



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:35 PM UTC

PDB ID : 8JKK / pdb_00008jkk
Title : Crystal Structure of the dioxygenase CcTet from Coprinopsis cinerea bound to 12bp 5-methylcytosine (5mC) containing duplex DNA
Authors : Zhang, L.; Zhang, L.
Deposited on : 2023-06-01
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 ⓘ 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
Mogul : 2022.3.0, CSD as543be (2022)
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

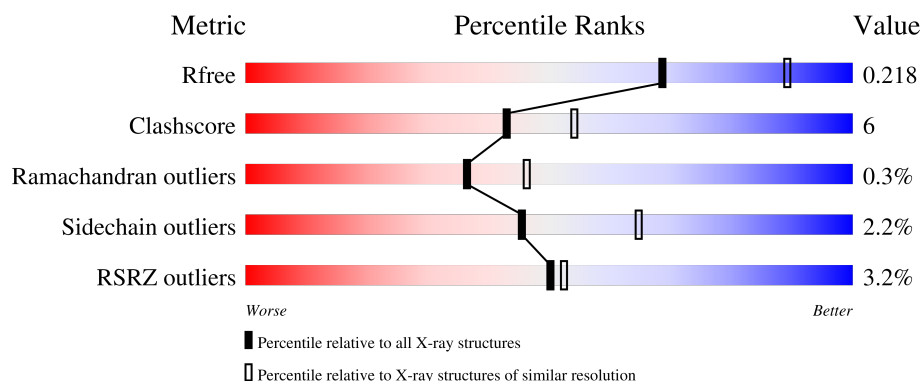
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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.

Mol	Chain	Length	Quality of chain
1	A	415	2% 78% 10% • 9%
1	D	415	• 66% 22% • • 8%
1	G	415	2% 75% 14% • 9%
1	J	415	5% 73% 17% • 8%
2	B	12	8% 50% 33% 17%

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Mol	Chain	Length	Quality of chain
2	E	12	33% 58% 8%
2	H	12	58% 42%
2	K	12	33% 58% 33% 8%
3	C	12	42% 58%
3	F	12	8% 25% 75%
3	I	12	17% 75% 8%
3	L	12	33% 17% 75% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14841 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 2OGFeDO JBP1/TET oxygenase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2955	1889	523	529	14			
1	D	383	Total	C	N	O	S	0	0	0
			3007	1921	535	536	15			
1	G	376	Total	C	N	O	S	0	0	0
			2947	1886	520	527	14			
1	J	383	Total	C	N	O	S	0	0	0
			3007	1921	533	538	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	P	0	0	0
			244	116	44	72	12			
2	E	12	Total	C	N	O	P	0	0	0
			244	116	44	72	12			
2	H	12	Total	C	N	O	P	0	0	0
			244	116	44	72	12			
2	K	12	Total	C	N	O	P	0	0	0
			244	116	44	72	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			247	117	45	73	12			
3	F	12	Total	C	N	O	P	0	0	0
			247	117	45	73	12			
3	I	12	Total	C	N	O	P	0	0	0
			247	117	45	73	12			

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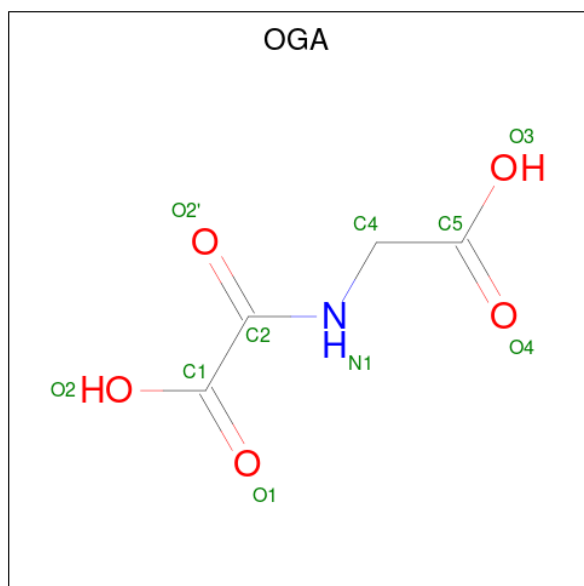
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	11	Total	C	N	O	P	0	0	0
			228	108	42	67	11			

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	D	1	Total	Mn	0	0
			1	1		
4	G	1	Total	Mn	0	0
			1	1		
4	J	1	Total	Mn	0	0
			1	1		

- Molecule 5 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: C₄H₅NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	4	1	5		
5	D	1	Total	C	N	O	0	0
			10	4	1	5		
5	G	1	Total	C	N	O	0	0
			10	4	1	5		
5	J	1	Total	C	N	O	0	0
			10	4	1	5		

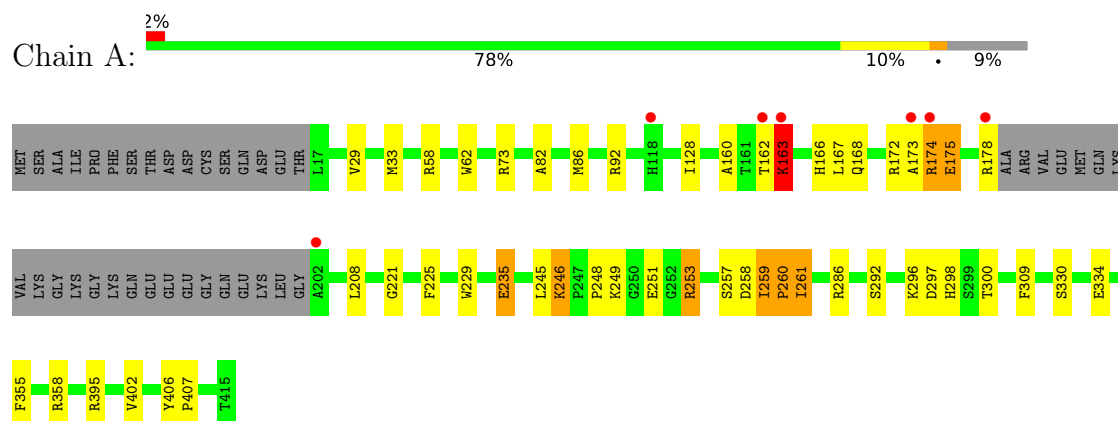
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	298	Total 298	O 298	0	0
6	B	16	Total 16	O 16	0	0
6	C	9	Total 9	O 9	0	0
6	D	275	Total 275	O 275	0	0
6	E	21	Total 21	O 21	0	0
6	F	23	Total 23	O 23	0	0
6	G	188	Total 188	O 188	0	0
6	H	22	Total 22	O 22	0	0
6	I	10	Total 10	O 10	0	0
6	J	70	Total 70	O 70	0	0
6	K	3	Total 3	O 3	0	0
6	L	1	Total 1	O 1	0	0

