



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:34 am BST

PDB ID : 4MD7  
Title : Crystal Structure of full-length symmetric CK2 holoenzyme  
Authors : Lolli, G.; Ranchio, A.; Battistutta, R.  
Deposited on : 2013-08-22  
Resolution : 3.10 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
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

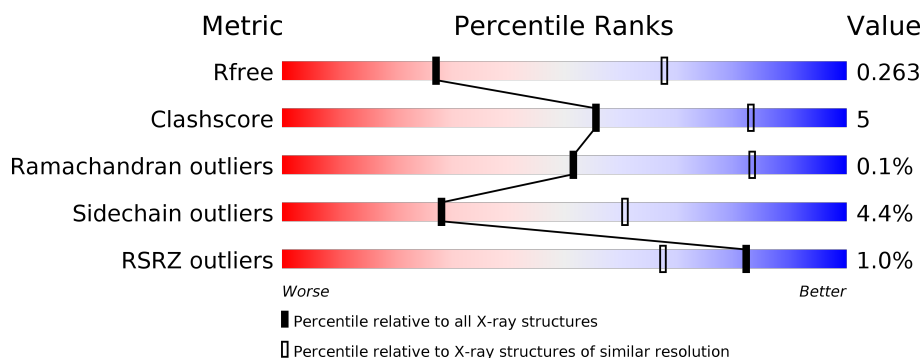
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	215	
1	B	215	
1	C	215	
1	D	215	
2	E	391	
2	F	391	

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Mol	Chain	Length	Quality of chain
2	G	391	<div><div>%</div><div><div></div><div>72%</div><div>12%</div><div>•</div><div>15%</div></div></div>
2	H	391	<div><div>3%</div><div><div></div><div>75%</div><div>9%</div><div>•</div><div>16%</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17621 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 Casein kinase II subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1622	1040	273	294	15			
1	B	195	Total	C	N	O	S	0	0	0
			1592	1024	268	285	15			
1	C	197	Total	C	N	O	S	0	0	0
			1605	1031	271	288	15			
1	D	195	Total	C	N	O	S	0	0	0
			1592	1024	268	285	15			

- Molecule 2 is a protein called Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	332	Total	C	N	O	S	0	0	0
			2804	1795	495	503	11			
2	F	332	Total	C	N	O	S	0	0	0
			2804	1795	495	503	11			
2	G	332	Total	C	N	O	S	0	0	0
			2804	1795	495	503	11			
2	H	330	Total	C	N	O	S	0	0	0
			2794	1790	493	500	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	344	GLU	THR	ENGINEERED MUTATION	UNP P68400
E	360	GLU	THR	ENGINEERED MUTATION	UNP P68400
E	362	GLU	SER	ENGINEERED MUTATION	UNP P68400
E	370	GLU	SER	ENGINEERED MUTATION	UNP P68400
F	344	GLU	THR	ENGINEERED MUTATION	UNP P68400
F	360	GLU	THR	ENGINEERED MUTATION	UNP P68400
F	362	GLU	SER	ENGINEERED MUTATION	UNP P68400
F	370	GLU	SER	ENGINEERED MUTATION	UNP P68400

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Chain	Residue	Modelled	Actual	Comment	Reference
G	344	GLU	THR	ENGINEERED MUTATION	UNP P68400
G	360	GLU	THR	ENGINEERED MUTATION	UNP P68400
G	362	GLU	SER	ENGINEERED MUTATION	UNP P68400
G	370	GLU	SER	ENGINEERED MUTATION	UNP P68400
H	344	GLU	THR	ENGINEERED MUTATION	UNP P68400
H	360	GLU	THR	ENGINEERED MUTATION	UNP P68400
H	362	GLU	SER	ENGINEERED MUTATION	UNP P68400
H	370	GLU	SER	ENGINEERED MUTATION	UNP P68400

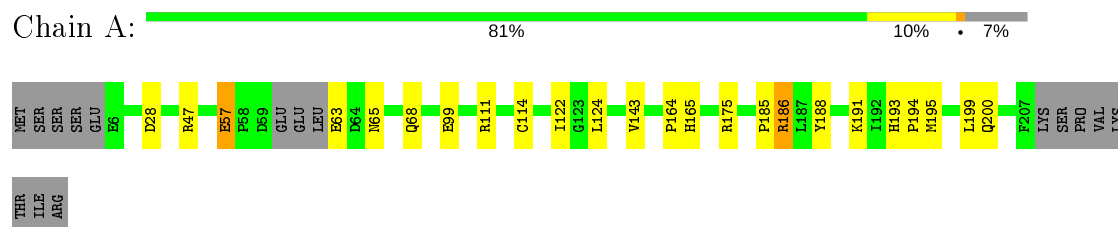
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

