



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:26 AM UTC

PDB ID : 1BF2 / pdb\_00001bf2  
Title : STRUCTURE OF PSEUDOMONAS ISOAMYLASE  
Authors : Katsuya, Y.; Mezaki, Y.; Kubota, M.; Matsuura, Y.  
Deposited on : 1998-05-26  
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

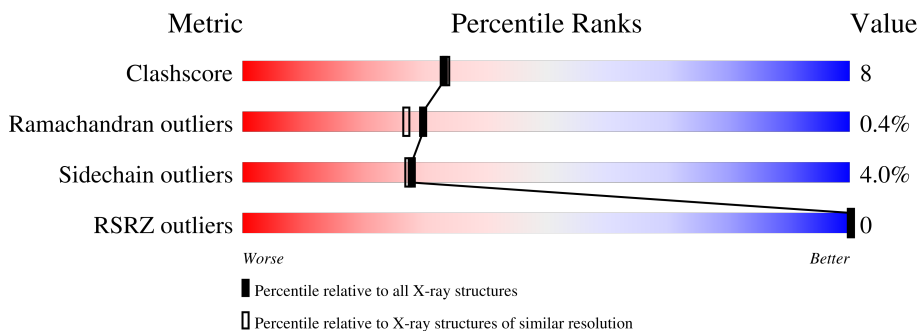
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

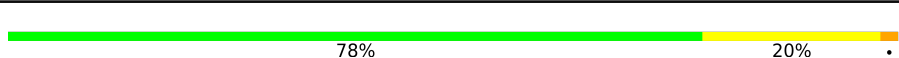
The reported resolution of this entry is 2.00 Å.

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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	750	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6143 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 ISOAMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	750	5735	3600	969	1149	17	0	0	0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

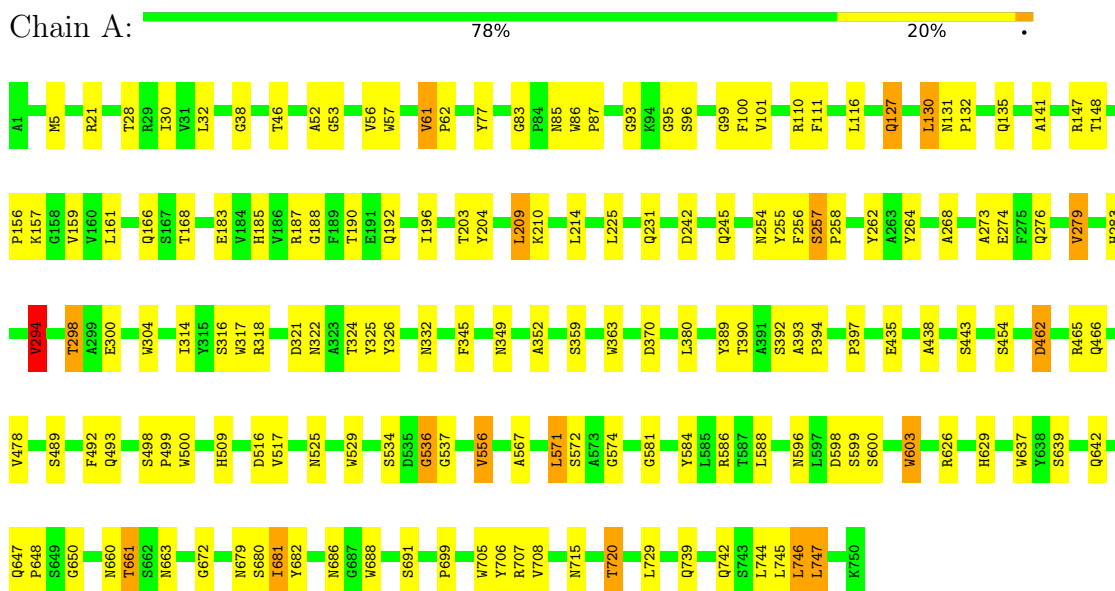
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	407	Total	O	0	0
			407	407		

