wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 12:44 AM EDT

PDB ID	:	1QU3
Title	:	INSIGHTS INTO EDITING FROM AN ILE-TRNA SYNTHETASE STRUCTURE WITH TRNA(ILE) AND MUPIROCIN
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Deposited on	:	1999-07-06
Resolution	:	2.90 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:

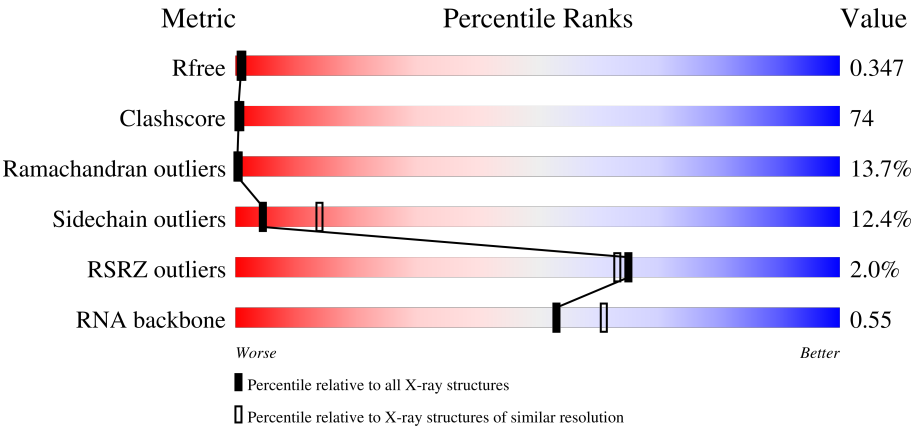
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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	T	75	3% 15% 55% 29%
2	A	917	2% 19% 58% 17%

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
4	MRC	A	993	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8870 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 RNA chain called ISOLEUCYL-TRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	75	Total	C	N	O	P	24	0	0
			1603	715	289	525	74			

- Molecule 2 is a protein called ISOLEUCYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	880	Total	C	N	O	S	0	0	0
			7113	4537	1198	1358	20			

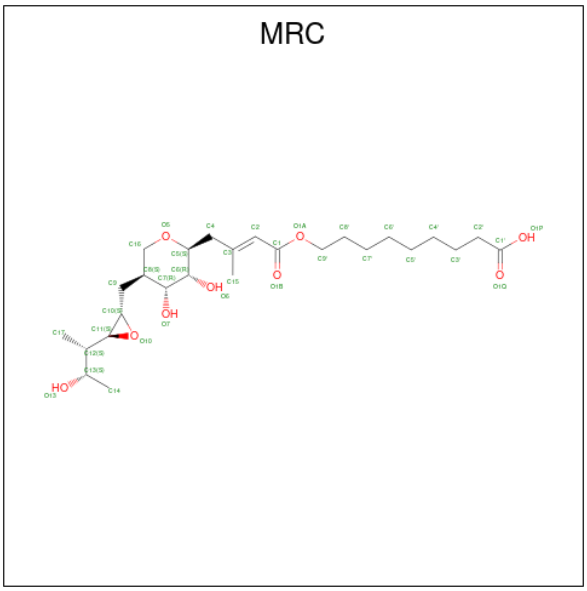
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLU	LYS	conflict	UNP P41972
A	5	LYS	GLU	conflict	UNP P41972
A	295	TRP	TYR	conflict	UNP P41972
A	340	GLN	LYS	conflict	UNP P41972
A	644	ASP	VAL	conflict	UNP P41972

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MUPIROCIN (three-letter code: MRC) (formula: $C_{26}H_{44}O_9$).



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

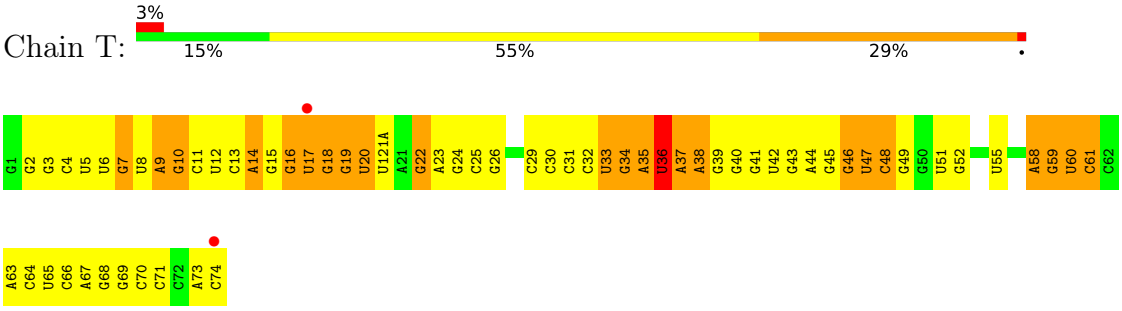
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	T	36	Total O 36 36	0	0
5	A	82	Total O 82 82	0	0

