



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 27, 2016 – 11:22 AM GMT

PDB ID : 3X3H  
Title : Crystal Structure of the Manihot esculenta Hydroxynitrile Lyase (MeHNL)  
3KP (K176P, K199P, K224P) triple mutant  
Authors : Cielo, C.B.C.; Yamane, T.; Asano, Y.; Dadashipour, M.; Suzuki, A.;  
Mizushima, T.; Komeda, H.; Okazaki, S.  
Deposited on : 2015-01-21  
Resolution : 2.88 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](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  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

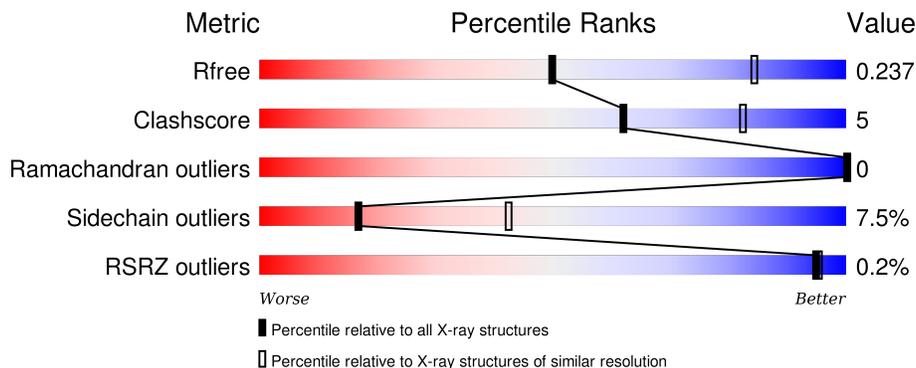
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.88 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	258	84% 14% .
1	B	258	81% 18% .
1	C	258	83% 15% .
1	D	258	83% 15% .
1	E	258	83% 16% .

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Mol	Chain	Length	Quality of chain
1	F	258	 84% 14% •
1	G	258	 86% 12% •
1	H	258	 83% 14% •

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16544 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 (S)-hydroxynitrile lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	2068	1336	341	383	8	0	0	0
1	B	258	2068	1336	341	383	8	0	0	0
1	C	258	2068	1336	341	383	8	0	0	0
1	D	258	2068	1336	341	383	8	0	0	0
1	E	258	2068	1336	341	383	8	0	0	0
1	F	258	2068	1336	341	383	8	0	0	0
1	G	258	2068	1336	341	383	8	0	0	0
1	H	258	2068	1336	341	383	8	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	PRO	LYS	ENGINEERED MUTATION	UNP P52705
A	199	PRO	LYS	ENGINEERED MUTATION	UNP P52705
A	224	PRO	LYS	ENGINEERED MUTATION	UNP P52705
B	176	PRO	LYS	ENGINEERED MUTATION	UNP P52705
B	199	PRO	LYS	ENGINEERED MUTATION	UNP P52705
B	224	PRO	LYS	ENGINEERED MUTATION	UNP P52705
C	176	PRO	LYS	ENGINEERED MUTATION	UNP P52705
C	199	PRO	LYS	ENGINEERED MUTATION	UNP P52705
C	224	PRO	LYS	ENGINEERED MUTATION	UNP P52705
D	176	PRO	LYS	ENGINEERED MUTATION	UNP P52705
D	199	PRO	LYS	ENGINEERED MUTATION	UNP P52705
D	224	PRO	LYS	ENGINEERED MUTATION	UNP P52705
E	176	PRO	LYS	ENGINEERED MUTATION	UNP P52705

