wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2023 – 08:29 AM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

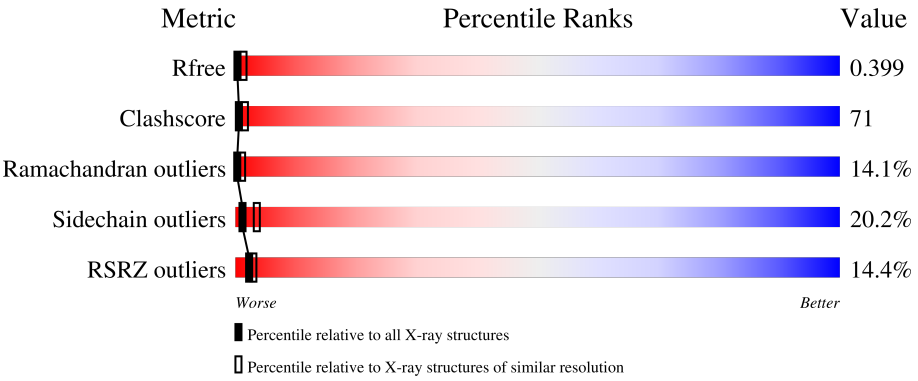
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (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 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	534	12% 25% 52% 20%
1	B	534	16% 20% 55% 21%
1	C	534	16% 23% 56% 19%

2 Entry composition (i)

There is only 1 type of molecule 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.

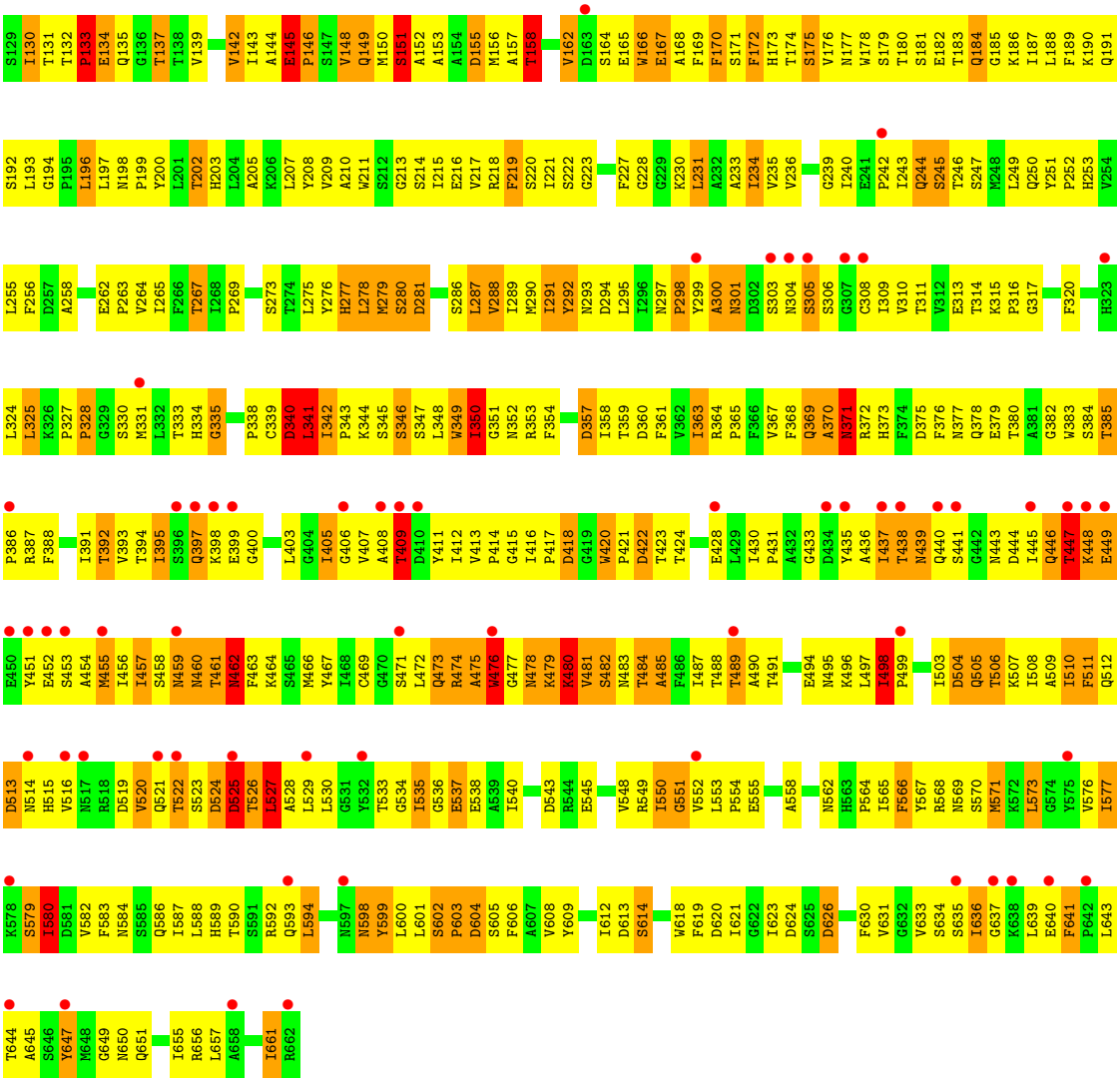
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4129	2632	687	796	14			
1	B	530	Total	C	N	O	S	0	0	0
			4101	2615	683	789	14			
1	C	534	Total	C	N	O	S	0	0	0
			4130	2632	687	797	14			