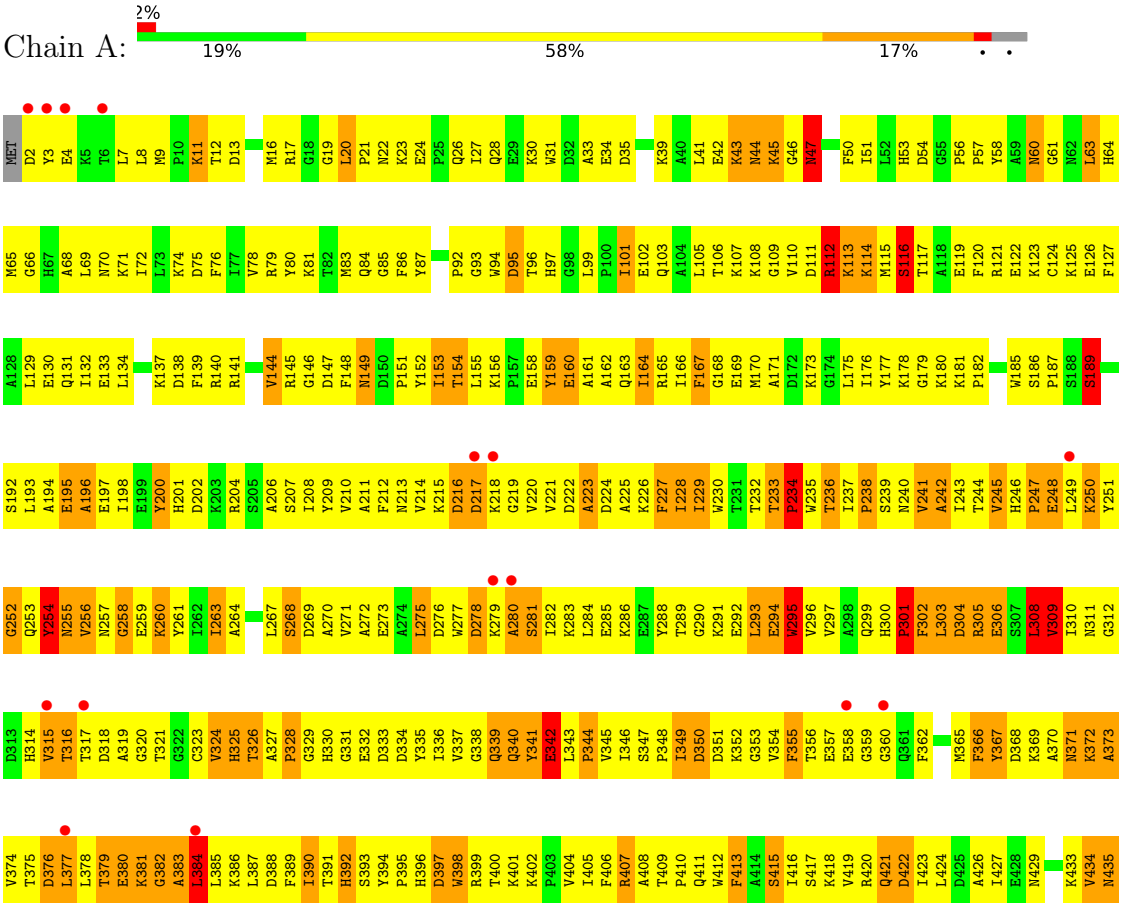
3 Residue-property plots (i)

