



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 03:56 pm BST

PDB ID : 2OIZ
Title : Crystal Structure of the Tryptamine-Derived (Indol-3-Acetamide)-TTQ Adduct of Aromatic Amine Dehydrogenase
Authors : Roujeinikova, A.; Leys, D.
Deposited on : 2007-01-12
Resolution : 1.05 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

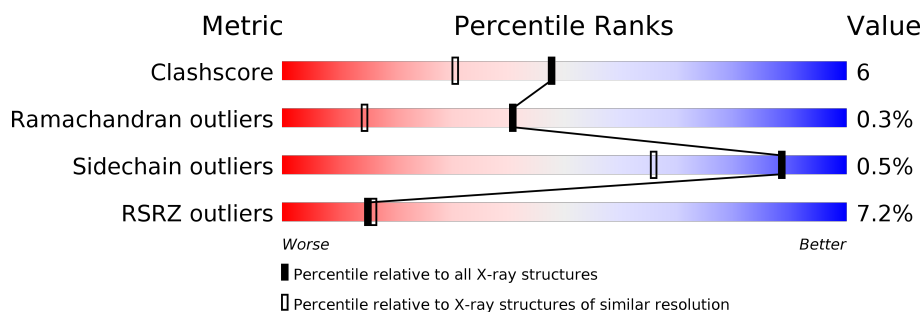
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.05 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))
Clashscore	141614	1252 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>11%</div> <div> <div></div> <div>62%</div> <div>19%</div> <div>19%</div> </div> </div>
1	H	135	<div> <div>17%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>• 10%</div> </div> </div>
2	A	361	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>•</div> </div> </div>
2	B	361	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9278 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
1	D	110	Total	C	N	O	S	0	15	0
			943	587	160	181	15			
1	H	122	Total	C	N	O	S	0	12	0
			992	608	170	199	15			

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

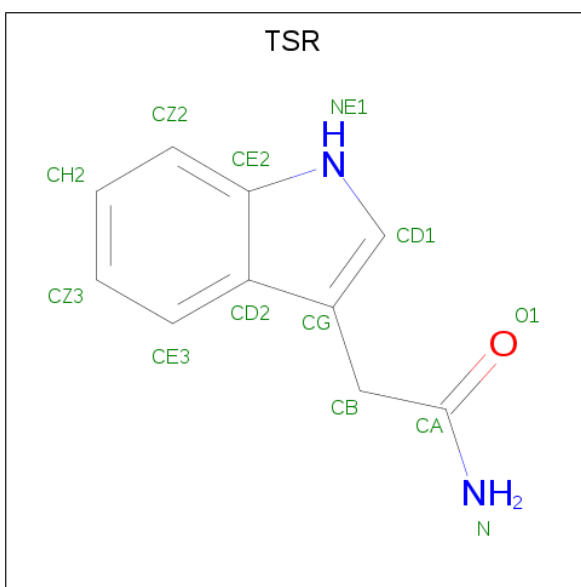
- Molecule 2 is a protein called Aromatic amine dehydrogenase, large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	360	Total	C	N	O	S	0	9	0
			2840	1796	492	538	14			
2	B	361	Total	C	N	O	S	0	5	0
			2826	1781	493	538	14			

There are 2 discrepancies between the modelled and reference sequences:

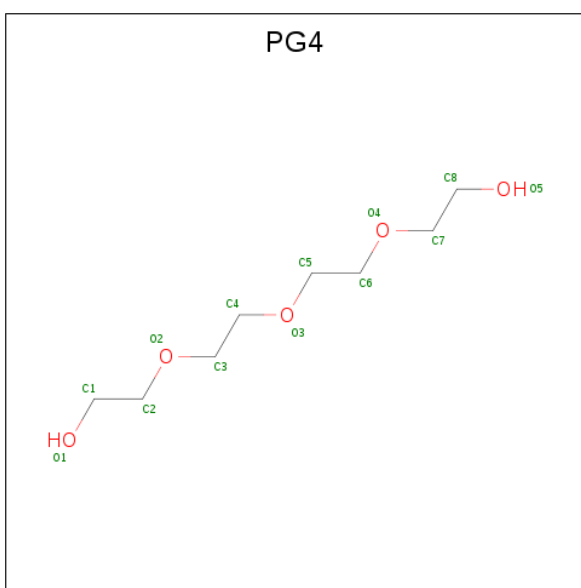
Chain	Residue	Modelled	Actual	Comment	Reference
A	433	THR	VAL	CONFLICT	UNP Q0VKG7
B	433	THR	VAL	CONFLICT	UNP Q0VKG7

- Molecule 3 is 2-(1H-INDOL-3-YL)ACETAMIDE (three-letter code: TSR) (formula: C₁₀H₁₀N₂O).



