wwPDB X-ray Structure Validation Summary Report (i)

Oct 9, 2023 – 10:28 PM EDT

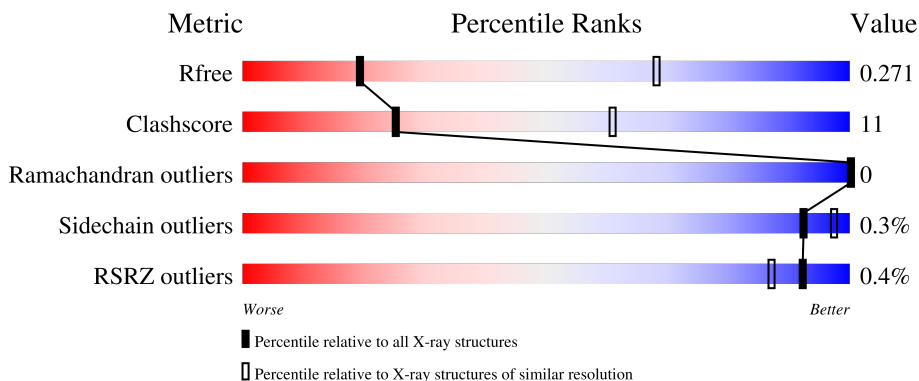|		
PDB ID	:	7RY1
Title	:	human Hsp90_MC domain structure
Authors	:	Peng, S.; Deng, J.; Matts, R.
Deposited on	:	2021-08-24
Resolution	:	3.52 Å(reported)

1 Overall quality at a glance ⓘ

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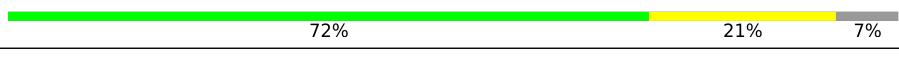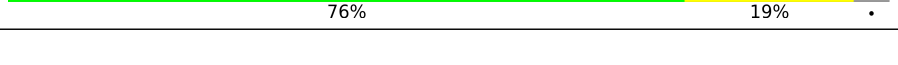*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.52 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	Percentile Ranks	Value
Rfree		0.271
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		0.3%
RSRZ outliers		0.4%

Worse .... *Better*

▌ 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}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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	425	73% 22% 5%
1	B	425	72% 21% 7%
1	C	425	76% 19% •

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
2	MDC	B	801	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10033 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 Heat shock protein HSP 90-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	1	0	0
			3340	2120	568	635	17			
1	B	396	Total	C	N	O	S	1	0	0
			3264	2072	555	620	17			
1	C	406	Total	C	N	O	S	1	0	0
			3345	2124	569	634	18			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	GLY	-	expression tag	UNP P07900
A	291	HIS	-	expression tag	UNP P07900
A	292	MET	-	expression tag	UNP P07900
B	290	GLY	-	expression tag	UNP P07900
B	291	HIS	-	expression tag	UNP P07900
B	292	MET	-	expression tag	UNP P07900
C	290	GLY	-	expression tag	UNP P07900
C	291	HIS	-	expression tag	UNP P07900
C	292	MET	-	expression tag	UNP P07900

- Molecule 2 is N-[2-(1-MALEIMIDYL)ETHYL]-7-DIETHYLAMINOCOUMARIN-3-C ARBOXAMIDE (three-letter code: MDC) (formula: $C_{20}H_{21}N_3O_5$) (labeled as "Ligand of Interest" by depositor).

MDC
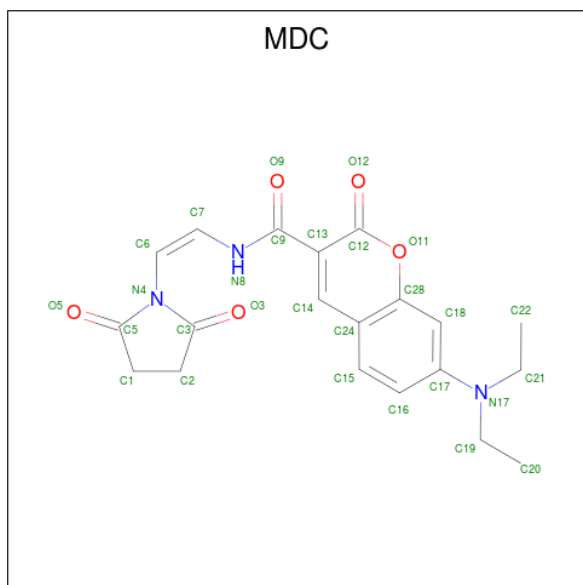
| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	20	3	5		
2	B	1	Total	C	N	O	0	0
			28	20	3	5		
2	C	1	Total	C	N	O	0	0
			28	20	3	5		