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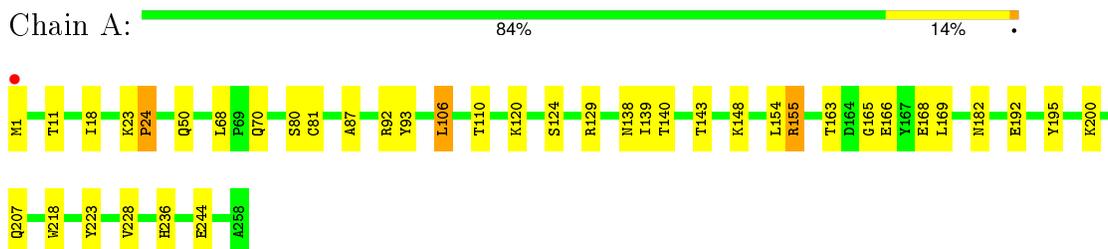
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<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
E	199	PRO	LYS	ENGINEERED MUTATION	UNP P52705
E	224	PRO	LYS	ENGINEERED MUTATION	UNP P52705
F	176	PRO	LYS	ENGINEERED MUTATION	UNP P52705
F	199	PRO	LYS	ENGINEERED MUTATION	UNP P52705
F	224	PRO	LYS	ENGINEERED MUTATION	UNP P52705
G	176	PRO	LYS	ENGINEERED MUTATION	UNP P52705
G	199	PRO	LYS	ENGINEERED MUTATION	UNP P52705
G	224	PRO	LYS	ENGINEERED MUTATION	UNP P52705
H	176	PRO	LYS	ENGINEERED MUTATION	UNP P52705
H	199	PRO	LYS	ENGINEERED MUTATION	UNP P52705
H	224	PRO	LYS	ENGINEERED MUTATION	UNP P52705

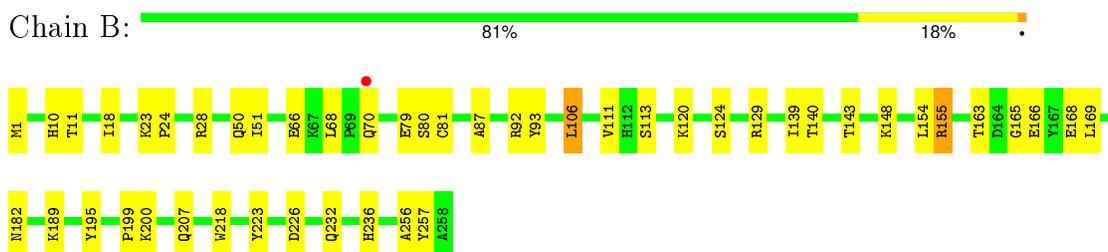
### 3 Residue-property plots [i](#)

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.

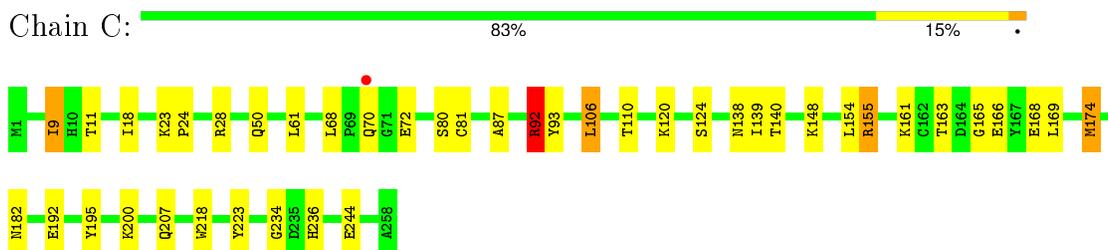
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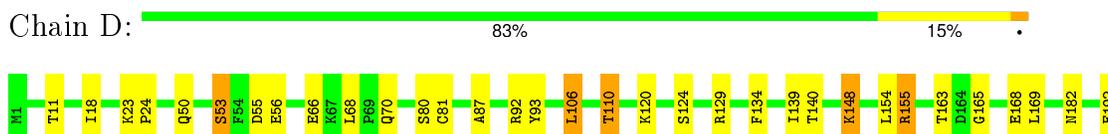
- Molecule 1: (S)-hydroxynitrile lyase



- Molecule 1: (S)-hydroxynitrile lyase

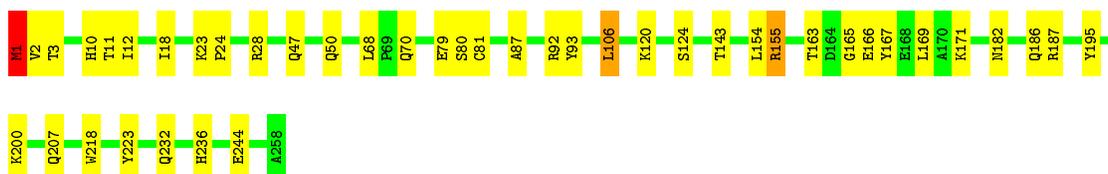
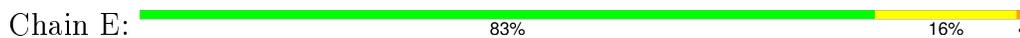


