



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:35 PM UTC

PDB ID : 4MD7 / pdb_00004md7
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

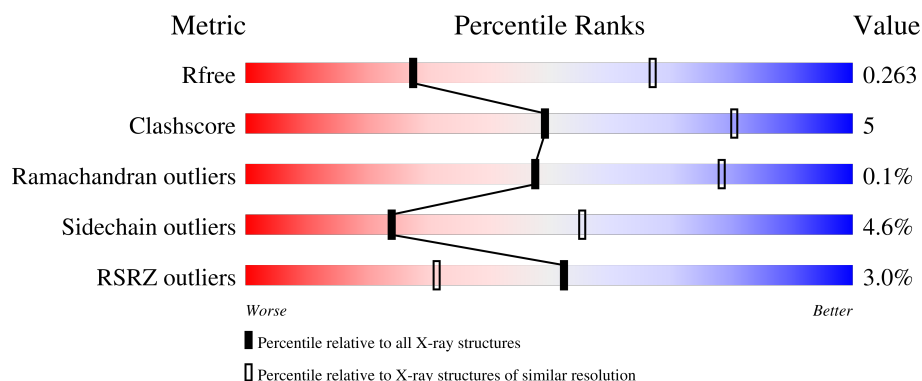
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	81% 10% • 7%
1	B	215	3% 77% 13% • 9%
1	C	215	3% 79% 11% • 8%
1	D	215	2% 76% 13% • 9%
2	E	391	70% 14% • 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	391	% 69% 15% • 15%
2	G	391	4% 71% 12% • 15%
2	H	391	8% 73% 10% • 16%

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

Continued on next page...

Continued from previous page...

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 (CCD ID: ZN) (formula: Zn).

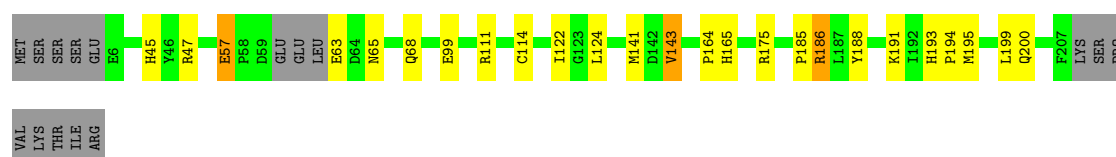
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

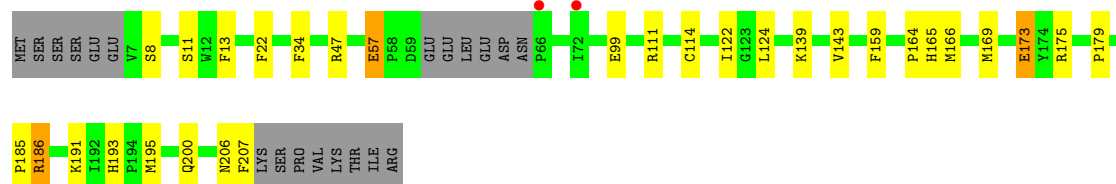
- Molecule 1: Casein kinase II subunit beta

Chain A: 



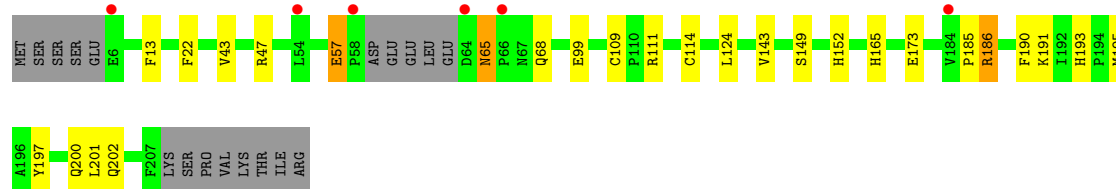
- Molecule 1: Casein kinase II subunit beta

Chain B: 



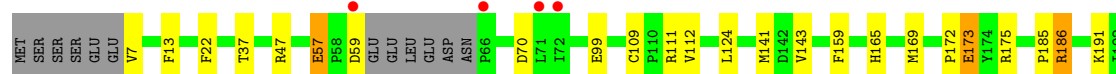
- Molecule 1: Casein kinase II subunit beta

