



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2024 – 04:07 PM JST

PDB ID : 8Z10  
Title : Human beta-catenin crystal structure  
Authors : Tim, F.  
Deposited on : 2024-04-10  
Resolution : 2.35 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36.2  
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) : 2.36.2

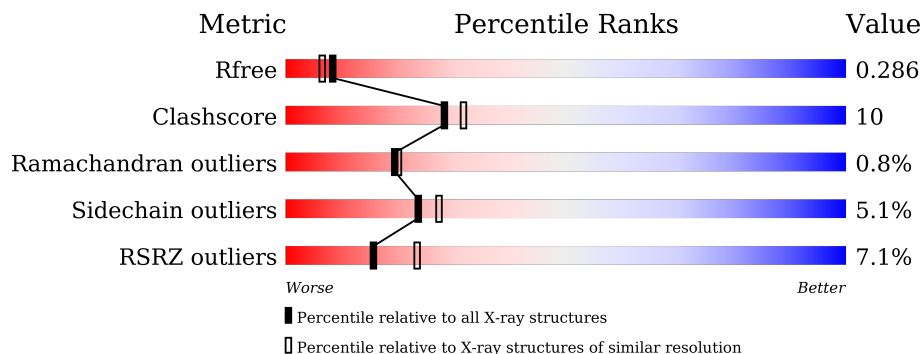
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	549	

## 2 Entry composition [i](#)

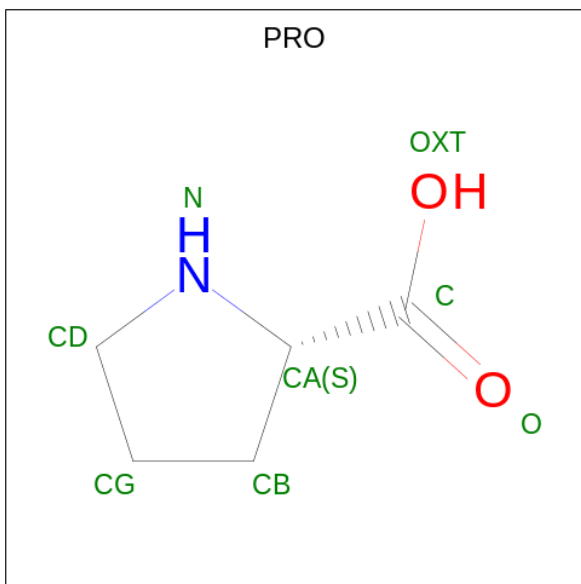
There are 2 unique types of molecules in this entry. The entry contains 3772 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catenin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	507	3756	2360	674	698	24	0	0	0

- Molecule 2 is PROLINE (three-letter code: PRO) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>2</sub>).

