



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:24 PM GMT

PDB ID : 1OU5
Title : Crystal structure of human CCA-adding enzyme
Authors : Augustin, M.A.; Reichert, A.S.; Betat, H.; Huber, R.; Moerl, M.; Steegborn, C.
Deposited on : 2003-03-24
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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

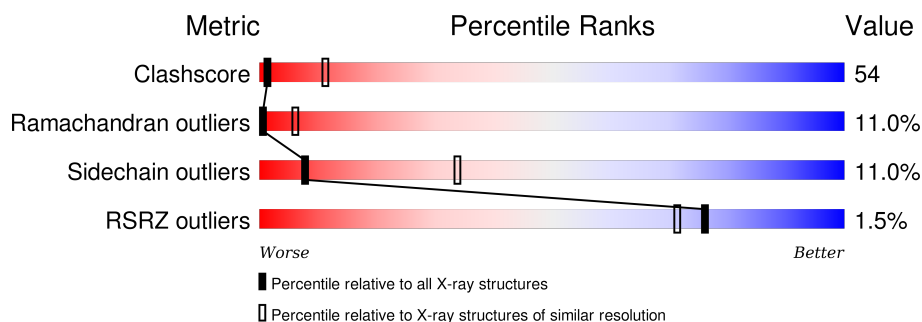
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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))
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 ≥ 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	448	
1	B	448	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5570 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 tRNA CCA-adding enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	266	0	0
			2785	1776	480	521	8			
1	B	344	Total	C	N	O	S	194	0	0
			2785	1776	480	521	8			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	CLONING ARTIFACT	UNP Q96Q11
A	-41	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-40	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-39	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-38	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-37	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-36	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-35	SER	-	CLONING ARTIFACT	UNP Q96Q11
A	-34	SER	-	CLONING ARTIFACT	UNP Q96Q11
A	-33	GLY	-	CLONING ARTIFACT	UNP Q96Q11
A	-32	LEU	-	CLONING ARTIFACT	UNP Q96Q11
A	-31	VAL	-	CLONING ARTIFACT	UNP Q96Q11
A	-30	PRO	-	CLONING ARTIFACT	UNP Q96Q11
A	-29	ARG	-	CLONING ARTIFACT	UNP Q96Q11
A	-28	GLY	-	CLONING ARTIFACT	UNP Q96Q11
A	-27	SER	-	CLONING ARTIFACT	UNP Q96Q11
A	-26	GLY	-	CLONING ARTIFACT	UNP Q96Q11
A	-25	MET	-	CLONING ARTIFACT	UNP Q96Q11
A	-24	LYS	-	CLONING ARTIFACT	UNP Q96Q11
A	-23	GLU	-	CLONING ARTIFACT	UNP Q96Q11
A	-22	THR	-	CLONING ARTIFACT	UNP Q96Q11
A	-21	ALA	-	CLONING ARTIFACT	UNP Q96Q11
A	-20	ALA	-	CLONING ARTIFACT	UNP Q96Q11
A	-19	ALA	-	CLONING ARTIFACT	UNP Q96Q11
A	-18	LYS	-	CLONING ARTIFACT	UNP Q96Q11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	PHE	-	CLONING ARTIFACT	UNP Q96Q11
A	-16	GLU	-	CLONING ARTIFACT	UNP Q96Q11
A	-15	ARG	-	CLONING ARTIFACT	UNP Q96Q11
A	-14	GLN	-	CLONING ARTIFACT	UNP Q96Q11
A	-13	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-12	MET	-	CLONING ARTIFACT	UNP Q96Q11
A	-11	ASP	-	CLONING ARTIFACT	UNP Q96Q11
A	-10	SER	-	CLONING ARTIFACT	UNP Q96Q11
A	-9	PRO	-	CLONING ARTIFACT	UNP Q96Q11
A	-8	ASP	-	CLONING ARTIFACT	UNP Q96Q11
A	-7	LEU	-	CLONING ARTIFACT	UNP Q96Q11
A	-6	GLY	-	CLONING ARTIFACT	UNP Q96Q11
A	-5	THR	-	CLONING ARTIFACT	UNP Q96Q11
A	-4	ASP	-	CLONING ARTIFACT	UNP Q96Q11
A	-3	ASP	-	CLONING ARTIFACT	UNP Q96Q11
A	-2	ASP	-	CLONING ARTIFACT	UNP Q96Q11
A	-1	ASP	-	CLONING ARTIFACT	UNP Q96Q11
A	0	LYS	-	CLONING ARTIFACT	UNP Q96Q11
B	-42	MET	-	CLONING ARTIFACT	UNP Q96Q11
B	-41	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-40	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-39	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-38	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-37	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-36	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-35	SER	-	CLONING ARTIFACT	UNP Q96Q11
B	-34	SER	-	CLONING ARTIFACT	UNP Q96Q11
B	-33	GLY	-	CLONING ARTIFACT	UNP Q96Q11
B	-32	LEU	-	CLONING ARTIFACT	UNP Q96Q11
B	-31	VAL	-	CLONING ARTIFACT	UNP Q96Q11
B	-30	PRO	-	CLONING ARTIFACT	UNP Q96Q11
B	-29	ARG	-	CLONING ARTIFACT	UNP Q96Q11
B	-28	GLY	-	CLONING ARTIFACT	UNP Q96Q11
B	-27	SER	-	CLONING ARTIFACT	UNP Q96Q11
B	-26	GLY	-	CLONING ARTIFACT	UNP Q96Q11
B	-25	MET	-	CLONING ARTIFACT	UNP Q96Q11
B	-24	LYS	-	CLONING ARTIFACT	UNP Q96Q11
B	-23	GLU	-	CLONING ARTIFACT	UNP Q96Q11
B	-22	THR	-	CLONING ARTIFACT	UNP Q96Q11
B	-21	ALA	-	CLONING ARTIFACT	UNP Q96Q11
B	-20	ALA	-	CLONING ARTIFACT	UNP Q96Q11
B	-19	ALA	-	CLONING ARTIFACT	UNP Q96Q11

