



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:33 PM UTC

PDB ID : 5D50 / pdb_00005d50
Title : Crystal structure of Rep-Ant complex from Salmonella-temperate phage
Authors : Son, S.H.; Yoon, H.J.; Ryu, S.; Lee, H.H.
Deposited on : 2015-08-10
Resolution : 2.49 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:

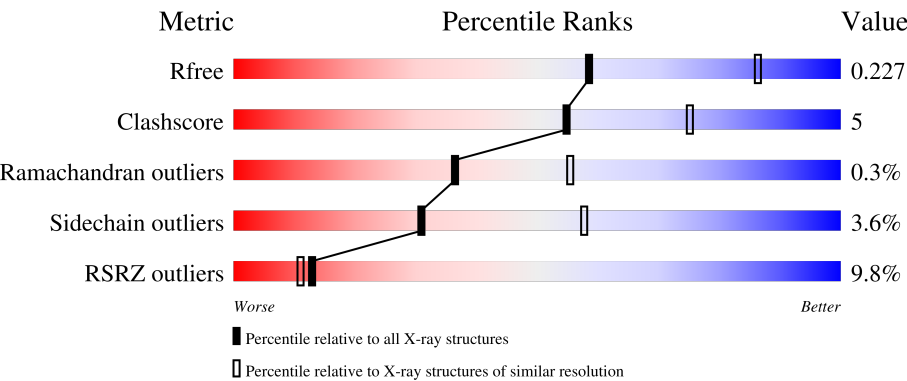
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	199	15% 72% 12% • 14%
1	B	199	9% 41% 11% • 47%
1	C	199	7% 71% 13% • 14%
1	D	199	6% 45% 7% 49%
1	I	199	9% 75% 11% 15%

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Mol	Chain	Length	Quality of chain
1	J	199	
1	K	199	
1	L	199	
2	E	86	
2	F	86	
2	G	86	
2	H	86	
2	M	86	
2	N	86	
2	O	86	
2	P	86	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13325 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 Repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1375	872	248	249	6			
1	B	105	Total	C	N	O	S	0	0	0
			816	521	139	152	4			
1	C	171	Total	C	N	O	S	0	0	0
			1375	872	248	249	6			
1	D	102	Total	C	N	O	S	0	0	0
			791	506	132	149	4			
1	I	170	Total	C	N	O	S	0	0	0
			1370	869	247	248	6			
1	J	103	Total	C	N	O	S	0	0	0
			806	515	137	150	4			
1	K	169	Total	C	N	O	S	0	0	0
			1361	863	245	247	6			
1	L	104	Total	C	N	O	S	0	0	0
			811	518	138	151	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP T1S9Z0
B	0	ALA	-	expression tag	UNP T1S9Z0
C	0	ALA	-	expression tag	UNP T1S9Z0
D	0	ALA	-	expression tag	UNP T1S9Z0
I	0	ALA	-	expression tag	UNP T1S9Z0
J	0	ALA	-	expression tag	UNP T1S9Z0
K	0	ALA	-	expression tag	UNP T1S9Z0
L	0	ALA	-	expression tag	UNP T1S9Z0

- Molecule 2 is a protein called Anti-repressor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	74	Total	C	N	O	S	0	0	0
			592	369	102	117	4			
2	G	77	Total	C	N	O	S	0	0	0
			614	381	105	124	4			
2	M	77	Total	C	N	O	S	0	0	0
			614	381	105	124	4			
2	O	77	Total	C	N	O	S	0	0	0
			614	381	105	124	4			
2	F	67	Total	C	N	O	S	0	0	0
			527	328	90	105	4			
2	H	68	Total	C	N	O	S	0	0	0
			534	332	91	107	4			
2	N	68	Total	C	N	O	S	0	0	0
			534	332	91	107	4			
2	P	67	Total	C	N	O	S	0	0	0
			527	328	90	105	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	5	Total	O	0	0
			5	5		
3	C	7	Total	O	0	0
			7	7		
3	D	4	Total	O	0	0
			4	4		
3	E	4	Total	O	0	0
			4	4		
3	G	3	Total	O	0	0
			3	3		
3	I	6	Total	O	0	0
			6	6		
3	J	4	Total	O	0	0
			4	4		
3	K	6	Total	O	0	0
			6	6		
3	L	4	Total	O	0	0
			4	4		
3	M	2	Total	O	0	0
			2	2		
3	O	2	Total	O	0	0
			2	2		

