Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 07:11 pm BST

PDB ID	:	8C8U
Title	:	Priestia megaterium mupirocin-resistant isoleucyl-tRNA synthetase 2 complexed with mupirocin
Authors	:	Brkic, A.; Leibundgut, M.; Jablonska, J.; Zanki, V.; Car, Z.; Petrovic Perokovic, V.; Gruic-Sovulj, I.; Ban, N.
Deposited on	:	2023-01-21
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

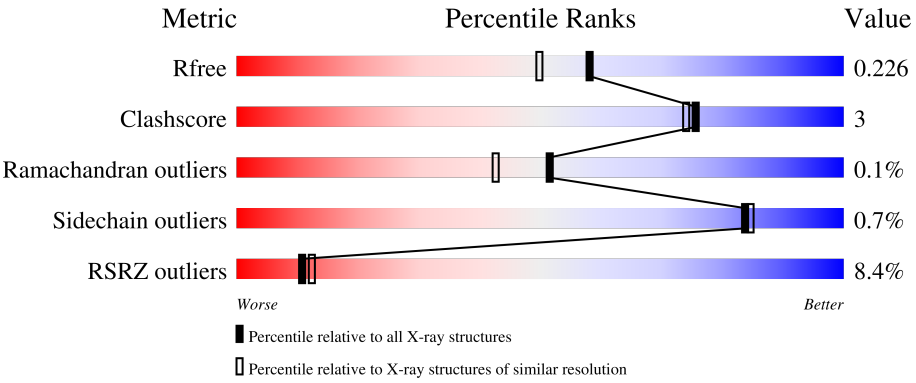
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	1032	8% 91% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9055 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 Isoleucine–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1028	Total	C	N	O	S	0	6	0
			8218	5229	1401	1564	24			

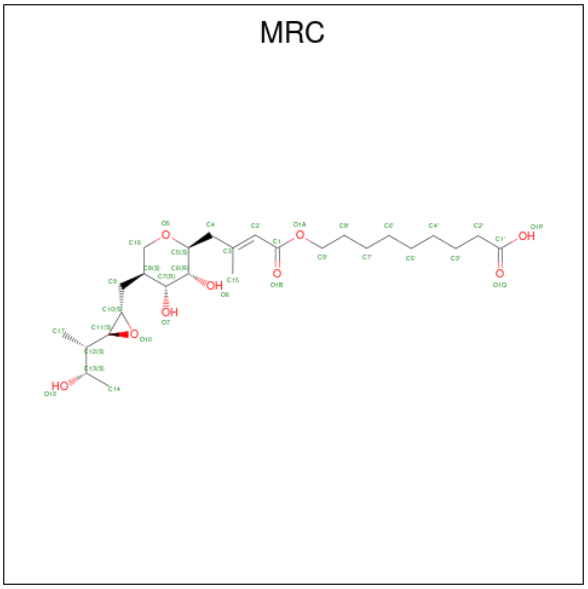
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	856	VAL	LEU	conflict	UNP A0A0B6AVD3
A	857	LEU	VAL	conflict	UNP A0A0B6AVD3

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

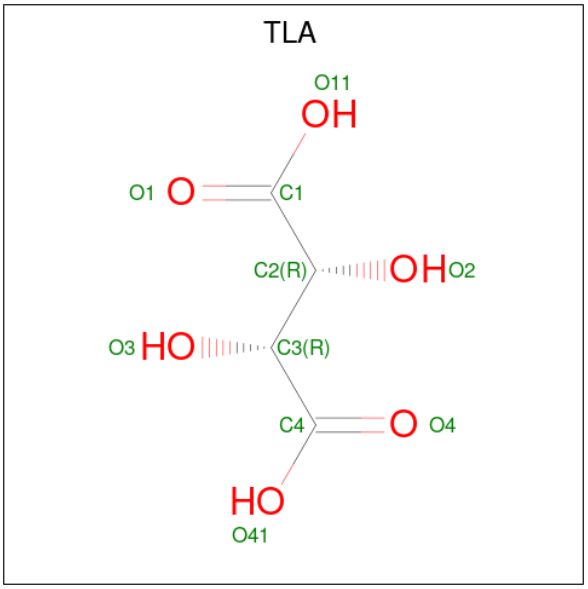
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is MUPIROCIN (three-letter code: MRC) (formula: $C_{26}H_{44}O_9$) (labeled as "Ligand of Interest" by depositor).



