



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:50 am BST

PDB ID : 4I2Y  
Title : Crystal Structure of the genetically encoded calcium indicator RGECO1  
Authors : Akerboom, J.; Looger, L.L.; Schreiter, E.R.  
Deposited on : 2012-11-23  
Resolution : 2.20 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

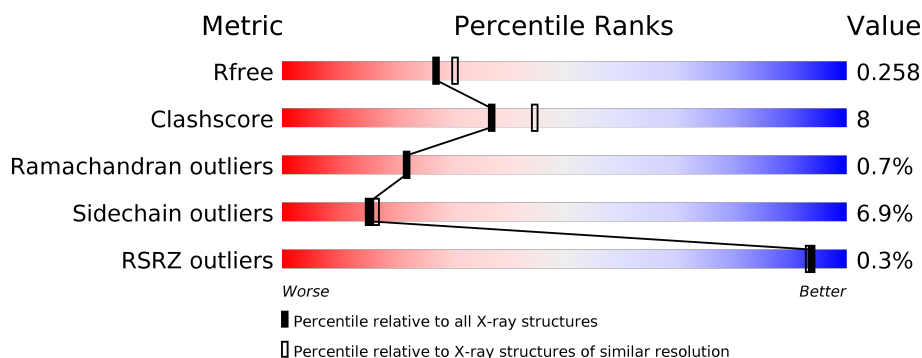
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	419	
1	B	419	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6199 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 RGECO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3060	1929	519	595	17			
1	B	379	Total	C	N	O	S	0	0	0
			3032	1911	512	592	17			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	EXPRESSION TAG	UNP Q6LDG3
A	32	HIS	-	EXPRESSION TAG	UNP Q6LDG3
A	33	HIS	-	EXPRESSION TAG	UNP Q6LDG3
A	34	HIS	-	EXPRESSION TAG	UNP Q6LDG3
A	35	HIS	-	EXPRESSION TAG	UNP Q6LDG3
A	36	HIS	-	EXPRESSION TAG	UNP Q6LDG3
A	37	HIS	-	EXPRESSION TAG	UNP Q6LDG3
A	38	SER	-	EXPRESSION TAG	UNP Q6LDG3
A	39	SER	-	EXPRESSION TAG	UNP Q6LDG3
A	44	ASN	GLN	ENGINEERED MUTATION	UNP Q6LDG3
A	46	ALA	THR	ENGINEERED MUTATION	UNP Q6LDG3
A	59	PRO	-	LINKER	UNP Q9U6Y8
A	60	VAL	-	LINKER	UNP Q9U6Y8
A	61	VAL	-	LINKER	UNP Q9U6Y8
A	62	SER	THR	ENGINEERED MUTATION	UNP Q9U6Y8
A	65	MET	LEU	ENGINEERED MUTATION	UNP Q9U6Y8
A	68	GLU	ARG	ENGINEERED MUTATION	UNP Q9U6Y8
A	71	ALA	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
A	74	SER	GLY	ENGINEERED MUTATION	UNP Q9U6Y8
A	77	LYS	HIS	ENGINEERED MUTATION	UNP Q9U6Y8
A	79	GLY	ALA	ENGINEERED MUTATION	UNP Q9U6Y8
A	81	ARG	LYS	ENGINEERED MUTATION	UNP Q9U6Y8
A	89	ALA	LEU	ENGINEERED MUTATION	UNP Q9U6Y8
A	90	ALA	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
A	92	VAL	PHE	ENGINEERED MUTATION	UNP Q9U6Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	94	THR	SER	ENGINEERED MUTATION	UNP Q9U6Y8
A	95	THR	ILE	ENGINEERED MUTATION	UNP Q9U6Y8
A	97	LYS	MET	ENGINEERED MUTATION	UNP Q9U6Y8
A	107	ALA	TYR	ENGINEERED MUTATION	UNP Q9U6Y8
A	109	ILE	TYR	ENGINEERED MUTATION	UNP Q9U6Y8
A	112	ILE	SER	ENGINEERED MUTATION	UNP Q9U6Y8
A	117	VAL	THR	ENGINEERED MUTATION	UNP Q9U6Y8
A	129	CYS	TYR	ENGINEERED MUTATION	UNP Q9U6Y8
A	132	ALA	THR	ENGINEERED MUTATION	UNP Q9U6Y8
A	137	SER	-	LINKER	UNP Q9U6Y8
A	138	THR	-	LINKER	UNP Q9U6Y8
A	139	GLY	-	LINKER	UNP Q9U6Y8
A	140	GLY	-	LINKER	UNP Q9U6Y8
A	141	MET	-	LINKER	UNP Q9U6Y8
A	142	ASP	-	LINKER	UNP Q9U6Y8
A	143	GLU	-	LINKER	UNP Q9U6Y8
A	144	LEU	-	LINKER	UNP Q9U6Y8
A	145	TYR	-	LINKER	UNP Q9U6Y8
A	146	LYS	-	LINKER	UNP Q9U6Y8
A	147	GLY	-	LINKER	UNP Q9U6Y8
A	148	GLY	-	LINKER	UNP Q9U6Y8
A	149	THR	-	LINKER	UNP Q9U6Y8
A	150	GLY	-	LINKER	UNP Q9U6Y8
A	151	GLY	-	LINKER	UNP Q9U6Y8
A	152	SER	-	LINKER	UNP Q9U6Y8
A	153	LEU	-	LINKER	UNP Q9U6Y8
A	154	VAL	-	LINKER	UNP Q9U6Y8
A	155	SER	-	LINKER	UNP Q9U6Y8
A	156	LYS	-	LINKER	UNP Q9U6Y8
