



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2025 – 02:30 am BST

PDB ID : 2IUQ / pdb\_00002iuq  
Title : CRYSTAL STRUCTURE OF DITHIONITE-REDUCED AROMATIC AMINE DEHYDROGENASE (AADH) FROM ALCALIGENES FAECALIS IN COMPLEX WITH TRYPTAMINE  
Authors : Roujeinikova, A.; Scrutton, N.; Leys, D.  
Deposited on : 2006-06-07  
Resolution : 1.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

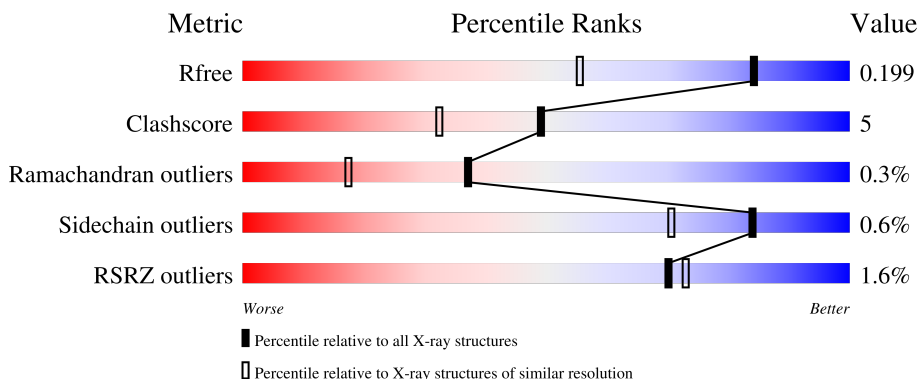
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	164625	3717 (1.50-1.50)
Clashscore	180529	4048 (1.50-1.50)
Ramachandran outliers	177936	3970 (1.50-1.50)
Sidechain outliers	177891	3967 (1.50-1.50)
RSRZ outliers	164620	3718 (1.50-1.50)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	A	361	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 2px auto;"> <span>89%</span> <span>10%</span> </div> </div>
1	B	361	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 2px auto;"> <span>90%</span> <span>9%</span> </div> </div>
2	D	135	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 71%, yellow 9%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 2px auto;"> <span>71%</span> <span>9%</span> <span>19%</span> </div> </div>
2	H	135	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 1%, green 93%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 2px auto;"> <span>76%</span> <span>12%</span> <span>12%</span> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8712 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.

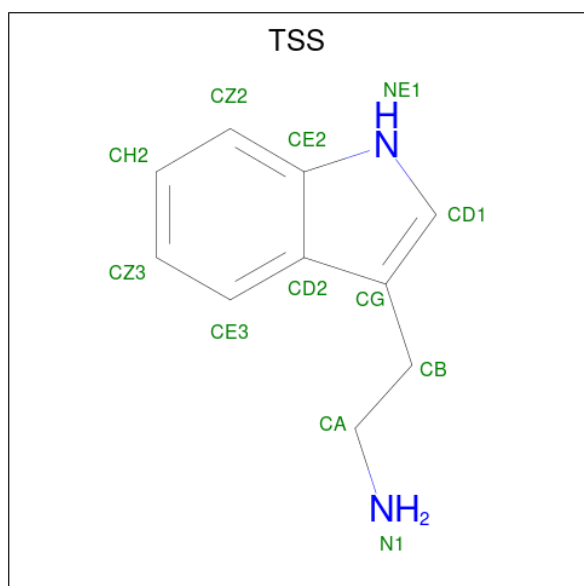
- Molecule 1 is a protein called AROMATIC AMINE DEHYDROGENASE ALPHA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	4	0
			2819	1778	491	536	14			
1	B	361	Total	C	N	O	S	0	2	0
			2796	1762	487	533	14			

- Molecule 2 is a protein called AROMATIC AMINE DEHYDROGENASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	109	Total	C	N	O	S	0	2	0
			851	522	148	166	15			
2	H	119	Total	C	N	O	S	0	1	0
			914	560	160	179	15			

- Molecule 3 is 2-(1H-INDOL-3-YL)ETHANAMINE (CCD ID: TSS) (formula: C<sub>10</sub>H<sub>12</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			12	10	2		
3	B	1	Total	C	N	0	0
			12	10	2		

