



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:38 am GMT

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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

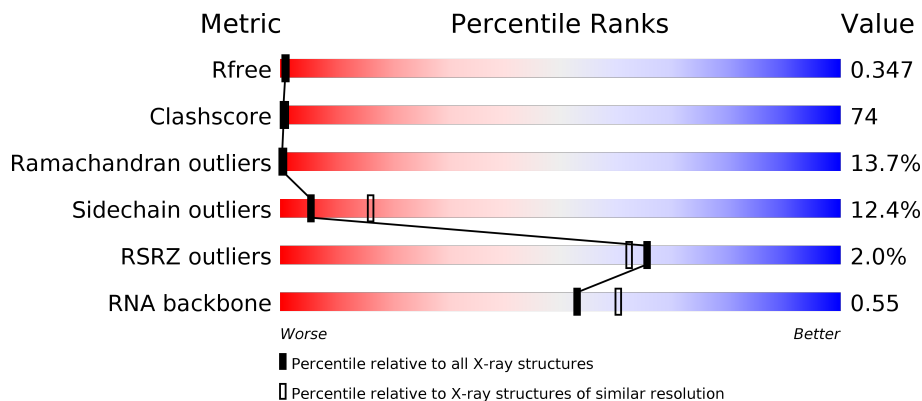
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)
RNA backbone	2435	1004 (3.20-2.60)

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. 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 $\leq 5\%$. 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	<div> <div>3%</div> <div>15%</div> <div>61%</div> <div>23%</div> <div>.</div> </div>
2	A	917	<div> <div>2%</div> <div>19%</div> <div>58%</div> <div>17%</div> <div>..</div> </div>

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	-	-	X

2 Entry composition

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			

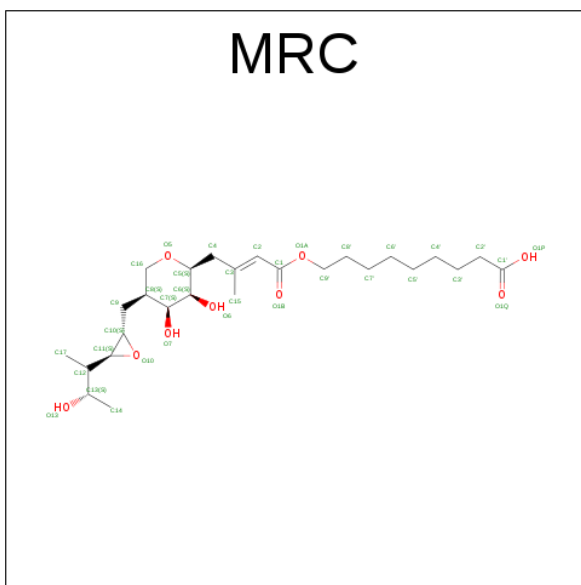
There are 5 discrepancies between the modelled and reference sequences:

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: C₂₆H₄₄O₉).



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

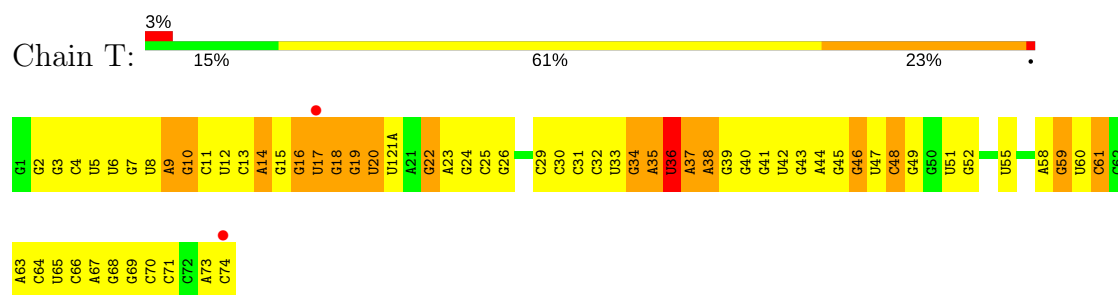
- Molecule 5 is water.

