



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:42 AM UTC

PDB ID : 3LEL / pdb_00003lel
Title : Structural Insight into the Sequence-Dependence of Nucleosome Positioning
Authors : Wu, B.; Vasudevan, D.; Davey, C.A.
Deposited on : 2010-01-15
Resolution : 2.95 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

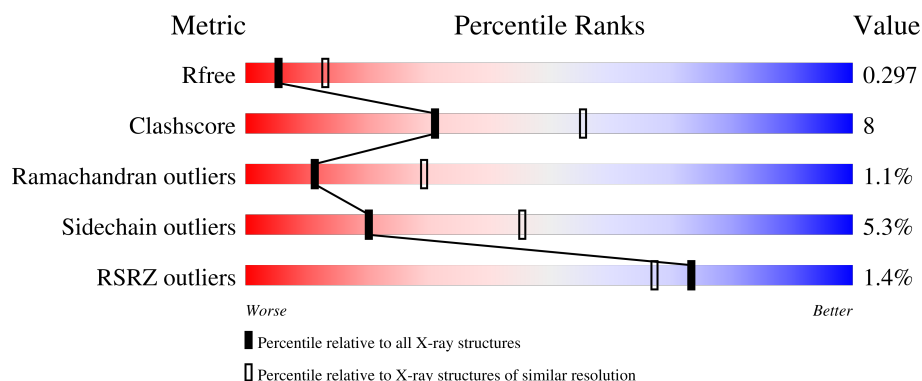
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	136	% 51% 18% • 28%
1	E	136	51% 21% • 28%
1	K	136	58% 12% • 27%
1	O	136	% 49% 22% • 28%
2	B	102	% 59% 19% 23%

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Mol	Chain	Length	Quality of chain
2	F	102	
2	L	102	
2	P	102	
3	C	128	
3	G	128	
3	M	128	
3	Q	128	
4	D	125	
4	H	125	
4	N	125	
4	R	125	
5	I	147	
5	S	147	
6	J	147	
6	T	147	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24335 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 Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			808	509	156	140	3			
1	E	98	Total	C	N	O	S	0	0	0
			808	509	156	140	3			
1	K	99	Total	C	N	O	S	0	0	0
			817	515	158	141	3			
1	O	98	Total	C	N	O	S	0	0	0
			808	509	156	140	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	SEE REMARK 999	UNP P84233
E	102	ALA	GLY	SEE REMARK 999	UNP P84233
K	102	ALA	GLY	SEE REMARK 999	UNP P84233
O	102	ALA	GLY	SEE REMARK 999	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
2	F	86	Total	C	N	O	S	0	0	0
			694	436	140	117	1			
2	L	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
2	P	87	Total	C	N	O	S	0	0	0
			703	442	142	118	1			

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	104	Total	C	N	O	0	0	0
			804	507	157	140			
3	G	109	Total	C	N	O	0	0	0
			843	531	164	148			
3	M	106	Total	C	N	O	0	0	0
			820	517	160	143			
3	Q	109	Total	C	N	O	0	0	0
			843	531	164	148			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ALA	deletion	UNP Q6AZJ8
G	?	-	ALA	deletion	UNP Q6AZJ8
M	?	-	ALA	deletion	UNP Q6AZJ8
Q	?	-	ALA	deletion	UNP Q6AZJ8

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	100	Total	C	N	O	S	0	0	0
			789	495	147	145	2			
4	H	96	Total	C	N	O	S	0	0	0
			756	475	138	141	2			
4	N	96	Total	C	N	O	S	0	0	0
			756	475	138	141	2			
4	R	96	Total	C	N	O	S	0	0	0
			756	475	138	141	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	SEE REMARK 999	UNP P02281
H	29	THR	SER	SEE REMARK 999	UNP P02281
N	29	THR	SER	SEE REMARK 999	UNP P02281
R	29	THR	SER	SEE REMARK 999	UNP P02281

- Molecule 5 is a DNA chain called 147-MER DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	147	Total	C	N	O	P	0	0	0
			3011	1445	541	879	146			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S	147	Total	C	N	O	P	0	0	0
			3011	1445	541	879	146			

- Molecule 6 is a DNA chain called 147-MER DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	147	Total	C	N	O	P	0	0	0
			3010	1445	538	881	146			
6	T	147	Total	C	N	O	P	0	0	0
			3010	1445	538	881	146			

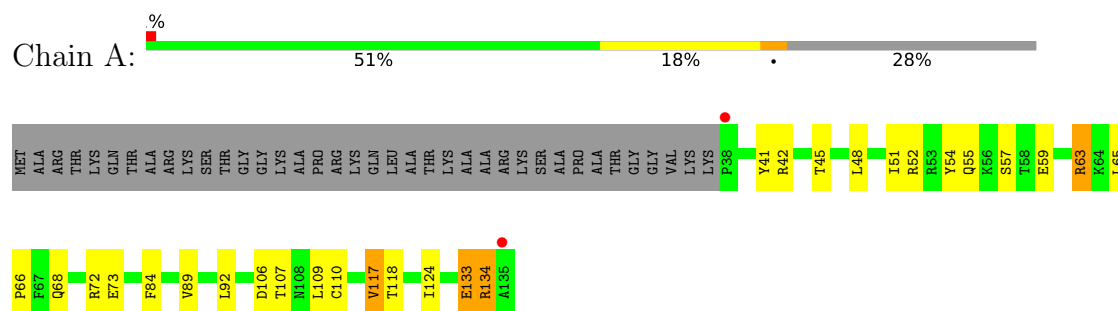
- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Mn	0	0
			1	1		
7	I	6	Total	Mn	0	0
			6	6		
7	J	8	Total	Mn	0	0
			8	8		
7	N	1	Total	Mn	0	0
			1	1		
7	O	1	Total	Mn	0	0
			1	1		
7	S	8	Total	Mn	0	0
			8	8		
7	T	9	Total	Mn	0	0
			9	9		

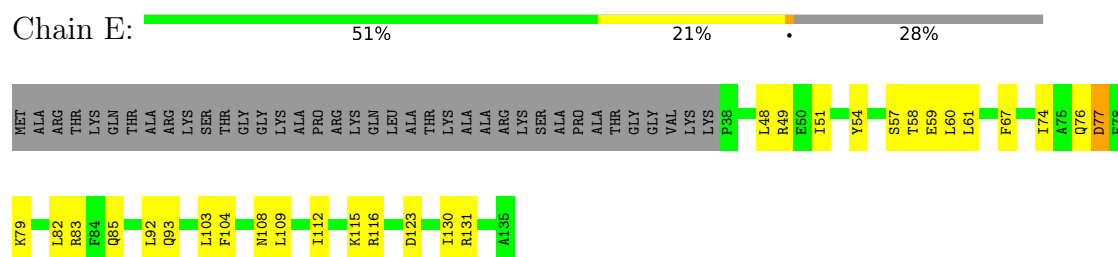
3 Residue-property plots [i](#)

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.