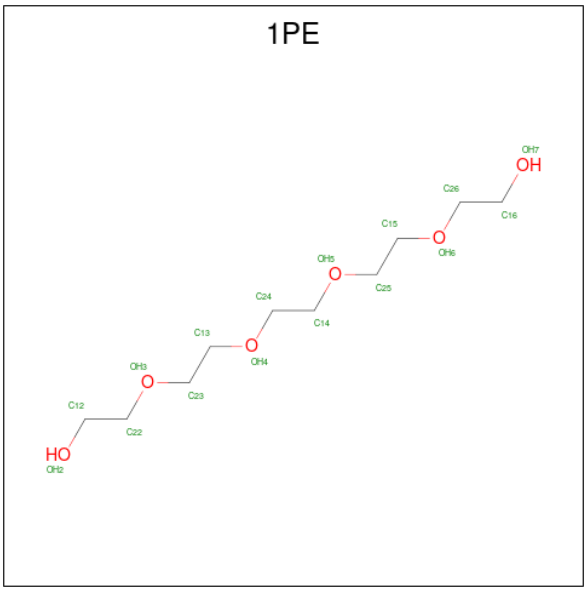
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 35 26 9	0	0

- Molecule 4 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 4 6	0	0
4	A	1	Total C O 10 4 6	0	0

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 6 is water.

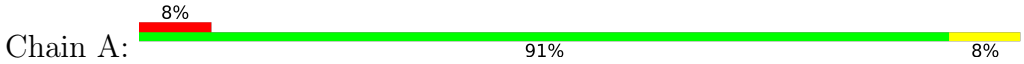
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	764	Total	O	0	0
			764	764		

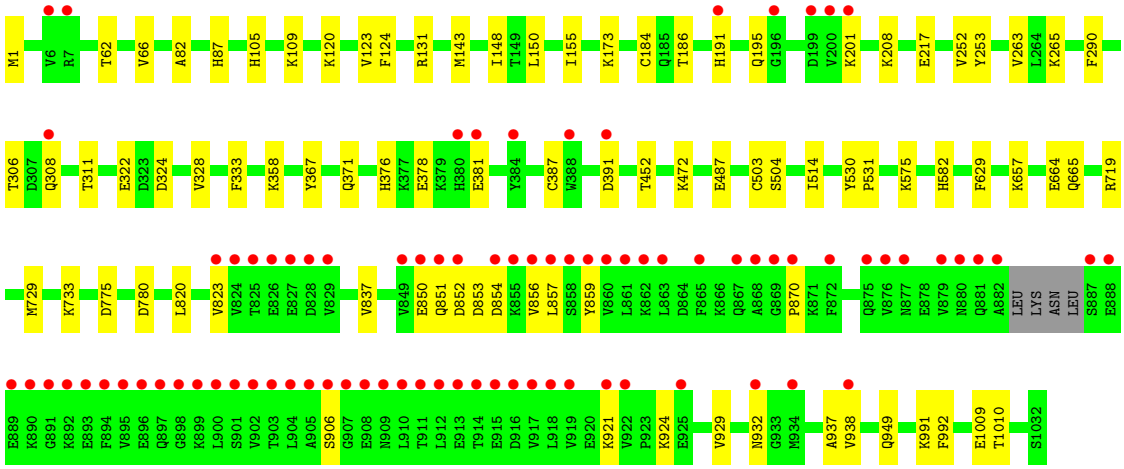
3 Residue-property plots (i)

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: Isoleucine–tRNA ligase

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	89.58Å 124.83Å 114.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.23 – 1.90 48.23 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.0 (48.23-1.90) 90.6 (48.23-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.183 , 0.222 0.185 , 0.226	Depositor DCC
R_{free} test set	4567 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9055	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: TLA, MRC, 1PE, ZN

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	0.42	0/8413	0.57	1/11416 (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	870	PRO	N-CA-CB	5.47	109.87	103.30

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	8218	0	7906	50	0
2	A	2	0	0	0	0
3	A	35	0	43	1	0
4	A	20	0	8	0	0
5	A	16	0	22	0	0
6	A	764	0	0	8	0
All	All	9055	0	7979	50	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 3.

