



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:32 am GMT

PDB ID : 4J7R  
Title : Crystal Structure of Chlamydomonas reinhardtii Isoamylase 1 (ISA1)  
Authors : Sim, L.; Palcic, M.  
Deposited on : 2013-02-14  
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.

---

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

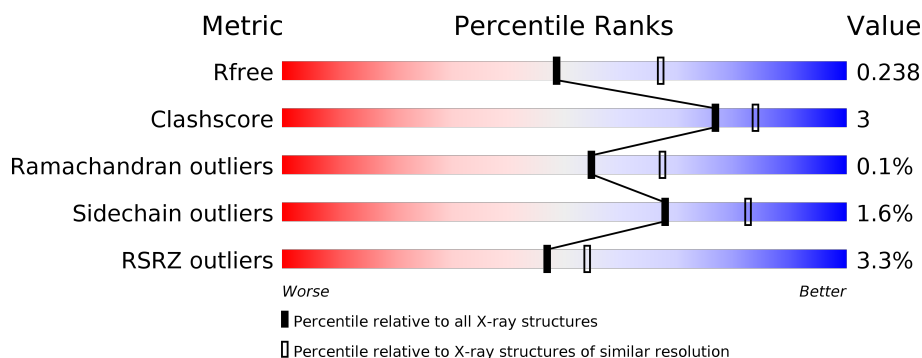
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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	840	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
1	B	840	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12892 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 Isoamylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	800	Total	C	N	O	S	0	0	0
			6212	3925	1092	1165	30			
1	B	797	Total	C	N	O	S	0	0	0
			6192	3907	1090	1165	30			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	MET	-	EXPRESSION TAG	UNP Q7X8Q2
A	37	GLY	-	EXPRESSION TAG	UNP Q7X8Q2
A	38	SER	-	EXPRESSION TAG	UNP Q7X8Q2
A	39	SER	-	EXPRESSION TAG	UNP Q7X8Q2
A	40	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	41	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	42	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	43	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	44	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	45	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	46	SER	-	EXPRESSION TAG	UNP Q7X8Q2
A	47	SER	-	EXPRESSION TAG	UNP Q7X8Q2
A	48	GLY	-	EXPRESSION TAG	UNP Q7X8Q2
A	49	LEU	-	EXPRESSION TAG	UNP Q7X8Q2
A	50	VAL	-	EXPRESSION TAG	UNP Q7X8Q2
A	51	PRO	-	EXPRESSION TAG	UNP Q7X8Q2
A	52	ARG	-	EXPRESSION TAG	UNP Q7X8Q2
A	53	GLY	-	EXPRESSION TAG	UNP Q7X8Q2
A	54	SER	-	EXPRESSION TAG	UNP Q7X8Q2
A	55	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
A	56	MET	-	EXPRESSION TAG	UNP Q7X8Q2
B	36	MET	-	EXPRESSION TAG	UNP Q7X8Q2
B	37	GLY	-	EXPRESSION TAG	UNP Q7X8Q2
B	38	SER	-	EXPRESSION TAG	UNP Q7X8Q2
B	39	SER	-	EXPRESSION TAG	UNP Q7X8Q2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	40	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	41	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	42	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	43	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	44	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	45	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	46	SER	-	EXPRESSION TAG	UNP Q7X8Q2
B	47	SER	-	EXPRESSION TAG	UNP Q7X8Q2
B	48	GLY	-	EXPRESSION TAG	UNP Q7X8Q2
B	49	LEU	-	EXPRESSION TAG	UNP Q7X8Q2
B	50	VAL	-	EXPRESSION TAG	UNP Q7X8Q2
B	51	PRO	-	EXPRESSION TAG	UNP Q7X8Q2
B	52	ARG	-	EXPRESSION TAG	UNP Q7X8Q2
B	53	GLY	-	EXPRESSION TAG	UNP Q7X8Q2
B	54	SER	-	EXPRESSION TAG	UNP Q7X8Q2
B	55	HIS	-	EXPRESSION TAG	UNP Q7X8Q2
B	56	MET	-	EXPRESSION TAG	UNP Q7X8Q2

