WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 14, 2024 – 12:05 pm GMT

PDB ID	:	6SKQ
Title	:	OXA-655_MEM. Structural insights into the enhanced carbapenemase efficiency of OXA-655 compared to OXA-10.
Authors	:	Leiros, H.-K.S.
Deposited on	:	2019-08-16
Resolution	:	2.10 Å(reported)

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

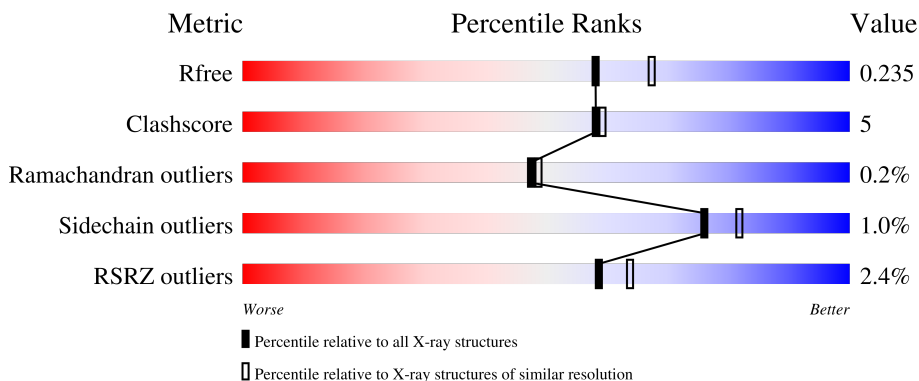|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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		0.235
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		1.0%
RSRZ outliers		2.4%

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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.

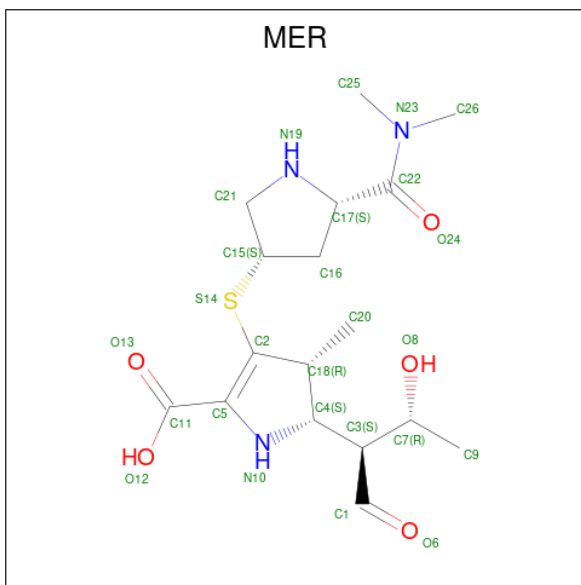| Mol	Chain	Length	Quality of chain
1	A	266	2% / 83% / 9% / 8%
1	B	266	2% / 79% / 12% / · / 8%
1	C	266	3% / 82% / 10% / 8%
1	D	266	.% / 83% / 8% / · / 8%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 16812 atoms, of which 7892 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 Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	245	Total	C	H	N	O	S	15	2	0
			3887	1246	1938	326	370	7			
1	B	245	Total	C	H	N	O	S	5	2	0
			3894	1247	1945	327	368	7			
1	C	245	Total	C	H	N	O	S	0	4	0
			3905	1251	1948	327	371	8			
1	D	245	Total	C	H	N	O	S	0	0	0
			3871	1241	1931	325	367	7			

- Molecule 2 is (4R,5S)-3-{[(3S,5S)-5-(dimethylcarbamoyl)pyrrolidin-3-yl]sulfanyl}-5-[(2S,3R)-3-hydroxy-1-oxobutan-2-yl]-4-methyl-4,5-d ihydro-1H-pyrrole-2-carboxylic acid (three-letter code: MER) (formula: $C_{17}H_{27}N_3O_5S$) (labeled as "Ligand of Interest" by depositor).
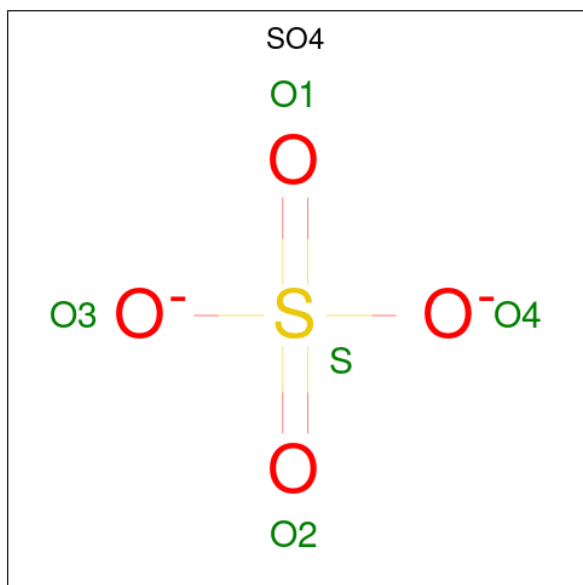

MER

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	1
			104	34	52	6	10	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	S	0	0
			52	17	26	3	5	1		
2	C	1	Total	C	H	N	O	S	0	0
			52	17	26	3	5	1		
2	D	1	Total	C	H	N	O	S	0	0
			52	17	26	3	5	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	239	Total	O	0	0
			239	239		

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	243	Total 243	O 243	0	0
4	C	225	Total 225	O 225	0	0
4	D	263	Total 263	O 263	0	0

