



Full wwPDB X-ray Structure Validation Report i

Jun 19, 2024 – 02:32 AM EDT

PDB ID : 4J3N
Title : Human Topoisomerase Iibeta in complex with DNA
Authors : Wu, C.C.; Li, T.K.; Li, Y.C.; Chan, N.L.
Deposited on : 2013-02-06
Resolution : 2.30 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 i 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

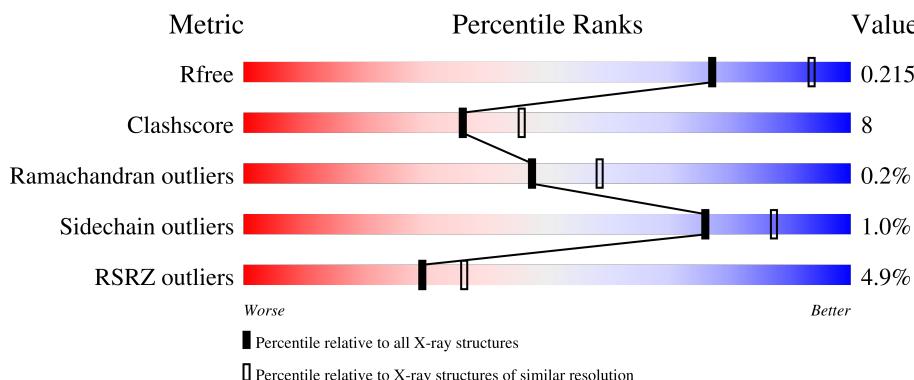
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

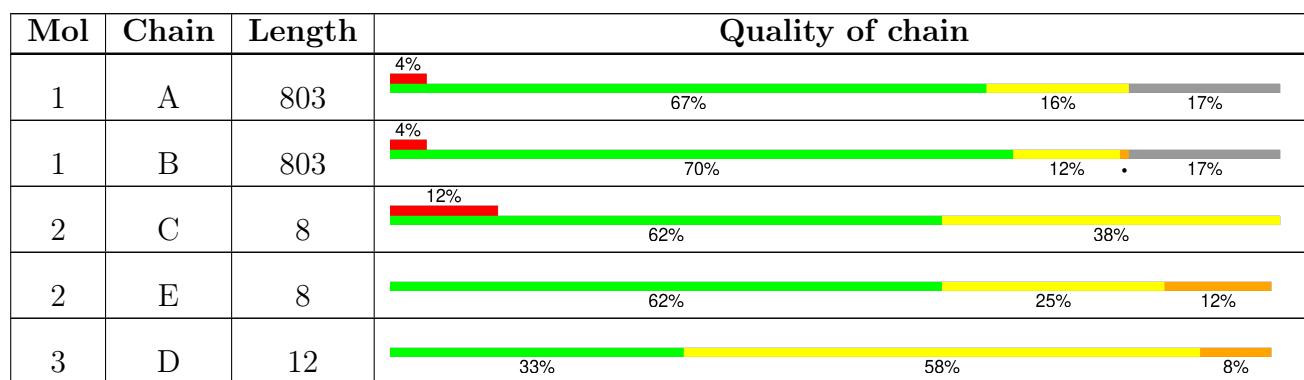
The reported resolution of this entry is 2.30 Å.

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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.



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2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12463 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 DNA topoisomerase 2-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	18	0
			5480	3501	941	1013	25			
1	B	670	Total	C	N	O	S	0	11	0
			5474	3491	950	1009	24			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	MET	-	expression tag	UNP Q02880
A	420	ALA	-	expression tag	UNP Q02880
A	421	SER	-	expression tag	UNP Q02880
A	422	TRP	-	expression tag	UNP Q02880
A	423	SER	-	expression tag	UNP Q02880
A	424	HIS	-	expression tag	UNP Q02880
A	425	PRO	-	expression tag	UNP Q02880
A	426	GLN	-	expression tag	UNP Q02880
A	427	PHE	-	expression tag	UNP Q02880
A	428	GLU	-	expression tag	UNP Q02880
A	429	LYS	-	expression tag	UNP Q02880
A	430	GLY	-	expression tag	UNP Q02880
A	431	ALA	-	expression tag	UNP Q02880
A	432	ASP	-	expression tag	UNP Q02880
A	433	ASP	-	expression tag	UNP Q02880
A	434	ASP	-	expression tag	UNP Q02880
A	435	ASP	-	expression tag	UNP Q02880
A	436	LYS	-	expression tag	UNP Q02880
A	437	VAL	-	expression tag	UNP Q02880
A	438	PRO	-	expression tag	UNP Q02880
A	439	ASP	-	expression tag	UNP Q02880
A	440	PRO	-	expression tag	UNP Q02880
A	441	THR	-	expression tag	UNP Q02880
A	442	SER	-	expression tag	UNP Q02880
A	443	VAL	-	expression tag	UNP Q02880

