



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:28 AM GMT

PDB ID : 3ILV  
Title : Crystal structure of a glutamine-dependent NAD(+) synthetase from *Cytophaga hutchinsonii*  
Authors : Palani, K.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2009-08-07  
Resolution : 1.79 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  
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

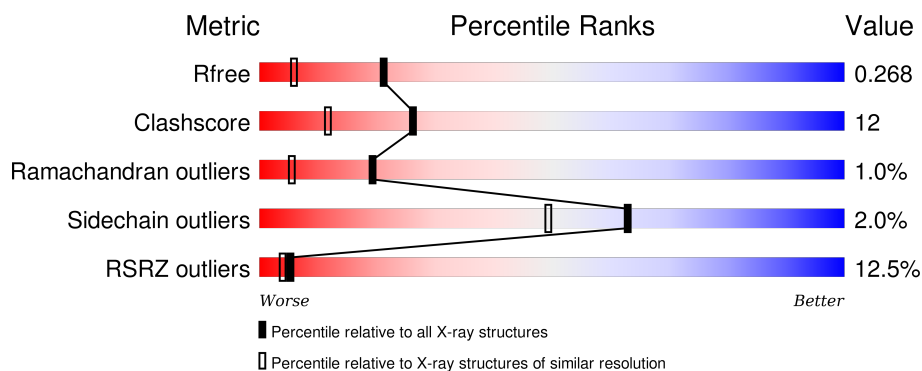
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	634	<div> <div>11%</div> <div>71%</div> <div>19%</div> <div>• 9%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4846 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 Glutamine-dependent NAD(+) synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	Se	0	0	0
			4638	2967	779	872	10	10			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP Q11SE1
A	0	SER	-	expression tag	UNP Q11SE1
A	1	LEU	-	expression tag	UNP Q11SE1
A	625	GLU	-	expression tag	UNP Q11SE1
A	626	GLY	-	expression tag	UNP Q11SE1
A	627	HIS	-	expression tag	UNP Q11SE1
A	628	HIS	-	expression tag	UNP Q11SE1
A	629	HIS	-	expression tag	UNP Q11SE1
A	630	HIS	-	expression tag	UNP Q11SE1
A	631	HIS	-	expression tag	UNP Q11SE1
A	632	HIS	-	expression tag	UNP Q11SE1

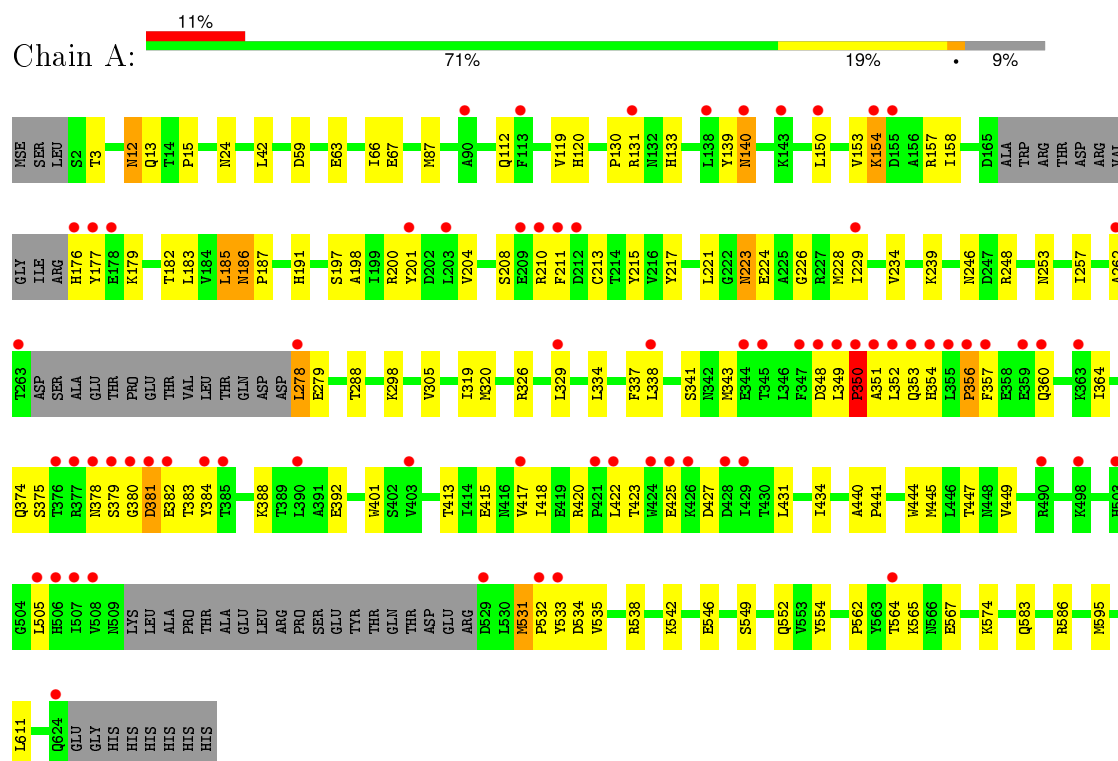
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	208	Total	O	0	0
			208	208		