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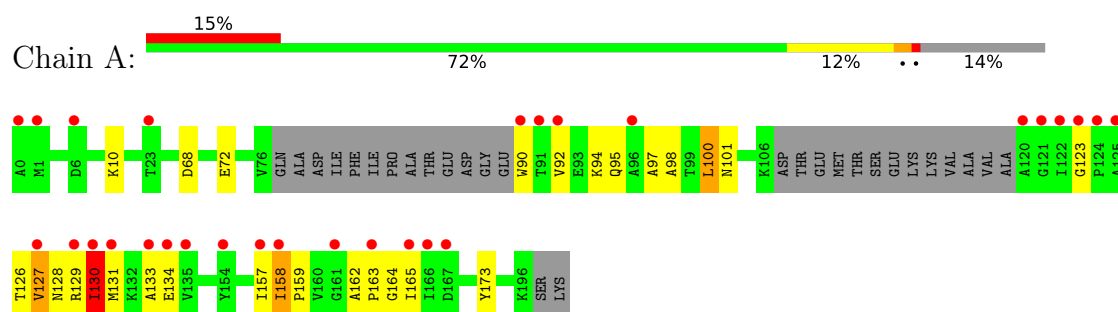
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total 2	O 2	0	0
3	H	1	Total 1	O 1	0	0
3	N	5	Total 5	O 5	0	0
3	P	5	Total 5	O 5	0	0

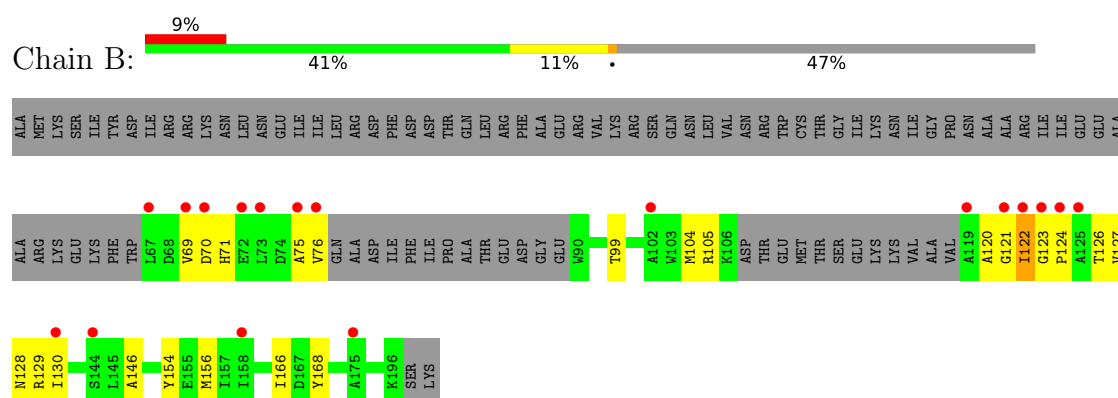
3 Residue-property plots [i](#)

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.