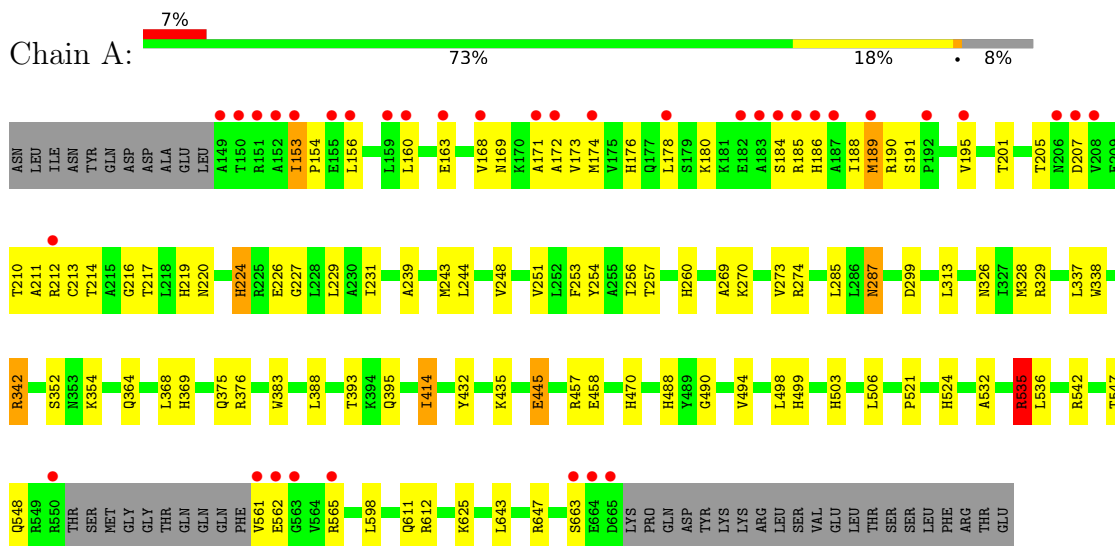


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	5	1	2	0	0
2	A	1	8	5	1	2	0	0

### 3 Residue-property plots

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: Catenin beta-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.95Å 103.05Å 185.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.37 – 2.35 39.62 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (6.37-2.35) 99.6 (39.62-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.34Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.218 , 0.275 0.227 , 0.286	Depositor DCC
$R_{free}$ test set	1317 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtrriage
Anisotropy	0.011	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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	0.73	1/3808 (0.0%)	0.83	5/5187 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	TRP	CD2-CE2	5.39	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	A	612	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	A	535	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	342	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	612	ARG	NE-CZ-NH2	5.18	122.89	120.30

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	3756	0	3792	74	0
2	A	16	0	14	1	0
All	All	3772	0	3806	74	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 10.