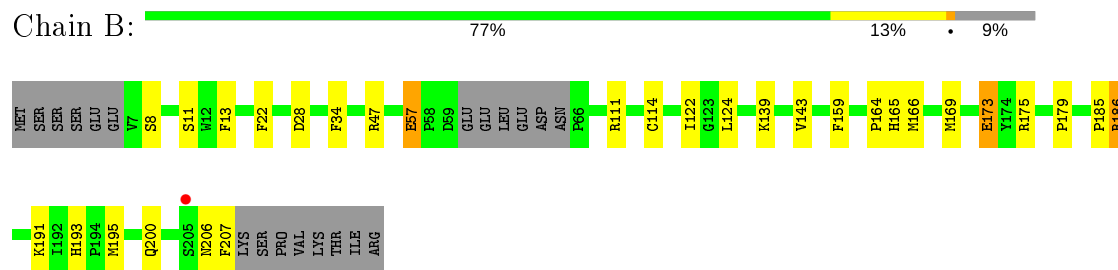
### 3 Residue-property plots [i](#)

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.

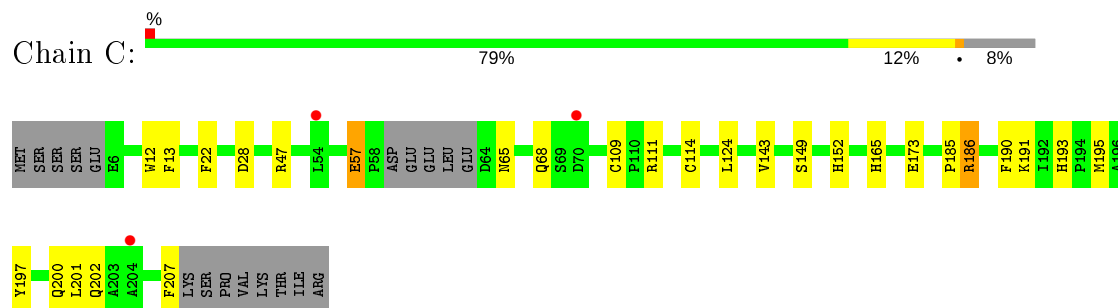
- Molecule 1: Casein kinase II subunit beta



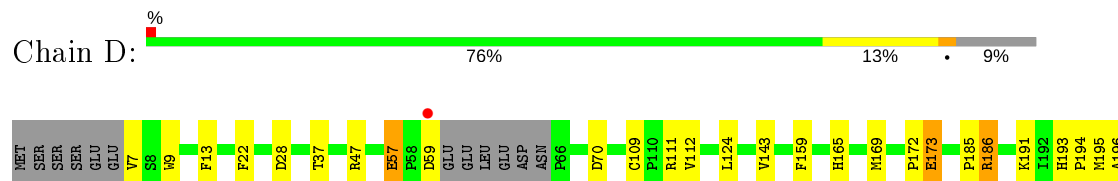
- Molecule 1: Casein kinase II subunit beta