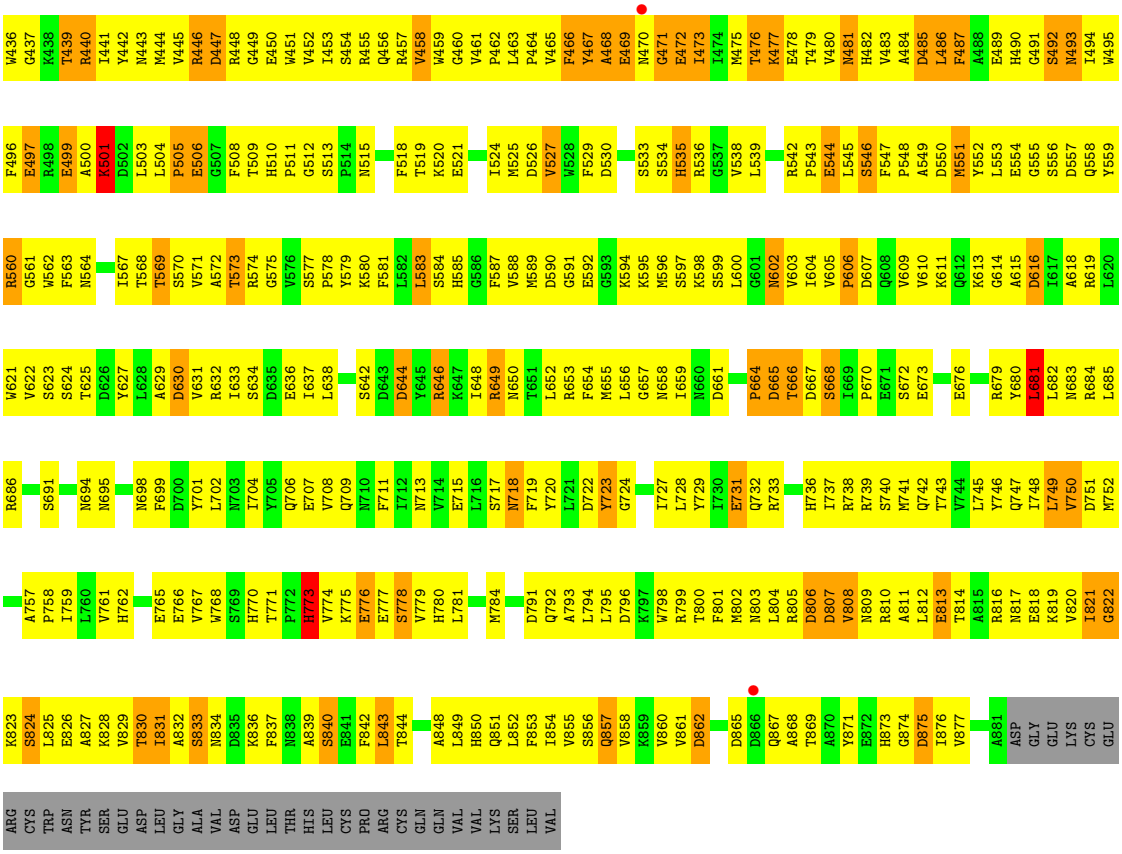
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ISOLEUCYL-TRNA