Chain C: 



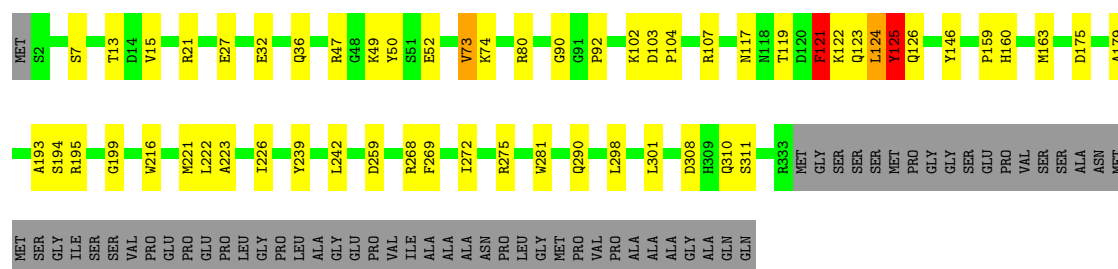
- Molecule 1: Casein kinase II subunit beta

Chain D: 

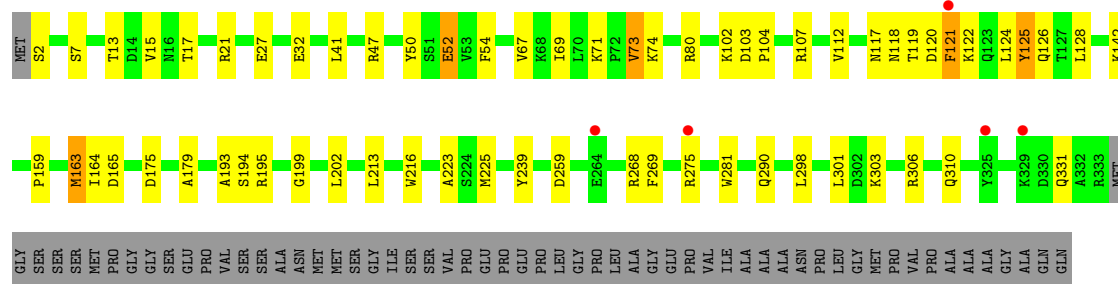




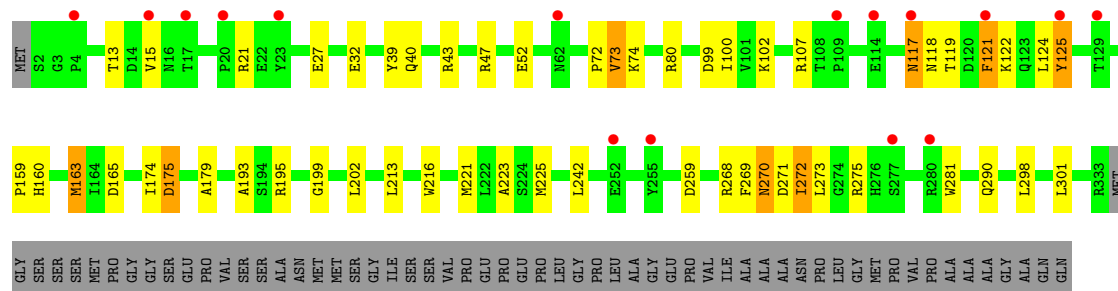
• Molecule 2: Casein kinase II subunit alpha



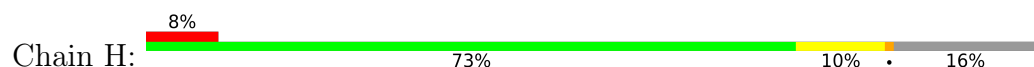
• Molecule 2: Casein kinase II subunit alpha