3 Residue-property plots ⓘ

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.
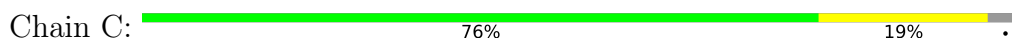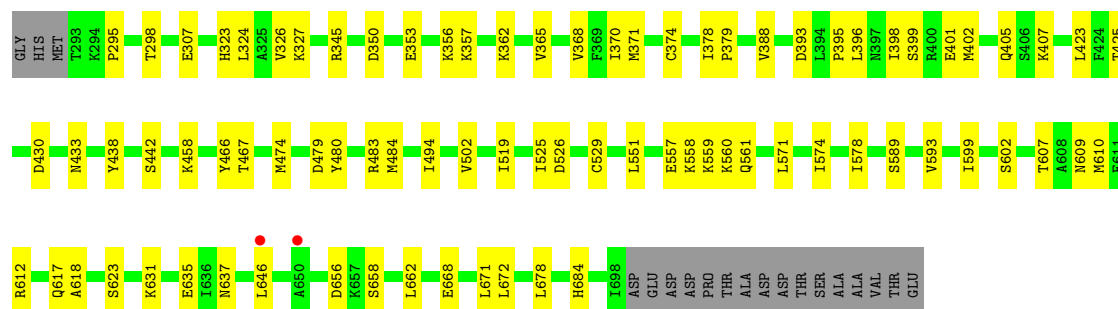
• Molecule 1: Heat shock protein HSP 90-alpha
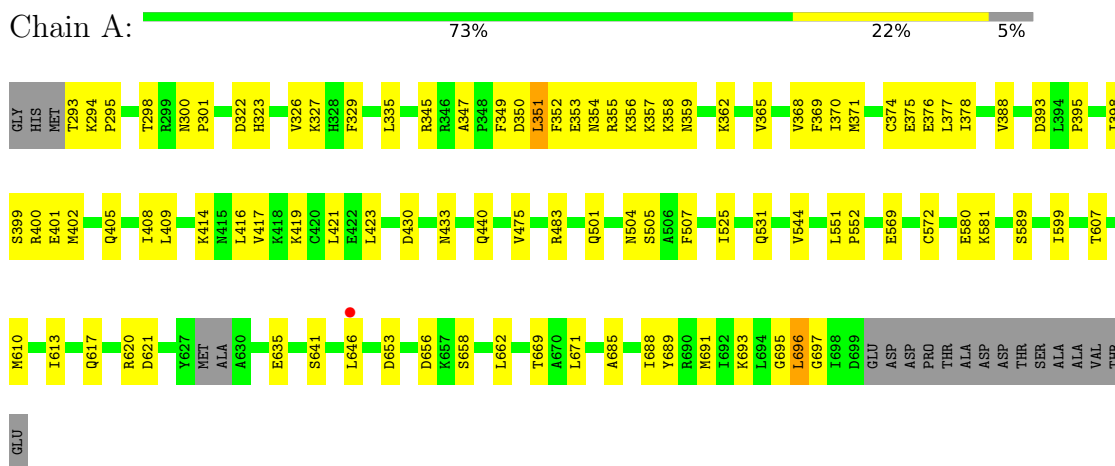
Chain A:

• Molecule 1: Heat shock protein HSP 90-alpha

Chain B:

• Molecule 1: Heat shock protein HSP 90-alpha

Chain C:
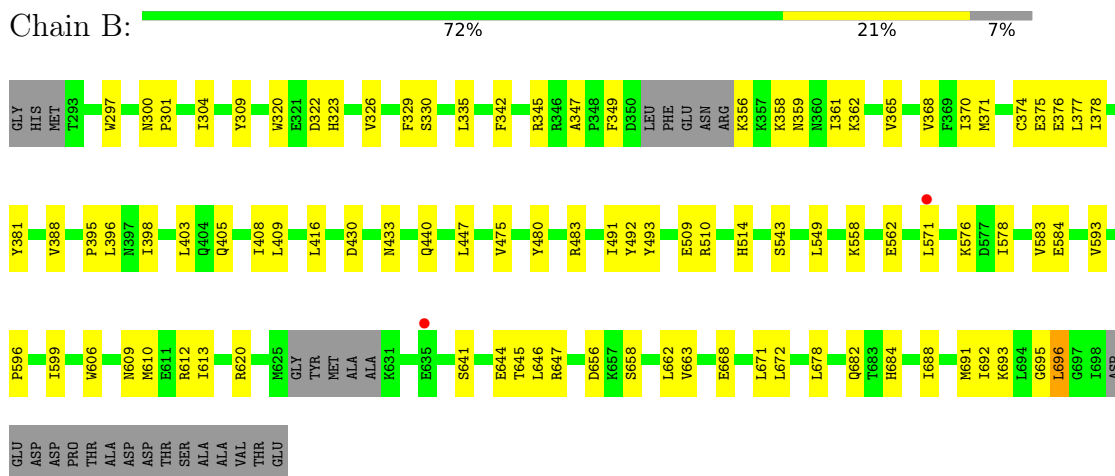
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	159.85Å 311.96Å 88.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.42 – 3.52 48.52 – 3.52	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.42-3.52) 92.9 (48.52-3.52)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.216 , 0.272 0.217 , 0.271	Depositor DCC
R_{free} test set	2000 reflections (7.29%)	wwPDB-VP
Wilson B-factor (Å^2)	117.1	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 75.3	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10033	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.26	0/3395	0.51	1/4558 (0.0%)
1	B	0.28	0/3316	0.49	0/4450
1	C	0.27	0/3401	0.52	0/4567
All	All	0.27	0/10112	0.51	1/13575 (0.0%)

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	C	0	1

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	351	LEU	CA-CB-CG	5.63	128.24	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	371	MET	Peptide

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	3340	0	3384	95	1
1	B	3264	0	3317	82	1
1	C	3345	0	3395	61	0
2	A	28	0	19	5	0
2	B	28	0	20	8	0
2	C	28	0	19	5	0
All	All	10033	0	10154	215	1

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 11.

The worst 5 of 215 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:374:CYS:HA	2:B:801:MDC:H22	1.26	1.09
1:A:696:LEU:HD12	1:A:697:GLY:N	1.72	1.05
1:A:352:PHE:HD2	1:A:354:ASN:HB3	1.24	1.00
1:A:354:ASN:OD1	1:A:356:LYS:CB	2.09	0.99
1:A:354:ASN:OD1	1:A:356:LYS:N	1.98	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:ASP:OD1	1:B:330:SER:OG[8_446]	2.02	0.18

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	401/425 (94%)	386 (96%)	15 (4%)	0	100	100
1	B	390/425 (92%)	374 (96%)	16 (4%)	0	100	100
1	C	404/425 (95%)	378 (94%)	26 (6%)	0	100	100
All	All	1195/1275 (94%)	1138 (95%)	57 (5%)	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	376/391 (96%)	375 (100%)	1 (0%)	92	97
1	B	369/391 (94%)	368 (100%)	1 (0%)	92	97
1	C	376/391 (96%)	375 (100%)	1 (0%)	92	97
All	All	1121/1173 (96%)	1118 (100%)	3 (0%)	92	97

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

Mol	Chain	Res	Type
1	A	696	LEU
1	B	696	LEU
1	C	551	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 ⓘ

