wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 10:25 PM EST

PDB ID	:	2OJY
Title	:	Crystal structure of indol-3-acetaldehyde derived TTQ-amide adduct of aromatic amine dehydrogenase
Authors	:	Roujeinikova, A.; Leys, D.
Deposited on	:	2007-01-15
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

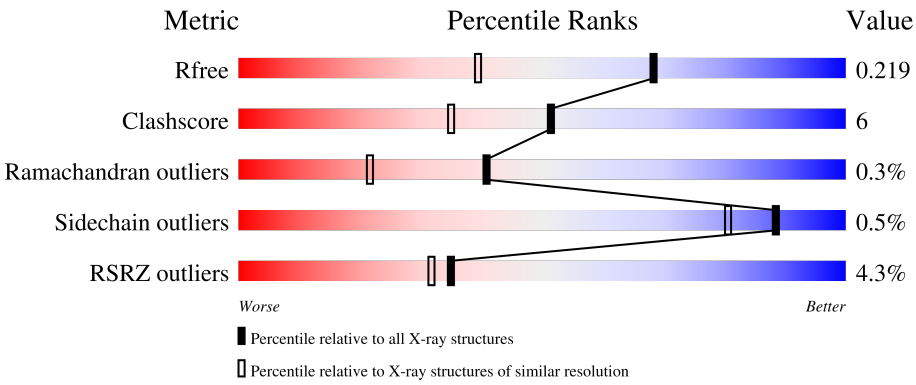
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (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	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 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	D	133	6% 71% 11% • 17%
1	H	133	10% 71% 17% • 11%
2	A	362	2% 93% 6% •
2	B	362	3% 92% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8609 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, small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	110	850	521	149	165	15	0	1	0
1	H	119	925	564	161	185	15	0	4	0

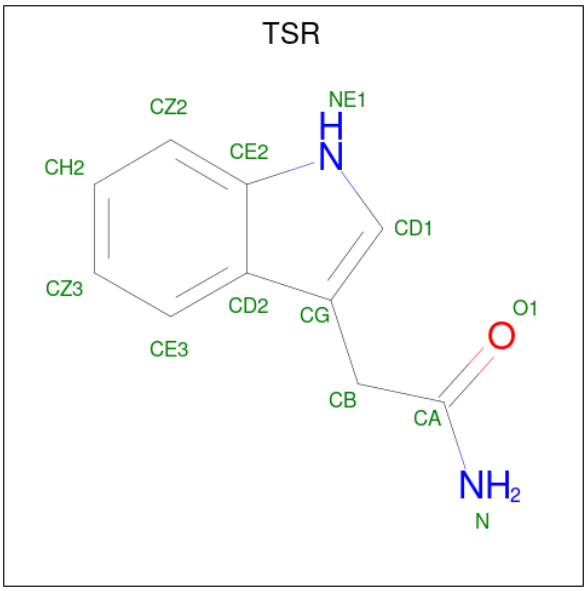
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	109	TRQ	TRP	modified residue	UNP Q0VKG6
H	109	TRQ	TRP	modified residue	UNP Q0VKG6

- Molecule 2 is a protein called Aromatic amine dehydrogenase, large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	360	2811	1773	491	533	14	0	2	0
2	B	361	2799	1764	488	533	14	0	2	0

- Molecule 3 is 2-(1H-INDOL-3-YL)ACETAMIDE (three-letter code: TSR) (formula: $C_{10}H_{10}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	D	1	26	20	4	2	0	1
			Total	C	N	O		
3	H	1	13	10	2	1	0	0

- Molecule 4 is water.

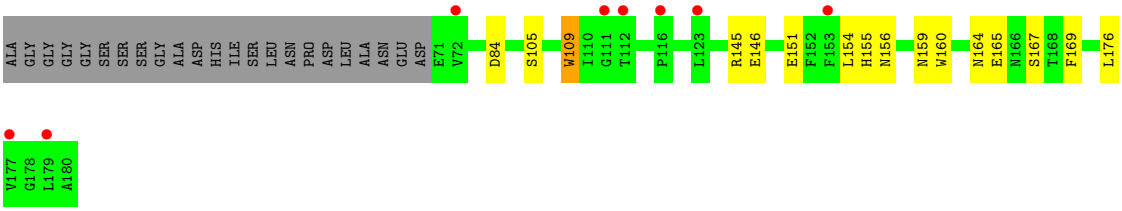
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	109	109	109	0	0
			Total	O		
4	H	134	134	134	0	0
			Total	O		
4	A	494	494	494	0	0
			Total	O		
4	B	448	448	448	0	0

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.