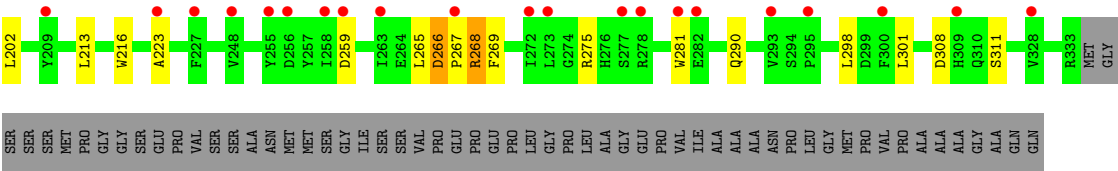


• Molecule 2: Casein kinase II subunit alpha



• Molecule 2: Casein kinase II subunit alpha





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	142.32Å 57.96Å 186.19Å 90.00° 102.42° 90.00°	Depositor
Resolution (Å)	181.83 – 3.10 181.83 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.9 (181.83-3.10) 96.1 (181.83-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.77	1/1671 (0.1%)	0.91	2/2265 (0.1%)
1	B	0.74	0/1641	0.92	3/2223 (0.1%)
1	C	0.68	0/1654	0.90	5/2242 (0.2%)
1	D	0.67	0/1641	0.86	2/2223 (0.1%)
2	E	0.77	0/2879	0.86	4/3893 (0.1%)
2	F	0.75	0/2879	0.84	2/3893 (0.1%)
2	G	0.73	0/2879	0.90	6/3893 (0.2%)
2	H	0.70	0/2869	0.87	7/3879 (0.2%)
All	All	0.73	1/18113 (0.0%)	0.88	31/24511 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	HIS	CG-CD2	5.22	1.41	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	270	ASN	N-CA-C	16.36	132.35	111.24
2	H	175	ASP	N-CA-C	10.49	124.14	111.02
2	G	175	ASP	N-CA-C	10.21	123.78	111.02
2	H	266	ASP	CA-C-N	9.66	131.92	119.84
2	H	266	ASP	C-N-CA	9.66	131.92	119.84
2	G	270	ASN	CB-CA-C	-9.17	95.73	110.86
2	F	193	ALA	N-CA-C	9.01	121.33	108.00
2	G	271	ASP	N-CA-C	-8.47	99.93	111.87
2	H	193	ALA	N-CA-C	8.25	120.21	108.00
2	E	193	ALA	N-CA-C	8.17	120.10	108.00
2	G	193	ALA	N-CA-C	8.14	120.05	108.00
2	H	266	ASP	N-CA-C	-8.03	100.36	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	266	ASP	CB-CA-C	7.52	121.90	109.56
1	C	47	ARG	NE-CZ-NH2	6.96	125.46	119.20
1	A	47	ARG	NE-CZ-NH2	6.76	125.29	119.20
1	C	65	ASN	CA-C-N	6.65	126.90	119.32
1	C	65	ASN	C-N-CA	6.65	126.90	119.32
1	A	47	ARG	NE-CZ-NH1	-6.47	115.03	121.50
2	E	117	ASN	CB-CA-C	6.40	119.87	110.26
1	D	173	GLU	CA-CB-CG	6.34	126.78	114.10
1	C	47	ARG	NE-CZ-NH1	-6.34	115.16	121.50
1	B	173	GLU	CA-CB-CG	6.15	126.40	114.10
2	E	121	PHE	N-CA-C	5.98	119.77	112.23
2	F	175	ASP	N-CA-C	5.98	123.53	110.80
2	G	117	ASN	N-CA-C	-5.94	98.14	110.80
2	E	175	ASP	N-CA-C	5.70	122.95	110.80
2	H	268	ARG	N-CA-C	5.61	120.40	113.50
1	D	47	ARG	CD-NE-CZ	5.38	131.93	124.40
1	B	47	ARG	NE-CZ-NH2	-5.35	114.39	119.20
1	B	47	ARG	CD-NE-CZ	5.33	131.86	124.40
1	C	43	VAL	N-CA-C	5.21	113.81	107.61