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.
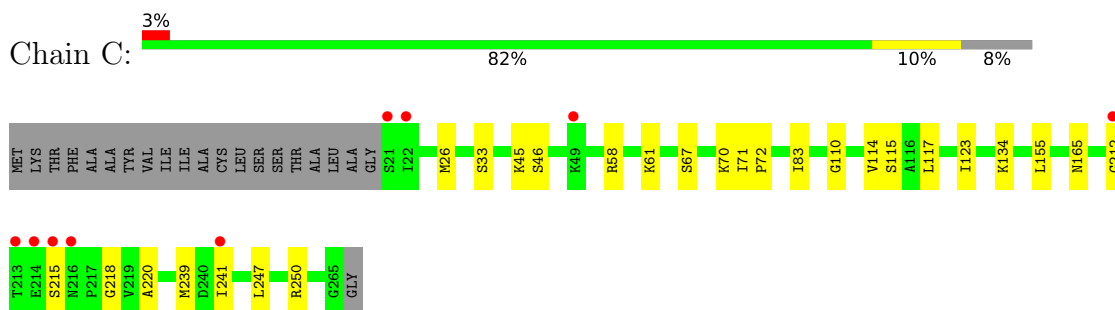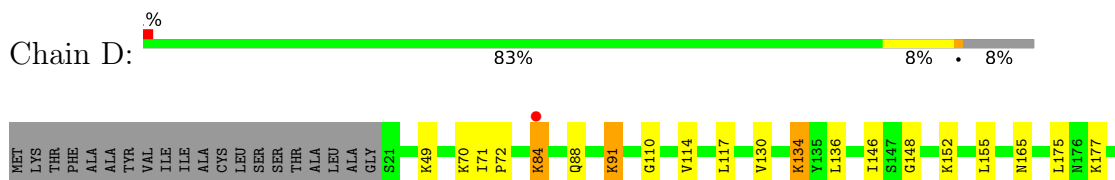
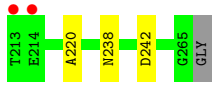• Molecule 1: Beta-lactamase
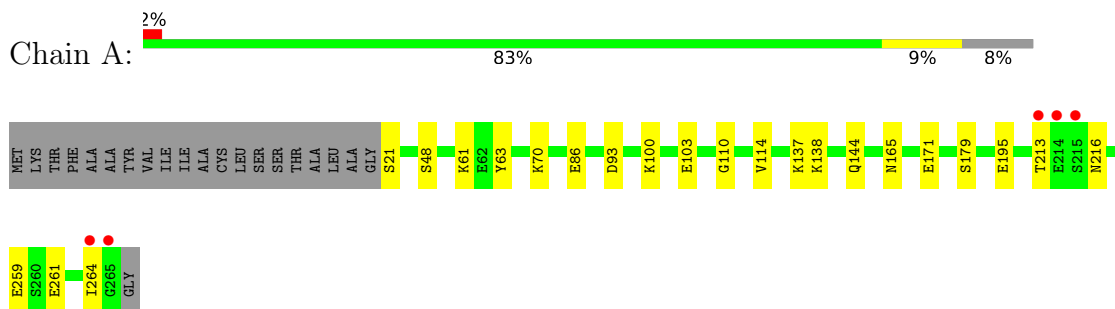
Chain A:

• Molecule 1: Beta-lactamase

Chain B:

• Molecule 1: Beta-lactamase

Chain C:

• Molecule 1: Beta-lactamase

Chain D:
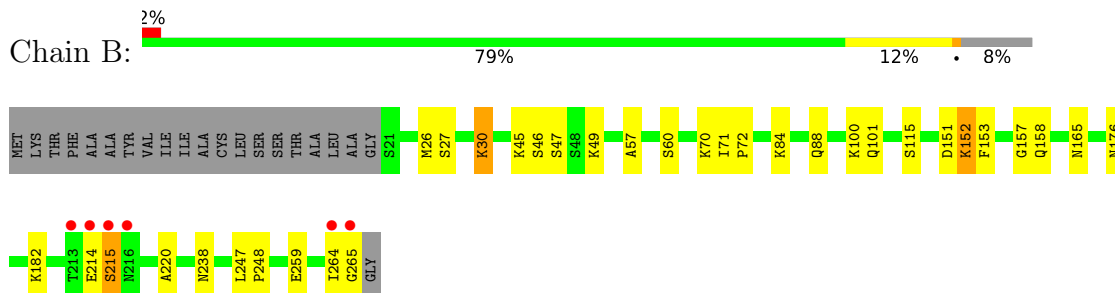
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.14Å 82.44Å 99.00Å 90.00° 97.01° 90.00°	Depositor
Resolution (Å)	24.05 – 2.10 24.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (24.05-2.10) 97.2 (24.05-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.14_3260, PHENIX 1.14_3260	Depositor
R, R_{free}	0.179 , 0.235 0.179 , 0.235	Depositor DCC
R_{free} test set	2426 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 52.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16812	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.28	0/1990	0.47	0/2687
1	B	0.33	1/1993 (0.1%)	0.48	0/2691
1	C	0.28	0/1998	0.47	0/2697
1	D	0.56	2/1968 (0.1%)	0.51	1/2657 (0.0%)
All	All	0.38	3/7949 (0.0%)	0.48	1/10732 (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	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	LYS	CE-NZ	-18.75	1.02	1.49
1	B	100	LYS	CE-NZ	-7.42	1.30	1.49
1	D	134	LYS	CD-CE	-5.04	1.38	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	LYS	CD-CE-NZ	-8.02	93.25	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	214	GLU	Peptide
1	B	215	SER	Peptide

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	1949	1938	1928	17	0
1	B	1949	1945	1933	18	0
1	C	1957	1948	1934	18	1
1	D	1940	1931	1931	15	0
2	A	52	52	50	3	0
2	B	26	26	25	2	0
2	C	26	26	25	4	0
2	D	26	26	25	0	0
3	A	5	0	0	0	0
3	B	10	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	239	0	0	10	0
4	B	243	0	0	7	2
4	C	225	0	0	6	1
4	D	263	0	0	5	1
All	All	8920	7892	7851	75	3

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 5.

The worst 5 of 75 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:86:GLU:OE1	4:A:401:HOH:O	1.91	0.86
1:C:134:LYS:NZ	4:C:402:HOH:O	2.09	0.83
2:A:301[B]:MER:O24	4:A:402:HOH:O	1.96	0.82
1:C:215:SER:O	4:C:401:HOH:O	2.00	0.79
1:A:261:GLU:OE2	4:A:403:HOH:O	2.03	0.77

All (3) 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)
4:B:466:HOH:O	4:C:573:HOH:O[1_655]	2.09	0.11
4:D:452:HOH:O	4:D:628:HOH:O[2_545]	2.13	0.07
1:C:33:SER:O	4:B:401:HOH:O[1_455]	2.14	0.06

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	244/266 (92%)	236 (97%)	7 (3%)	1 (0%)	34	32
1	B	244/266 (92%)	235 (96%)	8 (3%)	1 (0%)	34	32
1	C	246/266 (92%)	237 (96%)	9 (4%)	0	100	100
1	D	242/266 (91%)	234 (97%)	8 (3%)	0	100	100
All	All	976/1064 (92%)	942 (96%)	32 (3%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	ILE
1	B	215	SER