• Molecule 2: ISOLEUCYL-TRNA SYNTHETASE




W436 G437 K438 T439 R440 I441 Y442 N443 M444 V445 R446 D447 R448 G449 E450 W451 V452 I453 S454 R455 Q456 R457 V458 W459 G460 V461 P462 L463 P464 V465 F466 Y467 A468 E469 N470 G471 E472 I473 I474 M475 T476 K477 E478 T479 V480 N481 H482 V483 A484 D485 L486 F487 A488 E489 H490 G491 S492 N493 I494 W495
F496 E497 R498 E499 A500 K501 D502 L503 L504 P505 E506 G507 F508 T509 H510 P511 G512 S513 P514 N515 F518 T519 K520 E521 I524 M525 D526 V527 W528 F529 D530 S533 S534 H535 R536 G537 V538 L539 R542 P543 E544 L545 S546 F547 P548 A549 D550 M551 Y552 L553 E554 G555 S556 D557 Q558 Y559
R560 G561 W562 F563 N564 I567 T568 T569 S570 V571 A572 T573 R574 G575 V576 S577 P578 Y579 K580 F581 L582 L583 S584 H585 G586 F587 V588 M589 D590 G591 E592 G593 K594 K595 M596 S597 K598 S599 L600 G601 N602 V603 I604 V605 P606 D607 Q608 V609 V610 K611 Q612 K613 G614 A615 D616 I617 A618 R619 L620
W621 V622 S623 S624 T625 D626 Y627 L628 A629 D630 V631 R632 I633 S634 D635 E636 I637 L638 S642 D643 D644 Y645 R646 K647 I648 R649 N650 T651 L652 R653 F654 M655 L656 G657 N658 I659 N660 D661 P664 D665 T666 D667 S668 I669 P670 E671 S672 E673 E676 R679 Y680 L681 L682 N683 R684 L685
R686 S691 N694 N695 N698 F699 D700 Y701 L702 N703 I704 Y705 Q706 E707 V708 Q709 N710 F711 I712 N713 V714 E715 L716 S717 N718 F719 Y720 L721 D722 Y723 G724 I727 L728 Y729 I730 E731 Q732 R733 H736 I737 R738 R739 S740 M741 Q742 T743 V744 L745 Y746 Q747 I748 L749 V750 D751 M752
A757 P758 I759 L760 V761 H762 E765 E766 V767 W768 S769 H770 T771 P772 H773 V774 K775 E776 E777 S778 V779 H780 L781 M784 D791 Q792 A793 L794 L795 D796 K797 W798 R799 T800 F801 M802 N803 L804 R805 D806 D807 V808 N809 R810 A811 L812 E813 T814 A815 R816 N817 E818 K819 V820 I821 G822
K823 S824 L825 E826 A827 K828 V829 T830 I831 A832 S833 N834 D835 K836 F837 N838 A839 S840 E841 F842 L843 T844 A848 L849 H850 Q851 L852 F853 I854 V855 S856 Q857 V858 K859 V860 V861 D862 D865 D866 Q867 A868 T869 A870 Y871 E872 H873 G874 D875 I876 V877 A881 ASP GLY GLU LYS CYS GLU
ARG CYS TRP ASN TYR SER GLU ASP LEU GLY ALA VAL ASP GLU LEU THR HIS LEU CYS PRO ARG CYS GLN GLN VAL VAL LYS SER LEU VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.00Å 100.00Å 180.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 19.93 – 2.75	Depositor EDS
% Data completeness (in resolution range)	85.9 (10.00-2.90) 55.5 (19.93-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.75Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.234 , 0.345 0.233 , 0.347	Depositor DCC
R_{free} test set	956 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	43.7	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8870	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: ZN, MRC

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	T	0.53	0/1792	0.80	1/2794 (0.0%)
2	A	0.44	0/7287	0.72	3/9879 (0.0%)
All	All	0.46	0/9079	0.74	4/12673 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	471	GLY	N-CA-C	-6.82	96.06	113.10
2	A	681	LEU	CA-CB-CG	-5.37	102.94	115.30
1	T	36	U	N1-C1'-C2'	5.28	120.86	114.00
2	A	255	ASN	N-CA-C	5.25	125.18	111.00

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	T	1603	0	811	99	1
2	A	7113	0	6935	1135	1
3	A	1	0	0	0	0
4	A	35	0	40	5	0
5	A	82	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	36	0	0	2	0
All	All	8870	0	7786	1212	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 74.

The worst 5 of 1212 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:T:13:C:H2'	1:T:14:A:H5"	1.32	1.10
2:A:366:PHE:H	2:A:370:ALA:HB3	1.18	1.07
2:A:53:HIS:NE2	2:A:534:SER:HB3	1.73	1.02
2:A:250:LYS:HG2	2:A:290:GLY:N	1.77	1.00
2:A:302:PHE:HA	2:A:378:LEU:HD13	1.43	0.99

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:T:19:G:O2'	2:A:672:SER:O[4_576]	2.19	0.01

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
2	A	878/917 (96%)	572 (65%)	186 (21%)	120 (14%)	0 0

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	45	LYS

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Mol	Chain	Res	Type
2	A	47	ASN
2	A	112	ARG
2	A	114	LYS
2	A	195	GLU

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
2	A	772/806 (96%)	676 (88%)	96 (12%)	4 14

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	476	THR
2	A	569	THR
2	A	485	ASP
2	A	526	ASP
2	A	616	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	713	ASN
2	A	809	ASN
2	A	732	GLN
2	A	770	HIS
2	A	857	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	T	74/75 (98%)	21 (28%)	12 (16%)

5 of 21 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	T	8	U
1	T	9	A
1	T	10	G
1	T	14	A
1	T	16	G

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	T	37	A
1	T	47	U
1	T	60	U
1	T	48	C
1	T	19	G