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	22	0
1	B	1592	0	1517	26	0
1	C	1605	0	1524	27	0
1	D	1592	0	1517	26	1
2	E	2804	0	2748	29	0
2	F	2804	0	2748	36	0
2	G	2804	0	2748	28	1
2	H	2794	0	2741	18	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	17621	0	17077	187	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 (187) 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:HH11	1:A:186:ARG:HG2	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:HH11	1:C:186:ARG:CG	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:HH11	1:A:186:ARG:CG	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:F:122:LYS:HG3	2:F:159:PRO:HB2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:LYS:NZ	2:F:331:GLN:NE2	2.49	0.60
2:F:142:LYS:NZ	2:F:331:GLN:HE22	1.99	0.60
2:G:272:ILE:HG13	2:G:273:LEU:N	2.16	0.59
1:B:57:GLU:HA	1:B:57:GLU:OE1	2.03	0.59
1:D:186:ARG:HH11	1:D:186:ARG:CG	2.13	0.59
1:D:57:GLU:HA	1:D:57:GLU:OE1	2.03	0.58
1:B:186:ARG:HH11	1:B:186:ARG:CG	2.14	0.58
1:C:57:GLU:OE1	1:C:57:GLU:HA	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:13:PHE:HE2	1:B:22:PHE:CD1	2.22	0.56
1:B:193:HIS:CD2	1:B:195:MET:H	2.22	0.56
2:F:118:ASN:HD22	2:F:163:MET:HE2	1.70	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
2:F:142:LYS:HZ3	2:F:331:GLN:NE2	2.03	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:E:121:PHE:C	2:E:123:GLN:H	2.14	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: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
1:C:65:ASN:CG	1:C:68:GLN:HB2	2.33	0.52
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:B:34:PHE:CZ	2:F:50:TYR:CE2	2.99	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:80:ARG:HD3	2:H:179:ALA:O	2.11	0.50
2:F:119:THR:HB	2:F:164:ILE:O	2.11	0.50
2:E:121:PHE:HD2	2:E:221:MET:HE3	1.76	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
2:G:117:ASN:HD22	2:G:165:ASP:HA	1.77	0.50
2:G:125:TYR:CD1	2:G:225:MET:HG2	2.46	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:A:193:HIS:HB3	2:F:41:LEU:O	2.12	0.49
1:D:124:LEU:HD21	1:D:143:VAL:HG11	1.94	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:H	2:F:124:LEU:HD23	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:223:ALA:HB2	2:H:301:LEU:HD11	1.96	0.48
2:H:266:ASP:HA	2:H:267:PRO:HD2	1.68	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:E:125:TYR:C	2:E:125:TYR:CD2	2.93	0.47
2:G:73:VAL:HG12	2:G:74:LYS:N	2.28	0.47
2:G:242:LEU:HD23	2:G:269:PHE:CE2	2.49	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
1:D:141:MET:HE2	1:D:175:ARG:NH1	2.30	0.47
2:F:103:ASP:O	2:F:104:PRO:C	2.57	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:124:LEU:C	2:E:126:GLN:H	2.24	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:124:LEU:C	2:F:126:GLN:H	2.24	0.45
2:H:73:VAL:HG12	2:H:74:LYS:N	2.29	0.45
2:H:265:LEU:O	2:H:266:ASP:C	2.59	0.45
1:A:193:HIS:CD2	1:A:195:MET:H	2.34	0.45
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:73:VAL:HG12	2:E:74:LYS:N	2.31	0.45
2:E:199:GLY:HA2	2:E:216:TRP:CD1	2.51	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
2:E:121:PHE:CD2	2:E:221:MET:HE3	2.52	0.45
1:C:13:PHE:HE2	1:C:22:PHE:CD1	2.36	0.44
1:C:190:PHE:HD2	2:G:39:TYR:O	2.00	0.44
2:F:125:TYR:CD2	2:F:126:GLN:HG2	2.53	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:E:194:SER:O	2:E:195:ARG:C	2.61	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:C:173:GLU:HG3	1:D:207:PHE:CD2	2.53	0.43
1:D:186:ARG:HG2	1:D:186:ARG:NH1	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:99:ASP:OD1	2:G:100:ILE:N	2.52	0.43
2:H:103:ASP:O	2:H:104:PRO:C	2.60	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:22:PHE:CE2	1:B:159:PHE:CZ	3.07	0.42
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:A:141:MET:HE2	1:A:175:ARG:NH1	2.34	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:142:LYS:HZ1	2:F:331:GLN:HE22	1.66	0.42
2:E:223:ALA:HB2	2:E:301:LEU:HD11	2.02	0.42
2:H:194:SER:O	2:H:195:ARG:C	2.63	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
1:A:193:HIS:CB	2:F:41:LEU:O	2.68	0.41
2:E:92:PRO:HD2	2:E:146:TYR:CG	2.55	0.41
2:G:118:ASN:ND2	2:G:163:MET:HE2	2.35	0.41
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: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:121:PHE:CD2	2:G:221:MET:HE3	2.56	0.41
2:G:174:ILE:HD12	2:G:175:ASP:HB2	2.03	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
1:D:169:MET:SD	2:G:43:ARG:HA	2.62	0.40
2:F:194:SER:O	2:F:195:ARG:C	2.63	0.40
2:F:223:ALA:HB2	2:F:301:LEU:HD11	2.03	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
2	E	330/391 (84%)	310 (94%)	19 (6%)	1 (0%)	36	67
2	F	330/391 (84%)	313 (95%)	17 (5%)	0	100	100
2	G	330/391 (84%)	308 (93%)	21 (6%)	1 (0%)	36	67
2	H	328/391 (84%)	312 (95%)	15 (5%)	1 (0%)	36	67
All	All	2088/2424 (86%)	1991 (95%)	94 (4%)	3 (0%)	48	78