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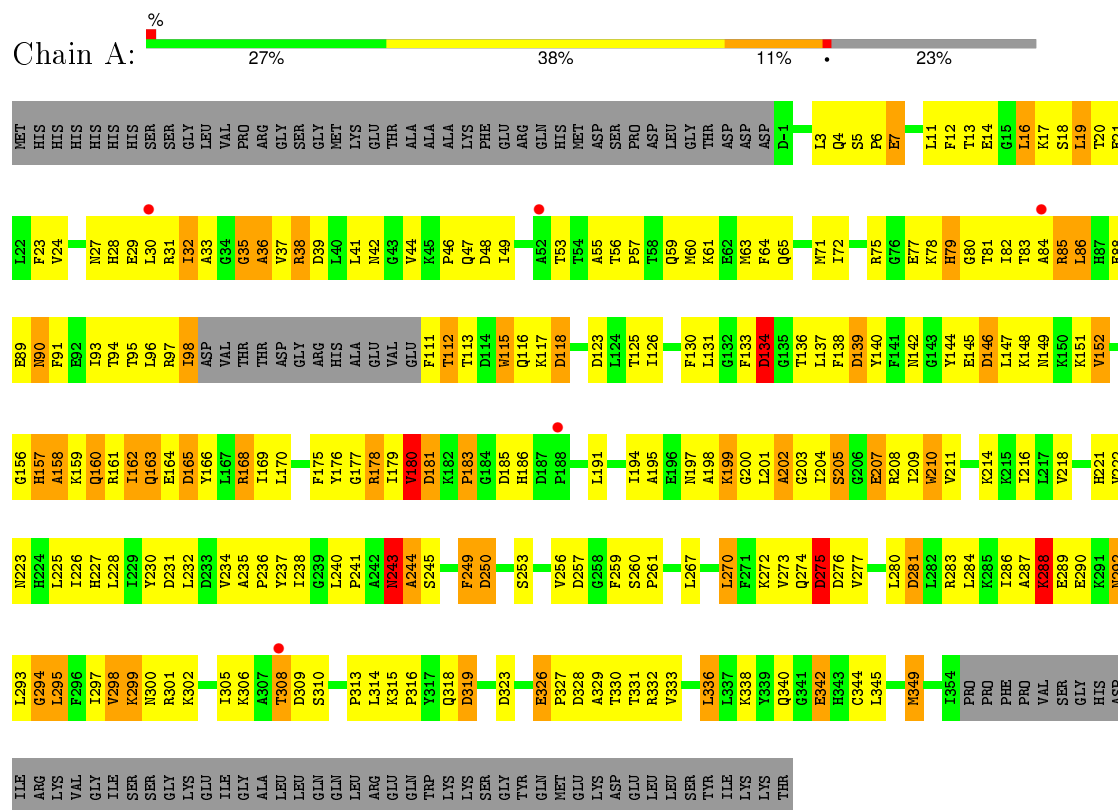
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	LYS	-	CLONING ARTIFACT	UNP Q96Q11
B	-17	PHE	-	CLONING ARTIFACT	UNP Q96Q11
B	-16	GLU	-	CLONING ARTIFACT	UNP Q96Q11
B	-15	ARG	-	CLONING ARTIFACT	UNP Q96Q11
B	-14	GLN	-	CLONING ARTIFACT	UNP Q96Q11
B	-13	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-12	MET	-	CLONING ARTIFACT	UNP Q96Q11
B	-11	ASP	-	CLONING ARTIFACT	UNP Q96Q11
B	-10	SER	-	CLONING ARTIFACT	UNP Q96Q11
B	-9	PRO	-	CLONING ARTIFACT	UNP Q96Q11
B	-8	ASP	-	CLONING ARTIFACT	UNP Q96Q11
B	-7	LEU	-	CLONING ARTIFACT	UNP Q96Q11
B	-6	GLY	-	CLONING ARTIFACT	UNP Q96Q11
B	-5	THR	-	CLONING ARTIFACT	UNP Q96Q11
B	-4	ASP	-	CLONING ARTIFACT	UNP Q96Q11
B	-3	ASP	-	CLONING ARTIFACT	UNP Q96Q11
B	-2	ASP	-	CLONING ARTIFACT	UNP Q96Q11
B	-1	ASP	-	CLONING ARTIFACT	UNP Q96Q11
B	0	LYS	-	CLONING ARTIFACT	UNP Q96Q11