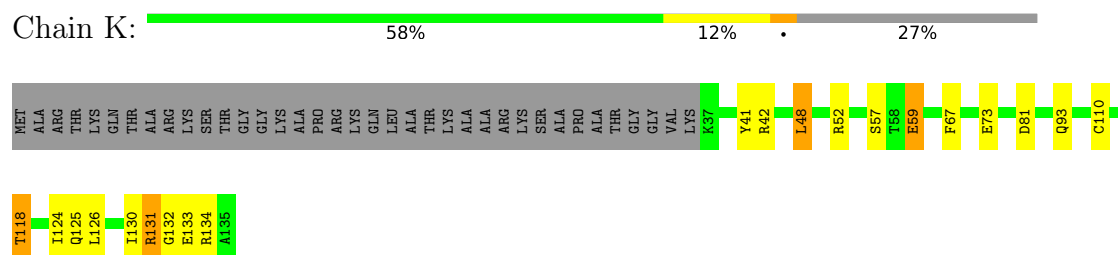
- Molecule 1: Histone H3.2



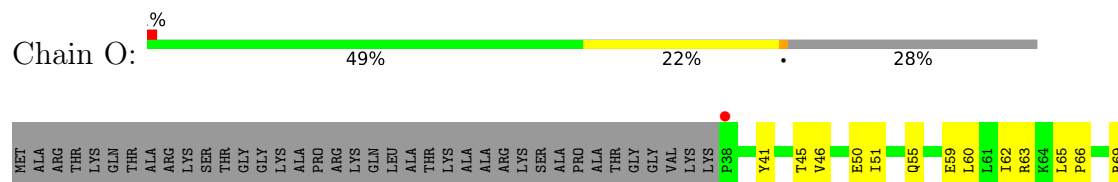
- Molecule 1: Histone H3.2

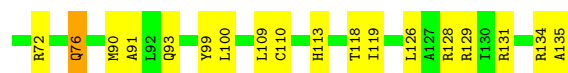


- Molecule 1: Histone H3.2

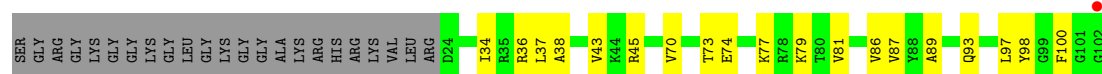


- Molecule 1: Histone H3.2

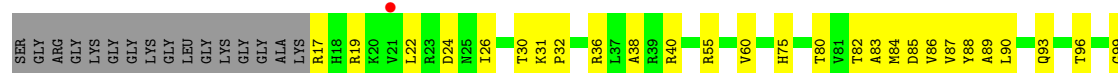




- Molecule 2: Histone H4



- Molecule 2: Histone H4



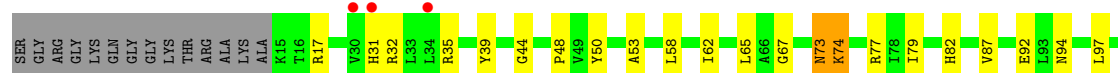
- Molecule 2: Histone H4



- Molecule 2: Histone H4

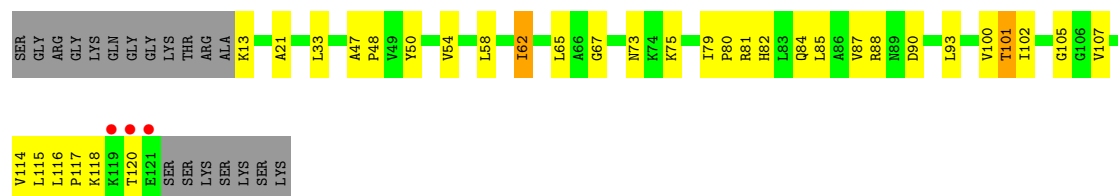


- Molecule 3: Histone H2A

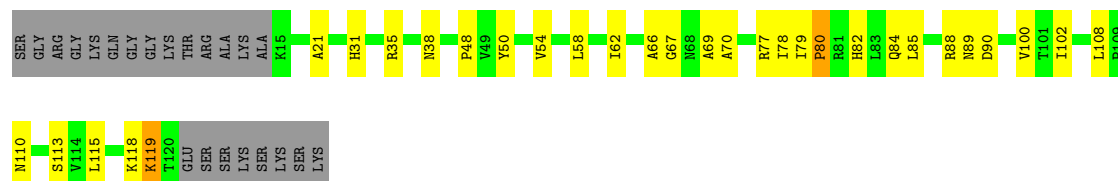


- Molecule 3: Histone H2A

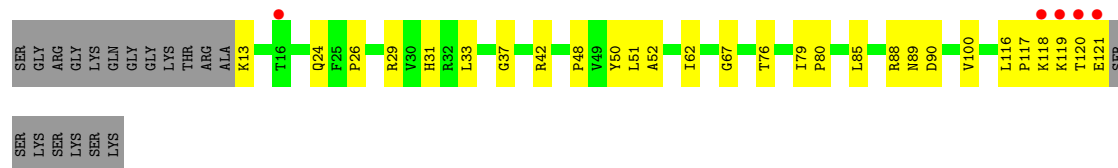




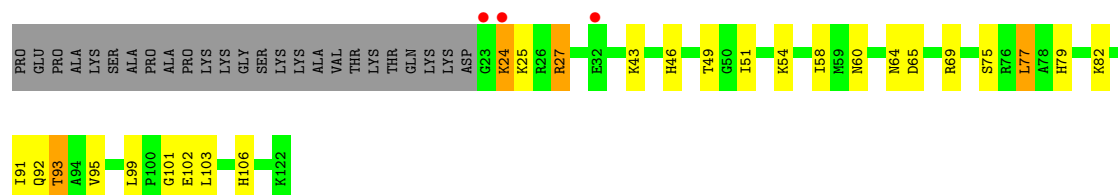
• Molecule 3: Histone H2A



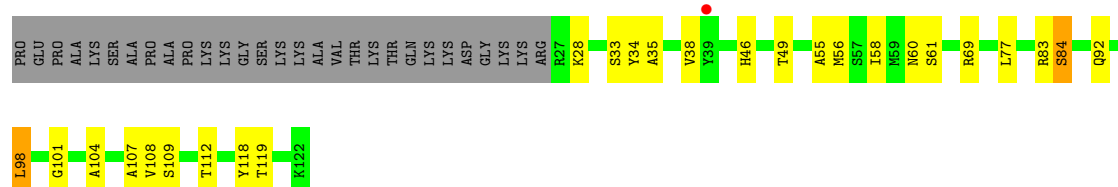
• Molecule 3: Histone H2A



• Molecule 4: Histone H2B 1.1

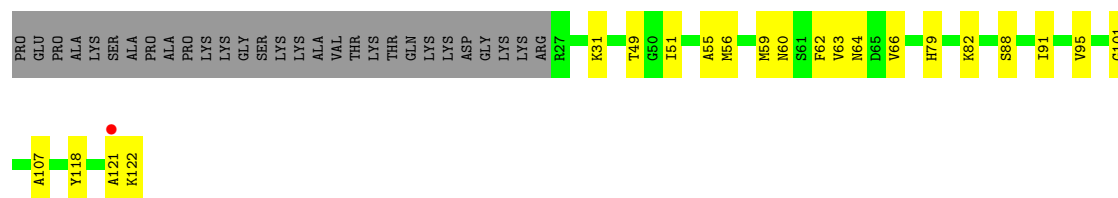


• Molecule 4: Histone H2B 1.1

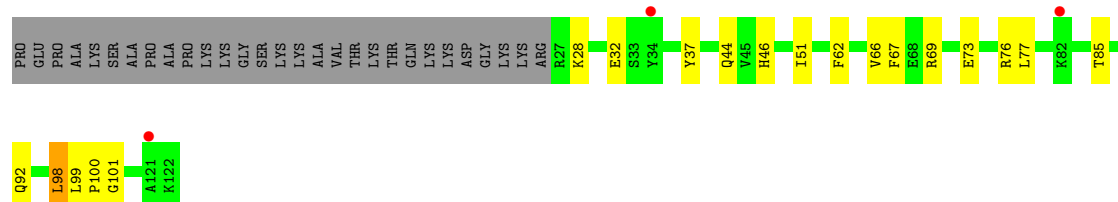


• Molecule 4: Histone H2B 1.1

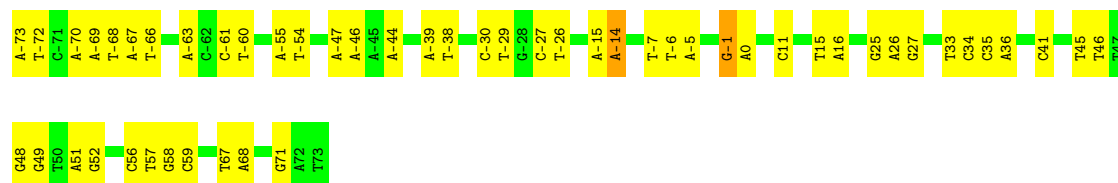




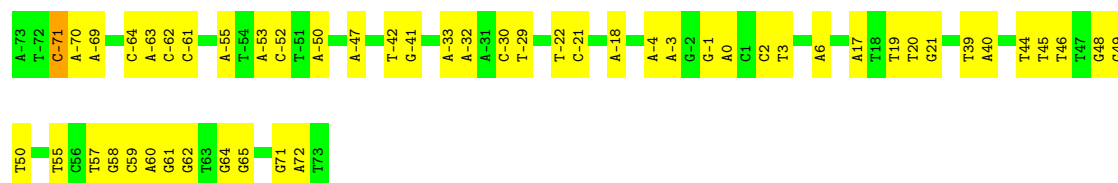
• Molecule 4: Histone H2B 1.1



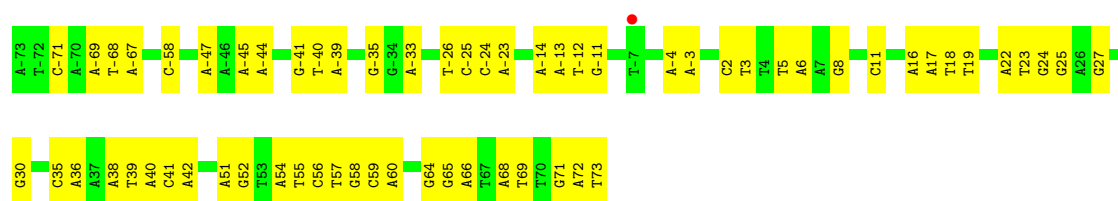
• Molecule 5: 147-MER DNA



• Molecule 5: 147-MER DNA



• Molecule 6: 147-MER DNA



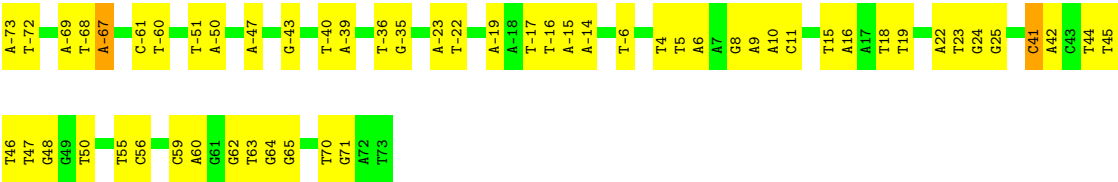
• Molecule 6: 147-MER DNA

Chain T:

62%

37%

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.75Å 178.51Å 110.41Å 90.00° 102.78° 90.00°	Depositor
Resolution (Å)	60.00 – 2.95 60.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	89.7 (60.00-2.95) 89.7 (60.00-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.229 , 0.300 0.224 , 0.297	Depositor DCC
R_{free} test set	1508 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	82.6	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24335	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: MN

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	0.60	0/820	0.90	0/1099
1	E	0.58	0/820	0.90	0/1099
1	K	0.57	0/829	0.89	0/1111
1	O	0.60	0/820	0.98	1/1099 (0.1%)
2	B	0.59	0/634	0.92	1/848 (0.1%)
2	F	0.57	0/702	0.90	0/937
2	L	0.56	0/634	0.96	0/848
2	P	0.60	0/711	0.90	0/948
3	C	0.61	0/814	0.89	1/1099 (0.1%)
3	G	0.56	0/853	0.95	3/1150 (0.3%)
3	M	0.55	0/830	0.96	0/1120
3	Q	0.63	0/853	0.92	2/1150 (0.2%)
4	D	0.59	0/800	0.94	0/1070
4	H	0.52	0/767	0.91	0/1029
4	N	0.55	0/767	0.95	0/1029
4	R	0.58	0/767	0.91	0/1029
5	I	0.28	0/3378	0.93	2/5212 (0.0%)
5	S	0.32	1/3378 (0.0%)	0.94	2/5212 (0.0%)
6	J	0.29	0/3376	0.94	1/5209 (0.0%)
6	T	0.29	0/3376	0.98	3/5209 (0.1%)
All	All	0.45	1/25929 (0.0%)	0.94	16/37507 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	-18	DA	P-OP2	5.05	1.58	1.48

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	100	PHE	N-CA-C	-7.73	105.00	114.75
3	G	116	LEU	CA-C-N	7.11	128.73	119.84
3	G	116	LEU	C-N-CA	7.11	128.73	119.84
3	Q	116	LEU	CA-C-N	6.70	128.22	119.84
3	Q	116	LEU	C-N-CA	6.70	128.22	119.84
5	I	-1	DG	P-O3'-C3'	5.66	128.69	120.20
5	S	-71	DC	P-O3'-C3'	5.55	128.52	120.20
6	T	11	DC	P-O3'-C3'	5.53	128.50	120.20
6	J	11	DC	P-O3'-C3'	5.35	128.23	120.20
5	S	55	DT	P-O3'-C3'	5.32	128.18	120.20
6	T	41	DC	P-O3'-C3'	5.23	128.05	120.20
1	O	69	ARG	N-CA-C	-5.14	105.37	110.97
3	C	67	GLY	N-CA-C	-5.09	106.48	112.64
6	T	-67	DA	C4'-C3'-O3'	-5.04	102.45	110.00
5	I	-14	DA	P-O3'-C3'	5.02	127.73	120.20
3	G	62	ILE	CB-CA-C	-5.01	105.48	112.04

