



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:31 AM GMT

PDB ID : 3M8L
Title : Crystal Structure Analysis of the Feline Calicivirus Capsid Protein
Authors : Zhou, Y.; Prasad, B.V.V.
Deposited on : 2010-03-18
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

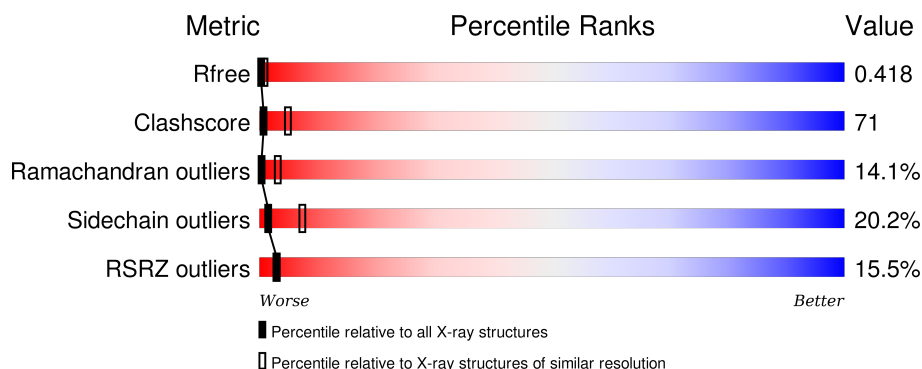
1 Overall quality at a glance

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))
R_{free}	91344	1476 (3.50-3.30)
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	534	<div> <div>13%</div> <div>25%</div> <div>52%</div> <div>20%</div> <div>.</div> </div>
1	C	534	<div> <div>16%</div> <div>23%</div> <div>56%</div> <div>19%</div> <div>.</div> </div>
2	B	530	<div> <div>18%</div> <div>20%</div> <div>55%</div> <div>21%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12360 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4129	2632	687	796	14			
1	C	534	Total	C	N	O	S	0	0	0
			4130	2632	687	797	14			

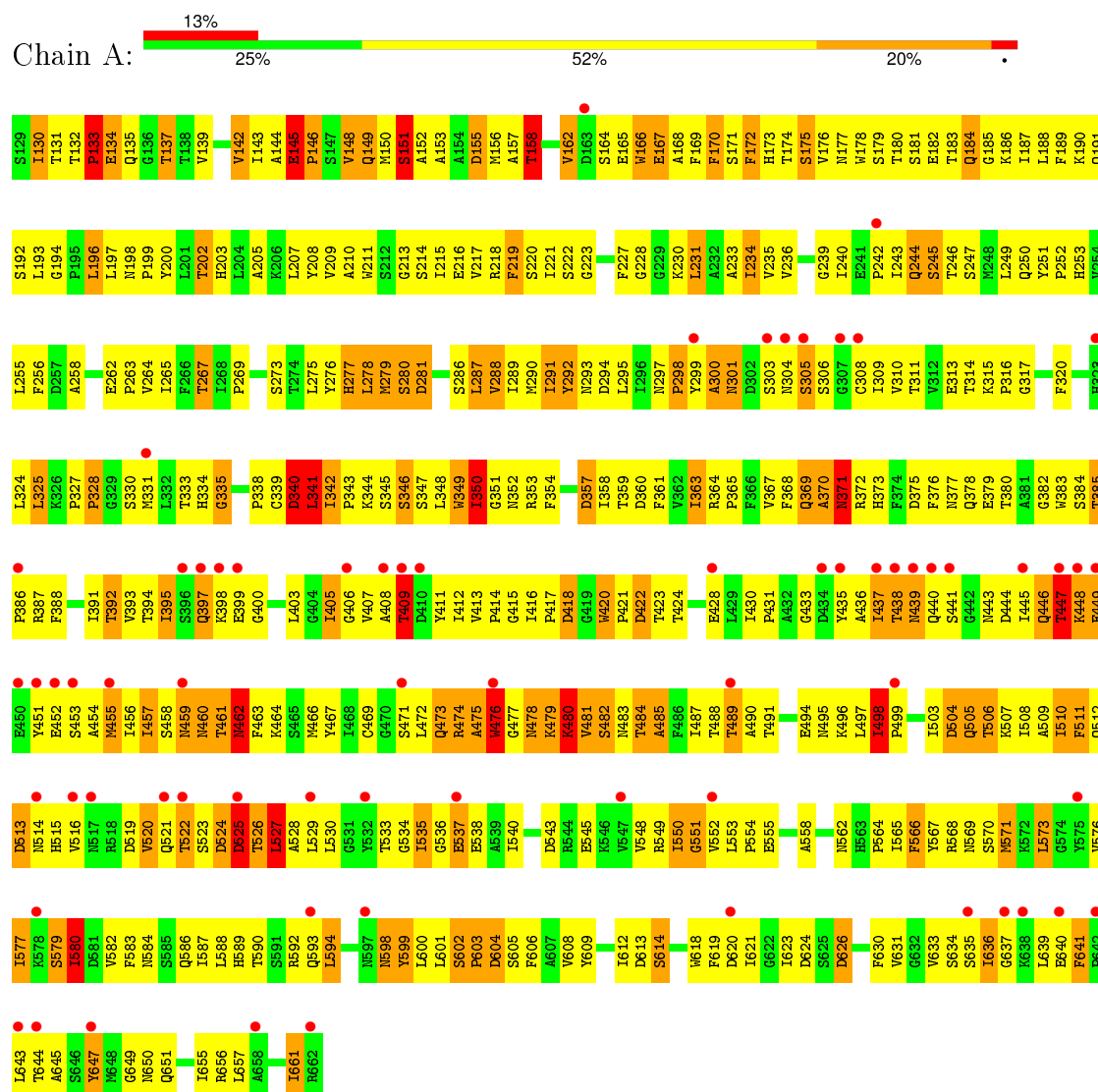
- Molecule 2 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	530	Total	C	N	O	S	0	0	0
			4101	2615	683	789	14			