### 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: ISOAMYLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.90Å 152.40Å 53.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 85.8 (10.00-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.20Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.161 , 0.214 0.156 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtrriage
Anisotropy	0.263	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
CA

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	0.61	1/5896 (0.0%)	1.04	31/8064 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	294	VAL	CA-CB	5.96	1.60	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	PHE	N-CA-C	-8.57	97.59	110.28
1	A	629	HIS	CA-C-N	8.35	129.15	119.47
1	A	629	HIS	C-N-CA	8.35	129.15	119.47
1	A	492	PHE	N-CA-C	8.19	123.57	113.50
1	A	435	GLU	N-CA-C	-8.11	92.69	108.59
1	A	556	VAL	CB-CA-C	-7.73	101.92	112.04
1	A	101	VAL	N-CA-C	-7.30	105.86	111.62
1	A	493	GLN	N-CA-C	6.59	118.55	111.36
1	A	680	SER	N-CA-C	-6.56	100.81	110.52
1	A	393	ALA	CA-C-N	6.50	126.73	119.32
1	A	393	ALA	C-N-CA	6.50	126.73	119.32
1	A	225	LEU	N-CA-C	-6.29	99.69	109.87
1	A	435	GLU	CA-C-N	6.23	127.62	119.84
1	A	435	GLU	C-N-CA	6.23	127.62	119.84
1	A	257	SER	N-CA-C	5.97	118.96	109.64
1	A	516	ASP	N-CA-C	5.90	118.50	111.71
1	A	255	TYR	N-CA-C	5.87	120.30	113.20
1	A	462	ASP	N-CA-C	5.82	117.30	111.07
1	A	325	TYR	N-CA-C	5.80	119.54	112.23
1	A	332	ASN	N-CA-C	5.78	120.14	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	537	GLY	N-CA-C	-5.76	104.41	112.13
1	A	465	ARG	N-CA-C	-5.75	105.10	111.36
1	A	294	VAL	N-CA-C	5.64	114.94	106.42
1	A	147	ARG	N-CA-C	5.63	118.18	111.71
1	A	454	SER	N-CA-C	-5.62	101.72	110.42
1	A	536	GLY	N-CA-C	5.58	126.40	113.18
1	A	647	GLN	N-CA-C	-5.37	102.22	110.07
1	A	77	TYR	N-CA-C	5.22	117.12	109.24
1	A	61	VAL	N-CA-C	5.12	113.47	107.89
1	A	264	TYR	N-CA-C	-5.12	105.34	112.45
1	A	650	GLY	N-CA-C	-5.03	108.38	115.32

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	5735	0	5289	86	0
2	A	1	0	0	0	0
3	A	407	0	0	7	0
All	All	6143	0	5289	86	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 8.