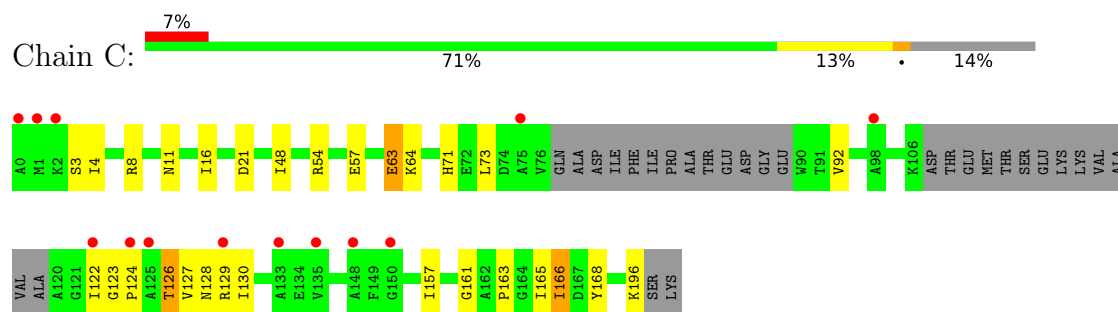
• Molecule 1: Repressor



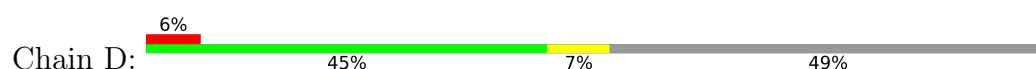
• Molecule 1: Repressor



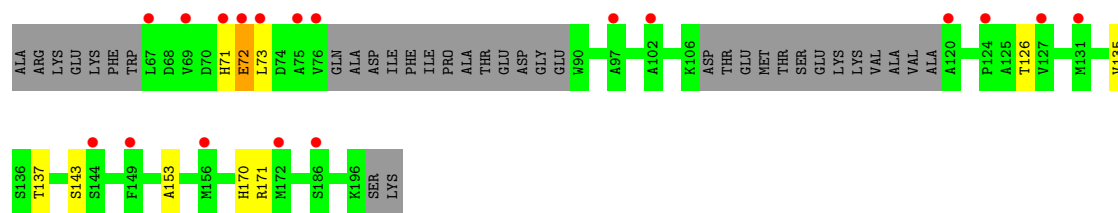
• Molecule 1: Repressor



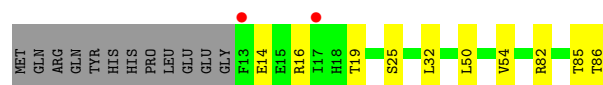
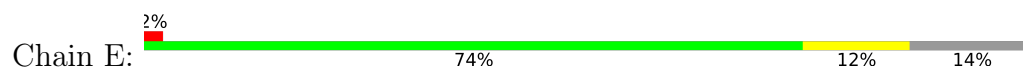
• Molecule 1: Repressor



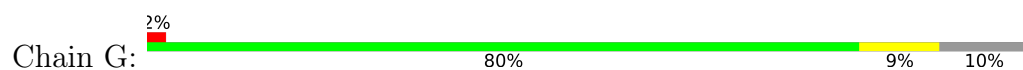




- Molecule 2: Anti-repressor protein



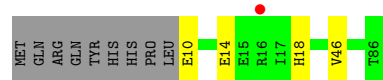
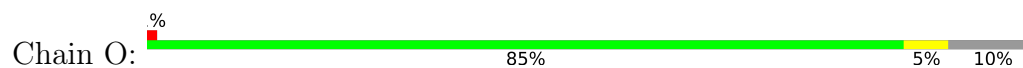
- Molecule 2: Anti-repressor protein



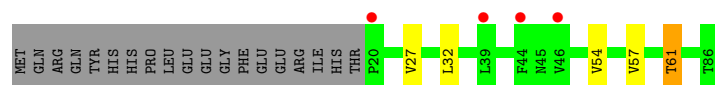
- Molecule 2: Anti-repressor protein



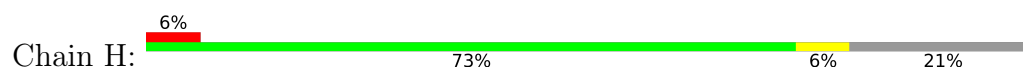
- Molecule 2: Anti-repressor protein

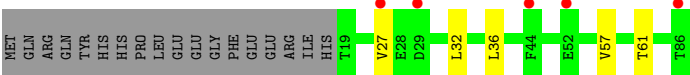


- Molecule 2: Anti-repressor protein

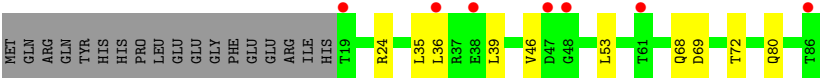


- Molecule 2: Anti-repressor protein

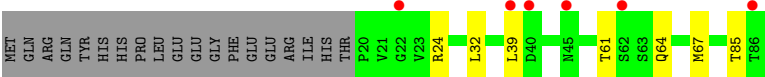




● Molecule 2: Anti-repressor protein



● Molecule 2: Anti-repressor protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	86.61Å 86.61Å 337.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.61 – 2.49 36.61 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.2 (36.61-2.49) 98.2 (36.61-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	54.36 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.201 , 0.210 (Not available) , 0.227	Depositor DCC
R_{free} test set	4785 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.103 for -h,-k,l 0.119 for h,-h-k,-l 0.117 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13325	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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

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	0.46	0/1399	0.83	1/1885 (0.1%)
1	B	0.49	0/831	0.83	0/1124
1	C	0.46	0/1399	0.80	1/1885 (0.1%)
1	D	0.47	0/806	0.78	0/1092
1	I	0.46	0/1394	0.80	0/1878
1	J	0.49	0/821	0.83	0/1110
1	K	0.45	0/1385	0.77	1/1867 (0.1%)
1	L	0.49	0/826	0.84	1/1117 (0.1%)
2	E	0.48	0/600	0.80	0/811
2	F	0.43	0/533	0.77	0/720
2	G	0.47	0/622	0.76	0/840
2	H	0.45	0/540	0.81	0/731
2	M	0.45	0/622	0.82	1/840 (0.1%)
2	N	0.44	0/540	0.85	0/731
2	O	0.46	0/622	0.74	0/840
2	P	0.40	0/533	0.77	0/720
All	All	0.46	0/13473	0.80	5/18191 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
2	M	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ILE	N-CA-C	7.10	117.81	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	ILE	N-CA-C	6.82	117.43	110.82
1	L	135	VAL	N-CA-C	6.02	116.19	110.53
2	M	70	LEU	N-CA-C	-5.57	105.36	111.82
1	K	141	VAL	N-CA-C	-5.42	100.61	108.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	73	LEU	Peptide
2	M	69	ASP	Peptide