### 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.

- Molecule 1: Glutamine-dependent NAD(+) synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.14Å 66.34Å 74.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.74 – 1.79 39.74 – 1.79	Depositor EDS
% Data completeness (in resolution range)	91.8 (39.74-1.79) 91.5 (39.74-1.79)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 1.78Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.244 , 0.268 0.243 , 0.268	Depositor DCC
$R_{free}$ test set	2903 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 61167 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4846	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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, 0.375 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	0.33	0/4731	0.59	0/6394

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4638	0	4551	113	0
2	A	208	0	0	3	0
All	All	4846	0	4551	113	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 12.

All (113) 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:374:GLN:HE21	1:A:401:TRP:HE1	1.29	0.78
1:A:423:THR:O	1:A:427:ASP:HB2	1.85	0.77
1:A:150:LEU:HD11	1:A:179:LYS:HB3	1.67	0.75
1:A:200:ARG:HD3	1:A:217:TYR:CE2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:GLN:HE21	1:A:586:ARG:HH21	1.36	0.74
1:A:549:SER:H	1:A:552:GLN:NE2	1.86	0.73
1:A:388:LYS:O	1:A:392:GLU:HG3	1.88	0.73
1:A:431:LEU:O	1:A:434:ILE:HG22	1.90	0.71
1:A:374:GLN:HG2	1:A:401:TRP:NE1	2.09	0.66
1:A:356:PRO:O	1:A:357:PHE:HB3	1.96	0.65
1:A:583:GLN:NE2	1:A:586:ARG:HH21	1.95	0.64
1:A:415:GLU:HG2	1:A:422:LEU:HG	1.80	0.64
1:A:150:LEU:HD11	1:A:179:LYS:HD3	1.80	0.64
1:A:549:SER:H	1:A:552:GLN:HE21	1.45	0.63
1:A:334:LEU:O	1:A:338:LEU:HD13	1.98	0.63
1:A:351:ALA:HA	1:A:354:HIS:HD2	1.65	0.62
1:A:349:LEU:HA	1:A:350:PRO:C	2.20	0.61
1:A:532:PRO:HA	2:A:779:HOH:O	2.00	0.61
1:A:150:LEU:HD12	1:A:157:ARG:HH21	1.64	0.61
1:A:176:HIS:CD2	1:A:177:TYR:H	2.18	0.61
1:A:531:MSE:HB3	1:A:535:VAL:CG1	2.31	0.61
1:A:150:LEU:CD1	1:A:157:ARG:HH21	2.14	0.60
1:A:204:VAL:HG13	1:A:215:TYR:CD2	2.36	0.60
1:A:380:GLY:O	1:A:382:GLU:N	2.32	0.60
1:A:66:ILE:HD12	1:A:87:MSE:HE3	1.84	0.59
1:A:334:LEU:HD22	1:A:352:LEU:N	2.17	0.59
1:A:63:GLU:O	1:A:67:GLU:HG3	2.04	0.58
1:A:176:HIS:HD2	1:A:177:TYR:H	1.51	0.57
1:A:59:ASP:O	1:A:63:GLU:HG3	2.04	0.57
1:A:177:TYR:HB2	1:A:211:PHE:CD2	2.39	0.57
1:A:229:ILE:HD12	1:A:595:MSE:HE1	1.88	0.56
1:A:380:GLY:C	1:A:382:GLU:H	2.10	0.55
1:A:229:ILE:HD12	1:A:595:MSE:CE	2.37	0.55
1:A:305:VAL:HG21	1:A:447:THR:HA	1.88	0.55
1:A:150:LEU:CD1	1:A:179:LYS:HB3	2.33	0.55
1:A:12:ASN:HD22	1:A:12:ASN:C	2.11	0.55
1:A:326:ARG:HG3	1:A:326:ARG:HH11	1.73	0.54
1:A:349:LEU:HA	1:A:351:ALA:N	2.23	0.54
1:A:139:TYR:O	1:A:140:ASN:HB2	2.08	0.53
1:A:210:ARG:HG3	1:A:211:PHE:CD2	2.44	0.53
1:A:533:TYR:O	1:A:534:ASP:HB3	2.09	0.53
1:A:360:GLN:O	1:A:364:ILE:HG13	2.08	0.53
1:A:176:HIS:HB3	1:A:179:LYS:HG3	1.90	0.53
1:A:418:ILE:HD12	1:A:420:ARG:HE	1.74	0.53
1:A:158:ILE:HG21	1:A:185:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:THR:O	1:A:417:VAL:HG23	2.09	0.52