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Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ASP	-	expression tag	UNP Q02880
A	1202	GLY	-	expression tag	UNP Q02880
A	1203	ALA	-	expression tag	UNP Q02880
A	1204	PRO	-	expression tag	UNP Q02880
A	1205	GLY	-	expression tag	UNP Q02880
A	1206	PHE	-	expression tag	UNP Q02880
A	1207	SER	-	expression tag	UNP Q02880
A	1208	SER	-	expression tag	UNP Q02880
A	1209	ILE	-	expression tag	UNP Q02880
A	1210	SER	-	expression tag	UNP Q02880
A	1211	ALA	-	expression tag	UNP Q02880
A	1212	HIS	-	expression tag	UNP Q02880
A	1213	HIS	-	expression tag	UNP Q02880
A	1214	HIS	-	expression tag	UNP Q02880
A	1215	HIS	-	expression tag	UNP Q02880
A	1216	HIS	-	expression tag	UNP Q02880
A	1217	HIS	-	expression tag	UNP Q02880
A	1218	HIS	-	expression tag	UNP Q02880
A	1219	HIS	-	expression tag	UNP Q02880
A	1220	HIS	-	expression tag	UNP Q02880
A	1221	HIS	-	expression tag	UNP Q02880
B	419	MET	-	expression tag	UNP Q02880
B	420	ALA	-	expression tag	UNP Q02880
B	421	SER	-	expression tag	UNP Q02880
B	422	TRP	-	expression tag	UNP Q02880
B	423	SER	-	expression tag	UNP Q02880
B	424	HIS	-	expression tag	UNP Q02880
B	425	PRO	-	expression tag	UNP Q02880
B	426	GLN	-	expression tag	UNP Q02880
B	427	PHE	-	expression tag	UNP Q02880
B	428	GLU	-	expression tag	UNP Q02880
B	429	LYS	-	expression tag	UNP Q02880
B	430	GLY	-	expression tag	UNP Q02880
B	431	ALA	-	expression tag	UNP Q02880
B	432	ASP	-	expression tag	UNP Q02880
B	433	ASP	-	expression tag	UNP Q02880
B	434	ASP	-	expression tag	UNP Q02880
B	435	ASP	-	expression tag	UNP Q02880
B	436	LYS	-	expression tag	UNP Q02880
B	437	VAL	-	expression tag	UNP Q02880
B	438	PRO	-	expression tag	UNP Q02880
B	439	ASP	-	expression tag	UNP Q02880

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Chain	Residue	Modelled	Actual	Comment	Reference
B	440	PRO	-	expression tag	UNP Q02880
B	441	THR	-	expression tag	UNP Q02880
B	442	SER	-	expression tag	UNP Q02880
B	443	VAL	-	expression tag	UNP Q02880
B	444	ASP	-	expression tag	UNP Q02880
B	1202	GLY	-	expression tag	UNP Q02880
B	1203	ALA	-	expression tag	UNP Q02880
B	1204	PRO	-	expression tag	UNP Q02880
B	1205	GLY	-	expression tag	UNP Q02880
B	1206	PHE	-	expression tag	UNP Q02880
B	1207	SER	-	expression tag	UNP Q02880
B	1208	SER	-	expression tag	UNP Q02880
B	1209	ILE	-	expression tag	UNP Q02880
B	1210	SER	-	expression tag	UNP Q02880
B	1211	ALA	-	expression tag	UNP Q02880
B	1212	HIS	-	expression tag	UNP Q02880
B	1213	HIS	-	expression tag	UNP Q02880
B	1214	HIS	-	expression tag	UNP Q02880
B	1215	HIS	-	expression tag	UNP Q02880
B	1216	HIS	-	expression tag	UNP Q02880
B	1217	HIS	-	expression tag	UNP Q02880
B	1218	HIS	-	expression tag	UNP Q02880
B	1219	HIS	-	expression tag	UNP Q02880
B	1220	HIS	-	expression tag	UNP Q02880
B	1221	HIS	-	expression tag	UNP Q02880

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			165	77	34	46	8			
2	E	8	Total	C	N	O	P	0	0	0
			165	77	34	46	8			

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*GP*CP*AP*GP*CP*TP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	12	Total	C	N	O	P	0	0	0
			245	116	43	74	12			
3	F	11	Total	C	N	O	P	0	0	0
			224	106	38	69	11			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Mg 3 3	0	0
4	B	2	Total Mg 2 2	0	0
4	D	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