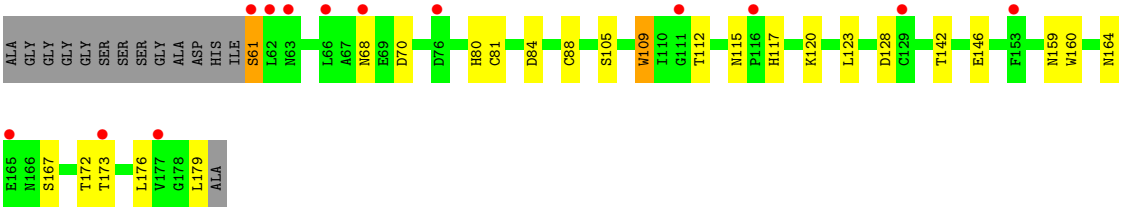
• Molecule 1: Aromatic amine dehydrogenase, small subunit

Chain D:



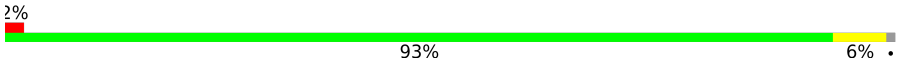
• Molecule 1: Aromatic amine dehydrogenase, small subunit

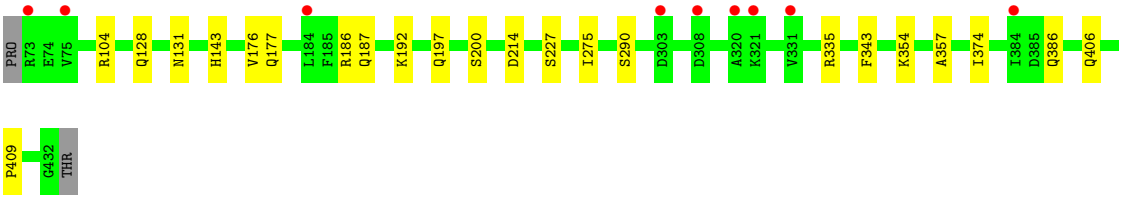
Chain H:



• Molecule 2: Aromatic amine dehydrogenase, large subunit

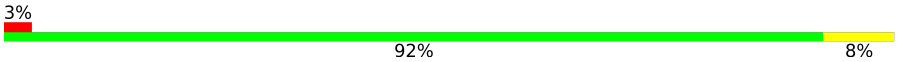
Chain A:

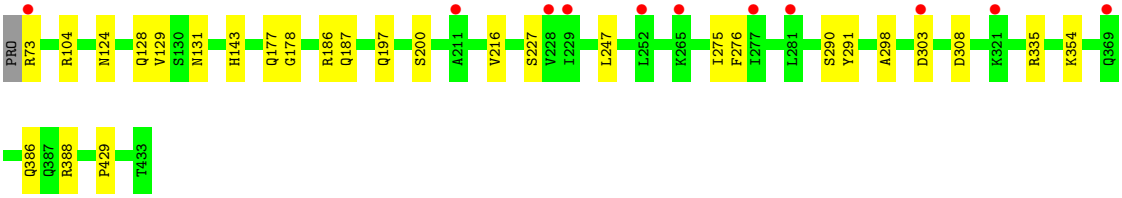




• Molecule 2: Aromatic amine dehydrogenase, large subunit

Chain B:




PRO
R73
R104
N124
Q128
V129
S130
N131
H143
Q177
G178
R186
Q187
Q197
S200
A211
V216
S227
V228
I229
L247
L252
K265
I275
F276
I277
L281
S290
Y291
A298
D303
D308
K321
R335
K354
Q369

Q386
Q387
R388
P429
T433

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.89Å 88.81Å 80.39Å 90.00° 90.62° 90.00°	Depositor
Resolution (Å)	15.00 – 1.60 29.80 – 1.60	Depositor EDS
% Data completeness (in resolution range)	88.2 (15.00-1.60) 88.2 (29.80-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.212 0.182 , 0.219	Depositor DCC
R_{free} test set	5829 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8609	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, TSR

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	0.75	0/846	0.83	2/1152 (0.2%)
1	H	0.71	1/941 (0.1%)	0.73	0/1284
2	A	0.73	0/2883	0.80	0/3907
2	B	0.72	0/2872	0.80	0/3895
All	All	0.73	1/7542 (0.0%)	0.79	2/10238 (0.0%)

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
1	D	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	61	SER	CA-CB	5.71	1.61	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	145	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	D	145	ARG	NE-CZ-NH2	-6.19	117.20	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	110	ILE	CB

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	850	0	738	15	0
1	H	925	0	809	28	0
2	A	2811	0	2752	23	0
2	B	2799	0	2713	20	0
3	D	26	0	17	4	0
3	H	13	0	9	2	0
4	A	494	0	0	6	0
4	B	448	0	0	8	0
4	D	109	0	0	2	1
4	H	134	0	0	7	1
All	All	8609	0	7038	81	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 6.