A	157	GLY	-	LINKER	UNP Q9U6Y8
A	158	GLU	-	LINKER	UNP Q9U6Y8
A	159	GLU	-	LINKER	UNP Q9U6Y8
A	160	ASP	-	LINKER	UNP Q9U6Y8
A	161	ASN	-	LINKER	UNP Q9U6Y8
A	162	MET	-	LINKER	UNP Q9U6Y8
A	163	ALA	-	LINKER	UNP Q9U6Y8
A	164	ILE	-	LINKER	UNP Q9U6Y8
A	174	HIS	ARG	ENGINEERED MUTATION	UNP Q9U6Y8
A	178	SER	THR	ENGINEERED MUTATION	UNP Q9U6Y8
A	197	ALA	GLY	ENGINEERED MUTATION	UNP Q9U6Y8
A	198	PHE	HIS	ENGINEERED MUTATION	UNP Q9U6Y8
A	199	GLN	ASN	ENGINEERED MUTATION	UNP Q9U6Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	201	ALA	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
A	224	NRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
A	224	NRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
A	224	NRQ	GLY	CHROMOPHORE	UNP Q9U6Y8
A	228	ALA	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
A	230	ILE	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
A	240	PHE	LYS	ENGINEERED MUTATION	UNP Q9U6Y8
A	249	ARG	LYS	ENGINEERED MUTATION	UNP Q9U6Y8
A	261	ILE	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
A	262	ILE	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
A	263	HIS	THR	ENGINEERED MUTATION	UNP Q9U6Y8
A	265	ASN	THR	ENGINEERED MUTATION	UNP Q9U6Y8
A	274	VAL	CYS	ENGINEERED MUTATION	UNP Q9U6Y8
A	281	LEU	PHE	ENGINEERED MUTATION	UNP Q9U6Y8
A	282	ARG	ILE	ENGINEERED MUTATION	UNP Q9U6Y8
A	284	THR	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
A	288	PRO	SER	ENGINEERED MUTATION	UNP Q9U6Y8
A	303	THR	-	LINKER	UNP P62161
A	304	ARG	-	LINKER	UNP P62161
A	363	ASP	ASN	ENGINEERED MUTATION	UNP P62161
A	366	PHE	ILE	ENGINEERED MUTATION	UNP P62161
A	380	ASN	LYS	ENGINEERED MUTATION	UNP P62161
A	404	GLY	SER	ENGINEERED MUTATION	UNP P62161
A	414	ASP	ASN	ENGINEERED MUTATION	UNP P62161
A	430	VAL	GLU	ENGINEERED MUTATION	UNP P62161
B	31	MET	-	EXPRESSION TAG	UNP Q6LDG3
B	32	HIS	-	EXPRESSION TAG	UNP Q6LDG3
B	33	HIS	-	EXPRESSION TAG	UNP Q6LDG3
B	34	HIS	-	EXPRESSION TAG	UNP Q6LDG3
B	35	HIS	-	EXPRESSION TAG	UNP Q6LDG3
B	36	HIS	-	EXPRESSION TAG	UNP Q6LDG3
B	37	HIS	-	EXPRESSION TAG	UNP Q6LDG3
B	38	SER	-	EXPRESSION TAG	UNP Q6LDG3
B	39	SER	-	EXPRESSION TAG	UNP Q6LDG3
B	44	ASN	GLN	ENGINEERED MUTATION	UNP Q6LDG3
B	46	ALA	THR	ENGINEERED MUTATION	UNP Q6LDG3
B	59	PRO	-	LINKER	UNP Q9U6Y8
B	60	VAL	-	LINKER	UNP Q9U6Y8
B	61	VAL	-	LINKER	UNP Q9U6Y8
B	62	SER	THR	ENGINEERED MUTATION	UNP Q9U6Y8
B	65	MET	LEU	ENGINEERED MUTATION	UNP Q9U6Y8
B	68	GLU	ARG	ENGINEERED MUTATION	UNP Q9U6Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	71	ALA	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
B	74	SER	GLY	ENGINEERED MUTATION	UNP Q9U6Y8
B	77	LYS	HIS	ENGINEERED MUTATION	UNP Q9U6Y8
B	79	GLY	ALA	ENGINEERED MUTATION	UNP Q9U6Y8
B	81	ARG	LYS	ENGINEERED MUTATION	UNP Q9U6Y8
B	89	ALA	LEU	ENGINEERED MUTATION	UNP Q9U6Y8
B	90	ALA	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
