



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:56 pm BST

PDB ID : 5WII
Title : TraE protein in complex with 2-Chloroisonicotinic Acid
Authors : Casu, B.; Arya, T.; Bessette, B.; Baron, C.
Deposited on : 2017-07-19
Resolution : 2.79 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

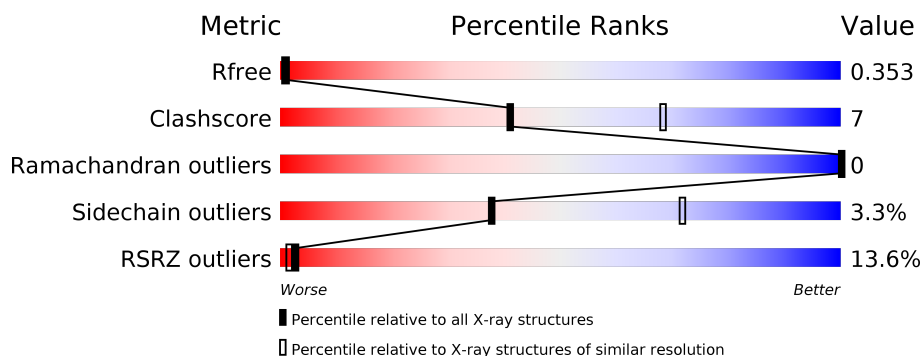
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	A	163	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	163	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	163	<div> <div>23%</div> <div> <div></div> <div>71%</div> <div>12%</div> <div>•</div> <div>17%</div> </div> </div>
1	D	163	<div> <div>14%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div>•</div> <div>14%</div> </div> </div>

2 Entry composition [i](#)

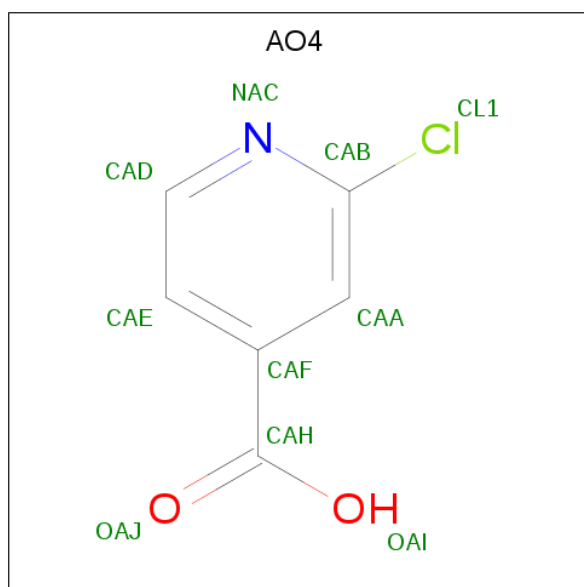
There are 3 unique types of molecules in this entry. The entry contains 8806 atoms, of which 4292 are hydrogens and 0 are deuteriums.

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 Conjugal transfer protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	141	Total	C	H	N	O	S	0	0	0
			2238	718	1100	198	219	3			
1	B	143	Total	C	H	N	O	S	0	0	0
			2285	728	1126	206	222	3			
1	C	136	Total	C	H	N	O	S	0	0	0
			2103	682	1021	187	210	3			
1	D	140	Total	C	H	N	O	S	0	0	0
			2146	697	1042	191	213	3			

- Molecule 2 is 2-chloropyridine-4-carboxylic acid (three-letter code: AO4) (formula: $C_6H_4ClNO_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	H	N	O	0	0
			13	6	1	3	1	2		


- Molecule 3 is water.

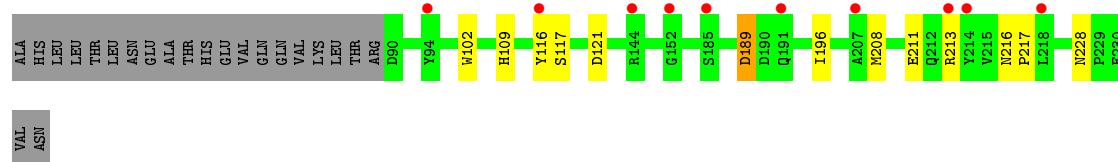
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	O 5	0	0
3	B	11	Total 11	O 11	0	0
3	C	4	Total 4	O 4	0	0
3	D	1	Total 1	O 1	0	0

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.