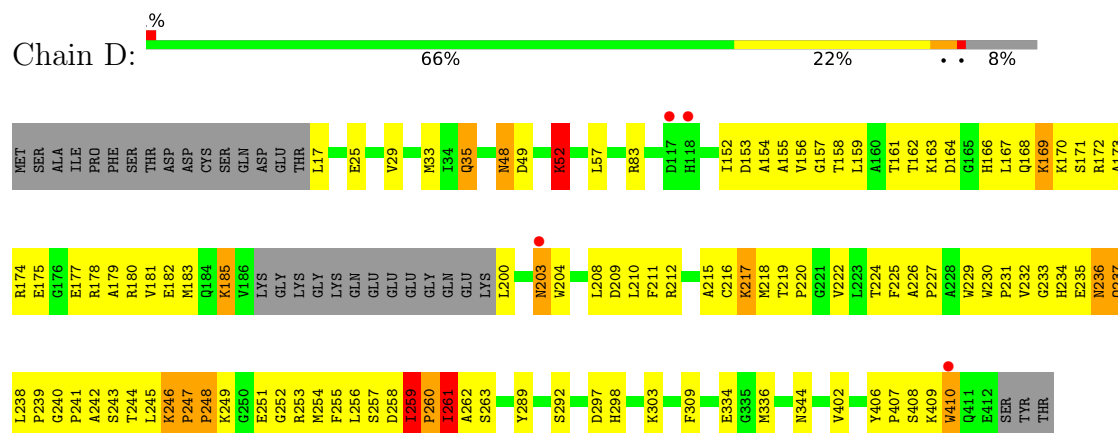
3 Residue-property plots [i](#)

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

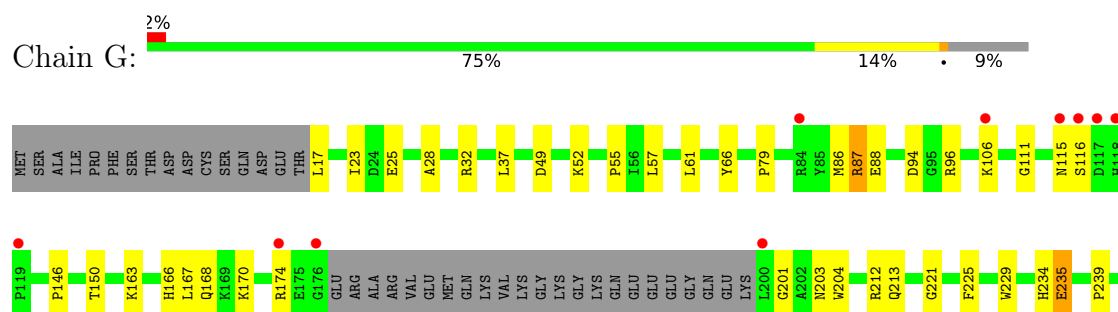
- Molecule 1: 2OGFeDO JBP1/TET oxygenase domain-containing protein



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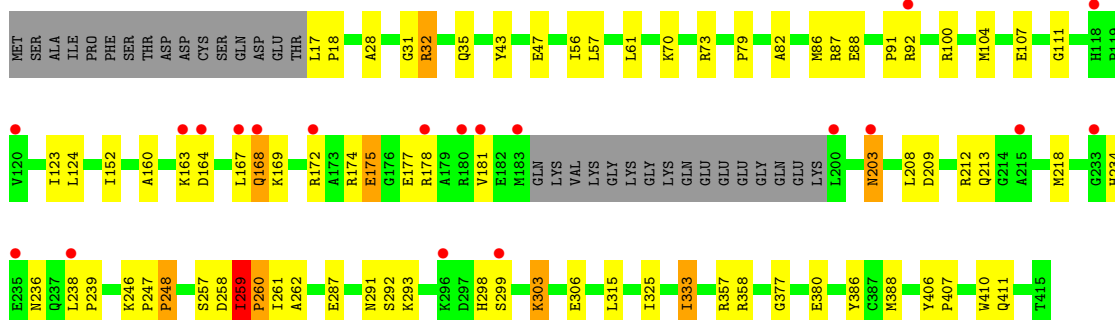


- Molecule 1: 2OGFeDO JBP1/TET oxygenase domain-containing protein





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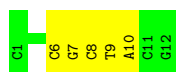
- Molecule 2: DNA (5'-D(P*CP*GP*AP*TP*CP*(5CM)P*GP*CP*TP*AP*CP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*GP*AP*TP*CP*(5CM)P*GP*CP*TP*AP*CP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*GP*AP*TP*CP*(5CM)P*GP*CP*TP*AP*CP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*GP*AP*TP*CP*(5CM)P*GP*CP*TP*AP*CP*G)-3')

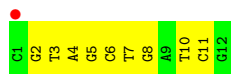
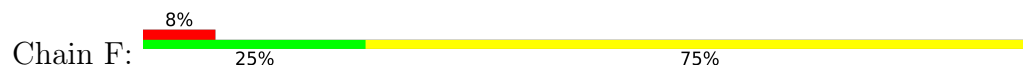


- Molecule 3: DNA (5'-D(P*CP*GP*TP*AP*GP*CP*TP*GP*AP*TP*CP*G)-3')





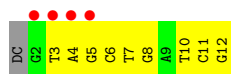
- Molecule 3: DNA (5'-D(P*CP*GP*TP*AP*GP*CP*TP*GP*AP*TP*CP*G)-3')



- Molecule 3: DNA (5'-D(P*CP*GP*TP*AP*GP*CP*TP*GP*AP*TP*CP*G)-3')



- Molecule 3: DNA (5'-D(P*CP*GP*TP*AP*GP*CP*TP*GP*AP*TP*CP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.57Å 127.63Å 212.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.98 – 2.30 21.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (21.98-2.30) 90.3 (21.98-2.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.98 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.187 , 0.216 0.190 , 0.218	Depositor DCC
R_{free} test set	4777 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14841	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, 5CM, OGA

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	0.73	8/3033 (0.3%)	0.85	9/4128 (0.2%)
1	D	1.58	94/3084 (3.0%)	1.07	17/4194 (0.4%)
1	G	0.76	16/3025 (0.5%)	0.85	8/4118 (0.2%)
1	J	0.89	15/3085 (0.5%)	1.13	39/4197 (0.9%)
2	B	0.43	0/249	0.99	2/379 (0.5%)
2	E	1.17	3/249 (1.2%)	1.25	1/379 (0.3%)
2	H	0.43	0/249	0.82	0/379
2	K	0.37	0/249	0.95	2/379 (0.5%)
3	C	0.45	0/276	0.73	0/424
3	F	0.51	0/276	0.82	0/424
3	I	0.74	2/276 (0.7%)	1.04	2/424 (0.5%)
3	L	0.51	0/255	1.06	2/392 (0.5%)
All	All	1.00	138/14306 (1.0%)	0.98	82/19817 (0.4%)