All (50) 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:201:LYS:HG2	1:A:381:GLU:HG2	1.65	0.78
1:A:856:VAL:HG12	1:A:857:LEU:HG	1.67	0.76
1:A:472:LYS:NZ	1:A:472:LYS:HB3	2.03	0.74
1:A:775:ASP:OD1	6:A:1201:HOH:O	2.10	0.69
1:A:729:MET:HA	1:A:733:LYS:HD3	1.77	0.65
1:A:217:GLU:HG2	1:A:252:VAL:HB	1.79	0.64
1:A:857:LEU:HD13	1:A:921:LYS:HB2	1.82	0.62
1:A:929:VAL:HG22	1:A:938:VAL:HG12	1.84	0.60
1:A:472:LYS:HB3	1:A:472:LYS:HZ3	1.66	0.59
1:A:949:GLN:OE1	1:A:991:LYS:HD2	2.07	0.55
1:A:780:ASP:OD2	6:A:1203:HOH:O	2.18	0.54
1:A:665:GLN:N	1:A:665:GLN:OE1	2.41	0.54
1:A:719:ARG:HD3	1:A:837:VAL:HG13	1.89	0.54
1:A:184:CYS:HB2	1:A:186:THR:HG22	1.92	0.52
1:A:1009:GLU:HG2	1:A:1010:THR:HG23	1.91	0.52
1:A:306:THR:HG23	1:A:308:GLN:H	1.74	0.52
1:A:173:LYS:NZ	6:A:1225:HOH:O	2.43	0.51
1:A:322:GLU:HG3	6:A:1438:HOH:O	2.10	0.51
1:A:82:ALA:HB3	6:A:1302:HOH:O	2.10	0.50
1:A:852:ASP:OD1	1:A:853:ASP:N	2.40	0.49
1:A:575:LYS:NZ	6:A:1228:HOH:O	2.46	0.48
1:A:991:LYS:HD3	1:A:992:PHE:CE2	2.49	0.47
1:A:582:HIS:HA	3:A:1102:MRC:H152	1.97	0.46
1:A:87:HIS:O	6:A:1204:HOH:O	2.21	0.46
1:A:358:LYS:NZ	6:A:1215:HOH:O	2.47	0.46
1:A:1:MET:O	1:A:657:LYS:NZ	2.36	0.45
1:A:929:VAL:HG13	1:A:938:VAL:HG12	1.98	0.44
1:A:387:CYS:O	1:A:391:ASP:N	2.43	0.44
1:A:191:HIS:O	1:A:195:GLN:HG3	2.17	0.44
1:A:853:ASP:OD2	1:A:859:TYR:OH	2.15	0.44
1:A:265:LYS:HE3	1:A:376:HIS:CE1	2.53	0.44
1:A:851:GLN:N	1:A:851:GLN:OE1	2.51	0.43
1:A:328:VAL:HG13	1:A:333:PHE:HB2	2.01	0.43
1:A:123:VAL:HG23	1:A:124:PHE:CD2	2.54	0.43
1:A:852:ASP:OD2	1:A:854:ASP:OD2	2.37	0.43
1:A:120:LYS:NZ	1:A:487:GLU:OE2	2.49	0.42
1:A:62:THR:O	1:A:66:VAL:HG23	2.20	0.42
1:A:263:VAL:HG11	1:A:311:THR:HG22	2.01	0.42
1:A:208:LYS:HD2	1:A:253:TYR:HE1	1.85	0.42
1:A:856:VAL:O	1:A:924:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:HA	1:A:143:MET:SD	2.60	0.41
1:A:148:ILE:HG22	1:A:150:LEU:HG	2.02	0.41
1:A:452:THR:HB	1:A:514:ILE:HG12	2.01	0.41
1:A:530:TYR:CD1	1:A:531:PRO:HA	2.54	0.41
1:A:823:VAL:HA	1:A:850:GLU:O	2.20	0.41
1:A:503:CYS:O	1:A:504:SER:OG	2.32	0.41
1:A:820:LEU:HD11	1:A:937:ALA:HB1	2.02	0.41
1:A:155:ILE:HG23	1:A:452:THR:HG23	2.02	0.41
1:A:105:HIS:CE1	1:A:109:LYS:HD2	2.57	0.41
1:A:367:TYR:CZ	1:A:371:GLN:HG3	2.56	0.40

