



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2017 – 02:59 PM EDT

PDB ID : 2I6Y  
Title : Structure and Mechanism of Mycobacterium tuberculosis Salicylate Synthase, MbtI  
Authors : Zwahlen, J.; Subramaniapillai, K.; Zhou, R.; Kisker, C.; Tonge, P.J.  
Deposited on : unknown  
Resolution : 2.50 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.

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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	:	rb-20030345
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)	:	rb-20030345

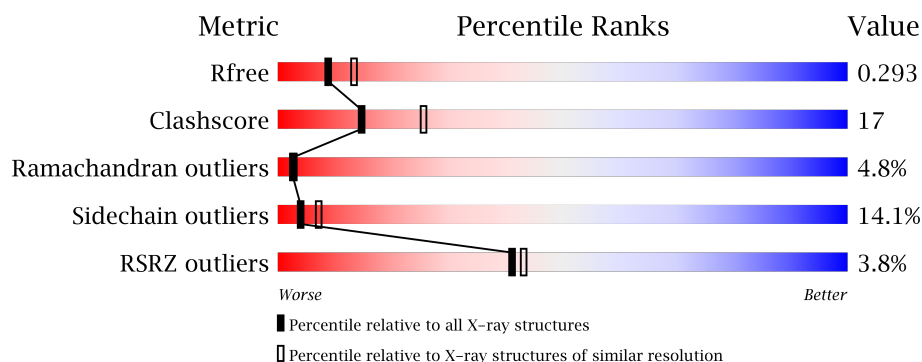
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	470	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3089 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 Anthranilate synthase component I, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3086	1941	547	588	10			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP Q7D785
A	-18	GLY	-	CLONING ARTIFACT	UNP Q7D785
A	-17	SER	-	CLONING ARTIFACT	UNP Q7D785
A	-16	SER	-	CLONING ARTIFACT	UNP Q7D785
A	-15	HIS	-	EXPRESSION TAG	UNP Q7D785
A	-14	HIS	-	EXPRESSION TAG	UNP Q7D785
A	-13	HIS	-	EXPRESSION TAG	UNP Q7D785
A	-12	HIS	-	EXPRESSION TAG	UNP Q7D785
A	-11	HIS	-	EXPRESSION TAG	UNP Q7D785
A	-10	HIS	-	EXPRESSION TAG	UNP Q7D785
A	-9	SER	-	CLONING ARTIFACT	UNP Q7D785
A	-8	SER	-	CLONING ARTIFACT	UNP Q7D785
A	-7	GLY	-	CLONING ARTIFACT	UNP Q7D785
A	-6	LEU	-	CLONING ARTIFACT	UNP Q7D785
A	-5	VAL	-	CLONING ARTIFACT	UNP Q7D785
A	-4	PRO	-	CLONING ARTIFACT	UNP Q7D785
A	-3	ARG	-	CLONING ARTIFACT	UNP Q7D785
A	-2	GLY	-	CLONING ARTIFACT	UNP Q7D785
A	-1	SER	-	CLONING ARTIFACT	UNP Q7D785
A	0	HIS	-	CLONING ARTIFACT	UNP Q7D785
A	1	VAL	-	CLONING ARTIFACT	UNP Q7D785

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		

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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A:
- 
- 3% 57% 26% 5% 11%
- MET GLY SER SER HIS HIS HIS HIS HIS VAL PRO ARG GLY SER HIS VAL SER GLU LEU SER VAL ALA THR GLY ALA VAL SER THR ALA SER SER S17 I18 P19 M20 P21 A22 G23 A27 D28 L29 V36 V41 D44 Y45 L46 L47 Y48 Y49 C50 D51 C52 Q53 M54 V55 L56 A57 A58 G59 V64 E65 L66 D69 E70 L71 R72 V73 I74 R75 T79 R80 R81 Q82 R87 T103 G108 A111 H117 H118 Y119 G120 L121 Q122 Q123 R124 L125 P127 L131 A132 R133 P137 R138 T139 R140 T141 M142 K146 E147 T148 R149 L150 E159 A160 L164 L165 A166 R170 E171 V172 V180 A181 D182 D183 P184 F187 R188 R189 R190 V191 Y203 T207 L208 S209 R210 C211 V212 E213 V214 P215 R225 L226 G227 R228 R229 H230 M231 R235 L238 G242 G243 T244 L247 C248 S251 V254 R258 V262 T265 E266 P267 L268 A269 G270 A273 L274 G275 ARG GLY PRO ALA ILE ASP ARG LEU ALA ARG ASP D287 L288 E289 S290 N291 S292 P298 T310 D311 I312 M324 T325 V326 R327 R329 GLU ARG GLY S331 S337 T338 I339 R340 E424 E427 P428 E429 R430 E433 E434 R438 L439 S440 T441 S442 D443 P444 S445 S446 S447 S448 S449 S450 S451 S452 S453 S454 S455 S456 S457 S458 S459 S460 S461 S462 S463 S464 S465 S466 S467 S468 S469 S470 S471 S472 S473 S474 S475 S476 S477 S478 S479 S480 S481 S482 S483 S484 S485 S486 S487 S488 S489 S490 S491 S492 S493 S494 S495 S496 S497 S498 S499 S500