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	808	0	846	22	0
1	E	808	0	846	21	0
1	K	817	0	858	13	0
1	O	808	0	846	22	0
2	B	627	0	663	12	0
2	F	694	0	742	17	0
2	L	627	0	663	7	0
2	P	703	0	755	16	0
3	C	804	0	859	25	0
3	G	843	0	903	23	0
3	M	820	0	879	23	0
3	Q	843	0	903	19	0
4	D	789	0	828	17	0
4	H	756	0	786	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	756	0	786	15	0
4	R	756	0	786	13	0
5	I	3011	0	1667	41	0
5	S	3011	0	1667	35	0
6	J	3010	0	1668	50	0
6	T	3010	0	1668	42	0
7	G	1	0	0	0	0
7	I	6	0	0	0	0
7	J	8	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	0	0
7	S	8	0	0	0	0
7	T	9	0	0	0	0
All	All	24335	0	19619	357	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 (357) 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)
6:T:-69:DA:H2''	6:T:-68:DT:H5''	1.50	0.93
3:C:17:ARG:HH12	3:C:31:HIS:HD2	1.25	0.85
3:Q:13:LYS:HD2	5:S:46:DT:H4'	1.59	0.84
1:O:129:ARG:HA	1:O:134:ARG:HB2	1.60	0.83
6:T:-68:DT:H2''	6:T:-67:DA:C8	2.16	0.80
5:S:-70:DA:H4'	5:S:-69:DA:OP1	1.80	0.78
3:M:31:HIS:HD2	3:M:48:PRO:HG3	1.47	0.78
3:Q:13:LYS:HG2	6:T:-43:DG:H4'	1.66	0.77
5:S:-22:DT:H3	6:T:22:DA:H61	1.32	0.77
5:S:-64:DC:H2'	5:S:-63:DA:C8	2.19	0.76
2:L:30:THR:HB	2:L:32:PRO:HD2	1.67	0.75
3:G:50:TYR:O	3:G:54:VAL:HG23	1.85	0.75
4:N:91:ILE:O	4:N:95:VAL:HG23	1.87	0.74
4:D:91:ILE:O	4:D:95:VAL:HG23	1.88	0.74
4:H:28:LYS:HE2	6:J:-47:DA:H4'	1.68	0.74
3:C:50:TYR:OH	4:D:92:GLN:HG3	1.88	0.73
5:I:-7:DT:O2	6:J:8:DG:N2	2.23	0.72
3:C:17:ARG:HH12	3:C:31:HIS:CD2	2.07	0.71
6:T:-16:DT:H4'	6:T:-15:DA:OP1	1.91	0.70
6:T:64:DG:H2''	6:T:65:DG:OP2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:6:DA:H61	6:T:-6:DT:H3	1.41	0.69
3:M:31:HIS:CD2	3:M:48:PRO:HG3	2.28	0.68
3:M:80:PRO:HD3	4:N:55:ALA:HB2	1.75	0.68
6:J:-69:DA:H2''	6:J:-68:DT:H5''	1.74	0.68
3:Q:29:ARG:HG2	3:Q:33:LEU:HD12	1.76	0.68
3:G:13:LYS:HD2	5:I:46:DT:H4'	1.76	0.67
3:Q:31:HIS:CD2	3:Q:48:PRO:HG3	2.30	0.66
1:O:50:GLU:HB3	2:P:39:ARG:HD2	1.78	0.65
1:O:99:TYR:HE1	1:O:131:ARG:NH1	1.95	0.65
1:A:51:ILE:O	1:A:55:GLN:HG3	1.96	0.64
6:J:65:DG:H2''	6:J:66:DA:OP2	1.98	0.64
3:G:73:ASN:O	3:G:75:LYS:HG3	1.98	0.63
5:I:-47:DA:H2''	5:I:-46:DA:C8	2.34	0.62
6:T:22:DA:H2''	6:T:23:DT:OP2	2.00	0.62
3:G:87:VAL:HG12	3:G:88:ARG:HD3	1.82	0.62
3:Q:50:TYR:OH	4:R:92:GLN:NE2	2.25	0.62
2:L:53:GLU:O	2:L:57:VAL:HG23	2.01	0.61
1:O:99:TYR:HE1	1:O:131:ARG:HH12	1.44	0.61
6:T:-69:DA:C2'	6:T:-68:DT:H5''	2.27	0.61
1:A:106:ASP:HA	1:A:109:LEU:HD12	1.82	0.61
3:C:73:ASN:N	3:C:73:ASN:HD22	1.99	0.61
1:A:41:TYR:OH	6:J:-67:DA:H5'	2.00	0.60
1:A:63:ARG:O	1:A:66:PRO:HD2	2.02	0.60
3:Q:31:HIS:HD2	3:Q:48:PRO:HG3	1.66	0.60
5:I:33:DT:H3	6:J:-33:DA:H61	1.48	0.59
6:J:57:DT:H2''	6:J:58:DG:N7	2.16	0.59
5:I:35:DC:H42	6:J:-35:DG:H1	1.51	0.59
6:J:68:DA:H1'	6:J:69:DT:H5'	1.85	0.59
1:K:73:GLU:OE1	2:L:25:ASN:ND2	2.35	0.59
5:S:39:DT:H2''	5:S:40:DA:H8	1.67	0.59
6:T:-40:DT:H2''	6:T:-39:DA:OP2	2.02	0.59
3:C:17:ARG:NH1	3:C:31:HIS:HD2	1.98	0.58
1:O:119:ILE:O	2:P:47:SER:HB3	2.02	0.58
3:M:85:LEU:O	3:M:89:ASN:HB2	2.04	0.57
6:J:72:DA:H2''	6:J:73:DT:H5''	1.86	0.57
1:O:63:ARG:O	1:O:66:PRO:HD2	2.05	0.57
3:C:31:HIS:CD2	3:C:48:PRO:HG3	2.39	0.57
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.40	0.56
1:O:110:CYS:SG	1:O:126:LEU:HD23	2.44	0.56
1:O:128:ARG:HH12	1:O:134:ARG:HE	1.53	0.56
1:E:103:LEU:HA	1:E:131:ARG:NH2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:79:ILE:HG12	3:M:82:HIS:CE1	2.40	0.56
4:D:24:LYS:H	6:J:51:DA:H4'	1.70	0.56
5:I:-61:DC:H2''	5:I:-60:DT:OP2	2.05	0.56
6:T:15:DT:H2''	6:T:16:DA:OP2	2.06	0.56
2:F:82:THR:O	2:F:85:ASP:HB2	2.06	0.56
1:O:100:LEU:HD11	2:P:58:LEU:HD13	1.88	0.56
4:N:121:ALA:O	4:N:122:LYS:HB2	2.06	0.55
1:K:67:PHE:CZ	1:K:93:GLN:HA	2.42	0.55
2:F:17:ARG:NH2	6:J:-23:DA:O3'	2.39	0.55
5:I:45:DT:H2''	5:I:46:DT:H6	1.72	0.55
5:S:-71:DC:H2''	5:S:-70:DA:OP2	2.06	0.55
4:D:54:LYS:O	4:D:58:ILE:HG12	2.06	0.54
1:A:42:ARG:CZ	1:A:42:ARG:HA	2.37	0.54
6:T:8:DG:H2''	6:T:9:DA:C8	2.42	0.54
5:I:15:DT:H2''	5:I:16:DA:OP2	2.08	0.54
6:J:35:DC:H2''	6:J:36:DA:N7	2.23	0.54
1:O:66:PRO:HG3	5:S:17:DA:OP1	2.08	0.54
6:T:18:DT:H2'	6:T:19:DT:H71	1.89	0.54
5:I:-67:DA:C2	6:J:68:DA:C2	2.95	0.54