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	1030/1032 (100%)	1008 (98%)	21 (2%)	1 (0%)	51 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	906	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	879/913 (96%)	873 (99%)	6 (1%)	84 84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	PHE
1	A	324	ASP
1	A	378	GLU
1	A	629	PHE
1	A	664	GLU
1	A	932	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	370	ASN
1	A	371	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	TLA	A	1104	-	9,9,9	1.24	0	12,12,12	1.39	2 (16%)
3	MRC	A	1102	-	35,36,36	2.13	5 (14%)	40,48,48	1.52	7 (17%)
4	TLA	A	1105	-	9,9,9	1.21	0	12,12,12	0.92	0
5	1PE	A	1106	-	15,15,15	0.66	0	14,14,14	0.39	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
4	TLA	A	1104	-	-	0/12/12/12	-
3	MRC	A	1102	-	-	5/32/54/54	0/2/2/2
4	TLA	A	1105	-	-	4/12/12/12	-
5	1PE	A	1106	-	-	5/13/13/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	MRC	C2-C3	10.50	1.53	1.33
3	A	1102	MRC	C11-C10	3.36	1.51	1.46
3	A	1102	MRC	C16-C8	3.28	1.56	1.51
3	A	1102	MRC	C2-C1	2.78	1.53	1.46
3	A	1102	MRC	C9-C10	2.09	1.56	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1102	MRC	C11-O10-C10	3.57	62.87	60.59
3	A	1102	MRC	C4-C5-C6	-3.51	110.09	113.01
3	A	1102	MRC	C9-C10-C11	-3.42	116.76	124.18
3	A	1102	MRC	C16-O5-C5	-3.08	108.02	112.19
3	A	1102	MRC	O1Q-C1'-C2'	-2.39	115.39	123.08
4	A	1104	TLA	O1-C1-C2	-2.36	115.44	121.63
3	A	1102	MRC	O5-C5-C4	2.31	112.86	107.50
3	A	1102	MRC	C15-C3-C4	2.31	120.95	115.27
4	A	1104	TLA	C3-C2-C1	-2.05	105.30	109.87

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1106	1PE	OH6-C15-C25-OH5
3	A	1102	MRC	C3'-C4'-C5'-C6'
3	A	1102	MRC	C5'-C6'-C7'-C8'
4	A	1105	TLA	O3-C3-C4-O41
3	A	1102	MRC	C1'-C2'-C3'-C4'
5	A	1106	1PE	C13-C23-OH3-C22
5	A	1106	1PE	OH2-C12-C22-OH3
4	A	1105	TLA	O3-C3-C4-O4
4	A	1105	TLA	C2-C3-C4-O41
4	A	1105	TLA	C2-C3-C4-O4
5	A	1106	1PE	OH5-C14-C24-OH4
3	A	1102	MRC	O1P-C1'-C2'-C3'
3	A	1102	MRC	O1Q-C1'-C2'-C3'
5	A	1106	1PE	C23-C13-OH4-C24

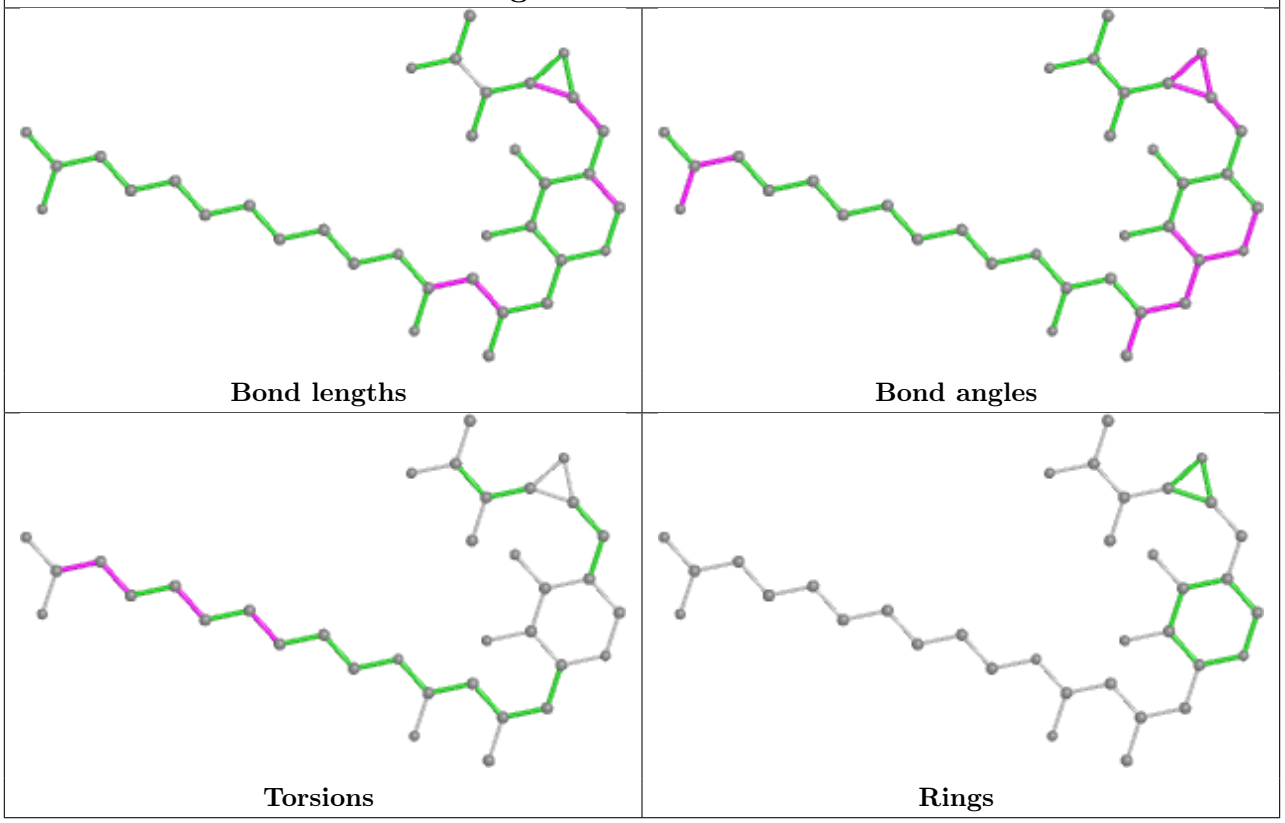
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	MRC	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 MRC A 1102