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	211/223 (95%)	210 (100%)	1 (0%)	88	92
1	B	211/223 (95%)	207 (98%)	4 (2%)	57	63
1	C	213/223 (96%)	211 (99%)	2 (1%)	78	84
1	D	209/223 (94%)	208 (100%)	1 (0%)	88	92
All	All	844/892 (95%)	836 (99%)	8 (1%)	76	84

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	165	ASN
1	C	165	ASN
1	B	165	ASN
1	B	152	LYS
1	C	115	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	87	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	#$|Z| > 2$
1	KCX	C	70	1	9,11,12	0.86	0	5,12,14	1.27	1 (20%)
1	KCX	B	70	1	9,11,12	0.87	0	5,12,14	1.46	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	KCX	D	70	1	9,11,12	0.87	0	5,12,14	1.54	1 (20%)
1	KCX	A	70	1	9,11,12	0.90	0	5,12,14	1.58	1 (20%)

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
1	KCX	C	70	1	-	0/9/10/12	-
1	KCX	B	70	1	-	0/9/10/12	-
1	KCX	D	70	1	-	0/9/10/12	-
1	KCX	A	70	1	-	0/9/10/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	KCX	OQ1-CX-NZ	-3.38	119.72	124.96
1	D	70	KCX	OQ1-CX-NZ	-3.36	119.74	124.96
1	B	70	KCX	OQ1-CX-NZ	-3.05	120.24	124.96
1	C	70	KCX	OQ1-CX-NZ	-2.73	120.72	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	MER	C	301	1	24,27,27	3.91	11 (45%)	17,39,39	1.21	3 (17%)
2	MER	A	301[A]	1	24,27,27	3.96	13 (54%)	17,39,39	1.50	4 (23%)
3	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.05	0
2	MER	D	301	1	24,27,27	3.94	11 (45%)	17,39,39	1.62	4 (23%)
2	MER	A	301[B]	1	24,27,27	3.89	11 (45%)	17,39,39	1.91	6 (35%)
3	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	D	302	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	303	-	4,4,4	0.15	0	6,6,6	0.06	0
2	MER	B	301	1	24,27,27	3.91	13 (54%)	17,39,39	1.79	6 (35%)
3	SO4	C	302	-	4,4,4	0.14	0	6,6,6	0.06	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	MER	C	301	1	-	8/23/51/51	0/2/2/2
2	MER	A	301[A]	1	-	8/23/51/51	0/2/2/2
2	MER	D	301	1	-	7/23/51/51	0/2/2/2
2	MER	A	301[B]	1	-	10/23/51/51	0/2/2/2
2	MER	B	301	1	-	9/23/51/51	0/2/2/2

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	MER	C16-C15	-9.29	1.28	1.52
2	A	301[A]	MER	C16-C15	-9.28	1.28	1.52
2	B	301	MER	C16-C15	-9.28	1.28	1.52
2	D	301	MER	C16-C15	-9.25	1.28	1.52
2	A	301[B]	MER	C16-C15	-8.90	1.29	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	MER	C11-C5-N10	3.90	125.29	120.38
2	D	301	MER	C11-C5-N10	3.89	125.28	120.38
2	A	301[B]	MER	C16-C17-C22	3.85	119.53	111.53
2	A	301[B]	MER	C11-C5-N10	3.57	124.88	120.38
2	A	301[B]	MER	C22-C17-N19	-3.15	106.04	111.74

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301[A]	MER	C7-C3-C4-C18
2	A	301[A]	MER	C1-C3-C7-O8
2	A	301[A]	MER	C1-C3-C7-C9
2	A	301[A]	MER	C4-C3-C7-O8
2	A	301[A]	MER	O12-C11-C5-C2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	MER	4	0
2	A	301[A]	MER	1	0
2	A	301[B]	MER	2	0
3	B	303	SO4	1	0
2	B	301	MER	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.
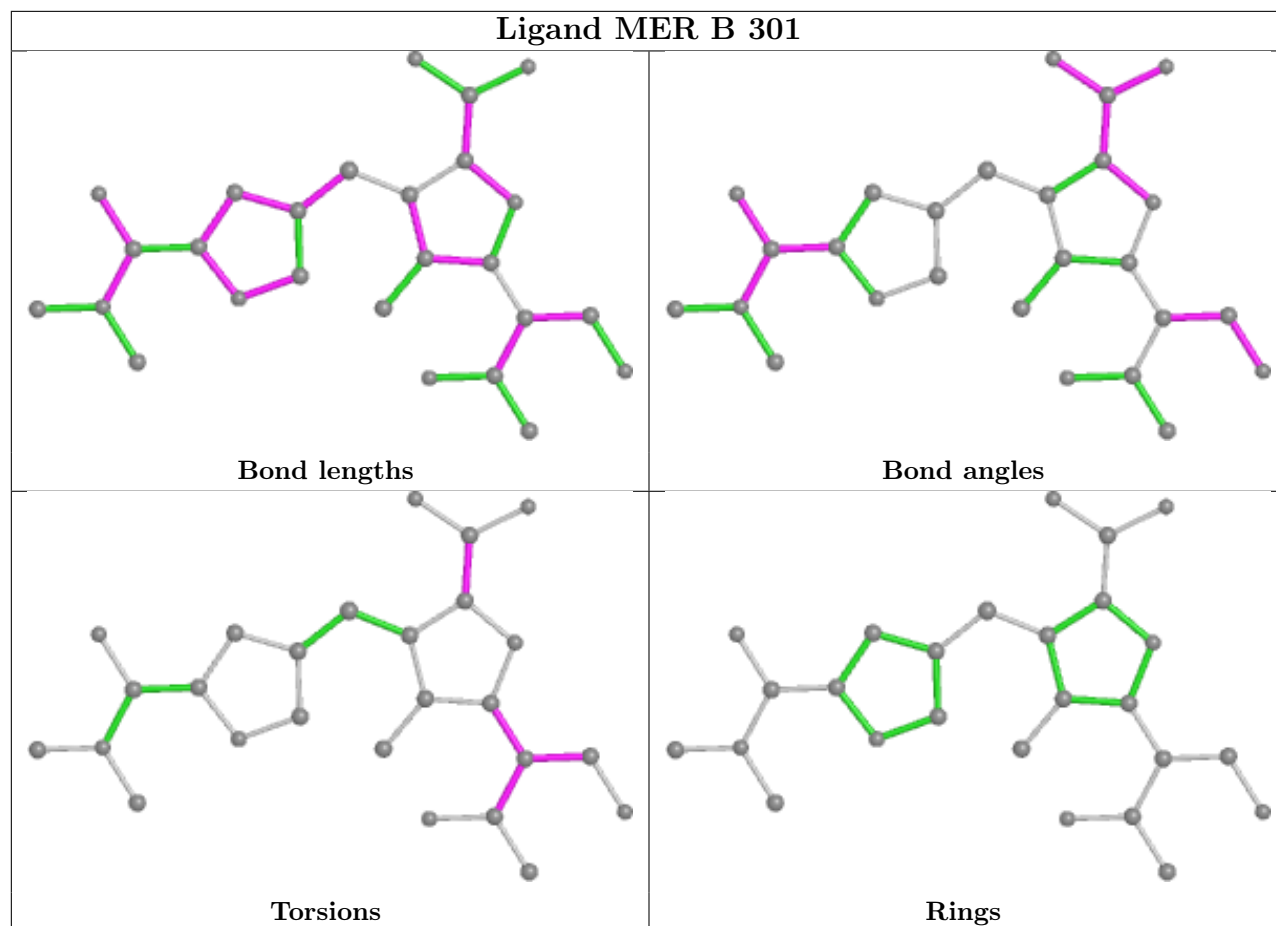
Ligand MER C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand MER A 301 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand MER D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand MER A 301 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand MER B 301