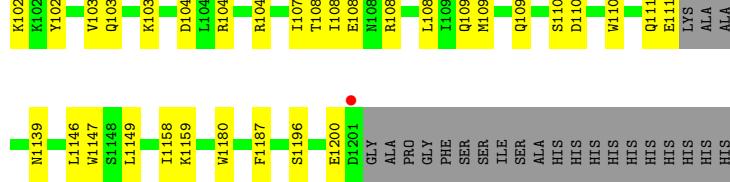
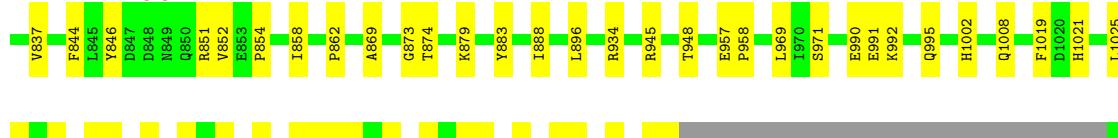
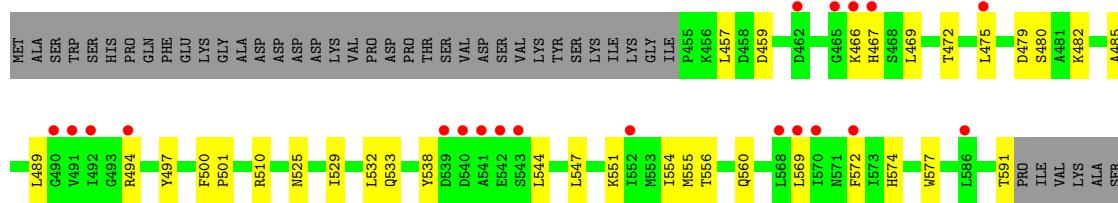
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	266	Total O 266 266	0	0
5	B	340	Total O 340 340	0	0
5	C	23	Total O 23 23	0	0
5	D	30	Total O 30 30	0	0
5	E	26	Total O 26 26	0	0
5	F	18	Total O 18 18	0	0

3 Residue-property plots

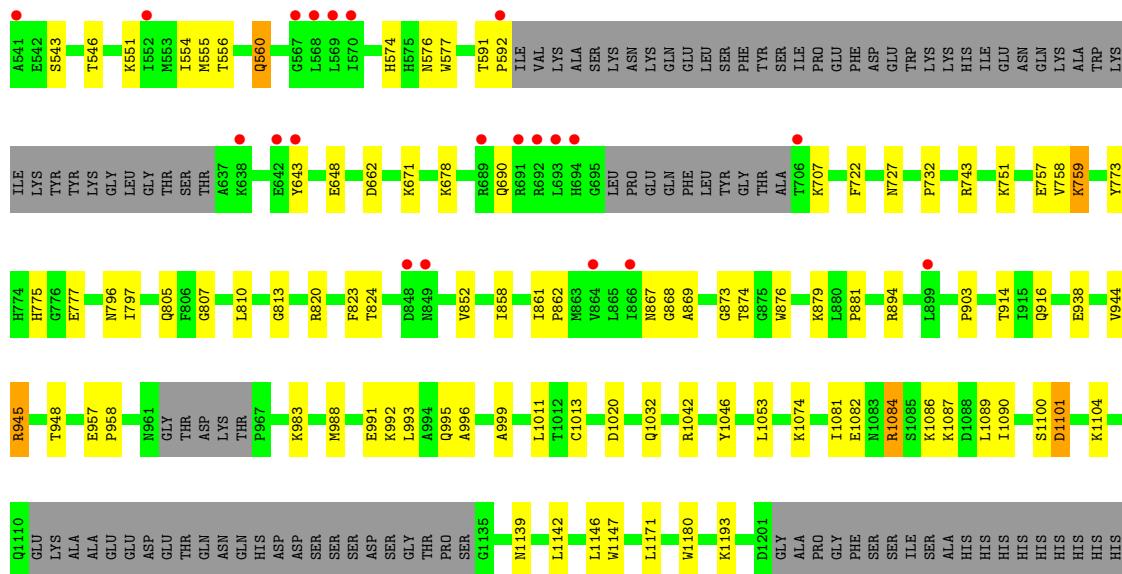
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA topoisomerase 2-beta



- Molecule 1: DNA topoisomerase 2-beta





- Molecule 2: DNA ($5'$ -D(P*AP*GP*CP*CP*GP*AP*GP*C)- $3'$)



- Molecule 2: DNA ($5'$ -D(P*AP*GP*CP*CP*GP*AP*GP*C)- $3'$)



- Molecule 3: DNA ($5'$ -D(P*TP*GP*CP*AP*GP*CP*TP*CP*GP*GP*CP*T)- $3'$)



- Molecule 3: DNA ($5'$ -D(P*TP*GP*CP*AP*GP*CP*TP*CP*GP*GP*CP*T)- $3'$)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.95 Å 176.37 Å 94.22 Å 90.00° 112.06° 90.00°	Depositor
Resolution (Å)	27.31 – 2.30 27.31 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.9 (27.31-2.30) 92.8 (27.31-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ ¹	2.63 (at 2.31 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R , R_{free}	0.176 , 0.218 0.174 , 0.215	Depositor DCC
R_{free} test set	5168 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12463	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
MG