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.

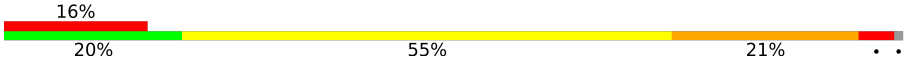
• Molecule 1: Capsid protein

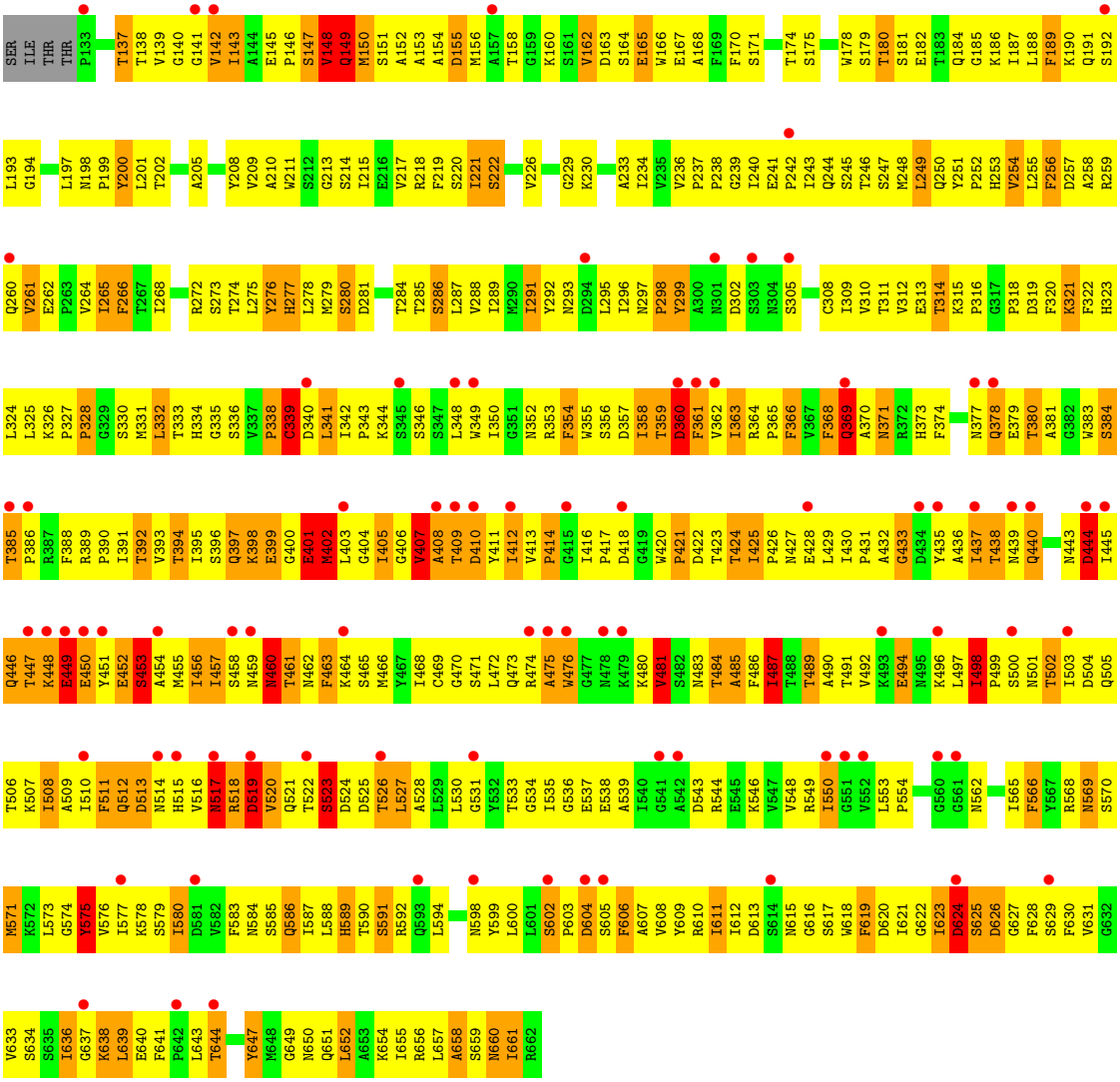
Chain A:



• Molecule 1: Capsid protein

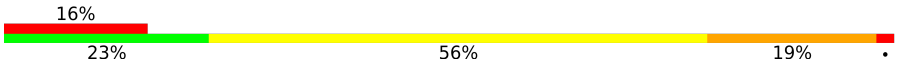
Chain B:

