W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 01:42 pm BST

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)

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

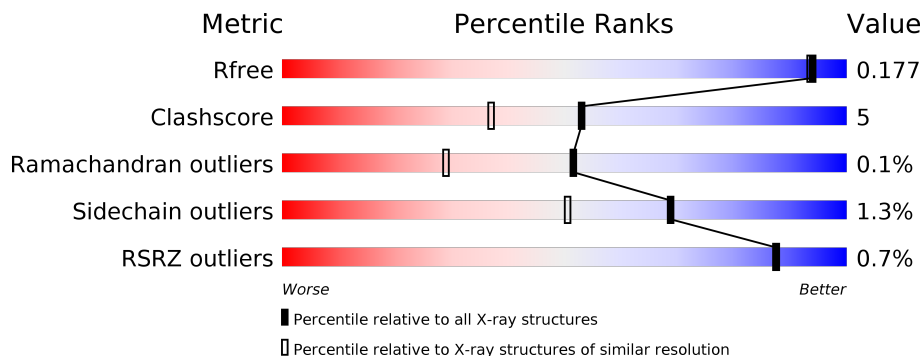|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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	Percentile Ranks	Value
Rfree		0.177
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		1.3%
RSRZ outliers		0.7%

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))
R$_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 >=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	D	135	70% 10% • 19%
1	H	135	2% 67% 19% 15%
2	A	361	90% 9% •
2	B	361	% 92% 6% •

2 Entry composition (i)

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 853	C 523	N 146	O 169	S 15	0	4	0
1	H	115	Total 871	C 530	N 154	O 172	S 15	0	0	0

- Molecule 2 is a protein called Aromatic amine dehydrogenase.

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

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

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

- Molecule 4 is (1S)-1-AMINO-2-(1H-INDOL-3-YL)ETHANOL (three-letter code: TSC) (formula: $C_{10}H_{12}N_2O$).

TSC

CZ2

CE2

NE1

H
N

CH2

CD1

CZ3

CD2

CG

N

NH₂

CE3

CA(S)

CB

OH

O1
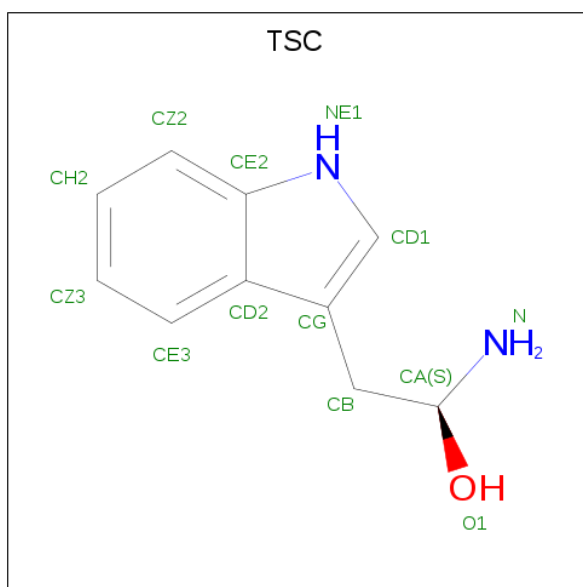
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total C N O 13　10　2　1				0	0
4	H	1	Total C N O 13　10　2　1				0	0

• Molecule 5 is water.

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

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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

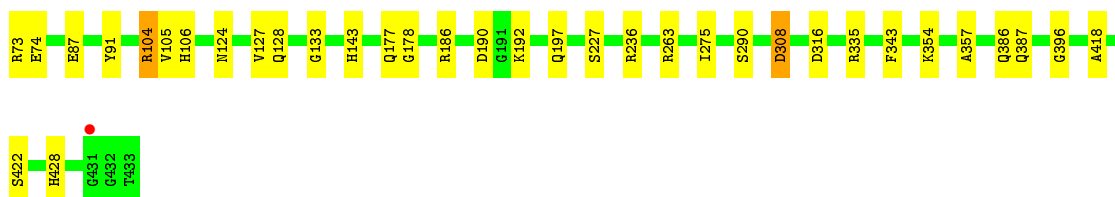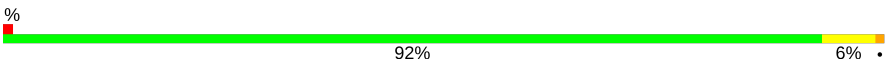- Molecule 1: Aromatic amine dehydrogenase