B	92	VAL	PHE	ENGINEERED MUTATION	UNP Q9U6Y8
B	94	THR	SER	ENGINEERED MUTATION	UNP Q9U6Y8
B	95	THR	ILE	ENGINEERED MUTATION	UNP Q9U6Y8
B	97	LYS	MET	ENGINEERED MUTATION	UNP Q9U6Y8
B	107	ALA	TYR	ENGINEERED MUTATION	UNP Q9U6Y8
B	109	ILE	TYR	ENGINEERED MUTATION	UNP Q9U6Y8
B	112	ILE	SER	ENGINEERED MUTATION	UNP Q9U6Y8
B	117	VAL	THR	ENGINEERED MUTATION	UNP Q9U6Y8
B	129	CYS	TYR	ENGINEERED MUTATION	UNP Q9U6Y8
B	132	ALA	THR	ENGINEERED MUTATION	UNP Q9U6Y8
B	137	SER	-	LINKER	UNP Q9U6Y8
B	138	THR	-	LINKER	UNP Q9U6Y8
B	139	GLY	-	LINKER	UNP Q9U6Y8
B	140	GLY	-	LINKER	UNP Q9U6Y8
B	141	MET	-	LINKER	UNP Q9U6Y8
B	142	ASP	-	LINKER	UNP Q9U6Y8
B	143	GLU	-	LINKER	UNP Q9U6Y8
B	144	LEU	-	LINKER	UNP Q9U6Y8
B	145	TYR	-	LINKER	UNP Q9U6Y8
B	146	LYS	-	LINKER	UNP Q9U6Y8
B	147	GLY	-	LINKER	UNP Q9U6Y8
B	148	GLY	-	LINKER	UNP Q9U6Y8
B	149	THR	-	LINKER	UNP Q9U6Y8
B	150	GLY	-	LINKER	UNP Q9U6Y8
B	151	GLY	-	LINKER	UNP Q9U6Y8
B	152	SER	-	LINKER	UNP Q9U6Y8
B	153	LEU	-	LINKER	UNP Q9U6Y8
B	154	VAL	-	LINKER	UNP Q9U6Y8
B	155	SER	-	LINKER	UNP Q9U6Y8
B	156	LYS	-	LINKER	UNP Q9U6Y8
B	157	GLY	-	LINKER	UNP Q9U6Y8
B	158	GLU	-	LINKER	UNP Q9U6Y8
B	159	GLU	-	LINKER	UNP Q9U6Y8
B	160	ASP	-	LINKER	UNP Q9U6Y8
B	161	ASN	-	LINKER	UNP Q9U6Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	162	MET	-	LINKER	UNP Q9U6Y8
B	163	ALA	-	LINKER	UNP Q9U6Y8
B	164	ILE	-	LINKER	UNP Q9U6Y8
B	174	HIS	ARG	ENGINEERED MUTATION	UNP Q9U6Y8
B	178	SER	THR	ENGINEERED MUTATION	UNP Q9U6Y8
B	197	ALA	GLY	ENGINEERED MUTATION	UNP Q9U6Y8
B	198	PHE	HIS	ENGINEERED MUTATION	UNP Q9U6Y8
B	199	GLN	ASN	ENGINEERED MUTATION	UNP Q9U6Y8
B	201	ALA	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
B	224	NRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
B	224	NRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
B	224	NRQ	GLY	CHROMOPHORE	UNP Q9U6Y8
B	228	ALA	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
B	230	ILE	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
B	240	PHE	LYS	ENGINEERED MUTATION	UNP Q9U6Y8
B	249	ARG	LYS	ENGINEERED MUTATION	UNP Q9U6Y8
B	261	ILE	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
B	262	ILE	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
B	263	HIS	THR	ENGINEERED MUTATION	UNP Q9U6Y8
B	265	ASN	THR	ENGINEERED MUTATION	UNP Q9U6Y8
B	274	VAL	CYS	ENGINEERED MUTATION	UNP Q9U6Y8
B	281	LEU	PHE	ENGINEERED MUTATION	UNP Q9U6Y8
B	282	ARG	ILE	ENGINEERED MUTATION	UNP Q9U6Y8
B	284	THR	VAL	ENGINEERED MUTATION	UNP Q9U6Y8
B	288	PRO	SER	ENGINEERED MUTATION	UNP Q9U6Y8
B	303	THR	-	LINKER	UNP P62161
B	304	ARG	-	LINKER	UNP P62161
B	363	ASP	ASN	ENGINEERED MUTATION	UNP P62161
B	366	PHE	ILE	ENGINEERED MUTATION	UNP P62161
B	380	ASN	LYS	ENGINEERED MUTATION	UNP P62161
B	404	GLY	SER	ENGINEERED MUTATION	UNP P62161
B	414	ASP	ASN	ENGINEERED MUTATION	UNP P62161
B	430	VAL	GLU	ENGINEERED MUTATION	UNP P62161

