



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:36 am GMT

PDB ID : 2AGX  
Title : Crystal structure of the Schiff base intermediate in the reductive half-reaction of aromatic amine dehydrogenase (AADH) with tryptamine. P212121 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 : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

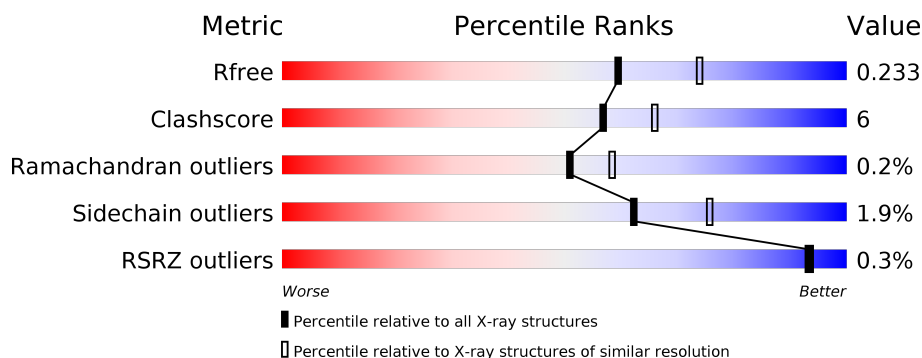
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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
3	TSH	D	2	-	-	-	X
3	TSH	H	1	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7929 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.

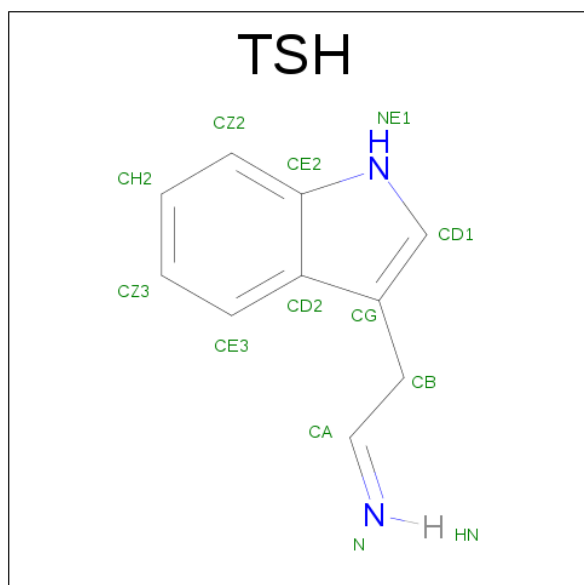
- Molecule 1 is a protein called Aromatic amine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	109	Total	C	N	O	S	0	0	0
			835	510	147	163	15			
1	H	121	Total	C	N	O	S	0	0	0
			912	557	161	179	15			

- Molecule 2 is a protein called Aromatic amine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	359	Total	C	N	O	S	0	0	0
			2798	1765	489	531	13			
2	B	359	Total	C	N	O	S	0	0	0
			2783	1755	486	529	13			

- Molecule 3 is 2-(1H-INDOL-3-YL)ETHANIMINE (three-letter code: TSH) (formula: C<sub>10</sub>H<sub>10</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	N	0	0
			12	10	2		
3	D	1	Total	C	N	0	0
			12	10	2		

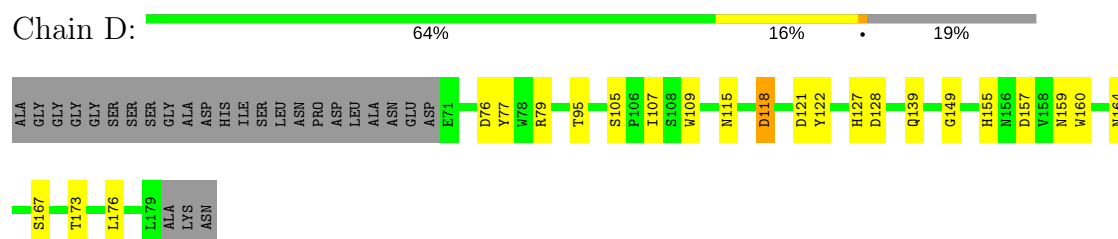
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	223	Total	O	0	0
			223	223		
4	B	239	Total	O	0	0
			239	239		
4	D	48	Total	O	0	0
			48	48		
4	H	67	Total	O	0	0
			67	67		

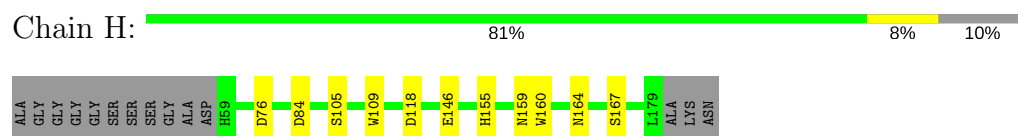
### 3 Residue-property plots

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.