3 Residue-property plots

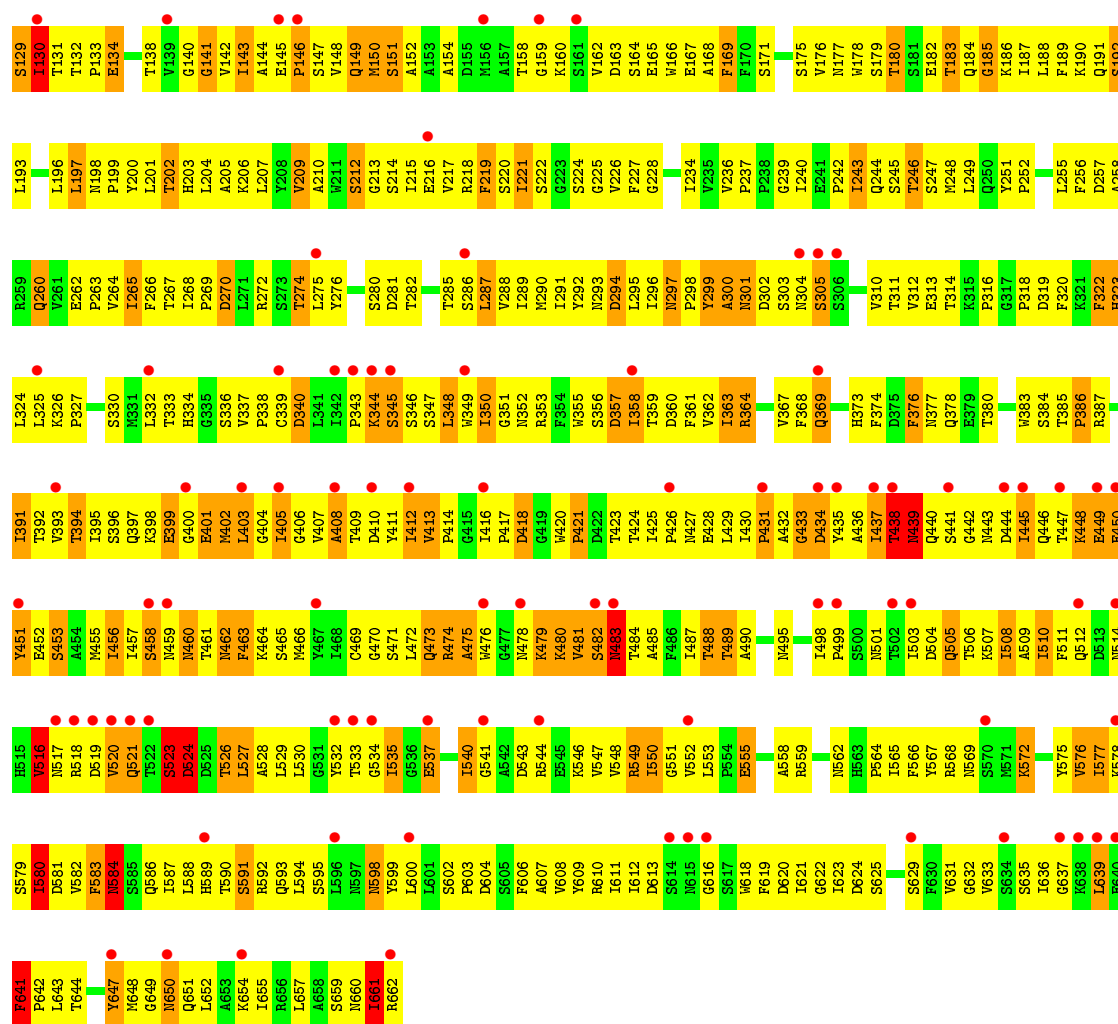
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: Capsid protein