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

There are no bond length outliers.
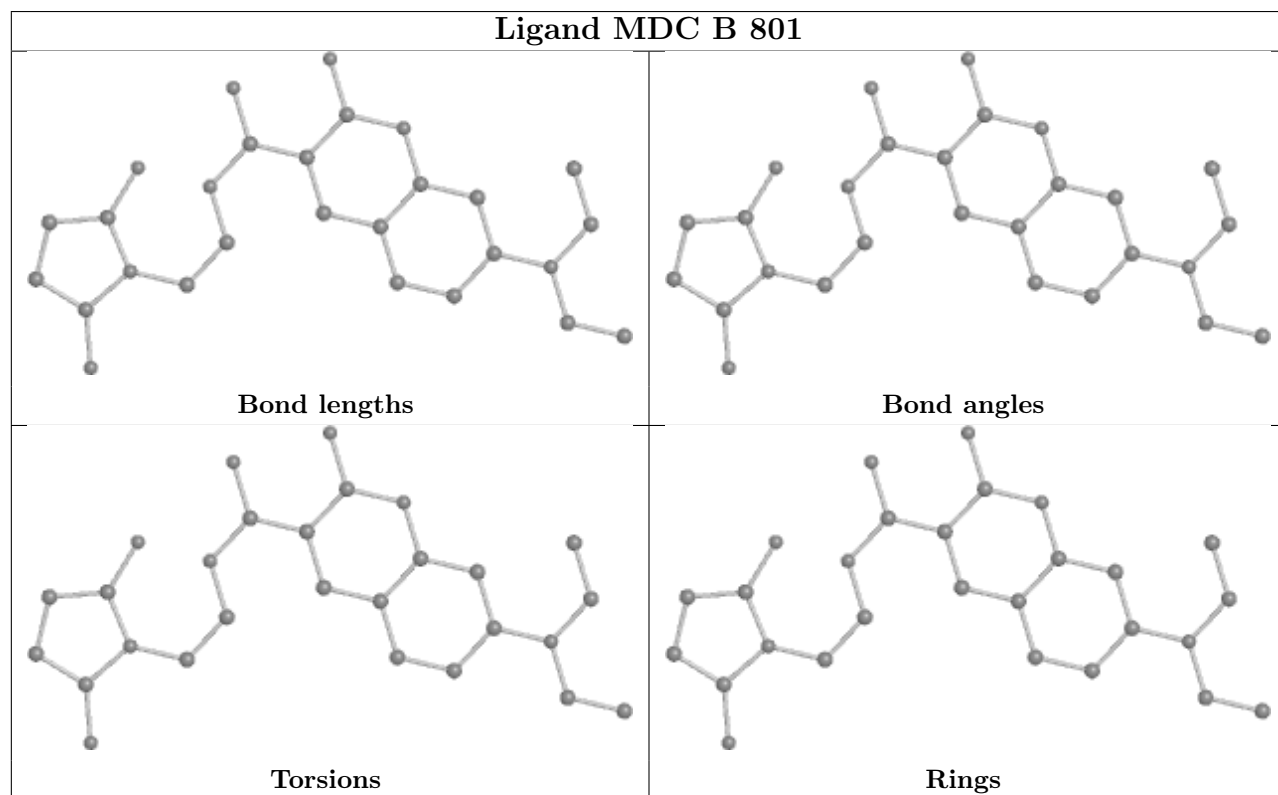