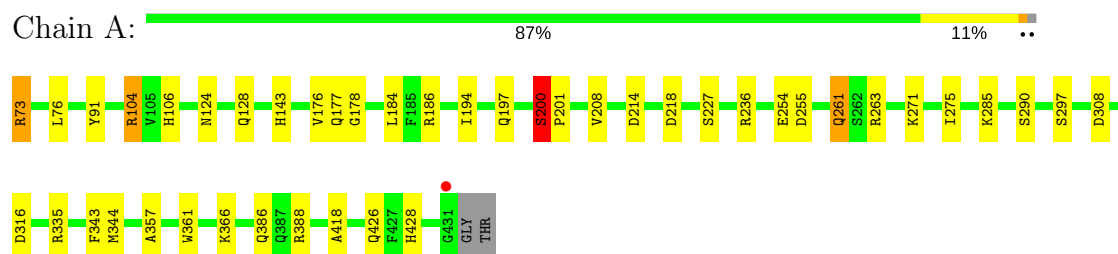
#### • Molecule 1: Aromatic amine dehydrogenase



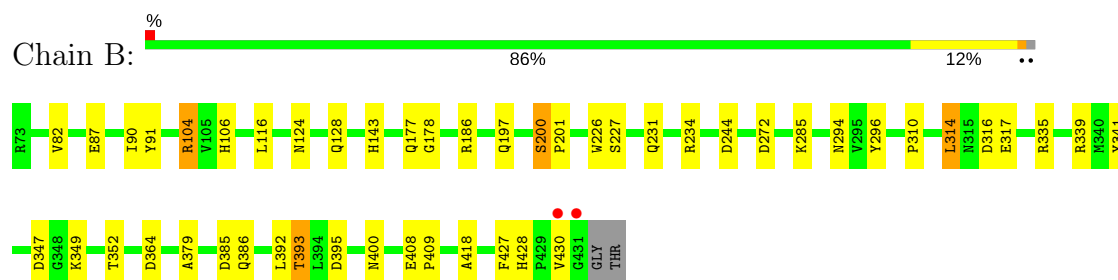
#### • Molecule 1: Aromatic amine dehydrogenase



#### • Molecule 2: Aromatic amine dehydrogenase



#### • Molecule 2: Aromatic amine dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.37Å 96.19Å 120.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 75.13 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.3 (15.00-2.20) 91.1 (75.13-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, $R_{free}$	0.159 , 0.225 0.165 , 0.233	Depositor DCC
$R_{free}$ test set	2490 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7929	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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, TSH

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	0.56	0/842	0.81	4/1146 (0.3%)
1	H	0.54	0/920	0.75	2/1255 (0.2%)
2	A	0.57	0/2862	0.81	5/3879 (0.1%)
2	B	0.59	0/2847	0.81	8/3863 (0.2%)
All	All	0.57	0/7471	0.80	19/10143 (0.2%)

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
2	A	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	244	ASP	CB-CG-OD2	6.86	124.47	118.30
2	A	214	ASP	CB-CG-OD2	6.57	124.21	118.30
2	A	316	ASP	CB-CG-OD2	6.46	124.12	118.30
2	A	308	ASP	CB-CG-OD2	6.45	124.11	118.30
1	D	118	ASP	CB-CG-OD2	6.32	123.99	118.30
2	B	314	LEU	CA-CB-CG	6.18	129.51	115.30
2	B	385	ASP	CB-CG-OD2	5.83	123.55	118.30
2	B	395	ASP	CB-CG-OD2	5.78	123.50	118.30
2	A	255	ASP	CB-CG-OD2	5.71	123.44	118.30
1	H	76	ASP	CB-CG-OD2	5.69	123.42	118.30
2	B	316	ASP	CB-CG-OD2	5.60	123.34	118.30
1	D	128	ASP	CB-CG-OD2	5.44	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	121	ASP	CB-CG-OD2	5.32	123.09	118.30
1	H	118	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	347	ASP	CB-CG-OD2	5.12	122.91	118.30
2	B	364	ASP	CB-CG-OD2	5.05	122.85	118.30
2	A	218	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	76	ASP	CB-CG-OD2	5.02	122.82	118.30
2	B	272	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	200	SER	Peptide