- Molecule 1: (S)-hydroxynitrile lyase

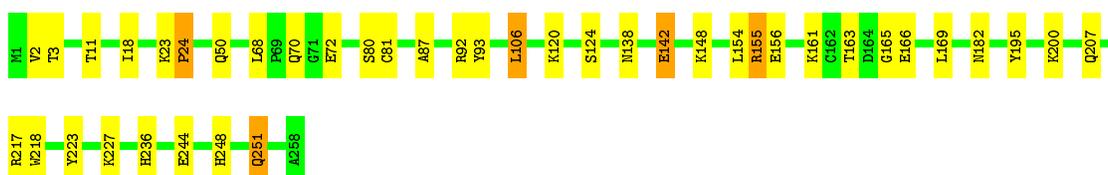
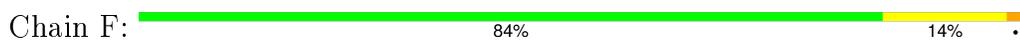




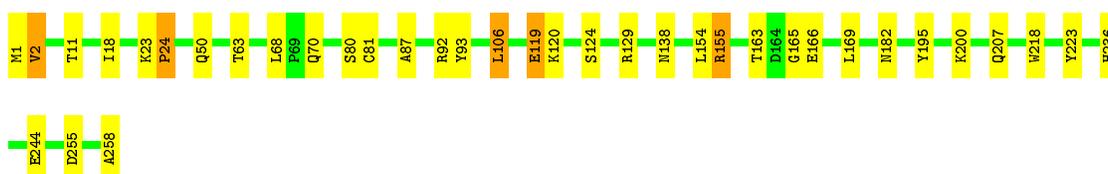
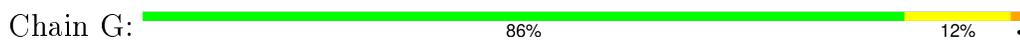
- Molecule 1: (S)-hydroxynitrile lyase



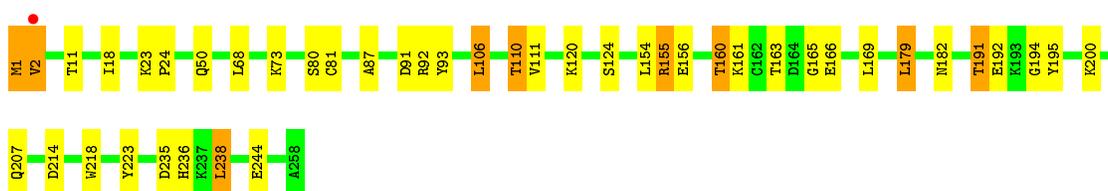
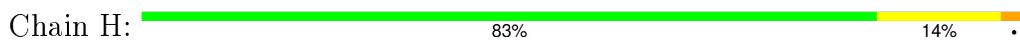
- Molecule 1: (S)-hydroxynitrile lyase



