



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:09 am BST

PDB ID : 1LGV  
Title : Structure of a Human Bence-Jones Dimer Crystallized in U.S. Space Shuttle Mission STS-95: 100K  
Authors : Terzyan, S.S.; DeWitt, C.R.; Ramsland, P.A.; Bourne, P.C.; Edmundson, A.B.  
Deposited on : 2002-04-16  
Resolution : 1.95 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.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

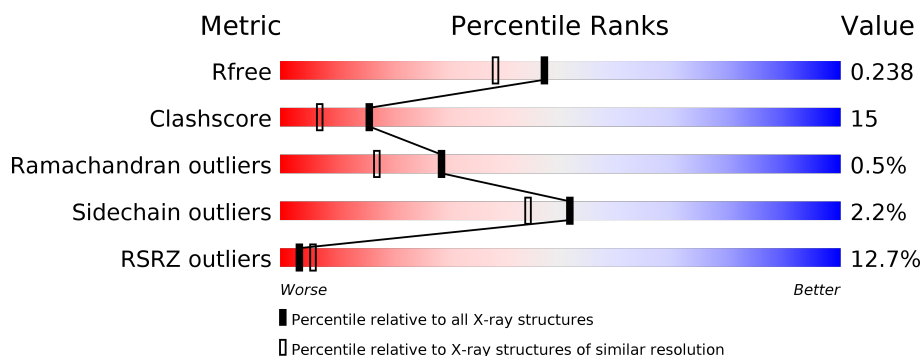
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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	216	<div> <div>10%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>..</div> </div> </div>
1	B	216	<div> <div>15%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3415 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 IMMUNOGLOBULIN LAMBDA LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1577	984	262	327	4			
1	B	214	Total	C	N	O	S	1	0	0
			1577	984	262	327	4			

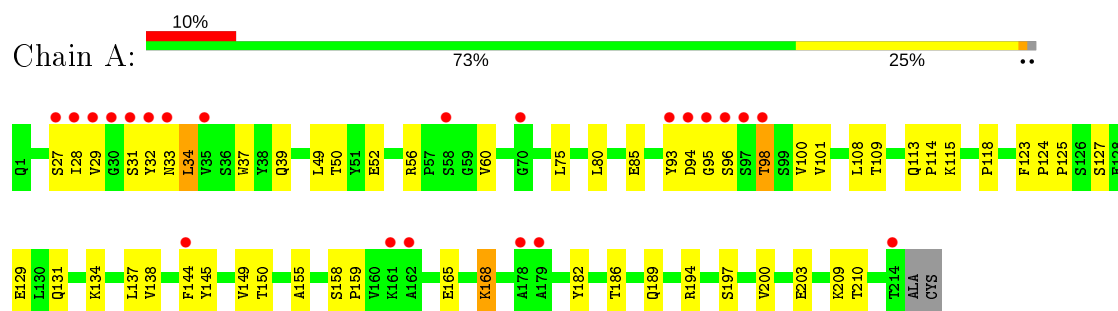
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	146	Total	O	0	0
			146	146		
2	B	115	Total	O	0	0
			115	115		

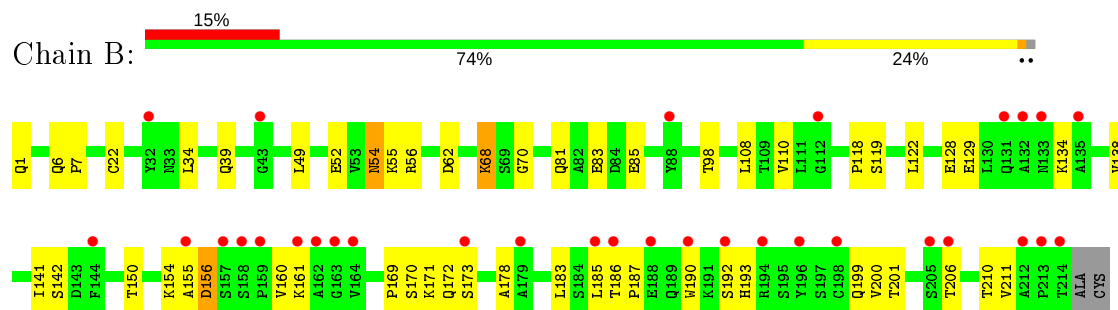
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: IMMUNOGLOBULIN LAMBDA LIGHT CHAIN



