



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:37 am GMT

PDB ID : 2AH0  
Title : Crystal structure of the carbinolamine intermediate in the reductive half-reaction of aromatic amine dehydrogenase (AADH) with tryptamine. Monoclinic 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 : 1.45 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

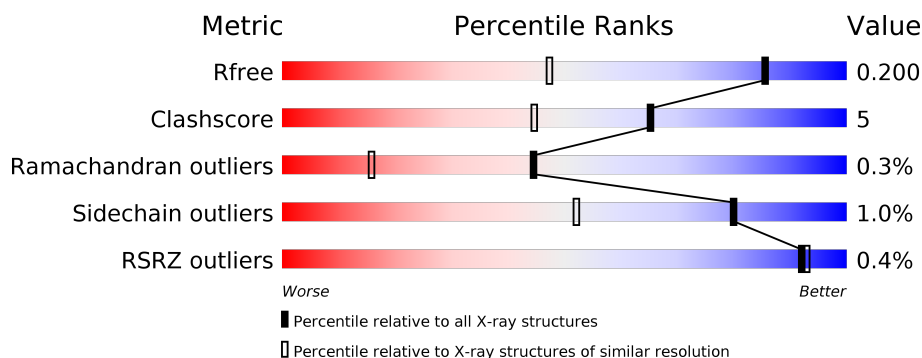
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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	1510 (1.48-1.44)
Clashscore	112137	1573 (1.48-1.44)
Ramachandran outliers	110173	1555 (1.48-1.44)
Sidechain outliers	110143	1555 (1.48-1.44)
RSRZ outliers	101464	1516 (1.48-1.44)

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	<div> <div style="width: 71%;"></div> <div style="width: 10%;"></div> <div style="width: 19%;"></div> </div>
1	H	135	<div> <div style="width: 67%;"></div> <div style="width: 13%;"></div> <div style="width: 19%;"></div> </div>
2	A	361	<div> <div style="width: 89%;"></div> <div style="width: 11%;"></div> </div>
2	B	361	<div> <div style="width: 91%;"></div> <div style="width: 9%;"></div> </div>

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	TSC	H	1	-	-	-	X
4	TSH	D	1	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8656 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.

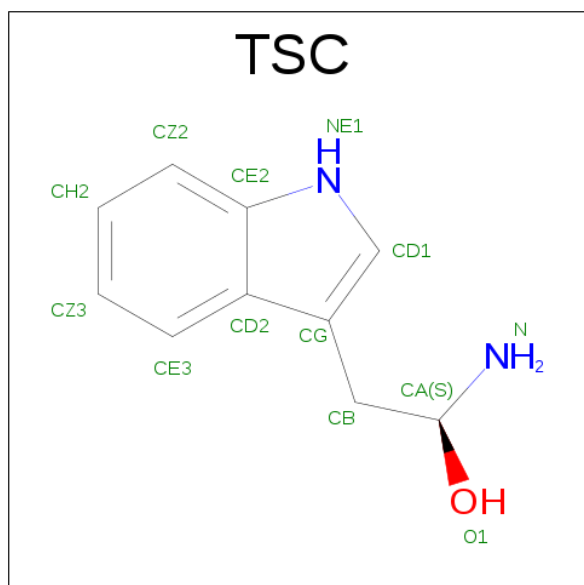
- Molecule 1 is a protein called Aromatic amine dehydrogenase.

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	109	Total	C	N	O	S	0	0	0
			831	508	147	161	15			

- Molecule 2 is a protein called Aromatic amine dehydrogenase.