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	247	PRO	C-O	-15.74	1.06	1.24
1	J	248	PRO	N-CA	15.18	1.66	1.47
1	J	246	LYS	C-N	13.03	1.48	1.33
1	D	260	PRO	C-O	-12.70	1.08	1.24
1	G	246	LYS	C-N	12.24	1.47	1.33
1	D	231	PRO	C-O	-11.86	1.10	1.23
1	J	238	LEU	C-N	11.51	1.48	1.33
1	D	241	PRO	C-O	-11.35	1.10	1.23
1	A	259	ILE	C-O	-11.16	1.10	1.24
1	D	154	ALA	C-O	-11.10	1.11	1.24
1	D	180	ARG	C-O	-10.53	1.11	1.24
1	J	260	PRO	C-O	-10.52	1.11	1.24
1	D	234	HIS	CE1-NE2	-10.51	1.22	1.32
1	D	230	TRP	C-O	-10.17	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	215	ALA	C-O	-10.03	1.11	1.23
2	E	5	DC	P-OP2	-9.91	1.28	1.48
1	D	217	LYS	C-O	-9.86	1.12	1.24
1	D	258	ASP	C-O	-9.78	1.11	1.24
1	D	172	ARG	C-O	-9.78	1.12	1.24
1	D	259	ILE	C-O	-9.53	1.12	1.24
1	D	208	LEU	C-O	-9.52	1.12	1.24
1	D	251	GLU	C-O	-9.48	1.13	1.24
1	A	261	ILE	C-O	-9.25	1.13	1.24
1	D	209	ASP	C-O	-9.25	1.12	1.24
1	A	257	SER	C-O	-9.14	1.12	1.24
1	A	260	PRO	C-O	-9.05	1.12	1.24
1	D	216	CYS	C-O	-9.04	1.13	1.24
1	D	226	ALA	C-O	-9.02	1.14	1.24
1	D	166	HIS	C-O	-8.98	1.13	1.24
1	G	259	ILE	C-O	-8.93	1.13	1.24
1	D	253	ARG	C-O	-8.79	1.13	1.24
1	D	244	THR	C-O	-8.78	1.13	1.24
1	D	402	VAL	CA-C	-8.76	1.45	1.53
1	D	155	ALA	C-O	-8.66	1.14	1.24
1	D	232	VAL	C-O	-8.64	1.15	1.24
1	D	262	ALA	C-O	-8.57	1.14	1.24
1	D	220	PRO	C-O	-8.56	1.14	1.23
1	D	224	THR	C-O	-8.56	1.13	1.24
1	J	259	ILE	C-O	-8.47	1.13	1.24
1	D	254	MET	C-O	-8.47	1.14	1.24
1	G	395	ARG	CZ-NH1	8.38	1.44	1.32
1	D	229	TRP	C-O	-8.29	1.15	1.24
1	D	211	PHE	C-O	-8.26	1.13	1.23
1	D	159	LEU	C-O	-8.21	1.14	1.24
1	D	156	VAL	C-O	-8.15	1.14	1.24
1	D	248	PRO	C-O	-7.98	1.15	1.24
1	D	261	ILE	C-O	-7.81	1.14	1.24
1	D	257	SER	C-O	-7.79	1.14	1.24
1	D	210	LEU	C-O	-7.79	1.14	1.24
1	D	246	LYS	C-O	-7.74	1.17	1.24
1	D	263	SER	C-O	-7.71	1.15	1.24
1	D	243	SER	C-O	-7.69	1.15	1.24
1	D	170	LYS	C-O	-7.68	1.15	1.24
1	D	240	GLY	C-O	-7.66	1.13	1.24
1	A	258	ASP	C-O	-7.65	1.14	1.24
1	D	161	THR	C-O	-7.64	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	VAL	CA-C	7.63	1.59	1.53
1	D	157	GLY	C-O	-7.60	1.14	1.23
1	D	252	GLY	C-O	-7.41	1.14	1.23
1	J	239	PRO	C-O	-7.37	1.15	1.23
1	D	222	VAL	C-O	-7.34	1.16	1.24
1	J	358	ARG	C-O	-7.31	1.15	1.24
1	G	246	LYS	C-O	-7.30	1.17	1.24
1	A	249	LYS	C-O	-7.27	1.13	1.24
1	G	260	PRO	C-O	-7.22	1.14	1.24
1	D	153	ASP	C-O	-7.16	1.15	1.24
1	D	239	PRO	C-O	-7.15	1.15	1.23
1	D	152	ILE	C-O	-7.13	1.15	1.24
1	D	153	ASP	CG-OD2	-7.11	1.11	1.25
1	D	227	PRO	C-O	-6.89	1.15	1.24
1	D	255	PHE	C-O	-6.88	1.16	1.24
1	G	204	TRP	C-O	-6.80	1.15	1.24
2	E	5	DC	P-OP1	-6.80	1.34	1.48
1	G	402	VAL	CA-C	6.73	1.58	1.53
1	D	173	ALA	C-O	-6.63	1.16	1.24
1	D	168	GLN	C-O	-6.55	1.16	1.24
1	D	35	GLN	C-O	-6.42	1.16	1.24
1	G	235	GLU	C-O	-6.41	1.16	1.24
1	G	290	SER	C-O	-6.39	1.16	1.24
1	J	333	ILE	C-O	-6.38	1.16	1.24
1	D	409	LYS	C-O	-6.33	1.15	1.23
1	D	174	ARG	C-O	-6.30	1.16	1.24
1	D	218	MET	C-O	-6.28	1.16	1.24
1	D	212	ARG	C-O	-6.24	1.16	1.23
1	D	153	ASP	CG-OD1	-6.22	1.13	1.25
1	D	182	GLU	C-O	-6.20	1.16	1.24
1	D	181	VAL	C-O	-6.13	1.15	1.24
1	G	287	GLU	C-O	-6.03	1.17	1.24
1	D	256	LEU	C-O	-6.03	1.17	1.24
1	D	169	LYS	C-O	-5.97	1.17	1.24
3	I	12	DG	P-OP2	-5.94	1.36	1.48
1	J	248	PRO	C-O	-5.93	1.16	1.24
1	D	52	LYS	C-O	-5.92	1.16	1.24
1	G	234	HIS	CE1-NE2	-5.91	1.26	1.32
1	D	178	ARG	C-O	-5.81	1.17	1.24
1	D	177	GLU	C-O	-5.80	1.17	1.24
1	D	171	SER	CA-CB	-5.79	1.44	1.53
1	D	234	HIS	CG-ND1	-5.78	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	234	HIS	C-O	-5.78	1.16	1.23
1	D	219	THR	C-O	-5.76	1.17	1.24
1	D	179	ALA	C-O	-5.75	1.17	1.24
1	D	175	GLU	C-O	-5.67	1.17	1.24
1	D	238	LEU	C-O	-5.66	1.16	1.24
1	J	246	LYS	C-O	-5.66	1.19	1.24
1	D	167	LEU	C-O	-5.64	1.17	1.24
1	J	257	SER	C-O	-5.61	1.17	1.24
1	D	234	HIS	CD2-NE2	-5.58	1.31	1.37
2	E	10	DA	O3'-P	-5.56	1.52	1.61
1	D	183	MET	C-O	-5.55	1.17	1.24
1	G	290	SER	CA-CB	-5.52	1.44	1.53
1	D	225	PHE	C-O	-5.51	1.17	1.23
1	G	88	GLU	C-O	-5.46	1.17	1.24
3	I	12	DG	P-OP1	-5.45	1.37	1.48
1	D	408	SER	CA-CB	-5.44	1.44	1.53
1	D	242	ALA	C-O	-5.41	1.17	1.23
1	D	263	SER	CA-CB	-5.39	1.44	1.53
1	A	163	LYS	C-O	-5.35	1.18	1.24
1	D	233	GLY	C-O	-5.32	1.16	1.23
1	D	251	GLU	CD-OE1	-5.32	1.15	1.25
1	J	32	ARG	CZ-NH2	5.31	1.40	1.33
1	D	185	LYS	C-O	-5.30	1.18	1.24
1	G	201	GLY	C-O	-5.27	1.18	1.23
1	D	163	LYS	C-O	-5.25	1.17	1.23
1	G	234	HIS	C-O	-5.23	1.17	1.23
1	G	258	ASP	C-O	-5.22	1.17	1.24
1	D	236	ASN	C-O	-5.16	1.15	1.23
1	J	258	ASP	C-O	-5.16	1.17	1.24
1	D	162	THR	C-O	-5.16	1.18	1.24
1	D	204	TRP	C-O	-5.15	1.17	1.24
1	J	303	LYS	C-O	-5.13	1.18	1.24
1	D	158	THR	C-O	-5.10	1.18	1.24
1	D	241	PRO	N-CA	-5.09	1.41	1.47
1	J	299	SER	C-O	-5.06	1.18	1.24
1	D	408	SER	C-O	-5.06	1.17	1.23
1	D	237	GLN	C-O	-5.05	1.17	1.23
1	D	410	TRP	C-O	-5.04	1.18	1.24
1	D	235	GLU	C-O	-5.03	1.18	1.24
1	D	245	LEU	C-O	-5.03	1.17	1.24