All (86) 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:298:THR:HG22	1:A:300:GLU:H	1.47	0.80
1:A:52:ALA:HB3	1:A:56:VAL:HG23	1.66	0.75
1:A:715:ASN:O	1:A:720:THR:HB	1.88	0.73
1:A:742:GLN:HG3	3:A:847:HOH:O	1.86	0.73
1:A:283:HIS:HE1	1:A:370:ASP:OD2	1.74	0.71
1:A:686:ASN:HD21	1:A:688:TRP:HB3	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ASN:HD22	1:A:352:ALA:H	1.40	0.69
1:A:28:THR:HG21	3:A:1131:HOH:O	1.95	0.66
1:A:720:THR:HG23	3:A:884:HOH:O	1.97	0.63
1:A:660:ASN:HB3	1:A:663:ASN:ND2	2.13	0.63
1:A:639:SER:H	1:A:642:GLN:NE2	1.98	0.62
1:A:681:ILE:HD12	1:A:746:LEU:HD21	1.83	0.60
1:A:600:SER:HA	1:A:603:TRP:CD1	2.36	0.60
1:A:254:ASN:ND2	1:A:256:PHE:H	2.00	0.59
1:A:707:ARG:HA	1:A:747:LEU:HD12	1.84	0.59
1:A:130:LEU:H	1:A:231:GLN:HE22	1.49	0.58
1:A:572:SER:O	1:A:626:ARG:NH2	2.36	0.58
1:A:298:THR:CG2	1:A:300:GLU:H	2.17	0.57
1:A:95:GLY:HA2	1:A:148:THR:O	2.04	0.57
1:A:498:SER:HB3	1:A:499:PRO:HD2	1.86	0.57
1:A:190:THR:HG22	1:A:210:LYS:HD2	1.86	0.56
1:A:85:ASN:HD21	1:A:111:PHE:H	1.53	0.56
1:A:681:ILE:HD12	1:A:746:LEU:CD2	2.36	0.56
1:A:183:GLU:OE2	1:A:509:HIS:HD2	1.89	0.56
1:A:298:THR:HG22	1:A:300:GLU:N	2.19	0.56
1:A:5:MET:O	1:A:21:ARG:NH1	2.39	0.55
1:A:739:GLN:NE2	1:A:745:LEU:HB2	2.22	0.55
1:A:598:ASP:OD1	1:A:603:TRP:HZ3	1.91	0.54
1:A:168:THR:O	1:A:283:HIS:HD2	1.91	0.54
1:A:298:THR:HG21	1:A:326:TYR:OH	2.07	0.54
1:A:586:ARG:HD2	3:A:770:HOH:O	2.08	0.53
1:A:196:ILE:HG23	1:A:209:LEU:HD23	1.90	0.53
1:A:188:GLY:HA2	1:A:603:TRP:HB3	1.90	0.53
1:A:87:PRO:HD2	1:A:99:GLY:O	2.10	0.52
1:A:598:ASP:OD1	1:A:603:TRP:CZ3	2.62	0.52
1:A:298:THR:HG23	1:A:317:TRP:CZ3	2.44	0.52
1:A:318:ARG:HD3	1:A:322:ASN:OD1	2.10	0.51
1:A:85:ASN:HD21	1:A:111:PHE:N	2.09	0.50
1:A:127:GLN:O	1:A:156:PRO:HB3	2.12	0.49
1:A:53:GLY:O	1:A:56:VAL:HG22	2.13	0.49
1:A:159:VAL:HG11	1:A:268:ALA:HB1	1.95	0.49
1:A:192:GLN:CD	1:A:603:TRP:HD1	2.21	0.49
1:A:462:ASP:O	1:A:466:GLN:HG3	2.14	0.48
1:A:500:TRP:HA	1:A:574:GLY:HA2	1.95	0.47
1:A:83:GLY:HA3	1:A:111:PHE:CD2	2.50	0.47
1:A:203:THR:HA	1:A:262:TYR:O	2.15	0.47
1:A:489:SER:HA	1:A:637:TRP:CH2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:TYR:CD1	1:A:397:PRO:HA	2.50	0.47
1:A:438:ALA:HB3	1:A:443:SER:HB2	1.96	0.47
1:A:639:SER:H	1:A:642:GLN:HE21	1.62	0.47
1:A:131:ASN:HB2	1:A:132:PRO:CD	2.46	0.46
1:A:168:THR:O	1:A:283:HIS:CD2	2.68	0.46
1:A:392:SER:C	1:A:394:PRO:HD3	2.41	0.45
1:A:478:VAL:HG12	3:A:1019:HOH:O	2.16	0.45
1:A:661:THR:O	1:A:661:THR:HG23	2.17	0.45
1:A:529:TRP:CH2	1:A:599:SER:HB3	2.52	0.45
1:A:567:ALA:O	1:A:571:LEU:HB2	2.17	0.45
1:A:314:ILE:HG12	1:A:318:ARG:HG2	1.99	0.45
1:A:242:ASP:HB2	1:A:596:ASN:O	2.17	0.45
1:A:204:TYR:HB2	1:A:274:GLU:HG2	1.98	0.44
1:A:324:THR:HG23	1:A:349:ASN:ND2	2.32	0.44
1:A:32:LEU:O	1:A:46:THR:HA	2.17	0.44
1:A:141:ALA:HB2	1:A:304:TRP:CZ2	2.52	0.44
1:A:273:ALA:HA	1:A:276:GLN:HE21	1.83	0.44
1:A:38:GLY:HA2	1:A:157:LYS:HG3	1.99	0.44
1:A:86:TRP:CE3	1:A:100:PHE:HD1	2.36	0.44
1:A:257:SER:HA	1:A:258:PRO:HD3	1.87	0.44
1:A:672:GLY:HA3	1:A:679:ASN:O	2.18	0.44
1:A:110:ARG:HD2	1:A:318:ARG:HD2	1.99	0.43
1:A:294:VAL:HG22	3:A:1138:HOH:O	2.19	0.43
1:A:93:GLY:O	1:A:96:SER:HB3	2.17	0.43
1:A:30:ILE:HD12	1:A:57:TRP:CG	2.53	0.43
1:A:708:VAL:HB	1:A:746:LEU:HD13	2.01	0.42
1:A:648:PRO:HD2	3:A:893:HOH:O	2.19	0.42
1:A:168:THR:HB	1:A:279:VAL:CG2	2.49	0.42
1:A:581:GLY:HA2	1:A:584:TYR:CE2	2.54	0.42
1:A:61:VAL:HA	1:A:62:PRO:HD3	1.87	0.42
1:A:525:ASN:HB3	1:A:534:SER:O	2.19	0.42
1:A:359:SER:O	1:A:363:TRP:HD1	2.03	0.42
1:A:185:HIS:CE1	1:A:187:ARG:HB3	2.55	0.42
1:A:166:GLN:HB3	1:A:276:GLN:NE2	2.34	0.42
1:A:245:GLN:NE2	1:A:598:ASP:H	2.18	0.42
1:A:294:VAL:HG22	1:A:294:VAL:O	2.20	0.42
1:A:699:PRO:HA	1:A:705:TRP:CZ2	2.55	0.41
1:A:706:TYR:CZ	1:A:729:LEU:HD23	2.55	0.41
1:A:681:ILE:HG13	1:A:682:TYR:N	2.33	0.41

