



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:41 am GMT

PDB ID : 2AGZ  
Title : Crystal structure of the carbinolamine intermediate in the reductive half-reaction of aromatic amine dehydrogenase (AADH) with tryptamine. F222 form  
Authors : Masgrau, L.; Roujeinikova, A.; Johannissen, L.O.; Hothi, P.; Basran, J.; Ranaghan, K.E.; Mulholland, A.J.; Sutcliffe, M.J.; Scrutton, N.S.; Leys, D.  
Deposited on : 2005-07-27  
Resolution : 1.60 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](mailto: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.

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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

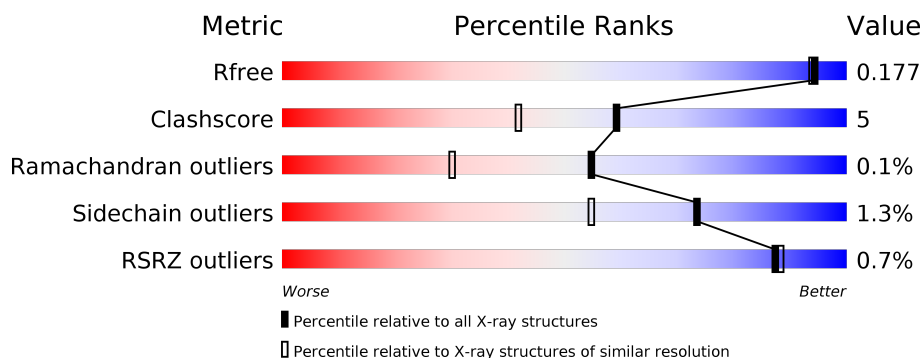
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	2696 (1.60-1.60)
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)
RSRZ outliers	101464	2714 (1.60-1.60)

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  $\geq 3$ , 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	D	135	
1	H	135	
2	A	361	
2	B	361	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TSC	D	190	-	-	-	X
4	TSC	H	191	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8662 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 Aromatic amine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	109	Total	C	N	O	S	0	4	0
			853	523	146	169	15			
1	H	115	Total	C	N	O	S	0	0	0
			871	530	154	172	15			

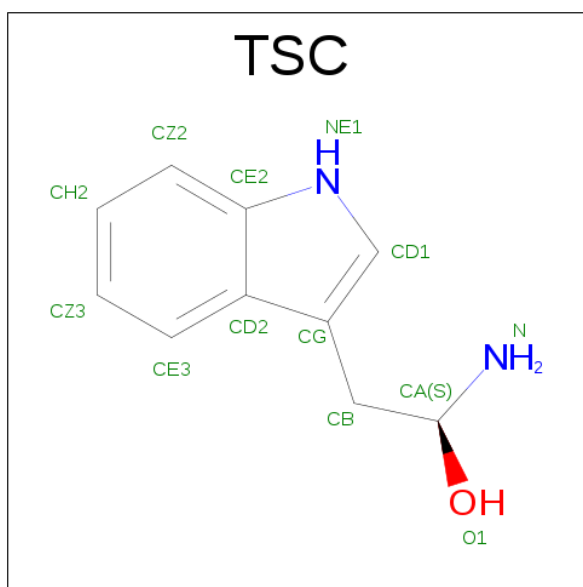
- Molecule 2 is a protein called Aromatic amine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	361	Total	C	N	O	S	0	1	0
			2816	1776	491	535	14			
2	B	361	Total	C	N	O	S	0	1	0
			2810	1772	490	534	14			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (1S)-1-AMINO-2-(1H-INDOL-3-YL)ETHANOL (three-letter code: TSC) (formula: C<sub>10</sub>H<sub>12</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			13	10	2	1		
4	H	1	Total	C	N	O	0	0
			13	10	2	1		

- Molecule 5 is water.

