



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:07 AM GMT

PDB ID : 2FP8  
Title : Structure of Strictosidine Synthase, the Biosynthetic Entry to the Monoterpenoid Indole Alkaloid Family  
Authors : Panjikar, S.  
Deposited on : 2006-01-16  
Resolution : 2.30 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

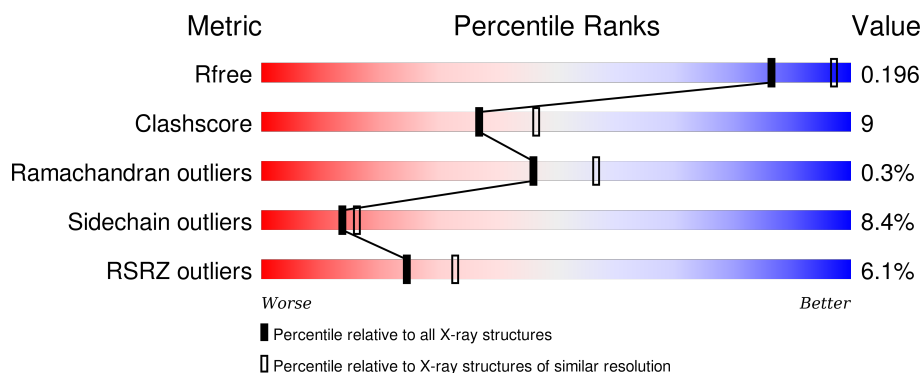
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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  $\geq 3$ , 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	322	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 6%</div> </div> </div>
1	B	322	<div> <div>11%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>•• 6%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5173 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 Strictosidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2382	1529	388	460	5			
1	B	303	Total	C	N	O	S	0	0	0
			2390	1535	389	461	5			

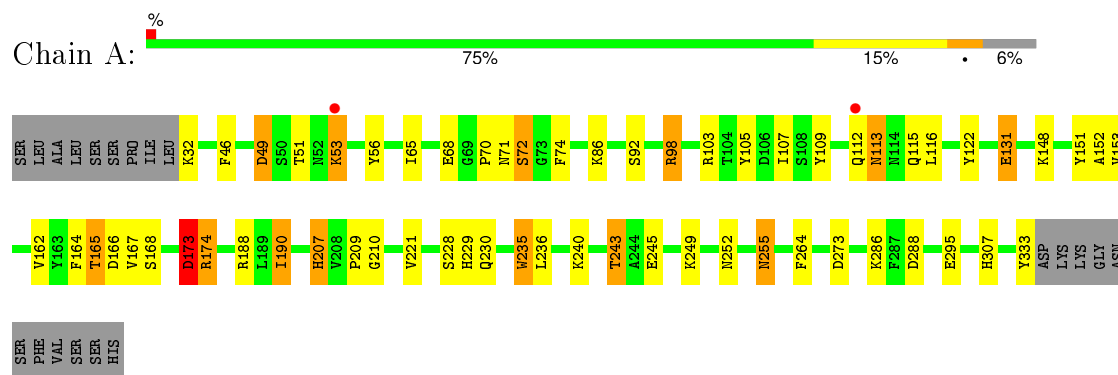
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	279	Total	O	0	0
			279	279		
2	B	122	Total	O	0	0
			122	122		

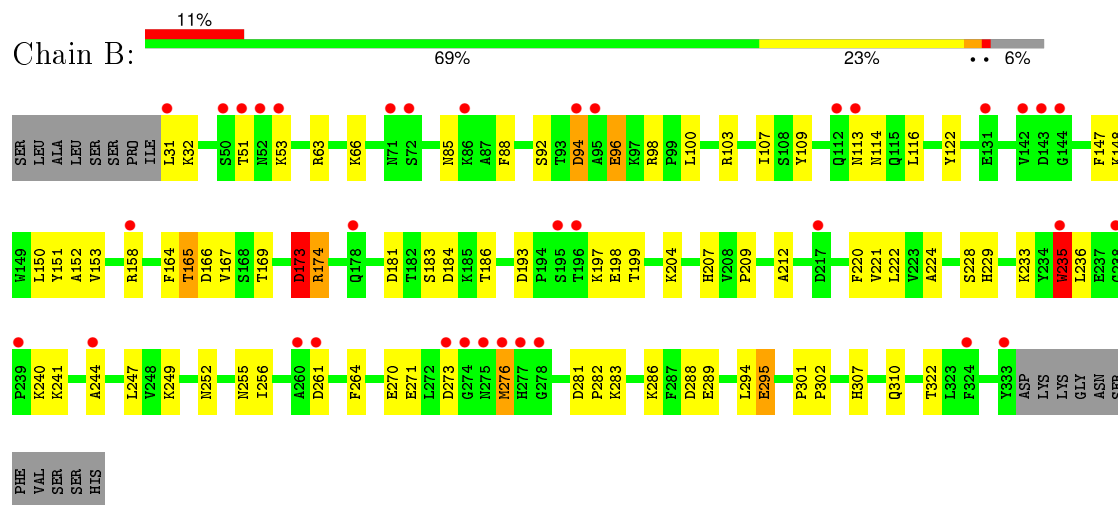
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Strictosidine synthase