- Molecule 2: Aromatic amine dehydrogenase

- Molecule 2: Aromatic amine dehydrogenase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	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
$<I/\sigma(I)>$ [1]	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 (4.69%)	wwPDB-VP
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.3	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	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^2)	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.*

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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 (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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 (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	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%)	41	21
All	All	942/992 (95%)	912 (97%)	29 (3%)	1 (0%)	51	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	200	SER

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	
1	D	98/112 (88%)	97 (99%)	1 (1%)	76	61
1	H	97/112 (87%)	93 (96%)	4 (4%)	30	9
2	A	305/305 (100%)	303 (99%)	2 (1%)	84	73
2	B	304/305 (100%)	301 (99%)	3 (1%)	76	61
All	All	804/834 (96%)	794 (99%)	10 (1%)	69	54

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 (i)

There are no RNA molecules in this entry.

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

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	H	109	1,4	11,16,18	4.64	3 (27%)	11,22,26	2.00	4 (36%)
1	TRQ	D	109	1,4	11,16,18	4.77	3 (27%)	11,22,26	1.91	3 (27%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	109	TRQ	O7-CZ2	13.98	1.44	1.22
1	H	109	TRQ	O7-CZ2	13.14	1.43	1.22
1	H	109	TRQ	CE3-CZ3	6.70	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	109	TRQ	CE3-CZ3	5.59	1.42	1.33
1	D	109	TRQ	CH2-CZ3	-3.52	1.39	1.48

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	109	TRQ	CG-CB-CA	3.90	120.55	114.53
1	H	109	TRQ	CG-CB-CA	3.40	119.79	114.53
1	D	109	TRQ	CZ3-CH2-CZ2	3.12	120.48	113.19
1	H	109	TRQ	CB-CG-CD1	-2.99	124.28	127.97
1	H	109	TRQ	CZ3-CH2-CZ2	2.84	119.82	113.19

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	H	109	TRQ	1	0
1	D	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	1.17	1 (8%)	13,19,19	2.68	3 (23%)

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	1.00	0	13,19,19	2.26	2 (15%)

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	-	2/3/4/4	0/2/2/2
4	TSC	H	191	1	-	2/3/4/4	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	-2.42	1.37	1.42

All (5) 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	D	190	TSC	CB-CG-CD2	5.51	134.82	126.25
4	H	191	TSC	CB-CG-CD2	4.60	133.41	126.25
4	D	190	TSC	O1-CA-N	-2.02	111.28	113.56

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	190	TSC	N-CA-CB-CG
4	H	191	TSC	O1-CA-CB-CG
4	H	191	TSC	N-CA-CB-CG
4	D	190	TSC	O1-CA-CB-CG

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 (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(Å²)	Q<0.9
1	D	108/135 (80%)	-0.60	0	100	100	11, 15, 24, 38	0
1	H	114/135 (84%)	-0.35	3 (2%)	56	53	12, 18, 41, 63	0
2	A	361/361 (100%)	-0.59	1 (0%)	94	93	10, 15, 31, 50	0
2	B	361/361 (100%)	-0.60	3 (0%)	86	86	11, 18, 32, 75	0
All	All	944/992 (95%)	-0.56	7 (0%)	87	87	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. 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	TRQ	D	109	15/17	0.96	0.07	11,12,15,18	0
1	TRQ	H	109	15/17	0.97	0.06	11,14,18,23	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. 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
4	TSC	H	191	13/13	0.91	0.12	21,24,29,35	0
4	TSC	D	190	13/13	0.94	0.11	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.