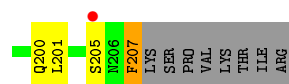


- Molecule 1: Casein kinase II subunit beta

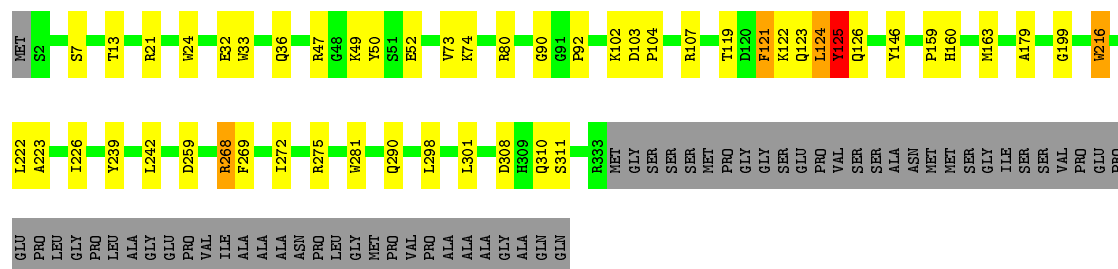


- Molecule 1: Casein kinase II subunit beta

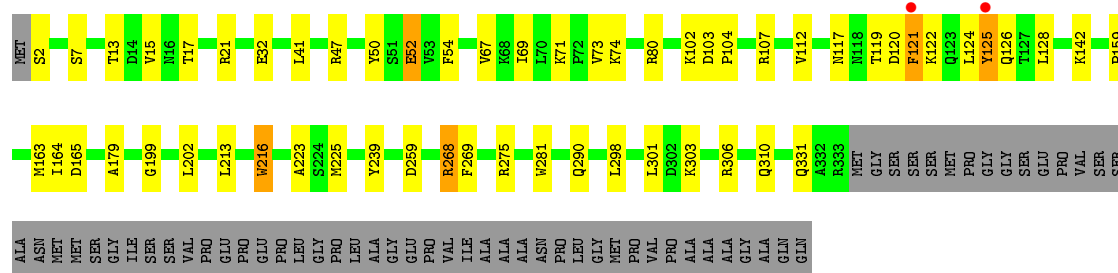




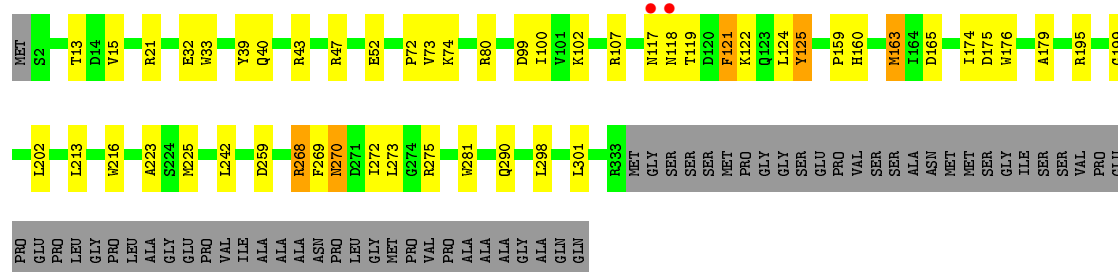
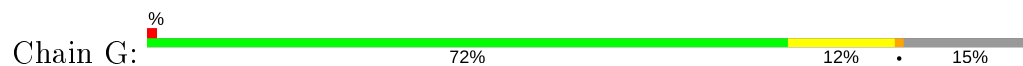
• Molecule 2: Casein kinase II subunit alpha



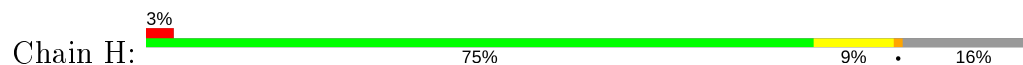
• Molecule 2: Casein kinase II subunit alpha

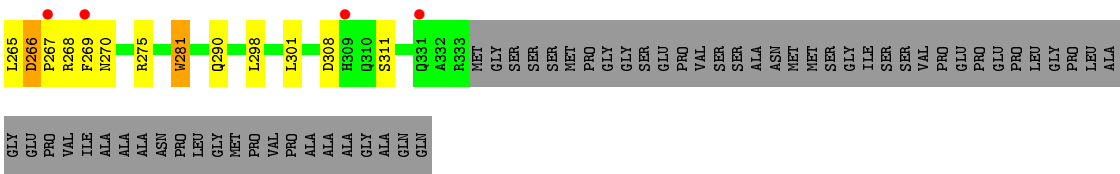


• Molecule 2: Casein kinase II subunit alpha



• Molecule 2: Casein kinase II subunit alpha





GLY  
GLU  
PRO  
VAL  
ILE  
ALA  
ALA  
ALA  
ASN  
PRO  
LEU  
GLY  
MET  
PRO  
VAL  
PRO  
ALA  
ALA  
ALA  
GLY  
ALA  
GLN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.32Å 57.96Å 186.19Å 90.00° 102.42° 90.00°	Depositor
Resolution (Å)	181.83 – 3.10 48.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.9 (181.83-3.10) 96.1 (48.87-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 3.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.233 , 0.263 0.234 , 0.263	Depositor DCC
$R_{free}$ test set	2681 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	17621	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% 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: ZN