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

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		

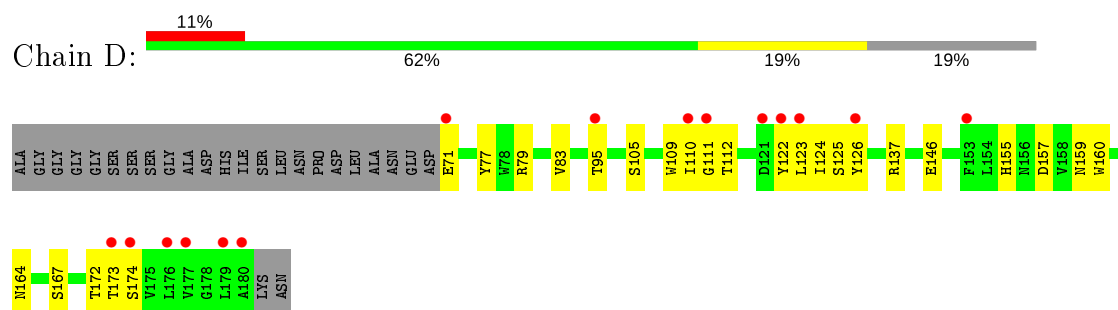
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	154	Total 154	O 154	0	1
5	H	160	Total 160	O 160	0	3
5	A	689	Total 689	O 689	0	0
5	B	622	Total 622	O 622	0	0

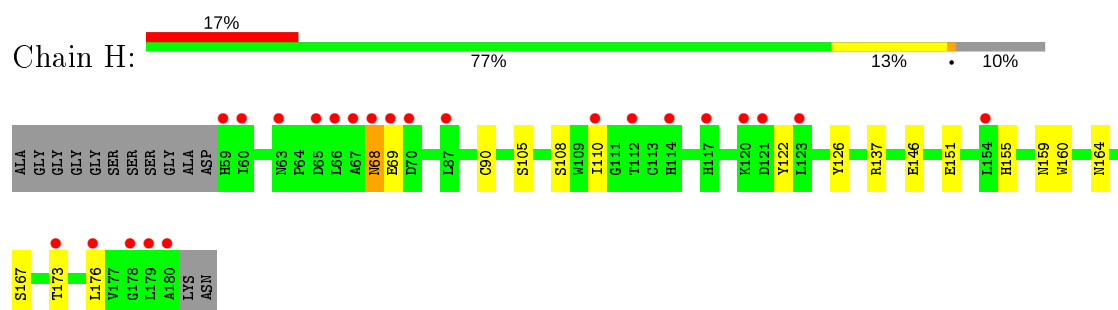
3 Residue-property plots [i](#)

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.

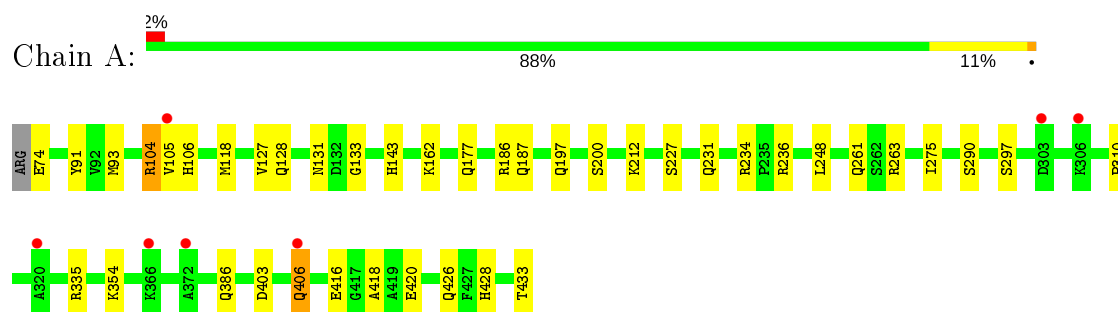
- Molecule 1: Aromatic amine dehydrogenase, small subunit