6:J:-4:DA:H2'	6:J:-3:DA:C8	2.43	0.54
6:J:2:DC:H2'	6:J:3:DT:C6	2.43	0.54
5:I:35:DC:H4'	5:I:36:DA:OP1	2.07	0.54
3:M:88:ARG:HB2	3:M:108:LEU:HD21	1.88	0.54
5:I:-39:DA:H2''	5:I:-38:DT:OP2	2.07	0.53
5:I:58:DG:H1	6:J:-58:DC:H42	1.55	0.53
4:R:69:ARG:HB3	4:R:98:LEU:HD21	1.88	0.53
2:F:83:ALA:O	2:F:87:VAL:HG23	2.08	0.53
1:A:42:ARG:HA	1:A:42:ARG:NE	2.24	0.53
5:S:-30:DC:H2''	5:S:-29:DT:OP2	2.08	0.53
3:G:58:LEU:O	3:G:62:ILE:HG13	2.09	0.53
5:I:-6:DT:H2''	5:I:-5:DA:C8	2.44	0.52
3:M:80:PRO:CD	4:N:55:ALA:HB2	2.39	0.52
1:O:65:LEU:HB3	1:O:66:PRO:HD3	1.91	0.52
3:Q:85:LEU:O	3:Q:89:ASN:HB2	2.08	0.52
6:T:55:DT:H2''	6:T:56:DC:OP2	2.07	0.52
4:D:65:ASP:O	4:D:69:ARG:HG3	2.08	0.52
5:S:57:DT:H2''	5:S:58:DG:N7	2.24	0.52
6:T:70:DT:H2''	6:T:71:DG:C8	2.45	0.52
3:G:102:ILE:HG23	4:H:58:ILE:HD12	1.91	0.52
1:O:41:TYR:HA	6:T:71:DG:H5''	1.90	0.52
1:E:49:ARG:HG3	5:I:-66:DT:OP1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:78:ILE:HG23	3:M:82:HIS:HB2	1.92	0.52
1:K:57:SER:OG	1:K:59:GLU:OE2	2.27	0.52
6:T:45:DT:H2''	6:T:46:DT:OP2	2.09	0.52
2:P:79:LYS:NZ	2:P:79:LYS:HB3	2.24	0.52
2:B:89:ALA:O	2:B:93:GLN:HG2	2.10	0.51
3:G:90:ASP:HB3	3:G:93:LEU:HB2	1.91	0.51
1:E:92:LEU:HG	2:F:86:VAL:HG11	1.91	0.51
5:I:-1:DG:H2''	5:I:0:DA:OP2	2.10	0.51
4:R:32:GLU:HA	5:S:49:DG:H5''	1.93	0.51
4:D:46:HIS:HB3	4:D:49:THR:OG1	2.09	0.51
3:M:78:ILE:HA	3:M:82:HIS:ND1	2.26	0.51
1:A:72:ARG:HH11	1:A:72:ARG:HG2	1.76	0.51
5:I:34:DC:H4'	5:I:35:DC:OP1	2.11	0.51
6:J:59:DC:H2''	6:J:60:DA:N7	2.26	0.51
6:T:63:DT:H2''	6:T:64:DG:OP2	2.09	0.51
4:H:33:SER:HB2	4:H:60:ASN:ND2	2.27	0.50
6:T:59:DC:H2''	6:T:60:DA:N7	2.26	0.50
2:B:98:TYR:CE2	3:G:100:VAL:HG11	2.47	0.50
3:G:84:GLN:HG2	3:G:105:GLY:O	2.11	0.50
6:J:-40:DT:H2''	6:J:-39:DA:OP2	2.11	0.50
5:S:64:DG:H2''	5:S:65:DG:OP2	2.11	0.50
2:B:79:LYS:NZ	6:J:27:DG:OP2	2.38	0.50
4:D:58:ILE:HD13	2:F:99:GLY:HA3	1.93	0.50
3:G:21:ALA:HB2	4:H:118:TYR:HB2	1.94	0.50
3:Q:120:THR:HG22	3:Q:120:THR:O	2.12	0.50
6:J:38:DA:H2'	6:J:39:DT:C6	2.47	0.50
3:M:66:ALA:O	3:M:69:ALA:HB3	2.11	0.50
3:Q:118:LYS:HG3	3:Q:121:GLU:HB2	1.92	0.50
5:S:-42:DT:H2''	5:S:-41:DG:OP2	2.12	0.50
5:I:67:DT:H4'	5:I:68:DA:OP1	2.10	0.50
6:J:-14:DA:H2''	6:J:-13:DA:OP2	2.11	0.49
1:K:126:LEU:HD22	1:O:113:HIS:CG	2.47	0.49
2:P:36:ARG:O	2:P:39:ARG:HB2	2.12	0.49
2:P:39:ARG:NH1	2:P:43:VAL:O	2.44	0.49
1:A:57:SER:HB2	1:A:59:GLU:OE2	2.12	0.49
1:E:54:TYR:OH	2:F:36:ARG:HD2	2.12	0.49
6:T:62:DG:H2''	6:T:63:DT:OP2	2.13	0.49
4:D:75:SER:O	4:D:79:HIS:HD2	1.95	0.49
4:N:51:ILE:HG21	4:N:56:MET:HE2	1.93	0.49
3:G:54:VAL:HG13	4:H:107:ALA:HB1	1.93	0.49
3:M:58:LEU:O	3:M:62:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:-70:DA:H1'	5:S:-69:DA:H5'	1.94	0.49
6:T:-17:DT:H2''	6:T:-16:DT:OP2	2.11	0.49
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.48	0.49
1:O:119:ILE:HG12	2:P:43:VAL:HG11	1.94	0.49
6:J:22:DA:H2''	6:J:23:DT:OP2	2.12	0.49
1:K:41:TYR:HD1	6:T:10:DA:OP1	1.95	0.49
5:S:-61:DC:N4	6:T:60:DA:N6	2.61	0.49
1:E:104:PHE:CD1	2:F:38:ALA:HA	2.47	0.49
6:J:64:DG:H2''	6:J:65:DG:C8	2.48	0.48
2:F:90:LEU:HA	2:F:93:GLN:HB2	1.95	0.48
6:J:5:DT:H4'	6:J:6:DA:H5'	1.95	0.48
6:J:54:DA:H2''	6:J:55:DT:OP2	2.13	0.48
6:J:18:DT:H2''	6:J:19:DT:C6	2.48	0.48
1:K:130:ILE:C	1:K:132:GLY:N	2.70	0.48
2:B:98:TYR:CD1	4:H:61:SER:HB3	2.48	0.48
4:H:35:ALA:HA	4:H:56:MET:SD	2.54	0.48
6:J:71:DG:H2''	6:J:72:DA:OP2	2.14	0.48
3:G:82:HIS:HA	3:G:85:LEU:HD12	1.95	0.48
3:Q:42:ARG:O	4:R:85:THR:HA	2.14	0.48
5:S:59:DC:H2''	5:S:60:DA:N7	2.28	0.48
3:G:67:GLY:HA3	4:H:46:HIS:CD2	2.49	0.47
2:P:90:LEU:HB3	2:P:95:ARG:O	2.15	0.47
3:Q:24:GLN:HG3	4:R:44:GLN:HE22	1.79	0.47
1:O:99:TYR:CE1	1:O:131:ARG:NH1	2.79	0.47
5:S:-50:DA:H61	6:T:50:DT:H3	1.61	0.47
5:S:-47:DA:N1	6:T:48:DG:N2	2.62	0.47
5:I:-73:DA:H4'	5:I:-72:DT:O5'	2.14	0.47
3:M:21:ALA:HB2	4:N:118:TYR:HB2	1.95	0.47
5:S:-1:DG:H2''	5:S:0:DA:C8	2.49	0.47
5:S:20:DT:H2''	5:S:21:DG:OP2	2.14	0.47
4:D:24:LYS:HE2	4:D:27:ARG:HD3	1.97	0.47
4:R:67:PHE:C	4:R:67:PHE:CD2	2.92	0.47
2:B:70:VAL:O	2:B:74:GLU:HG3	2.14	0.47
5:I:-55:DA:C2	5:I:-54:DT:C2	3.02	0.47
6:J:56:DC:H2'	6:J:57:DT:C6	2.50	0.47
3:M:54:VAL:HG13	4:N:107:ALA:HB1	1.96	0.47
3:C:106:GLY:HA3	1:E:58:THR:HG22	1.95	0.47