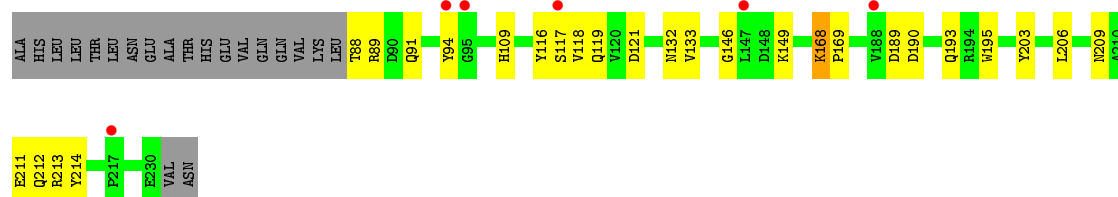
- Molecule 1: Conjugal transfer protein

Chain A: 



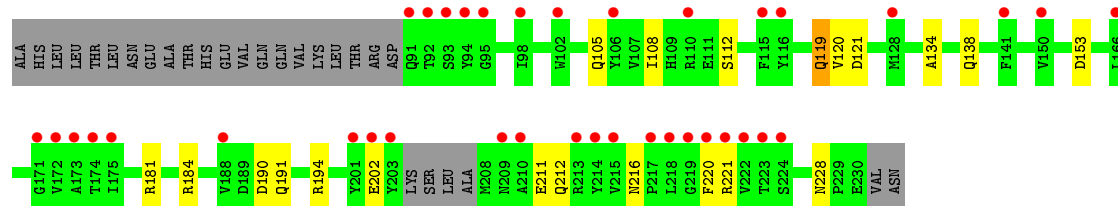
- Molecule 1: Conjugal transfer protein

Chain B: 



- Molecule 1: Conjugal transfer protein

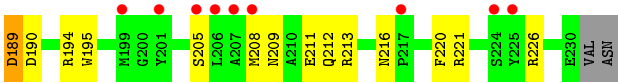
Chain C: 



- Molecule 1: Conjugal transfer protein

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	111.80Å 124.12Å 109.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.16 – 2.79 45.86 – 2.79	Depositor EDS
% Data completeness (in resolution range)	81.6 (41.16-2.79) 81.6 (45.86-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.298 , 0.357 0.308 , 0.353	Depositor DCC
R_{free} test set	1584 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8806	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AO4

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	0.37	0/1163	0.44	0/1578
1	B	0.47	0/1184	0.46	0/1605
1	C	0.39	0/1106	0.44	0/1503
1	D	0.41	0/1129	0.46	0/1537
All	All	0.41	0/4582	0.45	0/6223

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	A	1138	1100	1099	9	0
1	B	1159	1126	1125	23	0
1	C	1082	1021	1018	18	0
1	D	1104	1042	1041	13	0
2	A	10	3	0	0	0
3	A	5	0	0	0	0
3	B	11	0	0	1	0
3	C	4	0	0	0	0
3	D	1	0	0	0	0
All	All	4514	4292	4283	62	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 7.