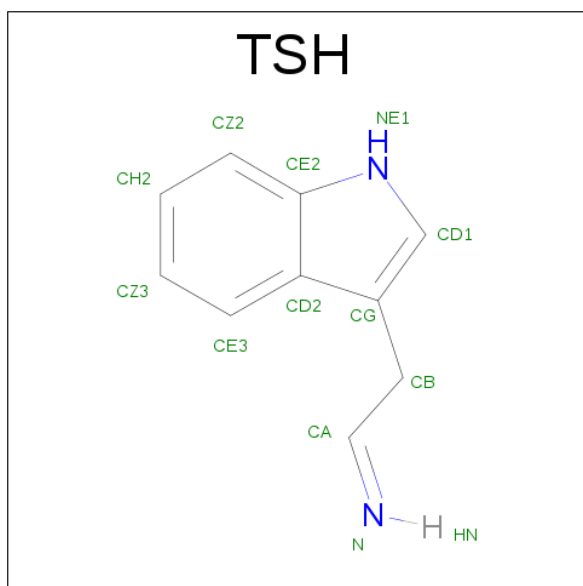
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	360	Total	C	N	O	S	0	2	0
			2812	1774	491	533	14			
2	B	361	Total	C	N	O	S	0	2	0
			2806	1768	489	535	14			

- Molecule 3 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
3	H	1	Total	C	N	O	0	0
			13	10	2	1		

- Molecule 4 is 2-(1H-INDOL-3-YL)ETHANIMINE (three-letter code: TSH) (formula:  $C_{10}H_{10}N_2$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	574	Total	O	0	0
			574	574		
5	B	493	Total	O	0	0
			493	493		
5	D	155	Total	O	0	0
			155	155		
5	H	125	Total	O	0	0
			125	125		

### 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 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.

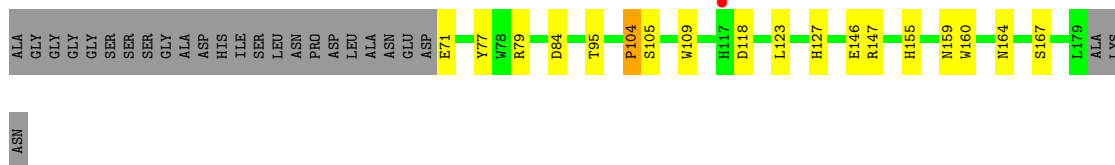
- Molecule 1: Aromatic amine dehydrogenase

Chain D: 



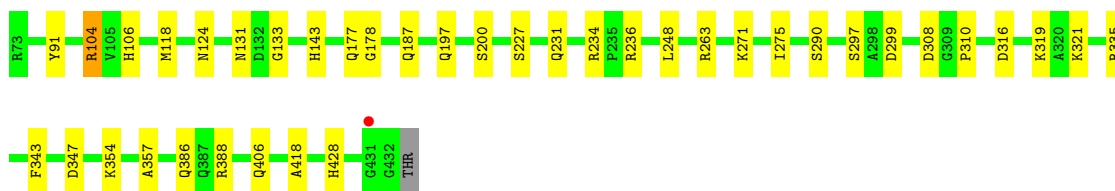
- Molecule 1: Aromatic amine dehydrogenase

Chain H: 




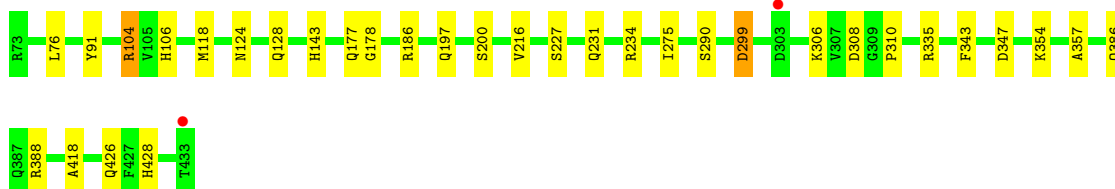
- Molecule 2: Aromatic amine dehydrogenase

Chain A: 



- Molecule 2: Aromatic amine dehydrogenase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.72Å 89.66Å 80.82Å 90.00° 90.41° 90.00°	Depositor
Resolution (Å)	15.00 – 1.45 80.82 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-1.45) 97.8 (80.82-1.45)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, $R_{free}$	0.167 , 0.200 0.168 , 0.200	Depositor DCC
$R_{free}$ test set	8744 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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, TSC, 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	0.59	0/842	0.76	1/1146 (0.1%)
1	H	0.57	0/838	0.77	2/1141 (0.2%)
2	A	0.65	0/2883	0.76	3/3907 (0.1%)
2	B	0.59	0/2879	0.75	3/3903 (0.1%)
All	All	0.61	0/7442	0.76	9/10097 (0.1%)