4:D:102:GLU:O	4:D:106:HIS:HD2	1.98	0.47
4:N:60:ASN:O	4:N:64:ASN:ND2	2.48	0.47
1:O:50:GLU:CB	2:P:39:ARG:HD2	2.43	0.47
6:T:-73:DA:H2''	6:T:-72:DT:OP2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:ILE:HD11	2:F:55:ARG:HB3	1.97	0.47
5:S:-53:DA:H2''	5:S:-52:DC:C6	2.50	0.47
1:A:118:THR:HA	2:B:45:ARG:O	2.14	0.47
1:O:62:ILE:HB	1:O:93:GLN:HE21	1.80	0.47
3:C:87:VAL:HG11	3:C:97:LEU:HD12	1.96	0.47
5:I:26:DA:H2''	5:I:27:DG:C8	2.50	0.47
5:I:-70:DA:C2	6:J:71:DG:N2	2.83	0.46
4:N:62:PHE:CE1	4:N:66:VAL:HG21	2.50	0.46
2:P:30:THR:HB	2:P:32:PRO:HD2	1.97	0.46
3:C:92:GLU:OE1	4:D:102:GLU:HB2	2.15	0.46
4:D:99:LEU:HD13	4:D:103:LEU:HB3	1.97	0.46
1:E:83:ARG:HH21	6:J:-24:DC:H1'	1.80	0.46
4:H:34:TYR:O	4:H:38:VAL:HG23	2.14	0.46
5:S:44:DT:H2'	5:S:45:DT:C6	2.50	0.46
6:T:47:DT:H2''	6:T:48:DG:N7	2.30	0.46
3:C:32:ARG:NH1	5:I:-44:DA:OP2	2.45	0.46
1:K:130:ILE:C	1:K:132:GLY:H	2.24	0.46
2:P:82:THR:O	2:P:85:ASP:HB2	2.15	0.46
2:L:83:ALA:O	2:L:87:VAL:HG23	2.16	0.46
2:P:84:MET:HB3	2:P:88:TYR:CE1	2.49	0.46
3:G:81:ARG:NH1	3:G:107:VAL:O	2.48	0.46
6:T:-51:DT:H2''	6:T:-50:DA:OP2	2.15	0.46
3:Q:26:PRO:HD3	4:R:37:TYR:CD2	2.51	0.46
3:M:31:HIS:CE1	3:M:35:ARG:HE	2.34	0.45
2:B:97:LEU:HD12	3:G:101:THR:O	2.15	0.45
2:B:34:ILE:HA	2:B:37:LEU:HD12	1.98	0.45
3:C:87:VAL:CG1	3:C:97:LEU:HD12	2.46	0.45
2:P:75:HIS:CD2	4:R:77:LEU:HD22	2.51	0.45
5:S:48:DG:N2	6:T:-47:DA:C2	2.84	0.45
1:A:117:VAL:HG12	3:G:115:LEU:HD23	1.99	0.45
3:C:31:HIS:CE1	3:C:35:ARG:NH1	2.84	0.45
1:K:131:ARG:NH1	1:K:133:GLU:OE2	2.49	0.45
3:Q:88:ARG:HA	3:Q:88:ARG:HD3	1.63	0.45
1:A:54:TYR:CZ	2:B:36:ARG:HG2	2.51	0.45
6:T:-61:DC:H2''	6:T:-60:DT:C6	2.51	0.45
4:R:28:LYS:HG3	5:S:50:DT:H4'	1.99	0.45
3:C:77:ARG:HH21	5:I:-55:DA:H4'	1.82	0.45
6:J:16:DA:H2''	6:J:17:DA:H8	1.81	0.45
3:M:84:GLN:OE1	3:M:102:ILE:HD12	2.17	0.45
1:E:57:SER:OG	1:E:59:GLU:OE2	2.32	0.45
1:K:48:LEU:HD12	1:K:52:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:THR:HB	2:F:32:PRO:HD2	1.98	0.45
4:H:104:ALA:O	4:H:108:VAL:HG23	2.17	0.45
5:I:11:DC:H42	6:J:-11:DG:H1	1.65	0.45
5:S:19:DT:H3	6:T:-19:DA:H61	1.65	0.45
4:D:60:ASN:O	4:D:64:ASN:ND2	2.50	0.45
6:J:41:DC:H2''	6:J:42:DA:OP2	2.17	0.45
3:M:67:GLY:HA2	3:M:78:ILE:HD11	1.99	0.44
3:M:77:ARG:NH2	5:S:-55:DA:H4'	2.32	0.44
1:E:116:ARG:HH22	1:E:123:ASP:CG	2.24	0.44
2:F:31:LYS:HB3	2:F:32:PRO:HD3	1.99	0.44
6:J:64:DG:H2''	6:J:65:DG:H8	1.83	0.44
6:T:4:DT:H1'	6:T:5:DT:H5'	1.98	0.44
6:T:44:DT:H2''	6:T:45:DT:OP2	2.17	0.44
5:I:-70:DA:H4'	5:I:-69:DA:OP1	2.18	0.44
1:A:84:PHE:HB3	1:A:89:VAL:HG23	1.99	0.44
3:G:75:LYS:HB3	5:I:59:DC:OP1	2.17	0.44
4:H:92:GLN:HE21	4:H:108:VAL:HG13	1.82	0.44
1:A:133:GLU:O	1:A:134:ARG:CB	2.65	0.44
1:A:72:ARG:HG2	1:A:72:ARG:NH1	2.32	0.44
1:E:54:TYR:CZ	2:F:36:ARG:HD2	2.53	0.44
6:J:-26:DT:H2''	6:J:-25:DC:C6	2.53	0.44
2:F:84:MET:HE1	2:F:102:GLY:HA3	2.00	0.43
6:J:39:DT:H2''	6:J:40:DA:H8	1.82	0.43
6:J:51:DA:H2''	6:J:52:DG:H8	1.82	0.43
6:T:-23:DA:C5	6:T:-22:DT:C4	3.06	0.43
3:M:70:ALA:HB2	3:M:78:ILE:HG12	2.00	0.43
3:M:100:VAL:HG11	2:P:98:TYR:CE2	2.54	0.43
1:E:79:LYS:HB3	1:E:82:LEU:HG	1.99	0.43
5:S:-62:DC:H2''	5:S:-61:DC:H5'	2.00	0.43
1:E:67:PHE:CZ	1:E:93:GLN:HA	2.54	0.43
2:F:88:TYR:O	2:F:89:ALA:C	2.61	0.43
1:O:51:ILE:O	1:O:55:GLN:HG3	2.18	0.43
3:C:50:TYR:O	3:C:53:ALA:HB3	2.18	0.43
5:I:41:DC:H6	5:I:41:DC:H2'	1.71	0.43
6:T:-36:DT:H2''	6:T:-35:DG:N7	2.34	0.43
2:B:73:THR:OG1	2:B:81:VAL:HA	2.18	0.43
3:C:115:LEU:HD11	1:E:108:ASN:HD21	1.84	0.43
6:J:-41:DG:H2''	6:J:-40:DT:OP2	2.18	0.43
6:J:30:DG:H8	6:J:30:DG:H5'	1.83	0.43
4:N:79:HIS:HE1	3:Q:37:GLY:HA2	1.82	0.43
1:A:133:GLU:O	1:A:134:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:GLY:HA2	6:J:38:DA:H5''	2.01	0.43
4:D:77:LEU:HD11	4:D:93:THR:CG2	2.48	0.43
1:E:108:ASN:O	1:E:112:ILE:HG13	2.18	0.43
5:I:45:DT:H2''	5:I:46:DT:C6	2.52	0.43
3:C:31:HIS:CE1	3:C:35:ARG:HH12	2.36	0.43
4:H:84:SER:OG	6:J:-35:DG:H3'	2.19	0.43
5:I:51:DA:H2''	5:I:52:DG:H8	1.83	0.43
5:I:56:DC:H2''	5:I:57:DT:OP2	2.18	0.43
1:O:72:ARG:O	1:O:76:GLN:HB2	2.19	0.43
3:C:77:ARG:NH1	6:J:59:DC:H5'	2.34	0.43
4:D:77:LEU:HD11	4:D:93:THR:HG21	2.00	0.43
1:E:61:LEU:HD21	2:F:40:ARG:NH2	2.33	0.43
3:G:79:ILE:C	4:H:55:ALA:HB2	2.43	0.43
