



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2017 – 09:08 AM EDT

PDB ID : 1VYA  
Title : Identification and characterization of the first plant G-quadruplex binding protein encoded by the Zea mays L. nucleoside diphosphate1 gene, ZmNDPK1  
Authors : Kopylov, M.; Stroupe, M.E.  
Deposited on : unknown  
Resolution : 2.05 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

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

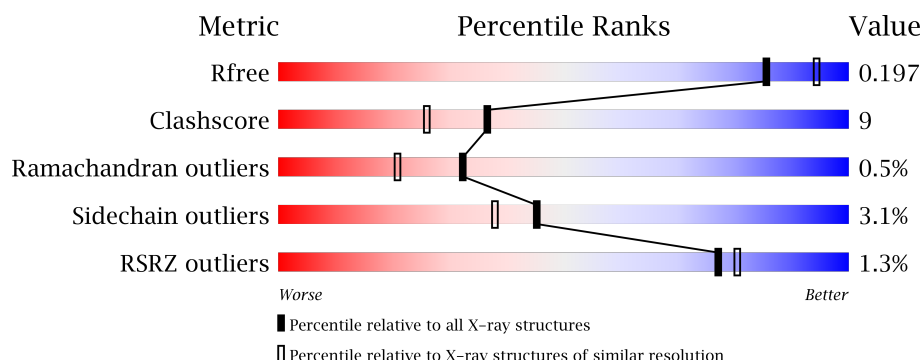
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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	149	<div> <div>0.1%</div> <div>87%</div> <div>13%</div> <div>0.1%</div> </div>
1	B	149	<div> <div>0.1%</div> <div>81%</div> <div>17%</div> <div>0.1%</div> </div>
1	C	149	<div> <div>0.1%</div> <div>80%</div> <div>20%</div> <div>0.1%</div> </div>
1	D	149	<div> <div>2%</div> <div>82%</div> <div>17%</div> <div>0.1%</div> </div>
1	E	149	<div> <div>0.1%</div> <div>80%</div> <div>18%</div> <div>0.1%</div> </div>

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Mol	Chain	Length	Quality of chain	
1	F	149	85%	15%
1	G	149	81%	18%
1	H	149	78%	21%
1	I	149	84%	15%
1	J	149	86%	13%
1	K	149	78%	21%
1	L	149	81%	17%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 16251 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	7	0
			1216	788	208	217	3			
1	B	149	Total	C	N	O	S	8	9	0
			1230	797	212	218	3			
1	C	149	Total	C	N	O	S	0	7	0
			1213	788	205	217	3			
1	D	149	Total	C	N	O	S	0	8	0
			1217	794	205	215	3			
1	E	149	Total	C	N	O	S	8	4	0
			1202	776	204	219	3			
1	F	149	Total	C	N	O	S	5	8	0
			1215	791	205	216	3			
1	G	149	Total	C	N	O	S	13	10	0
			1229	802	205	219	3			
1	H	149	Total	C	N	O	S	0	9	0
			1222	794	205	220	3			
1	I	149	Total	C	N	O	S	8	9	0
			1218	790	204	221	3			
1	J	149	Total	C	N	O	S	8	7	0
			1214	788	206	217	3			
1	K	149	Total	C	N	O	S	8	9	0
			1218	793	202	220	3			
1	L	149	Total	C	N	O	S	8	4	0
			1194	774	202	215	3			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	140	Total	O	0	0
			140	140		
2	B	147	Total	O	0	0
			147	147		

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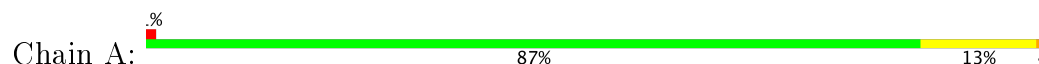
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	130	Total 130	O 130	0	0
2	D	130	Total 130	O 130	0	0
2	E	160	Total 160	O 160	0	0
2	F	145	Total 145	O 145	0	0
2	G	139	Total 139	O 139	0	0
2	H	152	Total 152	O 152	0	0
2	I	133	Total 133	O 133	0	0
2	J	143	Total 143	O 143	0	0
2	K	131	Total 131	O 131	0	0
2	L	113	Total 113	O 113	0	0

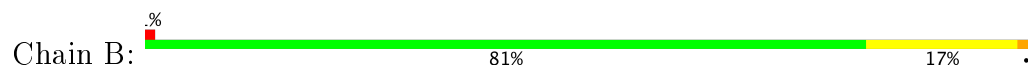
### 3 Residue-property plots [i](#)

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.