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.21Å 143.60Å 123.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 43.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (25.00-2.50) 99.1 (43.57-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.232 , 0.294 0.230 , 0.293	Depositor DCC
$R_{free}$ test set	776 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.5	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3089	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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	0.68	1/3140 (0.0%)	0.86	3/4277 (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	A	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	GLU	CD-OE2	8.73	1.35	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	LEU	CA-CB-CG	6.78	130.90	115.30
1	A	344	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	360	VAL	CB-CA-C	-5.28	101.38	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	344	ASP	Peptide
1	A	387	GLY	Peptide
1	A	388	ALA	Peptide
1	A	41	VAL	Peptide

## 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	3086	0	2987	104	0
2	A	3	0	0	2	0
All	All	3089	0	2987	104	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 17.

All (104) 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:388:ALA:HB2	1:A:403:THR:HG22	1.42	0.98
1:A:388:ALA:HB3	1:A:401:ALA:O	1.65	0.96
1:A:72:ARG:HG2	1:A:81:ARG:HG3	1.53	0.90
1:A:388:ALA:CB	1:A:401:ALA:O	2.22	0.86
1:A:405:ARG:HD3	1:A:438:LYS:O	1.79	0.83
1:A:389:VAL:O	1:A:390:VAL:HB	1.77	0.83
1:A:108:GLY:O	1:A:389:VAL:O	2.02	0.78
1:A:344:ASP:HB3	1:A:345:PRO:C	2.07	0.75
1:A:398:LEU:HD22	1:A:399:ASP:N	2.05	0.71
1:A:387:GLY:O	1:A:388:ALA:HB2	1.88	0.71
1:A:360:VAL:CG2	2:A:453:HOH:O	2.40	0.69
1:A:360:VAL:HG22	2:A:453:HOH:O	1.92	0.69
1:A:36:VAL:HG12	1:A:160:ALA:HB1	1.76	0.67
1:A:366:PRO:O	1:A:367:LYS:CB	2.43	0.66
1:A:213:GLU:OE1	1:A:413:ARG:NH1	2.30	0.65
1:A:390:VAL:HA	1:A:399:ASP:O	1.98	0.64
1:A:108:GLY:HA3	1:A:133:ARG:O	1.97	0.64
1:A:388:ALA:CB	1:A:403:THR:HG22	2.23	0.64
1:A:387:GLY:O	1:A:388:ALA:CB	2.46	0.62
1:A:266:GLU:OE2	1:A:327:ARG:NH1	2.32	0.62
1:A:183:ASP:HB3	1:A:184:PRO:HA	1.80	0.62
1:A:117:HIS:HA	1:A:122:GLN:HG3	1.81	0.60
1:A:268:LEU:HG	1:A:298:HIS:CD2	2.35	0.60
1:A:27:ALA:HB2	1:A:54:TRP:CZ2	2.36	0.60
1:A:183:ASP:CB	1:A:184:PRO:HA	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLY:H	1:A:244:ILE:CG2	2.16	0.59
1:A:191:VAL:HG22	1:A:422:ILE:CD1	2.33	0.59
1:A:235:ARG:O	1:A:251:PRO:HD2	2.03	0.58
1:A:250:SER:N	1:A:251:PRO:HD3	2.18	0.58
1:A:365:ILE:HA	1:A:366:PRO:C	2.24	0.58
1:A:389:VAL:O	1:A:390:VAL:CB	2.48	0.58
1:A:254:VAL:CG1	1:A:269:ALA:HB3	2.35	0.56
1:A:343:LEU:O	1:A:344:ASP:CB	2.54	0.55
1:A:55:VAL:HG22	1:A:142:MET:SD	2.46	0.55
1:A:183:ASP:HB3	1:A:184:PRO:CA	2.37	0.54
1:A:254:VAL:HG13	1:A:269:ALA:HB3	1.90	0.54
1:A:343:LEU:O	1:A:344:ASP:HB2	2.08	0.53
1:A:372:GLU:OE2	1:A:376:ARG:NH1	2.42	0.52