#### • Molecule 1: IMMUNOGLOBULIN LAMBDA LIGHT CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.34Å 83.25Å 112.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.95 15.96 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.7 (25.00-1.95) 94.9 (15.96-1.95)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 1.95Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.200 , 0.245 0.195 , 0.238	Depositor DCC
$R_{free}$ test set	2353 reflections (6.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% 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

### 5.1 Standard geometry

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

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	0.83	0/1606	0.93	2/2192 (0.1%)
1	B	0.69	0/1606	0.85	3/2192 (0.1%)
All	All	0.76	0/3212	0.89	5/4384 (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	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	22	CYS	CA-CB-SG	6.07	124.92	114.00
1	B	62	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	155	ALA	N-CA-C	-5.29	96.72	111.00
1	A	80	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	62	ASP	CB-CG-OD2	-5.06	113.75	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	TYR	Sidechain

## 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	1577	0	1535	59	0
1	B	1577	0	1535	38	0
2	A	146	0	0	1	0
2	B	115	0	0	5	0
All	All	3415	0	3070	91	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 15.

All (91) 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:B:122:LEU:HD23	1:B:211:VAL:HG13	1.61	0.81
1:A:29:VAL:HG22	1:A:95:GLY:CA	2.11	0.80
1:A:28:ILE:CG1	1:A:96:SER:HB3	2.13	0.79
1:A:28:ILE:HG13	1:A:96:SER:HB3	1.66	0.77
1:A:100:VAL:O	1:A:100:VAL:HG13	1.89	0.71
1:A:125:PRO:HD3	1:A:137:LEU:HD21	1.76	0.67
1:A:28:ILE:HB	1:A:96:SER:N	2.09	0.67
1:B:54:ASN:H	1:B:54:ASN:HD22	1.42	0.66
1:A:32:TYR:HB3	1:A:34:LEU:HG	1.77	0.65
1:A:125:PRO:HD3	1:A:137:LEU:CD2	2.29	0.62
1:B:155:ALA:O	1:B:156:ASP:HB2	2.00	0.61
1:A:32:TYR:CE1	1:A:93:TYR:CE2	2.89	0.59
1:A:123:PHE:HB2	1:A:138:VAL:HG13	1.85	0.59
1:A:29:VAL:HG22	1:A:95:GLY:C	2.24	0.58
1:B:129:GLU:HG2	1:B:134:LYS:O	2.03	0.58
1:A:29:VAL:HG22	1:A:95:GLY:O	2.03	0.58
1:B:150:THR:OG1	1:B:201:THR:HB	2.03	0.57
1:A:56:ARG:HD2	1:A:60:VAL:O	2.04	0.57
1:B:83:GLU:CD	1:B:83:GLU:H	2.08	0.56
1:B:6:GLN:HB2	1:B:7:PRO:HD2	1.87	0.56
1:A:123:PHE:CZ	1:B:138:VAL:HG23	2.40	0.56
1:B:183:LEU:HG	1:B:185:LEU:HD23	1.87	0.56
1:A:29:VAL:O	1:A:29:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:TYR:CE1	1:A:93:TYR:HE2	2.25	0.55
1:A:115:LYS:HE2	1:A:203:GLU:HG3	1.88	0.55
1:A:194:ARG:HG2	2:A:247:HOH:O	2.07	0.53
1:A:168:LYS:HD3	1:B:170:SER:OG	2.09	0.53
1:A:29:VAL:O	1:A:32:TYR:CE1	2.61	0.53
1:B:172:GLN:OE1	1:B:178:ALA:HB2	2.09	0.53
1:B:154:LYS:HD3	1:B:199:GLN:OE1	2.08	0.52
1:A:29:VAL:H	1:A:95:GLY:HA3	1.74	0.52
