



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:34 pm GMT

PDB ID : 1JLY
Title : CRYSTAL STRUCTURE OF AMARANTHUS CAUDATUS AGGLUTININ
Authors : Transue, T.R.; Smith, A.K.; Mo, H.; Goldstein, I.J.; Saper, M.A.
Deposited on : 1997-07-23
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

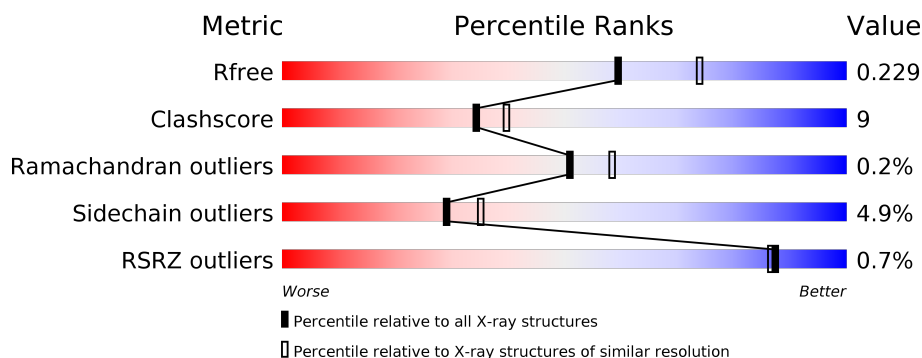
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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. 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	304	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 0; left: 0; width: 74%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 74%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 98%; height: 10px; background-color: red; width: 2%;"></div> <div style="position: absolute; top: 0; left: 99%; height: 10px; background-color: red; width: 2%;"></div> <div style="position: absolute; top: 0; left: 100%; height: 10px; background-color: red; width: 2%;"></div> <div style="position: absolute; top: 0; left: 74%; width: 100px; text-align: center;">74%</div> <div style="position: absolute; top: 0; left: 78%; width: 100px; text-align: center;">22%</div> <div style="position: absolute; top: 0; left: 95%; text-align: center;">...</div> </div> </div>
1	B	304	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 77%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 77%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 99%; height: 10px; background-color: red; width: 2%;"></div> <div style="position: absolute; top: 0; left: 100%; height: 10px; background-color: red; width: 2%;"></div> <div style="position: absolute; top: 0; left: 77%; width: 100px; text-align: center;">77%</div> <div style="position: absolute; top: 0; left: 79%; width: 100px; text-align: center;">21%</div> <div style="position: absolute; top: 0; left: 96%; text-align: center;">..</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5188 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 AGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	1
			2428	1560	407	450	11			
1	B	300	Total	C	N	O	S	0	0	1
			2428	1560	407	450	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	HIS	ASN	CONFLICT	UNP Q71QF2
A	122	GLN	GLU	CONFLICT	UNP Q71QF2
A	163	GLY	THR	CONFLICT	UNP Q71QF2
A	227	ASP	ASN	CONFLICT	UNP Q71QF2
A	276	GLY	GLU	CONFLICT	UNP Q71QF2
A	287	ASN	ILE	CONFLICT	UNP Q71QF2
A	301	GLN	SER	CONFLICT	UNP Q71QF2
B	14	HIS	ASN	CONFLICT	UNP Q71QF2
B	122	GLN	GLU	CONFLICT	UNP Q71QF2
B	163	GLY	THR	CONFLICT	UNP Q71QF2
B	227	ASP	ASN	CONFLICT	UNP Q71QF2
B	276	GLY	GLU	CONFLICT	UNP Q71QF2
B	287	ASN	ILE	CONFLICT	UNP Q71QF2
B	301	GLN	SER	CONFLICT	UNP Q71QF2