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	0.39	0/5637	0.51	0/7590
1	B	0.40	0/5609	0.52	1/7551 (0.0%)
2	C	0.71	0/185	1.35	1/283 (0.4%)
2	E	0.91	0/185	1.56	3/283 (1.1%)
3	D	0.74	0/273	1.55	7/419 (1.7%)
3	F	0.78	0/248	1.65	6/378 (1.6%)
All	All	0.43	0/12137	0.66	18/16504 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	13	DG	O4'-C1'-N9	9.30	114.51	108.00
2	E	2	DG	O4'-C1'-N9	9.14	114.40	108.00
3	D	19	DC	C1'-O4'-C4'	-8.73	101.37	110.10
3	D	17	DG	O4'-C1'-N9	-7.97	102.42	108.00
3	F	19	DC	C1'-O4'-C4'	-7.90	102.20	110.10
2	E	8	DC	O4'-C1'-N1	7.59	113.32	108.00
3	D	20	DT	O4'-C4'-C3'	-7.58	101.45	106.00
2	C	8	DC	O4'-C1'-N1	7.19	113.03	108.00
3	D	13	DG	O4'-C1'-N9	7.15	113.00	108.00
2	E	1	DA	C1'-O4'-C4'	-7.07	103.03	110.10
3	F	11	DC	O4'-C1'-N1	7.03	112.92	108.00
3	D	9	DT	N3-C4-O4	6.29	123.67	119.90
3	D	20	DT	C1'-O4'-C4'	-6.20	103.90	110.10
1	B	743	ARG	NE-CZ-NH2	-6.18	117.21	120.30
3	F	14	DC	O4'-C4'-C3'	-5.99	102.10	104.50
3	F	17	DG	O4'-C1'-N9	-5.85	103.90	108.00
3	D	9	DT	C5-C4-O4	-5.53	121.03	124.90
3	F	19	DC	P-O5'-C5'	-5.01	112.88	120.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5480	0	5564	92	0
1	B	5474	0	5554	92	0
2	C	165	0	89	4	0
2	E	165	0	89	1	0
3	D	245	0	136	11	0
3	F	224	0	126	3	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	A	266	0	0	4	0
5	B	340	0	0	15	0
5	C	23	0	0	2	0
5	D	30	0	0	1	0
5	E	26	0	0	1	0
5	F	18	0	0	1	0
All	All	12463	0	11558	186	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (186) 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:1032[A]:GLN:HG2	5:A:1582:HOH:O	1.58	1.03
1:B:510:ARG:HH22	1:B:574:HIS:HD2	1.14	0.93
1:A:805:GLN:HE21	1:A:807:GLY:H	1.15	0.89
1:B:560:GLN:H	1:B:560:GLN:HE21	1.22	0.87
1:B:797:ILE:H	1:B:867:ASN:HD21	1.20	0.86
1:B:805:GLN:HE21	1:B:807:GLY:H	1.27	0.82
3:D:10:DG:H2"	3:D:11:DC:H5"	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:GLU:HB2	1:B:820[B]:ARG:HH11	1.47	0.78
3:D:10:DG:C2'	3:D:11:DC:H5"	2.16	0.75
1:A:510:ARG:HH22	1:A:574:HIS:HD2	1.33	0.74
1:A:1139:ASN:HD22	1:B:1147:TRP:HE1	1.34	0.73
1:B:536:LYS:HZ2	1:B:546:THR:HG21	1.53	0.73
2:C:1:DA:C8	2:C:1:DA:H5'	2.25	0.72
1:B:944:VAL:HG12	1:B:945:ARG:HG2	1.71	0.72
1:A:805:GLN:NE2	1:A:807:GLY:H	1.85	0.71
1:A:846:TYR:CZ	1:A:851:ARG:HG3	2.25	0.71
1:B:536:LYS:NZ	1:B:546:THR:HG21	2.07	0.70
1:B:805:GLN:NE2	1:B:807:GLY:H	1.89	0.70
1:B:868:GLY:HA2	5:B:1681:HOH:O	1.91	0.69
1:A:466:LYS:HG3	1:A:467:HIS:CD2	2.28	0.68
1:B:868:GLY:CA	5:B:1681:HOH:O	2.42	0.68