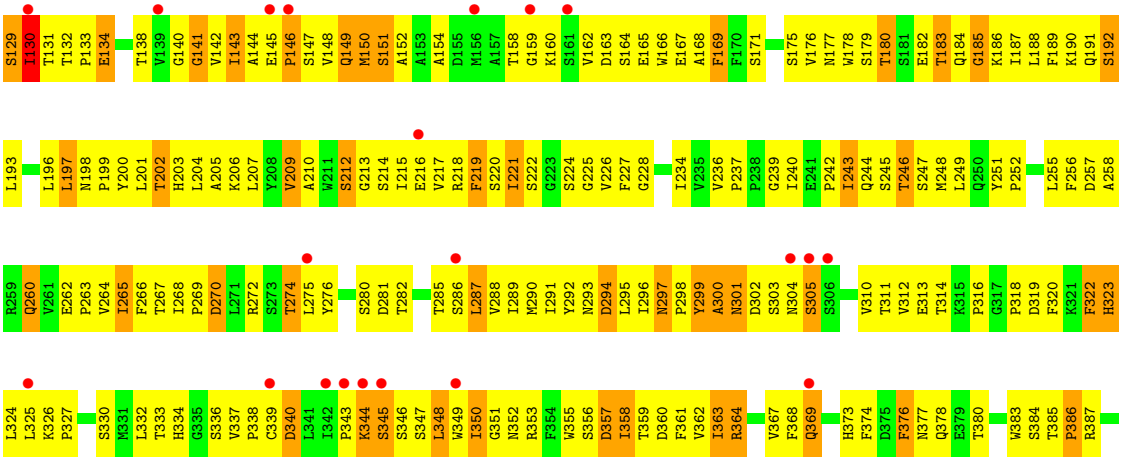


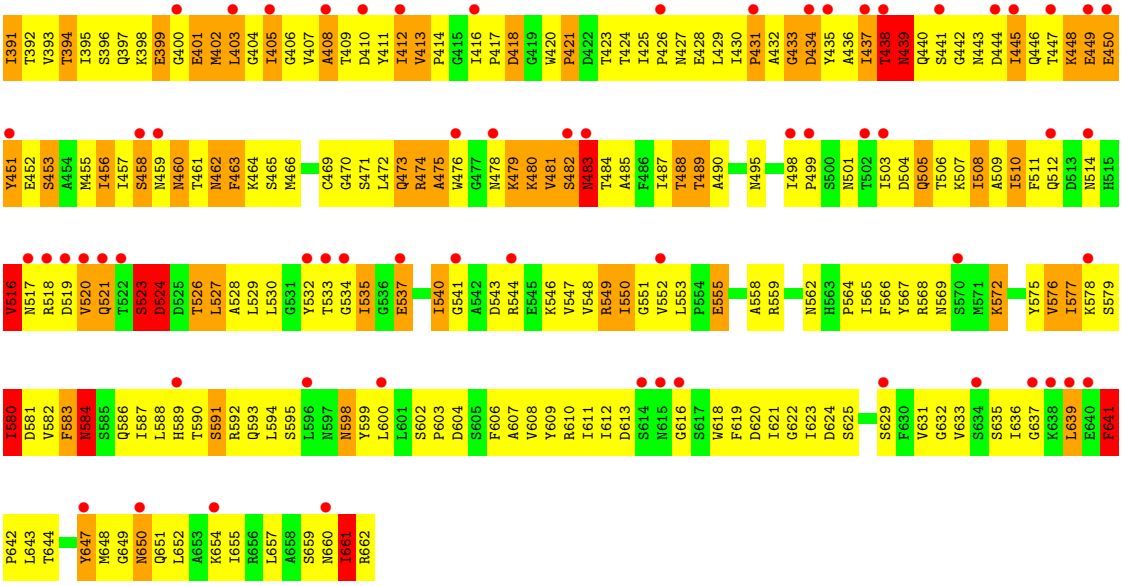


• Molecule 1: Capsid protein

Chain C:






I391 T392 V393 T394 I395 S396 Q397 K398 E399 G400 E401 M402 L403 G404 I405 G406 V407 A408 T409 D410 Y411 I412 V413 P414 G415 I416 P417 D418 G419 W420 P421 D422 T423 T424 I425 P426 N427 E428 L429 I430 P431 A432 G433 D434 Y435 A436 I437 T438 N439 Q440 S441 G442 N443 D444 I445 Q446 T447 K448 E449 E450
Y451 E452 S453 A454 M455 I456 I457 S458 N459 N460 T461 N462 F463 K464 S465 M466 C469 G470 S471 L472 Q473 R474 A475 W476 G477 N478 K479 K480 V481 S482 N483 T484 A485 F486 I487 T488 T489 A490 N495 I498 P499 S500 N501 T502 I503 D504 Q505 T506 K507 I508 A509 I510 F511 Q512 D513 N514 H515
V516 N517 R518 D519 V520 Q521 T522 S523 D524 D525 T526 L527 A528 L529 L530 G531 Y532 T533 G534 I535 G536 E537 I540 G541 A542 D543 R544 E545 K546 V547 V548 R549 I550 G551 V552 L553 P554 E555 A558 R559 N562 H563 P564 I565 F566 Y567 R568 N569 S570 M571 K572 Y575 V576 I577 K578 S579
I580 D581 V582 F583 N584 S585 Q586 I587 L588 H589 T590 S591 R592 Q593 L594 S595 L596 N597 N598 Y599 L600 L601 S602 P603 D604 S605 F606 A607 V608 Y609 R610 I611 I612 D613 S614 N615 G616 S617 W618 F619 D620 I621 G622 I623 D624 S625 S629 F630 V631 G632 V633 S634 S635 I636 G637 K638 L639 E640 F641
P642 L643 T644 Y647 M648 G649 N650 Q651 L652 A653 K654 I655 R656 L657 A658 S659 N660 I661 R662