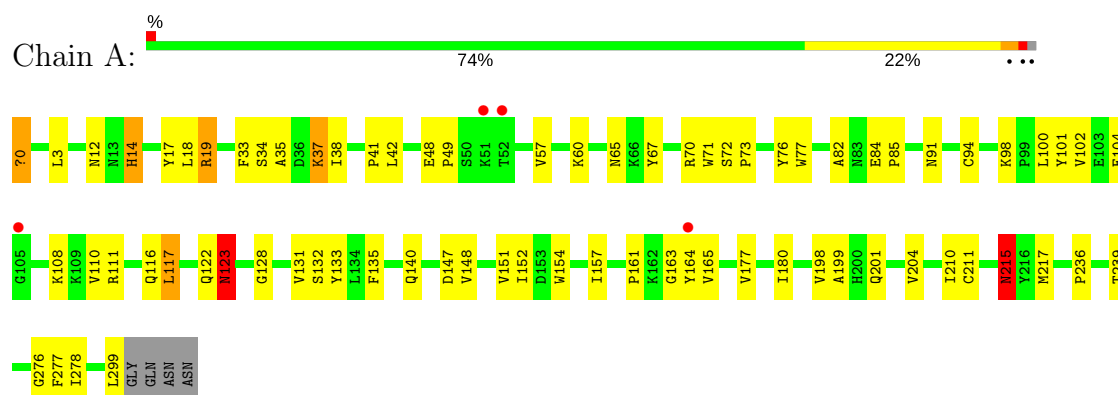
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	176	Total	O	0	0
			176	176		
2	B	156	Total	O	0	0
			156	156		

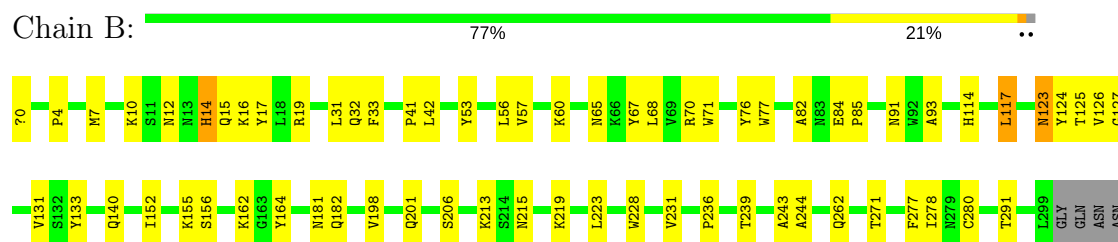
3 Residue-property plots [i](#)

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: AGGLUTININ



• Molecule 1: AGGLUTININ



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.30Å 99.10Å 66.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 33.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.20) 83.2 (33.20-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.10Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.174 , 0.246 0.164 , 0.229	Depositor DCC
R_{free} test set	3421 reflections (9.97%)	DCC
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 81.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5188	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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: FOR

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	0.61	2/2491 (0.1%)	0.81	4/3381 (0.1%)
1	B	0.60	0/2491	0.78	2/3381 (0.1%)
All	All	0.60	2/4982 (0.0%)	0.79	6/6762 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	CYS	CB-SG	-6.27	1.71	1.82
1	A	215	ASN	CB-CG	-5.62	1.38	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	GLY	N-CA-C	-6.82	96.05	113.10
1	A	123	ASN	N-CA-C	-5.53	96.06	111.00
1	A	0	FOR	O-C-N	-5.43	114.01	122.70
1	B	123	ASN	N-CA-C	-5.29	96.72	111.00
1	B	0	FOR	O-C-N	-5.13	114.49	122.70
1	A	111	ARG	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2428	0	2365	54	0
1	B	2428	0	2365	39	0
2	A	176	0	0	1	0
2	B	156	0	0	0	0
All	All	5188	0	4730	91	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 9.