1:A:820[A]:ARG:HD3	3:F:9:DT:OP2	1.95	0.66
1:B:1087:LYS:HE2	5:B:1732:HOH:O	1.97	0.65
1:A:777:GLU:HB2	1:B:820[B]:ARG:NH1	2.12	0.64
1:B:879:LYS:HE2	5:D:218:HOH:O	1.97	0.64
1:A:466:LYS:HG3	1:A:467:HIS:HD2	1.62	0.63
1:A:820[B]:ARG:NH1	1:B:777:GLU:HB2	2.13	0.63
1:A:485:ALA:O	1:A:489:LEU:HB2	2.00	0.61
1:B:592:PRO:HG2	1:B:643:TYR:OH	1.99	0.61
1:A:732:PRO:HG3	1:A:869:ALA:HB1	1.81	0.61
3:D:11:DC:H2"	3:D:12:DA:H5'	1.84	0.60
1:A:510:ARG:HH22	1:A:574:HIS:CD2	2.19	0.59
1:A:759:LYS:HE3	5:B:1480:HOH:O	2.02	0.59
1:B:540:ASP:HB2	1:B:543:SER:H	1.69	0.58
1:B:574:HIS:HE1	1:B:662:ASP:OD2	1.87	0.58
1:B:938:GLU:OE2	1:B:983:LYS:HE3	2.02	0.58
1:B:457:LEU:HD22	1:B:529:ILE:HG12	1.85	0.58
1:A:1079:ILE:HD11	1:A:1092:MET:HE3	1.86	0.57
1:B:732:PRO:HG2	1:B:869:ALA:HB1	1.86	0.57
3:F:10:DG:H2"	3:F:11:DC:OP2	2.04	0.57
1:B:868:GLY:N	5:B:1681:HOH:O	2.38	0.56
1:B:1086:LYS:O	1:B:1090:ILE:HG12	2.05	0.56
1:B:510:ARG:HH22	1:B:574:HIS:CD2	2.06	0.56
3:D:10:DG:H2"	3:D:11:DC:C5'	2.33	0.56
1:A:1147:TRP:HE1	1:B:1139:ASN:HD22	1.52	0.56
1:A:778[B]:GLN:HG2	5:C:110:HOH:O	2.06	0.55
3:D:10:DG:H1'	3:D:11:DC:H5"	1.89	0.55
1:A:457:LEU:HD13	1:A:529:ILE:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778[A]:GLN:HB2	3:D:9:DT:H73	1.88	0.55
1:A:820[B]:ARG:HH11	1:B:777:GLU:HB2	1.70	0.54
1:A:479:ASP:O	1:A:482:LYS:HB3	2.08	0.54
1:B:536:LYS:NZ	1:B:546:THR:CG2	2.71	0.54
1:B:560:GLN:HE21	1:B:560:GLN:N	1.98	0.54
1:A:1026:LYS:HD3	1:A:1028:TYR:CZ	2.44	0.53
1:A:746[B]:LEU:HG	1:A:750:PHE:CE2	2.42	0.53
1:B:881:PRO:HB3	1:B:1011:LEU:HD21	1.89	0.53
1:B:810[A]:LEU:HD12	1:B:948:THR:HB	1.91	0.53
1:A:883:TYR:CZ	1:A:1031[A]:VAL:HG21	2.44	0.53
1:B:858:ILE:HG13	1:B:1042:ARG:HD2	1.91	0.53
1:B:543:SER:HA	5:B:1690:HOH:O	2.08	0.53
1:B:820[A]:ARG:HH21	3:D:9:DT:H2'	1.74	0.52
1:B:510:ARG:NH2	1:B:574:HIS:HD2	1.97	0.52
1:A:459:ASP:O	1:A:494:ARG:NH1	2.40	0.52
1:B:751:LYS:HE3	5:B:1556:HOH:O	2.08	0.52
3:D:10:DG:C1'	3:D:11:DC:H5"	2.40	0.52
1:B:727:ASN:ND2	1:B:874:THR:H	2.08	0.52
1:A:1089:LEU:HD12	1:A:1092:MET:HE2	1.92	0.51
1:B:993:LEU:HD12	1:B:993:LEU:O	2.11	0.51
1:A:533:GLN:HA	5:A:1630:HOH:O	2.10	0.51
1:B:560:GLN:H	1:B:560:GLN:NE2	2.01	0.51
1:B:858:ILE:O	1:B:858:ILE:HG23	2.11	0.51
1:A:769:GLU:HG2	1:A:770:MET:HG3	1.93	0.51
1:A:879:LYS:HE2	5:F:206:HOH:O	2.09	0.51
1:A:1021:HIS:HD2	5:A:1659:HOH:O	1.93	0.51
1:B:727:ASN:HD21	1:B:874:THR:H	1.57	0.51
1:A:934:ARG:HB3	1:A:990:GLU:HG2	1.92	0.51
1:A:751:LYS:HD3	1:A:770:MET:HE3	1.92	0.50
1:B:758[A]:VAL:HG12	1:B:824:THR:O	2.12	0.50