- Molecule 1: Aromatic amine dehydrogenase, small subunit

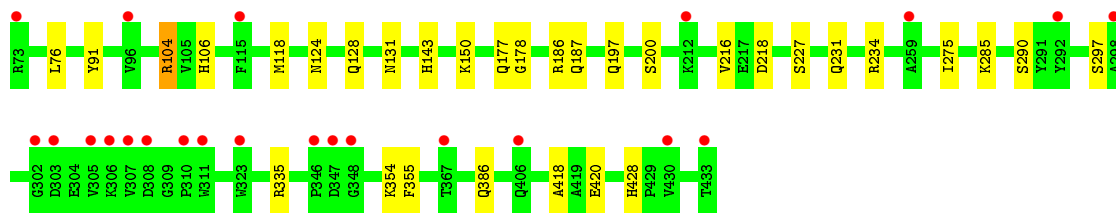


- Molecule 2: Aromatic amine dehydrogenase, large subunit



- Molecule 2: Aromatic amine dehydrogenase, large subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.94Å 88.70Å 80.22Å 90.00° 90.36° 90.00°	Depositor
Resolution (Å)	15.00 – 1.05 13.87 – 1.05	Depositor EDS
% Data completeness (in resolution range)	83.4 (15.00-1.05) 83.3 (13.87-1.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.05Å)	Xtriage
Refinement program	REFMAC 5.2.0011	Depositor
R, R_{free}	0.117 , 0.141 0.132 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	8.9	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9278	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, PG4, 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	0.70	0/961	0.85	2/1311 (0.2%)
1	H	0.64	1/1013 (0.1%)	0.79	2/1383 (0.1%)
2	A	0.66	1/2936 (0.0%)	0.80	2/3977 (0.1%)
2	B	0.63	1/2906 (0.0%)	0.80	3/3937 (0.1%)
All	All	0.65	3/7816 (0.0%)	0.80	9/10608 (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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	90	CYS	CB-SG	-5.59	1.72	1.81
2	A	420	GLU	CD-OE2	-5.22	1.20	1.25
2	B	420	GLU	CD-OE2	-5.09	1.20	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	ARG	NE-CZ-NH2	-8.46	116.07	120.30
2	A	403	ASP	CB-CG-OD1	6.71	124.34	118.30
1	H	137	ARG	NE-CZ-NH2	-6.29	117.15	120.30
2	B	218	ASP	CB-CG-OD1	5.80	123.53	118.30
2	A	236	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	B	218	ASP	CB-CG-OD2	-5.71	113.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	H	137	ARG	NE-CZ-NH1	5.67	123.13	120.30
2	B	355	PHE	CB-CG-CD1	5.45	124.61	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	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	943	0	847	21	0
1	H	992	0	867	16	0
2	A	2840	0	2805	36	1
2	B	2826	0	2758	26	0
3	D	26	0	17	2	0
3	H	13	0	9	0	0
4	A	13	0	18	0	0
5	A	689	0	0	12	0
5	B	622	0	0	6	1
5	D	154	0	0	6	0
5	H	160	0	0	4	0
All	All	9278	0	7321	91	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.