6:J:-45:DA:H2''	6:J:-44:DA:C8	2.53	0.43
5:S:61:DG:C4	5:S:62:DG:N7	2.87	0.43
3:C:58:LEU:O	3:C:62:ILE:HG22	2.18	0.42
1:E:48:LEU:HD23	1:E:51:ILE:HD12	2.01	0.42
1:K:124:ILE:HD11	2:L:50:ILE:HD12	2.01	0.42
2:L:35:ARG:O	2:L:39:ARG:HG2	2.19	0.42
6:T:5:DT:H1'	6:T:6:DA:C8	2.54	0.42
3:C:50:TYR:CZ	4:D:92:GLN:HG3	2.52	0.42
5:I:67:DT:C2	5:I:68:DA:C8	3.07	0.42
4:N:79:HIS:CE1	3:Q:37:GLY:HA2	2.54	0.42
5:I:-27:DC:H4'	5:I:-26:DT:H5'	2.02	0.42
5:I:71:DG:H1	6:J:-71:DC:H42	1.68	0.42
6:J:41:DC:H1'	6:J:42:DA:O5'	2.19	0.42
5:S:-33:DA:H2''	5:S:-32:DA:OP2	2.19	0.42
1:A:107:THR:HG21	1:A:124:ILE:HG12	2.00	0.42
3:C:39:TYR:HB3	4:D:75:SER:HB2	2.01	0.42
5:I:26:DA:H1'	5:I:27:DG:H5'	2.00	0.42
3:M:21:ALA:HB2	4:N:118:TYR:HD1	1.84	0.42
3:M:115:LEU:HD22	2:P:44:LYS:HD3	2.01	0.42
1:O:128:ARG:NH1	1:O:134:ARG:HE	2.15	0.42
3:Q:51:LEU:O	3:Q:52:ALA:C	2.62	0.42
1:A:59:GLU:OE2	1:A:59:GLU:N	2.51	0.42
5:S:2:DC:H2'	5:S:3:DT:C6	2.54	0.42
6:T:24:DG:C6	6:T:25:DG:C6	3.07	0.42
2:B:38:ALA:HB1	2:B:43:VAL:HB	2.00	0.42
3:G:114:VAL:HG22	3:G:114:VAL:O	2.19	0.42
4:H:33:SER:HB2	4:H:60:ASN:HD21	1.85	0.42
5:S:71:DG:H2''	5:S:72:DA:OP2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:48:DG:H2''	5:I:49:DG:OP2	2.19	0.42
1:O:129:ARG:NH1	1:O:135:ALA:HB3	2.34	0.42
6:T:23:DT:H2''	6:T:24:DG:C8	2.55	0.42
1:O:90:MET:O	1:O:91:ALA:C	2.62	0.42
5:I:-30:DC:H2''	5:I:-29:DT:H5'	2.02	0.42
4:N:59:MET:O	4:N:63:VAL:HG23	2.20	0.42
4:R:99:LEU:HA	4:R:100:PRO:HD3	1.89	0.42
1:A:110:CYS:SG	1:E:130:ILE:HD11	2.60	0.41
4:H:69:ARG:HD3	4:H:98:LEU:HD21	2.02	0.41
6:J:-12:DT:H2''	6:J:-11:DG:C8	2.55	0.41
6:T:-15:DA:C2	6:T:-14:DA:C4	3.08	0.41
1:A:65:LEU:O	1:A:66:PRO:C	2.62	0.41
4:N:79:HIS:HE1	3:Q:37:GLY:C	2.28	0.41
3:C:117:PRO:HD3	1:E:48:LEU:CD1	2.51	0.41
1:E:85:GLN:NE2	2:F:82:THR:HG22	2.35	0.41
2:F:75:HIS:CD2	4:H:77:LEU:HD22	2.56	0.41
5:I:-15:DA:C2	5:I:-14:DA:C4	3.09	0.41
4:R:73:GLU:HA	4:R:76:ARG:HH11	1.85	0.41
1:A:92:LEU:HG	2:B:86:VAL:HG11	2.01	0.41
3:C:73:ASN:C	3:C:74:LYS:HD2	2.45	0.41
3:G:93:LEU:HD23	3:G:93:LEU:HA	1.93	0.41
5:I:-47:DA:C2	5:I:-46:DA:C2	3.09	0.41
1:A:68:GLN:O	1:A:72:ARG:HG3	2.20	0.41
3:G:47:ALA:HB3	3:G:48:PRO:CD	2.51	0.41
3:Q:79:ILE:HB	3:Q:80:PRO:CD	2.50	0.41
1:E:77:ASP:OD1	1:E:77:ASP:N	2.52	0.41
1:K:125:GLN:HG2	1:K:134:ARG:NH1	2.36	0.41
3:M:115:LEU:HD22	2:P:44:LYS:HB3	2.03	0.41
5:I:-68:DT:H2''	5:I:-67:DA:OP2	2.21	0.41
5:I:25:DG:H2''	5:I:26:DA:OP2	2.21	0.41
6:J:24:DG:H2'	6:J:25:DG:C8	2.55	0.41
6:J:65:DG:H2'	6:J:65:DG:OP2	2.21	0.41
3:M:50:TYR:HD1	4:N:88:SER:HB2	1.86	0.41
4:H:83:ARG:HA	4:H:83:ARG:HD3	1.96	0.41
3:Q:67:GLY:HA3	4:R:46:HIS:CD2	2.56	0.41
6:T:41:DC:H1'	6:T:42:DA:C8	2.55	0.41
1:A:48:LEU:HB3	1:A:52:ARG:HH12	1.86	0.40
5:I:-63:DA:OP2	5:I:-63:DA:H2'	2.21	0.40
5:S:-22:DT:H2''	5:S:-21:DC:O4'	2.21	0.40
6:J:18:DT:H2''	6:J:19:DT:H6	1.84	0.40
1:K:118:THR:OG1	5:S:-3:DA:OP1	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:62:PHE:O	4:R:66:VAL:HG23	2.22	0.40
3:G:79:ILE:HB	3:G:80:PRO:CD	2.52	0.40
6:T:5:DT:H4'	6:T:6:DA:H5'	2.04	0.40
4:H:58:ILE:H	4:H:58:ILE:HG12	1.71	0.40
2:L:45:ARG:CZ	5:S:-4:DA:H4'	2.51	0.40
3:C:73:ASN:N	3:C:73:ASN:ND2	2.66	0.40
1:E:74:ILE:C	1:E:76:GLN:H	2.29	0.40
1:K:110:CYS:SG	1:K:126:LEU:HD23	2.61	0.40
5:S:-47:DA:C2	6:T:48:DG:N2	2.89	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	96/136 (71%)	90 (94%)	5 (5%)	1 (1%)	12	32
1	E	96/136 (71%)	90 (94%)	6 (6%)	0	100	100
1	K	97/136 (71%)	88 (91%)	9 (9%)	0	100	100
1	O	96/136 (71%)	90 (94%)	5 (5%)	1 (1%)	12	32
2	B	77/102 (76%)	71 (92%)	5 (6%)	1 (1%)	9	26
2	F	84/102 (82%)	78 (93%)	6 (7%)	0	100	100
2	L	77/102 (76%)	72 (94%)	5 (6%)	0	100	100
2	P	85/102 (83%)	78 (92%)	7 (8%)	0	100	100
3	C	102/128 (80%)	97 (95%)	5 (5%)	0	100	100
3	G	107/128 (84%)	95 (89%)	10 (9%)	2 (2%)	6	17
3	M	104/128 (81%)	96 (92%)	6 (6%)	2 (2%)	6	17
3	Q	107/128 (84%)	97 (91%)	8 (8%)	2 (2%)	6	17
4	D	98/125 (78%)	89 (91%)	5 (5%)	4 (4%)	2	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	94/125 (75%)	86 (92%)	7 (7%)	1 (1%)	11	29
4	N	94/125 (75%)	87 (93%)	6 (6%)	1 (1%)	11	29
4	R	94/125 (75%)	89 (95%)	3 (3%)	2 (2%)	5	16
All	All	1508/1964 (77%)	1393 (92%)	98 (6%)	17 (1%)	11	29