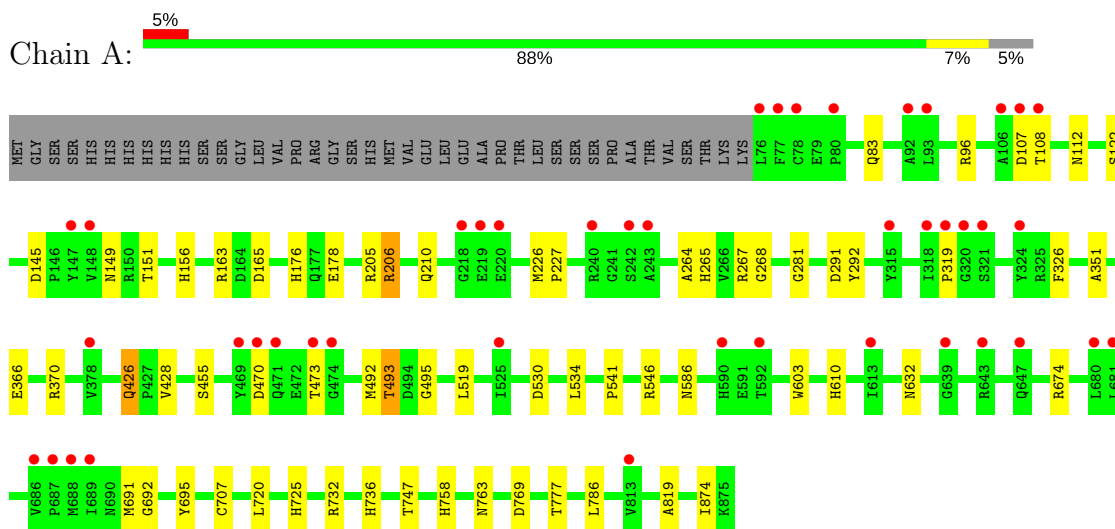
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	227	Total O 227 227	0	0
2	B	261	Total O 261 261	0	0

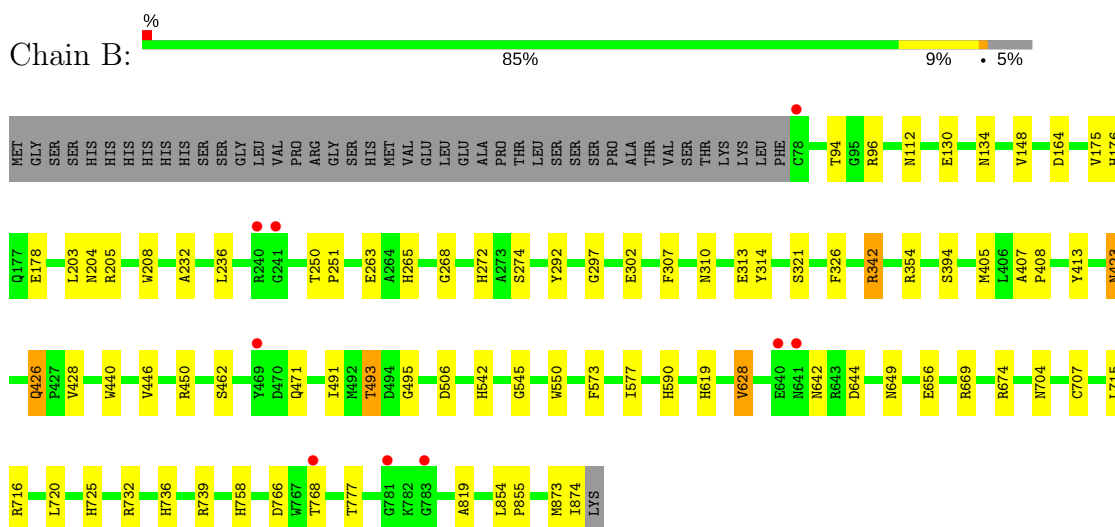
### 3 Residue-property plots [i](#)