#### • Molecule 1: Strictosidine synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.29 Å   147.29 Å   122.33 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.30) 99.7 (19.65-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.30 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.188 , 0.217 0.192 , 0.196	Depositor DCC
$R_{free}$ test set	1078 reflections (2.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.704	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.4	EDS
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43715 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5173	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.80	2/2447 (0.1%)	0.91	6/3329 (0.2%)
1	B	0.73	2/2455 (0.1%)	0.84	6/3340 (0.2%)
All	All	0.76	4/4902 (0.1%)	0.87	12/6669 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	240	LYS	CD-CE	6.70	1.68	1.51
1	A	173	ASP	CB-CG	-6.21	1.38	1.51
1	B	235	TRP	CB-CG	5.58	1.60	1.50
1	A	255	ASN	CG-OD1	5.05	1.35	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	A	166	ASP	CB-CG-OD2	7.04	124.63	118.30
1	B	94	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	174	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	A	273	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	49	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	288	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	273	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	261	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	193	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	184	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	181	ASP	CB-CG-OD2	5.02	122.81	118.30

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	2382	0	2287	41	0
1	B	2390	0	2298	48	0
2	A	279	0	0	8	0
2	B	122	0	0	8	0
All	All	5173	0	4585	88	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 (88) 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:A:49:ASP:OD1	1:A:51:THR:HG22	1.62	0.98
1:A:229:HIS:HD2	1:A:252:ASN:H	1.04	0.95
1:B:229:HIS:HD2	1:B:252:ASN:H	1.04	0.94
1:A:235:TRP:HZ3	1:A:245:GLU:OE2	1.51	0.92
1:A:162:VAL:HG12	2:A:511:HOH:O	1.70	0.89
1:A:122:TYR:OH	1:A:174:ARG:NH1	2.08	0.87
1:B:235:TRP:HE3	2:B:410:HOH:O	1.60	0.83
1:B:229:HIS:CD2	1:B:252:ASN:H	1.95	0.81
1:B:152:ALA:H	1:B:165:THR:HG22	1.45	0.79
1:A:229:HIS:CD2	1:A:252:ASN:H	1.96	0.78
1:A:235:TRP:CZ3	1:A:245:GLU:OE2	2.38	0.76
1:A:153:VAL:HG23	2:A:511:HOH:O	1.85	0.76
1:B:307:HIS:HD2	2:B:465:HOH:O	1.74	0.71
1:A:174:ARG:HH11	1:A:174:ARG:HG3	1.56	0.71
1:B:174:ARG:HG3	1:B:174:ARG:HH11	1.57	0.69
1:A:230:GLN:HE21	1:A:249:LYS:HE2	1.58	0.69
1:B:94:ASP:HB3	1:B:96:GLU:OE1	1.94	0.66
1:B:229:HIS:HD2	1:B:252:ASN:N	1.87	0.65
1:B:98:ARG:HH11	1:B:173:ASP:HB3	1.62	0.65
1:B:233:LYS:HD2	1:B:247:LEU:HD13	1.78	0.65
1:A:229:HIS:HD2	1:A:252:ASN:N	1.88	0.64
1:B:166:ASP:CG	2:B:408:HOH:O	2.35	0.64
1:A:307:HIS:HD2	2:A:406:HOH:O	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:VAL:HA	1:B:209:PRO:HD2	1.81	0.63
1:A:164:PHE:HB3	2:A:511:HOH:O	1.98	0.62