All (62) 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:91:GLN:O	1:D:92:THR:HG22	1.15	1.30
1:D:91:GLN:O	1:D:92:THR:CG2	2.05	1.04
1:B:116:TYR:O	1:B:117:SER:HB2	1.80	0.80
1:B:89:ARG:HD3	1:B:91:GLN:CD	2.09	0.73
1:C:202:GLU:OE2	1:C:221:ARG:NH2	2.21	0.73
1:C:181:ARG:NH1	1:C:190:ASP:OD2	2.27	0.68
1:C:119:GLN:HE21	1:C:120:VAL:HG13	1.58	0.67
1:C:119:GLN:HG3	1:C:120:VAL:N	2.10	0.66
1:B:91:GLN:O	1:B:203:TYR:O	2.15	0.66
1:B:89:ARG:HD3	1:B:91:GLN:OE1	1.97	0.65
1:C:105:GLN:OE1	1:C:105:GLN:N	2.30	0.64
1:D:211:GLU:OE2	1:D:211:GLU:N	2.31	0.64
1:A:208:MET:SD	1:A:213:ARG:NH1	2.71	0.63
1:A:211:GLU:OE1	1:A:211:GLU:N	2.34	0.61
1:B:88:THR:N	3:B:302:HOH:O	2.33	0.61
1:C:119:GLN:HE21	1:C:120:VAL:CG1	2.14	0.60
1:C:119:GLN:HG3	1:C:120:VAL:H	1.68	0.58
1:B:211:GLU:N	1:B:211:GLU:OE1	2.35	0.58
1:B:94:TYR:CD1	1:B:203:TYR:CD2	2.92	0.58
1:A:213:ARG:NH2	1:A:217:PRO:O	2.38	0.57
1:C:191:GLN:OE1	1:C:191:GLN:N	2.39	0.55
1:D:110:ARG:HH12	1:D:133:VAL:HG12	1.72	0.55
1:C:153:ASP:O	1:C:184:ARG:NH1	2.40	0.54
1:D:107:VAL:HG21	1:D:175:ILE:CD1	2.37	0.54
1:C:216:ASN:HD21	1:C:220:PHE:HB3	1.72	0.54
1:B:118:VAL:HG13	1:B:119:GLN:N	2.22	0.54
1:A:196:ILE:N	1:A:228:ASN:O	2.41	0.53
1:D:209:ASN:OD1	1:D:212:GLN:HG2	2.09	0.53
1:B:214:TYR:OH	1:D:96:ASP:OD1	2.22	0.53
1:B:209:ASN:OD1	1:B:212:GLN:HG3	2.09	0.53
1:C:120:VAL:HG23	1:C:121:ASP:N	2.23	0.53
1:D:208:MET:SD	1:D:213:ARG:NH1	2.82	0.53
1:D:216:ASN:HD21	1:D:220:PHE:N	2.09	0.50
1:A:116:TYR:O	1:A:117:SER:OG	2.19	0.50
1:C:212:GLN:O	1:C:216:ASN:O	2.29	0.49
1:D:212:GLN:O	1:D:216:ASN:O	2.30	0.49
1:C:120:VAL:HG23	1:C:121:ASP:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:TYR:CE1	1:B:203:TYR:CD2	3.02	0.48
1:B:203:TYR:CD1	1:B:203:TYR:N	2.82	0.46
1:C:202:GLU:OE2	1:C:221:ARG:NE	2.48	0.46
1:B:89:ARG:CD	1:B:91:GLN:CD	2.83	0.45
1:B:132:ASN:OD1	1:B:133:VAL:N	2.50	0.44
1:C:108:ILE:O	1:C:112:SER:OG	2.34	0.44
1:B:118:VAL:CG1	1:B:119:GLN:N	2.81	0.43
1:C:134:ALA:O	1:C:138:GLN:N	2.50	0.43
1:B:109:HIS:ND1	1:B:121:ASP:OD1	2.50	0.43
1:B:146:GLY:O	1:B:149:LYS:N	2.52	0.43
1:A:213:ARG:NH1	1:A:216:ASN:O	2.52	0.43
1:D:189:ASP:OD1	1:D:189:ASP:N	2.52	0.42
1:C:202:GLU:OE2	1:C:221:ARG:CZ	2.68	0.42
1:B:89:ARG:HG2	1:B:91:GLN:HG3	2.01	0.42
1:B:193:GLN:HB3	1:B:195:TRP:HE1	1.85	0.42
1:A:109:HIS:ND1	1:A:121:ASP:OD1	2.52	0.41
1:C:216:ASN:ND2	1:C:220:PHE:O	2.52	0.41
1:B:89:ARG:HB3	1:B:91:GLN:OE1	2.20	0.41
1:D:146:GLY:O	1:D:149:LYS:N	2.53	0.41
1:A:102:TRP:CH2	1:A:217:PRO:HD2	2.56	0.40
1:B:94:TYR:CD1	1:B:203:TYR:CG	3.09	0.40
1:D:194:ARG:C	1:D:195:TRP:CD1	2.94	0.40
1:A:189:ASP:N	1:A:189:ASP:OD1	2.55	0.40
1:B:193:GLN:HB3	1:B:195:TRP:NE1	2.37	0.40
1:B:168:LYS:N	1:B:169:PRO:CD	2.84	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	A	139/163 (85%)	138 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	141/163 (86%)	139 (99%)	2 (1%)	0	100	100
1	C	132/163 (81%)	129 (98%)	3 (2%)	0	100	100
1	D	138/163 (85%)	135 (98%)	3 (2%)	0	100	100
All	All	550/652 (84%)	541 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	124/147 (84%)	123 (99%)	1 (1%)	81	94
1	B	127/147 (86%)	122 (96%)	5 (4%)	32	66
1	C	116/147 (79%)	112 (97%)	4 (3%)	37	71
1	D	117/147 (80%)	111 (95%)	6 (5%)	24	55
All	All	484/588 (82%)	468 (97%)	16 (3%)	38	72