## 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	835	0	732	17	0
1	H	912	0	792	10	0
2	A	2798	0	2740	27	0
2	B	2783	0	2705	33	0
3	D	12	0	9	1	0
3	H	12	0	9	1	0
4	A	223	0	0	3	0
4	B	239	0	0	4	0
4	D	48	0	0	3	0
4	H	67	0	0	2	0
All	All	7929	0	6987	81	0

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 6.

All (81) 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:393:THR:HG21	4:B:479:HOH:O	1.74	0.86
2:B:393:THR:HG22	2:B:400:ASN:HD22	1.44	0.82
1:D:105:SER:HA	1:D:164:ASN:HD21	1.46	0.80
2:A:236:ARG:HD3	4:A:625:HOH:O	1.83	0.77
1:H:109:TRQ:HB2	1:H:160:TRP:HE1	1.51	0.76
2:B:124:ASN:HD21	2:B:178:GLY:H	1.33	0.75
1:H:109:TRQ:HB2	1:H:160:TRP:NE1	2.01	0.74
1:H:105:SER:HA	1:H:164:ASN:HD21	1.54	0.72
2:B:91:TYR:OH	2:B:428:HIS:HD2	1.73	0.71
1:D:109:TRQ:HB2	1:D:160:TRP:NE1	2.08	0.68
1:D:139:GLN:NE2	4:D:222:HOH:O	2.26	0.68
1:D:109:TRQ:HB2	1:D:160:TRP:HE1	1.57	0.67
2:A:104:ARG:HH11	2:A:106:HIS:HE1	1.44	0.64
2:B:335:ARG:H	2:B:386:GLN:HE22	1.45	0.64
2:B:104:ARG:HH11	2:B:106:HIS:HE1	1.45	0.64
2:A:124:ASN:HD21	2:A:178:GLY:H	1.46	0.63
1:D:167:SER:HB2	2:B:177:GLN:HE22	1.63	0.63
2:A:335:ARG:H	2:A:386:GLN:HE22	1.47	0.62
2:A:197:GLN:NE2	2:A:227:SER:H	2.00	0.60
2:B:335:ARG:H	2:B:386:GLN:NE2	2.00	0.59
1:D:77:TYR:CE1	1:D:79:ARG:HB2	2.38	0.59
2:A:186:ARG:HH22	2:A:426:GLN:NE2	2.01	0.58
2:B:124:ASN:ND2	2:B:178:GLY:H	2.02	0.58
2:A:91:TYR:OH	2:A:428:HIS:HD2	1.86	0.57
2:A:335:ARG:H	2:A:386:GLN:NE2	2.01	0.57
2:B:197:GLN:NE2	2:B:227:SER:H	2.02	0.57
2:B:231:GLN:NE2	2:B:234:ARG:HH11	2.03	0.56
1:D:159:ASN:HD22	2:B:177:GLN:NE2	2.05	0.55
2:A:128:GLN:HE22	2:A:186:ARG:C	2.10	0.54
1:H:159:ASN:HD22	2:A:177:GLN:NE2	2.06	0.54
2:A:200:SER:N	2:A:201:PRO:HA	2.22	0.54
2:A:197:GLN:HE21	2:A:227:SER:H	1.55	0.53
1:H:155:HIS:HE1	4:A:459:HOH:O	1.92	0.53
4:D:184:HOH:O	2:B:143:HIS:HE1	1.92	0.52
2:B:90:ILE:HG21	2:B:392:LEU:HD11	1.91	0.52
2:A:73:ARG:HA	2:A:73:ARG:HH11	1.76	0.51
1:H:84:ASP:OD2	3:H:1:TSH:HD1	2.12	0.50