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	MRC	A	993	-	35,36,36	2.19	10 (28%)	40,48,48	1.94	8 (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
4	MRC	A	993	-	3/3/11/12	15/32/54/54	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	993	MRC	C11-C10	-7.01	1.36	1.46
4	A	993	MRC	C8-C7	4.51	1.59	1.53
4	A	993	MRC	O1A-C1	3.92	1.43	1.34
4	A	993	MRC	C9-C8	3.44	1.60	1.53
4	A	993	MRC	C2-C3	3.24	1.39	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	993	MRC	C11-O10-C10	-5.02	57.39	60.59
4	A	993	MRC	C11-C12-C13	4.44	120.59	111.11
4	A	993	MRC	C9-C8-C7	4.23	119.33	113.32
4	A	993	MRC	O1A-C1-C2	4.07	118.98	110.60
4	A	993	MRC	C17-C12-C11	3.87	118.34	111.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	993	MRC	C7
4	A	993	MRC	C6
4	A	993	MRC	C12

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	993	MRC	C2-C1-O1A-C9'
4	A	993	MRC	O1B-C1-O1A-C9'
4	A	993	MRC	O10-C11-C12-C13
4	A	993	MRC	C1'-C2'-C3'-C4'
4	A	993	MRC	C6'-C7'-C8'-C9'

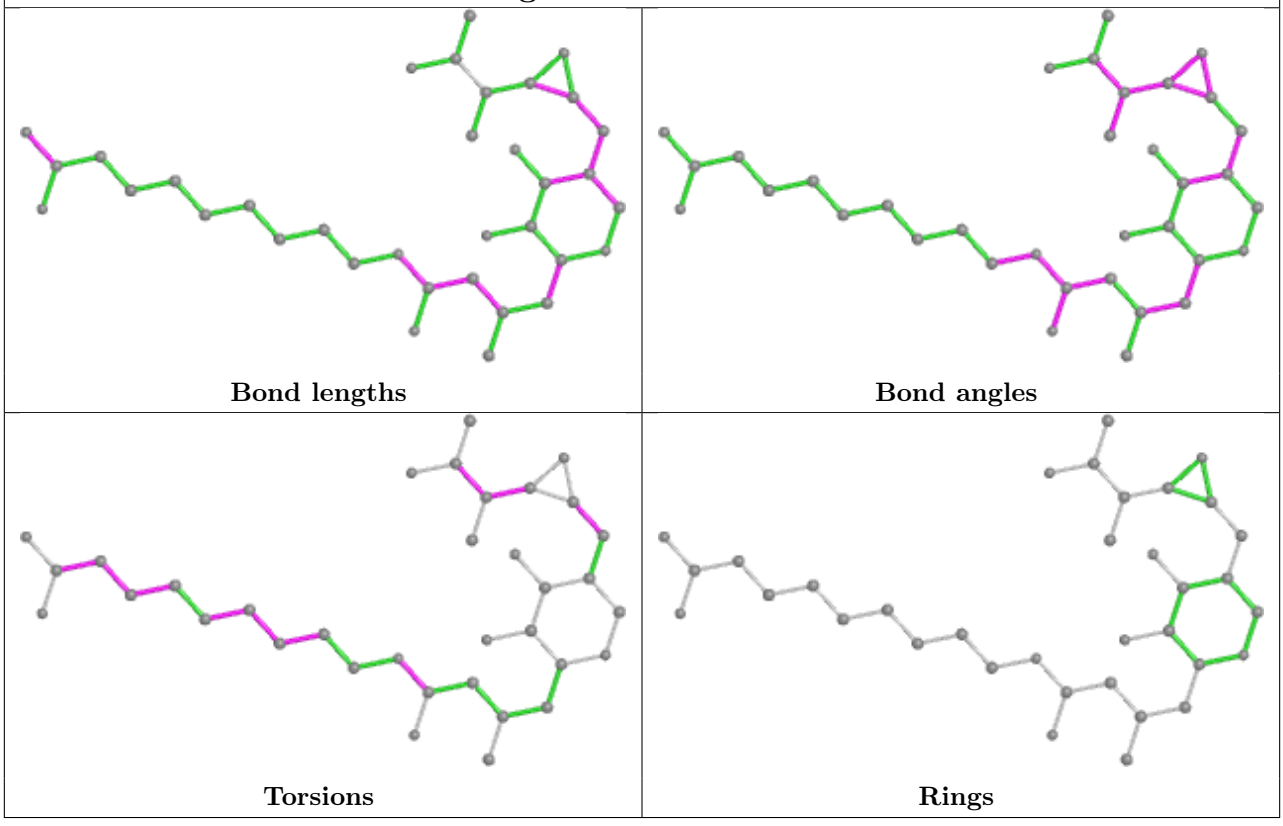
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	993	MRC	5	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 993