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	1028/1032 (99%)	0.39	86 (8%)	11	12	18, 36, 83, 105	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	887	SER	10.6
1	A	859	TYR	8.6
1	A	903	THR	7.8
1	A	894	PHE	7.7
1	A	868	ALA	7.6
1	A	904	LEU	7.4
1	A	879	VAL	6.9
1	A	863	LEU	6.8
1	A	902	VAL	6.7
1	A	882	ALA	6.7
1	A	824	VAL	6.6
1	A	861	LEU	6.4
1	A	891	GLY	6.2
1	A	900	LEU	6.2
1	A	898	GLY	6.0
1	A	889	GLU	6.0
1	A	895	VAL	6.0
1	A	910	LEU	5.9
1	A	876	VAL	5.8
1	A	893	GLU	5.8
1	A	875	GLN	5.8
1	A	857	LEU	5.6
1	A	916	ASP	5.6
1	A	7	ARG	5.5
1	A	6	VAL	5.5
1	A	860	VAL	5.4
1	A	919	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	899	LYS	5.2
1	A	911	THR	5.2
1	A	888	GLU	5.2
1	A	869	GLY	5.1
1	A	918	LEU	5.1
1	A	890	LYS	5.0
1	A	865	PHE	5.0
1	A	897	GLN	4.8
1	A	880	ASN	4.6
1	A	906	SER	4.5
1	A	308	GLN	4.3
1	A	862	LYS	4.2
1	A	921	LYS	4.1
1	A	851	GLN	4.1
1	A	870	PRO	4.0
1	A	825	THR	3.9
1	A	881	GLN	3.9
1	A	934	MET	3.9
1	A	827	GLU	3.9
1	A	855	LYS	3.9
1	A	901	SER	3.8
1	A	877	ASN	3.7
1	A	912	LEU	3.7
1	A	858	SER	3.7
1	A	892	LYS	3.6
1	A	199	ASP	3.6
1	A	905	ALA	3.6
1	A	852	ASP	3.6
1	A	854	ASP	3.4
1	A	381	GLU	3.4
1	A	823	VAL	3.3
1	A	201	LYS	3.3
1	A	913	GLU	3.3
1	A	867	GLN	3.2
1	A	872	PHE	3.2
1	A	384	TYR	3.1
1	A	907	GLY	3.1
1	A	196	GLY	3.0
1	A	380	HIS	3.0
1	A	388	TRP	2.9
1	A	917	VAL	2.7
1	A	896	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	856	VAL	2.7
1	A	191	HIS	2.6
1	A	922	VAL	2.5
1	A	391	ASP	2.5
1	A	909	ASN	2.5
1	A	850	GLU	2.5
1	A	200	VAL	2.4
1	A	908	GLU	2.4
1	A	828	ASP	2.3
1	A	829	VAL	2.3
1	A	914	THR	2.3
1	A	932	ASN	2.2
1	A	849	VAL	2.2
1	A	826	GLU	2.2
1	A	938	VAL	2.2
1	A	915	GLU	2.1
1	A	925	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