2:B:124:ASN:ND2	2:B:177:GLN:HA	2.26	0.50
2:B:128:GLN:HE22	2:B:186:ARG:C	2.15	0.50
4:H:211:HOH:O	2:A:143:HIS:HE1	1.95	0.49
1:D:122:TYR:CD2	1:D:176:LEU:HD21	2.47	0.49
2:B:341:TYR:N	2:B:341:TYR:CD1	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:SER:HB2	2:A:177:GLN:HE22	1.78	0.49
1:H:146:GLU:OE2	1:H:155:HIS:HD2	1.96	0.49
2:A:200:SER:N	2:A:201:PRO:CA	2.76	0.48
2:B:200:SER:N	2:B:201:PRO:HA	2.29	0.48
2:A:343:PHE:HB3	2:A:357:ALA:HB2	1.97	0.47
2:B:296:TYR:CZ	2:B:310:PRO:HB3	2.51	0.46
4:D:184:HOH:O	2:B:143:HIS:CE1	2.68	0.46
1:D:155:HIS:HE1	4:B:439:HOH:O	1.99	0.46
2:A:275:ILE:HA	2:A:290:SER:HA	1.97	0.46
2:B:197:GLN:HE21	2:B:227:SER:H	1.63	0.46
1:D:95:THR:O	1:D:173:THR:HB	2.17	0.45
2:B:393:THR:CG2	2:B:400:ASN:HD22	2.24	0.45
1:D:115:ASN:HD22	1:D:118:ASP:CG	2.20	0.44
2:B:200:SER:N	2:B:201:PRO:CA	2.81	0.44
2:B:294:ASN:HB3	2:B:310:PRO:HB2	2.00	0.44
2:B:379:ALA:HB2	2:B:393:THR:HG23	1.99	0.43
2:A:261:GLN:HE21	2:A:261:GLN:HB3	1.67	0.43
2:A:194:ILE:HB	2:A:208:VAL:HB	1.99	0.43
1:H:146:GLU:OE2	1:H:155:HIS:CD2	2.72	0.43
4:H:211:HOH:O	2:A:143:HIS:CE1	2.71	0.43
1:D:155:HIS:CE1	4:B:439:HOH:O	2.70	0.43
2:A:186:ARG:HH22	2:A:426:GLN:HE22	1.64	0.42
1:H:155:HIS:CE1	4:A:459:HOH:O	2.71	0.42
2:B:87:GLU:HA	2:B:430:VAL:HG11	2.01	0.42
1:D:159:ASN:HB2	3:D:2:TSH:CZ3	2.49	0.42
1:D:107:ILE:HD12	1:D:160:TRP:CE3	2.54	0.42
2:A:124:ASN:ND2	2:A:177:GLN:HA	2.35	0.42
2:B:408:GLU:HA	2:B:409:PRO:HD3	1.93	0.42
2:A:106:HIS:HD2	2:A:418:ALA:O	2.03	0.41
2:B:106:HIS:HD2	2:B:418:ALA:O	2.04	0.41
2:A:344:MET:HG3	2:A:361:TRP:CD2	2.55	0.41
1:D:127:HIS:HB2	2:A:76:LEU:CD2	2.50	0.41
2:B:82:VAL:HG13	2:B:116:LEU:HB3	2.03	0.41
2:B:339:ARG:HD3	4:B:619:HOH:O	2.21	0.41
2:B:392:LEU:HG	2:B:427:PHE:CE1	2.56	0.40
1:D:149:GLY:HA3	2:B:226:TRP:CD1	2.55	0.40
1:D:155:HIS:NE2	1:D:157:ASP:HB2	2.36	0.40
2:B:349:LYS:O	2:B:352:THR:HG23	2.21	0.40
2:A:176:VAL:HG11	2:A:184:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