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	0.56	0/1671	0.69	3/2265 (0.1%)
1	B	0.54	0/1641	0.73	4/2223 (0.2%)
1	C	0.50	1/1654 (0.1%)	0.65	3/2242 (0.1%)
1	D	0.49	1/1641 (0.1%)	0.68	4/2223 (0.2%)
2	E	0.56	3/2879 (0.1%)	0.62	0/3893
2	F	0.55	1/2879 (0.0%)	0.60	0/3893
2	G	0.52	2/2879 (0.1%)	0.61	2/3893 (0.1%)
2	H	0.51	2/2869 (0.1%)	0.57	1/3879 (0.0%)
All	All	0.53	10/18113 (0.1%)	0.63	17/24511 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	216	TRP	CD2-CE2	5.55	1.48	1.41
1	C	12	TRP	CD2-CE2	5.30	1.47	1.41
2	G	33	TRP	CD2-CE2	5.27	1.47	1.41
1	D	9	TRP	CD2-CE2	5.21	1.47	1.41
2	H	281	TRP	CD2-CE2	5.16	1.47	1.41
2	G	176	TRP	CD2-CE2	5.14	1.47	1.41
2	E	24	TRP	CD2-CE2	5.14	1.47	1.41
2	E	33	TRP	CD2-CE2	5.06	1.47	1.41
2	H	33	TRP	CD2-CE2	5.05	1.47	1.41
2	E	216	TRP	CD2-CE2	5.00	1.47	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	B	47	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	D	47	ARG	NE-CZ-NH2	-11.18	114.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	47	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	A	47	ARG	NE-CZ-NH1	-10.54	115.03	120.30
1	C	47	ARG	NE-CZ-NH2	10.32	125.46	120.30
1	C	47	ARG	NE-CZ-NH1	-10.27	115.16	120.30
1	A	47	ARG	NE-CZ-NH2	9.97	125.29	120.30
2	G	270	ASN	N-CA-C	7.91	132.35	111.00
2	G	270	ASN	CB-CA-C	-7.33	95.73	110.40
1	D	173	GLU	CA-CB-CG	6.08	126.78	113.40
1	D	47	ARG	CD-NE-CZ	5.95	131.93	123.60
1	B	173	GLU	CA-CB-CG	5.91	126.40	113.40
1	B	47	ARG	CD-NE-CZ	5.90	131.86	123.60
2	H	266	ASP	CB-CA-C	5.75	121.90	110.40
1	C	47	ARG	CD-NE-CZ	5.56	131.38	123.60
1	A	47	ARG	CD-NE-CZ	5.25	130.95	123.60

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	1622	0	1534	21	0
1	B	1592	0	1517	26	0
1	C	1605	0	1524	27	0
1	D	1592	0	1517	25	1
2	E	2804	0	2748	26	0
2	F	2804	0	2748	34	0
2	G	2804	0	2748	27	1
2	H	2794	0	2741	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	17621	0	17077	177	1

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 5.