1:A:246:ASN:HB3	1:A:257:ILE:HG21	1.92	0.51
1:A:130:PRO:HB2	1:A:133:HIS:CG	2.45	0.51
1:A:158:ILE:CG2	1:A:185:LEU:HD22	2.41	0.51
1:A:531:MSE:HB3	1:A:535:VAL:HG13	1.93	0.51
1:A:348:ASP:O	1:A:349:LEU:HB2	2.11	0.50
1:A:197:SER:HB2	1:A:248:ARG:NH1	2.27	0.50
1:A:382:GLU:HG3	1:A:383:THR:H	1.76	0.49
1:A:534:ASP:OD2	1:A:538:ARG:HD2	2.12	0.49
1:A:381:ASP:HA	1:A:384:TYR:HB3	1.94	0.49
1:A:574:LYS:HE2	2:A:783:HOH:O	2.11	0.49
1:A:182:THR:O	1:A:213:CYS:HB2	2.12	0.49
1:A:349:LEU:CA	1:A:350:PRO:C	2.80	0.49
1:A:440:ALA:HB3	1:A:441:PRO:HD3	1.94	0.48
1:A:183:LEU:HG	1:A:185:LEU:HD13	1.95	0.48
1:A:246:ASN:HB3	1:A:257:ILE:CG2	2.44	0.47
1:A:3:THR:HG22	1:A:262:ALA:HA	1.95	0.47
1:A:334:LEU:HD22	1:A:352:LEU:H	1.79	0.47
1:A:542:LYS:HA	1:A:546:GLU:HB2	1.95	0.47
1:A:191:HIS:CB	1:A:228:MSE:HE3	2.44	0.47
1:A:564:THR:HG22	1:A:567:GLU:OE1	2.14	0.47
1:A:120:HIS:HE1	2:A:720:HOH:O	1.97	0.47
1:A:564:THR:HG22	1:A:567:GLU:HG3	1.97	0.47
1:A:176:HIS:CD2	1:A:177:TYR:N	2.83	0.46
1:A:153:VAL:O	1:A:154:LYS:C	2.53	0.46
1:A:158:ILE:HG12	1:A:183:LEU:HD23	1.98	0.46
1:A:42:LEU:O	1:A:187:PRO:HB3	2.16	0.46
1:A:12:ASN:HD21	1:A:298:LYS:NZ	2.13	0.46
1:A:278:LEU:HD12	1:A:279:GLU:N	2.30	0.46
1:A:531:MSE:HB3	1:A:535:VAL:HG11	1.97	0.46
1:A:334:LEU:HD21	1:A:351:ALA:CB	2.47	0.45
1:A:13:GLN:NE2	1:A:24:ASN:HD22	2.14	0.45
1:A:351:ALA:HA	1:A:354:HIS:CD2	2.48	0.45
1:A:445:MSE:O	1:A:449:VAL:HG23	2.16	0.45
1:A:375:SER:HB2	1:A:379:SER:OG	2.17	0.45
1:A:329:LEU:HG	1:A:357:PHE:HE1	1.82	0.45
1:A:223:ASN:ND2	1:A:226:GLY:H	2.14	0.45
1:A:554:TYR:OH	1:A:565:LYS:HB3	2.16	0.44
1:A:186:ASN:HD22	1:A:186:ASN:C	2.20	0.44
1:A:334:LEU:HD21	1:A:351:ALA:HB1	1.99	0.44
1:A:208:SER:O	1:A:239:LYS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:MSE:CB	1:A:535:VAL:HG13	2.47	0.44
1:A:382:GLU:HG3	1:A:383:THR:N	2.32	0.44
1:A:349:LEU:HA	1:A:351:ALA:CB	2.48	0.44
1:A:583:GLN:NE2	1:A:586:ARG:HE	2.15	0.43
1:A:112:GLN:OE1	1:A:131:ARG:HG3	2.19	0.43
1:A:341:SER:HB3	1:A:343:MSE:HE3	2.01	0.43
1:A:12:ASN:HA	1:A:221:LEU:O	2.19	0.43
1:A:348:ASP:C	1:A:349:LEU:HD12	2.39	0.42
1:A:326:ARG:HG3	1:A:326:ARG:NH1	2.33	0.42
1:A:357:PHE:O	1:A:360:GLN:HG2	2.19	0.42
1:A:374:GLN:NE2	1:A:401:TRP:HE1	2.08	0.42
1:A:423:THR:C	1:A:425:GLU:H	2.22	0.42
1:A:337:PHE:HD2	1:A:338:LEU:HD12	1.83	0.42
1:A:349:LEU:HA	1:A:351:ALA:HB3	2.01	0.42
1:A:351:ALA:C	1:A:353:GLN:N	2.71	0.42
1:A:423:THR:C	1:A:425:GLU:N	2.73	0.41
1:A:319:ILE:HG13	1:A:505:LEU:HD11	2.02	0.41
1:A:288:THR:HG21	1:A:320:MSE:HE3	2.02	0.41
1:A:348:ASP:HB3	1:A:350:PRO:HB2	2.03	0.41
1:A:253:ASN:HA	1:A:253:ASN:HD22	1.66	0.41
1:A:564:THR:HG22	1:A:567:GLU:CG	2.50	0.41
1:A:349:LEU:HG	1:A:351:ALA:HB3	2.03	0.41
1:A:198:ALA:O	1:A:201:TYR:HB3	2.20	0.41
1:A:15:PRO:HD3	1:A:224:GLU:HG2	2.03	0.40
1:A:234:VAL:HG12	1:A:257:ILE:HD11	2.03	0.40
1:A:130:PRO:O	1:A:133:HIS:HB2	2.21	0.40
1:A:119:VAL:HG21	1:A:228:MSE:HE2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	572/634 (90%)	532 (93%)	34 (6%)	6 (1%)	19 5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	LYS
1	A	350	PRO
1	A	381	ASP
1	A	140	ASN
1	A	531	MSE
1	A	356	PRO