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	748/750 (100%)	716 (96%)	29 (4%)	3 (0%)	30 27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	536	GLY
1	A	316	SER
1	A	321	ASP

### 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	594/594 (100%)	570 (96%)	24 (4%)	28 27

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LEU
1	A	127	GLN
1	A	130	LEU
1	A	135	GLN
1	A	161	LEU
1	A	209	LEU
1	A	214	LEU
1	A	279	VAL

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Mol	Chain	Res	Type
1	A	294	VAL
1	A	298	THR
1	A	380	LEU
1	A	390	THR
1	A	517	VAL
1	A	556	VAL
1	A	571	LEU
1	A	588	LEU
1	A	603	TRP
1	A	661	THR
1	A	681	ILE
1	A	691	SER
1	A	720	THR
1	A	744	LEU
1	A	746	LEU
1	A	747	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	85	ASN
1	A	97	GLN
1	A	107	ASN
1	A	127	GLN
1	A	138	ASN
1	A	166	GLN
1	A	192	GLN
1	A	231	GLN
1	A	235	ASN
1	A	240	ASN
1	A	246	ASN
1	A	254	ASN
1	A	276	GLN
1	A	283	HIS
1	A	332	ASN
1	A	333	GLN
1	A	349	ASN
1	A	365	ASN
1	A	386	ASN
1	A	451	GLN
1	A	466	GLN

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Mol	Chain	Res	Type
1	A	480	GLN
1	A	483	ASN
1	A	509	HIS
1	A	527	GLN
1	A	558	GLN
1	A	589	GLN
1	A	614	ASN
1	A	620	GLN
1	A	642	GLN
1	A	659	ASN
1	A	686	ASN
1	A	739	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	750/750 (100%)	-0.92	0 <b>100</b> <b>100</b>	8, 16, 31, 49	0

There are no RSRZ outliers to report.

### 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	A	751	1/1	1.00	0.01	10,10,10,10	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.