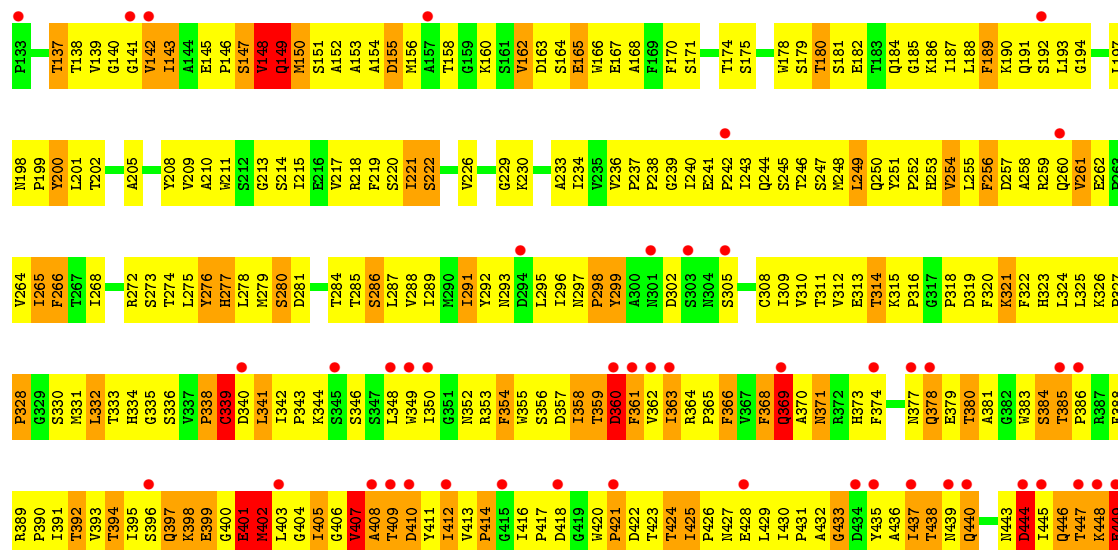


• Molecule 1: Capsid protein





• Molecule 2: Capsid protein



I636	Y575	I510	E450		
G637	V576	F511	Y451		
K638	I577	Q512	E452		
L639	K578	D513	S453		
E640	S579	N514	A454		
F641	I580	H515	M455		
P642	D581	V516	I456		
L643	V582	N517	I457		
T644	F583	R518	S458		
	N584	D519	M459		
Y647	S585	V520	M460		
M648	Q586	Q521	T461		
G649	I587	T522	N462		
N650	L588	S523	F463		
Q651	H589	D524	K464		
L652	T590	D525	S465		
A653	S591	T526	M466		
K654	R592	L527	Y467		
I655	Q593	A528	I468		
R656	L594	L529	C469		
L657		L530	G470		
A658	N597	G531	S471		
S659	N598	Y532	L472		
N660	Y599	T533	Q473		
I661	L600	G534	R474		
R662	L601	I535	A475		
	S602	G536	W476		
	P603	E537	G477		
	D604	E538	M478		
	S605	A539	K479		
	F606	T540	K480		
	A607	G541	Y683		
	V608	A542	S482		
	Y609	D543	M483		
	R610	R544	T484		
	I611	E545	A485		
	I612	K546	F486		
	D613	Y547	I487		
	S614	V548	T488		
	N615	R549	T489		
	G616	T550	A490		
	S617	G551	T491		
	W618	V552	V492		
	F619	L553	K493		
	D620	P554	E494		
	I621		N495		
	G622	G560	K496		
	I623	G561	L497		
	D624	N562	I498		
	S625		P499		
	D626	I565	S500		
	G627	F566	N501		
	F628	Y567	T502		
	S629	R568	I503		
	F630	N569	D504		
	V631	S570	Q505		
	G632	R571	T506		
	V633	L572	K507		
	S634	L573	I508		
	S635	G574	A509		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	427.08 Å 450.73 Å 467.59 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.40 29.98 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.40) 89.1 (29.98-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.39 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.390 , 0.370 0.419 , 0.418	Depositor DCC
R_{free} test set	27284 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	85.6	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , -9.8	EDS
Estimated twinning fraction	0.017 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	4 of 542437 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	12360	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 [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	0.68	1/4229 (0.0%)	0.84	4/5759 (0.1%)
1	C	0.71	1/4230 (0.0%)	0.89	7/5759 (0.1%)
2	B	1.17	11/4201 (0.3%)	0.89	6/5719 (0.1%)
All	All	0.88	13/12660 (0.1%)	0.87	17/17237 (0.1%)

