WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 10, 2024 – 08:14 AM EST

PDB ID	:	2TRA
Title	:	RESTRAINED REFINEMENT OF TWO CRYSTALLINE FORMS OF YEAST ASPARTIC ACID AND PHENYLALANINE TRANSFER RNA CRYSTALS
Authors	:	Westhof, E.; Dumas, P.; Moras, D.
Deposited on	:	1987-11-06
Resolution	:	3.00 Å(reported)

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

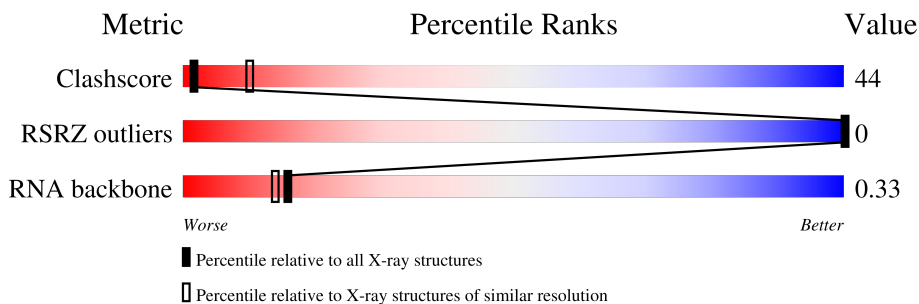|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.00 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
Clashscore		44
RSRZ outliers		0
RNA backbone		0.33

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))
Clashscore	141614	2416 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	75	7%　　　　　　　71%　　　　　　　20%　　・

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
1	H2U	A	19	-	-	-	X

2   Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1798 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 TRNAASP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	73	Total 1689	C 753	N 294	O 563	P 79	0	6	0

- Molecule 2 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).

SPM
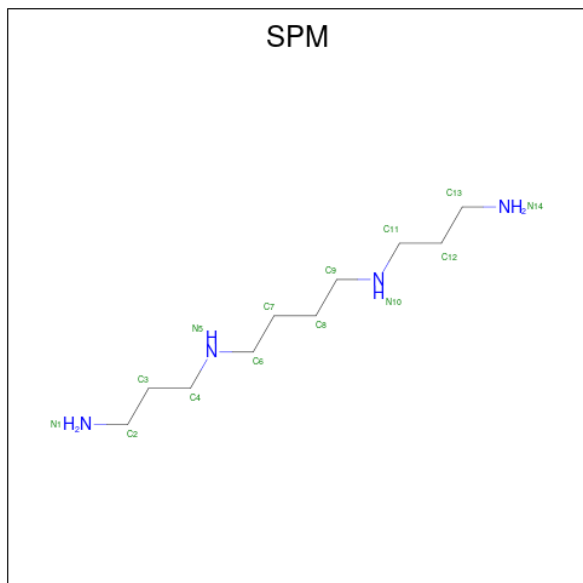
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 14	C 10	N 4	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total 94	O 94	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: TRNAASP
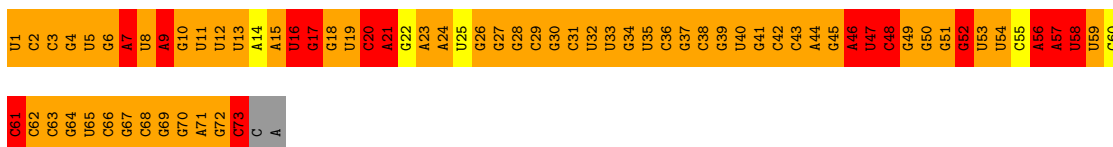
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	61.50Å 67.50Å 149.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 28.87 – 2.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.00) 70.1 (28.87-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 3.00Å)	Xtriage
Refinement program	NUCLSQ	Depositor
R, R_{free}	0.193 , (Not available) 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.02 , -4.5	EDS
L-test for twinning[2]	$< |L| > = 0.39, < L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	1798	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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: 5MC, PSU, MG, H2U, 5MU, 1MG, SPM

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	1.39	6/1679 (0.4%)	2.70	208/2614 (8.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	U	C4-O4	5.71	1.28	1.23
1	A	10	G	C4'-O4'	-5.38	1.38	1.45
1	A	42	C	C4'-O4'	-5.36	1.38	1.45
1	A	33	U	C4-O4	5.30	1.27	1.23
1	A	58	U	C4-O4	5.17	1.27	1.23

The worst 5 of 208 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
1	A	59	U	P-O3'-C3'	-15.85	100.68	119.70
1	A	45	G	O4'-C1'-N9	13.23	118.78	108.20
1	A	30	G	O4'-C1'-N9	9.89	116.11	108.20
1	A	12	U	C2-N3-C4	-9.66	121.20	127.00
1	A	65	U	C5-C4-O4	-9.54	120.18	125.90

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1689	0	862	114	2
2	A	14	0	26	2	0
3	A	1	0	0	0	0
4	A	94	0	0	3	0
All	All	1798	0	888	115	2

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 44.