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	N	101	GLY
4	R	101	GLY
4	D	51	ILE
4	D	101	GLY
3	M	119	LYS
2	B	77	LYS
3	G	117	PRO
3	Q	117	PRO
4	D	27	ARG
3	G	118	LYS
1	O	59	GLU
4	D	24	LYS
3	Q	119	LYS
1	A	134	ARG
4	R	51	ILE
4	H	101	GLY
3	M	80	PRO

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	85/111 (77%)	80 (94%)	5 (6%)	18	41
1	E	85/111 (77%)	81 (95%)	4 (5%)	23	49
1	K	86/111 (78%)	80 (93%)	6 (7%)	14	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	85/111 (77%)	79 (93%)	6 (7%)	13	33
2	B	64/78 (82%)	63 (98%)	1 (2%)	55	75
2	F	71/78 (91%)	65 (92%)	6 (8%)	10	25
2	L	64/78 (82%)	61 (95%)	3 (5%)	23	49
2	P	72/78 (92%)	70 (97%)	2 (3%)	38	62
3	C	83/101 (82%)	77 (93%)	6 (7%)	13	33
3	G	87/101 (86%)	83 (95%)	4 (5%)	24	50
3	M	85/101 (84%)	79 (93%)	6 (7%)	13	33
3	Q	87/101 (86%)	83 (95%)	4 (5%)	24	50
4	D	85/105 (81%)	80 (94%)	5 (6%)	18	41
4	H	82/105 (78%)	76 (93%)	6 (7%)	13	33
4	N	82/105 (78%)	79 (96%)	3 (4%)	30	55
4	R	82/105 (78%)	81 (99%)	1 (1%)	63	79
All	All	1285/1580 (81%)	1217 (95%)	68 (5%)	20	45