All (91) 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:A:74:GLU:N	5:A:2359:HOH:O	2.13	0.81
2:A:104:ARG:HH11	2:A:106:HIS:HE1	1.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ARG:HH11	2:B:106:HIS:HE1	1.31	0.78
1:D:95[B]:THR:CG2	5:D:1737:HOH:O	2.34	0.76
5:H:1758:HOH:O	2:B:118[B]:MET:SD	2.46	0.73
2:B:124:ASN:HD21	2:B:178:GLY:H	1.34	0.73
2:A:297[A]:SER:OG	5:A:2043:HOH:O	2.07	0.72
5:D:1813:HOH:O	2:A:118[A]:MET:SD	2.48	0.71
1:H:105:SER:HA	1:H:164:ASN:HD21	1.55	0.71
1:D:105:SER:HA	1:D:164:ASN:HD21	1.57	0.70
2:B:91:TYR:OH	2:B:428:HIS:HD2	1.75	0.69
1:H:108:SER:HB2	1:H:126[B]:TYR:O	1.93	0.68
1:D:77:TYR:CE1	1:D:79[B]:ARG:HG2	2.29	0.68
1:D:95[B]:THR:HG22	5:D:1737:HOH:O	1.92	0.65
2:B:197:GLN:NE2	2:B:227:SER:H	1.95	0.65
1:H:173[B]:THR:HG21	2:B:76:LEU:CD1	2.28	0.64
2:A:91:TYR:OH	2:A:428:HIS:HD2	1.81	0.64
1:D:109[B]:TRQ:HB2	1:D:160[B]:TRP:NE1	2.13	0.63
2:A:197:GLN:NE2	2:A:227:SER:H	1.97	0.63
2:A:335:ARG:H	2:A:386:GLN:HE22	1.44	0.62
2:A:105[B]:VAL:HG11	2:A:127:VAL:HG11	1.82	0.62
2:B:197:GLN:HE21	2:B:227:SER:H	1.48	0.61
1:D:109[B]:TRQ:HB2	1:D:160[B]:TRP:HE1	1.66	0.61
1:D:124:ILE:HG21	1:D:174[A]:SER:HB3	1.83	0.60
2:B:285:LYS:NZ	5:B:1054:HOH:O	2.36	0.59
2:A:335:ARG:H	2:A:386:GLN:NE2	2.00	0.58
2:A:197:GLN:HE21	2:A:227:SER:H	1.50	0.57
1:H:151:GLU:OE2	5:H:1804:HOH:O	2.17	0.57
1:H:68:ASN:HD22	1:H:69:GLU:N	2.04	0.56
2:B:297[B]:SER:OG	5:B:656:HOH:O	2.18	0.56
2:B:143:HIS:HD2	5:B:639:HOH:O	1.88	0.56
2:B:335:ARG:H	2:B:386:GLN:HE22	1.53	0.56
2:A:143:HIS:HD2	5:A:1890:HOH:O	1.89	0.55
1:H:167:SER:HB2	2:A:177:GLN:HE22	1.73	0.53
5:H:1739:HOH:O	2:A:143:HIS:HE1	1.91	0.53
2:B:106:HIS:HD2	2:B:418:ALA:O	1.91	0.53
1:D:167:SER:HB2	2:B:177:GLN:HE22	1.72	0.53
2:A:91:TYR:OH	2:A:428:HIS:CD2	2.61	0.53
2:A:93:MET:SD	2:A:105[B]:VAL:CG1	2.97	0.53
2:A:106:HIS:HD2	2:A:418:ALA:O	1.93	0.52
1:D:112[A]:THR:HA	1:D:122:TYR:O	2.09	0.52
1:H:173[B]:THR:HG21	2:B:76:LEU:HD13	1.91	0.52
2:A:416:GLU:CG	5:A:2140:HOH:O	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:ARG:H	2:B:386:GLN:NE2	2.09	0.50
5:D:1736:HOH:O	2:B:143:HIS:HE1	1.94	0.50
1:H:159:ASN:HD22	2:A:177:GLN:NE2	2.09	0.49
1:D:159:ASN:HD22	2:B:177:GLN:NE2	2.11	0.49
2:B:150:LYS:HE3	5:B:799:HOH:O	2.14	0.48
1:D:146:GLU:CD	2:B:354:LYS:HZ1	2.17	0.48
1:D:126[A]:TYR:HA	1:D:173[A]:THR:O	2.13	0.48
1:D:71:GLU:N	5:D:1787:HOH:O	2.47	0.48
2:A:133:GLY:O	2:A:428:HIS:HE1	1.97	0.47
2:A:162[B]:LYS:HD3	5:A:2178:HOH:O	2.14	0.47
2:A:162[B]:LYS:NZ	5:A:2248:HOH:O	2.48	0.47
2:A:131:ASN:H	2:A:187:GLN:HE22	1.61	0.47
1:D:111[A]:GLY:O	1:D:123:LEU:HA	2.14	0.47
1:D:124:ILE:CG2	1:D:174[A]:SER:HB3	2.45	0.47
2:A:128:GLN:HE22	2:A:186:ARG:C	2.18	0.47
2:A:261:GLN:NE2	5:A:1829:HOH:O	2.48	0.46
1:H:173[B]:THR:HG21	2:B:76:LEU:HD11	1.96	0.46
2:A:231:GLN:NE2	2:A:234:ARG:HH11	2.14	0.45
1:H:155:HIS:HE1	5:A:1724:HOH:O	1.99	0.45
1:H:146:GLU:CD	2:A:354:LYS:HZ1	2.20	0.45
2:B:91:TYR:OH	2:B:428:HIS:CD2	2.65	0.45
2:A:93:MET:HA	2:A:105[B]:VAL:HG12	1.99	0.44
1:H:173[B]:THR:OG1	2:B:76:LEU:HD22	2.17	0.44
1:D:95[B]:THR:HG23	5:D:1737:HOH:O	2.05	0.44
2:A:275:ILE:HA	2:A:290:SER:HA	2.00	0.43
2:A:416:GLU:HG3	5:A:2140:HOH:O	2.16	0.43
1:H:110[B]:ILE:HD12	5:H:1826:HOH:O	2.19	0.43
1:D:83:VAL:HG13	1:D:172[A]:THR:CG2	2.49	0.43
2:A:93:MET:SD	2:A:105[B]:VAL:HG12	2.59	0.43
2:B:128:GLN:HE22	2:B:186:ARG:C	2.22	0.42
1:D:109[B]:TRQ:HZ3	3:D:1702[B]:TSR:O1	2.18	0.42
1:H:122:TYR:HB3	1:H:176[A]:LEU:CD1	2.49	0.42
2:A:263:ARG:HG2	5:A:2181:HOH:O	2.18	0.42
2:B:131:ASN:H	2:B:187:GLN:HE22	1.68	0.42
1:D:172[A]:THR:HB	3:D:1702[A]:TSR:O1	2.19	0.42
2:A:212:LYS:NZ	5:A:2132:HOH:O	2.39	0.42
2:A:248:LEU:HD13	2:A:263:ARG:HD3	2.01	0.42
2:B:231:GLN:NE2	2:B:234:ARG:HH11	2.18	0.42
2:A:131:ASN:H	2:A:187:GLN:NE2	2.18	0.41
1:D:155:HIS:CE1	1:D:157:ASP:HB2	2.56	0.41
2:A:406[B]:GLN:NE2	5:A:1869:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:ILE:HA	2:B:290:SER:HA	2.03	0.41
2:A:186:ARG:HH22	2:A:426:GLN:NE2	2.19	0.40
1:D:110[B]:ILE:HD13	1:D:125[B]:SER:HA	2.03	0.40
1:H:68:ASN:C	1:H:68:ASN:HD22	2.25	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)
2:A:433:THR:C	5:B:800:HOH:O[1_655]	1.58	0.62