Bond lengths

Bond angles

Torsions

Rings
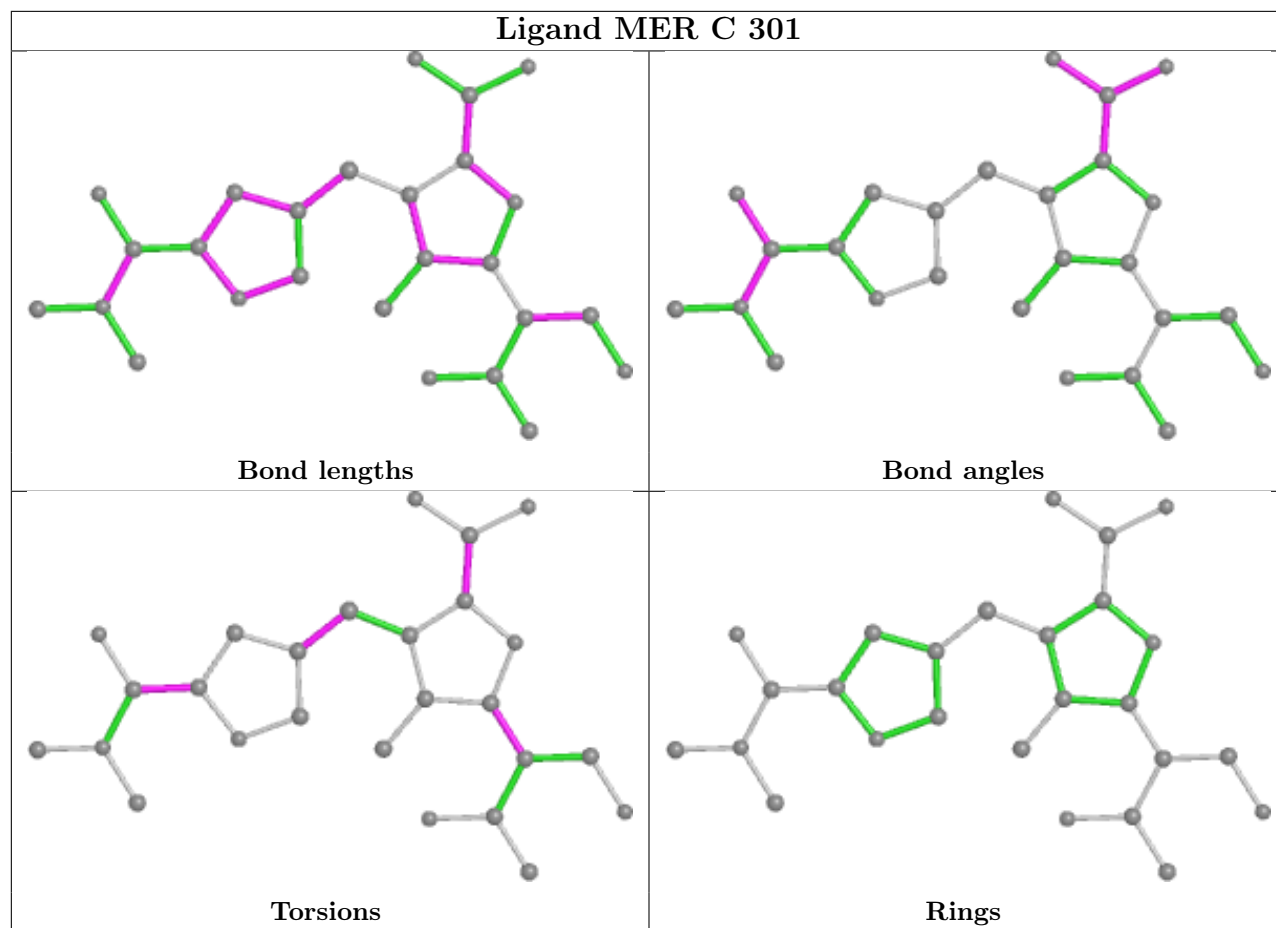