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)
1:B:14:HIS:HE1	1:B:33:PHE:HB3	1.39	0.84
1:A:101:TYR:CD1	1:A:110:VAL:HG12	2.18	0.79
1:B:67:TYR:HB2	1:B:82:ALA:HB3	1.67	0.75
1:A:14:HIS:CE1	1:A:33:PHE:HB3	2.23	0.73
1:A:154:TRP:O	1:A:157:ILE:HG22	1.89	0.72
1:A:14:HIS:HE1	1:A:33:PHE:HB3	1.55	0.72
1:B:14:HIS:CE1	1:B:33:PHE:HB3	2.25	0.72
1:B:14:HIS:CE1	1:B:16:LYS:HB2	2.27	0.69
1:A:102:VAL:HG21	1:A:148:VAL:HG13	1.76	0.68
1:A:17:TYR:HE1	1:A:152:ILE:HD12	1.59	0.67
1:B:164:TYR:HE1	1:B:215:ASN:ND2	1.92	0.66
1:B:10:LYS:HE2	1:B:15:GLN:HG3	1.79	0.65
1:A:164:TYR:HB3	1:A:299:LEU:HD12	1.77	0.65
1:A:164:TYR:HB2	1:A:299:LEU:HB2	1.81	0.63
1:B:124:TYR:CE2	1:B:126:VAL:HG22	2.35	0.62
1:A:67:TYR:HB2	1:A:82:ALA:HB3	1.80	0.61
1:B:125:THR:HG22	1:B:127:GLY:H	1.65	0.59
1:B:31:LEU:HD11	1:B:68:LEU:HD22	1.85	0.59
1:B:164:TYR:HE1	1:B:215:ASN:HD21	1.49	0.58
1:A:91:ASN:O	1:A:116:GLN:HG3	2.03	0.57
1:A:37:LYS:HE2	2:A:348:HOH:O	2.05	0.57
1:A:108:LYS:HE3	1:A:151:VAL:O	2.04	0.57
1:A:76:TYR:HB2	1:A:135:PHE:CE1	2.40	0.57
1:B:4:PRO:HG2	1:B:7:MET:HB3	1.86	0.56
1:B:76:TYR:CD1	1:B:117:LEU:HD21	2.40	0.56
1:A:123:ASN:ND2	1:A:132:SER:HA	2.20	0.55
1:B:124:TYR:HE2	1:B:126:VAL:HG22	1.72	0.55
1:A:17:TYR:HB2	1:A:35:ALA:HB3	1.90	0.54
1:A:60:LYS:NZ	1:A:65:ASN:HD21	2.06	0.54
1:A:38:ILE:CD1	1:A:152:ILE:HG21	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:TYR:CE1	1:B:215:ASN:ND2	2.75	0.54
1:B:228:TRP:CZ3	1:B:280:CYS:HB2	2.43	0.54
1:A:17:TYR:CE1	1:A:152:ILE:HD12	2.42	0.52
1:A:70:ARG:HD2	1:A:117:LEU:HD22	1.90	0.52
1:B:271:THR:HG23	1:B:278:ILE:HA	1.91	0.52
1:A:199:ALA:O	1:A:215:ASN:HB2	2.11	0.51
1:B:17:TYR:HE2	1:B:152:ILE:HD12	1.75	0.50
1:B:114:HIS:ND1	1:B:117:LEU:HB2	2.26	0.50
1:A:101:TYR:CE1	1:A:110:VAL:HG12	2.46	0.50
1:B:53:TYR:CB	1:B:56:LEU:HD12	2.42	0.50
1:B:84:GLU:HB2	1:B:85:PRO:HD2	1.94	0.50
1:A:84:GLU:HB2	1:A:85:PRO:HD2	1.94	0.49
1:A:19:ARG:HD2	1:A:34:SER:OG	2.12	0.49
1:A:180:ILE:HD13	1:A:276:GLY:O	2.12	0.49
1:A:72:SER:HB2	1:A:73:PRO:CD	2.43	0.49
1:A:177:VAL:HG21	1:A:217:MET:HG2	1.95	0.49
1:A:164:TYR:HE2	1:A:215:ASN:ND2	2.10	0.48
1:B:219:LYS:HB2	1:B:231:VAL:HG12	1.95	0.48
1:A:123:ASN:HD21	1:A:132:SER:HA	1.78	0.48
1:A:94:CYS:HB3	1:A:116:GLN:HB2	1.96	0.48
1:B:70:ARG:HD2	1:B:117:LEU:HD22	1.95	0.48
1:B:236:PRO:HB3	1:B:244:ALA:HB3	1.96	0.47
1:B:201:GLN:HG3	1:B:215:ASN:OD1	2.14	0.47
1:A:236:PRO:HA	1:A:239:THR:OG1	2.14	0.47
1:A:67:TYR:CE1	1:A:85:PRO:HD3	2.50	0.46
1:A:12:ASN:ND2	1:A:148:VAL:O	2.47	0.46
1:B:243:ALA:HA	1:B:262:GLN:HB2	1.98	0.46
1:A:277:PHE:C	1:A:278:ILE:HD12	2.37	0.45
1:A:38:ILE:HD11	1:A:152:ILE:HG21	1.97	0.45
1:A:60:LYS:HZ3	1:A:65:ASN:HD21	1.64	0.45
1:B:91:ASN:HD21	1:B:93:ALA:HB3	1.81	0.45
1:A:204:VAL:HG22	1:A:210:ILE:HG12	1.97	0.45
1:A:161:PRO:HG2	1:A:165:VAL:HG11	1.99	0.45
1:A:67:TYR:CZ	1:A:85:PRO:HD3	2.51	0.45
1:A:131:VAL:O	1:A:131:VAL:HG23	2.18	0.44
1:B:181:ASN:O	1:B:182:GLN:HB3	2.18	0.44
1:A:48:GLU:HA	1:A:49:PRO:HD2	1.77	0.44
1:B:60:LYS:NZ	1:B:65:ASN:HD21	2.16	0.44
1:A:101:TYR:CE1	1:A:110:VAL:CG1	3.01	0.43
1:B:124:TYR:CE2	1:B:126:VAL:CG2	3.02	0.43
1:A:38:ILE:HD12	1:A:152:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ASN:O	1:B:182:GLN:CB	2.66	0.43
1:B:14:HIS:NE2	1:B:33:PHE:O	2.51	0.43
1:B:181:ASN:HD22	1:B:277:PHE:HE2	1.67	0.43
1:A:164:TYR:CB	1:A:299:LEU:HB2	2.49	0.42
1:A:0:FOR:O	1:A:3:LEU:HB2	2.20	0.42
1:A:98:LYS:HE3	1:A:100:LEU:HD21	2.01	0.42
1:B:125:THR:HG23	1:B:131:VAL:HA	2.01	0.42
1:A:18:LEU:HD13	1:A:33:PHE:CE2	2.55	0.41
1:A:41:PRO:HB2	1:B:41:PRO:HB2	2.03	0.41
1:B:32:GLN:HB2	1:B:133:TYR:CE1	2.56	0.41
1:A:123:ASN:HD21	1:A:132:SER:CA	2.33	0.41
1:B:77:TRP:CZ3	1:B:133:TYR:HB2	2.56	0.41
1:A:77:TRP:CZ3	1:A:133:TYR:HB2	2.56	0.41
1:A:122:GLN:HG2	1:A:147:ASP:HB3	2.03	0.41
1:A:201:GLN:NE2	1:A:215:ASN:OD1	2.52	0.40
1:A:84:GLU:HG2	1:B:206:SER:HB2	2.03	0.40
1:B:236:PRO:HA	1:B:239:THR:OG1	2.20	0.40
1:A:123:ASN:HD22	1:A:123:ASN:C	2.25	0.40
1:B:155:LYS:HG2	1:B:156:SER:N	2.36	0.40
1:A:72:SER:CB	1:A:73:PRO:CD	3.00	0.40