1:A:695:GLY:O	1:A:696:LEU:HD23	2.11	0.49
1:A:1079:ILE:HD11	1:A:1092:MET:CE	2.42	0.49
1:A:1002:HIS:HB3	1:A:1008:GLN:HG3	1.94	0.49
1:A:858:ILE:O	1:A:858:ILE:HG23	2.12	0.49
1:A:769:GLU:HG2	1:A:770:MET:N	2.27	0.49
1:A:1082:GLU:OE2	1:B:1074:LYS:HE3	2.13	0.49
1:B:914:THR:HG22	1:B:916:GLN:HG3	1.95	0.49
1:A:1080:THR:O	1:A:1084:ARG:HD2	2.12	0.48
1:B:560:GLN:HB3	1:B:722:PHE:HA	1.95	0.48
1:A:457:LEU:HD22	1:A:529:ILE:HG12	1.96	0.48
1:B:648:GLU:O	1:B:707:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778[B]:GLN:HG2	1:A:779:ALA:N	2.27	0.48
1:B:1193:LYS:HE2	5:B:1738:HOH:O	2.12	0.48
1:B:546:THR:HG23	5:B:1433:HOH:O	2.14	0.48
1:A:560:GLN:HB3	1:A:722:PHE:HA	1.95	0.48
1:B:461:ASN:HB2	1:B:495:ASP:HA	1.96	0.47
1:B:903:PRO:HA	5:B:1717:HOH:O	2.14	0.47
1:A:727:ASN:ND2	1:A:874:THR:H	2.12	0.47
1:A:810[A]:LEU:HD12	1:A:948:THR:HB	1.95	0.47
1:B:820[A]:ARG:NH2	3:D:9:DT:H2'	2.30	0.47
1:A:732:PRO:CG	1:A:869:ALA:HB1	2.44	0.47
1:B:773:TYR:CZ	1:B:775:HIS:HB2	2.49	0.47
1:A:969:LEU:HD12	1:A:992:LYS:HD2	1.97	0.47
1:B:1081:ILE:HG22	1:B:1089:LEU:HD11	1.97	0.46
1:A:957:GLU:HB2	1:A:958:PRO:HD3	1.97	0.46
1:A:1036:LYS:HE3	1:A:1040:ASP:OD2	2.16	0.46
1:A:785:VAL:O	1:A:789:GLN:HG3	2.16	0.46
1:A:472:THR:HB	1:A:497:TYR:CD2	2.50	0.46
1:B:796:ASN:H	1:B:867:ASN:HD22	1.63	0.46
3:D:11:DC:H6	3:D:11:DC:H5'	1.80	0.46
1:A:480:SER:HB3	5:A:1593:HOH:O	2.15	0.46
1:A:489:LEU:HD21	1:A:497:TYR:CB	2.46	0.46
1:A:1146:LEU:HD23	1:B:1146:LEU:HD23	1.98	0.45
1:B:894:ARG:NH2	5:B:1713:HOH:O	2.49	0.45
2:C:1:DA:H5'	2:C:1:DA:H8	1.81	0.45
1:A:667:LEU:HD21	1:A:680:TRP:CG	2.52	0.45
1:A:1081:ILE:HG22	1:A:1089:LEU:HD11	1.98	0.45
1:A:469:LEU:HD11	1:A:544:LEU:O	2.17	0.45
1:B:957:GLU:HB2	1:B:958:PRO:HD3	1.97	0.45
1:A:727:ASN:HD22	1:A:873:GLY:HA3	1.83	0.45
1:A:1091:GLN:O	1:A:1095:GLN:HG3	2.17	0.45
2:C:1:DA:H2"	2:C:2:DG:O5'	2.18	0.44
2:E:1:DA:N7	5:E:120:HOH:O	2.36	0.44
1:A:858:ILE:HG13	1:A:1042:ARG:HD2	1.98	0.44
1:A:844:PHE:HA	1:A:854:PRO:HA	1.99	0.44
1:A:1100:SER:O	1:A:1101:ASP:C	2.54	0.44
1:A:1110:GLN:O	1:A:1111:GLU:CB	2.66	0.44
1:A:1110:GLN:O	1:A:1111:GLU:HB3	2.17	0.44
1:B:1032:GLN:HB2	5:B:1725:HOH:O	2.17	0.44
1:B:1082:GLU:OE1	1:B:1082:GLU:N	2.42	0.44
1:A:555:MET:HB2	1:A:555:MET:HE2	1.84	0.43
1:B:1053:LEU:HB3	1:B:1171:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:VAL:HG13	1:A:1049:ARG:HD2	1.98	0.43
1:A:525:ASN:O	1:A:529:ILE:HG13	2.19	0.43
1:A:532:LEU:HD13	1:A:577:TRP:CZ3	2.53	0.43
1:A:896:LEU:HD21	1:A:1180:TRP:CE3	2.54	0.43