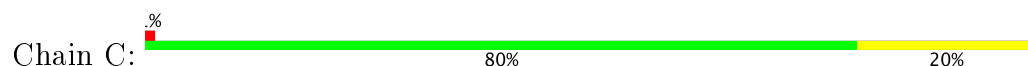
- Molecule 1: Nucleoside diphosphate kinase



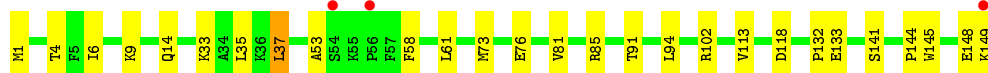
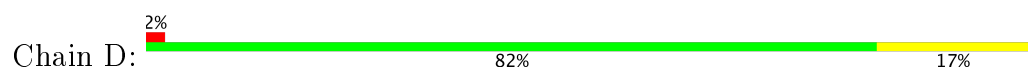
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



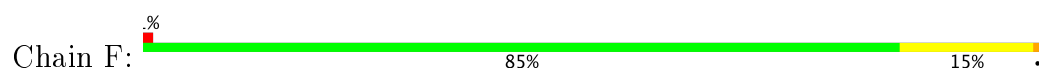
- Molecule 1: Nucleoside diphosphate kinase



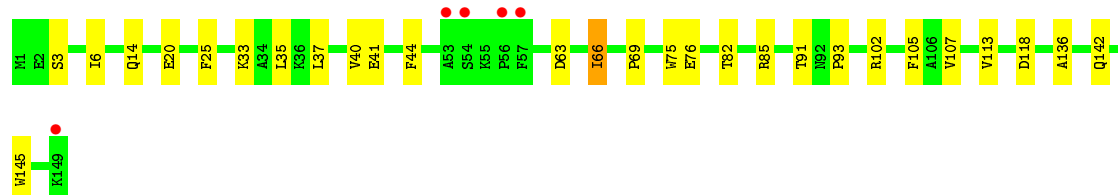
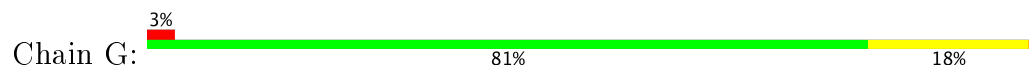
- Molecule 1: Nucleoside diphosphate kinase



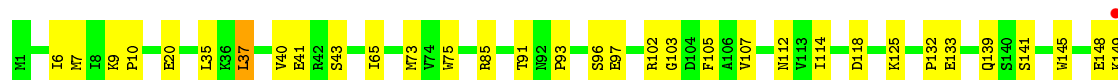
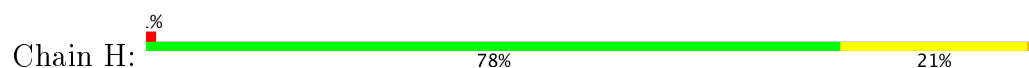
- Molecule 1: Nucleoside diphosphate kinase



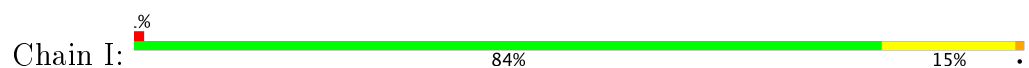
- Molecule 1: Nucleoside diphosphate kinase



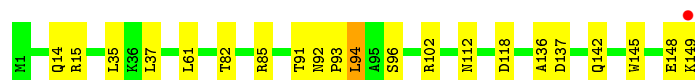
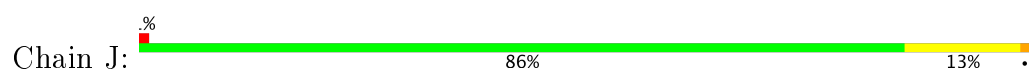
- Molecule 1: Nucleoside diphosphate kinase



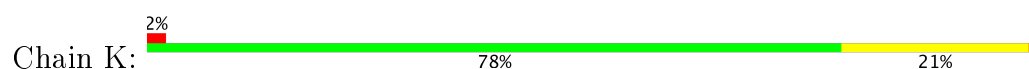
- Molecule 1: Nucleoside diphosphate kinase



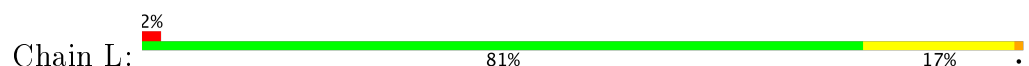
- Molecule 1: Nucleoside diphosphate kinase

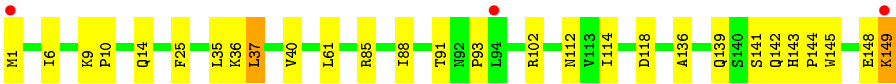


- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase





GLOBAL-STATISTICS INFOmissingINFO

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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	0.36	0/1266	0.49	0/1709
1	B	0.37	0/1286	0.50	0/1735
1	C	0.36	0/1263	0.49	0/1706
1	D	0.36	0/1270	0.50	0/1716
1	E	0.38	0/1237	0.53	0/1671
1	F	0.36	0/1268	0.52	0/1713
1	G	0.36	0/1288	0.48	0/1740
1	H	0.37	0/1278	0.51	0/1726
1	I	0.37	0/1274	0.53	0/1721
1	J	0.37	0/1264	0.50	0/1706
1	K	0.39	0/1274	0.55	0/1722
1	L	0.36	0/1235	0.53	0/1669
All	All	0.37	0/15203	0.51	0/20534