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	1375	0	1387	26	0
1	B	816	0	809	26	0
1	C	1375	0	1387	17	0
1	D	791	0	778	9	0
1	I	1370	0	1382	10	0
1	J	806	0	799	4	0
1	K	1361	0	1369	13	0
1	L	811	0	804	6	0
2	E	592	0	586	6	0
2	F	527	0	528	9	0
2	G	614	0	601	3	0
2	H	534	0	534	4	0
2	M	614	0	601	14	0
2	N	534	0	534	5	0
2	O	614	0	601	3	0
2	P	527	0	528	6	0
3	A	4	0	0	0	0
3	B	5	0	0	0	0
3	C	7	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	1	0	0	0	0
3	I	6	0	0	0	0
3	J	4	0	0	0	0
3	K	6	0	0	0	0
3	L	4	0	0	0	0
3	M	2	0	0	1	0
3	N	5	0	0	0	0
3	O	2	0	0	0	0
3	P	5	0	0	0	0
All	All	13325	0	13228	128	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 5.

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLY:HA2	1:A:127:VAL:HG11	1.50	0.93
1:B:71:HIS:ND1	2:F:61:THR:OG1	2.16	0.75
1:A:127:VAL:HG13	1:A:128:ASN:H	1.55	0.69
1:C:92:VAL:HG21	1:D:143:SER:HB2	1.75	0.69
1:C:73:LEU:HD12	2:G:27:VAL:HG21	1.76	0.68
1:C:54:ARG:NH1	1:C:57:GLU:OE2	2.27	0.67
1:K:130:ILE:O	1:K:131:MET:C	2.37	0.67
1:B:121:GLY:HA2	1:B:123:GLY:H	1.59	0.67
1:C:122:ILE:HA	1:C:124:PRO:HD3	1.77	0.67
2:M:24:ARG:NH1	2:P:85:THR:O	2.28	0.65
1:A:123:GLY:CA	1:A:127:VAL:HG11	2.24	0.63
2:M:33:MET:SD	2:M:50:LEU:HD11	2.38	0.63
1:B:69:VAL:HG12	1:B:71:HIS:CD2	2.34	0.62
1:A:130:ILE:HG13	1:A:131:MET:HA	1.82	0.62
1:B:127:VAL:O	1:B:129:ARG:N	2.30	0.62
1:A:163:PRO:HB2	1:B:154:TYR:OH	1.99	0.61
1:B:71:HIS:NE2	2:F:57:VAL:HG12	2.16	0.60
1:B:127:VAL:O	1:B:130:ILE:HG12	2.02	0.60
1:A:126:THR:OG1	1:A:127:VAL:N	2.34	0.60
2:N:69:ASP:HB3	2:N:72:THR:H	1.67	0.59
1:B:122:ILE:HG13	1:B:123:GLY:N	2.15	0.59
1:A:97:ALA:HA	1:A:100:LEU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:72:GLU:HG2	2:P:61:THR:HG23	1.86	0.57
2:M:69:ASP:HB3	2:M:72:THR:H	1.69	0.57
1:C:166:ILE:HG12	1:D:173:TYR:CZ	2.40	0.57
1:L:72:GLU:HG2	2:P:61:THR:CG2	2.35	0.57
1:A:97:ALA:HB2	1:A:133:ALA:HB2	1.87	0.57
2:M:79:GLU:OE1	2:M:82:ARG:NH1	2.37	0.56
1:B:104:MET:O	1:B:105:ARG:HB3	2.05	0.56
1:A:162:ALA:N	1:A:163:PRO:HD2	2.21	0.55
1:C:63:GLU:OE1	1:C:64:LYS:N	2.34	0.54
1:C:128:ASN:O	1:C:129:ARG:HG3	2.06	0.54
1:L:71:HIS:O	1:L:72:GLU:HG3	2.08	0.54
1:K:70:ASP:OD1	1:K:72:GLU:HG2	2.08	0.53
1:I:123:GLY:N	1:I:124:PRO:CD	2.72	0.53
2:F:27:VAL:HA	2:F:57:VAL:HG13	1.90	0.53
1:C:8:ARG:NH1	1:C:48:ILE:O	2.41	0.53
1:K:123:GLY:N	1:K:124:PRO:CD	2.73	0.52
1:K:4:ILE:HB	2:M:18:HIS:CE1	2.44	0.52
1:C:122:ILE:HG13	1:C:123:GLY:HA2	1.92	0.52
1:B:71:HIS:CE1	2:F:61:THR:HG1	2.19	0.52
2:M:85:THR:O	2:P:24:ARG:NH1	2.42	0.52
1:C:166:ILE:O	1:C:168:TYR:HD1	1.92	0.52
2:M:84:GLN:O	2:P:64:GLN:NE2	2.20	0.52
1:C:92:VAL:HG13	1:C:157:ILE:HB	1.92	0.51
1:B:127:VAL:C	1:B:129:ARG:H	2.18	0.51
1:A:97:ALA:O	1:A:101:ASN:N	2.33	0.51
1:B:71:HIS:HE2	2:F:57:VAL:HG12	1.75	0.50
1:B:126:THR:OG1	1:B:127:VAL:N	2.45	0.50
1:K:149:PHE:HD2	1:K:151:HIS:HD2	1.60	0.49
1:K:125:ALA:CB	1:K:145:LEU:HA	2.41	0.49
1:A:127:VAL:HG22	1:A:128:ASN:N	2.28	0.49
1:A:173:TYR:CZ	1:B:166:ILE:HG12	2.48	0.49
1:D:120:ALA:HA	1:D:121:GLY:C	2.37	0.49
2:E:16:ARG:O	2:E:19:THR:OG1	2.25	0.48
1:C:126:THR:HG23	1:C:127:VAL:HG23	1.96	0.48
2:M:83:LYS:NZ	3:M:101:HOH:O	2.46	0.48
1:I:104:MET:HG3	1:I:149:PHE:CG	2.48	0.48
2:F:32:LEU:HD21	2:H:32:LEU:HD21	1.96	0.48
1:A:130:ILE:N	1:A:131:MET:HA	2.29	0.47
1:D:160:VAL:HB	1:D:165:ILE:HG13	1.97	0.47
1:A:123:GLY:HA2	1:A:127:VAL:CG1	2.32	0.47
1:A:127:VAL:HG13	1:A:128:ASN:N	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:THR:HG21	1:B:156:MET:HA	1.97	0.47
1:I:158:ILE:HG22	1:I:159:PRO:O	2.15	0.47
1:K:163:PRO:HB2	1:L:170:HIS:HB3	1.96	0.47
1:I:168:TYR:OH	1:J:163:PRO:O	2.32	0.47