All (177) 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:C:186:ARG:HG2	1:C:186:ARG:HH11	1.36	0.90
1:A:186:ARG:HG2	1:A:186:ARG:HH11	1.37	0.89
1:B:186:ARG:HH11	1:B:186:ARG:HG2	1.38	0.85
1:D:186:ARG:HG2	1:D:186:ARG:HH11	1.39	0.85
2:E:90:GLY:O	2:H:18:HIS:CG	2.32	0.83
2:E:122:LYS:HE3	2:E:160:HIS:CD2	2.15	0.81
2:G:122:LYS:HE2	2:G:160:HIS:CD2	2.20	0.76
2:G:121:PHE:HB3	2:G:159:PRO:HB3	1.68	0.75
2:F:73:VAL:HG12	2:F:74:LYS:H	1.51	0.74
1:D:193:HIS:HD2	1:D:195:MET:HB3	1.51	0.73
1:A:186:ARG:NH1	1:A:191:LYS:HG3	2.03	0.73
1:A:186:ARG:HH12	1:A:191:LYS:HG3	1.55	0.70
1:C:186:ARG:NH1	1:C:191:LYS:HG3	2.07	0.70
1:C:186:ARG:HH12	1:C:191:LYS:HG3	1.59	0.68
2:G:73:VAL:HG12	2:G:74:LYS:H	1.59	0.67
2:H:73:VAL:HG12	2:H:74:LYS:H	1.60	0.67
1:B:186:ARG:NH1	1:B:191:LYS:HG3	2.10	0.66
1:D:186:ARG:NH1	1:D:191:LYS:HG3	2.10	0.66
1:D:186:ARG:HH12	1:D:191:LYS:HG3	1.61	0.66
1:D:13:PHE:HE2	1:D:22:PHE:CE1	2.15	0.65
2:E:73:VAL:HG12	2:E:74:LYS:H	1.63	0.64
1:C:186:ARG:CG	1:C:186:ARG:HH11	2.11	0.63
1:C:165:HIS:CE1	1:D:185:PRO:HB3	2.33	0.63
2:E:269:PHE:HA	2:E:272:ILE:HG12	1.81	0.62
1:B:13:PHE:HE2	1:B:22:PHE:CE1	2.18	0.62
1:B:186:ARG:HH12	1:B:191:LYS:HG3	1.65	0.61
1:D:196:ALA:O	1:D:200:GLN:HG3	2.01	0.61
1:A:186:ARG:CG	1:A:186:ARG:HH11	2.11	0.61
1:A:165:HIS:CE1	1:B:185:PRO:HB3	2.35	0.61
1:D:13:PHE:HE2	1:D:22:PHE:CD1	2.19	0.60
2:G:118:ASN:HA	2:G:163:MET:HE2	1.82	0.60
2:F:122:LYS:HG3	2:F:159:PRO:HB2	1.83	0.60
2:F:142:LYS:NZ	2:F:331:GLN:HE22	1.99	0.60
2:F:142:LYS:NZ	2:F:331:GLN:NE2	2.49	0.60
2:G:272:ILE:HG13	2:G:273:LEU:N	2.16	0.59
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.03	0.59
1:D:186:ARG:CG	1:D:186:ARG:HH11	2.13	0.59
1:D:57:GLU:OE1	1:D:57:GLU:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ARG:HH11	1:B:186:ARG:CG	2.14	0.58
1:C:57:GLU:HA	1:C:57:GLU:OE1	2.04	0.58
1:A:57:GLU:HA	1:A:57:GLU:OE1	2.04	0.57
2:G:269:PHE:HA	2:G:272:ILE:HG12	1.87	0.57
1:B:193:HIS:CD2	1:B:195:MET:H	2.22	0.56
1:B:13:PHE:HE2	1:B:22:PHE:CD1	2.22	0.56
2:F:117:ASN:HD22	2:F:165:ASP:HA	1.70	0.56
1:C:124:LEU:HD21	1:C:143:VAL:HG11	1.88	0.55
1:A:124:LEU:HD21	1:A:143:VAL:HG11	1.89	0.55
1:C:190:PHE:HE2	2:G:39:TYR:HB2	1.71	0.55
1:A:65:ASN:HB3	1:A:68:GLN:HB2	1.89	0.55
1:B:193:HIS:HD2	1:B:195:MET:HB3	1.71	0.55
2:E:281:TRP:HB3	2:E:298:LEU:HD22	1.88	0.54
2:F:124:LEU:HD12	2:F:128:LEU:HD21	1.89	0.54
1:A:200:GLN:OE1	1:B:175:ARG:NE	2.39	0.54
2:F:142:LYS:HZ1	2:F:331:GLN:HE22	1.56	0.54
2:E:122:LYS:HG3	2:E:159:PRO:HB2	1.90	0.54
2:G:121:PHE:CE2	2:G:225:MET:SD	3.01	0.53
2:F:73:VAL:HG12	2:F:74:LYS:N	2.23	0.52
1:D:37:THR:HB	2:G:72:PRO:HB2	1.92	0.52
2:E:36:GLN:NE2	2:E:104:PRO:HD3	2.25	0.52
1:A:193:HIS:HD2	1:A:195:MET:HB3	1.75	0.51
2:E:121:PHE:HB3	2:E:159:PRO:HB3	1.91	0.51
2:F:202:LEU:HD11	2:F:213:LEU:HD11	1.91	0.51
1:C:200:GLN:HG2	1:D:172:PRO:HB3	1.92	0.51
1:C:190:PHE:CE2	2:G:39:TYR:HB2	2.46	0.51
1:A:175:ARG:NE	1:B:200:GLN:OE1	2.36	0.51
1:A:195:MET:O	1:A:199:LEU:HG	2.10	0.51
1:A:111:ARG:NH1	1:A:114:CYS:SG	2.83	0.51
1:C:185:PRO:HB3	1:D:165:HIS:CE1	2.46	0.51
2:F:281:TRP:HB3	2:F:298:LEU:HD22	1.92	0.51
1:C:13:PHE:CE2	1:C:22:PHE:CE1	2.99	0.51
2:E:239:TYR:CZ	2:E:268:ARG:HD3	2.45	0.51
1:B:34:PHE:CZ	2:F:50:TYR:CE2	2.99	0.51
2:H:80:ARG:HD3	2:H:179:ALA:O	2.11	0.50
2:E:121:PHE:C	2:E:123:GLN:H	2.14	0.50
2:F:119:THR:HB	2:F:164:ILE:O	2.11	0.50
1:B:169:MET:HG3	2:F:54:PHE:HE2	1.77	0.50
2:H:281:TRP:HB3	2:H:298:LEU:HD22	1.94	0.50
1:C:191:LYS:HB2	2:G:40:GLN:HG2	1.94	0.50
2:F:7:SER:OG	2:F:310:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:125:TYR:CD1	2:G:225:MET:HG2	2.46	0.50
2:G:117:ASN:HD22	2:G:165:ASP:HA	1.77	0.50
1:A:193:HIS:CG	1:A:194:PRO:HD2	2.47	0.49
1:D:13:PHE:CE2	1:D:22:PHE:CE1	2.98	0.49
2:F:239:TYR:HA	2:F:269:PHE:CE2	2.48	0.49
1:C:13:PHE:HE2	1:C:22:PHE:CE1	2.31	0.49
2:G:102:LYS:HD3	2:G:107:ARG:HG2	1.94	0.49
1:D:124:LEU:HD21	1:D:143:VAL:HG11	1.94	0.49
1:A:193:HIS:HB3	2:F:41:LEU:O	2.12	0.49