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 4.2 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	1216	0	1247	20	0
1	B	1230	0	1268	34	1
1	C	1213	0	1245	21	0
1	D	1217	0	1261	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1202	0	1210	24	0
1	F	1215	0	1255	27	0
1	G	1229	0	1273	22	0
1	H	1222	0	1256	32	0
1	I	1218	0	1247	24	0
1	J	1214	0	1247	17	0
1	K	1218	0	1252	28	1
1	L	1194	0	1215	30	0
2	A	140	0	0	5	0
2	B	147	0	0	12	0
2	C	130	0	0	8	0
2	D	130	0	0	3	0
2	E	160	0	0	5	0
2	F	145	0	0	3	0
2	G	139	0	0	2	0
2	H	152	0	0	2	0
2	I	133	0	0	4	0
2	J	143	0	0	1	0
2	K	131	0	0	8	0
2	L	113	0	0	11	0
All	All	16251	0	14976	262	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 9.

All (262) 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:20[B]:GLU:OE2	2:B:266:HOH:O	1.66	1.12
1:A:85:ARG:NH2	2:A:284:HOH:O	1.82	1.09
1:I:102[B]:ARG:NH1	1:I:114:ILE:O	1.91	1.04
1:E:137:ASP:OD1	2:E:246:HOH:O	1.81	0.96
1:B:85[B]:ARG:NH1	2:B:309:HOH:O	1.95	0.93
1:H:141[A]:SER:OG	2:H:271:HOH:O	1.64	0.90
1:F:141:SER:OG	1:I:142[B]:GLN:NE2	2.04	0.89
1:A:110:GLY:O	1:A:111[A]:ARG:NH2	2.05	0.89
1:A:78:LYS:NZ	2:A:338:HOH:O	2.07	0.86
1:F:142:GLN:NE2	1:I:142[B]:GLN:HE21	1.73	0.86
1:L:1:MET:HG2	2:L:217:HOH:O	1.75	0.85
1:C:78:LYS:HE3	1:C:147:TYR:CD2	2.12	0.85
1:K:27:LYS:NZ	2:K:314:HOH:O	1.98	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1:MET:HB2	2:L:225:HOH:O	1.79	0.82
1:C:59:GLN:OE1	2:C:201:HOH:O	1.96	0.81
1:C:142:GLN:NE2	2:C:248:HOH:O	2.12	0.80
1:E:85:ARG:NH2	1:E:118:ASP:HA	1.98	0.78
1:A:42[A]:ARG:NH1	2:A:201:HOH:O	2.17	0.78
1:B:85[B]:ARG:NE	2:B:309:HOH:O	2.16	0.78
1:I:42:ARG:HA	1:I:66:ILE:HD11	1.66	0.77
1:E:85:ARG:HH21	1:E:118:ASP:HA	1.48	0.77
1:G:85[A]:ARG:HD2	1:G:118:ASP:HA	1.66	0.77
1:I:118:ASP:OD1	2:I:201:HOH:O	2.03	0.77
1:L:85:ARG:HD2	1:L:118:ASP:HA	1.67	0.75
1:D:76:GLU:OE2	2:D:264:HOH:O	2.03	0.75
1:D:85[A]:ARG:HD2	1:D:118:ASP:HA	1.70	0.74
1:F:76:GLU:OE2	2:F:303:HOH:O	2.05	0.74
1:H:37:LEU:HD13	1:L:136:ALA:HB3	1.70	0.74
1:C:20[A]:GLU:CD	2:C:235:HOH:O	2.25	0.74
1:E:148:GLU:O	1:E:149:LYS:HB3	1.86	0.73
1:B:142:GLN:NE2	1:L:142:GLN:HG2	2.03	0.73
1:B:111[A]:ARG:NH2	1:D:144:PRO:O	2.23	0.72
1:L:1:MET:SD	2:L:225:HOH:O	2.48	0.71
1:B:59[B]:GLN:NE2	2:B:201:HOH:O	2.16	0.71
1:G:85[B]:ARG:HD3	1:G:118:ASP:HA	1.71	0.71
1:K:78:LYS:NZ	2:K:319:HOH:O	2.24	0.71
1:C:97:GLU:OE2	2:C:308:HOH:O	2.09	0.70
1:H:102[A]:ARG:HD3	1:H:112:ASN:HB2	1.73	0.70
1:B:20[A]:GLU:CD	2:B:259:HOH:O	2.30	0.69
1:G:3:SER:HB3	1:G:76[B]:GLU:HG2	1.72	0.69
1:L:142:GLN:NE2	2:L:264:HOH:O	2.27	0.68
1:L:102[B]:ARG:NH1	1:L:114:ILE:O	2.25	0.68
1:E:20[A]:GLU:HG3	2:E:326:HOH:O	1.94	0.68
1:E:55:LYS:HD3	1:E:57:PHE:CZ	2.28	0.67
1:B:85[A]:ARG:NH1	2:B:280:HOH:O	2.27	0.67
1:L:91:THR:O	1:L:93:PRO:HD3	1.96	0.66
1:B:85[A]:ARG:HD2	1:B:118:ASP:HA	1.77	0.66
1:L:1:MET:CG	2:L:217:HOH:O	2.36	0.66
1:C:20[A]:GLU:OE2	2:C:235:HOH:O	2.13	0.65
1:B:115:HIS:ND1	2:B:258:HOH:O	2.27	0.65
1:J:91:THR:HA	1:J:102[B]:ARG:NH2	2.12	0.65
1:I:27:LYS:HD2	2:I:266:HOH:O	1.95	0.65
1:A:111[A]:ARG:HG2	1:A:111[A]:ARG:HH21	1.62	0.65