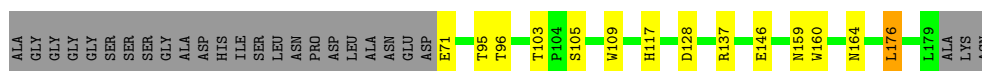
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	532	Total	O	0	0
			532	532		
5	B	481	Total	O	0	0
			481	481		
5	D	141	Total	O	0	0
			141	141		
5	H	130	Total	O	0	0
			130	130		

### 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.

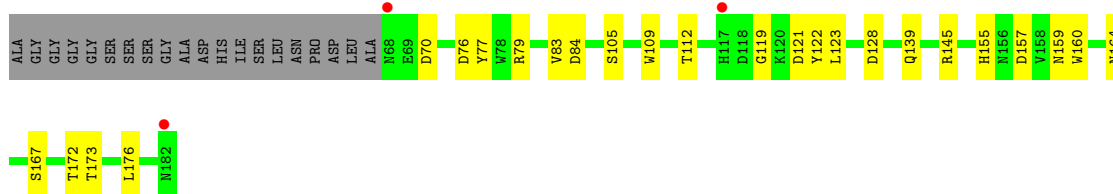
- Molecule 1: Aromatic amine dehydrogenase

Chain D: 




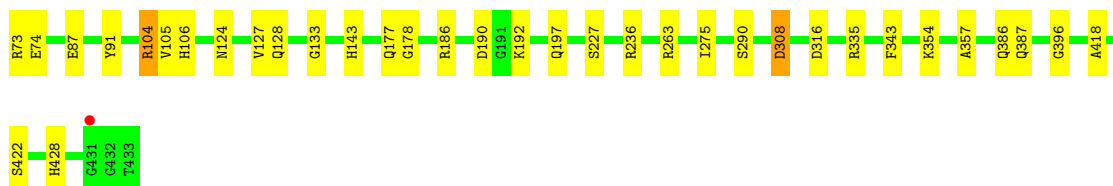
- Molecule 1: Aromatic amine dehydrogenase

Chain H: 




- Molecule 2: Aromatic amine dehydrogenase

Chain A: 



- Molecule 2: Aromatic amine dehydrogenase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.91Å 157.34Å 268.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.60 134.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.5 (15.00-1.60) 93.5 (134.00-1.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, $R_{free}$	0.142 , 0.169 0.151 , 0.177	Depositor DCC
$R_{free}$ test set	7752 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 67.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8662	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRQ, ZN, TSC

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	D	0.65	0/872	0.90	2/1188 (0.2%)
1	H	0.63	0/878	0.85	0/1196
2	A	0.63	0/2883	0.86	5/3906 (0.1%)
2	B	0.58	0/2877	0.82	4/3900 (0.1%)
All	All	0.62	0/7510	0.85	11/10190 (0.1%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	263	ARG	NE-CZ-NH1	7.91	124.26	120.30
2	A	263	ARG	NE-CZ-NH2	-7.44	116.58	120.30
2	A	316	ASP	CB-CG-OD2	6.33	124.00	118.30
1	D	176	LEU	CA-CB-CG	6.09	129.30	115.30
2	B	303	ASP	CB-CG-OD2	5.74	123.47	118.30

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	D	853	0	755	12	0
1	H	871	0	753	15	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2816	0	2758	30	0
2	B	2810	0	2748	28	0
3	D	1	0	0	0	0
3	H	1	0	0	0	0
4	D	13	0	10	1	0
4	H	13	0	10	2	0
5	A	532	0	0	10	0
5	B	481	0	0	9	0
5	D	141	0	0	5	0
5	H	130	0	0	4	0
All	All	8662	0	7034	78	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 5.

The worst 5 of 78 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)
2:B:217:GLU:HG3	2:B:257:LYS:HA	1.37	1.05
2:B:93:MET:SD	5:B:905:HOH:O	2.16	1.04
1:D:95[A]:THR:HG22	5:D:399:HOH:O	1.76	0.85
1:H:173:THR:HA	5:H:355:HOH:O	1.76	0.84
2:B:73:ARG:N	5:B:692:HOH:O	2.12	0.83

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:H:119:GLY:O	1:H:121:ASP:OD2[14_455]	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	
1	D	110/135 (82%)	107 (97%)	3 (3%)	0	100	100
1	H	112/135 (83%)	109 (97%)	3 (3%)	0	100	100
2	A	360/361 (100%)	347 (96%)	13 (4%)	0	100	100
2	B	360/361 (100%)	349 (97%)	10 (3%)	1 (0%)	44	22
All	All	942/992 (95%)	912 (97%)	29 (3%)	1 (0%)	55	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	200	SER