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

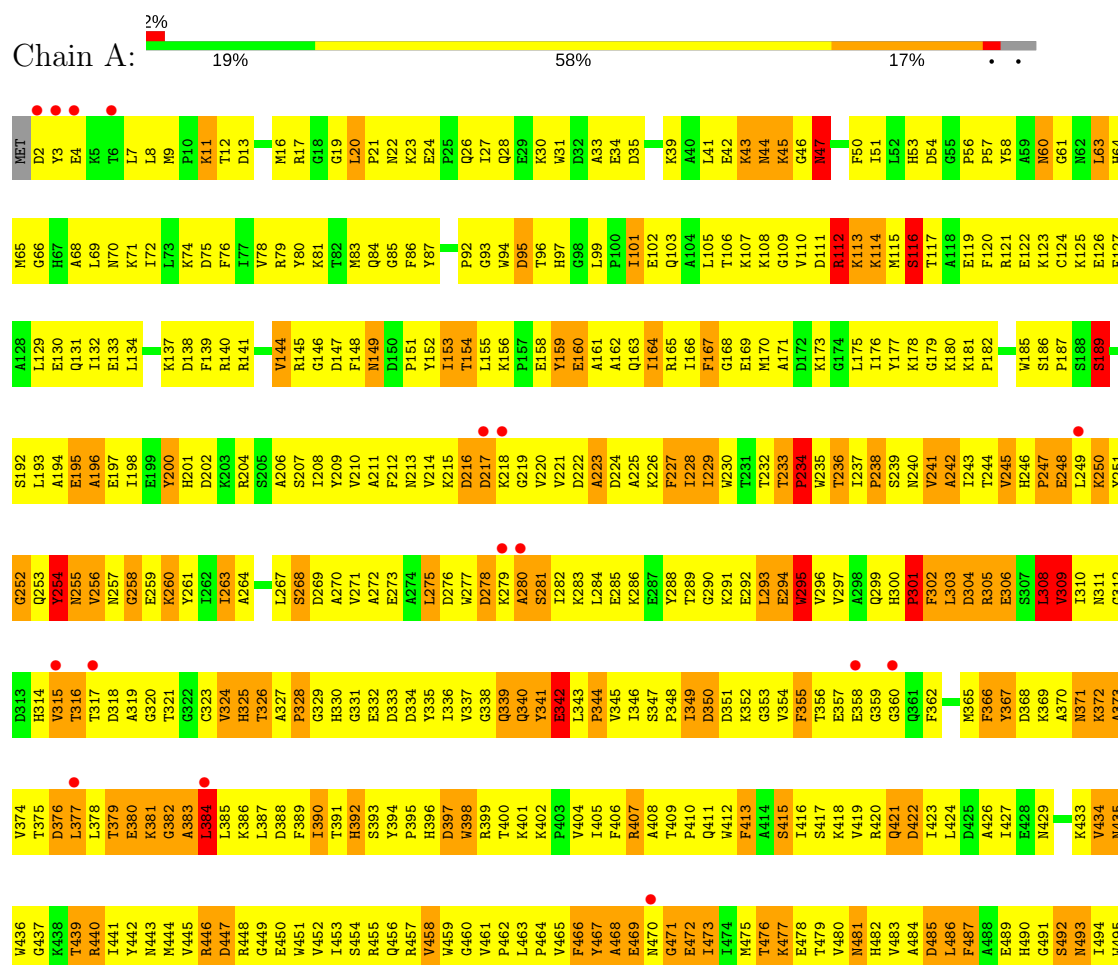
3 Residue-property plots

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: ISOLEUCYL-TRNA



• Molecule 2: ISOLEUCYL-TRNA SYNTHETASE



ARG	K823	A757	R686	V621	R560	F496
CYS	S824	P758	S691	V622	G561	E497
TRP	L825	I759		S623	W562	R498
ASN	E826	L760	N694	S624	F563	E499
TYR	A827	V761	N695	T625	N564	A500
SER	K828	H762		D626	K501	K501
GLU	V829			Y627	I567	D502
ASP	T830			L628	T568	L503
LEU	I831	E765	N698	A629	T569	L504
GLY	A832	E766	P699	D630	T568	P505
ALA	S833	V767	D700	V631	S570	E506
VAL	N834	V768	Y701	R632	V571	
ASP	D835	S769	L702	L633	A572	G507
GLU	K836	H770	N703	I633	T573	F508
LEU	F837	I771	I704	S634	R574	T509
THR	N838	P772	Q706	D635	V576	H510
HIS	A839	H773	E707	E636	S577	P511
LEU	S840	V774	V708	I637	P578	G512
CYS	F841	K775	Q709	L638	Y579	S513
PRO	F842	E776	N710		K580	P514
ARG	L843	E777	F711	S642	F581	N515
GLN	T844	S778	I712	D643	L582	F518
GLN	A848	V779	N713	D644	L583	T519
VAL	L849	H780	V714	R645	S584	K520
VAL	H850	L781	E715	K646	H585	E521
LYS	Q851	N784	L716	I643	G586	
LEU	F853	D791	R649	R649	F587	L624
	L854	Q792	N718	N650	V588	M525
S855	A793	Q792	F719	T651	M589	D526
S856	A793	Q792	Y720	L652	D590	V527
Q857	L794	D722	L721	R653	G591	K528
V858	L795	D723	D722	F654	E592	F529
K859	L796	G724	Y723	M655	G593	D530
V860	K797		L656	G657	K594	
V861	W798	I727	G657	L657	K595	S533
D862	V861	L728	N658	I659	M596	S534
		Y729	L659	N660	S597	H535
D865	D865	I730	N660	D661	K598	R536
D866	D866	E731	P664	P664	S599	G537
Q867	Q867	R732	D665	D665	L600	V538
A868	A868	R733	T666	T666	G601	L539
T869	T869	H736	D667	D667	V603	R542
A870	A870	I737	S668	S668	I604	P543
Y871	Y871	R738	I669	I669	V605	E544
E872	E872	R739	P670	P670	P606	L545
H873	H873	S740	E571	E571	D607	S546
G874	G874	M741	S672	S672	Q608	F547
D875	D875	Q742	E673	E673	V609	P548
I876	I876	T743			V610	A549
V877	V877	V744	E576	E576	K611	D550
A881	A881	L745			Q612	M551
ASP	ASP	Y746	R579	R579	K613	Y552
GLY	GLY	Q747	Y680	Y680	G614	L553
GLU	GLU	I748	L681	L681	A615	E554
LYS	LYS	L749	L682	L682	D616	G555
CYS	CYS	V750	N683	N683	I617	S556
GLU	GLU	I821	R684	R684	A618	D557
		G822	L685	L685	R619	Q558
					L620	Y559