1:D:33:LYS:HE3	1:D:76:GLU:OE2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:VAL:CG1	1:B:85[B]:ARG:HH22	2.11	0.63
1:D:81:VAL:HG12	1:D:85[B]:ARG:HH22	1.63	0.63
1:D:85[B]:ARG:HD3	1:D:118:ASP:HA	1.81	0.62
1:D:4:THR:HG23	1:D:6:ILE:CD1	2.29	0.62
1:A:35:LEU:HB3	1:F:37:LEU:HB2	1.80	0.62
1:E:102[B]:ARG:NH1	1:E:114:ILE:O	2.27	0.62
1:K:91:THR:HA	1:K:102[B]:ARG:NH2	2.14	0.62
1:A:110:GLY:C	1:A:111[A]:ARG:HH21	2.03	0.62
1:B:81:VAL:HG12	1:B:85[B]:ARG:HH22	1.64	0.62
1:G:91:THR:HA	1:G:102[B]:ARG:NH2	2.14	0.61
1:I:42:ARG:HA	1:I:66:ILE:CD1	2.31	0.61
1:K:85:ARG:HD2	1:K:118:ASP:HA	1.82	0.61
1:B:85[B]:ARG:HD3	1:B:118:ASP:HA	1.82	0.61
1:A:125:LYS:NZ	2:A:330:HOH:O	2.33	0.60
1:J:91:THR:O	1:J:93:PRO:HD3	2.00	0.60
1:D:148:GLU:O	1:D:149:LYS:HB2	2.00	0.60
1:D:4:THR:HG23	1:D:6:ILE:HD13	1.83	0.60
1:K:91:THR:O	1:K:93:PRO:HD3	2.02	0.60
1:C:85[A]:ARG:HD2	1:C:118:ASP:HA	1.84	0.59
1:D:94:LEU:HD12	2:D:247:HOH:O	2.02	0.59
1:H:91:THR:O	1:H:93:PRO:HD3	2.02	0.59
1:K:55:LYS:HB3	1:K:56:PRO:HD2	1.85	0.59
1:L:1:MET:HB3	2:L:217:HOH:O	2.01	0.59
1:G:102[A]:ARG:NH1	2:G:311:HOH:O	2.35	0.59
1:I:66:ILE:O	1:I:66:ILE:HG22	2.01	0.59
1:E:37:LEU:HD13	1:K:136:ALA:HB3	1.83	0.59
1:H:35:LEU:HB3	1:L:37:LEU:HB2	1.85	0.58
1:D:132:PRO:HD2	1:D:133:GLU:OE1	2.03	0.58
1:E:102[A]:ARG:NH1	2:E:274:HOH:O	2.29	0.58
1:B:111[A]:ARG:NH1	2:B:303:HOH:O	2.36	0.58
1:F:91:THR:HA	1:F:102[B]:ARG:NH2	2.18	0.58
1:F:97:GLU:OE2	2:F:296:HOH:O	2.17	0.58
1:L:1:MET:CG	2:L:225:HOH:O	2.51	0.57
1:K:42:ARG:NE	2:K:201:HOH:O	1.57	0.57
1:J:93:PRO:HA	1:J:96:SER:OG	2.04	0.57
1:A:111[A]:ARG:HG2	1:A:111[A]:ARG:NH2	2.18	0.57
1:B:37:LEU:HB2	1:G:35:LEU:HB3	1.86	0.56
1:L:1:MET:CB	2:L:217:HOH:O	2.52	0.56
1:G:41:GLU:C	1:G:66[A]:ILE:HD11	2.26	0.56
1:G:6[A]:ILE:HD12	1:G:75:TRP:CD1	2.41	0.56
1:D:81:VAL:HG12	1:D:85[B]:ARG:NH2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:LYS:HE2	2:D:253:HOH:O	2.05	0.55
1:D:37[A]:LEU:HB2	1:J:35:LEU:HB3	1.88	0.55
1:C:132:PRO:HD2	1:C:133:GLU:OE1	2.07	0.55
1:E:91:THR:HA	1:E:102[B]:ARG:NH2	2.22	0.55
1:E:92:ASN:OD1	1:E:94:LEU:HB2	2.07	0.54
1:H:85[B]:ARG:HH21	1:H:118:ASP:HA	1.72	0.54
1:G:40:VAL:HG13	1:G:44:PHE:HD2	1.73	0.54
1:A:85:ARG:HD2	1:A:118:ASP:HA	1.90	0.54
1:B:91:THR:HA	1:B:102[B]:ARG:NH2	2.23	0.54
1:C:85[B]:ARG:HD3	1:C:118:ASP:HA	1.90	0.54
1:H:148:GLU:O	1:H:149:LYS:HB2	2.07	0.54
1:J:92:ASN:OD1	1:J:94:LEU:HB2	2.08	0.54
1:F:142:GLN:NE2	1:F:142:GLN:HA	2.23	0.53
1:F:82[A]:THR:HG23	2:F:321:HOH:O	2.07	0.53
1:A:51:ASP:HB2	2:A:320:HOH:O	2.07	0.53
1:K:55:LYS:HE2	1:K:55:LYS:HA	1.91	0.53
1:H:141[B]:SER:HB2	2:H:271:HOH:O	2.09	0.53
1:K:86:LYS:HE3	2:K:307:HOH:O	2.07	0.53
1:K:92:ASN:HA	1:K:109[B]:ILE:HG12	1.90	0.53
1:B:148:GLU:HG2	1:B:149:LYS:HG3	1.91	0.52
1:H:93:PRO:HA	1:H:96:SER:OG	2.10	0.52
1:I:148:GLU:HG2	1:I:149:LYS:HG3	1.90	0.52
2:B:275:HOH:O	1:L:141:SER:HB2	2.08	0.52
1:I:91[A]:THR:HG21	2:I:223:HOH:O	2.09	0.52
1:H:37:LEU:HB2	1:L:35:LEU:HB3	1.92	0.51
1:C:125:LYS:HE2	2:C:264:HOH:O	2.09	0.51
1:F:142:GLN:CD	1:I:142[B]:GLN:HE21	2.14	0.51
1:J:91:THR:HA	1:J:102[B]:ARG:HH21	1.76	0.51