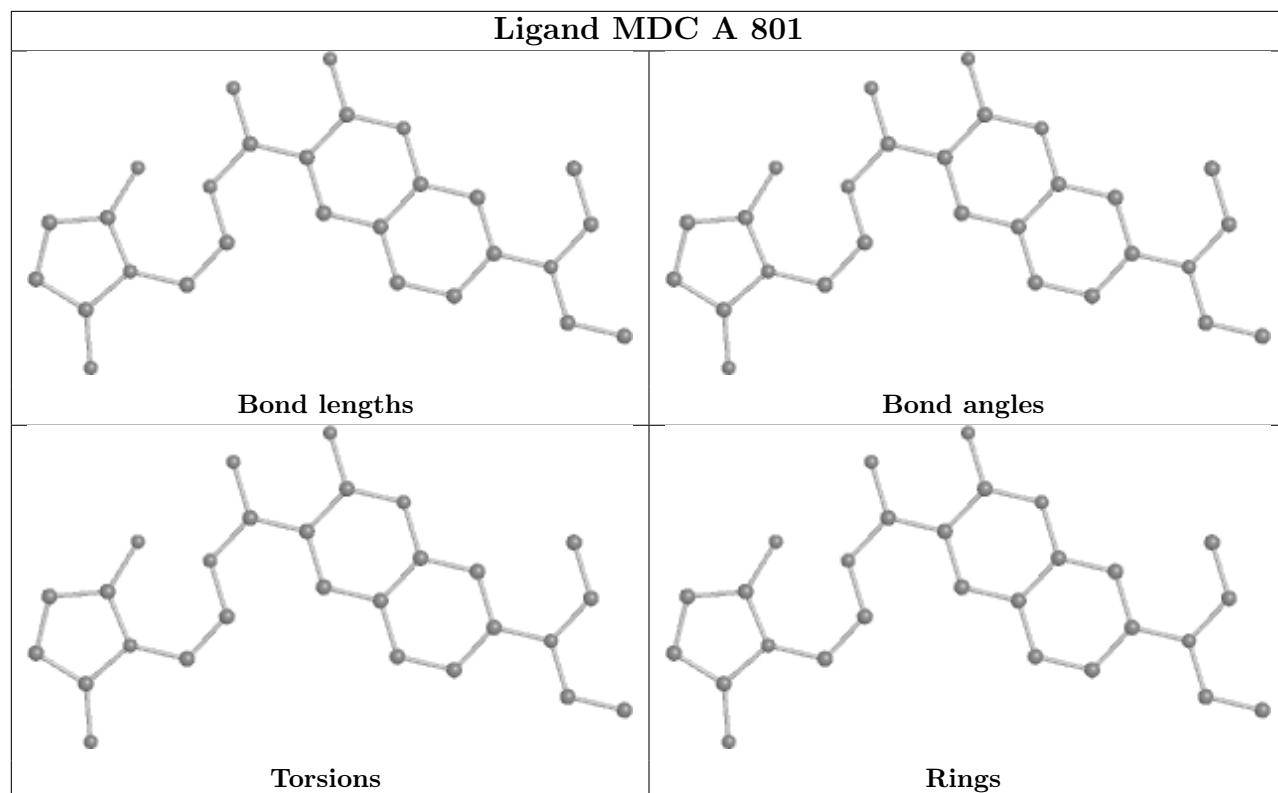
There are no bond angle outliers.
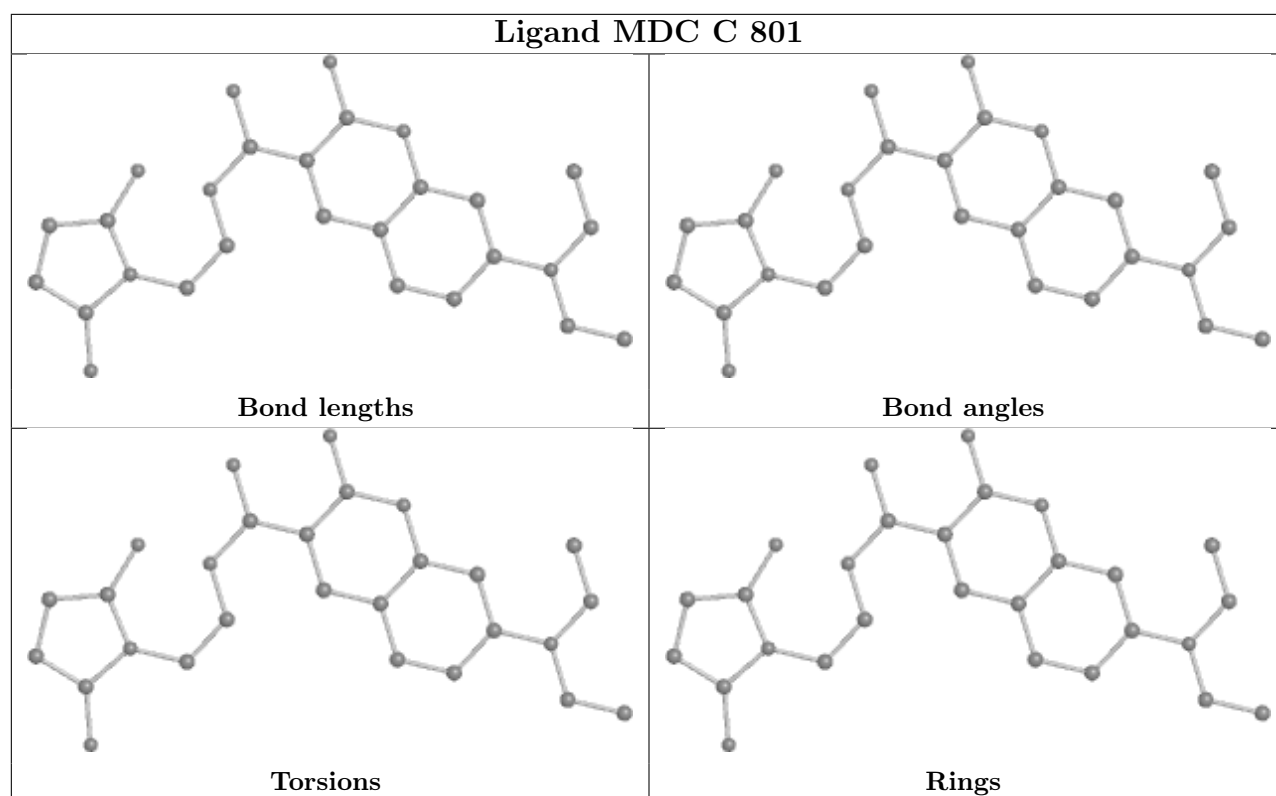
There are no chirality outliers.