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	4	Total Ca 4 4	0	0
2	A	4	Total Ca 4 4	0	0

- Molecule 3 is water.

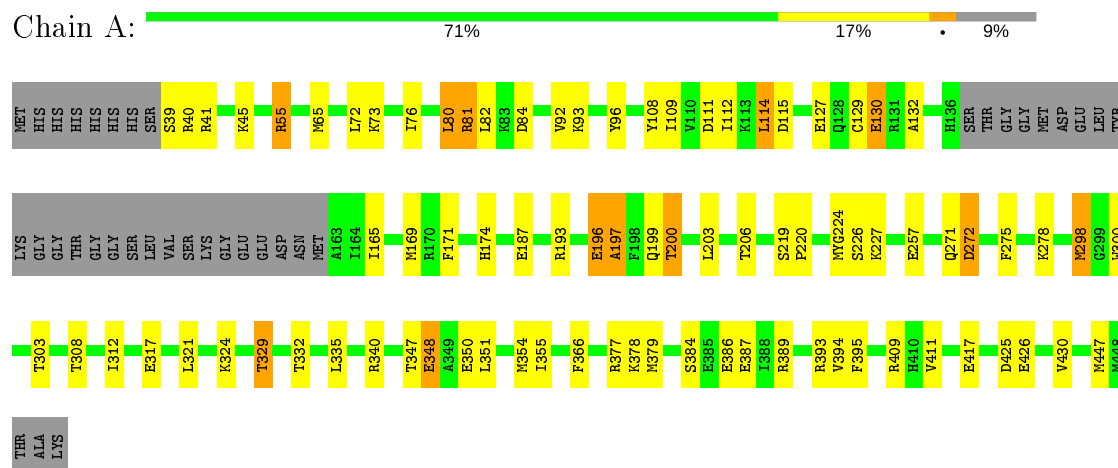
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total 65	O 65	0	0
3	B	34	Total 34	O 34	0	0