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	T	75/75 (100%)	-0.27	2 (2%)	54	50	5, 30, 78, 100	2 (2%)
2	A	880/917 (95%)	-0.39	17 (1%)	66	65	3, 32, 70, 83	0
All	All	955/992 (96%)	-0.38	19 (1%)	65	63	3, 32, 70, 100	2 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	2	ASP	4.0
1	T	74	C	3.9
2	A	4	GLU	3.9
2	A	280	ALA	3.7
2	A	3	TYR	3.6

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

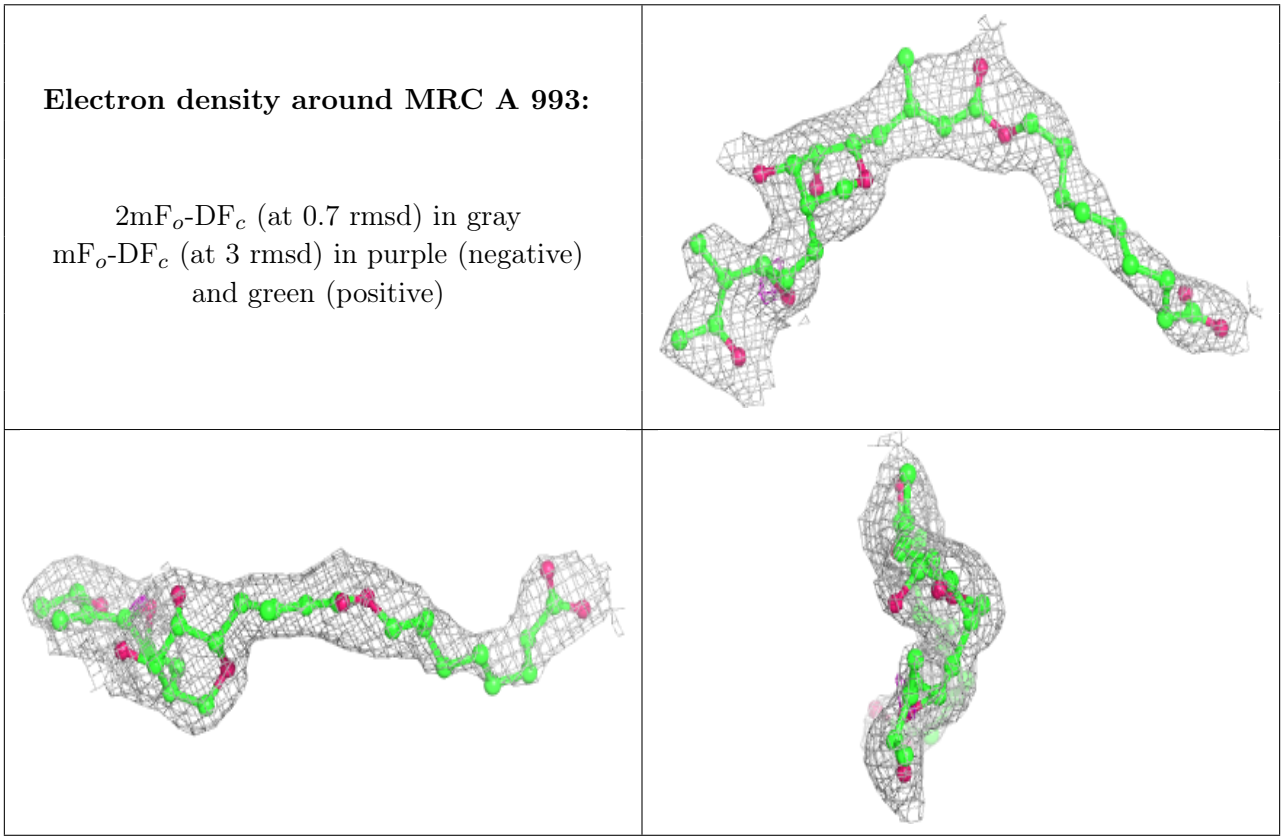
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MRC	A	993	35/35	0.90	0.21	22,29,57,58	0
3	ZN	A	992	1/1	1.00	0.04	35,35,35,35	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 993:

$2mF_o$-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.