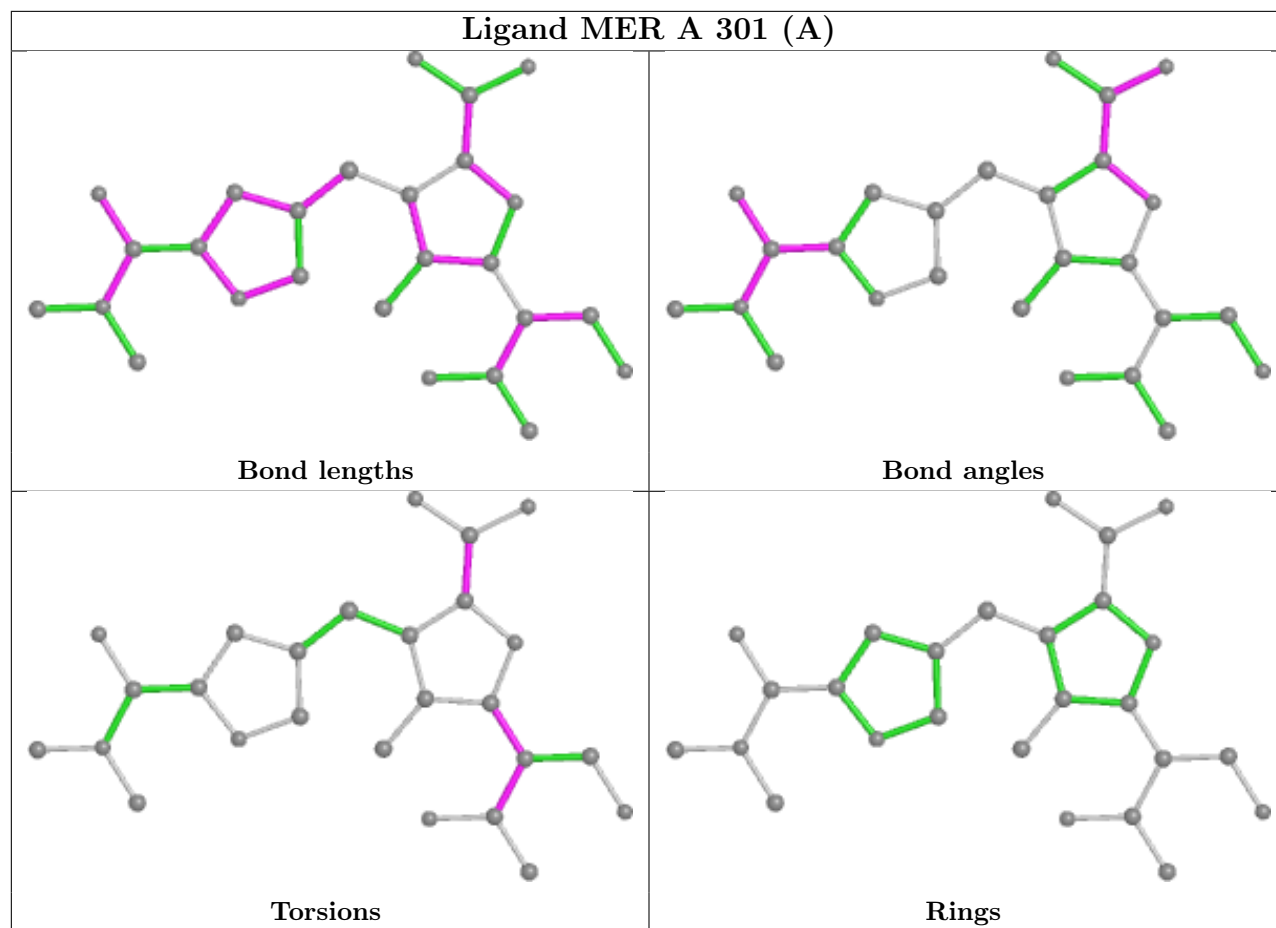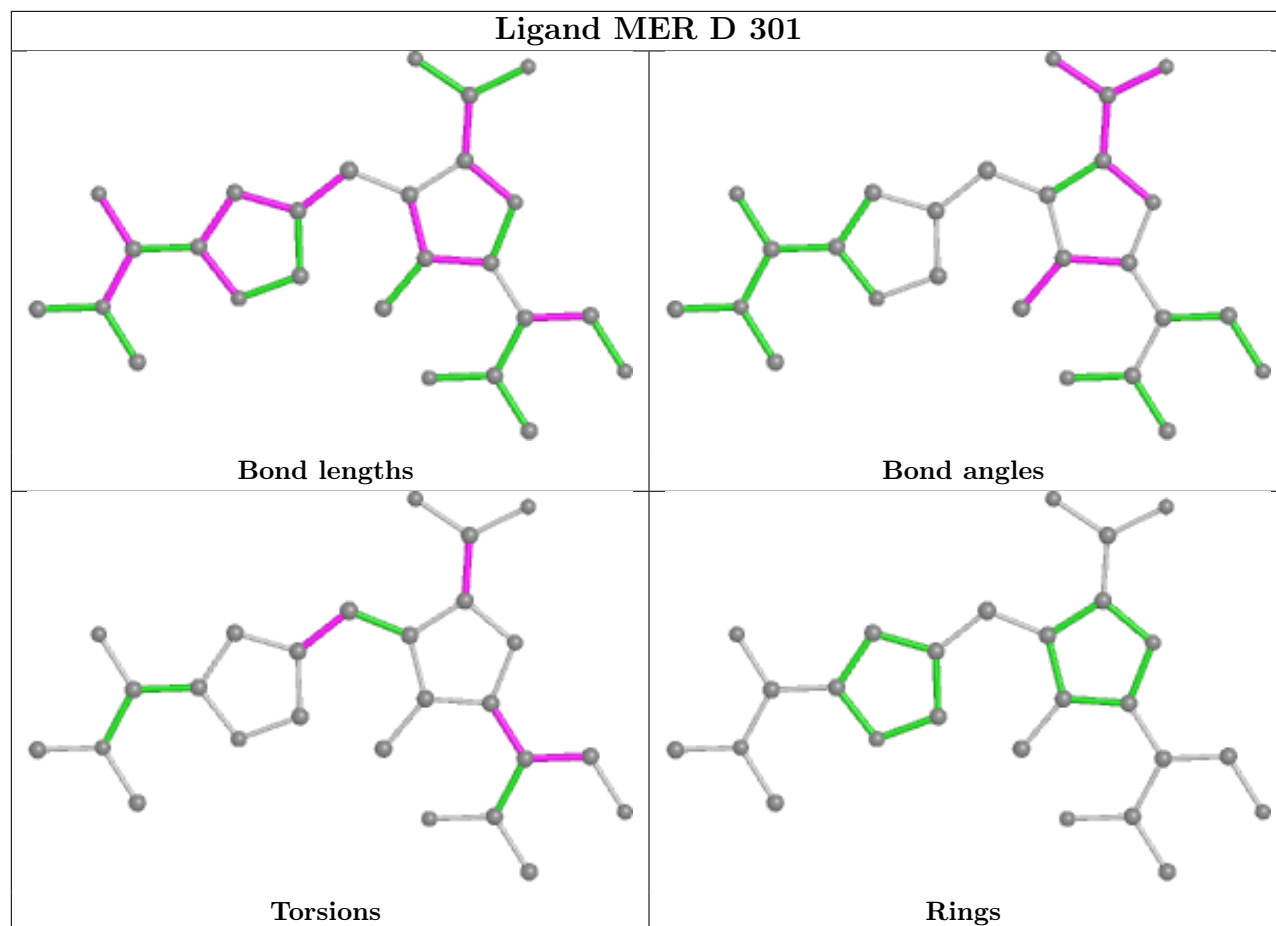