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	247	PRO	CA-C-N	14.15	137.52	119.84
1	J	247	PRO	C-N-CA	14.15	137.52	119.84
3	L	3	DT	C2'-C3'-O3'	-12.28	93.09	111.50
2	E	10	DA	C4'-C3'-O3'	-11.55	92.68	110.00
1	J	32	ARG	CA-CB-CG	11.19	136.49	114.10
1	G	106	LYS	CD-CE-NZ	11.16	147.62	111.90
1	J	238	LEU	CA-C-N	10.78	130.74	119.85
1	J	238	LEU	C-N-CA	10.78	130.74	119.85
1	J	246	LYS	CA-C-N	10.53	131.22	120.38
1	J	246	LYS	C-N-CA	10.53	131.22	120.38
1	G	106	LYS	CG-CD-CE	-9.48	89.49	111.30
1	G	246	LYS	O-C-N	-9.23	112.03	120.71
1	D	203	ASN	CB-CA-C	9.06	124.75	111.89
2	B	1	DC	OP1-P-O3'	-9.02	80.95	108.00
2	K	1	DC	OP1-P-O3'	-8.84	81.49	108.00
3	I	12	DG	C2'-C3'-O3'	-8.28	99.08	111.50
1	J	203	ASN	CB-CA-C	7.96	123.19	111.89
2	K	1	DC	OP2-P-O3'	-7.79	84.62	108.00
1	J	87	ARG	CB-CG-CD	-7.78	93.40	111.30
1	A	172	ARG	CB-CA-C	-7.73	97.71	110.85
1	G	246	LYS	CA-C-N	7.43	128.03	120.38
1	G	246	LYS	C-N-CA	7.43	128.03	120.38
2	B	1	DC	OP2-P-O3'	-7.40	85.79	108.00
1	J	91	PRO	CA-C-N	-7.21	111.04	122.79
1	J	91	PRO	C-N-CA	-7.21	111.04	122.79
1	J	32	ARG	NE-CZ-NH1	-7.12	114.38	121.50
1	A	246	LYS	CA-CB-CG	-6.91	100.28	114.10
1	D	164	ASP	CA-CB-CG	6.88	119.48	112.60
1	A	162	THR	CA-C-N	6.87	129.38	120.44
1	A	162	THR	C-N-CA	6.87	129.38	120.44
1	J	248	PRO	CB-CA-C	6.83	122.82	111.56
1	J	248	PRO	CA-N-CD	-6.78	102.52	112.00
1	J	163	LYS	CD-CE-NZ	-6.76	90.26	111.90
1	J	238	LEU	O-C-N	-6.74	113.89	121.43
1	J	236	ASN	CB-CA-C	-6.72	99.63	110.79
1	D	166	HIS	CA-CB-CG	6.63	120.43	113.80
1	D	179	ALA	CA-C-N	6.46	128.93	120.28
1	D	179	ALA	C-N-CA	6.46	128.93	120.28
1	J	248	PRO	N-CA-C	-6.40	99.29	112.47
1	J	32	ARG	N-CA-CB	-6.24	100.97	110.01
1	J	236	ASN	CA-CB-CG	-6.22	106.38	112.60
1	J	87	ARG	CG-CD-NE	6.19	125.62	112.00
1	J	203	ASN	CA-CB-CG	6.18	118.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	153	ASP	CA-CB-CG	6.09	118.69	112.60
1	D	234	HIS	CA-C-N	6.04	128.86	120.29
1	D	234	HIS	C-N-CA	6.04	128.86	120.29
1	G	87	ARG	CD-NE-CZ	-6.02	115.97	124.40
1	J	87	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	J	31	GLY	CA-C-N	5.93	128.15	120.44
1	J	31	GLY	C-N-CA	5.93	128.15	120.44
1	A	174	ARG	CB-CA-C	5.93	120.25	111.06
1	J	87	ARG	CA-CB-CG	5.88	125.86	114.10
1	D	48	ASN	CA-C-O	-5.82	115.12	122.63
1	J	163	LYS	CG-CD-CE	5.81	124.66	111.30
1	J	73	ARG	CG-CD-NE	-5.71	99.43	112.00
3	L	3	DT	C3'-C2'-C1'	5.69	110.13	101.60
3	I	10	DT	P-O3'-C3'	5.68	128.71	120.20
1	J	293	LYS	CD-CE-NZ	5.67	130.05	111.90
1	J	92	ARG	CA-CB-CG	-5.62	102.85	114.10
1	J	212	ARG	CA-C-N	5.60	130.99	122.65
1	J	212	ARG	C-N-CA	5.60	130.99	122.65
1	J	246	LYS	O-C-N	-5.56	115.27	120.55
1	A	246	LYS	CB-CG-CD	5.51	123.97	111.30
1	D	83	ARG	CA-CB-CG	5.42	124.94	114.10
1	J	175	GLU	CB-CA-C	5.38	119.99	110.85
1	J	47	GLU	CG-CD-OE2	-5.32	106.17	118.40
1	J	92	ARG	CD-NE-CZ	5.32	131.84	124.40
1	D	243	SER	CB-CA-C	5.28	119.56	110.79
1	A	296	LYS	CB-CA-C	-5.27	99.77	109.46
1	G	166	HIS	CA-CB-CG	5.25	119.05	113.80
1	J	168	GLN	CA-CB-CG	5.24	124.58	114.10
1	D	410	TRP	CA-CB-CG	-5.22	103.68	113.60
1	D	402	VAL	O-C-N	-5.21	116.27	121.12
1	J	47	GLU	CB-CG-CD	5.19	121.42	112.60
1	D	247	PRO	CB-CA-C	-5.14	104.65	110.92
1	J	87	ARG	N-CA-CB	-5.09	102.62	110.16
1	D	162	THR	CA-CB-OG1	-5.08	101.98	109.60
1	D	402	VAL	CA-C-N	5.07	124.98	119.76
1	D	402	VAL	C-N-CA	5.07	124.98	119.76
1	G	203	ASN	CB-CA-C	5.03	118.88	111.73
1	A	173	ALA	CA-C-N	-5.00	115.12	122.83
1	A	173	ALA	C-N-CA	-5.00	115.12	122.83

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	2955	0	2964	29	0
1	D	3007	0	3029	29	0
1	G	2947	0	2959	33	0
1	J	3007	0	3020	36	0
2	B	244	0	137	8	0
2	E	244	0	137	5	0
2	H	244	0	137	4	0
2	K	244	0	137	5	0
3	C	247	0	136	6	0
3	F	247	0	136	6	0
3	I	247	0	136	7	0
3	L	228	0	125	5	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	10	0	3	0	0
5	D	10	0	3	0	0
5	G	10	0	3	0	0
5	J	10	0	3	0	0
6	A	298	0	0	6	0
6	B	16	0	0	2	0
6	C	9	0	0	0	0
6	D	275	0	0	4	0
6	E	21	0	0	0	0
6	F	23	0	0	0	0
6	G	188	0	0	7	0
6	H	22	0	0	0	0
6	I	10	0	0	0	0
6	J	70	0	0	1	0
6	K	3	0	0	1	0
6	L	1	0	0	0	0
All	All	14841	0	13065	166	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 6.