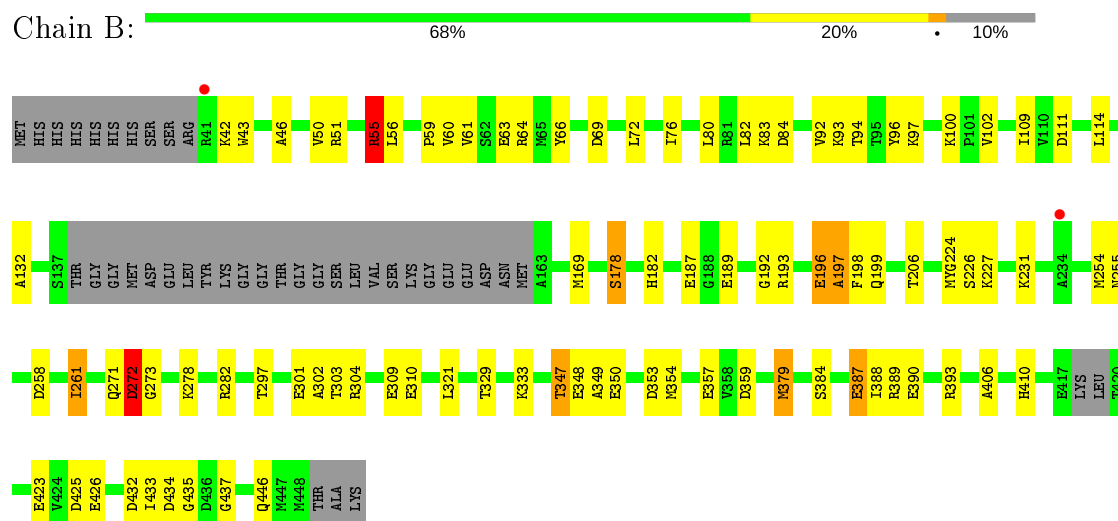
### 3 Residue-property plots

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: RGE01



#### • Molecule 1: RGE01



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.16Å 91.73Å 68.57Å 90.00° 95.29° 90.00°	Depositor
Resolution (Å)	68.28 – 2.20 54.77 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.28-2.20) 100.0 (54.77-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0111	Depositor
R, $R_{free}$	0.193 , 0.257 0.197 , 0.258	Depositor DCC
$R_{free}$ test set	2049 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 37.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6199	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 5.62% 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, NRQ

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	1.07	1/3099 (0.0%)	0.99	11/4167 (0.3%)
1	B	1.00	4/3070 (0.1%)	0.92	7/4128 (0.2%)
All	All	1.04	5/6169 (0.1%)	0.96	18/8295 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	309	GLU	CG-CD	5.27	1.59	1.51
1	A	394	VAL	CB-CG2	5.25	1.63	1.52
1	B	43	TRP	CD2-CE2	5.13	1.47	1.41
1	B	426	GLU	CG-CD	5.10	1.59	1.51
1	B	390	GLU	CG-CD	5.07	1.59	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	ARG	NE-CZ-NH2	9.07	124.83	120.30
1	A	340	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	55	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	409	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	A	298	MET	CA-CB-CG	6.00	123.50	113.30
1	B	193	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	258	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	B	55	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	193	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	B	359	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	40	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	193	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	55	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	393	ARG	NE-CZ-NH2	-5.36	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	MET	CG-SD-CE	5.34	108.75	100.20
1	A	393	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	81	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	304	ARG	CB-CA-C	-5.09	100.23	110.40