All (74) 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:178:LEU:HG	1:A:188:ILE:HD11	1.21	1.15
1:A:521:PRO:HA	1:A:524:HIS:CD2	1.81	1.14
1:A:207:ASP:HB3	1:A:210:THR:OG1	1.47	1.12
1:A:364:GLN:HE22	1:A:395:GLN:HE21	1.10	0.94
1:A:521:PRO:HA	1:A:524:HIS:NE2	1.82	0.94
1:A:414:ILE:HD12	1:A:414:ILE:H	1.36	0.90
1:A:364:GLN:HE22	1:A:395:GLN:NE2	1.80	0.80
1:A:328:MET:O	1:A:369:HIS:HE1	1.65	0.79
1:A:189:MET:HG2	1:A:189:MET:O	1.87	0.75
1:A:184:SER:O	1:A:188:ILE:HG13	1.88	0.72
1:A:521:PRO:CA	1:A:524:HIS:CD2	2.69	0.70
1:A:227:GLY:O	1:A:231:ILE:HD12	1.94	0.68
1:A:207:ASP:HB3	1:A:210:THR:HG1	1.60	0.67
1:A:153:ILE:HB	1:A:154:PRO:HD3	1.77	0.66
1:A:178:LEU:HG	1:A:188:ILE:CD1	2.12	0.64
1:A:253:PHE:O	1:A:257:THR:HG23	1.99	0.62
1:A:521:PRO:O	1:A:524:HIS:CD2	2.52	0.62
1:A:328:MET:O	1:A:369:HIS:CE1	2.51	0.60
1:A:458:GLU:HG2	1:A:506:LEU:HD22	1.83	0.60
1:A:178:LEU:CG	1:A:188:ILE:HD11	2.14	0.59
1:A:499:HIS:CE1	1:A:535:ARG:HD2	2.38	0.58
1:A:248:VAL:HG13	1:A:251:VAL:HB	1.84	0.58
1:A:160:LEU:HD21	1:A:172:ALA:N	2.19	0.57
1:A:611:GLN:NE2	1:A:643:LEU:HD21	2.22	0.55
1:A:414:ILE:H	1:A:414:ILE:CD1	2.07	0.55
1:A:163:GLU:O	1:A:163:GLU:HG2	2.05	0.54
1:A:260:HIS:HE1	1:A:299:ASP:OD2	1.91	0.54
1:A:160:LEU:HD21	1:A:171:ALA:C	2.28	0.54
1:A:176:HIS:CE1	1:A:180:LYS:HE3	2.43	0.54
1:A:499:HIS:NE2	1:A:535:ARG:HD2	2.24	0.53
1:A:498:LEU:HB3	1:A:535:ARG:HG2	1.92	0.52
1:A:364:GLN:NE2	1:A:395:GLN:HE21	1.93	0.51
1:A:160:LEU:HD23	1:A:168:VAL:O	2.11	0.51
1:A:213:CYS:O	1:A:217:THR:OG1	2.21	0.51
1:A:458:GLU:H	2:A:701:PRO:N	2.09	0.51
1:A:172:ALA:C	1:A:174:MET:H	2.14	0.50
1:A:521:PRO:O	1:A:524:HIS:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:SER:O	1:A:195:VAL:HG23	2.12	0.50
1:A:270:LYS:O	1:A:274:ARG:HG3	2.12	0.49
1:A:532:ALA:O	1:A:536:LEU:HG	2.14	0.48
1:A:561:VAL:HG12	1:A:562:GLU:N	2.29	0.48
1:A:216:GLY:HA2	1:A:254:TYR:CD1	2.49	0.47
1:A:287:ASN:HD22	1:A:287:ASN:H	1.63	0.47
1:A:458:GLU:OE2	1:A:503:HIS:HD2	1.98	0.47
1:A:445:GLU:HG3	1:A:488:HIS:CE1	2.49	0.46
1:A:163:GLU:N	1:A:163:GLU:OE1	2.47	0.46
1:A:338:TRP:CD1	1:A:376:ARG:HG3	2.51	0.46
1:A:287:ASN:HD22	1:A:287:ASN:N	2.14	0.46
1:A:326:ASN:ND2	1:A:329:ARG:HH21	2.13	0.46
1:A:224:HIS:C	1:A:226:GLU:H	2.19	0.46
1:A:354:LYS:HG3	1:A:388:LEU:HD23	1.98	0.45
1:A:185:ARG:HA	1:A:188:ILE:HD12	1.99	0.45
1:A:153:ILE:HB	1:A:154:PRO:CD	2.46	0.45
1:A:338:TRP:O	1:A:342:ARG:HG3	2.16	0.45
1:A:547:THR:HG22	1:A:548:GLN:NE2	2.33	0.44
1:A:211:ALA:O	1:A:212:ARG:C	2.55	0.44
1:A:156:LEU:CD2	1:A:174:MET:SD	3.06	0.43
1:A:239:ALA:O	1:A:243:MET:HG2	2.17	0.43
1:A:256:ILE:HD12	1:A:256:ILE:HA	1.80	0.43
1:A:435:LYS:HE2	1:A:470:HIS:O	2.17	0.43
1:A:445:GLU:CG	1:A:488:HIS:CE1	3.02	0.43
1:A:337:LEU:HA	1:A:337:LEU:HD23	1.83	0.43
1:A:547:THR:HG22	1:A:548:GLN:HE21	1.84	0.43
1:A:269:ALA:O	1:A:273:VAL:HG23	2.19	0.43
1:A:172:ALA:O	1:A:174:MET:N	2.48	0.42
1:A:207:ASP:HB3	1:A:210:THR:CB	2.45	0.42
1:A:224:HIS:C	1:A:226:GLU:N	2.71	0.42
1:A:432:TYR:HA	1:A:435:LYS:HD2	2.00	0.42
1:A:542:ARG:HD2	1:A:542:ARG:HA	1.76	0.42
1:A:244:LEU:HB3	1:A:285:LEU:HD11	2.03	0.41
1:A:201:THR:O	1:A:205:THR:HB	2.21	0.41
1:A:216:GLY:O	1:A:220:ASN:OD1	2.39	0.41
1:A:219:HIS:CB	1:A:254:TYR:HD1	2.34	0.40
1:A:490:GLY:O	1:A:494:VAL:HG23	2.22	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	503/549 (92%)	475 (94%)	24 (5%)	4 (1%)	19 20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	VAL
1	A	153	ILE
1	A	190	ARG
1	A	186	HIS