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: Isoamylase



#### • Molecule 1: Isoamylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.13Å 102.13Å 488.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.73 – 2.30 48.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.73-2.30) 97.6 (48.73-2.30)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.202 , 0.235 0.211 , 0.238	Depositor DCC
$R_{free}$ test set	5689 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 37.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.39	0/6396	0.60	0/8729
1	B	0.41	0/6374	0.63	4/8699 (0.0%)
All	All	0.40	0/12770	0.61	4/17428 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	B	342	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	342	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	205	ARG	NE-CZ-NH1	5.51	123.05	120.30

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	6212	0	5821	39	0
1	B	6192	0	5812	47	0
2	A	227	0	0	1	0
2	B	261	0	0	5	0
All	All	12892	0	11633	84	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 3.

All (84) 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:206:ARG:NH2	1:A:351:ALA:O	2.23	0.72
1:B:542:HIS:HD2	1:B:545:GLY:H	1.42	0.67
1:B:176:HIS:HD2	1:B:178:GLU:H	1.40	0.67
1:B:766:ASP:OD1	1:B:768:THR:HG22	1.96	0.65
1:B:644:ASP:HB3	1:B:704:ASN:HD22	1.61	0.63
1:B:590:HIS:CB	2:B:952:HOH:O	2.47	0.63
1:A:674:ARG:HH12	1:A:725:HIS:HD2	1.47	0.61
1:A:732:ARG:O	1:A:736:HIS:HD2	1.84	0.61
1:B:423:ASN:HD21	1:B:462:SER:H	1.47	0.60
1:B:94:THR:HG22	1:B:148:VAL:CG1	2.31	0.60
1:A:519:LEU:O	1:A:546:ARG:NH2	2.37	0.58
1:B:250:THR:HG22	1:B:251:PRO:O	2.04	0.57
1:A:819:ALA:O	1:B:874:ILE:HG12	2.05	0.57
1:A:96:ARG:H	1:A:112:ASN:HD21	1.53	0.57
1:B:732:ARG:O	1:B:736:HIS:HD2	1.88	0.57
1:A:493:THR:HG21	2:A:1021:HOH:O	2.05	0.56
1:B:326:PHE:O	1:B:707:CYS:HA	2.06	0.56
1:A:205:ARG:HD2	1:A:210:GLN:O	2.07	0.55
1:B:263:GLU:OE2	1:B:619:HIS:HD2	1.90	0.54
1:B:493:THR:HG21	2:B:921:HOH:O	2.07	0.54
1:B:674:ARG:HH12	1:B:725:HIS:CD2	2.24	0.54
1:A:493:THR:HG22	1:A:495:GLY:H	1.73	0.54
1:A:366:GLU:OE1	1:A:370:ARG:NH2	2.41	0.54
1:A:291:ASP:OD1	1:A:370:ARG:NH1	2.41	0.53
1:B:292:TYR:CE1	1:B:720:LEU:HD21	2.43	0.53
1:B:236:LEU:O	1:B:354:ARG:NH1	2.42	0.53
1:A:292:TYR:CE1	1:A:720:LEU:HD21	2.45	0.52
1:B:758:HIS:HE1	1:B:777:THR:OG1	1.92	0.52
1:A:226:MET:HB2	1:A:227:PRO:HD2	1.92	0.52
1:A:610:HIS:CD2	1:A:747:THR:HA	2.45	0.52
1:B:493:THR:HG23	1:B:495:GLY:H	1.74	0.51
1:B:176:HIS:CD2	1:B:178:GLU:H	2.25	0.51
1:B:426:GLN:NE2	1:B:428:VAL:H	2.09	0.51
1:B:310:ASN:O	1:B:313:GLU:HB2	2.11	0.51
1:B:208:TRP:N	1:B:342:ARG:HG2	2.26	0.50