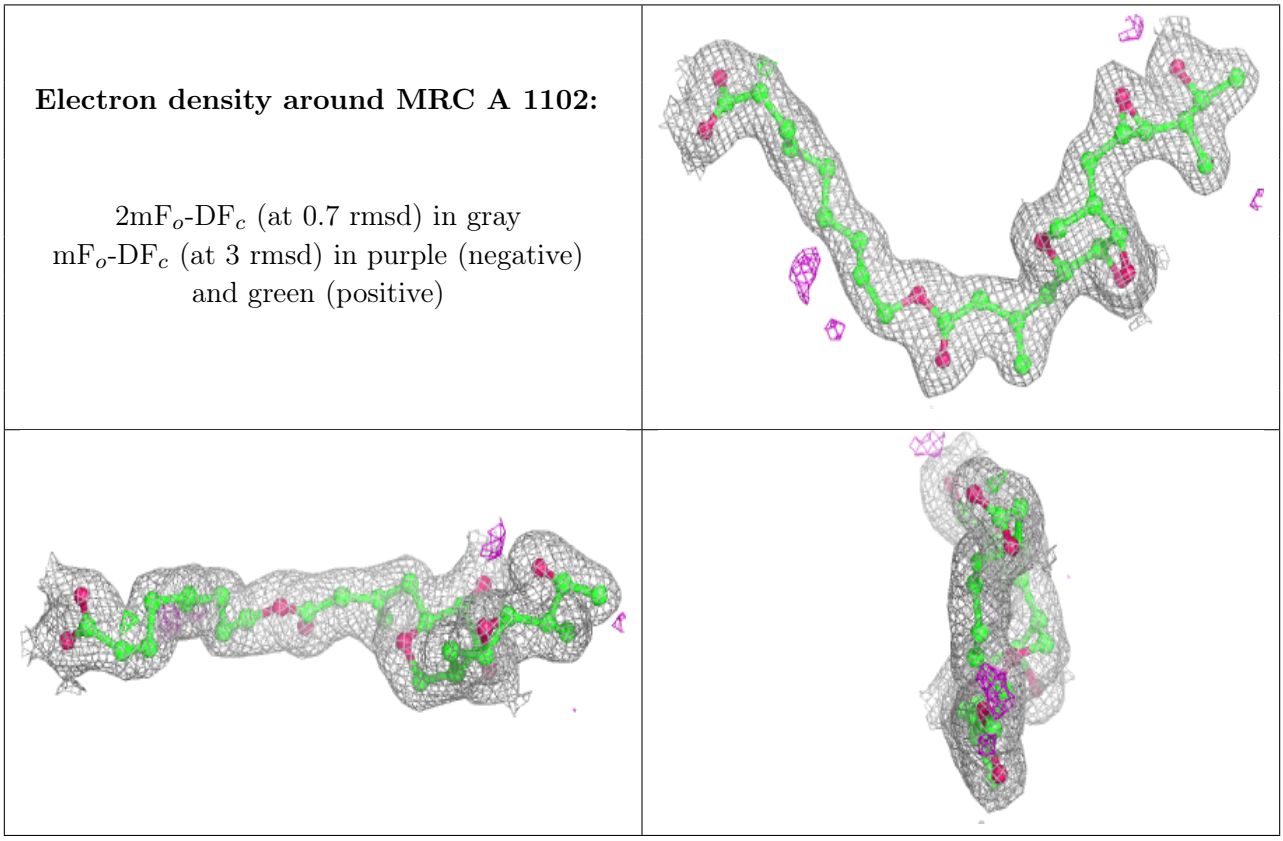
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	1PE	A	1106	16/16	0.81	0.29	51,65,72,74	0
4	TLA	A	1105	10/10	0.93	0.15	46,52,57,62	0
2	ZN	A	1103	1/1	0.94	0.06	60,60,60,60	0
3	MRC	A	1102	35/35	0.96	0.13	20,23,31,33	0
4	TLA	A	1104	10/10	0.96	0.10	26,32,45,45	0
2	ZN	A	1101	1/1	0.98	0.08	44,44,44,44	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 MRC A 1102:

$2mF_o$-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.