C33
2	B	502	FRM	C11-C17-C20-C23

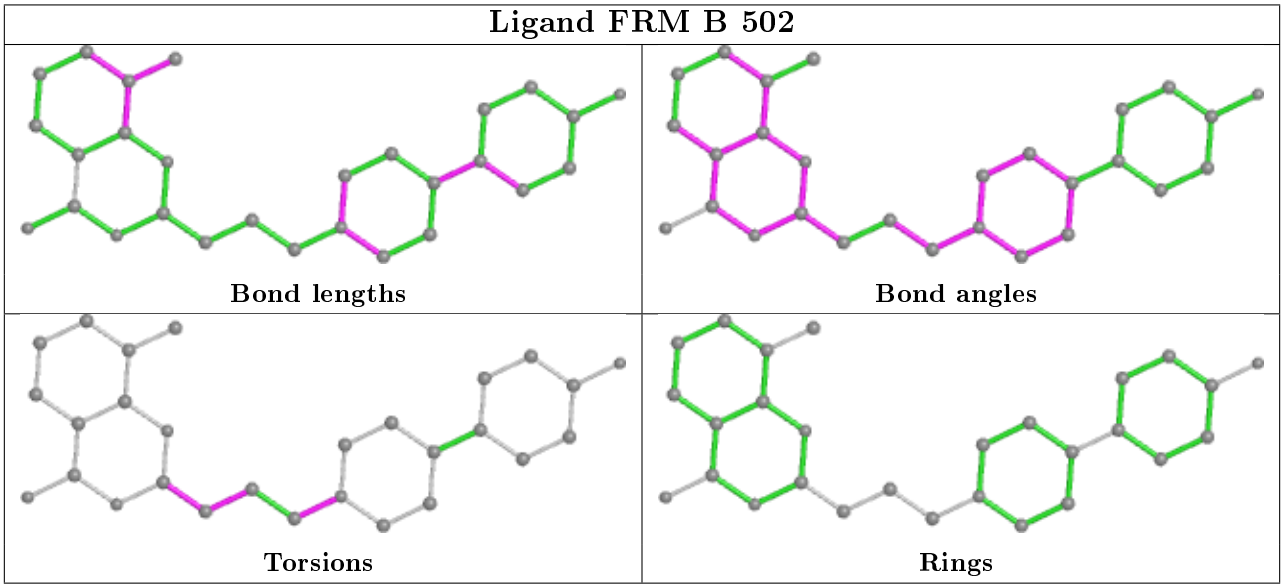
There are no ring outliers.

1 monomer is involved in 2 short contacts:

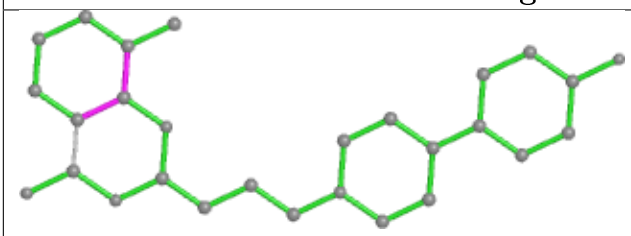
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FRM	2	0

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.

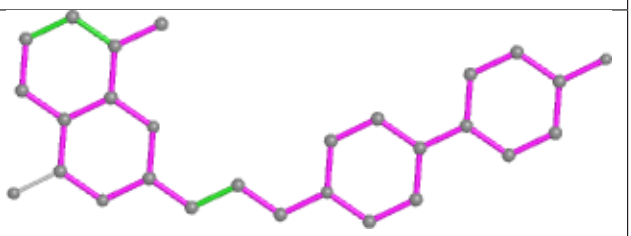
Ligand FRM B 502



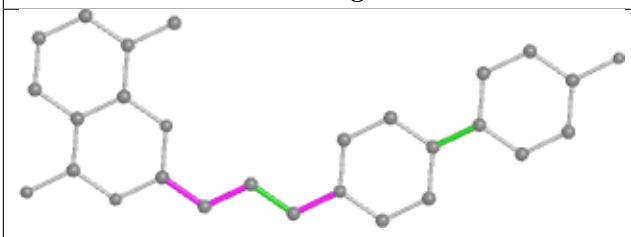
Ligand FRM A 501



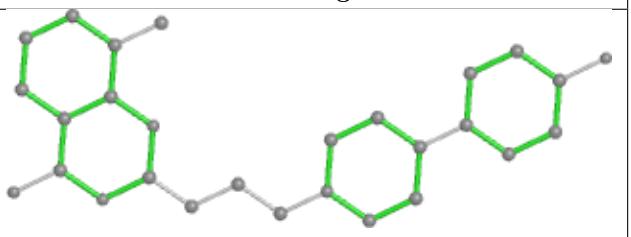
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	350/350 (100%)	-0.44	2 (0%)	89	72	2, 10, 26, 38	0
1	B	350/350 (100%)	-0.31	3 (0%)	84	63	3, 12, 28, 43	0
All	All	700/700 (100%)	-0.37	5 (0%)	87	69	2, 11, 27, 43	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	SER	3.3
1	A	125	SER	2.3
1	A	2	SER	2.2
1	B	123	ASP	2.1
1	B	126	LYS	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