1:G:82[B]:THR:HG22	1:G:85[B]:ARG:HH11	1.76	0.50
1:J:85:ARG:HD3	1:J:118[A]:ASP:HA	1.93	0.50
1:H:7:MET:SD	1:H:65:ILE:HD11	2.51	0.50
1:F:142:GLN:HE21	1:F:142:GLN:HA	1.76	0.50
1:B:91:THR:HA	1:B:102[B]:ARG:HH21	1.77	0.49
1:H:85[A]:ARG:HD3	1:H:118:ASP:HA	1.94	0.49
1:B:42[A]:ARG:HG2	1:B:66:ILE:HD13	1.94	0.49
1:G:6[A]:ILE:HD13	1:G:25:PHE:CE1	2.48	0.49
1:B:137:ASP:CG	2:B:254:HOH:O	2.50	0.49
1:G:20[A]:GLU:HG2	1:G:105:PHE:CZ	2.47	0.49
1:G:91:THR:HA	1:G:102[B]:ARG:HH21	1.76	0.49
1:I:132:PRO:HD2	1:I:133:GLU:OE1	2.13	0.49
1:J:102[A]:ARG:CD	1:J:112:ASN:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:85:ARG:HD3	1:J:118[B]:ASP:HA	1.95	0.49
1:L:40[A]:VAL:HG23	2:L:236:HOH:O	2.13	0.48
1:H:85[B]:ARG:HH22	1:H:118:ASP:HB3	1.78	0.48
1:C:148:GLU:O	1:C:149:LYS:HB2	2.13	0.48
1:B:143:HIS:N	1:B:144:PRO:HD2	2.29	0.48
1:B:20[A]:GLU:OE2	2:B:259:HOH:O	2.19	0.48
1:C:78:LYS:HE3	1:C:147:TYR:HD2	1.71	0.48
1:B:81:VAL:HG12	1:B:85[B]:ARG:NH2	2.28	0.48
1:E:53:ALA:HA	1:E:58:PHE:CD1	2.48	0.48
1:H:6[A]:ILE:HG12	1:H:75:TRP:CD1	2.49	0.48
1:H:132:PRO:HD2	1:H:133:GLU:OE1	2.14	0.48
1:E:35:LEU:HB3	1:K:37:LEU:HB2	1.95	0.48
1:K:55:LYS:CA	1:K:55:LYS:HE2	2.43	0.48
1:H:35:LEU:O	1:L:36:LYS:HA	2.14	0.48
1:A:136:ALA:HB3	1:F:37:LEU:HD13	1.95	0.47
1:G:91:THR:O	1:G:93:PRO:HD3	2.13	0.47
1:J:148:GLU:HG2	1:J:149:LYS:HG3	1.95	0.47
1:D:53:ALA:HA	1:D:58:PHE:CD1	2.49	0.47
1:D:14:GLN:HG3	1:H:145:TRP:CE2	2.49	0.47
1:F:85[B]:ARG:CZ	1:F:118:ASP:O	2.62	0.47
1:G:14:GLN:HG3	1:L:145:TRP:CE2	2.49	0.47
1:K:42:ARG:HH22	1:K:59:GLN:HG3	1.78	0.47
1:E:82[B]:THR:HG23	2:E:250:HOH:O	2.13	0.47
1:L:102[A]:ARG:HD2	1:L:112:ASN:HB2	1.96	0.47
1:E:1:MET:N	2:E:310:HOH:O	2.47	0.47
1:J:82[B]:THR:HG23	2:J:244:HOH:O	2.14	0.47
1:K:53:ALA:HA	1:K:58:PHE:CD1	2.50	0.47
1:A:37:LEU:HB2	1:F:35:LEU:HB3	1.96	0.47
1:C:36:LYS:HA	1:I:35:LEU:O	2.14	0.47
1:G:145:TRP:CE2	1:J:14:GLN:HG3	2.50	0.47
1:E:37:LEU:HB2	1:K:35:LEU:HB3	1.96	0.47
1:I:98:PRO:HD3	1:K:86:LYS:HD3	1.97	0.47
1:L:91:THR:HA	1:L:102[A]:ARG:NH1	2.30	0.47
1:H:6[A]:ILE:HD11	1:H:75:TRP:HE1	1.80	0.47
1:A:102[B]:ARG:NH1	1:A:114:ILE:O	2.41	0.46
1:D:141:SER:HB3	2:G:327:HOH:O	2.14	0.46
1:E:91:THR:HA	1:E:102[B]:ARG:HH21	1.78	0.46
1:E:91:THR:O	1:E:93:PRO:HD3	2.14	0.46
1:H:20[A]:GLU:HG2	1:H:105:PHE:CZ	2.50	0.46
1:D:81:VAL:CG1	1:D:85[B]:ARG:HH22	2.28	0.46
1:J:142:GLN:HA	1:J:142:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLY:C	1:A:111[A]:ARG:NH2	2.64	0.46
1:D:91:THR:HA	1:D:102[B]:ARG:NH2	2.30	0.46
1:F:91:THR:HA	1:F:102[B]:ARG:HH21	1.81	0.46
1:L:1:MET:CB	2:L:225:HOH:O	2.48	0.46
1:E:93:PRO:HA	1:E:96:SER:OG	2.16	0.46
1:F:148:GLU:O	1:F:149:LYS:HB2	2.16	0.46
1:J:145:TRP:CE2	1:L:14:GLN:HG3	2.50	0.46
1:F:85[B]:ARG:HD3	1:F:118:ASP:HA	1.97	0.46
1:H:37:LEU:HD13	1:L:136:ALA:CB	2.44	0.46
1:B:37:LEU:HD13	1:G:136:ALA:HB3	1.98	0.45
1:E:85:ARG:HD3	1:E:117:SER:O	2.17	0.45
1:L:88:ILE:O	1:L:102[A]:ARG:HG3	2.16	0.45
1:C:20[A]:GLU:HG2	1:C:105:PHE:CZ	2.52	0.45
1:F:142:GLN:HG2	1:I:142[B]:GLN:NE2	2.31	0.45
1:K:94:LEU:HD12	2:K:282:HOH:O	2.17	0.45
1:H:6[A]:ILE:HD11	1:H:75:TRP:NE1	2.31	0.45