The worst 5 of 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)
1:H:112:THR:HG22	1:H:123:LEU:HD23	1.32	1.10
1:H:128:ASP:OD1	1:H:172[B]:THR:HG23	1.67	0.94
1:H:80:HIS:O	1:H:142[A]:THR:HG21	1.75	0.86
2:B:73:ARG:N	4:B:866:HOH:O	2.16	0.78
2:B:291:TYR:CE2	4:B:839:HOH:O	2.37	0.78

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)
4:D:349:HOH:O	4:H:408:HOH:O[1_554]	2.18	0.02

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	107/133 (80%)	103 (96%)	4 (4%)	0	100	100
1	H	120/133 (90%)	117 (98%)	3 (2%)	0	100	100
2	A	360/362 (99%)	348 (97%)	11 (3%)	1 (0%)	41	21
2	B	360/362 (99%)	346 (96%)	12 (3%)	2 (1%)	25	8
All	All	947/990 (96%)	914 (96%)	30 (3%)	3 (0%)	41	21

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 (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	94/110 (86%)	94 (100%)	0	100	100
1	H	106/110 (96%)	106 (100%)	0	100	100
2	A	305/306 (100%)	304 (100%)	1 (0%)	92	87
2	B	302/306 (99%)	299 (99%)	3 (1%)	76	61
All	All	807/832 (97%)	803 (100%)	4 (0%)	88	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	104	ARG
2	B	104	ARG
2	B	303	ASP
2	B	388	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	187	GLN
2	B	197	GLN
2	B	406	GLN
2	A	177	GLN
2	A	143	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)

3 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[B]	1,3	11,16,18	3.48	2 (18%)	11,22,26	2.14	3 (27%)
1	TRQ	H	109	1,3	11,16,18	3.78	3 (27%)	11,22,26	2.56	5 (45%)
1	TRQ	D	109[A]	1,3	11,16,18	3.88	4 (36%)	11,22,26	3.31	4 (36%)

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[B]	1,3	-	0/4/16/21	0/2/2/2
1	TRQ	H	109	1,3	-	0/4/16/21	0/2/2/2
1	TRQ	D	109[A]	1,3	-	0/4/16/21	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[A]	TRQ	O7-CZ2	8.92	1.36	1.22
1	H	109	TRQ	CE3-CZ3	8.39	1.46	1.33
1	H	109	TRQ	O7-CZ2	8.10	1.35	1.22
1	D	109[B]	TRQ	CE3-CZ3	8.01	1.45	1.33
1	D	109[B]	TRQ	O7-CZ2	7.78	1.34	1.22

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	109[A]	TRQ	CG-CB-CA	8.19	127.19	114.53
1	D	109[B]	TRQ	CD2-CE3-CZ3	-5.36	113.56	119.88
1	D	109[A]	TRQ	CD2-CE3-CZ3	-5.14	113.81	119.88
1	H	109	TRQ	CD2-CE3-CZ3	-5.10	113.86	119.88
1	H	109	TRQ	CG-CB-CA	3.99	120.69	114.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	109[B]	TRQ	1	0
1	H	109	TRQ	1	0
1	D	109[A]	TRQ	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	TSR	H	291	1	13,14,14	1.19	1 (7%)	14,19,19	1.53	2 (14%)
3	TSR	D	292[A]	1	13,14,14	0.95	0	14,19,19	2.07	4 (28%)
3	TSR	D	292[B]	1	13,14,14	0.97	0	14,19,19	1.36	2 (14%)

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	TSR	H	291	1	-	0/4/4/4	0/2/2/2
3	TSR	D	292[A]	1	-	2/4/4/4	0/2/2/2
3	TSR	D	292[B]	1	-	0/4/4/4	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	291	TSR	CZ3-CE3	2.31	1.42	1.36

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	291	TSR	CB-CG-CD2	4.37	135.07	126.50
3	D	292[A]	TSR	CG-CB-CA	4.17	120.37	112.98
3	D	292[A]	TSR	CB-CG-CD2	3.57	133.49	126.50
3	D	292[A]	TSR	CB-CA-N	3.37	122.39	116.49
3	D	292[B]	TSR	CB-CG-CD2	3.16	132.69	126.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	292[A]	TSR	O1-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	292[A]	TSR	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	291	TSR	2	0
3	D	292[A]	TSR	3	0
3	D	292[B]	TSR	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, 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(Å^2)	Q<0.9
1	D	109/133 (81%)	0.71	8 (7%)	15	13	23, 28, 39, 41	0
1	H	118/133 (88%)	0.71	13 (11%)	5	4	24, 28, 40, 47	0
2	A	360/362 (99%)	0.43	9 (2%)	57	55	23, 26, 34, 49	0
2	B	361/362 (99%)	0.52	11 (3%)	50	48	23, 28, 37, 46	0
All	All	948/990 (95%)	0.53	41 (4%)	35	32	23, 27, 37, 49	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	303	ASP	6.5
1	D	111	GLY	5.7
2	A	303	ASP	4.6
2	B	73	ARG	4.2
2	A	75	VAL	3.6

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(Å^2)	Q<0.9
1	TRQ	H	109	15/17	0.91	0.09	20,26,27,28	0
1	TRQ	D	109[B]	15/17	0.92	0.11	22,25,28,29	11
1	TRQ	D	109[A]	15/17	0.92	0.11	22,25,28,29	11

6.3 Carbohydrates (i)

There are no monosaccharides 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
3	TSR	D	292[A]	13/13	0.85	0.17	26,27,28,29	13
3	TSR	D	292[B]	13/13	0.85	0.17	26,26,27,28	13
3	TSR	H	291	13/13	0.87	0.56	21,22,23,24	13

6.5 Other polymers (i)

There are no such residues in this entry.