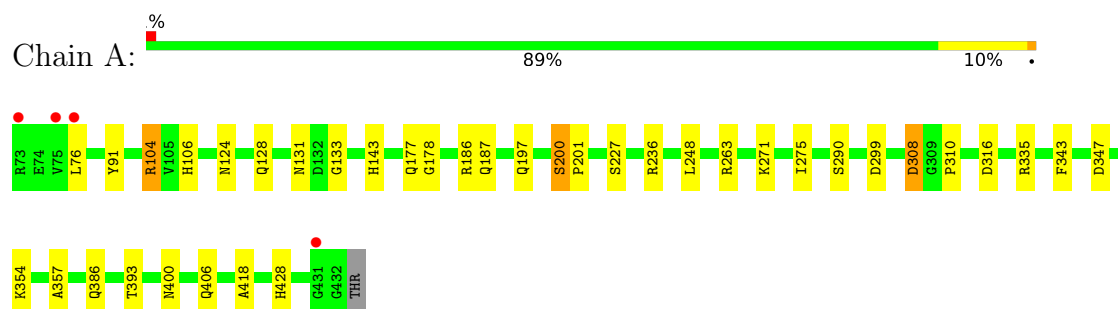
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	550	Total	O	0	0
			550	550		
4	B	472	Total	O	0	0
			472	472		
4	D	154	Total	O	0	0
			154	154		
4	H	132	Total	O	0	0
			132	132		

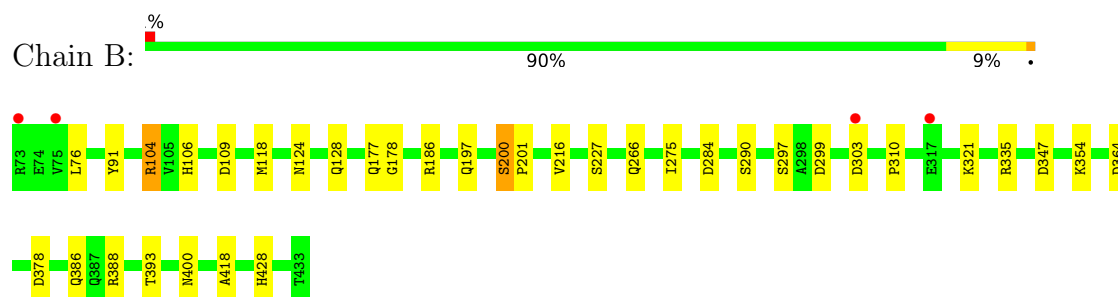
### 3 Residue-property plots [i](#)

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.

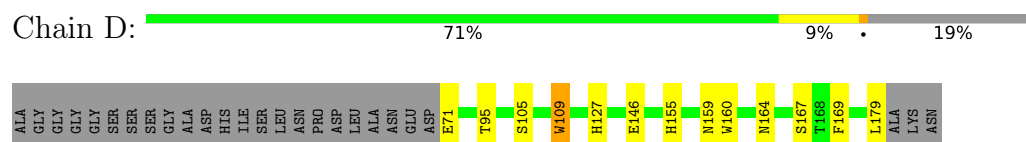
- Molecule 1: AROMATIC AMINE DEHYDROGENASE ALPHA SUBUNIT



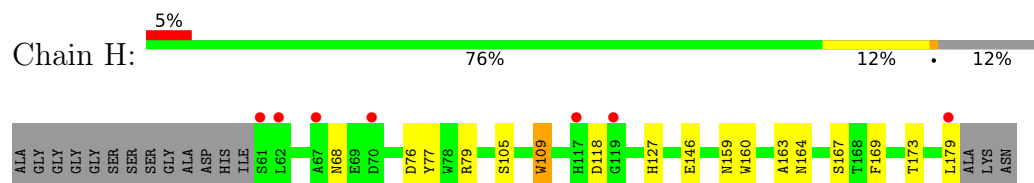
- Molecule 1: AROMATIC AMINE DEHYDROGENASE ALPHA SUBUNIT



- Molecule 2: AROMATIC AMINE DEHYDROGENASE BETA SUBUNIT



- Molecule 2: AROMATIC AMINE DEHYDROGENASE BETA SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.14Å 89.03Å 80.73Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	15.00 – 1.50 15.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	91.2 (15.00-1.50) 91.1 (15.00-1.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, $R_{free}$	0.157 , 0.190 0.167 , 0.199	Depositor DCC
$R_{free}$ test set	7357 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.5	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8712	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: TSS, TRQ