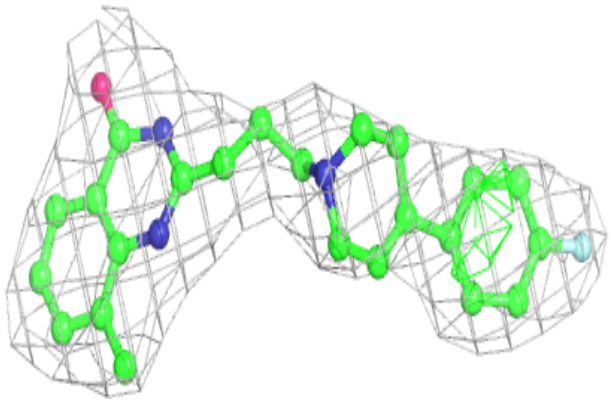
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

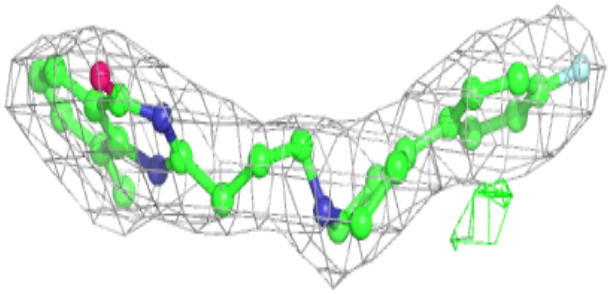
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FRM	A	501	28/28	0.96	0.16	2,7,16,17	0
2	FRM	B	502	28/28	0.97	0.15	2,2,6,9	0

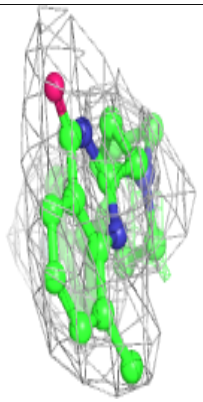
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FRM 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)

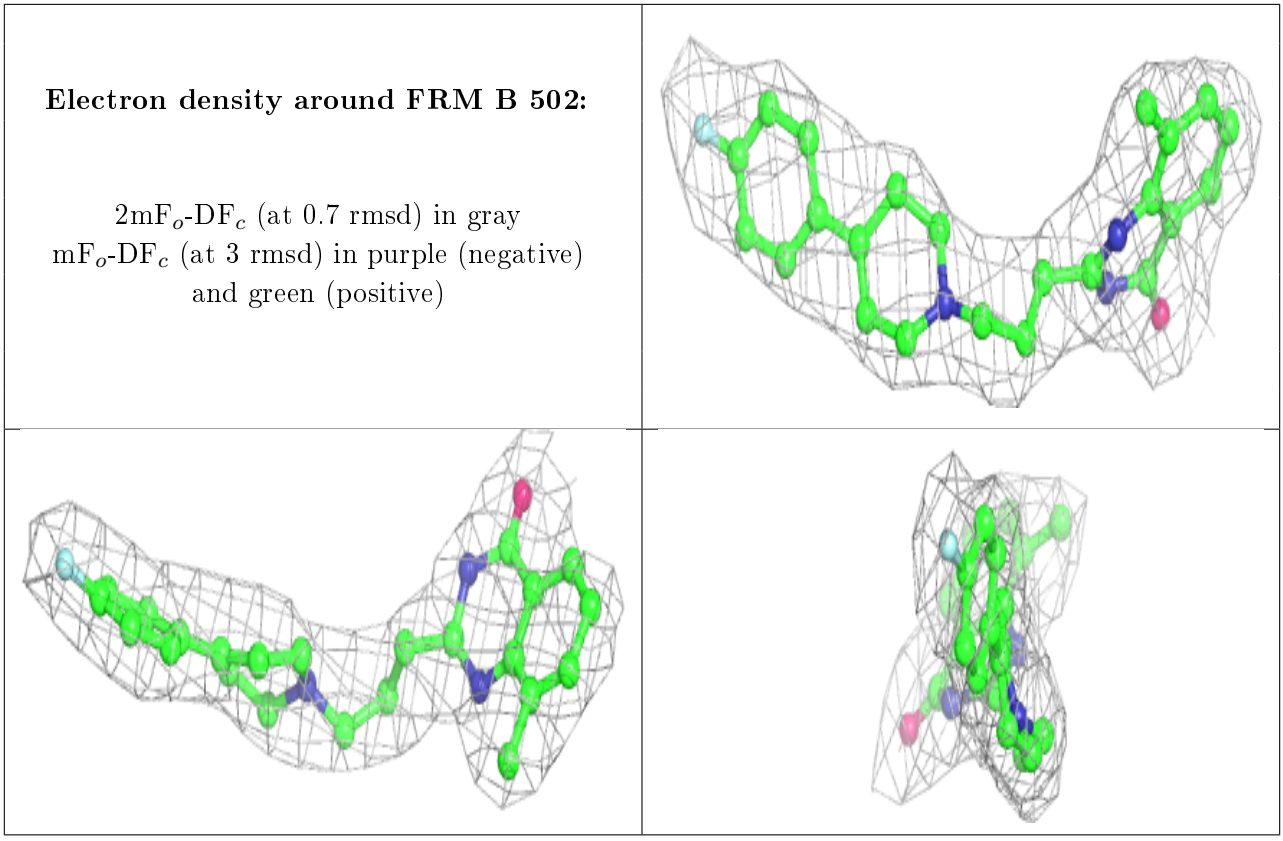






Electron density around FRM B 502:

$2mF_o$-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

There are no such residues in this entry.