1:J:73:LEU:HD11	2:N:24:ARG:HD2	1.96	0.47
1:D:70:ASP:HB3	2:H:61:THR:HG21	1.97	0.47
2:E:85:THR:O	2:E:86:THR:C	2.57	0.47
2:E:82:ARG:O	2:E:86:THR:N	2.43	0.46
1:K:130:ILE:O	1:K:130:ILE:HG22	2.16	0.46
1:A:97:ALA:CB	1:A:133:ALA:HB2	2.46	0.46
2:M:14:GLU:O	2:M:18:HIS:CE1	2.69	0.46
1:B:69:VAL:HG12	1:B:71:HIS:HD2	1.80	0.46
1:I:162:ALA:N	1:I:163:PRO:CD	2.79	0.46
1:D:69:VAL:HG11	2:H:57:VAL:HG11	1.97	0.46
1:A:123:GLY:CA	1:A:127:VAL:CG1	2.93	0.45
1:A:90:TRP:HZ2	1:A:157:ILE:O	1.99	0.45
1:I:73:LEU:HG	2:M:61:THR:HG23	1.99	0.45
1:A:94:LYS:HA	1:A:133:ALA:HB1	1.98	0.45
2:M:13:PHE:CE2	2:M:17:ILE:HD11	2.52	0.44
2:N:68:GLN:HA	2:N:69:ASP:HA	1.63	0.44
1:I:122:ILE:HB	1:I:123:GLY:C	2.42	0.44
2:M:45:ASN:ND2	2:O:10:GLU:OE1	2.50	0.44
2:G:68:GLN:OE1	2:G:71:GLN:NE2	2.51	0.44
1:C:128:ASN:O	1:C:129:ARG:CG	2.66	0.44
1:C:161:GLY:O	1:C:163:PRO:HD3	2.17	0.43
1:A:68:ASP:HB3	2:E:54:VAL:HG11	2.00	0.43
1:B:69:VAL:HG22	2:F:54:VAL:HG13	1.99	0.43
1:A:162:ALA:N	1:A:163:PRO:CD	2.80	0.43
1:B:75:ALA:O	1:B:76:VAL:HB	2.19	0.43
1:B:121:GLY:HA2	1:B:123:GLY:N	2.31	0.43
1:B:70:ASP:O	1:B:71:HIS:CD2	2.71	0.43
1:B:70:ASP:C	1:B:71:HIS:CD2	2.97	0.43
1:B:71:HIS:CG	2:F:61:THR:HG1	2.23	0.43
1:K:12:LEU:CD2	1:K:41:TRP:HB3	2.49	0.43
1:J:176:LEU:O	1:J:181:LYS:NZ	2.52	0.43
1:A:10:LYS:NZ	1:A:72:GLU:OE1	2.52	0.42
1:A:95:GLN:HA	1:A:98:ALA:HB3	2.01	0.42
1:B:71:HIS:CE1	2:F:27:VAL:HG13	2.54	0.42
1:L:143:SER:HA	1:L:153:ALA:HB2	2.02	0.42
1:J:70:ASP:OD1	1:J:70:ASP:C	2.62	0.42
1:B:146:ALA:HB2	1:B:156:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ALA:C	1:B:122:ILE:HG23	2.45	0.42
1:A:90:TRP:CE2	1:A:159:PRO:HD3	2.54	0.42
2:H:27:VAL:HA	2:H:57:VAL:HG13	2.01	0.42
1:C:4:ILE:CD1	2:E:14:GLU:HG2	2.50	0.41
1:D:155:GLU:O	1:D:158:ILE:HG22	2.20	0.41
1:D:166:ILE:HG22	1:D:168:TYR:CD1	2.56	0.41
1:A:164:GLY:HA2	1:B:168:TYR:OH	2.20	0.41
2:E:32:LEU:HD11	2:G:32:LEU:HD11	2.02	0.41
1:I:8:ARG:NH2	2:O:14:GLU:OE1	2.54	0.41
1:K:163:PRO:HB3	1:L:170:HIS:O	2.21	0.41
2:M:68:GLN:HA	2:M:69:ASP:HA	1.71	0.41
1:D:165:ILE:HG12	1:D:165:ILE:O	2.21	0.41
1:K:142:LEU:HD22	1:K:156:MET:SD	2.60	0.41
1:K:162:ALA:N	1:K:163:PRO:HD3	2.35	0.41
2:O:14:GLU:O	2:O:18:HIS:ND1	2.45	0.41
2:M:84:GLN:HB2	2:P:67:MET:SD	2.61	0.41
2:N:36:LEU:HD12	2:N:53:LEU:HD22	2.02	0.41
1:C:11:ASN:OD1	1:C:71:HIS:HD2	2.04	0.40
1:I:165:ILE:O	1:I:168:TYR:HB3	2.21	0.40
1:I:33:ARG:HB3	1:I:37:LEU:HD23	2.03	0.40
2:N:35:LEU:O	2:N:39:LEU:HB2	2.21	0.40
1:C:16:ILE:O	1:C:21:ASP:N	2.55	0.40
1:A:158:ILE:HG22	1:A:159:PRO:HD2	2.04	0.40
1:K:91:THR:OG1	1:K:92:VAL:N	2.54	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	165/199 (83%)	158 (96%)	6 (4%)	1 (1%)	21 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	99/199 (50%)	92 (93%)	5 (5%)	2 (2%)	6	10
1	C	165/199 (83%)	155 (94%)	9 (6%)	1 (1%)	21	38
1	D	96/199 (48%)	85 (88%)	11 (12%)	0	100	100
1	I	164/199 (82%)	154 (94%)	10 (6%)	0	100	100
1	J	97/199 (49%)	91 (94%)	5 (5%)	1 (1%)	12	24
1	K	163/199 (82%)	149 (91%)	14 (9%)	0	100	100
1	L	98/199 (49%)	89 (91%)	9 (9%)	0	100	100
2	E	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
2	F	65/86 (76%)	63 (97%)	2 (3%)	0	100	100
2	G	75/86 (87%)	73 (97%)	2 (3%)	0	100	100
2	H	66/86 (77%)	64 (97%)	2 (3%)	0	100	100
2	M	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
2	N	66/86 (77%)	66 (100%)	0	0	100	100
2	O	75/86 (87%)	73 (97%)	2 (3%)	0	100	100
2	P	65/86 (76%)	61 (94%)	4 (6%)	0	100	100
All	All	1606/2280 (70%)	1513 (94%)	88 (6%)	5 (0%)	36	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	128	ASN
1	A	127	VAL
1	J	153	ALA
1	B	124	PRO
1	C	166	ILE