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	121/135 (90%)	118 (98%)	3 (2%)	0	100	100
1	H	130/135 (96%)	127 (98%)	3 (2%)	0	100	100
2	A	367/361 (102%)	355 (97%)	11 (3%)	1 (0%)	41	14
2	B	362/361 (100%)	348 (96%)	12 (3%)	2 (1%)	25	5
All	All	980/992 (99%)	948 (97%)	29 (3%)	3 (0%)	41	14

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	108/112 (96%)	108 (100%)	0	100	100
1	H	114/112 (102%)	113 (99%)	1 (1%)	78	49
2	A	313/305 (103%)	310 (99%)	3 (1%)	76	44
2	B	308/305 (101%)	307 (100%)	1 (0%)	92	75
All	All	843/834 (101%)	838 (99%)	5 (1%)	88	62

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

Mol	Chain	Res	Type
1	H	68	ASN
2	A	104	ARG
2	A	406[A]	GLN
2	A	406[B]	GLN
2	B	104	ARG

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	139	GLN
1	D	143	GLN
1	D	164	ASN
1	H	68	ASN
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	128	GLN
2	A	143	HIS
2	A	177	GLN
2	A	180	ASN

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Mol	Chain	Res	Type
2	A	187	GLN
2	A	197	GLN
2	A	231	GLN
2	A	261	GLN
2	A	386	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	406	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 ⓘ

4 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	3.55	4 (36%)	11,22,26	2.54	4 (36%)
1	TRQ	D	109[A]	1,3	11,16,18	3.24	4 (36%)	11,22,26	1.79	3 (27%)
1	TRQ	H	109[B]	1	11,16,18	3.50	3 (27%)	11,22,26	2.17	5 (45%)
1	TRQ	H	109[A]	1	11,16,18	3.51	3 (27%)	11,22,26	2.20	6 (54%)