1:A:209:LYS:HD2	1:B:128:GLU:OE2	2.10	0.51
1:A:123:PHE:HB2	1:A:138:VAL:CG1	2.41	0.51
1:A:29:VAL:HG22	1:A:95:GLY:HA3	1.89	0.51
1:B:68:LYS:HE3	1:B:70:GLY:O	2.11	0.51
1:B:39:GLN:HB2	1:B:49:LEU:HD11	1.93	0.50
1:A:168:LYS:HD3	1:A:168:LYS:H	1.76	0.50
1:B:70:GLY:HA3	2:B:283:HOH:O	2.10	0.50
1:A:32:TYR:CD1	1:A:93:TYR:CD2	3.01	0.49
1:B:141:ILE:HG12	1:B:200:VAL:HG21	1.94	0.49
1:B:52:GLU:OE1	1:B:55:LYS:HE2	2.12	0.49
1:A:28:ILE:CB	1:A:96:SER:HB3	2.43	0.49
1:A:34:LEU:HD23	1:A:34:LEU:N	2.28	0.49
1:A:118:PRO:HB3	1:A:144:PHE:HB3	1.93	0.48
1:A:56:ARG:HG3	1:A:60:VAL:HB	1.94	0.48
1:B:81:GLN:O	1:B:110:VAL:HG21	2.14	0.48
1:A:129:GLU:OE2	1:A:134:LYS:HG3	2.12	0.48
1:B:187:PRO:O	1:B:190:TRP:HB3	2.14	0.47
1:A:186:THR:OG1	1:A:189:GLN:HG3	2.14	0.47
1:B:185:LEU:HD12	1:B:186:THR:O	2.15	0.47
1:A:33:ASN:C	1:A:34:LEU:HD23	2.35	0.47
1:A:149:VAL:HG21	1:A:200:VAL:HG13	1.97	0.47
1:B:54:ASN:N	1:B:54:ASN:HD22	2.07	0.47
1:A:85:GLU:HG3	1:A:109:THR:HA	1.97	0.46
1:B:156:ASP:HB3	2:B:326:HOH:O	2.16	0.46
1:B:206:THR:O	1:B:206:THR:HG23	2.15	0.46
1:A:49:LEU:O	1:A:50:THR:HG23	2.16	0.46
1:B:85:GLU:HG3	1:B:108:LEU:O	2.16	0.46
1:B:122:LEU:CD2	1:B:211:VAL:HG13	2.39	0.46
1:A:98:THR:HG23	1:A:98:THR:O	2.15	0.46
1:B:1:PCA:HA	2:B:318:HOH:O	2.16	0.46
1:B:119:SER:HB2	1:B:142:SER:OG	2.16	0.45
1:A:37:TRP:CD2	1:A:75:LEU:HB2	2.51	0.45
1:B:171:LYS:HD2	1:B:172:GLN:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:VAL:O	1:A:100:VAL:CG1	2.60	0.45
1:B:160:VAL:HG12	1:B:161:LYS:N	2.32	0.45
1:A:149:VAL:HG22	1:A:150:THR:N	2.31	0.45
1:B:156:ASP:OD2	1:B:193:HIS:CD2	2.70	0.45
1:A:94:ASP:HB2	1:A:101:VAL:HG23	1.98	0.45
1:A:165:GLU:OE2	1:B:173:SER:OG	2.34	0.45
1:B:169:PRO:HG2	2:B:311:HOH:O	2.16	0.44
1:B:201:THR:HA	1:B:206:THR:HA	2.00	0.44
1:A:124:PRO:HA	1:A:137:LEU:HD22	1.98	0.44
1:A:149:VAL:CG2	1:A:200:VAL:HG13	2.48	0.43
1:B:56:ARG:NE	2:B:321:HOH:O	2.29	0.43
1:A:165:GLU:HB2	1:A:182:TYR:CE1	2.54	0.43
1:A:39:GLN:HB2	1:A:49:LEU:HD11	2.00	0.43
1:A:129:GLU:HG2	1:A:134:LYS:CG	2.48	0.42
1:A:149:VAL:HG21	1:A:200:VAL:CG1	2.48	0.42
1:A:32:TYR:CD1	1:A:93:TYR:HD2	2.37	0.42
1:B:118:PRO:HB2	1:B:141:ILE:HG23	2.02	0.41
1:A:27:SER:HB2	1:A:32:TYR:HD1	1.85	0.41
1:A:49:LEU:O	1:A:50:THR:CG2	2.69	0.41
1:A:113:GLN:HB3	1:A:114:PRO:HD2	2.01	0.41
1:A:108:LEU:HD23	1:A:108:LEU:C	2.41	0.40
1:A:158:SER:HA	1:A:159:PRO:HD3	1.93	0.40
1:A:28:ILE:HB	1:A:96:SER:CA	2.52	0.40
1:A:127:SER:O	1:A:131:GLN:HG3	2.21	0.40
1:A:123:PHE:CZ	1:B:138:VAL:CG2	3.04	0.40
1:A:197:SER:OG	1:A:210:THR:HG23	2.22	0.40
1:A:52:GLU:HG3	1:B:98:THR:OG1	2.20	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	212/216 (98%)	206 (97%)	6 (3%)	0	100	100
1	B	212/216 (98%)	202 (95%)	8 (4%)	2 (1%)	17	8
All	All	424/432 (98%)	408 (96%)	14 (3%)	2 (0%)	29	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	ASP
1	B	192	SER