1:A:111[A]:ARG:NH2	1:I:148:GLU:HB2	2.32	0.45
1:G:142:GLN:HE22	1:J:15[B]:ARG:HA	1.81	0.45
1:J:102[A]:ARG:HD3	1:J:112:ASN:HB2	1.98	0.45
1:L:148:GLU:HG2	1:L:149:LYS:HG3	1.98	0.45
1:I:141[A]:SER:OG	2:I:259:HOH:O	2.06	0.44
1:L:6:ILE:HD13	1:L:25:PHE:CZ	2.52	0.44
1:K:91:THR:HA	1:K:102[B]:ARG:HH21	1.81	0.44
1:C:8:ILE:HB	1:C:71:VAL:HB	2.00	0.44
1:H:125:LYS:HB3	1:H:125:LYS:HE2	1.73	0.44
1:H:6[A]:ILE:HG12	1:H:75:TRP:HD1	1.82	0.44
1:H:97:GLU:O	1:H:103:GLY:HA3	2.17	0.44
1:E:36:LYS:HA	1:K:35:LEU:O	2.17	0.44
1:C:34:ALA:HB1	1:C:131:PHE:CE2	2.53	0.44
1:K:42:ARG:NH2	2:K:201:HOH:O	2.45	0.44
1:C:69:PRO:HD2	2:C:237:HOH:O	2.18	0.43
1:C:81:VAL:HG12	1:C:85[B]:ARG:HH22	1.82	0.43
1:H:102[B]:ARG:NH1	1:H:114:ILE:O	2.46	0.43
1:I:15[B]:ARG:HA	1:K:142:GLN:NE2	2.33	0.43
1:A:111[A]:ARG:CG	1:A:111[A]:ARG:HH21	2.31	0.43
1:E:85:ARG:NH2	1:E:118:ASP:CA	2.78	0.43
1:G:63:ASP:O	1:G:66[B]:ILE:HG12	2.18	0.43
1:I:66:ILE:CG2	1:I:66:ILE:O	2.66	0.43
1:F:52:LEU:O	1:F:58:PHE:HB2	2.19	0.43
1:H:37:LEU:CD1	1:L:136:ALA:HB3	2.46	0.43
1:B:102[A]:ARG:CD	1:B:112:ASN:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LYS:HA	1:F:35:LEU:O	2.19	0.42
1:H:85[A]:ARG:HG3	1:H:85[A]:ARG:HH21	1.84	0.42
1:L:9:LYS:HB3	1:L:10:PRO:CD	2.49	0.42
1:F:141:SER:HG	1:I:142[B]:GLN:HE22	1.59	0.42
1:B:85[B]:ARG:CZ	2:B:309:HOH:O	2.33	0.42
1:B:36:LYS:HG3	1:B:38:VAL:HG23	2.00	0.42
1:B:78:LYS:HB2	1:B:78:LYS:HE2	1.72	0.42
1:I:102[A]:ARG:HD2	1:I:112[A]:ASN:OD1	2.19	0.42
1:F:85[B]:ARG:NH1	1:F:118:ASP:O	2.53	0.42
1:E:52:LEU:O	1:E:55:LYS:HB2	2.20	0.42
1:K:102[A]:ARG:CD	1:K:112:ASN:HB2	2.50	0.42
1:F:34:ALA:HB1	1:F:131:PHE:CE2	2.54	0.42
1:G:6[A]:ILE:HD12	1:G:75:TRP:HD1	1.81	0.42
1:B:28:LYS:O	1:H:107[B]:VAL:HG13	2.20	0.42
1:D:35:LEU:HD12	1:D:73:MET:HG2	2.02	0.42
1:E:9:LYS:HB3	1:E:10:PRO:CD	2.50	0.41
1:H:41[A]:GLU:OE1	1:H:43:SER:HB3	2.20	0.41
1:F:7:MET:SD	1:F:65:ILE:HD11	2.59	0.41
1:I:9:LYS:HB3	1:I:10:PRO:HD2	2.01	0.41
1:H:9:LYS:HB3	1:H:10:PRO:CD	2.50	0.41
1:L:143:HIS:N	1:L:144:PRO:HD2	2.34	0.41
1:H:20[B]:GLU:HG3	2:L:207:HOH:O	2.20	0.41
1:D:85[B]:ARG:NH2	1:D:118:ASP:C	2.74	0.41
1:A:9:LYS:HB3	1:A:10:PRO:HD2	2.03	0.41
1:D:37[A]:LEU:HD13	1:J:136:ALA:HB3	2.03	0.41
1:B:17:LEU:HA	1:B:20[B]:GLU:OE1	2.21	0.41
1:C:94:LEU:HD13	1:F:79:SER:HB2	2.03	0.41
1:K:36:LYS:HG3	1:K:38:VAL:CG2	2.51	0.41
1:K:41[B]:GLU:HG2	2:K:213:HOH:O	2.21	0.41
1:K:53:ALA:HA	1:K:58:PHE:CG	2.56	0.41
1:B:85[B]:ARG:NH2	1:B:118:ASP:C	2.75	0.41
1:C:24:ARG:HD2	2:C:216:HOH:O	2.21	0.41
1:G:33:LYS:HG3	1:G:76[B]:GLU:CD	2.41	0.41
1:C:143:HIS:N	1:C:144:PRO:HD2	2.36	0.40
1:B:14:GLN:HG3	1:D:145:TRP:CE2	2.56	0.40
1:H:6[A]:ILE:HG13	1:H:73:MET:HE3	2.02	0.40
1:K:108:ASP:OD2	2:K:316:HOH:O	2.21	0.40
1:B:125:LYS:HE3	1:B:125:LYS:HB3	1.84	0.40
1:I:14:GLN:HG3	1:K:145:TRP:CE2	2.56	0.40
1:I:8:ILE:HB	1:I:71:VAL:HB	2.03	0.40
1:A:35:LEU:O	1:F:36:LYS:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:TRP:HB3	1:G:69:PRO:HD3	2.03	0.40
1:F:148:GLU:HG2	1:F:149:LYS:HG3	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:B:59[B]:GLN:NE2	1:K:43:SER:OG[2_555]	1.87	0.33