### 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	
1	D	98/112 (88%)	97 (99%)	1 (1%)	80	65
1	H	97/112 (87%)	93 (96%)	4 (4%)	35	11
2	A	305/305 (100%)	303 (99%)	2 (1%)	87	77
2	B	304/305 (100%)	301 (99%)	3 (1%)	80	65
All	All	804/834 (96%)	794 (99%)	10 (1%)	73	58

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	145	ARG
2	A	104	ARG
2	B	73	ARG
1	H	123	LEU
2	A	308	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	386	GLN
2	A	426	GLN
2	B	406	GLN
2	A	406	GLN
2	A	428	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	TRQ	D	109	1,4	14,16,18	4.77	4 (28%)	13,22,26	1.63	3 (23%)
1	TRQ	H	109	1,4	14,16,18	4.61	5 (35%)	13,22,26	1.79	4 (30%)

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	TRQ	D	109	1,4	-	0/3/16/21	0/2/2/2
1	TRQ	H	109	1,4	-	0/3/16/21	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	109	TRQ	CE2-CZ2	-9.20	1.39	1.50
1	H	109	TRQ	CE2-CZ2	-8.85	1.40	1.50
1	D	109	TRQ	CH2-CZ3	-4.32	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	109	TRQ	CH2-CZ3	-3.77	1.40	1.49
1	H	109	TRQ	CA-C	3.62	1.55	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	109	TRQ	O7-CZ2-CE2	-3.32	116.64	122.33
1	D	109	TRQ	O7-CZ2-CE2	-3.17	116.91	122.33
1	H	109	TRQ	CB-CG-CD1	-2.99	124.28	127.97
1	D	109	TRQ	CB-CG-CD1	-2.12	125.35	127.97
1	H	109	TRQ	O7-CZ2-CH2	2.28	124.04	120.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	109	TRQ	1	0
1	H	109	TRQ	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	TSC	D	190	1	12,14,14	1.15	1 (8%)	13,19,19	2.94	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	TSC	H	191	1	12,14,14	0.98	0	13,19,19	2.73	3 (23%)

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	TSC	D	190	1	-	0/3/4/4	0/2/2/2
4	TSC	H	191	1	-	0/3/4/4	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	190	TSC	CE3-CD2	-2.37	1.37	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	190	TSC	CB-CG-CD1	-7.39	118.83	127.97
4	H	191	TSC	CB-CG-CD1	-6.08	120.46	127.97
4	H	191	TSC	CG-CB-CA	-5.47	104.87	112.73
4	D	190	TSC	CG-CB-CA	-4.35	106.48	112.73
4	D	190	TSC	O1-CA-N	-2.02	111.28	113.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	190	TSC	1	0
4	H	191	TSC	2	0

## 5.7 Other polymers ⓘ

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	D	108/135 (80%)	-0.60	0 <b>100</b> <b>100</b>	11, 15, 24, 38	0
1	H	114/135 (84%)	-0.35	3 (2%) 56 55	12, 18, 41, 63	0
2	A	361/361 (100%)	-0.59	1 (0%) <b>93</b> <b>93</b>	10, 15, 31, 50	0
2	B	361/361 (100%)	-0.60	3 (0%) <b>86</b> <b>87</b>	11, 18, 32, 75	0
All	All	944/992 (95%)	-0.56	7 (0%) <b>87</b> <b>88</b>	10, 17, 32, 75	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	433	THR	8.8
2	B	432	GLY	5.1
2	B	431	GLY	4.2
1	H	68	ASN	3.9
1	H	182	ASN	3.4

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
1	TRQ	H	109	15/17	0.97	0.06	-	11,14,18,23	0
1	TRQ	D	109	15/17	0.96	0.07	-	11,12,15,18	0

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	TSC	H	191	13/13	0.91	0.12	12.68	21,24,29,35	0
4	TSC	D	190	13/13	0.94	0.11	6.46	17,21,26,28	0
3	ZN	H	300	1/1	0.98	0.11	-	20,20,20,20	1
3	ZN	D	301	1/1	0.99	0.07	-	15,15,15,15	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.