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	812 reflections (4.92%)	DCC
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	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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(°)	Ideal(°)
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 [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	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 ⓘ

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%)	5 16

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

Mol	Chain	Res	Type
2	A	371	ASN
2	A	450	GLU
2	A	813	GLU
2	A	384	LEU
2	A	398	TRP

Some 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	456	GLN
2	A	493	ASN
2	A	851	GLN
2	A	481	ASN
2	A	482	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	T	74/75 (98%)	21 (28%)	0

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

There are no RNA pucker outliers to report.

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 carbohydrates 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	-	32,36,36	2.22	9 (28%)	35,48,48	2.05	7 (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	-	1/1/11/12	0/30/54/54	0/1/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	993	MRC	C11-C10	-7.11	1.36	1.46
4	A	993	MRC	C2-C1	-2.87	1.39	1.46
4	A	993	MRC	C9-C10	2.02	1.56	1.52
4	A	993	MRC	C4-C5	2.26	1.58	1.52
4	A	993	MRC	C16-C8	2.58	1.55	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	993	MRC	C11-O10-C10	-5.05	57.39	60.58
4	A	993	MRC	C9'-O1A-C1	-3.29	110.72	116.49
4	A	993	MRC	C5-C4-C3	2.92	120.99	113.11
4	A	993	MRC	C17-C12-C11	3.75	118.34	111.43
4	A	993	MRC	O1A-C1-C2	3.77	118.98	110.61

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	993	MRC	C12

There are no torsion outliers.

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	T	75/75 (100%)	-0.27	2 (2%) 55 50	5, 30, 78, 100	2 (2%)
2	A	880/917 (95%)	-0.39	17 (1%) 67 64	3, 32, 70, 83	0
All	All	955/992 (96%)	-0.38	19 (1%) 65 62	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 [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	MRC	A	993	35/35	0.90	0.21	2.49	22,29,57,58	0
3	ZN	A	992	1/1	1.00	0.04	-1.35	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.