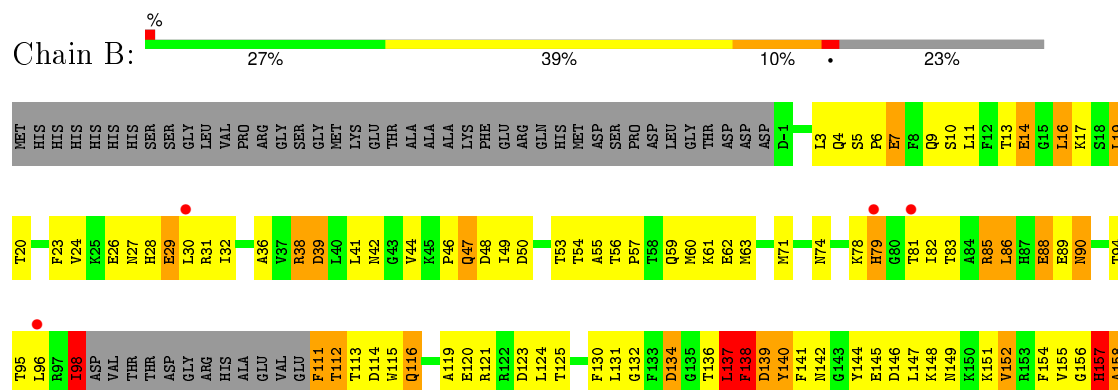
3 Residue-property plots

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: tRNA CCA-adding enzyme



• Molecule 1: tRNA CCA-adding enzyme



Lys	K299	D233	K159
	GLU	V234	K160
	ILE	A235	R161
	GLY	P236	I162
	ALA	Y237	Q163
	LEU	I238	E164
	LEU	Q239	D165
	GLN	L240	Y166
	GLN	P241	L167
	LEU	A242	K168
Arg	ARG	I243	I169
	GLU	A244	L170
	GLN	S245	R171
	TRP	L246	R171
	Lys	E247	F175
	Lys	F248	Y176
	Lys	E249	G177
	Ser	D250	R178
	GLY	K251	I179
	Tyr	V252	R180
Gln	I321	V256	D181
	I322	D257	H186
	D323	G258	D187
	S324	F259	
	ASP	S260	T190
	Lys	P261	
	LEU	K262	A193
	LEU	P263	I194
	Ser		
	Tyr		
Ile	E335	L267	N197
	Lys	K336	A198
	Lys	L337	K199
	Lys	K338	G200
	Lys	Y339	L201
	GLU	Q340	A202
		V273	G203
	L345	Q274	I204
	M349	D276	S205
		V277	G206
Pro	I354	T278	E207
	PRO	K279	R208
	PRO	L280	I209
	PHE	D281	W210
	VAL	L282	V211
	VAL	R283	
	SER	L284	I216
	GLY	A287	
	His	K288	N220
	ASP	E289	H221
Ile	ILE	R293	N223
	ARG	E290	H224
	Lys		L225
	VAL	L293	I226
	GLY	G294	H227
	ILE	L295	L228
	Ser	F296	L229
	Ser	T297	Y230
	GLY	V298	

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.52Å 102.52Å 206.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.40 44.65 – 3.25	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-3.40) 98.3 (44.65-3.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.278 , 0.318 0.296 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.0	EDS
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 20358 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5570	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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, 0.375 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	0.78	5/2839 (0.2%)	1.02	21/3826 (0.5%)
1	B	0.61	1/2839 (0.0%)	0.95	16/3826 (0.4%)
All	All	0.70	6/5678 (0.1%)	0.99	37/7652 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	ILE	C-N	22.89	1.86	1.34
1	B	98	ILE	CB-CG2	12.08	1.90	1.52
1	A	98	ILE	CB-CG2	8.71	1.79	1.52
1	A	342	GLU	CG-CD	7.60	1.63	1.51