1:B:206:ASN:O	1:B:207:PHE:HB2	2.12	0.48
2:E:90:GLY:O	2:H:18:HIS:CD2	2.67	0.48
2:F:102:LYS:HD3	2:F:107:ARG:HG2	1.95	0.48
1:C:193:HIS:CD2	1:C:195:MET:H	2.31	0.48
1:B:193:HIS:HD2	1:B:195:MET:CB	2.27	0.48
1:D:22:PHE:CE2	1:D:159:PHE:CZ	3.01	0.48
2:F:124:LEU:HD23	2:F:124:LEU:H	1.78	0.48
1:B:8:SER:OG	1:B:11:SER:HB3	2.13	0.48
1:B:124:LEU:HD21	1:B:143:VAL:HG11	1.94	0.48
2:H:266:ASP:HA	2:H:267:PRO:HD2	1.68	0.48
2:H:223:ALA:HB2	2:H:301:LEU:HD11	1.96	0.48
1:C:65:ASN:CG	1:C:68:GLN:HB2	2.33	0.48
1:D:191:LYS:HB2	2:H:40:GLN:HG2	1.96	0.48
2:G:281:TRP:HB3	2:G:298:LEU:HD22	1.96	0.47
1:A:188:TYR:CD2	2:F:69:ILE:HG21	2.49	0.47
2:G:242:LEU:HD23	2:G:269:PHE:CE2	2.49	0.47
2:G:73:VAL:HG12	2:G:74:LYS:N	2.28	0.47
1:C:65:ASN:HB3	1:C:68:GLN:HB2	1.96	0.47
1:C:197:TYR:O	1:C:201:LEU:HG	2.15	0.47
2:F:121:PHE:CE2	2:F:225:MET:SD	3.08	0.47
2:F:303:LYS:HA	2:F:306:ARG:HE	1.80	0.47
2:E:222:LEU:O	2:E:226:ILE:HG12	2.15	0.46
2:G:80:ARG:HD3	2:G:179:ALA:O	2.15	0.46
1:D:193:HIS:CG	1:D:194:PRO:HD2	2.51	0.46
2:F:80:ARG:HD3	2:F:179:ALA:O	2.15	0.46
2:F:52:GLU:OE1	2:F:71:LYS:HE2	2.16	0.46
1:C:109:CYS:SG	1:C:111:ARG:HB2	2.56	0.46
2:F:239:TYR:CZ	2:F:268:ARG:HD3	2.50	0.46
2:H:102:LYS:HD3	2:H:107:ARG:HG2	1.98	0.46
2:F:142:LYS:HZ3	2:F:331:GLN:NE2	2.13	0.45
2:H:73:VAL:HG12	2:H:74:LYS:N	2.29	0.45
1:A:193:HIS:CD2	1:A:195:MET:H	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:CYS:SG	1:D:111:ARG:HB2	2.57	0.45
1:C:124:LEU:HD11	1:D:112:VAL:HG11	1.98	0.45
2:E:102:LYS:HD3	2:E:107:ARG:HG2	1.99	0.45
2:E:90:GLY:O	2:H:18:HIS:CB	2.64	0.45
2:F:199:GLY:HA2	2:F:216:TRP:CD1	2.52	0.45
2:E:199:GLY:HA2	2:E:216:TRP:CD1	2.51	0.45
2:E:73:VAL:HG12	2:E:74:LYS:N	2.31	0.45
2:E:80:ARG:HD3	2:E:179:ALA:O	2.17	0.45
1:A:185:PRO:HB3	1:B:165:HIS:CE1	2.52	0.45
1:C:13:PHE:HE2	1:C:22:PHE:CD1	2.36	0.44
2:F:125:TYR:CD2	2:F:126:GLN:HG2	2.53	0.44
1:C:190:PHE:HD2	2:G:39:TYR:O	2.00	0.44
2:E:242:LEU:HD23	2:E:269:PHE:CE2	2.53	0.44
1:B:139:LYS:HG2	1:B:179:PRO:HG3	2.00	0.44
1:A:186:ARG:HG2	1:A:186:ARG:NH1	2.18	0.44
1:A:122:ILE:HD12	1:A:164:PRO:HG2	2.00	0.44
2:G:202:LEU:HD11	2:G:213:LEU:HD11	2.00	0.43
2:H:199:GLY:HA2	2:H:216:TRP:CD1	2.53	0.43
1:D:186:ARG:NH1	1:D:186:ARG:HG2	2.21	0.43
1:C:173:GLU:HG3	1:D:207:PHE:CD2	2.53	0.43
2:G:121:PHE:HE2	2:G:225:MET:SD	2.40	0.43
1:C:111:ARG:NH1	1:C:114:CYS:SG	2.91	0.43
2:G:223:ALA:HB2	2:G:301:LEU:HD11	2.01	0.43
2:H:202:LEU:HD11	2:H:213:LEU:HD11	2.01	0.43
1:C:149:SER:HA	1:C:152:HIS:CE1	2.54	0.43
2:H:308:ASP:HB3	2:H:311:SER:OG	2.19	0.43
2:G:99:ASP:OD1	2:G:100:ILE:N	2.52	0.43
1:B:13:PHE:CE2	1:B:22:PHE:CE1	3.02	0.43
2:E:7:SER:OG	2:E:310:GLN:NE2	2.52	0.43
1:B:111:ARG:NH1	1:B:114:CYS:SG	2.92	0.42
1:B:166:MET:O	1:B:169:MET:HB2	2.19	0.42
1:B:22:PHE:CE2	1:B:159:PHE:CZ	3.07	0.42
2:E:125:TYR:CD2	2:E:125:TYR:C	2.93	0.42
1:D:193:HIS:CD2	1:D:195:MET:HB3	2.42	0.42
2:E:308:ASP:HB3	2:E:311:SER:OG	2.20	0.42
2:F:103:ASP:O	2:F:104:PRO:C	2.57	0.42
2:E:223:ALA:HB2	2:E:301:LEU:HD11	2.02	0.42
2:F:122:LYS:HG3	2:F:159:PRO:CB	2.50	0.42
1:C:13:PHE:CE2	1:C:22:PHE:CD1	3.08	0.41
2:E:92:PRO:HD2	2:E:146:TYR:CG	2.55	0.41
1:A:193:HIS:CB	2:F:41:LEU:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ASN:CB	1:C:68:GLN:HB2	2.50	0.41
2:E:103:ASP:O	2:E:107:ARG:N	2.50	0.41
2:E:124:LEU:C	2:E:126:GLN:H	2.24	0.41
2:F:142:LYS:HZ1	2:F:331:GLN:NE2	2.15	0.41
2:G:199:GLY:HA2	2:G:216:TRP:CD1	2.55	0.41
1:B:193:HIS:HD2	1:B:195:MET:H	1.68	0.41
2:F:67:VAL:HG22	2:F:112:VAL:HG22	2.01	0.41
2:G:117:ASN:HB3	2:G:165:ASP:HB2	2.02	0.41
2:F:119:THR:HG22	2:F:124:LEU:HD22	2.01	0.41
2:G:174:ILE:HD12	2:G:175:ASP:HB2	2.03	0.41
2:H:265:LEU:O	2:H:266:ASP:C	2.59	0.41
2:E:49:LYS:HD3	2:E:50:TYR:CE1	2.56	0.41
1:B:122:ILE:HD12	1:B:164:PRO:HG2	2.02	0.40
1:D:196:ALA:HB2	2:H:42:VAL:HA	2.03	0.40
2:F:223:ALA:HB2	2:F:301:LEU:HD11	2.03	0.40
1:D:169:MET:SD	2:G:43:ARG:HA	2.62	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ASP:OD1	2:G:195:ARG:NH1[2_546]	2.12	0.08