1:A:203:TYR:CB	1:A:366:PRO:HD2	2.38	0.52
1:A:231:ASN:OD1	1:A:441:THR:HB	2.10	0.52
1:A:119:TYR:OH	1:A:367:LYS:HE2	2.11	0.51
1:A:49:GLU:HB2	1:A:54:TRP:CD1	2.46	0.51
1:A:209:SER:OG	1:A:417:ARG:NE	2.41	0.51
1:A:49:GLU:HB2	1:A:54:TRP:NE1	2.25	0.51
1:A:117:HIS:ND1	1:A:122:GLN:HG2	2.25	0.51
1:A:176:ARG:O	1:A:446:LEU:HB2	2.10	0.50
1:A:251:PRO:HA	1:A:402:LEU:O	2.10	0.50
1:A:191:VAL:HG22	1:A:422:ILE:HD11	1.92	0.50
1:A:383:GLY:O	1:A:384:LEU:CB	2.60	0.49
1:A:298:HIS:HE1	1:A:337:SER:OG	1.95	0.49
1:A:366:PRO:O	1:A:367:LYS:HB3	2.12	0.49
1:A:180:VAL:HG12	1:A:212:VAL:HG11	1.95	0.49
1:A:190:ARG:HD2	1:A:377:LEU:O	2.13	0.49
1:A:182:ASP:OD1	1:A:182:ASP:N	2.47	0.48
1:A:64:VAL:HG22	1:A:73:VAL:HG22	1.95	0.48
1:A:348:ASP:OD2	1:A:350:MET:HB2	2.14	0.48
1:A:267:PRO:HD2	1:A:337:SER:O	2.14	0.47
1:A:267:PRO:HG3	1:A:339:ILE:HD12	1.96	0.47
1:A:175:SER:HB3	1:A:226:LEU:CD1	2.43	0.47
1:A:120:GLY:HA2	1:A:122:GLN:OE1	2.14	0.47
1:A:254:VAL:O	1:A:265:THR:HA	2.15	0.47
1:A:258:ARG:HD3	1:A:262:VAL:CG2	2.44	0.47
1:A:312:ILE:HD13	1:A:347:SER:OG	2.15	0.46
1:A:59:GLY:HA3	1:A:138:ARG:HB2	1.97	0.46
1:A:187:PHE:O	1:A:188:ARG:HG2	2.15	0.46
1:A:345:PRO:O	1:A:346:SER:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ILE:HG13	1:A:421:GLY:HA2	1.98	0.46
1:A:242:GLY:H	1:A:244:ILE:HG22	1.81	0.46
1:A:388:ALA:HB1	1:A:401:ALA:O	2.11	0.46
1:A:211:CYS:SG	1:A:417:ARG:HG2	2.55	0.46
1:A:430:ARG:O	1:A:433:GLU:HG2	2.15	0.46
1:A:74:ILE:HG23	1:A:79:THR:HG22	1.98	0.46
1:A:247:LEU:HD22	1:A:407:ALA:HB3	1.98	0.46
1:A:250:SER:N	1:A:251:PRO:CD	2.78	0.45
1:A:203:TYR:HB2	1:A:366:PRO:HD2	1.97	0.45
1:A:230:HIS:HB3	1:A:445:TYR:CZ	2.52	0.45
1:A:310:THR:C	1:A:312:ILE:H	2.19	0.45
1:A:288:LEU:O	1:A:292:SER:HB3	2.16	0.45
1:A:57:ALA:HB1	1:A:137:PRO:HB3	2.00	0.44
1:A:226:LEU:HD22	1:A:445:TYR:HB3	2.00	0.43
1:A:59:GLY:HA3	1:A:138:ARG:HD2	2.00	0.43
1:A:172:VAL:HG22	1:A:225:ARG:HH11	1.84	0.43
1:A:111:ALA:HB1	1:A:383:GLY:HA2	2.01	0.43
1:A:427:GLU:O	1:A:428:PRO:C	2.57	0.43
1:A:183:ASP:CB	1:A:184:PRO:CA	2.97	0.43
1:A:191:VAL:HG22	1:A:422:ILE:HD13	1.99	0.43
1:A:212:VAL:HG21	1:A:439:LEU:HD13	2.00	0.43
1:A:366:PRO:O	1:A:367:LYS:HB2	2.19	0.42
1:A:188:ARG:HH11	1:A:188:ARG:HG3	1.84	0.42
1:A:408:TYR:HE1	1:A:417:ARG:HB2	1.84	0.42
1:A:424:GLU:HA	1:A:424:GLU:OE2	2.19	0.42
1:A:69:ASP:CG	1:A:127:PRO:O	2.58	0.42
1:A:58:ALA:HB3	1:A:139:THR:HB	2.01	0.42
1:A:254:VAL:HG12	1:A:269:ALA:HB3	2.02	0.41
1:A:124:ARG:HH11	1:A:124:ARG:HG2	1.86	0.41
1:A:273:ALA:O	1:A:438:LYS:HE2	2.20	0.41
1:A:180:VAL:O	1:A:210:ARG:NH2	2.49	0.41
1:A:44:ASP:O	1:A:58:ALA:O	2.38	0.41
1:A:122:GLN:O	1:A:125:LEU:HB2	2.20	0.41
1:A:383:GLY:O	1:A:384:LEU:HB3	2.21	0.41
1:A:270:GLY:O	1:A:274:LEU:HB2	2.20	0.41
1:A:372:GLU:OE1	1:A:376:ARG:HD3	2.21	0.40
1:A:122:GLN:H	1:A:122:GLN:CD	2.24	0.40
1:A:70:GLU:CD	1:A:81:ARG:HG2	2.42	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	413/470 (88%)	359 (87%)	34 (8%)	20 (5%)	<b>2</b> <b>3</b>