All (166) 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:D:57:LEU:HB2	1:D:261:ILE:HD11	1.31	1.06
1:D:57:LEU:CB	1:D:261:ILE:HD11	2.01	0.90
1:A:178:ARG:HG2	1:A:208:LEU:HD21	1.61	0.80
1:D:57:LEU:HB2	1:D:261:ILE:CD1	2.14	0.75
1:J:123:ILE:HG13	1:J:124:LEU:HD22	1.76	0.68
1:D:246:LYS:NZ	1:D:297:ASP:OD2	2.23	0.68
1:A:175:GLU:O	1:A:175:GLU:HG3	1.95	0.66
3:L:11:DC:H2''	3:L:12:DG:C8	2.30	0.66
1:D:57:LEU:CA	1:D:261:ILE:HD11	2.25	0.66
3:I:10:DT:H2'	3:I:11:DC:C6	2.31	0.66
1:J:303:LYS:NZ	1:J:306:GLU:OE2	2.29	0.65
1:G:285:LEU:CD2	6:G:647:HOH:O	2.44	0.65
3:L:10:DT:H2''	3:L:11:DC:H5''	1.78	0.65
2:B:1:DC:H2'	2:B:2:DG:C8	2.31	0.65
1:A:246:LYS:HE3	6:A:642:HOH:O	1.97	0.63
1:J:292:SER:HA	1:J:298:HIS:CD2	2.34	0.63
3:I:10:DT:H2''	3:I:11:DC:O5'	1.99	0.63
1:G:94:ASP:OD1	1:G:96:ARG:HG2	1.98	0.62
1:J:57:LEU:HB2	1:J:261:ILE:HG23	1.83	0.61
1:G:86:MET:HG2	1:G:333:ILE:CD1	2.30	0.60
1:J:218:MET:HE1	1:J:386:TYR:HD2	1.66	0.60
3:L:7:DT:H2'	3:L:8:DG:C8	2.36	0.60
1:G:86:MET:HG2	1:G:333:ILE:HD13	1.83	0.59
2:K:1:DC:H2'	2:K:2:DG:C8	2.38	0.59
1:J:325:ILE:HD13	1:J:377:GLY:HA3	1.85	0.59
1:J:32:ARG:HG3	1:J:43:TYR:CE1	2.39	0.58
1:J:56:ILE:HD12	1:J:56:ILE:H	1.68	0.58
1:D:406:TYR:CG	1:D:407:PRO:HD2	2.38	0.58
1:A:246:LYS:HG3	1:A:300:THR:HG21	1.85	0.57
1:G:167:LEU:HD22	1:G:221:GLY:HA3	1.85	0.57
1:J:175:GLU:OE2	1:J:175:GLU:HA	2.02	0.57
1:J:160:ALA:HA	1:J:167:LEU:HD12	1.85	0.56
2:B:6:5CM:H3'	6:B:101:HOH:O	2.04	0.56
1:D:52:LYS:HB2	1:D:52:LYS:NZ	2.21	0.56
1:D:292:SER:HA	1:D:298:HIS:CD2	2.41	0.56
2:H:9:DT:H2''	2:H:10:DA:C8	2.40	0.56
3:I:2:DG:H2'	3:I:3:DT:H72	1.88	0.56
3:I:7:DT:H2'	3:I:8:DG:C8	2.42	0.56
1:A:246:LYS:NZ	1:A:297:ASP:OD2	2.35	0.55
2:K:9:DT:H2''	2:K:10:DA:C8	2.41	0.55
3:C:1:DC:H2'	3:C:2:DG:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLU:HB3	1:A:407:PRO:HD3	1.88	0.55
1:J:259:ILE:N	1:J:260:PRO:HD3	2.21	0.55
1:D:410:TRP:CD2	1:D:410:TRP:C	2.85	0.54
1:G:23:ILE:HG22	1:G:264:ALA:HA	1.88	0.54
1:D:344:ASN:O	1:D:344:ASN:OD1	2.25	0.54
3:I:3:DT:H2''	3:I:4:DA:C8	2.43	0.54
1:G:225:PHE:HB3	1:G:245:LEU:HD11	1.90	0.53
1:A:235:GLU:HB2	1:A:395:ARG:NH1	2.24	0.53
1:D:260:PRO:HB3	1:D:309:PHE:CD1	2.43	0.53
1:A:82:ALA:O	1:A:86:MET:HG2	2.08	0.53
1:A:128:ILE:HD13	1:A:355:PHE:CD2	2.44	0.53
1:A:260:PRO:HB3	1:A:309:PHE:CD1	2.44	0.52
2:E:10:DA:H2''	2:E:11:DC:H5''	1.91	0.52
1:J:82:ALA:O	1:J:86:MET:HG3	2.08	0.52
1:D:336:MET:HE2	6:D:740:HOH:O	2.08	0.52
2:E:1:DC:H2'	2:E:2:DG:C8	2.44	0.52
1:A:261:ILE:HG22	6:A:720:HOH:O	2.08	0.52
3:F:7:DT:H2'	3:F:8:DG:C8	2.45	0.51
2:K:2:DG:N7	6:K:102:HOH:O	2.33	0.51
1:J:164:ASP:H	1:J:168:GLN:HG3	1.75	0.51
1:D:410:TRP:CD2	1:D:410:TRP:O	2.64	0.51
1:D:410:TRP:HD1	6:D:807:HOH:O	1.94	0.51
1:A:358:ARG:NH1	6:A:607:HOH:O	2.37	0.51
1:G:163:LYS:HA	1:G:168:GLN:NE2	2.27	0.50
1:G:239:PRO:HG2	1:G:295:THR:HG22	1.93	0.50
1:J:88:GLU:HG3	1:J:104:MET:SD	2.52	0.50
1:J:28:ALA:O	1:J:32:ARG:HB2	2.11	0.50
3:C:12:DG:H2''	2:K:1:DC:H5''	1.94	0.49
2:E:10:DA:H2''	2:E:11:DC:C5'	2.42	0.49
3:I:4:DA:H2''	3:I:5:DG:O5'	2.12	0.49
1:D:410:TRP:HB3	6:D:807:HOH:O	2.13	0.49
2:B:1:DC:H5''	2:B:1:DC:H6	1.76	0.49
1:D:25:GLU:CD	1:D:49:ASP:HB2	2.37	0.49
3:C:1:DC:H3'	3:C:1:DC:OP1	2.12	0.48
1:D:259:ILE:N	1:D:260:PRO:HD3	2.29	0.48
3:F:5:DG:H2''	3:F:6:DC:C6	2.48	0.48
2:E:9:DT:H2''	2:E:10:DA:C8	2.48	0.48
1:G:260:PRO:HB3	1:G:309:PHE:CD1	2.49	0.48
1:J:380:GLU:O	6:J:601:HOH:O	2.20	0.48
1:J:410:TRP:CE2	1:J:411:GLN:OE1	2.67	0.48
1:D:25:GLU:OE1	1:D:49:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3:DT:H2''	3:F:4:DA:C8	2.48	0.48
1:J:410:TRP:CZ3	1:J:411:GLN:HG3	2.50	0.47
1:A:168:GLN:HB2	6:A:608:HOH:O	2.13	0.47
1:A:166:HIS:ND1	1:A:251:GLU:OE1	2.46	0.47
1:G:358:ARG:NE	6:G:601:HOH:O	2.22	0.47
1:G:79:PRO:HD3	1:G:111:GLY:HA3	1.97	0.47