1:A:131:GLU:HB3	2:A:492:HOH:O	2.00	0.61
1:A:255:ASN:ND2	2:A:502:HOH:O	2.33	0.60
1:B:152:ALA:N	1:B:165:THR:HG22	2.16	0.59
1:B:235:TRP:CE3	2:B:410:HOH:O	2.42	0.59
1:A:221:VAL:HG23	1:A:236:LEU:HD11	1.85	0.58
1:B:174:ARG:HG3	1:B:174:ARG:NH1	2.19	0.55
1:B:252:ASN:ND2	1:B:271:GLU:H	2.06	0.54
1:A:174:ARG:NH1	1:A:174:ARG:HG3	2.22	0.54
1:B:98:ARG:NH1	1:B:173:ASP:HB3	2.23	0.54
1:B:221:VAL:HG23	1:B:236:LEU:HD11	1.90	0.53
1:B:147:PHE:HB3	2:B:408:HOH:O	2.08	0.53
1:A:98:ARG:HD3	1:A:173:ASP:OD1	2.09	0.52
1:A:71:ASN:ND2	1:A:72:SER:H	2.08	0.52
1:A:113:ASN:ND2	1:A:115:GLN:HG3	2.25	0.52
1:A:207:HIS:HD2	1:A:228:SER:OG	1.93	0.51
1:B:255:ASN:HD22	1:B:310:GLN:HB2	1.76	0.51
1:B:236:LEU:O	1:B:241:LYS:HG3	2.12	0.50
1:B:85:ASN:HD22	1:B:88:PHE:H	1.60	0.50
1:A:51:THR:HG23	1:A:53:LYS:H	1.76	0.49
1:A:221:VAL:CG2	1:A:236:LEU:HD11	2.42	0.48
1:B:151:TYR:HB2	1:B:167:VAL:HG13	1.95	0.48
1:B:224:ALA:HB2	1:B:256:ILE:HD11	1.96	0.48
1:B:264:PHE:O	1:B:286:LYS:HA	2.14	0.47
1:B:158:ARG:CB	1:B:158:ARG:HH11	2.27	0.47
1:A:65:ILE:HD12	1:A:74:PHE:CD2	2.50	0.47
1:B:282:PRO:HD2	2:B:362:HOH:O	2.15	0.47
1:B:252:ASN:HD22	1:B:270:GLU:HA	1.80	0.47
1:B:153:VAL:HG23	1:B:164:PHE:HB3	1.97	0.47
1:A:105:TYR:OH	1:A:173:ASP:OD2	2.21	0.46
1:B:301:PRO:HA	2:B:351:HOH:O	2.15	0.46
1:A:295:GLU:OE2	1:A:333:TYR:OH	2.21	0.46
1:B:122:TYR:OH	1:B:174:ARG:NH1	2.49	0.46
1:B:158:ARG:HB2	1:B:158:ARG:NH1	2.31	0.45
1:B:286:LYS:HB3	1:B:295:GLU:HB2	1.98	0.45
1:A:210:GLY:N	2:A:421:HOH:O	2.49	0.45
1:B:276:MET:HG2	1:B:276:MET:O	2.15	0.45
1:A:107:ILE:HB	1:A:116:LEU:HD11	1.99	0.44
1:A:148:LYS:HD2	1:A:148:LYS:HA	1.69	0.44
1:A:264:PHE:O	1:A:286:LYS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:HB2	1:A:168:SER:O	2.18	0.44
1:A:210:GLY:CA	2:A:421:HOH:O	2.66	0.44
1:A:240:LYS:O	1:A:243:THR:HB	2.17	0.44
1:A:152:ALA:H	1:A:165:THR:HG22	1.84	0.43
1:A:151:TYR:HB2	1:A:167:VAL:HG13	2.01	0.43
1:B:212:ALA:HA	1:B:222:LEU:O	2.18	0.43
1:B:288:ASP:HB3	1:B:294:LEU:HD11	2.00	0.43
1:B:150:LEU:HD23	1:B:166:ASP:HB2	2.00	0.42
1:B:322:THR:HG22	2:B:352:HOH:O	2.19	0.42
1:A:70:PRO:HG2	1:B:302:PRO:HB3	2.01	0.42
1:B:249:LYS:HB3	1:B:249:LYS:HE3	1.74	0.42
1:A:46:PHE:HA	1:A:56:TYR:O	2.19	0.42
1:B:122:TYR:OH	1:B:173:ASP:HB2	2.18	0.42
1:B:270:GLU:HB3	1:B:281:ASP:HB3	2.02	0.42
1:A:122:TYR:OH	1:A:173:ASP:HB2	2.20	0.41
1:B:220:PHE:HZ	1:B:289:GLU:HB3	1.85	0.41
1:B:233:LYS:O	1:B:244:ALA:HA	2.20	0.41
1:A:165:THR:HG21	1:A:209:PRO:O	2.20	0.41
1:A:188:ARG:HB3	1:A:190:ILE:CD1	2.51	0.40
1:B:148:LYS:HD3	1:B:148:LYS:HA	1.94	0.40
1:B:107:ILE:HB	1:B:116:LEU:HD21	2.04	0.40
1:A:122:TYR:CZ	1:A:174:ARG:NH1	2.88	0.40
1:B:169:THR:HG23	1:B:186:THR:O	2.20	0.40
1:B:221:VAL:CG2	1:B:236:LEU:HD11	2.51	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	300/322 (93%)	288 (96%)	11 (4%)	1 (0%)	46 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	301/322 (94%)	288 (96%)	12 (4%)	1 (0%)	46	57
All	All	601/644 (93%)	576 (96%)	23 (4%)	2 (0%)	46	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ASP
1	B	173	ASP