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%)	37	66
1	B	171/191 (90%)	167 (98%)	4 (2%)	44	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	172/191 (90%)	168 (98%)	4 (2%)	44	70
1	D	171/191 (90%)	163 (95%)	8 (5%)	23	55
2	E	305/347 (88%)	289 (95%)	16 (5%)	21	51
2	F	305/347 (88%)	288 (94%)	17 (6%)	19	49
2	G	305/347 (88%)	287 (94%)	18 (6%)	18	48
2	H	304/347 (88%)	289 (95%)	15 (5%)	22	53
All	All	1907/2152 (89%)	1820 (95%)	87 (5%)	24	55

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	63	GLU
1	A	99	GLU
1	A	143	VAL
1	A	186	ARG
1	B	57	GLU
1	B	99	GLU
1	B	173	GLU
1	B	186	ARG
1	C	57	GLU
1	C	99	GLU
1	C	186	ARG
1	C	202	GLN
1	D	7	VAL
1	D	57	GLU
1	D	59	ASP
1	D	99	GLU
1	D	173	GLU
1	D	186	ARG
1	D	201	LEU
1	D	205	SER
2	E	13	THR
2	E	15	VAL
2	E	21	ARG
2	E	27	GLU
2	E	32	GLU
2	E	47	ARG
2	E	52	GLU
2	E	73	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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	27	GLU
2	F	32	GLU
2	F	47	ARG
2	F	52	GLU
2	F	73	VAL
2	F	120	ASP
2	F	121	PHE
2	F	125	TYR
2	F	163	MET
2	F	259	ASP
2	F	275	ARG
2	F	290	GLN
2	G	13	THR
2	G	15	VAL
2	G	21	ARG
2	G	27	GLU
2	G	32	GLU
2	G	47	ARG
2	G	52	GLU
2	G	73	VAL
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	270	ASN
2	G	272	ILE
2	G	275	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	290	GLN
2	H	13	THR
2	H	21	ARG
2	H	27	GLU
2	H	32	GLU
2	H	47	ARG
2	H	52	GLU
2	H	73	VAL
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	275	ARG
2	H	290	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	117	GLN
1	A	151	HIS
1	A	165	HIS
1	A	171	HIS
1	A	193	HIS
1	B	165	HIS
1	B	171	HIS
1	B	193	HIS
1	C	165	HIS
1	C	193	HIS
1	D	165	HIS
1	D	193	HIS
2	E	35	ASN
2	E	36	GLN
2	E	160	HIS
2	E	270	ASN
2	E	290	GLN
2	E	291	HIS
2	E	310	GLN
2	F	29	HIS
2	F	35	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	36	GLN
2	F	40	GLN
2	F	117	ASN
2	F	118	ASN
2	F	160	HIS
2	F	270	ASN
2	F	291	HIS
2	F	310	GLN
2	F	331	GLN
2	G	29	HIS
2	G	35	ASN
2	G	36	GLN
2	G	93	ASN
2	G	117	ASN
2	G	118	ASN
2	G	160	HIS
2	G	270	ASN
2	G	290	GLN
2	G	291	HIS
2	G	310	GLN
2	H	35	ASN
2	H	36	GLN
2	H	117	ASN
2	H	123	GLN