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	63	ARG
1	A	73	GLU
1	A	117	VAL
1	A	133	GLU
2	B	87	VAL
3	C	65	LEU
3	C	73	ASN
3	C	74	LYS
3	C	94	ASN
3	C	100	VAL
3	C	118	LYS
4	D	25	LYS
4	D	43	LYS
4	D	77	LEU
4	D	82	LYS
4	D	93	THR
1	E	60	LEU
1	E	77	ASP

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Mol	Chain	Res	Type
1	E	109	LEU
1	E	115	LYS
2	F	19	ARG
2	F	22	LEU
2	F	24	ASP
2	F	60	VAL
2	F	80	THR
2	F	96	THR
3	G	33	LEU
3	G	65	LEU
3	G	101	THR
3	G	120	THR
4	H	49	THR
4	H	84	SER
4	H	98	LEU
4	H	109	SER
4	H	112	THR
4	H	119	THR
1	K	42	ARG
1	K	48	LEU
1	K	59	GLU
1	K	81	ASP
1	K	118	THR
1	K	131	ARG
2	L	49	LEU
2	L	73	THR
2	L	95	ARG
3	M	38	ASN
3	M	90	ASP
3	M	110	ASN
3	M	113	SER
3	M	118	LYS
3	M	119	LYS
4	N	31	LYS
4	N	49	THR
4	N	82	LYS
1	O	45	THR
1	O	46	VAL
1	O	60	LEU
1	O	76	GLN
1	O	109	LEU
1	O	118	THR

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Mol	Chain	Res	Type
2	P	21	VAL
2	P	47	SER
3	Q	62	ILE
3	Q	76	THR
3	Q	90	ASP
3	Q	100	VAL
4	R	98	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	93	GLN
3	C	31	HIS
3	C	73	ASN
3	C	94	ASN
4	D	44	GLN
4	D	79	HIS
4	D	106	HIS
1	E	39	HIS
1	E	93	GLN
1	E	108	ASN
1	E	125	GLN
2	F	64	ASN
3	G	31	HIS
3	G	38	ASN
3	G	89	ASN
4	H	92	GLN
3	M	31	HIS
3	M	38	ASN
4	N	46	HIS
4	N	79	HIS
4	N	106	HIS
1	O	68	GLN
2	P	93	GLN
3	Q	31	HIS
4	R	81	ASN
4	R	92	GLN

5.3.3 RNA ⓘ

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](#)

Of 34 ligands modelled in this entry, 34 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 ⓘ

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	98/136 (72%)	-0.13	2 (2%) 65 57	55, 71, 104, 114	0
1	E	98/136 (72%)	-0.38	0 100 100	48, 64, 85, 100	0
1	K	99/136 (72%)	-0.27	0 100 100	53, 68, 93, 105	0
1	O	98/136 (72%)	-0.13	1 (1%) 79 74	51, 63, 95, 108	0
2	B	79/102 (77%)	-0.23	1 (1%) 75 69	55, 64, 80, 89	0
2	F	86/102 (84%)	-0.22	1 (1%) 76 71	52, 61, 113, 126	0
2	L	79/102 (77%)	-0.18	2 (2%) 58 50	57, 67, 82, 84	0
2	P	87/102 (85%)	0.02	3 (3%) 48 41	49, 62, 90, 113	0
3	C	104/128 (81%)	-0.11	3 (2%) 53 46	50, 61, 81, 89	0
3	G	109/128 (85%)	0.23	3 (2%) 55 47	63, 82, 116, 123	0
3	M	106/128 (82%)	0.02	0 100 100	59, 83, 103, 108	0
3	Q	109/128 (85%)	0.03	5 (4%) 37 31	52, 67, 103, 112	0
4	D	100/125 (80%)	-0.03	3 (3%) 52 45	48, 65, 113, 123	0
4	H	96/125 (76%)	0.13	1 (1%) 79 74	61, 79, 110, 115	0
4	N	96/125 (76%)	0.15	1 (1%) 79 74	70, 88, 110, 116	0
4	R	96/125 (76%)	0.09	3 (3%) 51 44	58, 74, 102, 115	0
5	I	147/147 (100%)	-0.32	0 100 100	78, 123, 151, 163	0
5	S	147/147 (100%)	-0.38	0 100 100	70, 123, 161, 171	0
6	J	147/147 (100%)	-0.40	1 (0%) 84 80	77, 119, 161, 172	0
6	T	147/147 (100%)	-0.44	0 100 100	70, 121, 157, 164	0
All	All	2128/2552 (83%)	-0.15	30 (1%) 73 67	48, 77, 143, 172	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	120	THR	6.4
3	G	120	THR	5.1
3	Q	119	LYS	5.0
2	L	102	GLY	4.7
3	G	119	LYS	4.5
2	B	102	GLY	4.2
2	P	102	GLY	3.7
3	G	121	GLU	3.7
4	R	82	LYS	3.5
4	R	121	ALA	3.4
2	L	101	GLY	3.3
1	A	38	PRO	2.9
3	C	30	VAL	2.9
3	Q	121	GLU	2.8
1	A	135	ALA	2.8
1	O	38	PRO	2.8
2	F	21	VAL	2.7
4	D	24	LYS	2.6
4	D	32	GLU	2.5
3	C	31	HIS	2.5
4	R	34	TYR	2.5
4	N	121	ALA	2.4
6	J	-7	DT	2.4
3	C	34	LEU	2.4
4	D	23	GLY	2.4
3	Q	16	THR	2.1
2	P	16	LYS	2.1
3	Q	118	LYS	2.1
4	H	39	TYR	2.1
2	P	77	LYS	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 ⓘ

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
7	MN	N	3132	1/1	0.62	0.24	174,174,174,174	0
7	MN	T	3154	1/1	0.68	0.13	187,187,187,187	0
7	MN	G	3140	1/1	0.72	0.26	153,153,153,153	0
7	MN	T	3143	1/1	0.73	0.19	177,177,177,177	0
7	MN	J	3148	1/1	0.75	0.20	180,180,180,180	0
7	MN	I	3136	1/1	0.75	0.17	147,147,147,147	0
7	MN	T	3156	1/1	0.81	0.09	171,171,171,171	0
7	MN	S	3157	1/1	0.83	0.14	156,156,156,156	0
7	MN	T	3147	1/1	0.83	0.12	147,147,147,147	0
7	MN	S	3146	1/1	0.85	0.11	137,137,137,137	0
7	MN	I	3142	1/1	0.85	0.12	132,132,132,132	0
7	MN	S	3151	1/1	0.87	0.13	126,126,126,126	0
7	MN	I	3144	1/1	0.87	0.08	143,143,143,143	0
7	MN	J	3166	1/1	0.87	0.09	74,74,74,74	0
7	MN	T	3139	1/1	0.88	0.15	133,133,133,133	0
7	MN	T	3162	1/1	0.88	0.08	74,74,74,74	0
7	MN	S	3158	1/1	0.90	0.10	142,142,142,142	0
7	MN	S	3163	1/1	0.91	0.09	75,75,75,75	0
7	MN	T	3145	1/1	0.91	0.08	135,135,135,135	0
7	MN	T	3159	1/1	0.93	0.07	149,149,149,149	0
7	MN	J	3135	1/1	0.93	0.16	107,107,107,107	0
7	MN	S	3155	1/1	0.94	0.07	116,116,116,116	0
7	MN	J	3165	1/1	0.94	0.08	75,75,75,75	0
7	MN	I	3150	1/1	0.94	0.09	122,122,122,122	0
7	MN	J	3138	1/1	0.94	0.14	117,117,117,117	0
7	MN	I	3161	1/1	0.94	0.08	121,121,121,121	0
7	MN	J	3149	1/1	0.94	0.10	134,134,134,134	0
7	MN	O	3152	1/1	0.95	0.17	67,67,67,67	0
7	MN	T	3134	1/1	0.96	0.10	95,95,95,95	0
7	MN	I	3160	1/1	0.96	0.05	145,145,145,145	0
7	MN	J	3164	1/1	0.96	0.08	76,76,76,76	0
7	MN	S	3133	1/1	0.97	0.24	91,91,91,91	0
7	MN	J	3137	1/1	0.97	0.13	85,85,85,85	0
7	MN	S	3153	1/1	0.98	0.04	95,95,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.