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	A	0.62	0/2897	0.72	5/3926 (0.1%)
1	B	0.59	0/2869	0.68	7/3892 (0.2%)
2	D	0.57	0/861	0.69	0/1172
2	H	0.59	0/922	0.70	2/1257 (0.2%)
All	All	0.60	0/7549	0.70	14/10247 (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
1	A	1	1
1	B	1	1
All	All	2	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	364	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	347	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	308[A]	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	308[B]	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	347	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	299	ASP	CB-CG-OD2	5.38	123.15	118.30
2	H	118	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	303	ASP	CB-CG-OD2	5.19	122.97	118.30
2	H	76	ASP	CB-CG-OD2	5.18	122.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	284	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	378	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	109	ASP	CB-CG-OD2	5.00	122.81	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	393	THR	CB
1	B	393	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	PRO	Peptide
1	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	A	2819	0	2761	34	0
1	B	2796	0	2704	25	0
2	D	851	0	747	14	0
2	H	914	0	796	14	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
4	A	550	0	0	6	0
4	B	472	0	0	4	1
4	D	154	0	0	6	1
4	H	132	0	0	6	0
All	All	8712	0	7032	77	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.

All (77) 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:H:169[B]:PHE:CZ	4:H:2018:HOH:O	2.11	1.03
2:D:169[A]:PHE:CZ	4:D:2017:HOH:O	2.12	1.02
1:A:393:THR:HG21	4:A:2470:HOH:O	1.71	0.90
1:B:393:THR:HG21	4:B:2398:HOH:O	1.76	0.86
1:B:118[B]:MET:SD	4:H:2089:HOH:O	2.40	0.79
1:A:393:THR:HG22	1:A:400:ASN:HB2	1.68	0.75
1:B:393:THR:HG22	1:B:400:ASN:HB2	1.69	0.72
1:A:393:THR:HG23	1:A:400:ASN:HD22	1.54	0.72
1:B:104:ARG:HH11	1:B:106:HIS:HE1	1.38	0.71
1:A:104:ARG:HH11	1:A:106:HIS:HE1	1.38	0.70
1:A:308[A]:ASP:OD2	4:A:2384:HOH:O	2.08	0.69
2:D:71:GLU:N	4:D:2003:HOH:O	2.25	0.69
2:H:105:SER:HA	2:H:164:ASN:HD21	1.58	0.69
1:B:393:THR:HG23	1:B:400:ASN:HD22	1.60	0.67
1:B:91:TYR:OH	1:B:428:HIS:HD2	1.79	0.65
2:H:179:LEU:C	4:H:2132:HOH:O	2.33	0.65
1:A:124:ASN:HD21	1:A:178:GLY:H	1.45	0.64
2:D:95[A]:THR:HG22	4:D:2028:HOH:O	1.96	0.64
1:A:335:ARG:H	1:A:386:GLN:HE22	1.43	0.64
1:B:124:ASN:HD21	1:B:178:GLY:H	1.45	0.63
1:B:177:GLN:HE22	2:D:167:SER:HB2	1.65	0.61
1:B:197:GLN:NE2	1:B:227:SER:H	1.98	0.61
2:D:105:SER:HA	2:D:164:ASN:HD21	1.63	0.61
1:A:91:TYR:OH	1:A:428:HIS:HD2	1.83	0.61
2:D:95[A]:THR:HG23	4:D:2029:HOH:O	2.00	0.61
1:A:197:GLN:NE2	1:A:227:SER:H	1.98	0.61
1:A:177:GLN:HE22	2:H:167:SER:HB2	1.66	0.61
1:A:248:LEU:HD13	1:A:263:ARG:HD3	1.81	0.60
2:D:179:LEU:C	4:D:2154:HOH:O	2.39	0.60
1:A:335:ARG:H	1:A:386:GLN:NE2	2.01	0.58
1:A:197:GLN:HE21	1:A:227:SER:H	1.50	0.58
2:D:109:TRQ:HB2	2:D:160:TRP:NE1	2.19	0.57
2:H:109:TRQ:HB2	2:H:160:TRP:NE1	2.20	0.57
1:B:106:HIS:HD2	1:B:418:ALA:O	1.89	0.56
1:B:266:GLN:NE2	4:B:2293:HOH:O	2.39	0.55
1:A:393:THR:CG2	1:A:400:ASN:HD22	2.19	0.55
1:B:335:ARG:H	1:B:386:GLN:HE22	1.54	0.55
1:A:177:GLN:NE2	2:H:159:ASN:HD22	2.05	0.55
1:A:91:TYR:OH	1:A:428:HIS:CD2	2.62	0.52
1:B:197:GLN:HE21	1:B:227:SER:H	1.58	0.51
1:B:335:ARG:H	1:B:386:GLN:NE2	2.08	0.51
1:A:143:HIS:HD2	4:A:2128:HOH:O	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:HIS:HD2	1:A:418:ALA:O	1.95	0.50
1:B:124:ASN:ND2	1:B:178:GLY:H	2.10	0.50
1:B:393:THR:CG2	1:B:400:ASN:HD22	2.24	0.49
1:B:177:GLN:NE2	2:D:159:ASN:HD22	2.10	0.49
2:H:169[B]:PHE:CE2	4:H:2018:HOH:O	2.51	0.49
1:A:200:SER:N	1:A:201:PRO:HA	2.28	0.48
2:H:163:ALA:HB3	4:H:2119:HOH:O	2.12	0.48
2:H:77:TYR:CE1	2:H:79:ARG:HG2	2.48	0.48
1:A:124:ASN:ND2	1:A:178:GLY:H	2.10	0.48
1:A:76:LEU:HD22	2:D:127:HIS:HB2	1.96	0.47
4:B:2258:HOH:O	2:D:155:HIS:HE1	1.97	0.46
2:H:109:TRQ:HB2	2:H:160:TRP:HE1	1.81	0.46
1:B:200:SER:N	1:B:201:PRO:HA	2.31	0.46
1:B:354:LYS:HZ1	2:D:146:GLU:CD	2.19	0.46
1:A:128:GLN:HE22	1:A:186:ARG:C	2.19	0.45
1:A:236:ARG:HD3	4:A:2225:HOH:O	2.17	0.45
1:A:200:SER:N	1:A:201:PRO:CA	2.80	0.45
1:B:275:ILE:HA	1:B:290:SER:HA	1.99	0.45
1:A:133:GLY:O	1:A:428:HIS:HE1	1.99	0.45
1:B:128:GLN:HE22	1:B:186:ARG:C	2.20	0.45
1:B:200:SER:N	1:B:201:PRO:CA	2.81	0.44
1:A:406[B]:GLN:NE2	4:A:2510:HOH:O	2.51	0.44
1:A:271:LYS:HE2	4:H:2078:HOH:O	2.18	0.43
1:B:76:LEU:HD22	2:H:127:HIS:HB2	1.99	0.43
1:B:321:LYS:HA	4:B:2339:HOH:O	2.18	0.43
1:A:275:ILE:HA	1:A:290:SER:HA	2.01	0.43
2:D:169[A]:PHE:CE2	4:D:2017:HOH:O	2.58	0.42
1:A:177:GLN:HE21	2:H:159:ASN:HD22	1.67	0.42
2:D:109:TRQ:HB2	2:D:160:TRP:HE1	1.82	0.41
1:A:131:ASN:H	1:A:187:GLN:HE22	1.68	0.41
1:A:354:LYS:HZ1	2:H:146:GLU:CD	2.23	0.41
1:A:343:PHE:HB3	1:A:357:ALA:HB2	2.02	0.41
1:A:393:THR:CG2	1:A:400:ASN:HB2	2.45	0.40
1:A:406[A]:GLN:NE2	4:A:2511:HOH:O	2.54	0.40
1:B:76:LEU:HD13	2:H:173:THR:HG21	2.04	0.40

