



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:13 PM GMT

PDB ID : 4YGA  
Title : CDPK1, from *Toxoplasma gondii*, bound to inhibitory VHH-1B7  
Authors : Knockenhauer, K.E.; Schwartz, T.U.  
Deposited on : 2015-02-26  
Resolution : 2.94 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

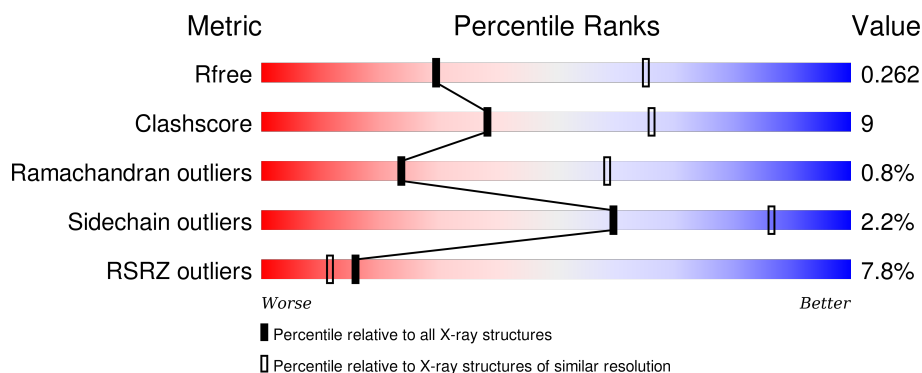
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.94 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	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (2.98-2.90)

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	516	 6% 69% 16% • 13%
1	C	516	 8% 70% 16% • 13%
1	E	516	 7% 70% 15% • 14%
1	G	516	 6% 67% 19% • 13%
2	B	141	 15% 70% 18% • 12%

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Mol	Chain	Length	Quality of chain
2	D	141	<div><div><div></div><div></div><div></div></div><div><div>7%</div><div>64%</div><div>23%</div><div>•</div><div>13%</div></div></div>
2	F	141	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>67%</div><div>20%</div><div>•</div><div>13%</div></div></div>
2	H	141	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>56%</div><div>30%</div><div>•</div><div>13%</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17348 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 Calmodulin-domain protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3419	2177	559	667	16			
1	C	449	Total	C	N	O	S	0	0	0
			3404	2170	553	664	17			
1	E	442	Total	C	N	O	S	0	0	0
			3395	2163	560	656	16			
1	G	447	Total	C	N	O	S	0	0	0
			3409	2170	558	664	17			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q9BJF5
A	508	LEU	-	expression tag	UNP Q9BJF5
A	509	GLU	-	expression tag	UNP Q9BJF5
A	510	HIS	-	expression tag	UNP Q9BJF5
A	511	HIS	-	expression tag	UNP Q9BJF5
A	512	HIS	-	expression tag	UNP Q9BJF5
A	513	HIS	-	expression tag	UNP Q9BJF5
A	514	HIS	-	expression tag	UNP Q9BJF5
A	515	HIS	-	expression tag	UNP Q9BJF5
C	0	MET	-	initiating methionine	UNP Q9BJF5
C	508	LEU	-	expression tag	UNP Q9BJF5
C	509	GLU	-	expression tag	UNP Q9BJF5
C	510	HIS	-	expression tag	UNP Q9BJF5
C	511	HIS	-	expression tag	UNP Q9BJF5
C	512	HIS	-	expression tag	UNP Q9BJF5
C	513	HIS	-	expression tag	UNP Q9BJF5
C	514	HIS	-	expression tag	UNP Q9BJF5
C	515	HIS	-	expression tag	UNP Q9BJF5
E	0	MET	-	initiating methionine	UNP Q9BJF5
E	508	LEU	-	expression tag	UNP Q9BJF5
E	509	GLU	-	expression tag	UNP Q9BJF5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	510	HIS	-	expression tag	UNP Q9BJF5
E	511	HIS	-	expression tag	UNP Q9BJF5
E	512	HIS	-	expression tag	UNP Q9BJF5
E	513	HIS	-	expression tag	UNP Q9BJF5
E	514	HIS	-	expression tag	UNP Q9BJF5
E	515	HIS	-	expression tag	UNP Q9BJF5
G	0	MET	-	initiating methionine	UNP Q9BJF5
G	508	LEU	-	expression tag	UNP Q9BJF5
G	509	GLU	-	expression tag	UNP Q9BJF5
G	510	HIS	-	expression tag	UNP Q9BJF5
G	511	HIS	-	expression tag	UNP Q9BJF5
G	512	HIS	-	expression tag	UNP Q9BJF5
G	513	HIS	-	expression tag	UNP Q9BJF5
G	514	HIS	-	expression tag	UNP Q9BJF5
G	515	HIS	-	expression tag	UNP Q9BJF5