1:A:692:GLY:HA2	1:A:695:TYR:CE2	2.47	0.50
1:A:758:HIS:HD2	1:A:763:ASN:H	1.60	0.50
1:B:493:THR:CG2	1:B:495:GLY:H	2.26	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLN:HE22	1:A:149:ASN:ND2	2.10	0.49
1:A:326:PHE:O	1:A:707:CYS:HA	2.12	0.49
1:A:674:ARG:HH12	1:A:725:HIS:CD2	2.29	0.48
1:B:674:ARG:HH12	1:B:725:HIS:HD2	1.61	0.48
1:B:642:ASN:HD22	1:B:644:ASP:H	1.62	0.48
1:A:758:HIS:CD2	1:A:763:ASN:H	2.32	0.47
1:A:176:HIS:HD2	1:A:178:GLU:H	1.61	0.47
1:B:573:PHE:CE2	1:B:577:ILE:HD11	2.48	0.47
1:B:204:ASN:HD22	1:B:232:ALA:HB2	1.79	0.47
1:B:297:GLY:O	1:B:739:ARG:NH1	2.45	0.47
1:A:145:ASP:H	1:A:149:ASN:HD22	1.61	0.46
1:A:265:HIS:HD2	1:A:268:GLY:H	1.62	0.46
1:A:267:ARG:HA	1:A:281:GLY:HA2	1.98	0.46
1:A:874:ILE:HG12	1:B:819:ALA:O	2.15	0.46
1:B:628:VAL:HG13	1:B:669:ARG:HG2	1.97	0.46
1:B:491:ILE:HD12	2:B:1146:HOH:O	2.16	0.46
1:B:272:HIS:HD2	1:B:274:SER:OG	1.99	0.46
1:A:264:ALA:CB	1:A:691:MET:HE3	2.46	0.46
1:A:493:THR:CG2	1:A:495:GLY:H	2.29	0.45
1:A:530:ASP:OD1	1:A:530:ASP:C	2.54	0.45
1:B:134:ASN:ND2	2:B:1069:HOH:O	2.43	0.45
1:B:302:GLU:OE2	1:B:450:ARG:HD3	2.16	0.45
1:B:656:GLU:O	1:B:669:ARG:NH2	2.50	0.45
1:B:96:ARG:H	1:B:112:ASN:HD21	1.64	0.45
1:B:405:MET:HE1	1:B:413:TYR:CG	2.52	0.44
1:A:163:ARG:HD2	1:A:165:ASP:OD1	2.17	0.44
1:A:264:ALA:HB1	1:A:691:MET:HE3	2.00	0.44
1:A:96:ARG:N	1:A:112:ASN:HD21	2.16	0.44
1:A:541:PRO:HA	1:A:603:TRP:CD2	2.53	0.43
1:B:307:PHE:CE1	1:B:440:TRP:CE2	3.06	0.43
1:B:715:LEU:HD23	1:B:716:ARG:N	2.33	0.43
1:B:644:ASP:HB3	1:B:704:ASN:ND2	2.32	0.43
1:A:151:THR:OG1	1:A:156:HIS:HE1	2.02	0.42
1:A:777:THR:HA	1:A:786:LEU:O	2.18	0.42
1:A:455:SER:HB3	1:A:534:LEU:HD23	2.01	0.42
1:B:450:ARG:HD2	1:B:550:TRP:CE2	2.54	0.42
1:B:854:LEU:HG	1:B:855:PRO:HD2	2.01	0.42
1:B:542:HIS:CD2	1:B:545:GLY:H	2.30	0.42
1:A:470:ASP:OD1	1:A:473:THR:N	2.52	0.41
1:B:649:ASN:ND2	2:B:942:HOH:O	2.46	0.41
1:B:265:HIS:HD2	1:B:268:GLY:H	1.67	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:GLN:NE2	1:A:428:VAL:H	2.19	0.41
1:A:610:HIS:CD2	1:A:610:HIS:H	2.38	0.41
1:B:407:ALA:HB1	1:B:408:PRO:CD	2.51	0.41
1:B:130:GLU:HG3	1:B:203:LEU:HD21	2.04	0.40
1:A:107:ASP:OD1	1:A:108:THR:HG23	2.21	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	798/840 (95%)	761 (95%)	36 (4%)	1 (0%)	55	67
1	B	795/840 (95%)	758 (95%)	36 (4%)	1 (0%)	55	67
All	All	1593/1680 (95%)	1519 (95%)	72 (4%)	2 (0%)	55	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	PRO
1	B	394	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	637/686 (93%)	629 (99%)	8 (1%)	73	86
1	B	638/686 (93%)	626 (98%)	12 (2%)	62	78
All	All	1275/1372 (93%)	1255 (98%)	20 (2%)	68	82