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	D	109[A]	1,3	-	0/4/16/21	0/2/2/2
1	TRQ	H	109[B]	1	-	0/4/16/21	0/2/2/2
1	TRQ	H	109[A]	1	-	0/4/16/21	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	109[B]	TRQ	O7-CZ2	10.00	1.38	1.22
1	H	109[A]	TRQ	O7-CZ2	10.00	1.38	1.22
1	D	109[B]	TRQ	O7-CZ2	9.86	1.38	1.22
1	D	109[A]	TRQ	O7-CZ2	8.65	1.36	1.22
1	D	109[B]	TRQ	CE3-CZ3	4.80	1.41	1.33
1	D	109[A]	TRQ	CE3-CZ3	4.56	1.40	1.33
1	H	109[B]	TRQ	CE3-CZ3	4.40	1.40	1.33
1	H	109[A]	TRQ	CE3-CZ3	4.40	1.40	1.33
1	D	109[A]	TRQ	CH2-CZ3	-3.35	1.40	1.48
1	D	109[B]	TRQ	CH2-CZ3	-3.13	1.40	1.48
1	H	109[B]	TRQ	CH2-CZ3	-2.79	1.41	1.48
1	H	109[A]	TRQ	CH2-CZ3	-2.79	1.41	1.48
1	D	109[A]	TRQ	CD2-CE3	-2.31	1.39	1.44
1	D	109[B]	TRQ	CD2-CE3	-2.20	1.40	1.44

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	109[B]	TRQ	O7-CZ2-CH2	5.90	129.08	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	109[B]	TRQ	CB-CG-CD1	-4.01	123.02	127.97
1	H	109[A]	TRQ	CB-CG-CD1	-4.01	123.02	127.97
1	D	109[B]	TRQ	CB-CG-CD1	-3.60	123.52	127.97
1	D	109[A]	TRQ	CZ3-CH2-CZ2	3.53	121.42	113.19
1	H	109[B]	TRQ	CZ3-CH2-CZ2	3.36	121.02	113.19
1	H	109[A]	TRQ	CZ3-CH2-CZ2	3.36	121.02	113.19
1	D	109[A]	TRQ	CG-CB-CA	3.35	119.71	114.53
1	D	109[B]	TRQ	CZ3-CH2-CZ2	3.28	120.85	113.19
1	H	109[B]	TRQ	CG-CB-CA	2.56	118.48	114.53
1	H	109[A]	TRQ	CG-CB-CA	2.56	118.48	114.53
1	H	109[B]	TRQ	O7-CZ2-CH2	2.47	124.26	120.79
1	H	109[A]	TRQ	O7-CZ2-CH2	2.47	124.26	120.79
1	D	109[A]	TRQ	CB-CG-CD1	-2.36	125.05	127.97
1	H	109[B]	TRQ	CB-CG-CD2	2.21	131.89	127.09
1	H	109[A]	TRQ	CB-CG-CD2	2.21	131.89	127.09
1	H	109[A]	TRQ	CB-CA-C	2.14	115.48	111.47
1	D	109[B]	TRQ	CG-CB-CA	2.13	117.81	114.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	109[B]	TRQ	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	D	1702[A]	1	13,14,14	0.96	0	14,19,19	2.47	5 (35%)
3	TSR	H	1701	1	13,14,14	1.01	0	14,19,19	1.58	4 (28%)
3	TSR	D	1702[B]	1	13,14,14	1.03	0	14,19,19	1.39	2 (14%)
4	PG4	A	1700	-	12,12,12	0.40	0	11,11,11	0.51	0

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	D	1702[A]	1	-	2/4/4/4	0/2/2/2
3	TSR	H	1701	1	-	0/4/4/4	0/2/2/2
3	TSR	D	1702[B]	1	-	0/4/4/4	0/2/2/2
4	PG4	A	1700	-	-	0/10/10/10	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	D	1702[A]	TSR	CB-CA-N	6.72	128.28	116.49
3	D	1702[A]	TSR	O1-CA-N	-3.74	112.29	122.50
3	D	1702[B]	TSR	CB-CG-CD2	2.98	132.34	126.50
3	D	1702[A]	TSR	CG-CB-CA	2.96	118.23	112.98
3	H	1701	TSR	CZ3-CE3-CD2	-2.71	117.13	120.89
3	H	1701	TSR	CB-CA-N	2.67	121.18	116.49
3	D	1702[A]	TSR	CE3-CD2-CE2	2.55	121.55	118.17
3	H	1701	TSR	CE3-CD2-CE2	2.43	121.39	118.17
3	D	1702[B]	TSR	CE3-CD2-CE2	2.21	121.10	118.17
3	H	1701	TSR	CB-CG-CD2	2.20	130.81	126.50
3	D	1702[A]	TSR	CE3-CD2-CG	-2.15	130.47	134.42