### 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	260/278 (94%)	243 (94%)	17 (6%)	21	27
1	B	261/278 (94%)	234 (90%)	27 (10%)	9	10
All	All	521/556 (94%)	477 (92%)	44 (8%)	14	16

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	53	LYS
1	A	68	GLU
1	A	72	SER
1	A	86	LYS
1	A	92	SER
1	A	103	ARG
1	A	109	TYR
1	A	112	GLN
1	A	113	ASN
1	A	131	GLU
1	A	165	THR
1	A	173	ASP
1	A	190	ILE

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Mol	Chain	Res	Type
1	A	207	HIS
1	A	235	TRP
1	A	243	THR
1	B	31	LEU
1	B	32	LYS
1	B	51	THR
1	B	53	LYS
1	B	63	ARG
1	B	66	LYS
1	B	92	SER
1	B	96	GLU
1	B	100	LEU
1	B	103	ARG
1	B	109	TYR
1	B	113	ASN
1	B	114	ASN
1	B	165	THR
1	B	173	ASP
1	B	174	ARG
1	B	183	SER
1	B	197	LYS
1	B	198	GLU
1	B	199	THR
1	B	204	LYS
1	B	207	HIS
1	B	228	SER
1	B	235	TRP
1	B	276	MET
1	B	283	LYS
1	B	295	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	91	ASN
1	A	112	GLN
1	A	113	ASN
1	A	207	HIS
1	A	229	HIS
1	A	230	GLN
1	A	252	ASN

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Mol	Chain	Res	Type
1	A	255	ASN
1	A	310	GLN
1	A	312	GLN
1	B	85	ASN
1	B	91	ASN
1	B	113	ASN
1	B	229	HIS
1	B	230	GLN
1	B	252	ASN
1	B	255	ASN
1	B	275	ASN
1	B	310	GLN
1	B	312	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 ⓘ

### 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	302/322 (93%)	-0.25	2 (0%) 89 92	16, 21, 28, 33	0
1	B	303/322 (94%)	0.55	35 (11%) 6 10	16, 22, 29, 50	0
All	All	605/644 (93%)	0.15	37 (6%) 25 33	16, 22, 29, 50	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	GLY	9.3
1	B	275	ASN	5.5
1	B	276	MET	5.5
1	B	112	GLN	5.1
1	B	196	THR	5.1
1	B	278	GLY	4.8
1	B	195	SER	4.3
1	B	239	PRO	4.3
1	B	277	HIS	4.2
1	B	51	THR	4.0
1	B	95	ALA	3.9
1	B	143	ASP	3.8
1	B	158	ARG	3.7
1	B	333	TYR	3.6
1	B	50	SER	3.5
1	B	144	GLY	3.5
1	B	244	ALA	3.5
1	B	238	GLY	3.4
1	B	72	SER	3.2
1	B	261	ASP	3.2
1	B	235	TRP	3.2
1	B	178	GLN	3.1
1	B	260	ALA	3.1
1	B	94	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	71	ASN	2.6
1	B	217	ASP	2.5
1	B	113	ASN	2.4
1	A	53	LYS	2.4
1	B	52	ASN	2.3
1	B	273	ASP	2.2
1	B	53	LYS	2.2
1	B	142	VAL	2.2
1	B	131	GLU	2.1
1	A	112	GLN	2.1
1	B	31	LEU	2.0
1	B	324	PHE	2.0
1	B	86	LYS	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.