The worst 5 of 115 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:71:A:C2'	1:A:72[B]:G:H5"	1.20	1.57
1:A:71:A:H2'	1:A:72[B]:G:C5'	1.49	1.43
1:A:71:A:C2'	1:A:72[B]:G:C5'	2.09	1.21
1:A:71:A:C3'	1:A:72[B]:G:H5"	1.95	0.95
1:A:52:G:H3'	1:A:53:5MU:H71	1.47	0.94

All (2) 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:A:33:U:O3'	1:A:34[B]:G:OP1[3_554]	1.77	0.43
1:A:56:A:N6	1:A:73:C:N3[5_455]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	66/75 (88%)	23 (34%)	0

5 of 23 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	C
1	A	7	A
1	A	8	U
1	A	9	A
1	A	16	H2U

There are no RNA pucker outliers to report.

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

9 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	5MC	A	48	1	18,22,23	0.64	0	26,32,35	1.24	2 (7%)
1	H2U	A	19	1	18,21,22	0.73	0	21,30,33	0.93	0
1	PSU	A	13	1	18,21,22	1.01	1 (5%)	22,30,33	1.13	2 (9%)
1	1MG	A	37	1	18,26,27	1.06	1 (5%)	19,39,42	0.88	1 (5%)
1	PSU	A	54[B]	1	18,21,22	0.58	0	22,30,33	0.75	0
1	5MU	A	53	1	19,22,23	0.87	0	28,32,35	1.66	7 (25%)
1	PSU	A	32	1	18,21,22	0.87	1 (5%)	22,30,33	0.99	1 (4%)
1	PSU	A	54[A]	1	18,21,22	0.55	0	22,30,33	0.83	0
1	H2U	A	16	1	18,21,22	0.59	0	21,30,33	0.99	2 (9%)

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	5MC	A	48	1	-	2/7/25/26	0/2/2/2
1	H2U	A	19	1	-	2/7/38/39	0/2/2/2
1	PSU	A	13	1	-	0/7/25/26	0/2/2/2
1	1MG	A	37	1	-	0/3/25/26	0/3/3/3
1	PSU	A	54[B]	1	-	3/7/25/26	0/2/2/2
1	5MU	A	53	1	-	0/7/25/26	0/2/2/2
1	PSU	A	32	1	-	4/7/25/26	0/2/2/2
1	PSU	A	54[A]	1	-	2/7/25/26	0/2/2/2
1	H2U	A	16	1	-	3/7/38/39	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	PSU	O4'-C1'	-2.63	1.40	1.43
1	A	32	PSU	C2'-C1'	-2.41	1.50	1.53
1	A	37	1MG	C8-N7	-2.33	1.31	1.35

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	5MU	C5-C4-N3	3.59	118.38	115.31
1	A	53	5MU	C4-N3-C2	-3.34	123.03	127.35
1	A	48	5MC	O4'-C1'-N1	2.97	115.16	108.36
1	A	53	5MU	O2-C2-N3	-2.94	116.03	121.50
1	A	48	5MC	C2'-C1'-N1	-2.70	105.57	113.22

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	16	H2U	C3'-C4'-C5'-O5'
1	A	54[B]	PSU	C3'-C4'-C5'-O5'
1	A	54[B]	PSU	O4'-C4'-C5'-O5'
1	A	16	H2U	O4'-C4'-C5'-O5'
1	A	48	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	48	5MC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	19	H2U	2	0
1	A	13	PSU	3	0
1	A	37	1MG	8	0
1	A	53	5MU	5	0
1	A	32	PSU	3	0
1	A	54[A]	PSU	1	0
1	A	16	H2U	3	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
2	SPM	A	76	-	13,13,13	1.44	4 (30%)	12,12,12	0.48	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	SPM	A	76	-	-	7/11/11/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	76	SPM	C4-N5	2.45	1.55	1.46
2	A	76	SPM	C6-N5	2.31	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	76	SPM	C11-N10	2.27	1.54	1.46
2	A	76	SPM	C9-N10	2.13	1.54	1.46

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	76	SPM	N10-C11-C12-C13
2	A	76	SPM	N5-C6-C7-C8
2	A	76	SPM	N1-C2-C3-C4
2	A	76	SPM	C7-C8-C9-N10
2	A	76	SPM	C3-C4-N5-C6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	76	SPM	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	33:U	O3'	34[B]:G	P	14.39
1	A	72[B]:G	O3'	73:C	P	3.94
1	A	54[B]:PSU	O3'	55:C	P	1.96
1	A	53:5MU	O3'	54[B]:PSU	P	1.26
1	A	71:A	O3'	72[B]:G	P	1.24

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(Å²)	Q<0.9
1	A	65/75 (86%)	-0.65	0	100	100	2, 10, 45, 52	4 (6%)

There are no RSRZ outliers to report.

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(Å²)	Q<0.9
1	H2U	A	19	20/21	0.74	0.50	46,48,49,50	20
1	H2U	A	16	20/21	0.89	0.33	17,30,32,33	20
1	PSU	A	54[A]	20/21	0.94	0.16	21,28,34,36	8
1	PSU	A	54[B]	20/21	0.94	0.16	34,34,35,35	20
1	5MU	A	53	21/22	0.95	0.11	15,22,26,27	0
1	PSU	A	13	20/21	0.95	0.11	1,4,13,17	0
1	1MG	A	37	24/25	0.95	0.13	20,23,34,40	0
1	PSU	A	32	20/21	0.96	0.12	2,14,22,22	0
1	5MC	A	48	21/22	0.97	0.13	1,1,7,12	0

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	MG	A	77	1/1	0.80	0.35	30,30,30,30	1
2	SPM	A	76	14/14	0.81	0.38	25,25,25,25	13

6.5 Other polymers ⓘ

There are no such residues in this entry.