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	143/166 (86%)	136 (95%)	7 (5%)	22	45
1	B	84/166 (51%)	83 (99%)	1 (1%)	63	83
1	C	143/166 (86%)	138 (96%)	5 (4%)	32	58
1	D	82/166 (49%)	81 (99%)	1 (1%)	63	83
1	I	143/166 (86%)	137 (96%)	6 (4%)	26	52
1	J	84/166 (51%)	80 (95%)	4 (5%)	23	46
1	K	142/166 (86%)	135 (95%)	7 (5%)	22	45
1	L	84/166 (51%)	80 (95%)	4 (5%)	23	46
2	E	68/79 (86%)	66 (97%)	2 (3%)	37	65
2	F	61/79 (77%)	60 (98%)	1 (2%)	55	79
2	G	70/79 (89%)	66 (94%)	4 (6%)	18	39
2	H	62/79 (78%)	61 (98%)	1 (2%)	55	79
2	M	70/79 (89%)	66 (94%)	4 (6%)	18	39
2	N	62/79 (78%)	60 (97%)	2 (3%)	34	62
2	O	70/79 (89%)	69 (99%)	1 (1%)	59	81
2	P	61/79 (77%)	59 (97%)	2 (3%)	33	61
All	All	1429/1960 (73%)	1377 (96%)	52 (4%)	31	58