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	3060	0	2949	53	0
1	B	3032	0	2911	41	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	65	0	0	1	0
3	B	34	0	0	0	0
All	All	6199	0	5860	93	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 (93) 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:384:SER:O	1:B:388:ILE:HD12	1.74	0.87
1:B:169:MET:HE1	1:B:273:GLY:O	1.77	0.85
1:A:332:THR:HG22	1:A:355:ILE:HD13	1.60	0.81
1:A:174:HIS:ND1	1:A:187:GLU:OE1	2.13	0.80
1:B:379:MET:HE1	1:B:387:GLU:OE1	1.85	0.76
1:B:301:GLU:HG3	1:B:302:ALA:O	1.85	0.76
1:B:55:ARG:HD3	1:B:387:GLU:OE2	1.86	0.76
1:A:351:LEU:O	1:A:355:ILE:HD12	1.90	0.71
1:A:196:GLU:O	1:A:197:ALA:CB	2.40	0.69
1:B:196:GLU:O	1:B:197:ALA:CB	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:MET:CE	1:B:273:GLY:O	2.43	0.67
1:A:41:ARG:HD3	1:A:317:GLU:OE1	1.96	0.65
1:B:92:VAL:HG13	1:B:254:MET:HG2	1.81	0.62
1:A:129:CYS:HB3	1:A:200:THR:HG23	1.82	0.61
1:B:196:GLU:O	1:B:197:ALA:HB3	2.00	0.61
1:A:332:THR:CG2	1:A:355:ILE:HD13	2.31	0.60
1:A:355:ILE:HG23	1:A:366:PHE:HB2	1.85	0.59
1:A:335:LEU:HD21	1:A:354:MET:CE	2.33	0.58
1:B:46:ALA:O	1:B:50:VAL:HG23	2.04	0.58
1:A:199:GLN:HE22	1:A:226:SER:HB3	1.68	0.58
1:A:196:GLU:O	1:A:197:ALA:HB3	2.05	0.57
1:A:187:GLU:HG3	1:A:206:THR:HG21	1.86	0.56
1:B:94:THR:HG21	1:B:96:TYR:CZ	2.41	0.56
1:A:332:THR:HG22	1:A:355:ILE:CD1	2.32	0.55
1:B:178:SER:HA	1:B:182:HIS:O	2.06	0.55
1:A:108:TYR:C	1:A:109:ILE:HD12	2.27	0.55
1:B:347:THR:HG22	1:B:350:GLU:H	1.72	0.54
1:B:63:GLU:OE1	1:B:227:LYS:NZ	2.41	0.54
1:A:303:THR:HG22	1:A:378:LYS:HD3	1.90	0.53
1:B:56:LEU:C	1:B:354:MET:HE2	2.28	0.53
1:B:199:GLN:HE22	1:B:226:SER:HB3	1.73	0.53
1:A:65:MET:CE	1:A:72:LEU:HG	2.39	0.52
1:A:303:THR:CG2	1:A:378:LYS:HD3	2.40	0.52
1:A:80:LEU:HD11	1:A:300:TRP:CE2	2.45	0.51
1:A:347:THR:OG1	1:A:350:GLU:HG3	2.10	0.51
1:A:129:CYS:CB	1:A:200:THR:HG23	2.41	0.51
1:B:61:VAL:HG22	1:B:109:ILE:HD12	1.92	0.51
1:B:347:THR:HG22	1:B:349:ALA:N	2.26	0.51
1:B:224:NRQ:N2	1:B:224:NRQ:HD1	2.26	0.51
1:B:432:ASP:OD2	1:B:437:GLY:N	2.44	0.51
1:A:165:ILE:HD12	1:A:275:PHE:CZ	2.47	0.50
1:A:335:LEU:HD21	1:A:354:MET:HE2	1.94	0.49
1:A:96:TYR:OH	1:A:227:LYS:HE2	2.12	0.49
1:A:112:ILE:HD12	1:A:224:NRQ:CD2	2.43	0.49
1:A:335:LEU:HD21	1:A:354:MET:HE1	1.95	0.48
1:B:446:GLN:HA	1:B:446:GLN:OE1	2.13	0.48
1:A:308:THR:O	1:A:312:ILE:HD12	2.13	0.48
1:A:395:PHE:HA	1:A:411:VAL:HG21	1.95	0.48
1:A:45:LYS:HE2	1:A:321:LEU:HD21	1.96	0.48
1:B:51:ARG:O	1:B:55:ARG:HG2	2.14	0.48
1:A:65:MET:HE3	1:A:73:LYS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD22	1:A:203:LEU:N	2.30	0.46
1:B:433:ILE:O	1:B:435:GLY:N	2.48	0.46
1:A:165:ILE:HD12	1:A:275:PHE:HZ	1.81	0.46
1:B:100:LYS:NZ	1:B:102:VAL:HG22	2.31	0.46
1:B:82:LEU:C	1:B:84:ASP:H	2.19	0.46
1:A:114:LEU:HD12	1:A:114:LEU:C	2.37	0.45
1:B:80:LEU:HD13	1:B:297:THR:HG21	1.97	0.45
1:A:224:NRQ:HD1	1:A:224:NRQ:N2	2.32	0.45
1:A:426:GLU:O	1:A:430:VAL:HG13	2.16	0.45
1:A:81:ARG:HG2	1:A:298:MET:HE3	1.98	0.45
1:B:76:ILE:HD13	1:B:224:NRQ:HD2	1.98	0.45
1:B:187:GLU:HG3	1:B:206:THR:HG21	1.98	0.44
1:A:55:ARG:NH2	1:A:379:MET:HE2	2.32	0.44
1:B:114:LEU:C	1:B:114:LEU:HD23	2.37	0.44
1:B:66:TYR:O	1:B:72:LEU:HD12	2.17	0.44
1:B:192:GLY:HA3	1:B:198:PHE:O	2.18	0.43
1:A:111:ASP:O	1:A:132:ALA:HA	2.19	0.43
1:A:76:ILE:HB	1:A:92:VAL:HB	2.01	0.43
1:B:406:ALA:O	1:B:410:HIS:HB2	2.18	0.43
1:B:197:ALA:HB2	1:B:231:LYS:HB2	2.00	0.42
1:A:65:MET:HE2	1:A:72:LEU:HG	2.01	0.42
1:A:379:MET:HE3	1:A:384:SER:HA	2.01	0.42
1:A:199:GLN:NE2	1:A:226:SER:HB3	2.32	0.42
1:B:347:THR:CG2	1:B:348:GLU:N	2.82	0.42
1:A:114:LEU:HD12	1:A:115:ASP:N	2.34	0.42
1:B:61:VAL:HG13	1:B:109:ILE:HB	2.01	0.42
1:B:255:ASN:OD1	1:B:261:ILE:HD12	2.19	0.42
1:B:271:GLN:O	1:B:272:ASP:CB	2.67	0.41
1:B:111:ASP:O	1:B:132:ALA:HA	2.20	0.41
1:A:108:TYR:O	1:A:109:ILE:HD12	2.21	0.41
1:A:219:SER:N	1:A:220:PRO:CD	2.84	0.41
1:B:59:PRO:HB3	1:B:357:GLU:HG2	2.01	0.41
1:A:324:LYS:HE2	3:A:618:HOH:O	2.21	0.41
1:B:42:LYS:NZ	1:B:423:GLU:HG2	2.36	0.41
1:A:329:THR:O	1:A:329:THR:HG22	2.21	0.41
1:A:84:ASP:OD1	1:A:84:ASP:C	2.59	0.41
1:A:171:PHE:CB	1:A:275:PHE:HB2	2.51	0.41
1:A:348:GLU:O	1:A:348:GLU:OE2	2.39	0.41
1:A:130:GLU:HG3	1:A:130:GLU:O	2.21	0.40
1:A:82:LEU:O	1:A:298:MET:HE3	2.22	0.40
1:A:271:GLN:O	1:A:272:ASP:CB	2.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:THR:HG21	1:B:282:ARG:NH2	2.36	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	375/419 (90%)	369 (98%)	5 (1%)	1 (0%)	41	46
1	B	370/419 (88%)	359 (97%)	7 (2%)	4 (1%)	14	12
All	All	745/838 (89%)	728 (98%)	12 (2%)	5 (1%)	22	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	ALA
1	B	83	LYS
1	B	197	ALA
1	B	272	ASP
1	B	434	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/351 (92%)	302 (94%)	20 (6%)	18	21
1	B	319/351 (91%)	295 (92%)	24 (8%)	13	14
All	All	641/702 (91%)	597 (93%)	44 (7%)	15	16