1:B:991:GLU:O	1:B:995:GLN:HG3	2.19	0.43
1:B:1100:SER:O	1:B:1101:ASP:C	2.57	0.43
1:B:881:PRO:HD3	1:B:1013:CYS:SG	2.58	0.43
1:B:944:VAL:O	1:B:945:ARG:HB2	2.19	0.43
1:B:671:LYS:HE3	5:B:1740:HOH:O	2.19	0.43
1:B:1104:LYS:HE3	1:B:1104:LYS:HB2	1.91	0.43
1:A:757:GLU:HB2	1:A:823:PHE:HB3	2.00	0.42
1:B:861:ILE:HB	1:B:862:PRO:HD2	2.00	0.42
1:B:678:LYS:HE3	1:B:876:TRP:CD1	2.53	0.42
1:B:1081:ILE:O	1:B:1084:ARG:HB2	2.20	0.42
2:C:1:DA:H2	3:F:20:DT:H3	1.57	0.42
1:A:554[A]:ILE:HG13	1:A:556:THR:HG23	2.01	0.42
1:B:690:GLN:HA	1:B:690:GLN:OE1	2.19	0.42
1:A:862:PRO:HD2	1:A:888:ILE:CG2	2.49	0.42
1:B:554[A]:ILE:HG13	1:B:556:THR:HG23	2.02	0.42
1:A:475:LEU:HD12	1:A:569[A]:LEU:HD11	2.01	0.42
1:B:450:LYS:O	1:B:451:ILE:HD13	2.19	0.42
1:A:819:PRO:HA	1:A:822:ILE:HG12	2.01	0.42
1:A:1019:PHE:CZ	1:A:1025:LEU:HD13	2.55	0.42
1:A:1106:TRP:O	1:A:1110:GLN:HG2	2.20	0.42
1:A:1149:LEU:HD12	1:B:1081:ILE:HD11	2.01	0.42
1:B:988:MET:CE	1:B:993:LEU:HD13	2.50	0.42
1:B:536:LYS:HZ3	1:B:546:THR:CG2	2.33	0.42
1:A:538:TYR:CE1	1:A:547:LEU:HD21	2.54	0.42
1:A:1196:SER:O	1:A:1200:GLU:HG3	2.20	0.42
1:B:757:GLU:HB2	1:B:823:PHE:HB3	2.01	0.42
1:A:489:LEU:HD21	1:A:497:TYR:HB2	2.02	0.41
1:B:992:LYS:HE3	5:B:1723:HOH:O	2.20	0.41
1:B:576:ASN:HB2	1:B:577:TRP:CE3	2.55	0.41
1:B:555:MET:HB2	1:B:555:MET:HE3	1.96	0.41
1:A:644:PHE:O	1:A:647:MET:HB2	2.21	0.41
1:A:820[B]:ARG:NH1	1:B:777:GLU:CB	2.81	0.41
1:B:807:GLY:HA3	1:B:813:GLY:HA2	2.02	0.41
1:B:996:ALA:O	1:B:999:ALA:O	2.39	0.41
1:B:999:ALA:HB1	5:B:1724:HOH:O	2.18	0.41
1:B:1020:ASP:OD1	1:B:1020:ASP:C	2.59	0.41
1:A:833:LEU:HD21	1:A:1187:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:991[B]:GLU:HG2	1:A:995:GLN:HE21	1.85	0.41
1:A:1158:ILE:HG22	1:A:1159:LYS:N	2.36	0.41
1:B:591:THR:HB	1:B:592:PRO:HD2	2.03	0.41
1:B:727:ASN:HD22	1:B:873:GLY:HA3	1.86	0.41
1:A:500:PHE:HA	1:A:501:PRO:HD3	1.87	0.40
1:B:1046:TYR:CZ	1:B:1180:TRP:HA	2.56	0.40
1:B:759:LYS:HE3	1:B:759:LYS:HB2	1.91	0.40
1:B:1046:TYR:CE2	1:B:1180:TRP:CG	3.09	0.40
1:A:778[B]:GLN:CG	5:C:110:HOH:O	2.65	0.40
1:A:778[B]:GLN:HB3	3:D:9:DT:H73	2.03	0.40
1:A:1147:TRP:CZ2	1:B:1142:LEU:HD12	2.57	0.40
1:B:500:PHE:HA	1:B:501:PRO:HD3	1.98	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	676/803 (84%)	654 (97%)	21 (3%)	1 (0%)	51 64
1	B	671/803 (84%)	650 (97%)	19 (3%)	2 (0%)	41 50
All	All	1347/1606 (84%)	1304 (97%)	40 (3%)	3 (0%)	47 58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	852	VAL
1	A	852	VAL
1	B	1101	ASP