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
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	316	ASP	CB-CG-OD2	5.89	123.60	118.30
1	H	147	ARG	NE-CZ-NH1	5.85	123.23	120.30
2	B	308	ASP	CB-CG-OD2	5.72	123.44	118.30
2	B	299	ASP	CB-CG-OD2	5.61	123.34	118.30
1	D	84	ASP	CB-CG-OD2	5.54	123.28	118.30
2	B	347	ASP	CB-CG-OD2	5.50	123.25	118.30
1	H	118	ASP	CB-CG-OD2	5.22	123.00	118.30
2	A	299	ASP	CB-CG-OD2	5.18	122.96	118.30
2	A	347	ASP	CB-CG-OD2	5.05	122.84	118.30



There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	310	PRO	Peptide
2	B	310	PRO	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	11	0
1	H	831	0	728	13	0
2	A	2812	0	2756	27	0
2	B	2806	0	2726	24	0
3	H	13	0	10	1	0
4	D	12	0	9	1	0
5	A	574	0	0	5	0
5	B	493	0	0	2	0
5	D	155	0	0	6	0
5	H	125	0	0	2	0
All	All	8656	0	6961	67	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 5.

All (67) 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:D:95:THR:HG22	5:D:265:HOH:O	1.83	0.79
2:A:104:ARG:HH11	2:A:106:HIS:HE1	1.32	0.76
2:B:124:ASN:HD21	2:B:178:GLY:H	1.32	0.75
5:D:306:HOH:O	2:A:118[A]:MET:SD	2.44	0.75
2:A:124:ASN:HD21	2:A:178:GLY:H	1.35	0.75
2:B:104:ARG:HH11	2:B:106:HIS:HE1	1.33	0.74
2:A:91:TYR:OH	2:A:428:HIS:HD2	1.72	0.72
5:H:248:HOH:O	2:B:118[B]:MET:SD	2.49	0.70
2:B:91:TYR:OH	2:B:428:HIS:HD2	1.76	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:SER:HA	1:D:164:ASN:HD21	1.59	0.68
1:H:105:SER:HA	1:H:164:ASN:HD21	1.60	0.67
2:A:197:GLN:NE2	2:A:227:SER:H	1.94	0.66
2:B:197:GLN:NE2	2:B:227:SER:H	1.96	0.64
2:A:335:ARG:H	2:A:386:GLN:HE22	1.44	0.63
2:B:197:GLN:HE21	2:B:227:SER:H	1.50	0.59
2:A:335:ARG:H	2:A:386:GLN:NE2	1.99	0.59
2:B:335:ARG:H	2:B:386:GLN:HE22	1.49	0.59
1:D:167:SER:HB2	2:B:177:GLN:HE22	1.68	0.58
2:A:91:TYR:OH	2:A:428:HIS:CD2	2.56	0.57
1:H:77:TYR:CE1	1:H:79:ARG:HG2	2.39	0.57
2:A:197:GLN:HE21	2:A:227:SER:H	1.52	0.56
2:B:335:ARG:H	2:B:386:GLN:NE2	2.05	0.55
1:H:127:HIS:HB2	2:B:76:LEU:HD22	1.88	0.54
1:D:179:LEU:C	5:D:274:HOH:O	2.45	0.54
2:B:106:HIS:HD2	2:B:418:ALA:O	1.92	0.53
1:H:109:TRQ:HB2	1:H:160:TRP:NE1	2.23	0.53
2:A:248:LEU:HD13	2:A:263:ARG:HD3	1.90	0.53
2:B:124:ASN:HD21	2:B:178:GLY:N	2.05	0.53
2:A:106:HIS:HD2	2:A:418:ALA:O	1.94	0.51
2:B:143:HIS:HD2	5:B:542:HOH:O	1.92	0.51