There are no torsion outliers.

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 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 MDC A 801

Bond lengths

Bond angles

Torsions

Rings

Ligand MDC B 801

Bond lengths

Bond angles

Torsions

Rings

Ligand MDC C 801

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, 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(Å²)	Q<0.9
1	A	405/425 (95%)	-0.21	1 (0%)	95	91	78, 138, 222, 272	1 (0%)
1	B	396/425 (93%)	-0.21	2 (0%)	91	84	76, 138, 222, 286	1 (0%)
1	C	406/425 (95%)	-0.26	2 (0%)	91	84	84, 130, 211, 313	1 (0%)
All	All	1207/1275 (94%)	-0.22	5 (0%)	92	87	76, 135, 220, 313	3 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	650	ALA	2.3
1	C	646	LEU	2.2
1	A	646	LEU	2.2
1	B	635	GLU	2.2
1	B	571	LEU	2.0

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

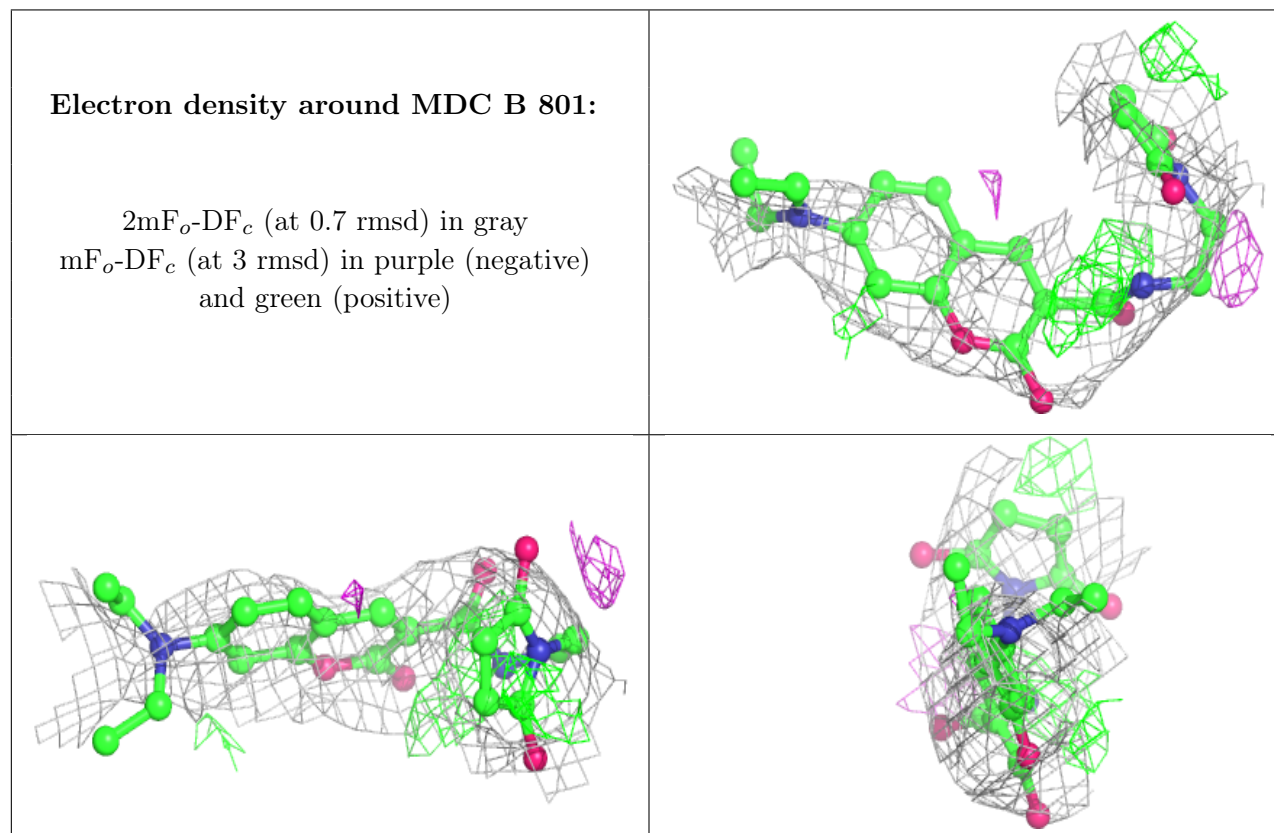There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 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
2	MDC	B	801	28/28	0.69	0.45	188,208,223,235	0
2	MDC	A	801	28/28	0.81	0.32	162,173,200,207	0
2	MDC	C	801	28/28	0.82	0.31	116,162,173,174	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.
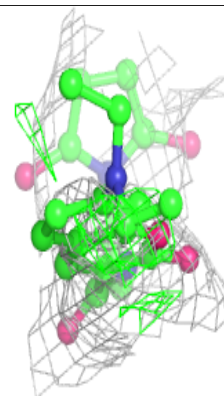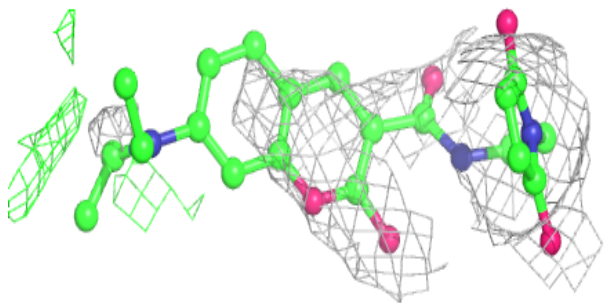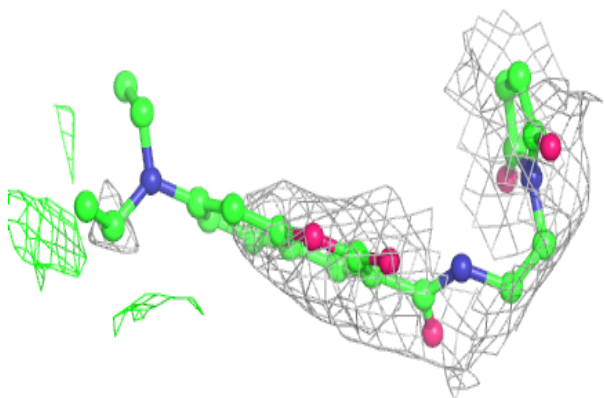