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	SER
1	A	206	ARG
1	A	426	GLN
1	A	492	MET
1	A	493	THR
1	A	586	ASN
1	A	632	ASN
1	A	769	ASP
1	B	164	ASP
1	B	175	VAL
1	B	314	TYR
1	B	321	SER
1	B	423	ASN
1	B	426	GLN
1	B	446	VAL
1	B	471	GLN
1	B	493	THR
1	B	506	ASP
1	B	628	VAL
1	B	873	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	149	ASN
1	A	156	HIS
1	A	176	HIS
1	A	265	HIS
1	A	272	HIS
1	A	381	ASN
1	A	400	ASN
1	A	425	ASN
1	A	426	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	521	ASN
1	A	535	ASN
1	A	597	ASN
1	A	598	ASN
1	A	602	GLN
1	A	610	HIS
1	A	641	ASN
1	A	704	ASN
1	A	713	ASN
1	A	725	HIS
1	A	728	ASN
1	A	736	HIS
1	A	758	HIS
1	A	849	HIS
1	B	112	ASN
1	B	176	HIS
1	B	177	GLN
1	B	188	HIS
1	B	265	HIS
1	B	272	HIS
1	B	381	ASN
1	B	400	ASN
1	B	423	ASN
1	B	425	ASN
1	B	426	GLN
1	B	471	GLN
1	B	535	ASN
1	B	542	HIS
1	B	619	HIS
1	B	638	ASN
1	B	642	ASN
1	B	649	ASN
1	B	704	ASN
1	B	713	ASN
1	B	725	HIS
1	B	728	ASN
1	B	736	HIS
1	B	758	HIS

### 5.3.3 RNA ⓘ

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	800/840 (95%)	0.12	43 (5%) 26 33	23, 35, 61, 86	0
1	B	797/840 (94%)	-0.14	9 (1%) 80 84	22, 32, 50, 76	0
All	All	1597/1680 (95%)	-0.01	52 (3%) 47 54	22, 33, 56, 86	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	GLY	4.9
1	A	147	TYR	4.2
1	A	107	ASP	3.8
1	A	78	CYS	3.7
1	A	319	PRO	3.7
1	A	240	ARG	3.6
1	B	240	ARG	3.5
1	A	106	ALA	3.4
1	A	473	THR	3.3
1	B	241	GLY	3.2
1	A	471	GLN	3.1
1	A	76	LEU	3.0
1	B	78	CYS	3.0
1	A	592	THR	3.0
1	A	647	GLN	2.9
1	A	470	ASP	2.7
1	A	469	TYR	2.7
1	A	378	VAL	2.7
1	A	320	GLY	2.6
1	A	324	TYR	2.6
1	A	321	SER	2.6
1	A	687	PRO	2.6
1	B	781	GLY	2.6
1	A	681	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	220	GLU	2.5
1	A	525	ILE	2.4
1	A	680	LEU	2.4
1	A	590	HIS	2.4
1	A	813	VAL	2.4
1	A	318	ILE	2.4
1	B	641	ASN	2.4
1	A	93	LEU	2.3
1	A	243	ALA	2.3
1	B	469	TYR	2.3
1	A	474	GLY	2.3
1	B	640	GLU	2.2
1	A	689	ILE	2.2
1	B	783	GLY	2.2
1	A	242	SER	2.2
1	A	80	PRO	2.2
1	A	108	THR	2.2
1	A	643	ARG	2.2
1	A	613	ILE	2.2
1	A	148	VAL	2.1
1	A	688	MET	2.1
1	A	219	GLU	2.1
1	A	315	TYR	2.1
1	A	77	PHE	2.1
1	B	768	THR	2.1
1	A	686	VAL	2.1
1	A	92	ALA	2.1
1	A	639	GLY	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.