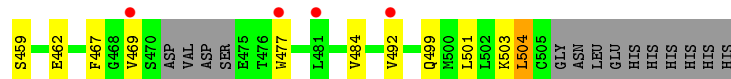
- Molecule 2 is a protein called VHH-1B7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	124	Total	C	N	O	S	0	0	0
			924	573	160	186	5			
2	D	123	Total	C	N	O	S	0	0	0
			932	581	163	183	5			
2	F	123	Total	C	N	O	S	0	0	0
			925	573	162	185	5			
2	H	123	Total	C	N	O	S	0	0	0
			924	576	162	181	5			

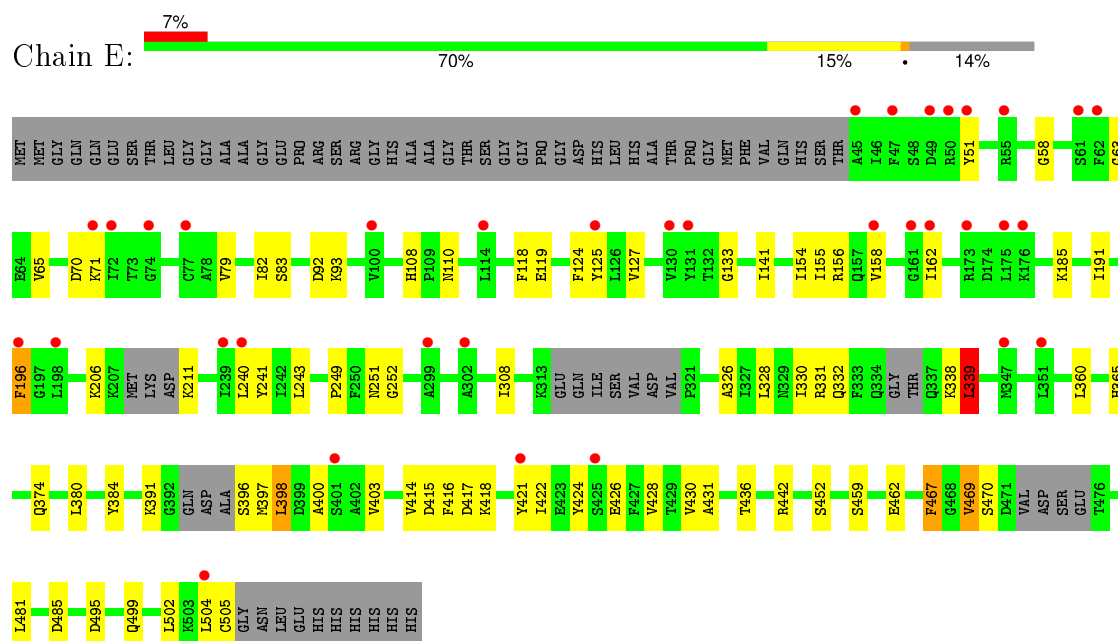
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	4	Total	Ca	0	0
			4	4		
3	A	4	Total	Ca	0	0
			4	4		
3	C	4	Total	Ca	0	0
			4	4		
3	E	4	Total	Ca	0	0
			4	4		