2	H	160	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 oligosaccharides 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, 95th 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 ²)	Q<0.9
1	A	199/215 (92%)	-0.37	0 100 100	14, 31, 61, 88	0
1	B	195/215 (90%)	-0.02	2 (1%) 79 61	21, 41, 71, 97	0
1	C	197/215 (91%)	0.42	6 (3%) 52 31	39, 65, 109, 155	0
1	D	195/215 (90%)	0.28	4 (2%) 63 42	36, 61, 90, 116	0
2	E	332/391 (84%)	-0.18	0 100 100	21, 36, 61, 95	0
2	F	332/391 (84%)	0.13	5 (1%) 72 52	25, 45, 81, 100	0
2	G	332/391 (84%)	0.42	16 (4%) 35 19	30, 61, 98, 123	0
2	H	330/391 (84%)	0.96	31 (9%) 14 8	51, 86, 116, 131	0
All	All	2112/2424 (87%)	0.24	64 (3%) 52 31	14, 52, 103, 155	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	4	PRO	5.1
1	B	66	PRO	4.0
1	D	66	PRO	4.0
1	C	58	PRO	3.9
2	H	227	PHE	3.3
2	H	125	TYR	3.3
2	H	281	TRP	3.2
2	H	258	ILE	3.1
1	C	6	GLU	3.1
2	H	263	ILE	3.0
2	H	256	ASP	3.0
2	H	273	LEU	3.0
2	H	20	PRO	2.9
2	H	18	HIS	2.9
2	H	121	PHE	2.9
2	H	272	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	109	PRO	2.7
2	H	267	PRO	2.6
1	D	59	ASP	2.6
2	G	252	GLU	2.6
2	H	223	ALA	2.6
2	G	125	TYR	2.5
1	D	72	ILE	2.5
2	F	121	PHE	2.5
1	C	66	PRO	2.5
2	H	295	PRO	2.5
2	H	282	GLU	2.4
2	H	309	HIS	2.4
2	G	117	ASN	2.4
2	F	325	TYR	2.4
2	H	293	VAL	2.4
2	H	186	GLN	2.4
2	G	20	PRO	2.4
2	F	329	LYS	2.3
1	C	54	LEU	2.3
2	G	23	TYR	2.3
2	H	128	LEU	2.3
1	B	72	ILE	2.2
2	H	278	ARG	2.2
2	G	280	ARG	2.2
2	G	15	VAL	2.2
2	H	259	ASP	2.2
2	G	17	THR	2.2
2	G	129	THR	2.2
2	H	5	VAL	2.2
1	C	184	VAL	2.1
2	H	277	SER	2.1
2	F	264	GLU	2.1
2	H	187	GLU	2.1
2	G	4	PRO	2.1
2	G	121	PHE	2.1
2	H	209	TYR	2.1
2	G	114	GLU	2.1
2	H	328	VAL	2.1
2	G	255	TYR	2.1
2	F	275	ARG	2.1
2	H	300	PHE	2.1
2	G	277	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	255	TYR	2.1
2	G	62	ASN	2.0
1	C	64	ASP	2.0
2	H	22	GLU	2.0
2	H	248	VAL	2.0
1	D	71	LEU	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 oligosaccharides 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, 95th 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	A	301	1/1	1.00	0.02	14,14,14,14	0
3	ZN	B	301	1/1	1.00	0.02	17,17,17,17	0
3	ZN	C	301	1/1	1.00	0.01	32,32,32,32	0
3	ZN	D	301	1/1	1.00	0.02	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.