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	ASP
1	A	188	ARG
1	A	344	ASP
1	A	345	PRO
1	A	367	LYS
1	A	384	LEU
1	A	447	VAL
1	A	41	VAL
1	A	346	SER
1	A	366	PRO
1	A	383	GLY
1	A	388	ALA
1	A	21	PRO
1	A	87	ARG
1	A	311	ASP
1	A	390	VAL
1	A	215	PRO
1	A	291	ASN
1	A	405	ARG
1	A	52	GLY

### 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	304/375 (81%)	261 (86%)	43 (14%)	<b>4</b> <b>7</b>

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	47	LEU
1	A	66	LEU
1	A	71	LEU
1	A	75	ARG
1	A	81	ARG
1	A	82	GLN
1	A	103	THR
1	A	122	GLN
1	A	124	ARG
1	A	125	LEU
1	A	131	LEU
1	A	140	ARG
1	A	150	LEU
1	A	164	LEU
1	A	170	ARG
1	A	171	GLU
1	A	182	ASP
1	A	183	ASP
1	A	188	ARG
1	A	228	ARG
1	A	231	ASN
1	A	238	LEU
1	A	247	LEU
1	A	254	VAL
1	A	290	SER
1	A	312	ILE
1	A	324	MET
1	A	326	VAL
1	A	340	ARG
1	A	343	LEU
1	A	350	MET
1	A	357	PHE
1	A	360	VAL
1	A	365	ILE
1	A	366	PRO

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Mol	Chain	Res	Type
1	A	376	ARG
1	A	378	ASP
1	A	384	LEU
1	A	398	LEU
1	A	417	ARG
1	A	424	GLU
1	A	434	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	82	GLN
1	A	240	GLN
1	A	298	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 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 ⓘ

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, 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	419/470 (89%)	0.39	16 (3%) 41 43	39, 51, 63, 70	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	ILE	5.2
1	A	345	PRO	4.2
1	A	23	GLY	4.2
1	A	19	PRO	3.6
1	A	164	LEU	3.1
1	A	22	ALA	2.9
1	A	148	ILE	2.7
1	A	51	ASP	2.7
1	A	166	ALA	2.6
1	A	171	GLU	2.6
1	A	146	LYS	2.4
1	A	21	PRO	2.4
1	A	446	LEU	2.3
1	A	58	ALA	2.1
1	A	29	LEU	2.1
1	A	388	ALA	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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.