2:H:8:DC:H2'	2:H:9:DT:H71	1.97	0.46
1:D:17:LEU:HD11	1:D:289:TYR:CZ	2.50	0.46
2:K:1:DC:H5''	2:K:1:DC:H6	1.81	0.46
1:J:152:ILE:HD11	1:J:262:ALA:HB1	1.98	0.46
1:G:229:TRP:CH2	2:H:7:DG:H5''	2.50	0.46
1:A:406:TYR:CG	1:A:407:PRO:HD2	2.51	0.46
2:B:7:DG:O5'	6:B:101:HOH:O	2.21	0.46
1:D:410:TRP:CD1	6:D:807:HOH:O	2.67	0.46
1:D:410:TRP:O	1:D:410:TRP:CE3	2.69	0.46
1:D:169:LYS:HG2	3:F:2:DG:OP1	2.17	0.45
1:G:332:PRO:HB3	1:G:394:GLU:HB2	1.98	0.45
2:H:8:DC:C2'	2:H:9:DT:H71	2.46	0.45
1:J:315:LEU:HD11	1:J:388:MET:HB3	1.97	0.45
1:G:37:LEU:HD21	1:G:66:TYR:CE1	2.52	0.45
1:A:225:PHE:HB3	1:A:245:LEU:HD11	1.97	0.45
1:J:406:TYR:CG	1:J:407:PRO:HD2	2.51	0.45
1:A:286:ARG:HD2	6:A:601:HOH:O	2.16	0.45
1:A:229:TRP:CH2	2:B:7:DG:H5''	2.52	0.45
1:G:55:PRO:HD2	6:G:748:HOH:O	2.16	0.45
1:J:79:PRO:HD3	1:J:111:GLY:HA3	1.98	0.45
1:G:52:LYS:NZ	6:G:609:HOH:O	2.50	0.45
3:C:4:DA:H2''	3:C:5:DG:O5'	2.17	0.44
1:J:169:LYS:HA	1:J:172:ARG:HD3	1.98	0.44
1:A:160:ALA:HA	1:A:167:LEU:HD12	1.98	0.44
1:J:234:HIS:HE1	3:L:6:DC:O2	2.00	0.44
1:G:57:LEU:O	1:G:61:LEU:HG	2.18	0.44
1:A:29:VAL:O	1:A:33:MET:HG3	2.18	0.44
1:A:330:SER:OG	2:B:6:5CM:OP1	2.25	0.44
2:E:11:DC:H2'	2:E:12:DG:C8	2.52	0.44
3:F:4:DA:H2''	3:F:5:DG:O5'	2.17	0.44
1:G:87:ARG:HH11	1:G:87:ARG:HD3	1.49	0.44
1:D:406:TYR:CD2	1:D:407:PRO:HD2	2.52	0.44
1:G:115:ASN:O	1:G:115:ASN:OD1	2.36	0.44
1:A:248:PRO:HA	1:A:253:ARG:CZ	2.48	0.44
1:G:17:LEU:HA	1:G:17:LEU:HD23	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:LYS:O	1:G:174:ARG:HG3	2.17	0.43
1:A:92:ARG:HD3	3:C:10:DT:H4'	2.00	0.43
1:D:17:LEU:HD11	1:D:289:TYR:CE2	2.52	0.43
1:J:100:ARG:O	1:J:104:MET:HG2	2.18	0.43
1:J:178:ARG:HH21	1:J:208:LEU:HD22	1.81	0.43
3:I:1:DC:P	3:I:1:DC:H3'	2.58	0.43
1:A:73:ARG:HH11	1:A:73:ARG:HD2	1.71	0.43
2:B:8:DC:H2'	2:B:9:DT:H71	1.99	0.43
1:A:33:MET:HE2	1:A:62:TRP:CE2	2.53	0.43
1:G:260:PRO:HB3	1:G:309:PHE:CG	2.54	0.43
1:J:410:TRP:CE3	1:J:411:GLN:HG3	2.52	0.43
1:A:167:LEU:HD22	1:A:221:GLY:HA3	2.00	0.43
1:G:94:ASP:OD1	1:G:96:ARG:CG	2.66	0.43
1:G:212:ARG:NH1	6:G:602:HOH:O	2.47	0.43
1:J:287:GLU:OE2	1:J:291:ASN:HB2	2.19	0.43
1:D:406:TYR:CD1	1:D:407:PRO:HD2	2.54	0.43
1:G:406:TYR:CG	1:G:407:PRO:HD2	2.54	0.42
1:J:174:ARG:HH21	1:J:174:ARG:HD2	1.68	0.42
1:D:334:GLU:HB3	1:D:407:PRO:HD3	2.01	0.42
3:L:4:DA:H2''	3:L:5:DG:O5'	2.18	0.42
1:J:410:TRP:CD2	1:J:411:GLN:OE1	2.73	0.42
1:G:146:PRO:O	1:G:150:THR:HG23	2.18	0.42
3:F:10:DT:H2''	3:F:11:DC:O5'	2.19	0.42
1:G:28:ALA:O	1:G:32:ARG:HG3	2.19	0.42
1:G:212:ARG:NE	6:G:602:HOH:O	2.28	0.42
1:J:177:GLU:HG3	1:J:181:VAL:HG23	2.02	0.42
1:A:292:SER:HA	1:A:298:HIS:CD2	2.55	0.42
1:J:57:LEU:O	1:J:61:LEU:HG	2.20	0.42
1:A:58:ARG:NH1	6:A:620:HOH:O	2.52	0.41
1:G:116:SER:HB2	6:G:714:HOH:O	2.19	0.41
1:G:300:THR:O	1:G:304:ILE:HG13	2.20	0.41
3:C:10:DT:H2''	3:C:11:DC:H5'	2.02	0.41
1:D:247:PRO:HA	1:D:248:PRO:HD3	1.83	0.41
1:J:357:ARG:HD3	1:J:357:ARG:HA	1.92	0.41
1:D:57:LEU:HB2	1:D:261:ILE:CG1	2.49	0.41
1:D:29:VAL:HG12	1:D:33:MET:HE3	2.03	0.41
1:G:266:VAL:HG13	1:G:338:ILE:HG21	2.02	0.41
1:J:104:MET:HE3	1:J:104:MET:HB3	1.87	0.41
1:J:17:LEU:HA	1:J:18:PRO:HD3	1.94	0.41
1:A:163:LYS:H	1:A:163:LYS:HG2	1.41	0.41
1:J:209:ASP:OD1	1:J:209:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:DC:C2'	2:B:9:DT:H71	2.51	0.40
1:G:25:GLU:OE1	1:G:49:ASP:HB2	2.21	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	372/415 (90%)	360 (97%)	11 (3%)	1 (0%)	36	46
1	D	379/415 (91%)	368 (97%)	10 (3%)	1 (0%)	36	46
1	G	372/415 (90%)	361 (97%)	10 (3%)	1 (0%)	36	46
1	J	379/415 (91%)	367 (97%)	11 (3%)	1 (0%)	36	46
All	All	1502/1660 (90%)	1456 (97%)	42 (3%)	4 (0%)	36	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	ILE
1	G	259	ILE
1	D	259	ILE
1	J	259	ILE