## 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	106/135 (78%)	98 (92%)	8 (8%)	0	100	100
1	H	118/135 (87%)	113 (96%)	5 (4%)	0	100	100
2	A	357/361 (99%)	341 (96%)	15 (4%)	1 (0%)	44	49
2	B	357/361 (99%)	341 (96%)	15 (4%)	1 (0%)	44	49
All	All	938/992 (95%)	893 (95%)	43 (5%)	2 (0%)	51	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	200	SER
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	95/112 (85%)	95 (100%)	0	100	100
1	H	101/112 (90%)	101 (100%)	0	100	100
2	A	303/305 (99%)	293 (97%)	10 (3%)	43	54
2	B	299/305 (98%)	294 (98%)	5 (2%)	66	79
All	All	798/834 (96%)	783 (98%)	15 (2%)	62	76

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	73	ARG
2	A	104	ARG
2	A	254	GLU
2	A	261	GLN
2	A	263	ARG
2	A	271	LYS
2	A	285	LYS
2	A	297	SER
2	A	366	LYS
2	A	388	ARG
2	B	104	ARG
2	B	285	LYS
2	B	314	LEU
2	B	317	GLU
2	B	393	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	115	ASN
1	D	117	HIS
1	D	143	GLN
1	D	155	HIS
1	D	164	ASN
1	H	143	GLN
1	H	155	HIS
1	H	164	ASN
2	A	106	HIS
2	A	124	ASN
2	A	128	GLN
2	A	143	HIS
2	A	177	GLN
2	A	180	ASN
2	A	187	GLN
2	A	197	GLN
2	A	231	GLN
2	A	261	GLN
2	A	266	GLN
2	A	386	GLN
2	A	424	GLN
2	A	426	GLN
2	A	428	HIS
2	B	86	GLN

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Mol	Chain	Res	Type
2	B	106	HIS
2	B	124	ASN
2	B	128	GLN
2	B	143	HIS
2	B	177	GLN
2	B	187	GLN
2	B	197	GLN
2	B	231	GLN
2	B	386	GLN
2	B	400	ASN
2	B	424	GLN
2	B	426	GLN
2	B	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	1,3	14,16,18	4.30	5 (35%)	13,22,26	1.31	1 (7%)
1	TRQ	H	109	1,3	14,16,18	4.66	5 (35%)	13,22,26	2.07	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
1	TRQ	D	109	1,3	-	0/3/16/21	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TRQ	H	109	1,3	-	0/3/16/21	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	109	TRQ	CE2-CZ2	-9.58	1.39	1.50
1	D	109	TRQ	CE2-CZ2	-8.68	1.40	1.50
1	H	109	TRQ	CH2-CZ3	-3.96	1.40	1.49
1	D	109	TRQ	CH2-CZ3	-3.49	1.41	1.49
1	D	109	TRQ	CA-C	2.11	1.53	1.50
1	H	109	TRQ	CA-C	3.13	1.54	1.50
1	D	109	TRQ	CD2-CG	3.77	1.45	1.40
1	H	109	TRQ	CD2-CG	4.23	1.46	1.40
1	D	109	TRQ	O7-CZ2	12.02	1.42	1.22
1	H	109	TRQ	O7-CZ2	12.80	1.43	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	109	TRQ	O7-CZ2-CE2	-4.21	115.11	122.33
1	H	109	TRQ	CZ3-CH2-CZ2	3.20	121.00	113.16
1	D	109	TRQ	CZ3-CH2-CZ2	3.20	121.01	113.16
1	H	109	TRQ	O7-CZ2-CH2	4.21	126.83	120.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	109	TRQ	2	0
1	H	109	TRQ	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands 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	$\# Z  > 2$
3	TSH	D	2	1	10,13,13	1.09	0	9,17,17	1.49	3 (33%)
3	TSH	H	1	1	10,13,13	0.95	0	9,17,17	1.42	3 (33%)

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
3	TSH	D	2	1	-	0/0/3/3	0/2/2/2
3	TSH	H	1	1	-	0/0/3/3	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	TSH	CE3-CD2-CG	-2.47	129.88	134.42
3	H	1	TSH	CE3-CD2-CG	-2.29	130.21	134.42
3	D	2	TSH	CZ3-CE3-CD2	-2.22	117.70	120.88
3	H	1	TSH	CZ3-CE3-CD2	-2.04	117.97	120.88
3	H	1	TSH	CE3-CD2-CE2	2.55	121.55	118.17
3	D	2	TSH	CE3-CD2-CE2	2.59	121.61	118.17

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
3	D	2	TSH	1	0
3	H	1	TSH	1	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, 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%)	-0.58	0	100 100	15, 23, 48, 61	0
1	H	120/135 (88%)	-0.68	0	100 100	14, 20, 39, 53	0
2	A	359/361 (99%)	-0.77	1 (0%)	93 93	11, 21, 35, 71	0
2	B	359/361 (99%)	-0.80	2 (0%)	89 88	11, 19, 32, 55	0
All	All	946/992 (95%)	-0.75	3 (0%)	93 93	11, 20, 36, 71	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	431	GLY	3.5
2	B	431	GLY	3.1
2	B	430	VAL	2.2

### 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	0.10	-	16,20,26,26	0
1	TRQ	D	109	15/17	0.96	0.10	-	17,21,26,30	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
3	TSH	D	2	12/12	0.88	0.16	9.58	26,31,35,35	0
3	TSH	H	1	12/12	0.82	0.20	9.48	23,34,41,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.