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	ASP
1	B	168	LYS
1	B	189	ASP
1	B	190	ASP
1	B	206	LEU
1	B	213	ARG
1	C	119	GLN
1	C	194	ARG
1	C	211	GLU
1	C	228	ASN
1	D	158	ARG
1	D	189	ASP
1	D	190	ASP

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Mol	Chain	Res	Type
1	D	205	SER
1	D	221	ARG
1	D	226	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	119	GLN
1	C	162	ASN
1	C	216	ASN
1	D	162	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	AO4	A	301	-	8,10,10	3.81	5 (62%)	10,13,13	0.85	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
2	AO4	A	301	-	-	0/0/4/4	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	AO4	CAF-CAH	6.86	1.54	1.47
2	A	301	AO4	CAA-CAB	4.87	1.46	1.38
2	A	301	AO4	CAE-CAD	4.02	1.46	1.38
2	A	301	AO4	CAB-NAC	3.77	1.40	1.32
2	A	301	AO4	CAB-CL1	3.45	1.81	1.74

There are no bond angle outliers.

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 [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	A	141/163 (86%)	0.67	10 (7%) 16 9	36, 49, 67, 73	0
1	B	143/163 (87%)	0.68	6 (4%) 36 26	42, 55, 67, 73	0
1	C	136/163 (83%)	1.45	37 (27%) 0 0	61, 79, 94, 102	0
1	D	140/163 (85%)	1.01	23 (16%) 1 1	62, 80, 88, 100	0
All	All	560/652 (85%)	0.95	76 (13%) 3 1	36, 66, 88, 102	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	91	GLN	6.4
1	C	210	ALA	6.0
1	C	203	TYR	5.7
1	C	150	VAL	5.7
1	C	201	TYR	5.4
1	D	205	SER	5.2
1	D	206	LEU	4.8
1	C	218	LEU	4.7
1	C	102	TRP	4.6
1	D	175	ILE	4.6
1	C	220	PHE	4.2
1	C	188	VAL	4.1
1	D	207	ALA	4.1
1	C	98	ILE	3.9
1	C	214	TYR	3.9
1	D	224	SER	3.8
1	C	94	TYR	3.7
1	D	225	TYR	3.7
1	C	213	ARG	3.7
1	C	215	VAL	3.6
1	A	94	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	175	ILE	3.5
1	C	219	GLY	3.5
1	C	92	THR	3.5
1	C	171	GLY	3.4
1	C	222	VAL	3.4
1	C	128	MET	3.4
1	A	144	ARG	3.3
1	C	223	THR	3.2
1	D	199	MET	3.0
1	C	173	ALA	3.0
1	D	208	MET	3.0
1	D	181	ARG	2.9
1	D	110	ARG	2.9
1	D	165	ILE	2.9
1	C	141	PHE	2.9
1	C	166	LEU	2.8
1	C	110	ARG	2.7
1	A	152	GLY	2.7
1	C	115	PHE	2.7
1	C	202	GLU	2.7
1	A	185	SER	2.7
1	C	106	TYR	2.6
1	A	218	LEU	2.6
1	A	207	ALA	2.6
1	D	201	TYR	2.6
1	C	116	TYR	2.5
1	C	93	SER	2.5
1	A	214	TYR	2.5
1	C	217	PRO	2.4
1	C	172	VAL	2.4
1	C	221	ARG	2.4
1	D	113	TYR	2.4
1	C	174	THR	2.4
1	C	209	ASN	2.4
1	B	217	PRO	2.4
1	D	126	GLY	2.3
1	B	94	TYR	2.3
1	D	94	TYR	2.2
1	B	117	SER	2.2
1	A	116	TYR	2.2
1	D	118	VAL	2.2
1	B	147	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	103	LEU	2.2
1	D	217	PRO	2.2
1	C	224	SER	2.2
1	D	184	ARG	2.2
1	B	188	VAL	2.1
1	A	191	GLN	2.1
1	B	95	GLY	2.1
1	C	95	GLY	2.1
1	D	107	VAL	2.1
1	D	127	LEU	2.1
1	D	132	ASN	2.1
1	A	213	ARG	2.1
1	D	141	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
2	AO4	A	301	10/10	0.88	0.45	39,44,53,55	1

6.5 Other polymers [i](#)

There are no such residues in this entry.