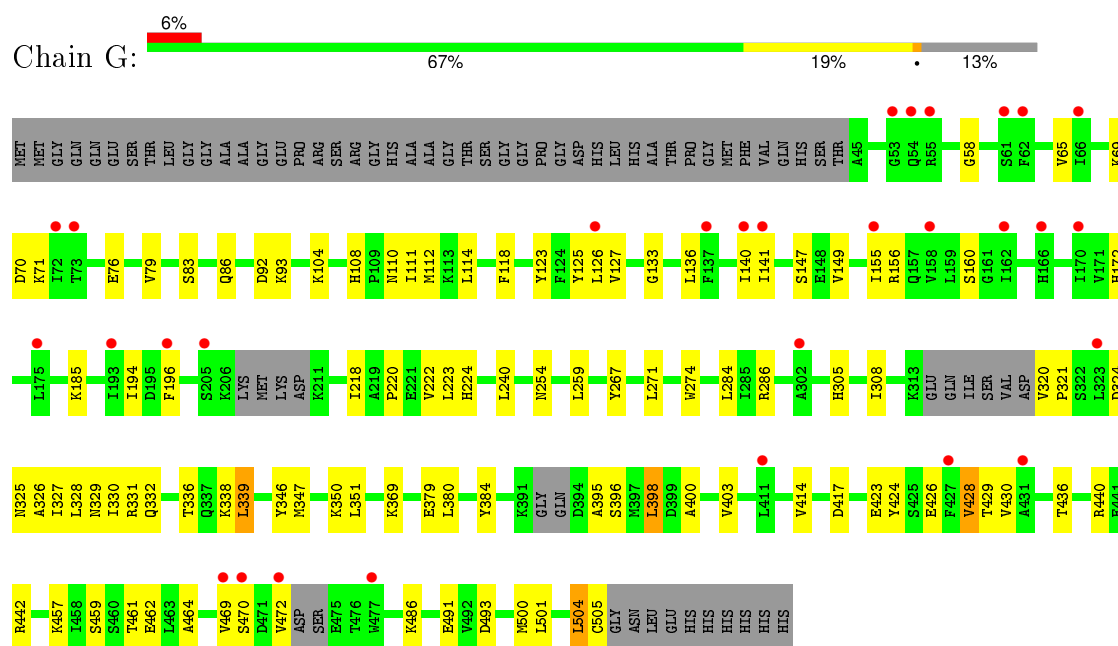




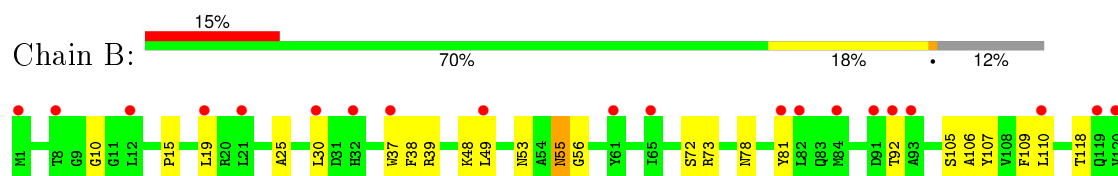
• Molecule 1: Calmodulin-domain protein kinase 1

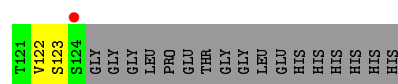


• Molecule 1: Calmodulin-domain protein kinase 1

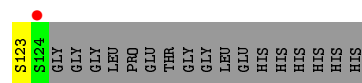
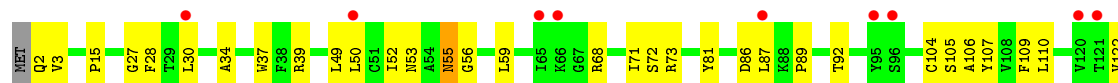


• Molecule 2: VHH-1B7

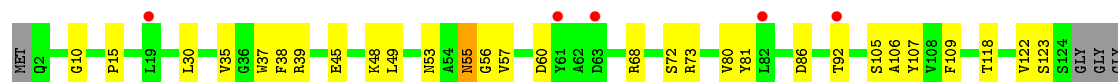




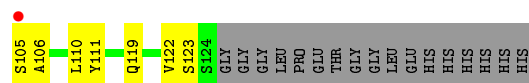
• Molecule 2: VHH-1B7



• Molecule 2: VHH-1B7



• Molecule 2: VHH-1B7





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.92Å 91.07Å 106.64Å 88.71° 108.27° 90.26°	Depositor
Resolution (Å)	70.67 – 2.94 70.67 – 2.94	Depositor EDS
% Data completeness (in resolution range)	92.3 (70.67-2.94) 88.9 (70.67-2.94)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.226 , 0.262 0.226 , 0.262	Depositor DCC
$R_{free}$ test set	1715 reflections (3.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.0	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 101.6	EDS
Estimated twinning fraction	0.287 for -h,k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53984 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17348	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% 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 ⓘ

### 5.1 Standard geometry ⓘ

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	0.23	0/3476	0.42	0/4702
1	C	0.23	0/3460	0.44	1/4682 (0.0%)
1	E	0.24	0/3449	0.46	2/4657 (0.0%)
1	G	0.23	0/3465	0.43	1/4689 (0.0%)
2	B	0.24	0/941	0.43	0/1279
2	D	0.23	0/949	0.46	0/1287
2	F	0.24	0/942	0.44	0/1279
2	H	0.24	0/941	0.47	0/1278
All	All	0.24	0/17623	0.44	4/23853 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	398	LEU	CA-CB-CG	6.25	129.67	115.30
1	C	398	LEU	CA-CB-CG	6.00	129.09	115.30
1	E	339	LEU	CA-CB-CG	5.83	128.72	115.30
1	G	339	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3419	0	3233	57	0
1	C	3404	0	3200	58	0
1	E	3395	0	3238	47	0
1	G	3409	0	3214	68	0
2	B	924	0	853	15	0
2	D	932	0	886	24	0
2	F	925	0	859	17	0
2	H	924	0	871	29	0
3	A	4	0	0	0	0
3	C	4	0	0	0	0
3	E	4	0	0	0	0
3	G	4	0	0	0	0
All	All	17348	0	16354	305	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 9.