### 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	493/530 (93%)	483 (98%)	10 (2%)	63 49

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	185	LEU
1	A	186	ASN
1	A	223	ASN
1	A	278	LEU
1	A	350	PRO
1	A	378	ASN
1	A	444	TRP
1	A	562	PRO
1	A	611	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	GLN
1	A	20	ASN
1	A	116	ASN
1	A	120	HIS
1	A	132	ASN
1	A	176	HIS
1	A	186	ASN
1	A	223	ASN
1	A	253	ASN
1	A	339	GLN
1	A	342	ASN
1	A	354	HIS
1	A	374	GLN
1	A	552	GLN
1	A	583	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 ⓘ

### 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<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	570/634 (89%)	0.94	71 (12%) 5 4	11, 27, 54, 67	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	533	TYR	16.1
1	A	355	LEU	14.2
1	A	356	PRO	13.1
1	A	532	PRO	10.7
1	A	352	LEU	9.0
1	A	349	LEU	8.5
1	A	177	TYR	8.1
1	A	424	TRP	8.1
1	A	154	LYS	6.5
1	A	263	THR	5.6
1	A	380	GLY	5.5
1	A	278	LEU	5.4
1	A	138	LEU	5.2
1	A	350	PRO	5.2
1	A	113	PHE	5.1
1	A	211	PHE	5.0
1	A	210	ARG	4.8
1	A	624	GLN	4.7
1	A	354	HIS	4.6
1	A	201	TYR	4.5
1	A	381	ASP	4.4
1	A	508	VAL	4.3
1	A	178	GLU	4.1
1	A	150	LEU	3.8
1	A	426	LYS	3.7
1	A	359	GLU	3.7
1	A	382	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	351	ALA	3.5
1	A	357	PHE	3.5
1	A	385	THR	3.3
1	A	506	HIS	3.3
1	A	422	LEU	3.2
1	A	425	GLU	3.2
1	A	345	THR	3.1
1	A	421	PRO	3.0
1	A	428	ASP	2.9
1	A	155	ASP	2.9
1	A	360	GLN	2.9
1	A	176	HIS	2.8
1	A	203	LEU	2.8
1	A	503	HIS	2.7
1	A	140	ASN	2.7
1	A	262	ALA	2.7
1	A	348	ASP	2.7
1	A	131	ARG	2.7
1	A	378	ASN	2.6
1	A	347	PHE	2.6
1	A	390	LEU	2.6
1	A	143	LYS	2.6
1	A	379	SER	2.5
1	A	209	GLU	2.5
1	A	507	ILE	2.5
1	A	353	GLN	2.5
1	A	212	ASP	2.4
1	A	417	VAL	2.4
1	A	384	TYR	2.4
1	A	329	LEU	2.4
1	A	429	ILE	2.3
1	A	363	LYS	2.3
1	A	377	ARG	2.3
1	A	490	ARG	2.3
1	A	338	LEU	2.3
1	A	90	ALA	2.2
1	A	564	THR	2.2
1	A	376	THR	2.1
1	A	229	ILE	2.1
1	A	529	ASP	2.1
1	A	344	GLU	2.1
1	A	505	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	498	LYS	2.0
1	A	403	VAL	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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.