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
2	B	0	1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	624	ASP	CB-CG	33.85	2.22	1.51
2	B	606	PHE	CE1-CZ	24.62	1.84	1.37
2	B	606	PHE	CE2-CZ	22.49	1.80	1.37
2	B	606	PHE	CD2-CE2	20.22	1.79	1.39
2	B	606	PHE	CD1-CE1	20.20	1.79	1.39

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	THR	CB-CA-C	13.09	146.94	111.60
1	A	439	ASN	N-CA-CB	-13.07	87.07	110.60
2	B	624	ASP	CB-CG-OD1	9.58	126.92	118.30
1	C	451	TYR	CB-CA-C	-8.87	92.67	110.40
2	B	360	ASP	N-CA-C	8.51	133.98	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	200	TYR	Sidechain

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	4129	0	4062	602	0
1	C	4130	0	4062	563	7
2	B	4101	0	4033	615	6
All	All	12360	0	12157	1731	7

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 71.

The worst 5 of 1731 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)
2:B:606:PHE:CE1	2:B:606:PHE:CZ	1.84	1.62
2:B:606:PHE:CD2	2:B:606:PHE:CE2	1.79	1.62
2:B:606:PHE:CD1	2:B:606:PHE:CE1	1.79	1.62
2:B:606:PHE:CZ	2:B:606:PHE:CE2	1.80	1.61
2:B:606:PHE:CZ	2:B:624:ASP:CB	1.88	1.51

The worst 5 of 7 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)
2:B:299:TYR:CE1	1:C:299:TYR:OH[2_555]	1.77	0.43
2:B:299:TYR:CD1	1:C:299:TYR:CZ[2_555]	1.97	0.23
2:B:229:GLY:N	1:C:222:SER:OG[2_555]	2.06	0.14
2:B:292:TYR:OH	1:C:313:GLU:OE1[2_555]	2.07	0.13
2:B:252:PRO:N	1:C:169:PHE:CE1[2_555]	2.10	0.10

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	532/534 (100%)	310 (58%)	147 (28%)	75 (14%)	0	3
1	C	532/534 (100%)	332 (62%)	126 (24%)	74 (14%)	0	3
2	B	528/530 (100%)	321 (61%)	132 (25%)	75 (14%)	0	3
All	All	1592/1598 (100%)	963 (60%)	405 (25%)	224 (14%)	0	3

5 of 224 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	PRO
1	A	145	GLU
1	A	146	PRO
1	A	151	SER
1	A	279	MET

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	461/461 (100%)	370 (80%)	91 (20%)	1	8
1	C	461/461 (100%)	377 (82%)	84 (18%)	2	11
2	B	457/457 (100%)	354 (78%)	103 (22%)	1	5
All	All	1379/1379 (100%)	1101 (80%)	278 (20%)	1	7

5 of 278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	369	GLN
2	B	487	ILE
1	C	523	SER
2	B	384	SER
2	B	435	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	277	HIS
2	B	443	ASN
1	C	569	ASN
2	B	369	GLN
2	B	514	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	534/534 (100%)	0.89	67 (12%) 5 5	48, 97, 120, 143	0
1	C	534/534 (100%)	1.07	88 (16%) 2 2	49, 95, 113, 123	0
2	B	530/530 (100%)	1.03	93 (17%) 2 2	48, 97, 112, 129	0
All	All	1598/1598 (100%)	1.00	248 (15%) 3 3	48, 96, 115, 143	0

The worst 5 of 248 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	522	THR	8.2
1	C	146	PRO	7.4
1	A	447	THR	7.0
1	A	450	GLU	6.4
2	B	451	TYR	6.4

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.