## 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	195/215 (91%)	190 (97%)	5 (3%)	0	100	100
1	B	191/215 (89%)	186 (97%)	5 (3%)	0	100	100
1	C	193/215 (90%)	187 (97%)	6 (3%)	0	100	100
1	D	191/215 (89%)	185 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	330/391 (84%)	310 (94%)	19 (6%)	1 (0%)	41	73
2	F	330/391 (84%)	313 (95%)	17 (5%)	0	100	100
2	G	330/391 (84%)	308 (93%)	21 (6%)	1 (0%)	41	73
2	H	328/391 (84%)	312 (95%)	15 (5%)	1 (0%)	41	73
All	All	2088/2424 (86%)	1991 (95%)	94 (4%)	3 (0%)	51	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	268	ARG
2	H	269	PHE
2	E	125	TYR

### 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	174/191 (91%)	169 (97%)	5 (3%)	42	72
1	B	171/191 (90%)	167 (98%)	4 (2%)	50	77
1	C	172/191 (90%)	167 (97%)	5 (3%)	42	72
1	D	171/191 (90%)	162 (95%)	9 (5%)	22	54
2	E	305/347 (88%)	291 (95%)	14 (5%)	27	59
2	F	305/347 (88%)	289 (95%)	16 (5%)	23	55
2	G	305/347 (88%)	289 (95%)	16 (5%)	23	55
2	H	304/347 (88%)	290 (95%)	14 (5%)	27	59
All	All	1907/2152 (89%)	1824 (96%)	83 (4%)	28	61