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:B:2235:HOH:O	4:D:2081:HOH:O[2_545]	1.89	0.31

### 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	A	362/361 (100%)	349 (96%)	12 (3%)	1 (0%)	37	17
1	B	360/361 (100%)	345 (96%)	13 (4%)	2 (1%)	22	6
2	D	108/135 (80%)	106 (98%)	2 (2%)	0	100	100
2	H	117/135 (87%)	115 (98%)	2 (2%)	0	100	100
All	All	947/992 (96%)	915 (97%)	29 (3%)	3 (0%)	37	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	216	VAL
1	A	200	SER
1	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	A	307/305 (101%)	306 (100%)	1 (0%)	91	82
1	B	301/305 (99%)	298 (99%)	3 (1%)	73	53
2	D	97/112 (87%)	97 (100%)	0	100	100
2	H	102/112 (91%)	101 (99%)	1 (1%)	73	53
All	All	807/834 (97%)	802 (99%)	5 (1%)	84	70

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	B	104	ARG
1	B	297	SER
1	B	388	ARG
2	H	68	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	106	HIS
1	A	124	ASN
1	A	128	GLN
1	A	143	HIS
1	A	177	GLN
1	A	180	ASN
1	A	187	GLN
1	A	197	GLN
1	A	231	GLN
1	A	266	GLN
1	A	386	GLN
1	A	400	ASN
1	A	424	GLN
1	A	426	GLN
1	A	428	HIS
1	B	86	GLN
1	B	106	HIS
1	B	124	ASN
1	B	128	GLN
1	B	143	HIS
1	B	177	GLN
1	B	180	ASN
1	B	187	GLN
1	B	197	GLN
1	B	231	GLN
1	B	386	GLN
1	B	400	ASN
1	B	424	GLN
1	B	426	GLN
1	B	428	HIS
2	D	139	GLN
2	D	143	GLN
2	D	155	HIS

