wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 06:01 PM GMT

PDB ID	:	2D6F
Title	:	Crystal structure of Glu-tRNA(Gln) amidotransferase in the complex with tRNA(Gln)
Authors	:	Nureki, O.
Deposited on	:	2005-11-13
Resolution	:	3.15 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html

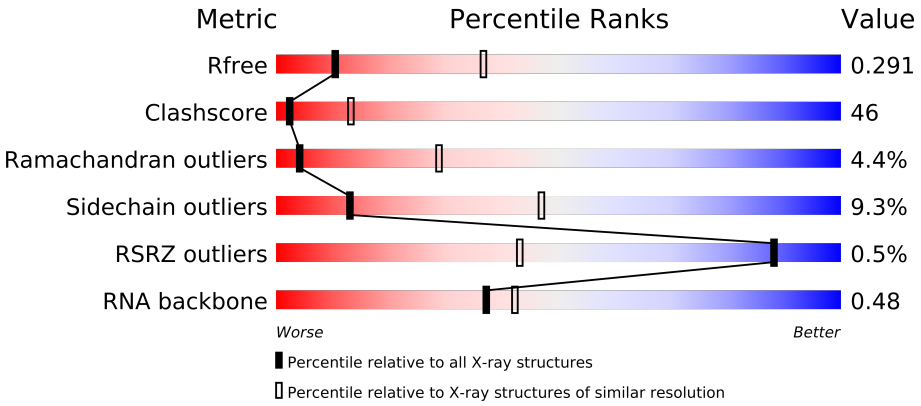
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.15 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}	66092	1360 (3.22-3.10)
Clashscore	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RSRZ outliers	66119	1361 (3.22-3.10)
RNA backbone	1838	1000 (3.68-2.64)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	E	74	
1	F	74	
2	A	435	
2	B	435	
3	C	619	
3	D	619	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17816 atoms, of which 0 are hydrogen and 0 are deuterium.

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 tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	72	Total	C	N	O	P	0	0	0
			1539	684	272	511	72			
1	F	74	Total	C	N	O	P	0	0	0
			1579	702	278	525	74			

- Molecule 2 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	424	Total	C	N	O	S	0	0	0
			3268	2028	575	641	24			
2	B	424	Total	C	N	O	S	0	0	0
			3274	2032	575	643	24			

- Molecule 3 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	485	Total	C	N	O	S	0	0	0
			3847	2390	690	752	15			
3	D	522	Total	C	N	O	S	0	0	0
			4127	2563	741	808	15			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

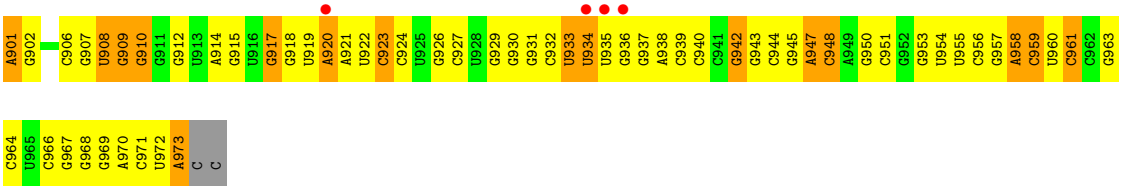
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	31	Total O 31 31	0	0
5	B	24	Total O 24 24	0	0
5	C	36	Total O 36 36	0	0
5	D	49	Total O 49 49	0	0
5	E	16	Total O 16 16	0	0
5	F	24	Total O 24 24	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: tRNA

Chain E:

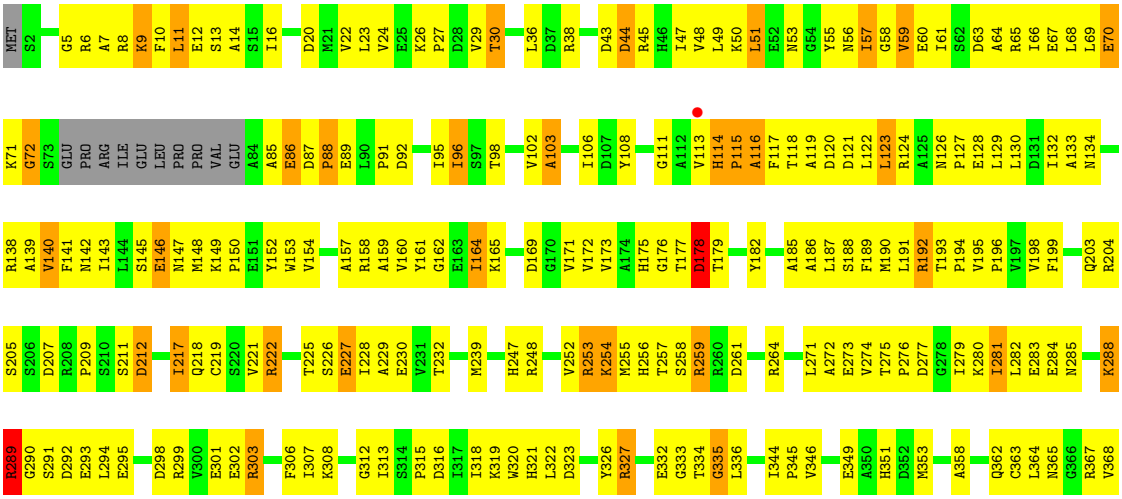


• Molecule 1: tRNA

Chain F:

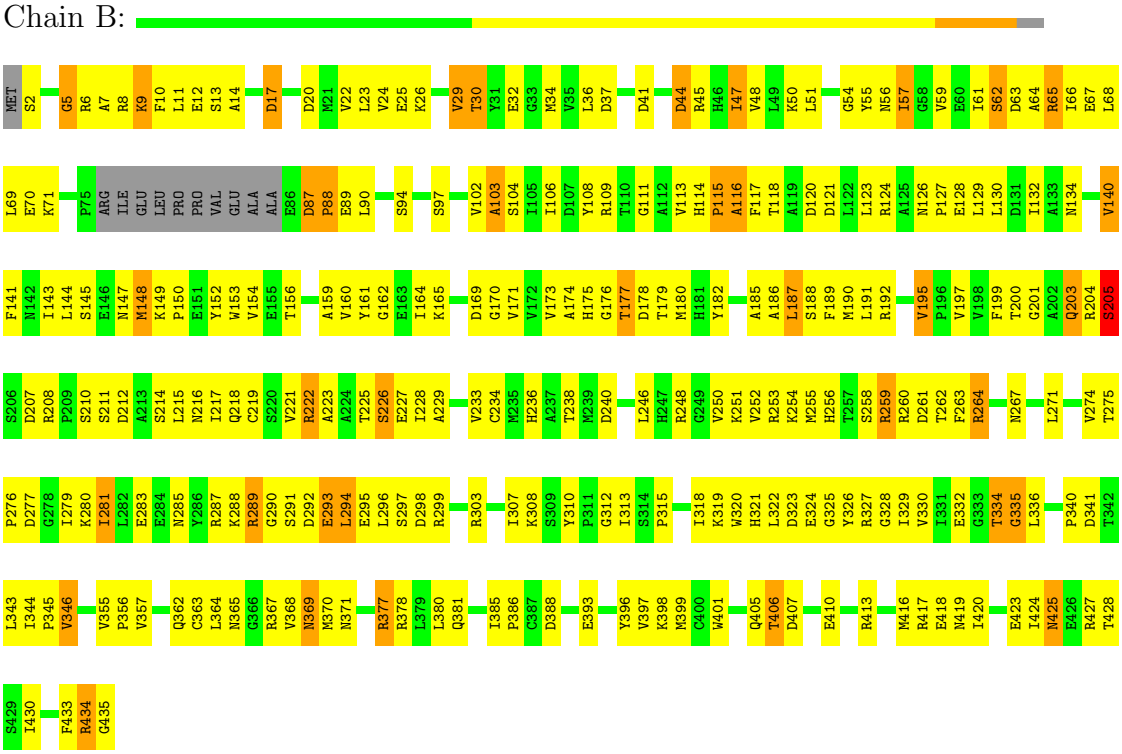
• Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit D