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	427.08Å 450.73Å 467.59Å 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
$< I/\sigma(I) >$ [1]	1.28 (at 3.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.390 , 0.370 0.402 , 0.399	Depositor DCC
R_{free} test set	27284 reflections (5.03%)	wwPDB-VP
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 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.017 for -h,-l,-k	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 $< |L| >$, $< L^2 >$ 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	0.68	1/4229 (0.0%)	0.84	4/5759 (0.1%)
1	B	1.17	11/4201 (0.3%)	0.89	6/5719 (0.1%)
1	C	0.71	1/4230 (0.0%)	0.89	7/5759 (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
1	B	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	624	ASP	CB-CG	33.85	2.22	1.51
1	B	606	PHE	CE1-CZ	24.62	1.84	1.37
1	B	606	PHE	CE2-CZ	22.49	1.80	1.37
1	B	606	PHE	CD2-CE2	20.22	1.79	1.39
1	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(^{o})	Ideal(^{o})
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
1	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
1	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
1	B	200	TYR	Sidechain

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	4129	0	4062	602	0
1	B	4101	0	4033	615	6
1	C	4130	0	4062	563	7
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)
1:B:606:PHE:CE1	1:B:606:PHE:CZ	1.84	1.62
1:B:606:PHE:CE1	1:B:606:PHE:CD1	1.79	1.62
1:B:606:PHE:CE2	1:B:606:PHE:CD2	1.79	1.62
1:B:606:PHE:CZ	1:B:606:PHE:CE2	1.80	1.61
1:B:606:PHE:CZ	1: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)
1:B:299:TYR:CE1	1:C:299:TYR:OH[2_555]	1.77	0.43
1:B:299:TYR:CD1	1:C:299:TYR:CZ[2_555]	1.97	0.23
1:B:229:GLY:N	1:C:222:SER:OG[2_555]	2.06	0.14
1:B:292:TYR:OH	1:C:313:GLU:OE1[2_555]	2.07	0.13
1: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 1
1	B	528/534 (99%)	321 (61%)	132 (25%)	75 (14%)	0 1
1	C	532/534 (100%)	332 (62%)	126 (24%)	74 (14%)	0 1
All	All	1592/1602 (99%)	963 (60%)	405 (25%)	224 (14%)	0 1

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 4
1	B	457/461 (99%)	354 (78%)	103 (22%)	1 2
1	C	461/461 (100%)	377 (82%)	84 (18%)	1 6
All	All	1379/1383 (100%)	1101 (80%)	278 (20%)	1 3

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

Mol	Chain	Res	Type
1	C	369	GLN
1	C	402	MET
1	C	537	GLU
1	B	180	THR
1	B	149	GLN

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

Mol	Chain	Res	Type
1	B	277	HIS
1	C	514	ASN
1	B	473	GLN
1	C	505	GLN
1	C	589	HIS

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 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	534/534 (100%)	0.85	62 (11%)	4 5	48, 97, 120, 143	0
1	B	530/534 (99%)	0.99	84 (15%)	2 2	48, 97, 112, 129	0
1	C	534/534 (100%)	1.02	84 (15%)	2 2	49, 95, 113, 123	0
All	All	1598/1602 (99%)	0.95	230 (14%)	2 3	48, 96, 115, 143	0

The worst 5 of 230 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	146	PRO	7.3
1	A	522	THR	7.1
1	A	447	THR	6.7
1	A	450	GLU	6.4
1	B	412	ILE	6.2

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.