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	100	LEU
1	A	129	ARG
1	A	130	ILE
1	A	134	GLU
1	A	158	ILE
1	A	165	ILE
1	B	122	ILE
1	C	3	SER
1	C	63	GLU
1	C	126	THR
1	C	130	ILE
1	C	196	LYS
1	D	137	THR
2	E	25	SER
2	E	50	LEU

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Mol	Chain	Res	Type
2	G	13	PHE
2	G	17	ILE
2	G	28	GLU
2	G	57	VAL
1	I	103	TRP
1	I	105	ARG
1	I	137	THR
1	I	138	THR
1	I	166	ILE
1	I	195	ASN
1	J	67	LEU
1	J	69	VAL
1	J	138	THR
1	J	156	MET
1	K	15	ILE
1	K	18	ARG
1	K	46	LYS
1	K	72	GLU
1	K	105	ARG
1	K	160	VAL
1	K	166	ILE
1	L	72	GLU
1	L	126	THR
1	L	137	THR
1	L	171	ARG
2	M	38	GLU
2	M	70	LEU
2	M	79	GLU
2	M	84	GLN
2	O	46	VAL
2	F	61	THR
2	H	36	LEU
2	N	46	VAL
2	N	80	GLN
2	P	32	LEU
2	P	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	B	178	GLN

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Mol	Chain	Res	Type
1	B	194	GLN
1	B	195	ASN
1	C	178	GLN
1	D	194	GLN
2	E	45	ASN
2	E	64	GLN
2	E	84	GLN
2	G	71	GLN
1	I	24	GLN
1	J	71	HIS
1	K	71	HIS
1	L	194	GLN
2	M	18	HIS
2	O	71	GLN
2	F	31	HIS
2	F	80	GLN
2	F	84	GLN
2	H	80	GLN
2	H	84	GLN
2	N	71	GLN
2	N	80	GLN
2	P	71	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	171/199 (85%)	0.89	29 (16%) 4 3	40, 63, 100, 112	0
1	B	105/199 (52%)	0.89	18 (17%) 4 3	35, 65, 102, 110	0
1	C	171/199 (85%)	0.68	13 (7%) 20 17	45, 61, 89, 108	0
1	D	102/199 (51%)	0.84	11 (10%) 11 9	39, 67, 89, 108	0
1	I	170/199 (85%)	0.81	17 (10%) 12 10	41, 62, 94, 124	0
1	J	103/199 (51%)	0.76	8 (7%) 19 17	40, 67, 90, 98	0
1	K	169/199 (84%)	0.80	18 (10%) 11 9	42, 63, 101, 117	0
1	L	104/199 (52%)	0.93	18 (17%) 4 3	37, 69, 111, 140	0
2	E	74/86 (86%)	0.38	2 (2%) 56 51	36, 57, 79, 93	0
2	F	67/86 (77%)	0.79	4 (5%) 27 24	38, 66, 103, 111	0
2	G	77/86 (89%)	0.54	2 (2%) 57 52	36, 61, 99, 119	0
2	H	68/86 (79%)	0.75	5 (7%) 20 18	40, 66, 94, 110	0
2	M	77/86 (89%)	0.53	4 (5%) 33 29	40, 57, 88, 109	0
2	N	68/86 (79%)	0.92	7 (10%) 12 10	43, 66, 93, 97	0
2	O	77/86 (89%)	0.46	1 (1%) 75 71	40, 56, 82, 98	0
2	P	67/86 (77%)	0.70	6 (8%) 15 13	43, 63, 88, 92	0
All	All	1670/2280 (73%)	0.75	163 (9%) 13 11	35, 63, 97, 140	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	ILE	8.6
1	B	122	ILE	6.3
1	B	102	ALA	6.1
1	L	120	ALA	5.7
1	L	72	GLU	5.4

