Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 04:20 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

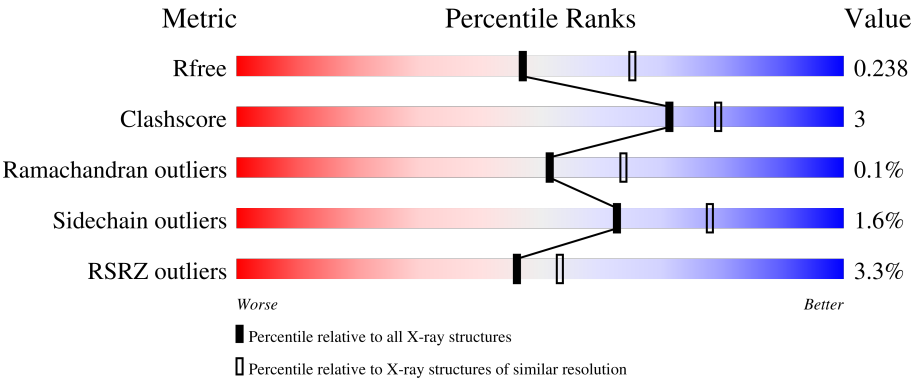
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 of 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 <=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	5% 88% 7% 5%
1	B	840	% 85% 9% • 5%

2 Entry composition (i)

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

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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.

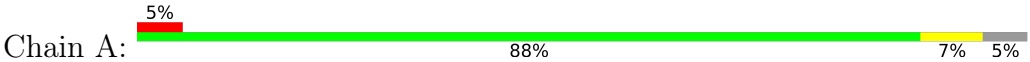
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	227	Total O 227 227	0	0
2	B	261	Total O 261 261	0	0

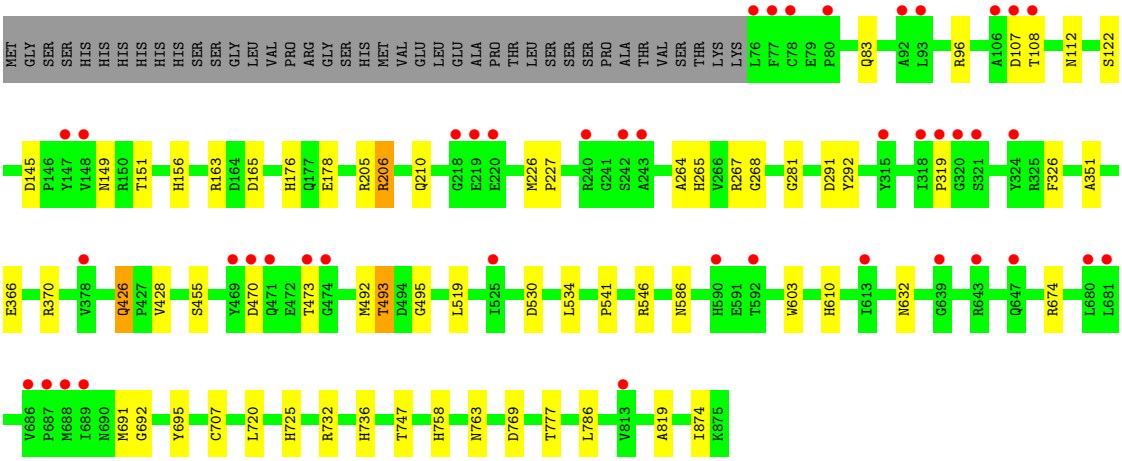
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

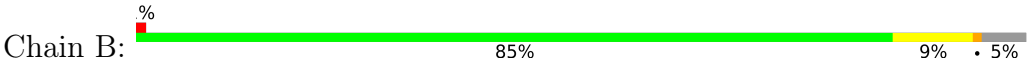
Chain A:

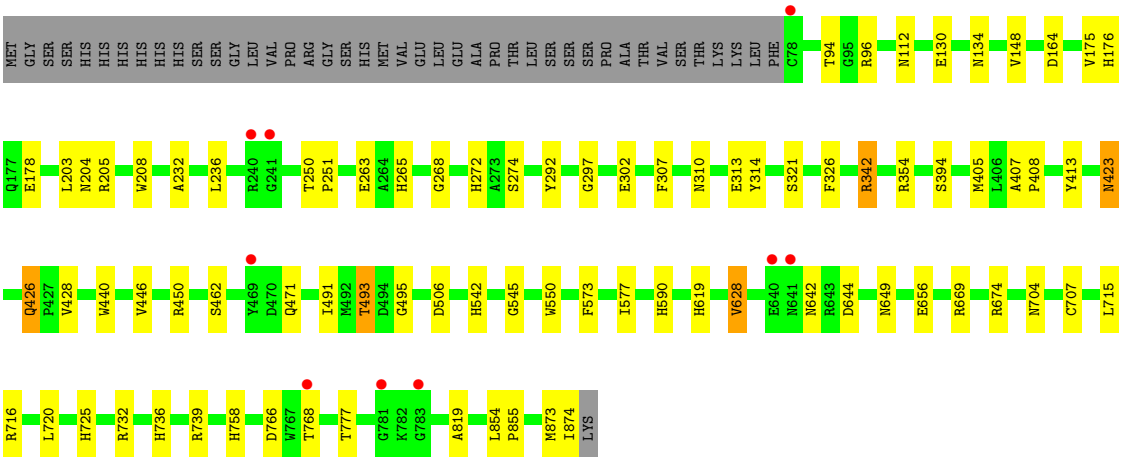




• Molecule 1: Isoamylase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.65 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.235 0.211 , 0.238	Depositor DCC
R_{free} test set	5702 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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(^{o})	Ideal(^{o})
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

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

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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

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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%)	51	64
1	B	795/840 (95%)	758 (95%)	36 (4%)	1 (0%)	51	64
All	All	1593/1680 (95%)	1519 (95%)	72 (4%)	2 (0%)	51	64

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%)	69	82
1	B	638/686 (93%)	626 (98%)	12 (2%)	57	73
All	All	1275/1372 (93%)	1255 (98%)	20 (2%)	62	78

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

Sometimes 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

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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 monosaccharides 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^{th} 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	800/840 (95%)	0.13	43 (5%) 25 32	23, 35, 61, 86	0
1	B	797/840 (94%)	-0.14	9 (1%) 80 85	22, 32, 50, 76	0
All	All	1597/1680 (95%)	-0.01	52 (3%) 46 53	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	319	PRO	3.7
1	A	78	CYS	3.7
1	A	240	ARG	3.6
1	A	106	ALA	3.4
1	B	240	ARG	3.4
1	A	473	THR	3.3
1	B	241	GLY	3.2
1	A	471	GLN	3.2
1	A	76	LEU	3.1
1	A	592	THR	3.0
1	B	78	CYS	3.0
1	A	647	GLN	2.9
1	A	470	ASP	2.7
1	A	378	VAL	2.7
1	A	469	TYR	2.7
1	A	324	TYR	2.6
1	A	320	GLY	2.6
1	A	687	PRO	2.6
1	A	321	SER	2.6
1	A	681	LEU	2.6
1	B	781	GLY	2.5

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