## 4.3 Torsion angles [i](#)

### 4.3.1 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	154/149 (103%)	151 (98%)	2 (1%)	1 (1%)	28	17
1	B	156/149 (105%)	153 (98%)	2 (1%)	1 (1%)	28	17
1	C	154/149 (103%)	150 (97%)	3 (2%)	1 (1%)	28	17
1	D	155/149 (104%)	151 (97%)	3 (2%)	1 (1%)	28	17
1	E	151/149 (101%)	147 (97%)	3 (2%)	1 (1%)	25	14
1	F	155/149 (104%)	153 (99%)	2 (1%)	0	100	100
1	G	157/149 (105%)	153 (98%)	3 (2%)	1 (1%)	28	17
1	H	156/149 (105%)	152 (97%)	4 (3%)	0	100	100
1	I	156/149 (105%)	153 (98%)	3 (2%)	0	100	100
1	J	154/149 (103%)	151 (98%)	3 (2%)	0	100	100
1	K	156/149 (105%)	148 (95%)	6 (4%)	2 (1%)	14	5
1	L	151/149 (101%)	148 (98%)	3 (2%)	0	100	100
All	All	1855/1788 (104%)	1810 (98%)	37 (2%)	8 (0%)	32	27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	51	ASP
1	D	113	VAL
1	C	113	VAL
1	B	113	VAL
1	E	113	VAL
1	K	113	VAL
1	A	113	VAL
1	G	113	VAL