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Mol	Chain	Res	Type	RSRZ
1	K	149	PHE	5.3
2	F	44	PHE	5.3
1	B	130	ILE	5.1
1	J	67	LEU	4.9
2	G	13	PHE	4.7
2	H	29	ASP	4.5
1	C	1	MET	4.4
1	J	69	VAL	4.3
1	L	67	LEU	4.2
1	C	0	ALA	4.2
2	M	17	ILE	4.2
1	I	104	MET	4.2
2	P	22	GLY	4.0
1	A	135	VAL	4.0
1	B	73	LEU	4.0
1	A	0	ALA	3.9
1	A	130	ILE	3.8
1	L	69	VAL	3.7
1	I	102	ALA	3.7
1	K	104	MET	3.7
1	K	105	ARG	3.5
1	D	123	GLY	3.5
1	K	19	ASP	3.4
1	D	104	MET	3.3
1	A	129	ARG	3.3
1	A	158	ILE	3.3
1	A	167	ASP	3.3
1	B	119	ALA	3.3
1	A	121	GLY	3.3
1	L	149	PHE	3.2
1	C	148	ALA	3.1
1	D	120	ALA	3.1
1	I	120	ALA	3.1
1	B	67	LEU	3.1
1	A	91	THR	3.0
2	G	44	PHE	3.0
1	A	157	ILE	3.0
1	L	71	HIS	3.0
2	H	52	GLU	3.0
1	A	133	ALA	2.9
1	B	124	PRO	2.9
2	P	40	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	135	VAL	2.9
1	A	1	MET	2.9
1	L	156	MET	2.9
1	D	69	VAL	2.9
2	N	19	THR	2.8
1	B	125	ALA	2.8
1	C	125	ALA	2.8
1	B	121	GLY	2.8
2	M	18	HIS	2.8
2	N	86	THR	2.8
1	A	125	ALA	2.8
1	K	100	LEU	2.8
2	H	44	PHE	2.8
1	K	133	ALA	2.8
1	C	122	ILE	2.8
1	I	76	VAL	2.7
1	D	102	ALA	2.7
1	I	130	ILE	2.7
1	L	124	PRO	2.7
2	P	45	ASN	2.7
1	I	103	TRP	2.7
1	D	67	LEU	2.7
2	N	47	ASP	2.7
1	B	158	ILE	2.7
1	I	1	MET	2.6
1	K	99	THR	2.6
1	L	97	ALA	2.6
2	P	86	THR	2.6
1	I	166	ILE	2.6
1	C	133	ALA	2.6
1	C	2	LYS	2.6
2	N	48	GLY	2.6
2	F	20	PRO	2.6
1	I	125	ALA	2.5
1	J	163	PRO	2.5
2	N	38	GLU	2.5
1	L	75	ALA	2.5
1	A	124	PRO	2.5
1	K	130	ILE	2.5
1	L	127	VAL	2.5
2	F	46	VAL	2.5
1	J	121	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	P	39	LEU	2.5
2	H	27	VAL	2.5
1	I	44	GLY	2.4
1	I	160	VAL	2.4
1	C	98	ALA	2.4
2	N	61	THR	2.4
1	J	166	ILE	2.4
1	J	169	ASP	2.4
2	N	36	LEU	2.4
1	J	141	VAL	2.4
1	L	186	SER	2.4
2	P	62	SER	2.4
1	K	44	GLY	2.4
1	A	165	ILE	2.4
1	D	130	ILE	2.4
2	M	19	THR	2.3
2	O	16	ARG	2.3
1	I	135	VAL	2.3
1	B	72	GLU	2.3
2	H	86	THR	2.3
1	I	161	GLY	2.3
1	A	127	VAL	2.3
1	B	76	VAL	2.3
1	A	90	TRP	2.3
1	A	134	GLU	2.3
1	K	98	ALA	2.3
1	C	129	ARG	2.3
1	A	23	THR	2.3
1	C	150	GLY	2.3
1	A	120	ALA	2.2
1	B	75	ALA	2.2
1	I	136	SER	2.2
2	E	17	ILE	2.2
1	A	6	ASP	2.2
1	A	123	GLY	2.2
1	B	123	GLY	2.2
1	K	167	ASP	2.2
1	A	92	VAL	2.2
1	K	102	ALA	2.2
1	L	102	ALA	2.2
1	B	144	SER	2.2
2	E	13	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	160	VAL	2.2
1	K	146	ALA	2.2
1	A	122	ILE	2.2
1	K	122	ILE	2.2
1	C	124	PRO	2.2
1	A	131	MET	2.1
1	A	154	TYR	2.1
1	J	158	ILE	2.1
1	D	144	SER	2.1
1	D	169	ASP	2.1
1	C	75	ALA	2.1
1	K	120	ALA	2.1
1	I	128	ASN	2.1
1	A	161	GLY	2.1
1	A	96	ALA	2.1
1	D	162	ALA	2.1
1	K	128	ASN	2.1
1	I	126	THR	2.1
1	B	70	ASP	2.1
1	L	172	MET	2.1
1	B	69	VAL	2.1
1	L	73	LEU	2.1
1	L	144	SER	2.1
1	L	131	MET	2.1
2	M	84	GLN	2.0
1	L	76	VAL	2.0
1	B	175	ALA	2.0
1	D	164	GLY	2.0
1	I	165	ILE	2.0
1	A	163	PRO	2.0
1	K	127	VAL	2.0
2	F	39	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.