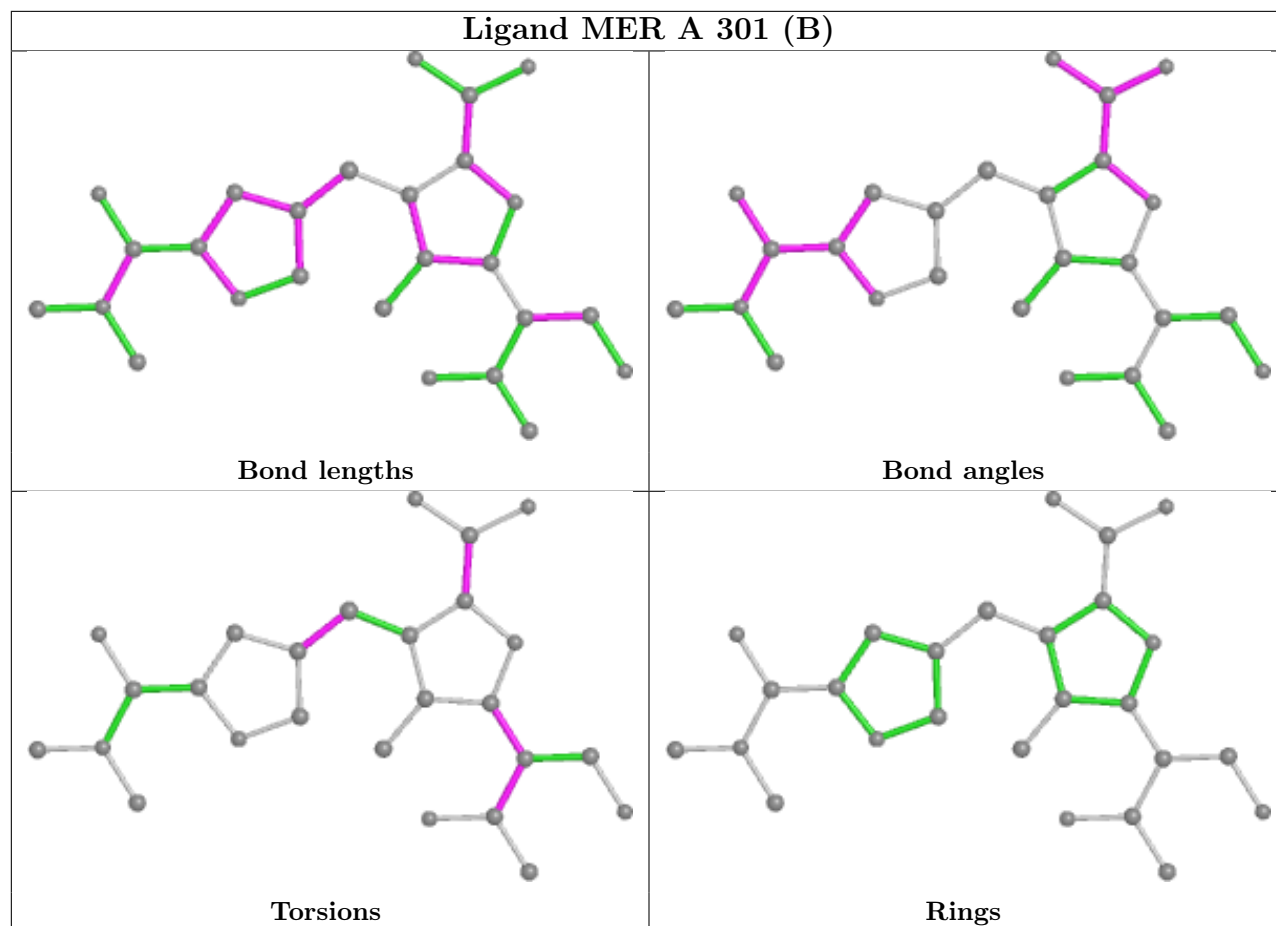
5.7 Other polymers ⓘ