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	80	LEU
1	A	93	LYS
1	A	114	LEU
1	A	127	GLU
1	A	130	GLU
1	A	196	GLU
1	A	200	THR
1	A	257	GLU
1	A	272	ASP
1	A	278	LYS
1	A	329	THR
1	A	348	GLU
1	A	377	ARG
1	A	386	GLU
1	A	387	GLU
1	A	389	ARG
1	A	417	GLU
1	A	425	ASP
1	A	447	MET
1	B	55	ARG
1	B	60	VAL
1	B	64	ARG
1	B	69	ASP
1	B	93	LYS
1	B	97	LYS
1	B	178	SER
1	B	189	GLU
1	B	196	GLU
1	B	261	ILE
1	B	272	ASP
1	B	278	LYS

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Mol	Chain	Res	Type
1	B	303	THR
1	B	310	GLU
1	B	321	LEU
1	B	329	THR
1	B	333	LYS
1	B	347	THR
1	B	353	ASP
1	B	379	MET
1	B	387	GLU
1	B	389	ARG
1	B	393	ARG
1	B	425	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	NRQ	A	224	1	23,24,25	4.39	5 (21%)	23,32,34	5.64	8 (34%)
1	NRQ	B	224	1	23,24,25	3.99	6 (26%)	23,32,34	3.94	9 (39%)