1	A	98	ILE	CA-C	5.91	1.68	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	ILE	N-CA-C	-10.57	82.46	111.00
1	B	111	PHE	N-CA-CB	9.77	128.19	110.60
1	A	98	ILE	CA-C-N	9.36	137.80	117.20
1	A	98	ILE	N-CA-C	-9.33	85.80	111.00
1	B	98	ILE	CG1-CB-CG2	-9.10	91.38	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	98	ILE	Peptide

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	2785	0	2799	252	1
1	B	2785	0	2803	286	1
All	All	5570	0	5602	537	1

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 54.

The worst 5 of 537 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:199:LYS:HA	1:B:237:TYR:CE1	1.46	1.45
1:B:199:LYS:HA	1:B:237:TYR:CD1	1.69	1.24
1:B:241:PRO:HG3	1:B:271:PHE:HB3	1.35	1.06
1:B:209:ILE:HD11	1:B:284:LEU:HD11	1.34	1.05
1:B:199:LYS:CA	1:B:237:TYR:CE1	2.39	1.05

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:SER:OG	1:B:328:ASP:OD2[4_565]	2.17	0.03

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	342/448 (76%)	229 (67%)	78 (23%)	35 (10%)	1	7
1	B	342/448 (76%)	227 (66%)	75 (22%)	40 (12%)	0	5
All	All	684/896 (76%)	456 (67%)	153 (22%)	75 (11%)	0	6

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	79	HIS
1	A	80	GLY
1	A	86	LEU
1	A	112	THR

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	304/393 (77%)	270 (89%)	34 (11%)	7	32
1	B	304/393 (77%)	271 (89%)	33 (11%)	8	34
All	All	608/786 (77%)	541 (89%)	67 (11%)	8	34

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	LEU
1	B	14	GLU
1	B	237	TYR
1	A	326	GLU
1	B	4	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	ASN
1	B	90	ASN
1	B	340	GLN
1	B	65	GLN
1	B	73	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](#)

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	340/448 (75%)	0.12	5 (1%) 76 71	26, 26, 26, 26	56 (16%)
1	B	344/448 (76%)	0.11	5 (1%) 76 71	26, 26, 26, 26	47 (13%)
All	All	684/896 (76%)	0.12	10 (1%) 76 71	26, 26, 26, 26	103 (15%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	THR	4.3
1	A	188	PRO	3.2
1	A	84	ALA	3.1
1	B	321	ILE	3.1
1	B	30	LEU	2.6

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.