Chain A:



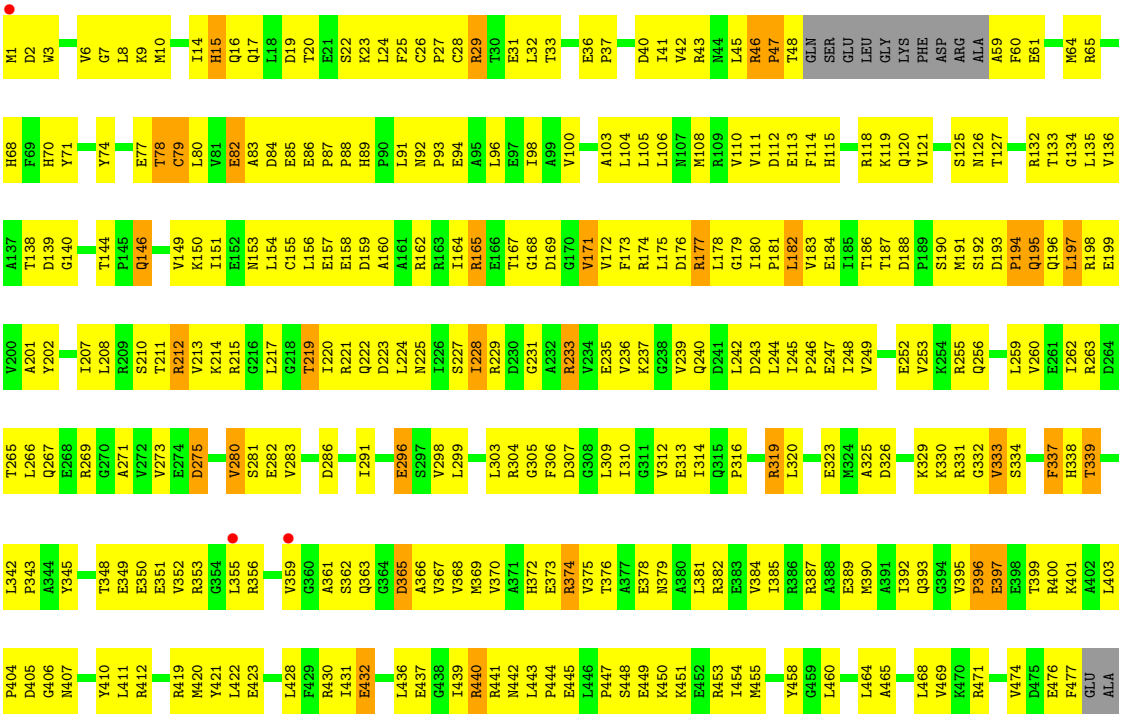
• Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit D

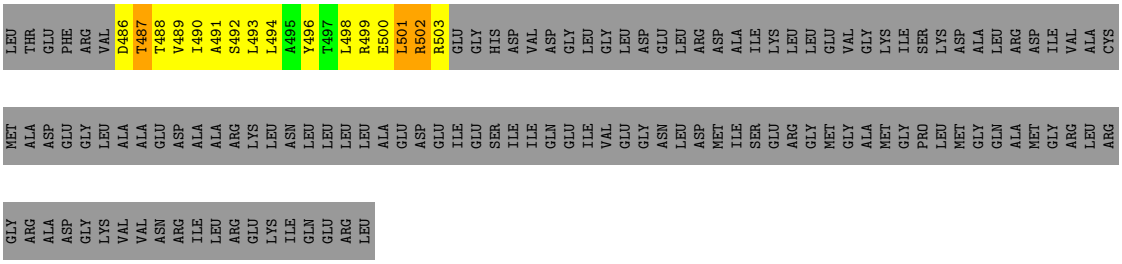
Chain B:



• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit E

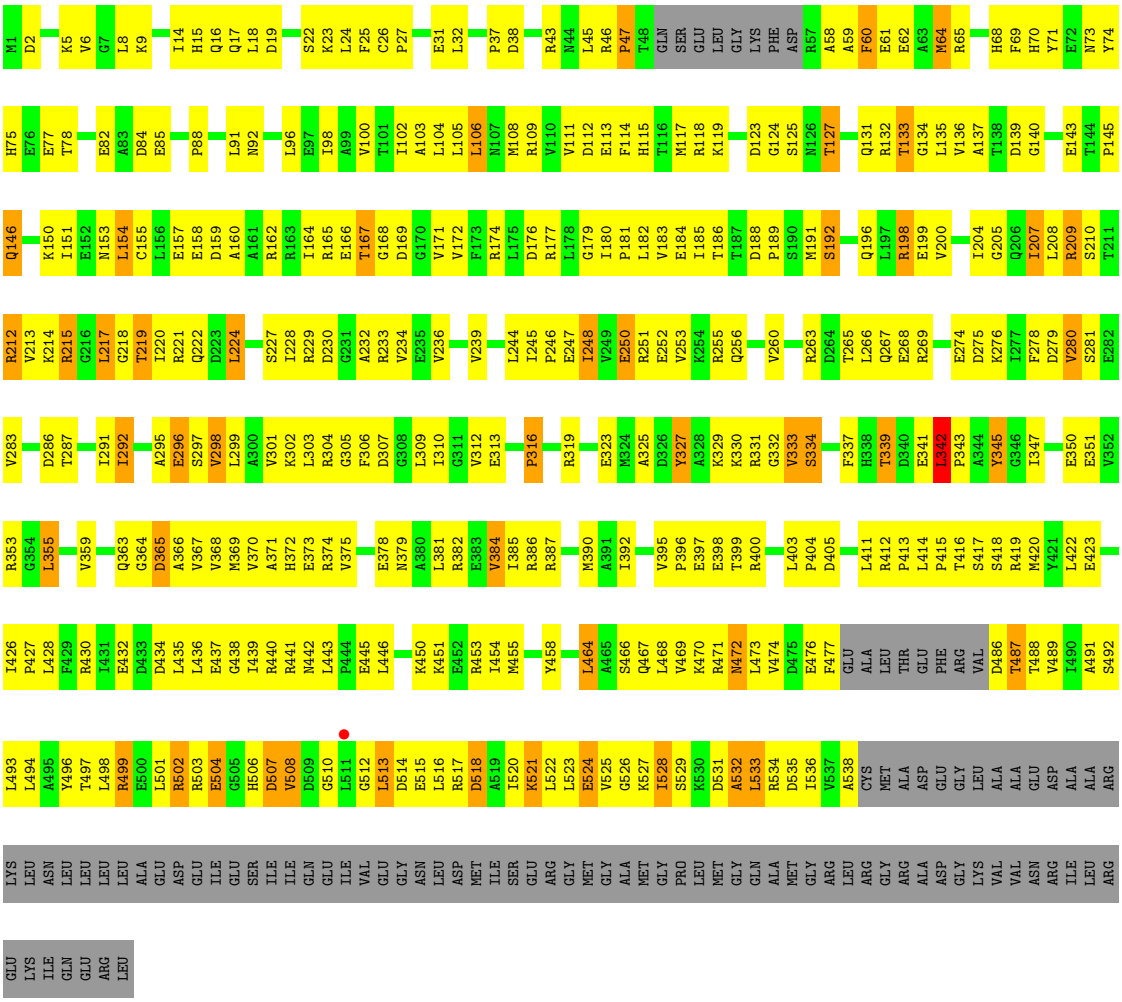
Chain C:





• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit E

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.81Å 140.71Å 186.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.52 – 3.15 70.35 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.52-3.15) 98.9 (70.35-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.13Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.292 0.228 , 0.291	Depositor DCC
R_{free} test set	2728 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	60.0	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 18.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 53863 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	17816	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	E	0.37	1/1718 (0.1%)	0.69	0/2676
1	F	0.40	1/1762 (0.1%)	0.72	0/2744
2	A	0.44	0/3323	0.71	1/4501 (0.0%)
2	B	0.45	0/3330	0.71	0/4511
3	C	0.36	0/3898	0.64	0/5265
3	D	0.44	0/4179	0.68	0/5642
All	All	0.42	2/18210 (0.0%)	0.69	1/25339 (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	F	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	901	A	OP3-P	-7.11	1.52	1.61
1	F	901	A	OP3-P	-6.87	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	192	ARG	N-CA-C	-5.15	97.09	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	960	U	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1539	0	777	77	0
1	F	1579	0	799	68	0
2	A	3268	0	3217	332	0
2	B	3274	0	3220	318	0
3	C	3847	0	3861	425	1
3	D	4127	0	4152	399	1
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	0	0	11	0
5	B	24	0	0	5	0
5	C	36	0	0	9	0
5	D	49	0	0	14	0
5	E	16	0	0	2	0
5	F	24	0	0	6	0
All	All	17816	0	16026	1543	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 46.

The worst 5 of 1543 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:133:THR:HG23	3:D:157:GLU:HB3	1.26	1.10
2:A:301:GLU:HG3	2:A:303:ARG:NH1	1.67	1.10
2:B:238:THR:HG23	2:B:240:ASP:H	1.12	1.08
3:D:43:ARG:HH11	3:D:43:ARG:HG2	1.19	1.06
3:C:233:ARG:HG3	3:C:397:GLU:HB3	1.37	1.06

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	Distance(Å)	Clash(Å)
3:C:169:ASP:OD2	3:D:268:GLU:OE1[4_556]	2.08	0.12

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
2	A	420/435 (97%)	349 (83%)	50 (12%)	21 (5%)	3 26
2	B	420/435 (97%)	337 (80%)	65 (16%)	18 (4%)	4 30
3	C	479/619 (77%)	411 (86%)	52 (11%)	16 (3%)	6 38
3	D	516/619 (83%)	436 (84%)	55 (11%)	25 (5%)	4 27
All	All	1835/2108 (87%)	1533 (84%)	222 (12%)	80 (4%)	4 29

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	13	SER
2	A	115	PRO
2	A	140	VAL
2	A	281	ILE
2	B	44	ASP

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	356/367 (97%)	320 (90%)	36 (10%)	11 41
2	B	358/367 (98%)	325 (91%)	33 (9%)	13 47
3	C	423/529 (80%)	388 (92%)	35 (8%)	16 55
3	D	452/529 (85%)	408 (90%)	44 (10%)	12 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1589/1792 (89%)	1441 (91%)	148 (9%)	13 47

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	425	ASN
3	C	171	VAL
3	D	384	VAL
2	B	434	ARG
3	C	82	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	425	ASN
3	C	131	GLN
3	D	267	GLN
3	C	73	ASN
3	C	146	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	71/74 (95%)	16 (22%)	1 (1%)
1	F	73/74 (98%)	19 (26%)	4 (5%)
All	All	144/148 (97%)	35 (24%)	5 (3%)

5 of 35 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	908	U
1	E	909	G
1	E	910	G
1	E	917	G
1	E	920	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	958	A

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Mol	Chain	Res	Type
1	F	907	G
1	F	909	G
1	F	958	A
1	F	960	U

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, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers (i)

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, 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	E	72/74 (97%)	-0.02	4 (5%) 24 4	83, 122, 174, 192	0
1	F	74/74 (100%)	0.06	1 (1%) 72 19	55, 88, 139, 152	0
2	A	424/435 (97%)	-0.35	1 (0%) 93 64	7, 33, 81, 113	0
2	B	424/435 (97%)	-0.35	0 100 100	12, 36, 68, 93	0
3	C	485/619 (78%)	-0.11	3 (0%) 86 39	23, 76, 133, 143	0
3	D	522/619 (84%)	-0.34	1 (0%) 93 64	9, 41, 102, 122	0
All	All	2001/2256 (88%)	-0.26	10 (0%) 88 43	7, 46, 127, 192	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	935	U	11.0
1	E	934	U	6.0
3	D	511	LEU	4.7
1	E	936	G	3.4
3	C	359	VAL	3.3

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 carbohydrates 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. 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, 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ZN	C	900	1/1	0.13	-1.15	41,41,41,41	0
4	ZN	D	1900	1/1	0.10	-1.54	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.