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	315/348 (90%)	310 (98%)	5 (2%)	55	73
1	D	320/348 (92%)	308 (96%)	12 (4%)	29	44
1	G	314/348 (90%)	310 (99%)	4 (1%)	61	77
1	J	320/348 (92%)	313 (98%)	7 (2%)	45	65
All	All	1269/1392 (91%)	1241 (98%)	28 (2%)	45	65

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	LYS
1	A	174	ARG
1	A	175	GLU
1	A	235	GLU
1	A	253	ARG
1	D	35	GLN
1	D	48	ASN
1	D	52	LYS
1	D	185	LYS
1	D	200	LEU
1	D	203	ASN
1	D	217	LYS
1	D	236	ASN
1	D	237	GLN
1	D	249	LYS
1	D	261	ILE
1	D	303	LYS
1	G	213	GLN
1	G	235	GLU
1	G	287	GLU
1	G	290	SER
1	J	35	GLN
1	J	70	LYS
1	J	107	GLU
1	J	203	ASN
1	J	213	GLN
1	J	248	PRO
1	J	333	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
1	D	237	GLN
1	D	298	HIS
1	D	344	ASN
1	G	115	ASN
1	G	118	HIS
1	G	134	HIS
1	G	168	GLN
1	G	203	ASN
1	J	35	GLN
1	J	121	GLN
1	J	234	HIS
1	J	298	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5CM	B	6	2	18,21,22	2.06	7 (38%)	24,30,33	2.42	10 (41%)
2	5CM	H	6	2	18,21,22	1.84	6 (33%)	24,30,33	2.33	9 (37%)
2	5CM	K	6	2	18,21,22	2.03	6 (33%)	24,30,33	2.43	11 (45%)
2	5CM	E	6	2	18,21,22	2.95	9 (50%)	24,30,33	2.54	11 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5CM	B	6	2	-	6/7/21/22	0/2/2/2
2	5CM	H	6	2	-	6/7/21/22	0/2/2/2
2	5CM	K	6	2	-	6/7/21/22	0/2/2/2
2	5CM	E	6	2	-	6/7/21/22	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	6	5CM	C6-N1	-6.27	1.27	1.38
2	E	6	5CM	O2-C2	-5.80	1.12	1.23
2	B	6	5CM	C4-N3	-4.21	1.27	1.34
2	E	6	5CM	C2-N3	-4.03	1.28	1.36
2	E	6	5CM	C4-N3	-3.96	1.27	1.34
2	K	6	5CM	C4-N3	-3.87	1.28	1.34
2	E	6	5CM	O4'-C1'	-3.84	1.33	1.42
2	B	6	5CM	O3'-C3'	-3.65	1.35	1.43
2	H	6	5CM	C6-N1	-3.47	1.32	1.38
2	K	6	5CM	O3'-C3'	-3.34	1.36	1.43
2	H	6	5CM	C4-N3	-3.32	1.28	1.34
2	K	6	5CM	C6-N1	-3.30	1.32	1.38
2	B	6	5CM	C6-C5	2.84	1.39	1.34
2	K	6	5CM	C2-N3	-2.80	1.30	1.36
2	H	6	5CM	O3'-C3'	-2.80	1.37	1.43
2	B	6	5CM	C6-N1	-2.74	1.33	1.38
2	B	6	5CM	O4'-C1'	-2.69	1.36	1.42
2	E	6	5CM	O4'-C4'	-2.67	1.39	1.45
2	E	6	5CM	O5'-C5'	-2.61	1.36	1.44
2	H	6	5CM	O4'-C1'	-2.60	1.36	1.42
2	K	6	5CM	O2-C2	-2.58	1.18	1.23
2	B	6	5CM	C2-N3	-2.57	1.31	1.36
2	H	6	5CM	C6-C5	2.54	1.38	1.34
2	K	6	5CM	O4'-C1'	-2.44	1.36	1.42
2	E	6	5CM	C1'-N1	-2.31	1.42	1.48
2	B	6	5CM	O2-C2	-2.24	1.19	1.23
2	E	6	5CM	C2-N1	-2.04	1.35	1.40
2	H	6	5CM	C2-N3	-2.02	1.32	1.36

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	5CM	O3'-C3'-C2'	-5.50	91.76	110.88
2	E	6	5CM	C1'-N1-C2	5.45	127.18	117.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	6	5CM	O2-C2-N3	-5.26	114.03	122.33
2	B	6	5CM	O2-C2-N3	-5.21	114.12	122.33
2	K	6	5CM	O3'-C3'-C2'	-5.15	92.98	110.88
2	H	6	5CM	O3'-C3'-C2'	-4.57	94.99	110.88
2	K	6	5CM	C1'-N1-C2	4.32	125.24	117.83
2	H	6	5CM	O2-C2-N3	-4.26	115.61	122.33
2	H	6	5CM	C1'-N1-C2	4.23	125.09	117.83
2	E	6	5CM	O3'-C3'-C2'	-4.18	96.34	110.88
2	H	6	5CM	C5-C4-N3	-4.13	117.52	121.75
2	E	6	5CM	O2-C2-N3	-4.13	115.82	122.33
2	E	6	5CM	C5-C4-N3	-4.12	117.54	121.75
2	B	6	5CM	C5-C4-N3	-3.72	117.94	121.75
2	K	6	5CM	C5-C4-N3	-3.32	118.35	121.75
2	B	6	5CM	C1'-N1-C2	3.27	123.45	117.83
2	B	6	5CM	C6-N1-C2	-3.23	116.64	120.95
2	E	6	5CM	C2'-C1'-N1	3.22	121.86	113.81
2	K	6	5CM	N1-C2-N3	3.08	124.14	118.80
2	E	6	5CM	C6-N1-C2	-2.97	116.99	120.95
2	B	6	5CM	N1-C2-N3	2.96	123.94	118.80
2	H	6	5CM	C6-N1-C2	-2.94	117.03	120.95
2	E	6	5CM	C1'-N1-C6	-2.93	115.83	120.74
2	B	6	5CM	O4'-C4'-C3'	2.91	112.27	105.65
2	E	6	5CM	C3'-C2'-C1'	2.90	109.70	102.60
2	E	6	5CM	N4-C4-N3	2.83	123.62	118.51
2	K	6	5CM	C6-N1-C2	-2.82	117.20	120.95
2	K	6	5CM	C2'-C1'-N1	2.79	120.79	113.81
2	K	6	5CM	C5-C6-N1	-2.77	120.30	123.31
2	H	6	5CM	O4'-C4'-C3'	2.65	111.69	105.65
2	E	6	5CM	N1-C2-N3	2.58	123.27	118.80
2	H	6	5CM	O4'-C1'-N1	-2.48	103.45	107.86
2	B	6	5CM	C5-C6-N1	-2.47	120.63	123.31
2	H	6	5CM	N1-C2-N3	2.47	123.09	118.80
2	K	6	5CM	O3'-C3'-C4'	-2.43	100.84	110.07
2	B	6	5CM	O4'-C1'-N1	-2.16	104.03	107.86
2	B	6	5CM	C3'-C2'-C1'	2.12	107.78	102.60
2	H	6	5CM	C5-C6-N1	-2.11	121.03	123.31
2	K	6	5CM	O4'-C1'-N1	-2.08	104.17	107.86
2	E	6	5CM	C2'-C3'-C4'	-2.02	98.69	102.80
2	K	6	5CM	O4'-C4'-C3'	2.00	110.21	105.65