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(Å^2)	Q<0.9
1	A	244/266 (91%)	-0.16	5 (2%)	65	69	8, 17, 34, 71	2 (0%)
1	B	244/266 (91%)	-0.13	6 (2%)	57	62	8, 18, 35, 59	0
1	C	244/266 (91%)	-0.14	9 (3%)	41	48	10, 18, 39, 95	0
1	D	244/266 (91%)	-0.23	3 (1%)	79	82	9, 17, 34, 67	0
All	All	976/1064 (91%)	-0.17	23 (2%)	59	64	8, 18, 37, 95	2 (0%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	GLY	5.8
1	C	215	SER	5.8
1	B	215	SER	3.9
1	C	21	SER	3.7
1	C	214	GLU	3.7

## 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, 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
1	KCX	B	70	12/13	0.96	0.15	8,14,19,19	0
1	KCX	D	70	12/13	0.96	0.13	9,14,17,17	0
1	KCX	C	70	12/13	0.97	0.12	5,13,23,29	0
1	KCX	A	70	12/13	0.97	0.15	7,10,17,18	0

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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
3	SO4	A	302	5/5	0.87	0.45	46,53,60,89	0
3	SO4	B	303	5/5	0.87	0.31	35,36,51,66	0
2	MER	A	301[A]	26/26	0.90	0.17	15,28,42,45	52
2	MER	A	301[B]	26/26	0.90	0.17	17,29,44,45	52
2	MER	C	301	26/26	0.92	0.14	15,32,48,52	0
3	SO4	B	302	5/5	0.93	0.14	36,37,55,64	0
3	SO4	C	302	5/5	0.93	0.15	43,54,72,75	0