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	NRQ	A	224	1	-	3/9/31/32	0/2/2/2
1	NRQ	B	224	1	-	4/9/31/32	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	NRQ	CA2-C2	-15.16	1.33	1.48
1	B	224	NRQ	CB2-CA2	12.98	1.46	1.35
1	A	224	NRQ	CB2-CA2	11.99	1.45	1.35
1	B	224	NRQ	CA2-C2	-11.20	1.37	1.48
1	B	224	NRQ	CA1-N1	5.95	1.41	1.27
1	A	224	NRQ	CA1-N1	5.73	1.41	1.27
1	A	224	NRQ	C2-N3	-4.71	1.28	1.39
1	B	224	NRQ	C2-N3	-3.64	1.31	1.39
1	A	224	NRQ	CA2-N2	-2.46	1.33	1.38
1	B	224	NRQ	O2-C2	2.45	1.28	1.23
1	B	224	NRQ	CA2-N2	-2.41	1.33	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	NRQ	CA2-C2-N3	20.17	112.91	103.37
1	A	224	NRQ	O2-C2-CA2	-15.64	122.18	130.96
1	B	224	NRQ	CA2-C2-N3	15.18	110.55	103.37
1	B	224	NRQ	O2-C2-CA2	-6.91	127.08	130.96
1	B	224	NRQ	CG2-CB2-CA2	-4.46	124.48	129.94
1	A	224	NRQ	CA3-N3-C1	4.45	136.94	128.22
1	A	224	NRQ	CG2-CB2-CA2	-3.67	125.45	129.94
1	B	224	NRQ	CB2-CA2-N2	-3.27	124.30	128.83
1	B	224	NRQ	O3-C3-CA3	-3.17	116.82	126.39
1	A	224	NRQ	CD1-CG2-CD2	3.06	122.17	117.64
1	B	224	NRQ	CB2-CA2-C2	3.02	125.88	122.28
1	A	224	NRQ	O3-C3-CA3	-2.88	117.69	126.39
1	A	224	NRQ	CE-SD-CG1	-2.86	90.56	100.40
1	B	224	NRQ	CA3-N3-C1	2.72	133.54	128.22
1	A	224	NRQ	CE1-CD1-CG2	-2.70	117.73	121.25
1	B	224	NRQ	CE2-CD2-CG2	-2.17	118.42	121.25
1	B	224	NRQ	CD1-CG2-CD2	2.00	120.61	117.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	224	NRQ	CA1-CB1-CG1-SD
1	A	224	NRQ	C1-CA1-CB1-CG1
1	B	224	NRQ	CA1-CB1-CG1-SD
1	B	224	NRQ	C2-CA2-CB2-CG2
1	A	224	NRQ	C3-CA3-N3-C1
1	B	224	NRQ	C1-CA1-CB1-CG1
1	B	224	NRQ	C3-CA3-N3-C1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	224	NRQ	2	0
1	B	224	NRQ	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 [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	381/419 (90%)	-0.18	0	100   100	12, 25, 43, 63	0
1	B	378/419 (90%)	-0.01	2 (0%)	91   90	17, 33, 56, 78	0
All	All	759/838 (90%)	-0.09	2 (0%)	94   93	12, 29, 51, 78	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	ARG	3.2
1	B	234	ALA	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	NRQ	B	224	23/24	0.95	0.16	27,32,36,38	0
1	NRQ	A	224	23/24	0.96	0.13	16,22,26,33	0

### 6.3 Carbohydrates [i](#)

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. 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( $\text{\AA}^2$ )	Q<0.9
2	CA	B	504	1/1	0.98	0.06	43,43,43,43	0
2	CA	B	503	1/1	0.98	0.06	37,37,37,37	0
2	CA	A	500	1/1	0.98	0.08	27,27,27,27	0
2	CA	A	503	1/1	0.99	0.10	17,17,17,17	0
2	CA	A	502	1/1	0.99	0.10	24,24,24,24	0
2	CA	B	501	1/1	1.00	0.08	22,22,22,22	0
2	CA	A	501	1/1	1.00	0.06	26,26,26,26	0
2	CA	B	502	1/1	1.00	0.09	21,21,21,21	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.