- Molecule 1: (S)-hydroxynitrile lyase



- Molecule 1: (S)-hydroxynitrile lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.04Å 84.21Å 134.90Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	15.26 – 2.88 15.26 – 2.88	Depositor EDS
% Data completeness (in resolution range)	95.9 (15.26-2.88) 96.2 (15.26-2.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.204 , 0.238 0.208 , 0.237	Depositor DCC
$R_{free}$ test set	2100 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , -10.4	EDS
Estimated twinning fraction	0.002 for k,h,-l 0.004 for -k,-h,-l 0.448 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 41590 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.22 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.0348e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 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	0.58	0/2122	0.71	0/2883
1	B	0.63	2/2122 (0.1%)	0.75	2/2883 (0.1%)
1	C	0.59	0/2122	0.79	4/2883 (0.1%)
1	D	0.58	0/2122	0.73	3/2883 (0.1%)
1	E	0.64	0/2122	0.75	2/2883 (0.1%)
1	F	0.61	0/2122	0.74	1/2883 (0.0%)
1	G	0.61	1/2122 (0.0%)	0.73	0/2883
1	H	0.62	0/2122	0.75	2/2883 (0.1%)
All	All	0.61	3/16976 (0.0%)	0.74	14/23064 (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	E	0	1
1	H	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	GLU	CD-OE1	5.83	1.32	1.25
1	B	66	GLU	CG-CD	5.56	1.60	1.51
1	G	119	GLU	CA-CB	5.22	1.65	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	ILE	CG1-CB-CG2	-10.43	88.44	111.40
1	D	53	SER	CB-CA-C	-9.47	92.10	110.10
1	C	174	MET	CG-SD-CE	-8.67	86.33	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	179	LEU	CB-CA-C	8.13	125.65	110.20
1	C	9	ILE	CA-CB-CG1	-7.78	96.21	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	1	MET	Peptide
1	H	1	MET	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	2068	0	2047	24	0
1	B	2068	0	2047	23	0
1	C	2068	0	2047	21	0
1	D	2068	0	2047	28	0
1	E	2068	0	2047	22	0
1	F	2068	0	2047	22	0
1	G	2068	0	2047	22	0
1	H	2068	0	2047	26	1
All	All	16544	0	16376	176	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 5.

The worst 5 of 176 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:D:205:THR:HG21	1:D:233:GLY:O	1.52	1.09
1:H:91:ASP:OD1	1:H:191:THR:HG22	1.76	0.85
1:C:110:THR:HG21	1:C:192:GLU:OE2	1.89	0.73
1:A:110:THR:HG21	1:A:192:GLU:OE2	1.88	0.73
1:A:228:VAL:O	1:H:111:VAL:CG1	2.38	0.72

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:H:2:VAL:CG2	1:H:214:ASP:OD2[2_746]	2.12	0.08

## 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	256/258 (99%)	246 (96%)	10 (4%)	0	100	100
1	B	256/258 (99%)	248 (97%)	8 (3%)	0	100	100
1	C	256/258 (99%)	248 (97%)	8 (3%)	0	100	100
1	D	256/258 (99%)	246 (96%)	10 (4%)	0	100	100
1	E	256/258 (99%)	246 (96%)	10 (4%)	0	100	100
1	F	256/258 (99%)	248 (97%)	8 (3%)	0	100	100
1	G	256/258 (99%)	248 (97%)	8 (3%)	0	100	100
1	H	256/258 (99%)	247 (96%)	9 (4%)	0	100	100
All	All	2048/2064 (99%)	1977 (96%)	71 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	223/223 (100%)	207 (93%)	16 (7%)	18	44
1	B	223/223 (100%)	206 (92%)	17 (8%)	16	42
1	C	223/223 (100%)	207 (93%)	16 (7%)	18	44
1	D	223/223 (100%)	209 (94%)	14 (6%)	22	52
1	E	223/223 (100%)	206 (92%)	17 (8%)	16	42
1	F	223/223 (100%)	204 (92%)	19 (8%)	13	35
1	G	223/223 (100%)	207 (93%)	16 (7%)	18	44
1	H	223/223 (100%)	204 (92%)	19 (8%)	13	35
All	All	1784/1784 (100%)	1650 (92%)	134 (8%)	17	42

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	169	LEU
1	E	169	LEU
1	H	124	SER
1	D	244	GLU
1	E	68	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	207	GLN

### 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, 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	258/258 (100%)	-0.38	1 (0%) 93   92	12, 23, 42, 59	0
1	B	258/258 (100%)	-0.37	1 (0%) 93   92	13, 21, 41, 75	0
1	C	258/258 (100%)	-0.39	1 (0%) 93   92	12, 22, 41, 73	0
1	D	258/258 (100%)	-0.39	0 100   100	12, 23, 41, 59	0
1	E	258/258 (100%)	-0.45	0 100   100	11, 20, 33, 48	0
1	F	258/258 (100%)	-0.44	0 100   100	11, 20, 32, 62	0
1	G	258/258 (100%)	-0.50	0 100   100	12, 20, 34, 52	0
1	H	258/258 (100%)	-0.49	1 (0%) 93   92	10, 19, 35, 50	0
All	All	2064/2064 (100%)	-0.43	4 (0%) 95   95	10, 21, 39, 75	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	GLN	2.8
1	H	2	VAL	2.5
1	C	70	GLN	2.2
1	A	1	MET	2.1

### 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.