### 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	393/459 (86%)	373 (95%)	20 (5%)	24 27

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	189	MET
1	A	214	THR
1	A	224	HIS
1	A	229	LEU
1	A	287	ASN
1	A	313	LEU

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Mol	Chain	Res	Type
1	A	352	SER
1	A	368	LEU
1	A	375	GLN
1	A	393	THR
1	A	414	ILE
1	A	445	GLU
1	A	457	ARG
1	A	535	ARG
1	A	565	ARG
1	A	598	LEU
1	A	625	LYS
1	A	647	ARG
1	A	663	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	176	HIS
1	A	177	GLN
1	A	220	ASN
1	A	260	HIS
1	A	287	ASN
1	A	326	ASN
1	A	369	HIS
1	A	395	GLN
1	A	407	GLN
1	A	488	HIS
1	A	503	HIS
1	A	524	HIS
1	A	538	GLN
1	A	544	HIS
1	A	548	GLN
1	A	578	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PRO	A	702	-	8,8,8	0.84	0	10,10,10	1.57	3 (30%)
2	PRO	A	701	-	8,8,8	0.84	1 (12%)	10,10,10	1.66	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PRO	A	702	-	-	1/4/11/11	0/1/1/1
2	PRO	A	701	-	-	4/4/11/11	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PRO	OXT-C	-2.00	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	PRO	OXT-C-O	-3.56	116.00	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	702	PRO	OXT-C-O	-3.18	116.87	124.09
2	A	701	PRO	OXT-C-CA	2.56	121.91	113.40
2	A	702	PRO	OXT-C-CA	2.17	120.61	113.40
2	A	702	PRO	C-CA-N	2.07	114.88	106.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	PRO	O-C-CA-N
2	A	701	PRO	OXT-C-CA-N
2	A	701	PRO	O-C-CA-CB
2	A	701	PRO	OXT-C-CA-CB
2	A	702	PRO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	PRO	1	0

## 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	507/549 (92%)	0.25	36 (7%) <b>16</b> <b>23</b>	31, 48, 110, 148	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	LEU	6.9
1	A	160	LEU	6.7
1	A	178	LEU	6.4
1	A	149	ALA	5.6
1	A	155	GLU	5.5
1	A	152	ALA	5.4
1	A	159	LEU	5.3
1	A	174	MET	5.2
1	A	208	VAL	5.1
1	A	163	GLU	4.9
1	A	182	GLU	4.7
1	A	665	ASP	4.3
1	A	153	ILE	4.2
1	A	172	ALA	4.2
1	A	151	ARG	4.1
1	A	550	ARG	3.4
1	A	183	ALA	3.3
1	A	664	GLU	3.2
1	A	561	VAL	3.1
1	A	168	VAL	3.0
1	A	207	ASP	3.0
1	A	184	SER	3.0
1	A	192	PRO	2.9
1	A	195	VAL	2.8
1	A	206	ASN	2.8
1	A	185	ARG	2.7
1	A	150	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	187	ALA	2.5
1	A	563	GLY	2.5
1	A	171	ALA	2.4
1	A	562	GLU	2.2
1	A	189	MET	2.2
1	A	663	SER	2.2
1	A	212	ARG	2.1
1	A	565	ARG	2.1
1	A	186	HIS	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 monosaccharides 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	PRO	A	702	8/8	0.68	0.29	77,89,98,102	0
2	PRO	A	701	8/8	0.79	0.37	91,96,108,113	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.