### 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	179/180 (99%)	175 (98%)	4 (2%)	52	44
1	B	179/180 (99%)	175 (98%)	4 (2%)	52	44
All	All	358/360 (99%)	350 (98%)	8 (2%)	52	44

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	34	LEU
1	A	98	THR
1	A	168	LYS
1	B	34	LEU
1	B	54	ASN
1	B	68	LYS
1	B	210	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	54	ASN

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Mol	Chain	Res	Type
1	B	131	GLN
1	B	193	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	PCA	B	1	1	7,8,9	2.50	4 (57%)	9,10,12	2.85	3 (33%)
1	PCA	A	1	1	7,8,9	2.73	3 (42%)	9,10,12	3.02	4 (44%)

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
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CB-CG	-4.98	1.41	1.53
1	B	1	PCA	CB-CG	-4.69	1.42	1.53
1	A	1	PCA	CA-N	3.52	1.50	1.46
1	B	1	PCA	OE-CD	2.67	1.28	1.23
1	B	1	PCA	CD-N	2.64	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	OE-CD	2.56	1.28	1.23
1	B	1	PCA	CG-CD	-2.14	1.44	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CB-CG-CD	7.36	116.26	104.40
1	B	1	PCA	CB-CG-CD	7.27	116.12	104.40
1	B	1	PCA	OE-CD-CG	3.30	132.52	126.76
1	A	1	PCA	CB-CA-C	-3.28	108.19	112.70
1	A	1	PCA	OE-CD-CG	3.18	132.32	126.76
1	B	1	PCA	CG-CD-N	-2.20	102.68	108.39
1	A	1	PCA	CG-CD-N	-2.12	102.91	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1	PCA	1	0

## 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	213/216 (98%)	0.72	22 (10%) 6 10	22, 39, 80, 101	4 (1%)
1	B	213/216 (98%)	0.78	32 (15%) 2 3	25, 52, 94, 105	2 (0%)
All	All	426/432 (98%)	0.75	54 (12%) 3 6	22, 43, 90, 105	6 (1%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	ILE	22.2
1	A	27	SER	16.2
1	A	29	VAL	15.5
1	A	96	SER	9.6
1	A	95	GLY	7.9
1	B	214	THR	7.5
1	A	98	THR	5.9
1	B	196	TYR	5.5
1	B	162	ALA	5.4
1	B	157	SER	5.2
1	A	93	TYR	4.8
1	A	31	SER	4.7
1	A	30	GLY	4.4
1	A	97	SER	4.4
1	A	32	TYR	4.4
1	B	32	TYR	4.1
1	B	161	LYS	3.8
1	B	163	GLY	3.8
1	A	161	LYS	3.7
1	A	214	THR	3.5
1	A	144	PHE	3.4
1	B	88	TYR	3.1
1	B	155	ALA	3.1
1	A	94	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	186	THR	3.0
1	B	135	ALA	2.9
1	B	159	PRO	2.9
1	B	131	GLN	2.8
1	B	173	SER	2.8
1	B	185	LEU	2.8
1	B	188	GLU	2.8
1	B	190	TRP	2.7
1	B	144	PHE	2.7
1	B	212	ALA	2.7
1	B	133	ASN	2.7
1	B	112	GLY	2.7
1	A	162	ALA	2.7
1	A	58	SER	2.6
1	B	158	SER	2.6
1	B	213	PRO	2.5
1	B	206	THR	2.5
1	A	35	VAL	2.4
1	B	164	VAL	2.4
1	B	205	SER	2.3
1	A	179	ALA	2.3
1	A	178	ALA	2.2
1	B	179	ALA	2.2
1	A	70	GLY	2.2
1	B	194	ARG	2.2
1	B	132	ALA	2.2
1	B	43	GLY	2.2
1	A	33	ASN	2.1
1	B	198	CYS	2.1
1	B	192	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	PCA	B	1	8/9	0.66	0.35	76,85,87,90	0
1	PCA	A	1	8/9	0.94	0.12	35,41,46,47	0

### 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.