1:D:159:ASN:HD22	2:B:177:GLN:NE2	2.08	0.50
2:B:104:ARG:HH11	2:B:106:HIS:CE1	2.23	0.50
2:B:299:ASP:HB3	2:B:306:LYS:HG3	1.94	0.49
2:A:236:ARG:HD3	5:A:772:HOH:O	2.13	0.49
1:H:71:GLU:N	5:H:275:HOH:O	2.45	0.49
1:H:79:ARG:HD2	1:H:95:THR:HG21	1.94	0.49
1:H:167:SER:HB2	2:A:177:GLN:HE22	1.78	0.48
1:H:155:HIS:HE1	5:A:441:HOH:O	1.94	0.48
1:H:104:PRO:HB3	2:B:76:LEU:CD2	2.43	0.48
1:H:159:ASN:HD22	2:A:177:GLN:NE2	2.11	0.47
1:D:109:TRQ:HB2	1:D:160:TRP:NE1	2.28	0.47
2:B:231:GLN:NE2	2:B:234:ARG:HH11	2.13	0.47
1:H:84:ASP:O	3:H:1:TSC:HB1	2.15	0.47
1:D:114:HIS:HE1	5:D:240:HOH:O	1.97	0.47
2:B:275:ILE:HA	2:B:290:SER:HA	1.97	0.47
2:A:104:ARG:HH11	2:A:106:HIS:CE1	2.23	0.46
2:A:275:ILE:HA	2:A:290:SER:HA	1.98	0.46
1:H:146:GLU:CD	2:A:354:LYS:HZ1	2.18	0.46
5:D:210:HOH:O	2:B:143:HIS:HE1	1.98	0.46
2:B:343:PHE:HB3	2:B:357:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:231:GLN:NE2	2:A:234:ARG:HH11	2.14	0.45
1:H:109:TRQ:HB2	1:H:160:TRP:HE1	1.82	0.45
2:A:124:ASN:HD21	2:A:178:GLY:N	2.11	0.44
2:B:128:GLN:HE22	2:B:186:ARG:C	2.21	0.44
1:D:146:GLU:CD	2:B:354:LYS:HZ1	2.21	0.44
2:A:297:SER:HB2	2:A:308:ASP:OD1	2.18	0.43
2:A:321:LYS:HD3	5:A:714:HOH:O	2.18	0.43
2:A:319:LYS:CE	5:A:900:HOH:O	2.66	0.43
2:A:133:GLY:O	2:A:428:HIS:HE1	2.01	0.42
1:D:155:HIS:HE1	5:B:444:HOH:O	2.01	0.42
2:A:343:PHE:HB3	2:A:357:ALA:HB2	2.01	0.42
2:A:131:ASN:H	2:A:187:GLN:HE22	1.67	0.42
1:D:71:GLU:N	5:D:238:HOH:O	2.52	0.42
2:A:143:HIS:HD2	5:A:656:HOH:O	2.03	0.41
1:D:159:ASN:HB2	4:D:1:TSH:CZ3	2.51	0.41
2:B:186:ARG:HH22	2:B:426:GLN:NE2	2.19	0.40
2:A:131:ASN:H	2:A:187:GLN:NE2	2.19	0.40

There are no symmetry-related clashes.

## 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	
1	D	106/135 (78%)	104 (98%)	2 (2%)	0	100	100
1	H	106/135 (78%)	104 (98%)	2 (2%)	0	100	100
2	A	360/361 (100%)	348 (97%)	11 (3%)	1 (0%)	44	16
2	B	360/361 (100%)	347 (96%)	11 (3%)	2 (1%)	28	6
All	All	932/992 (94%)	903 (97%)	26 (3%)	3 (0%)	44	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	216	VAL
2	A	200	SER
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	95/112 (85%)	95 (100%)	0	100	100
1	H	94/112 (84%)	92 (98%)	2 (2%)	59	21
2	A	305/305 (100%)	300 (98%)	5 (2%)	68	32
2	B	304/305 (100%)	302 (99%)	2 (1%)	87	66
All	All	798/834 (96%)	789 (99%)	9 (1%)	80	48