Electron density around MDC B 801:

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

Electron density around MDC A 801:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
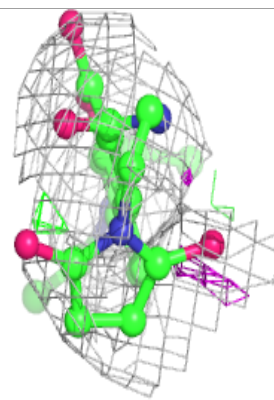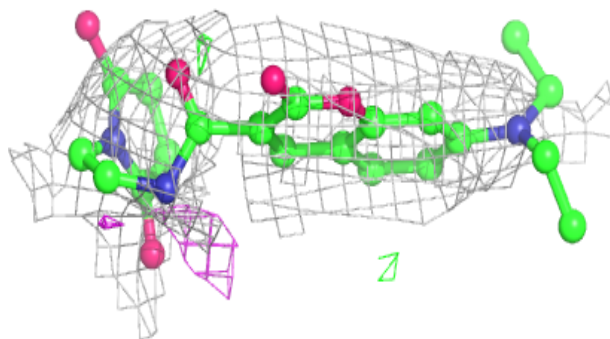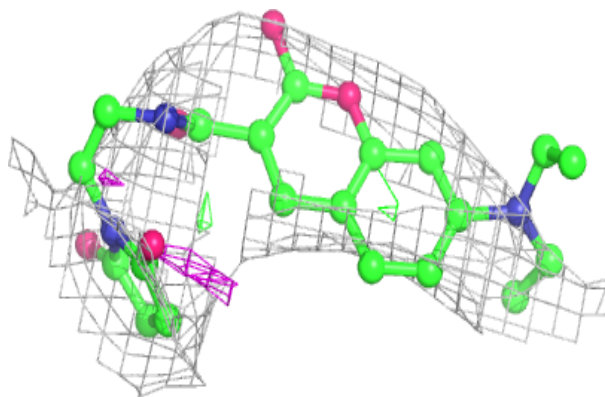
Electron density around MDC C 801:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.