2	MER	B	301	26/26	0.95	0.14	13,30,43,51	0
2	MER	D	301	26/26	0.95	0.12	10,31,50,51	0
3	SO4	D	302	5/5	0.97	0.18	40,41,53,61	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 MER A 301 (A):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
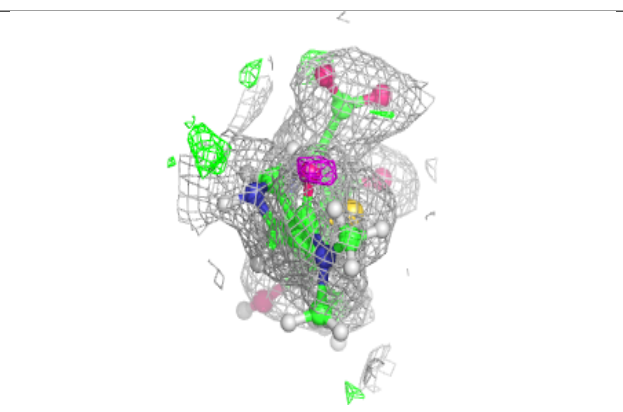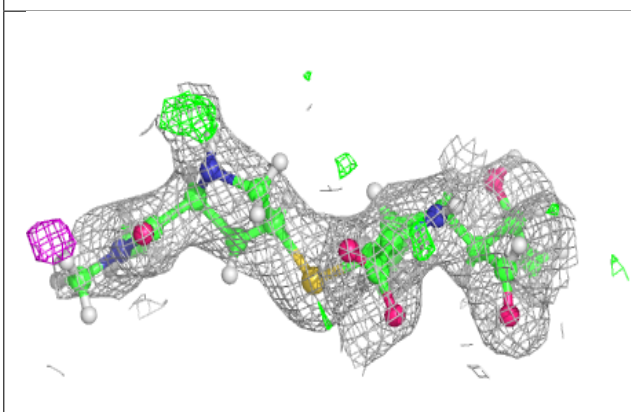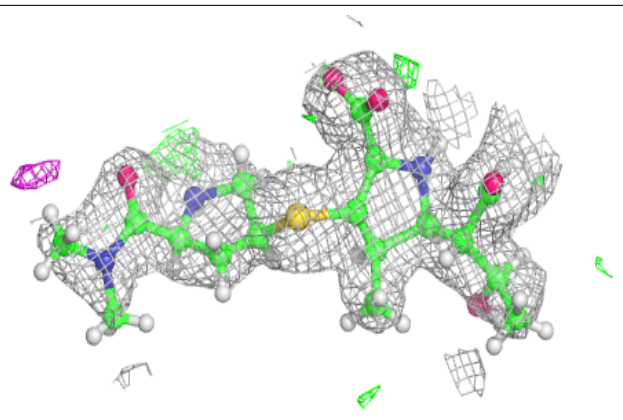
Electron density around MER A 301 (B):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
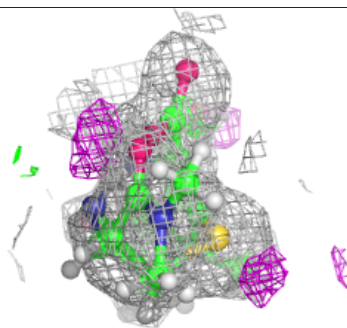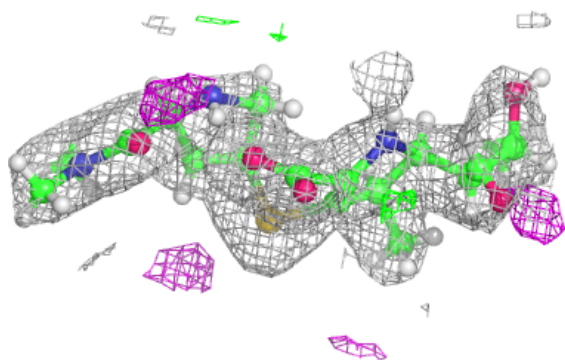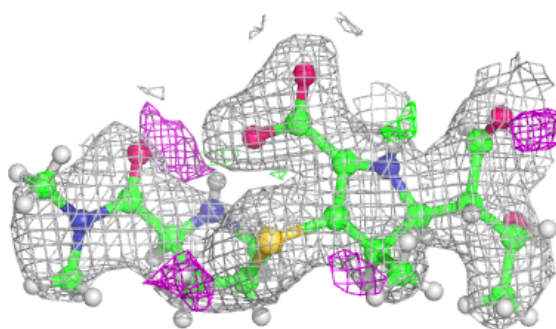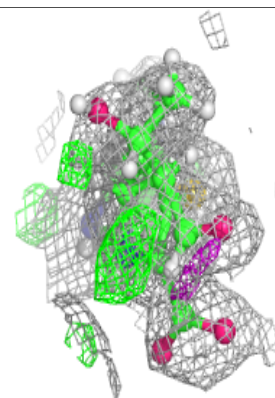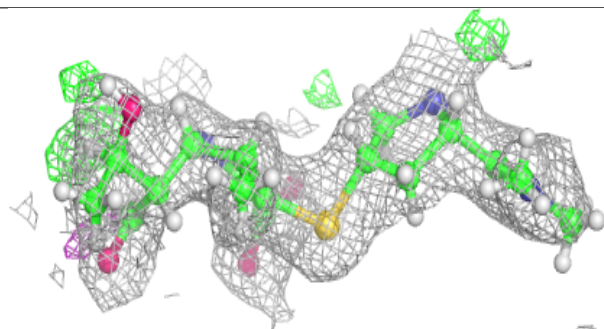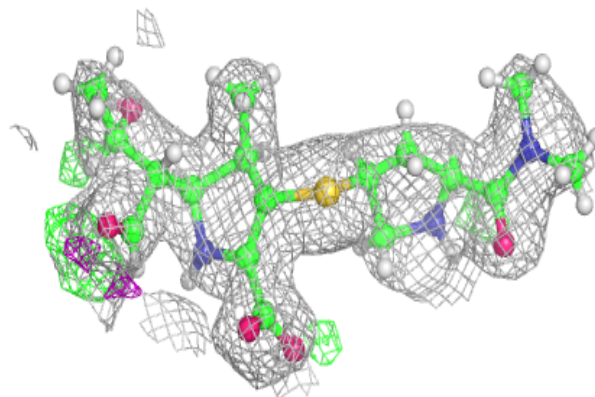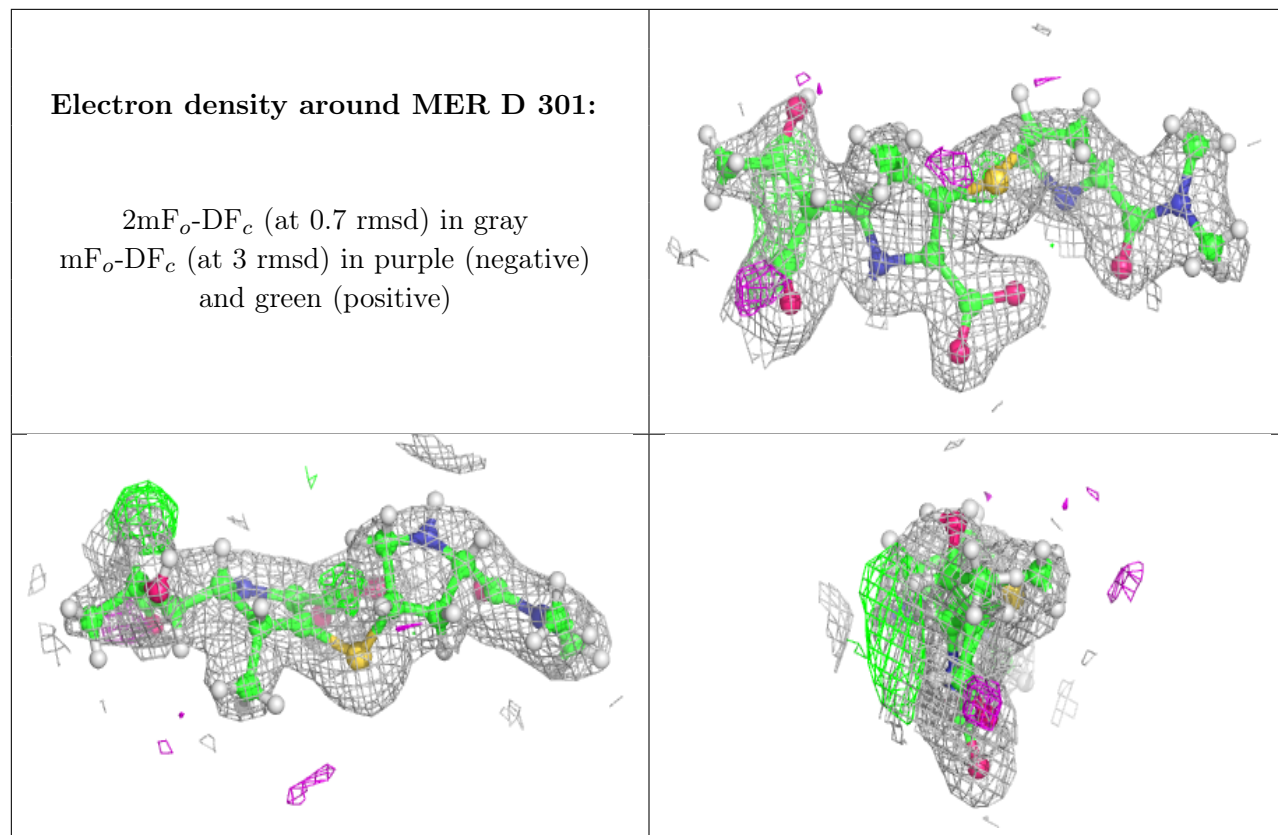and green (positive)
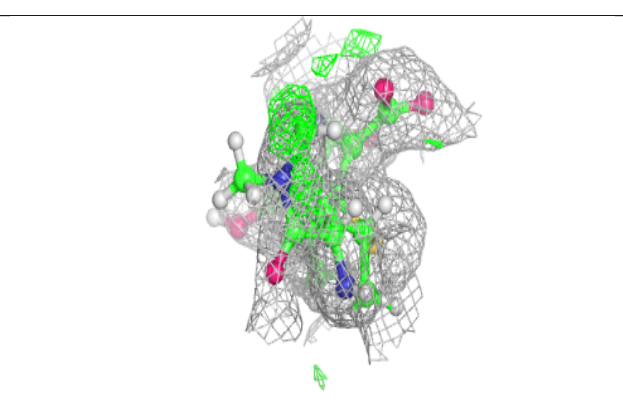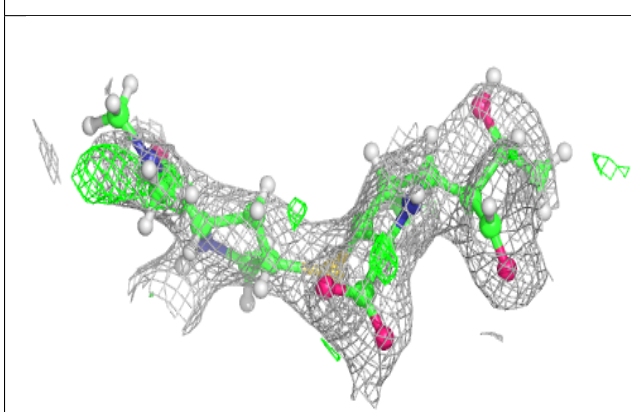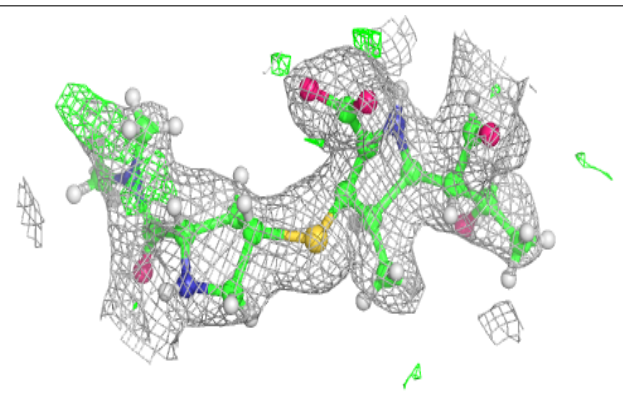
Electron density around MER C 301:

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

Electron density around MER B 301:

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

Electron density around MER D 301:

$2mF_o$-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.