There are no symmetry-related clashes.

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	298/304 (98%)	282 (95%)	15 (5%)	1 (0%)	44	49
1	B	298/304 (98%)	281 (94%)	17 (6%)	0	100	100
All	All	596/608 (98%)	563 (94%)	32 (5%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLY

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	268/271 (99%)	256 (96%)	12 (4%)	32	39
1	B	268/271 (99%)	254 (95%)	14 (5%)	27	32
All	All	536/542 (99%)	510 (95%)	26 (5%)	29	35

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	19	ARG
1	A	37	LYS
1	A	42	LEU
1	A	57	VAL
1	A	71	TRP
1	A	104	GLU
1	A	117	LEU
1	A	123	ASN
1	A	140	GLN
1	A	198	VAL
1	A	215	ASN
1	B	12	ASN
1	B	14	HIS
1	B	19	ARG
1	B	42	LEU
1	B	57	VAL
1	B	71	TRP
1	B	117	LEU
1	B	123	ASN
1	B	140	GLN
1	B	162	LYS
1	B	198	VAL

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Mol	Chain	Res	Type
1	B	213	LYS
1	B	223	LEU
1	B	291	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	65	ASN
1	A	123	ASN
1	A	140	GLN
1	A	159	GLN
1	A	262	GLN
1	B	13	ASN
1	B	65	ASN
1	B	74	ASN
1	B	91	ASN
1	B	123	ASN
1	B	140	GLN

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](#)

There are no ligands in this entry.

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	A	299/304 (98%)	-0.52	4 (1%) 77 75	4, 14, 38, 44	0
1	B	299/304 (98%)	-0.53	0 100 100	4, 15, 36, 51	0
All	All	598/608 (98%)	-0.52	4 (0%) 87 86	4, 15, 37, 51	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	TYR	3.8
1	A	52	THR	2.7
1	A	51	LYS	2.5
1	A	105	GLY	2.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.