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Mol	Chain	Res	Type
2	D	164	ASN
2	H	68	ASN
2	H	143	GLN
2	H	155	HIS
2	H	164	ASN

### 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
2	TRQ	D	109	2	13,17,18	6.13	5 (38%)	14,24,26	2.41	4 (28%)
2	TRQ	H	109	2	13,17,18	6.17	6 (46%)	14,24,26	2.15	3 (21%)

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
2	TRQ	D	109	2	-	0/4/19/21	0/2/2/2
2	TRQ	H	109	2	-	0/4/19/21	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	109	TRQ	CH2-CZ2	-15.99	1.36	1.54
2	H	109	TRQ	CH2-CZ2	-15.52	1.36	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	109	TRQ	O7-CZ2	9.83	1.44	1.23
2	D	109	TRQ	O7-CZ2	9.39	1.43	1.23
2	D	109	TRQ	O6-CH2	8.22	1.46	1.24
2	H	109	TRQ	O6-CH2	8.16	1.46	1.24
2	H	109	TRQ	CE2-CZ2	-7.48	1.40	1.50
2	D	109	TRQ	CE2-CZ2	-6.90	1.41	1.50
2	D	109	TRQ	CZ3-CE3	4.73	1.42	1.34
2	H	109	TRQ	CZ3-CE3	4.14	1.41	1.34
2	H	109	TRQ	CZ3-CH2	-2.10	1.40	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	109	TRQ	CZ2-CE2-NE1	6.13	129.73	119.94
2	D	109	TRQ	CZ2-CE2-NE1	6.08	129.65	119.94
2	D	109	TRQ	O7-CZ2-CE2	4.14	126.22	121.84
2	D	109	TRQ	O7-CZ2-CH2	-3.16	115.27	119.00
2	H	109	TRQ	CD2-CE3-CZ3	-2.20	118.43	121.09
2	H	109	TRQ	O7-CZ2-CH2	2.20	121.58	119.00
2	D	109	TRQ	CD2-CE3-CZ3	-2.15	118.49	121.09

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z  > 2$
3	TSS	A	1433	-	11,13,13	1.05	0	11,17,17	1.57	3 (27%)
3	TSS	B	1434	-	11,13,13	1.08	0	11,17,17	1.46	2 (18%)

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	TSS	A	1433	-	-	0/3/3/3	0/2/2/2
3	TSS	B	1434	-	-	0/3/3/3	0/2/2/2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1433	TSS	CE3-CD2-CE2	3.22	122.44	118.17
3	B	1434	TSS	CE3-CD2-CE2	3.07	122.24	118.17
3	B	1434	TSS	CE3-CD2-CG	-2.87	129.15	134.42
3	A	1433	TSS	CE3-CD2-CG	-2.80	129.28	134.42
3	A	1433	TSS	CZ3-CE3-CD2	-2.57	117.33	120.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	A	360/361 (99%)	-0.48	4 (1%) 77 80	7, 12, 22, 58	4 (1%)
1	B	361/361 (100%)	0.03	4 (1%) 77 80	7, 18, 32, 52	2 (0%)
2	D	108/135 (80%)	-0.15	0 100 100	6, 15, 25, 33	2 (1%)
2	H	118/135 (87%)	0.16	7 (5%) 29 30	6, 16, 41, 51	1 (0%)
All	All	947/992 (95%)	-0.16	15 (1%) 70 73	6, 15, 31, 58	9 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	ARG	2.7
1	A	75	VAL	2.7
1	B	303	ASP	2.6
1	A	76	LEU	2.5
2	H	117	HIS	2.5
1	B	73	ARG	2.5
2	H	61	SER	2.5
2	H	62	LEU	2.4
1	A	431	GLY	2.3
1	B	317	GLU	2.3
2	H	179	LEU	2.2
2	H	67	ALA	2.2
1	B	75	VAL	2.1
2	H	70	ASP	2.0
2	H	119	GLY	2.0

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

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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TRQ	D	109	16/17	0.96	0.06	13,14,18,20	0
2	TRQ	H	109	16/17	0.96	0.06	11,12,16,20	0

### 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TSS	B	1434	12/12	0.81	0.13	8,10,13,14	12
3	TSS	A	1433	12/12	0.90	0.10	9,10,12,12	12

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

There are no such residues in this entry.