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	104	PRO
1	H	123	LEU
2	A	104	ARG
2	A	271	LYS
2	A	388	ARG
2	A	406[A]	GLN
2	A	406[B]	GLN
2	B	104	ARG
2	B	388	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	114	HIS
1	D	139	GLN
1	D	143	GLN
1	D	155	HIS
1	D	164	ASN

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Mol	Chain	Res	Type
1	H	139	GLN
1	H	143	GLN
1	H	155	HIS
1	H	164	ASN
2	A	86	GLN
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	386	GLN
2	A	387	GLN
2	A	424	GLN
2	A	426	GLN
2	A	428	HIS
2	B	86	GLN
2	B	106	HIS
2	B	124	ASN
2	B	128	GLN
2	B	143	HIS
2	B	177	GLN
2	B	180	ASN
2	B	187	GLN
2	B	197	GLN
2	B	231	GLN
2	B	386	GLN
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	1,4	14,16,18	4.33	5 (35%)	13,22,26	1.21	1 (7%)
1	TRQ	H	109	1,3	14,16,18	4.55	5 (35%)	13,22,26	1.56	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	1,4	-	0/3/16/21	0/2/2/2
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	-9.87	1.38	1.50
1	D	109	TRQ	CE2-CZ2	-7.88	1.41	1.50
1	H	109	TRQ	CH2-CZ3	-3.70	1.41	1.49
1	D	109	TRQ	CH2-CZ3	-3.70	1.41	1.49
1	D	109	TRQ	CA-C	2.78	1.53	1.50
1	H	109	TRQ	CA-C	3.04	1.54	1.50
1	H	109	TRQ	CD2-CG	4.63	1.46	1.40
1	D	109	TRQ	CD2-CG	4.91	1.46	1.40
1	H	109	TRQ	O7-CZ2	11.91	1.42	1.22
1	D	109	TRQ	O7-CZ2	12.14	1.42	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	-2.65	117.79	122.33
1	H	109	TRQ	O7-CZ2-CH2	2.15	123.86	120.74
1	H	109	TRQ	CZ3-CH2-CZ2	3.09	120.73	113.16
1	D	109	TRQ	CZ3-CH2-CZ2	3.11	120.78	113.16

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
1	D	109	TRQ	1	0
1	H	109	TRQ	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
4	TSH	D	1	1	10,13,13	1.07	0	9,17,17	1.30	2 (22%)
3	TSC	H	1	1	12,14,14	1.17	0	13,19,19	2.10	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
4	TSH	D	1	1	-	0/0/3/3	0/2/2/2
3	TSC	H	1	1	-	0/3/4/4	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	H	1	TSC	O1-CA-N	-4.78	108.16	113.56
3	H	1	TSC	CG-CB-CA	-4.03	106.94	112.73
4	D	1	TSH	CE3-CD2-CG	-2.27	130.25	134.42
3	H	1	TSC	CE3-CD2-CG	-2.17	130.43	134.42
3	H	1	TSC	CE3-CD2-CE2	2.30	121.21	118.17
4	D	1	TSH	CE3-CD2-CE2	2.38	121.32	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
4	D	1	TSH	1	0
3	H	1	TSC	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%)	-0.32	0 <b>100</b> <b>100</b>	10, 17, 28, 35	0
1	H	108/135 (80%)	-0.26	1 (0%) <b>84</b> <b>84</b>	11, 17, 35, 52	0
2	A	360/361 (99%)	-0.51	1 (0%) <b>93</b> <b>95</b>	8, 14, 27, 51	0
2	B	361/361 (100%)	-0.24	2 (0%) <b>89</b> <b>91</b>	9, 20, 34, 57	0
All	All	937/992 (94%)	-0.36	4 (0%) <b>92</b> <b>93</b>	8, 16, 32, 57	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	433[A]	THR	3.3
2	A	431	GLY	3.2
2	B	303	ASP	2.4
1	H	117	HIS	2.3

### 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	-	13,14,20,21	0
1	TRQ	D	109	15/17	0.94	0.07	-	15,17,23,25	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	TSC	H	1	13/13	0.83	0.20	16.06	23,31,35,36	0
4	TSH	D	1	12/12	0.82	0.16	12.33	26,33,37,38	0

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

There are no such residues in this entry.