#### 4.3.2 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	131/124 (106%)	127 (97%)	4 (3%)	45	38
1	B	133/124 (107%)	129 (97%)	4 (3%)	46	39
1	C	131/124 (106%)	125 (95%)	6 (5%)	31	22
1	D	132/124 (106%)	127 (96%)	5 (4%)	38	30
1	E	128/124 (103%)	122 (95%)	6 (5%)	30	21
1	F	132/124 (106%)	128 (97%)	4 (3%)	46	39
1	G	134/124 (108%)	128 (96%)	6 (4%)	32	23
1	H	133/124 (107%)	130 (98%)	3 (2%)	56	49
1	I	133/124 (107%)	126 (95%)	7 (5%)	26	16
1	J	131/124 (106%)	127 (97%)	4 (3%)	45	38
1	K	133/124 (107%)	129 (97%)	4 (3%)	46	39
1	L	128/124 (103%)	124 (97%)	4 (3%)	45	38
All	All	1579/1488 (106%)	1522 (96%)	57 (4%)	45	32

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	37	LEU
1	A	61	LEU

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Mol	Chain	Res	Type
1	A	92	ASN
1	B	37	LEU
1	B	61	LEU
1	B	125	LYS
1	B	137	ASP
1	C	37[A]	LEU
1	C	37[B]	LEU
1	C	38[A]	VAL
1	C	38[B]	VAL
1	C	47	LYS
1	C	61	LEU
1	D	1	MET
1	D	37[A]	LEU
1	D	37[B]	LEU
1	D	61[A]	LEU
1	D	61[B]	LEU
1	E	37	LEU
1	E	42	ARG
1	E	61	LEU
1	E	94	LEU
1	E	121	GLU
1	E	137	ASP
1	F	37	LEU
1	F	61	LEU
1	F	114[A]	ILE
1	F	114[B]	ILE
1	G	37[A]	LEU
1	G	37[B]	LEU
1	G	66[A]	ILE
1	G	66[B]	ILE
1	G	107[A]	VAL
1	G	107[B]	VAL
1	H	37	LEU
1	H	40	VAL
1	H	139	GLN
1	I	37[A]	LEU
1	I	37[B]	LEU
1	I	61	LEU
1	I	91[A]	THR
1	I	91[B]	THR
1	I	142[A]	GLN
1	I	142[B]	GLN

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Mol	Chain	Res	Type
1	J	37	LEU
1	J	61	LEU
1	J	94	LEU
1	J	137	ASP
1	K	1	MET
1	K	37	LEU
1	K	61	LEU
1	K	64	TYR
1	L	37	LEU
1	L	61	LEU
1	L	139	GLN
1	L	149	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	142	GLN

#### 4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

#### 4.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

#### 4.6 Ligand geometry ⓘ

There are no ligands in this entry.

#### 4.7 Other polymers ⓘ

There are no such residues in this entry.

## 4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 5 Fit of model and data ⓘ

### 5.1 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	149/149 (100%)	-0.60	1 (0%) 87 89	12, 21, 41, 66	0
1	B	149/149 (100%)	-0.49	2 (1%) 77 80	14, 21, 43, 62	0
1	C	149/149 (100%)	-0.60	1 (0%) 87 89	13, 24, 43, 64	0
1	D	149/149 (100%)	-0.52	3 (2%) 65 70	14, 23, 43, 63	0
1	E	149/149 (100%)	-0.61	2 (1%) 77 80	12, 20, 44, 68	0
1	F	149/149 (100%)	-0.68	1 (0%) 87 89	12, 19, 40, 65	0
1	G	149/149 (100%)	-0.44	5 (3%) 46 50	14, 21, 43, 64	0
1	H	149/149 (100%)	-0.68	1 (0%) 87 89	13, 20, 36, 66	0
1	I	149/149 (100%)	-0.60	1 (0%) 87 89	13, 21, 42, 58	0
1	J	149/149 (100%)	-0.62	1 (0%) 87 89	15, 21, 42, 67	0
1	K	149/149 (100%)	-0.57	3 (2%) 65 70	12, 20, 47, 70	0
1	L	149/149 (100%)	-0.63	3 (2%) 65 70	13, 22, 48, 63	0
All	All	1788/1788 (100%)	-0.59	24 (1%) 77 80	12, 21, 43, 70	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	149	LYS	3.8
1	H	149	LYS	3.6
1	D	149	LYS	3.3
1	E	54	SER	3.3
1	L	149	LYS	3.2
1	K	54	SER	3.1
1	D	54	SER	3.0
1	C	149	LYS	3.0
1	G	149	LYS	3.0
1	G	56	PRO	2.9
1	B	149	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	54	SER	2.8
1	K	56	PRO	2.8
1	I	149	LYS	2.8
1	D	56	PRO	2.6
1	A	149	LYS	2.6
1	J	149	LYS	2.6
1	K	94	LEU	2.3
1	E	57	PHE	2.1
1	G	57	PHE	2.1
1	L	1	MET	2.1
1	B	56	PRO	2.1
1	G	53	ALA	2.0
1	L	94	LEU	2.0

## 5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.4 Ligands [i](#)

There are no ligands in this entry.

## 5.5 Other polymers [i](#)

There are no such residues in this entry.