The worst 5 of 305 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:467:PHE:HB2	2:B:109:PHE:HB2	1.42	0.99
1:C:332:GLN:HE22	1:C:504:LEU:H	1.30	0.79
1:C:155:ILE:HG13	1:C:240:LEU:HD13	1.68	0.76
2:H:30:LEU:O	2:H:73:ARG:NH2	2.19	0.74
1:E:467:PHE:HB2	2:F:109:PHE:HB2	1.68	0.74

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	440/516 (85%)	416 (94%)	19 (4%)	5 (1%)	17 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	439/516 (85%)	420 (96%)	16 (4%)	3 (1%)	26	62
1	E	430/516 (83%)	415 (96%)	14 (3%)	1 (0%)	52	83
1	G	437/516 (85%)	416 (95%)	18 (4%)	3 (1%)	26	62
2	B	122/141 (86%)	114 (93%)	7 (6%)	1 (1%)	24	58
2	D	121/141 (86%)	112 (93%)	8 (7%)	1 (1%)	24	58
2	F	121/141 (86%)	114 (94%)	5 (4%)	2 (2%)	11	37
2	H	121/141 (86%)	110 (91%)	9 (7%)	2 (2%)	11	37
All	All	2231/2628 (85%)	2117 (95%)	96 (4%)	18 (1%)	24	58

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
1	A	336	THR
1	A	337	GLN
1	A	473	ASP
1	C	503	LYS

### 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	350/448 (78%)	345 (99%)	5 (1%)	74	92
1	C	345/448 (77%)	337 (98%)	8 (2%)	58	86
1	E	349/448 (78%)	340 (97%)	9 (3%)	54	84
1	G	348/448 (78%)	342 (98%)	6 (2%)	68	90
2	B	96/116 (83%)	93 (97%)	3 (3%)	47	81
2	D	99/116 (85%)	97 (98%)	2 (2%)	63	87
2	F	97/116 (84%)	94 (97%)	3 (3%)	47	81
2	H	97/116 (84%)	93 (96%)	4 (4%)	37	72
All	All	1781/2256 (79%)	1741 (98%)	40 (2%)	60	86

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	83	SER
1	E	365	HIS
2	H	19	LEU
1	E	328	LEU
1	E	398	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	332	GLN
2	H	55	ASN
2	D	55	ASN
2	B	55	ASN
2	F	55	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 are 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 ⓘ

### 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	448/516 (86%)	0.32	30 (6%) 21 16	60, 107, 192, 296	1 (0%)
1	C	449/516 (87%)	0.45	43 (9%) 10 7	59, 104, 198, 345	1 (0%)
1	E	442/516 (85%)	0.41	35 (7%) 15 11	59, 106, 185, 287	1 (0%)
1	G	447/516 (86%)	0.33	30 (6%) 21 16	60, 104, 182, 289	1 (0%)
2	B	124/141 (87%)	0.72	21 (16%) 2 1	65, 102, 171, 199	0
2	D	123/141 (87%)	0.50	10 (8%) 15 10	64, 109, 192, 251	0
2	F	123/141 (87%)	0.33	5 (4%) 41 37	65, 88, 184, 267	0
2	H	123/141 (87%)	0.29	4 (3%) 50 45	62, 99, 159, 219	0
All	All	2279/2628 (86%)	0.40	178 (7%) 16 11	59, 105, 189, 345	4 (0%)

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	72	ILE	12.7
1	C	73	THR	7.7
1	E	72	ILE	7.6
1	A	72	ILE	7.4
1	C	131	TYR	7.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	E	604	1/1	0.98	0.23	1.83	82,82,82,82	0
3	CA	A	601	1/1	0.99	0.20	0.98	80,80,80,80	0
3	CA	G	603	1/1	0.96	0.20	0.67	79,79,79,79	0
3	CA	C	603	1/1	0.90	0.18	0.13	89,89,89,89	0
3	CA	A	602	1/1	0.99	0.21	0.06	81,81,81,81	0
3	CA	E	601	1/1	0.98	0.18	0.00	79,79,79,79	0
3	CA	E	603	1/1	0.91	0.17	-0.07	80,80,80,80	0
3	CA	G	602	1/1	0.97	0.20	-0.08	75,75,75,75	0
3	CA	G	604	1/1	0.91	0.15	-0.21	90,90,90,90	0
3	CA	A	604	1/1	0.96	0.15	-0.27	94,94,94,94	0
3	CA	G	601	1/1	0.98	0.15	-0.35	100,100,100,100	0
3	CA	E	602	1/1	0.98	0.17	-0.43	75,75,75,75	0
3	CA	C	601	1/1	0.82	0.14	-0.47	96,96,96,96	0
3	CA	C	604	1/1	0.97	0.12	-0.89	82,82,82,82	0
3	CA	C	602	1/1	0.98	0.13	-1.13	81,81,81,81	0
3	CA	A	603	1/1	0.96	0.11	-1.22	80,80,80,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.