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP

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Mol	Chain	Res	Type
1	A	57	GLU
1	A	63	GLU
1	A	99	GLU
1	A	186	ARG
1	B	28	ASP
1	B	57	GLU
1	B	173	GLU
1	B	186	ARG
1	C	28	ASP
1	C	57	GLU
1	C	186	ARG
1	C	202	GLN
1	C	207	PHE
1	D	7	VAL
1	D	28	ASP
1	D	57	GLU
1	D	59	ASP
1	D	173	GLU
1	D	186	ARG
1	D	201	LEU
1	D	205	SER
1	D	207	PHE
2	E	13	THR
2	E	21	ARG
2	E	32	GLU
2	E	47	ARG
2	E	52	GLU
2	E	119	THR
2	E	121	PHE
2	E	124	LEU
2	E	125	TYR
2	E	163	MET
2	E	259	ASP
2	E	268	ARG
2	E	275	ARG
2	E	290	GLN
2	F	2	SER
2	F	13	THR
2	F	15	VAL
2	F	17	THR
2	F	21	ARG
2	F	32	GLU

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Mol	Chain	Res	Type
2	F	47	ARG
2	F	52	GLU
2	F	120	ASP
2	F	121	PHE
2	F	125	TYR
2	F	163	MET
2	F	259	ASP
2	F	268	ARG
2	F	275	ARG
2	F	290	GLN
2	G	13	THR
2	G	15	VAL
2	G	21	ARG
2	G	32	GLU
2	G	47	ARG
2	G	52	GLU
2	G	119	THR
2	G	121	PHE
2	G	124	LEU
2	G	125	TYR
2	G	163	MET
2	G	259	ASP
2	G	268	ARG
2	G	270	ASN
2	G	275	ARG
2	G	290	GLN
2	H	13	THR
2	H	21	ARG
2	H	32	GLU
2	H	47	ARG
2	H	52	GLU
2	H	119	THR
2	H	121	PHE
2	H	125	TYR
2	H	163	MET
2	H	259	ASP
2	H	268	ARG
2	H	270	ASN
2	H	275	ARG
2	H	290	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	HIS
1	A	193	HIS
1	B	165	HIS
1	B	193	HIS
1	C	165	HIS
1	C	193	HIS
1	D	165	HIS
1	D	193	HIS
2	E	118	ASN
2	E	160	HIS
2	E	234	HIS
2	E	310	GLN
2	F	36	GLN
2	F	117	ASN
2	F	118	ASN
2	F	234	HIS
2	F	310	GLN
2	F	331	GLN
2	G	36	GLN
2	G	117	ASN
2	G	118	ASN
2	G	160	HIS
2	G	234	HIS
2	G	270	ASN
2	G	310	GLN
2	H	36	GLN
2	H	117	ASN
2	H	234	HIS
2	H	310	GLN

### 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 4 ligands modelled in this entry, 4 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	199/215 (92%)	-0.52	0 100 100	14, 31, 61, 88	0
1	B	195/215 (90%)	-0.32	1 (0%) 91 81	21, 41, 71, 97	0
1	C	197/215 (91%)	-0.11	3 (1%) 73 54	39, 65, 109, 155	0
1	D	195/215 (90%)	-0.17	2 (1%) 82 67	36, 61, 90, 116	0
2	E	332/391 (84%)	-0.49	0 100 100	21, 36, 61, 95	0
2	F	332/391 (84%)	-0.29	2 (0%) 89 78	25, 45, 81, 100	0
2	G	332/391 (84%)	-0.14	2 (0%) 89 78	30, 61, 98, 123	0
2	H	330/391 (84%)	0.28	11 (3%) 46 24	51, 86, 116, 131	0
All	All	2112/2424 (87%)	-0.20	21 (0%) 82 67	14, 52, 103, 155	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	267	PRO	4.4
1	C	70	ASP	3.9
2	H	125	TYR	3.5
2	H	128	LEU	3.4
2	F	121	PHE	3.1
2	H	126	GLN	3.1
1	D	59	ASP	3.0
2	H	121	PHE	3.0
2	H	263	ILE	2.6
1	B	205	SER	2.6
2	H	18	HIS	2.6
2	F	125	TYR	2.5
2	G	117	ASN	2.4
2	G	118	ASN	2.3
1	C	54	LEU	2.3
2	H	331	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	245	ILE	2.1
1	D	205	SER	2.1
2	H	269	PHE	2.1
1	C	204	ALA	2.0
2	H	309	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 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
3	ZN	B	301	1/1	0.99	0.12	17,17,17,17	0
3	ZN	A	301	1/1	0.99	0.11	14,14,14,14	0
3	ZN	D	301	1/1	0.99	0.10	36,36,36,36	0
3	ZN	C	301	1/1	1.00	0.12	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.