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1702[A]	TSR	O1-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
3	D	1702[A]	TSR	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1702[A]	TSR	1	0
3	D	1702[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 ⓘ

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, 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	109/135 (80%)	1.32	15 (13%) 2 5	8, 12, 22, 30	0
1	H	121/135 (89%)	1.47	23 (19%) 1 3	8, 12, 27, 36	0
2	A	360/361 (99%)	0.99	7 (1%) 66 60	6, 10, 19, 28	0
2	B	361/361 (100%)	0.99	23 (6%) 19 19	7, 12, 23, 33	0
All	All	951/992 (95%)	1.09	68 (7%) 15 16	6, 11, 23, 36	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	60	ILE	7.3
1	D	180	ALA	6.7
1	H	66	LEU	6.7
1	H	70	ASP	5.5
1	H	180	ALA	4.8
1	D	179	LEU	4.2
1	H	68	ASN	4.2
1	H	123	LEU	3.9
1	H	179	LEU	3.8
1	D	177	VAL	3.5
2	B	303	ASP	3.5
2	B	73[A]	ARG	3.4
1	D	110[A]	ILE	3.4
1	D	176[A]	LEU	3.2
1	H	173[A]	THR	3.2
1	H	67	ALA	3.2
2	B	307	VAL	3.2
1	H	110[A]	ILE	3.1
1	D	123	LEU	3.0
1	D	126[A]	TYR	3.0
1	H	117	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	433[A]	THR	2.8
1	D	121	ASP	2.8
2	B	212	LYS	2.7
1	H	121	ASP	2.7
2	B	306	LYS	2.7
2	B	308	ASP	2.7
1	H	178	GLY	2.6
1	H	120	LYS	2.6
1	D	95[A]	THR	2.5
2	B	305	VAL	2.5
2	B	346	PRO	2.5
2	B	367	THR	2.5
2	B	292	TYR	2.5
2	B	302	GLY	2.4
1	H	69	GLU	2.3
1	H	87	LEU	2.3
2	A	366	LYS	2.3
1	H	59	HIS	2.3
2	B	323	TRP	2.3
1	H	114	HIS	2.3
1	D	71	GLU	2.2
2	A	303	ASP	2.2
2	B	298	ALA	2.2
2	B	310	PRO	2.2
2	B	430	VAL	2.2
1	H	65	ASP	2.2
1	D	174[A]	SER	2.2
2	A	105[A]	VAL	2.2
2	B	406	GLN	2.1
2	B	96	VAL	2.1
2	A	320	ALA	2.1
2	B	311	TRP	2.1
2	B	115	PHE	2.1
1	H	176[A]	LEU	2.1
2	A	406[A]	GLN	2.1
2	B	347	ASP	2.1
1	H	112[A]	THR	2.1
1	D	111[A]	GLY	2.1
1	H	154	LEU	2.1
2	B	259	ALA	2.0
1	D	122	TYR	2.0
1	H	63	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	153	PHE	2.0
2	B	348	GLY	2.0
1	D	173[A]	THR	2.0
2	A	372	ALA	2.0
2	A	306	LYS	2.0

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	D	109[B]	15/17	0.95	0.16	5,8,10,12	14
1	TRQ	D	109[A]	15/17	0.95	0.16	5,8,10,12	14
1	TRQ	H	109[B]	15/17	0.96	0.10	9,10,11,14	2
1	TRQ	H	109[A]	15/17	0.96	0.10	9,9,11,14	2

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TSR	D	1702[A]	13/13	0.86	0.19	9,12,17,18	13
3	TSR	D	1702[B]	13/13	0.86	0.19	10,11,12,13	13
3	TSR	H	1701	13/13	0.89	0.14	9,12,14,15	13
4	PG4	A	1700	13/13	0.92	0.12	14,16,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.