5.3.2 Protein sidechains [\(i\)](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	603/704 (86%)	596 (99%)	7 (1%)	71 84
1	B	599/704 (85%)	594 (99%)	5 (1%)	81 91
All	All	1202/1408 (85%)	1190 (99%)	12 (1%)	76 87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	551	LYS
1	A	591	THR
1	A	769	GLU
1	A	818	SER
1	A	825	MET
1	A	945	ARG
1	A	971	SER
1	B	551	LYS
1	B	560	GLN
1	B	759	LYS
1	B	945	ARG
1	B	1084	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	467	HIS
1	A	558	GLN
1	A	574	HIS
1	A	576	ASN
1	A	727	ASN
1	A	805	GLN
1	A	882	ASN
1	A	922	GLN
1	A	995	GLN
1	A	1067	GLN

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Mol	Chain	Res	Type
1	A	1083	ASN
1	A	1091	GLN
1	A	1139	ASN
1	A	1160	GLN
1	A	1197	GLN
1	B	467	HIS
1	B	560	GLN
1	B	574	HIS
1	B	583	HIS
1	B	694	HIS
1	B	727	ASN
1	B	805	GLN
1	B	867	ASN
1	B	882	ASN
1	B	949	GLN
1	B	1014	ASN
1	B	1021	HIS
1	B	1067	GLN
1	B	1076	GLN
1	B	1095	GLN
1	B	1139	ASN
1	B	1169	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	666/803 (82%)	-0.08	36 (5%) 25 32	24, 44, 81, 112	0
1	B	670/803 (83%)	-0.14	29 (4%) 35 42	25, 40, 72, 96	0
2	C	8/8 (100%)	-0.43	1 (12%) 3 5	37, 40, 62, 82	0
2	E	8/8 (100%)	-0.62	0 100 100	30, 33, 55, 78	0
3	D	12/12 (100%)	-0.30	0 100 100	29, 38, 80, 88	0
3	F	11/12 (91%)	-0.17	1 (9%) 9 12	37, 49, 72, 86	0
All	All	1375/1646 (83%)	-0.12	67 (4%) 29 36	24, 42, 77, 112	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	491	VAL	5.8
1	A	849	ASN	5.0
1	A	490	GLY	4.6
1	A	693	LEU	4.4
1	A	643	TYR	4.4
1	A	542	GLU	4.3
1	A	492	ILE	4.2
1	B	849	ASN	4.2
1	B	592	PRO	4.2
1	B	643	TYR	4.1
1	B	693	LEU	4.1
1	A	848	ASP	4.0
1	B	848	ASP	3.9
1	A	657	ALA	3.7
1	A	466	LYS	3.7
1	A	642	GLU	3.6
1	A	543	SER	3.5
1	A	568	LEU	3.5
1	B	706	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	695	GLY	3.5
1	B	568	LEU	3.4
1	B	638	LYS	3.2
1	B	694	HIS	3.2
1	B	569[A]	LEU	3.1
1	A	552	ILE	3.0
1	A	540	ASP	3.0
1	A	645	ALA	3.0
1	B	452	LYS	2.9
1	A	541	ALA	2.9
1	B	491	VAL	2.8
1	B	692	ARG	2.8
1	A	696	LEU	2.8
1	B	899	LEU	2.8
1	B	466	LYS	2.7
1	A	690	GLN	2.7
1	B	570	ILE	2.7
1	A	569[A]	LEU	2.7
1	B	689[A]	ARG	2.6
1	B	866	ILE	2.6
1	B	453	GLY	2.6
1	A	570	ILE	2.6
2	C	1	DA	2.5
1	A	462	ASP	2.4
1	A	467	HIS	2.4
1	A	539	ASP	2.4
1	A	694	HIS	2.4
1	B	449	SER	2.4
1	A	465	GLY	2.3
1	A	644	PHE	2.3
1	B	541	ALA	2.3
1	A	1201	ASP	2.3
1	B	864	VAL	2.3
1	B	490	GLY	2.3
1	A	641	LYS	2.3
1	B	642	GLU	2.3
1	B	506	ILE	2.3
1	A	475	LEU	2.2
1	B	691	ARG	2.2
1	A	572	PHE	2.2
1	A	692	ARG	2.2
1	B	552	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	11	DC	2.2
1	A	494	ARG	2.1
1	A	586	LEU	2.1
1	B	567	GLY	2.1
1	B	492	ILE	2.1
1	A	659	PRO	2.1

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 monosaccharides 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(Å ²)	Q<0.9
4	MG	F	101	1/1	0.71	0.07	62,62,62,62	0
4	MG	B	1301	1/1	0.87	0.04	38,38,38,38	0
4	MG	D	101	1/1	0.89	0.13	55,55,55,55	0
4	MG	A	1302	1/1	0.93	0.51	67,67,67,67	0
4	MG	B	1302	1/1	0.94	0.10	61,61,61,61	0
4	MG	A	1301	1/1	0.96	0.04	46,46,46,46	0
4	MG	A	1303	1/1	0.96	0.13	56,56,56,56	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.