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	6	5CM	O4'-C4'-C5'-O5'
2	B	6	5CM	O4'-C4'-C5'-O5'
2	H	6	5CM	C3'-C4'-C5'-O5'
2	E	6	5CM	C2'-C1'-N1-C2
2	K	6	5CM	C2'-C1'-N1-C2
2	E	6	5CM	C3'-C4'-C5'-O5'
2	B	6	5CM	C3'-C4'-C5'-O5'
2	K	6	5CM	C2'-C1'-N1-C6
2	B	6	5CM	C2'-C1'-N1-C2
2	E	6	5CM	C2'-C1'-N1-C6
2	H	6	5CM	C2'-C1'-N1-C2
2	B	6	5CM	O4'-C1'-N1-C6
2	H	6	5CM	O4'-C1'-N1-C6
2	H	6	5CM	C2'-C1'-N1-C6
2	E	6	5CM	O4'-C4'-C5'-O5'
2	K	6	5CM	C3'-C4'-C5'-O5'
2	E	6	5CM	O4'-C1'-N1-C6
2	B	6	5CM	C2'-C1'-N1-C6
2	K	6	5CM	O4'-C1'-N1-C6
2	H	6	5CM	O4'-C1'-N1-C2
2	B	6	5CM	O4'-C1'-N1-C2
2	K	6	5CM	O4'-C1'-N1-C2
2	E	6	5CM	O4'-C1'-N1-C2
2	K	6	5CM	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6	5CM	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OGA	J	502	4	9,9,9	1.24	0	8,11,11	1.33	1 (12%)
5	OGA	G	502	4	9,9,9	1.17	1 (11%)	8,11,11	1.26	0
5	OGA	A	502	4	9,9,9	1.29	0	8,11,11	1.38	1 (12%)
5	OGA	D	502	4	9,9,9	1.15	0	8,11,11	1.56	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OGA	J	502	4	-	1/8/9/9	-
5	OGA	G	502	4	-	1/8/9/9	-
5	OGA	A	502	4	-	1/8/9/9	-
5	OGA	D	502	4	-	1/8/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	502	OGA	O3-C5	-2.20	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	OGA	O2'-C2-C1	-2.40	118.20	121.36
5	D	502	OGA	O2'-C2-C1	-2.04	118.68	121.36
5	J	502	OGA	O2-C1-O1	-2.00	119.14	123.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	OGA	O2-C1-C2-O2'
5	G	502	OGA	O2-C1-C2-O2'
5	D	502	OGA	N1-C4-C5-O4
5	J	502	OGA	N1-C4-C5-O4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	376/415 (90%)	-0.35	7 (1%) 66 68	18, 28, 51, 89	0
1	D	383/415 (92%)	-0.32	4 (1%) 79 80	19, 29, 50, 79	0
1	G	376/415 (90%)	-0.12	10 (2%) 56 58	24, 38, 56, 94	0
1	J	383/415 (92%)	0.44	20 (5%) 33 34	36, 51, 76, 105	0
2	B	11/12 (91%)	-0.21	1 (9%) 15 16	34, 42, 50, 64	0
2	E	11/12 (91%)	-0.01	0 100 100	30, 33, 65, 73	0
2	H	11/12 (91%)	-0.18	0 100 100	33, 37, 53, 59	0
2	K	11/12 (91%)	1.48	4 (36%) 1 1	54, 61, 108, 111	0
3	C	12/12 (100%)	-0.32	0 100 100	39, 46, 49, 50	0
3	F	12/12 (100%)	0.13	1 (8%) 17 19	28, 45, 70, 81	0
3	I	12/12 (100%)	0.00	0 100 100	44, 47, 49, 51	0
3	L	11/12 (91%)	1.25	4 (36%) 1 1	57, 62, 119, 123	0
All	All	1609/1756 (91%)	-0.06	51 (3%) 50 52	18, 38, 65, 123	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	410	TRP	4.5
1	J	183	MET	4.0
2	K	12	DG	3.9
1	A	173	ALA	3.7
1	D	203	ASN	3.7
1	G	176	GLY	3.7
1	J	92	ARG	3.4
2	K	11	DC	3.2
1	J	172	ARG	3.1
1	J	181	VAL	3.1
2	K	9	DT	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	163	LYS	3.0
3	L	3	DT	3.0
1	D	118	HIS	2.9
1	A	118	HIS	2.9
1	A	178	ARG	2.9
1	J	200	LEU	2.8
1	J	163	LYS	2.8
1	J	178	ARG	2.8
2	K	10	DA	2.7
1	G	174	ARG	2.5
1	J	168	GLN	2.5
1	J	120	VAL	2.5
3	F	1	DC	2.5
1	J	215	ALA	2.4
1	G	106	LYS	2.4
1	A	174	ARG	2.4
3	L	2	DG	2.3
3	L	5	DG	2.3
1	J	118	HIS	2.3
1	G	117	ASP	2.3
1	J	203	ASN	2.3
1	J	167	LEU	2.3
1	J	235	GLU	2.3
1	G	200	LEU	2.2
1	A	162	THR	2.2
1	J	164	ASP	2.2
1	J	233	GLY	2.2
1	J	238	LEU	2.1
1	J	296	LYS	2.1
1	G	84	ARG	2.1
3	L	4	DA	2.1
1	D	117	ASP	2.1
1	G	118	HIS	2.1
2	B	1	DC	2.1
1	G	116	SER	2.0
1	A	202	ALA	2.0
1	G	119	PRO	2.0
1	J	299	SER	2.0
1	G	115	ASN	2.0
1	J	180	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	5CM	H	6	20/21	0.87	0.10	29,37,48,54	0
2	5CM	K	6	20/21	0.92	0.08	39,45,57,63	0
2	5CM	B	6	20/21	0.93	0.08	25,32,50,52	0
2	5CM	E	6	20/21	0.96	0.06	20,28,36,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	OGA	J	502	10/10	0.93	0.09	36,41,44,44	0
5	OGA	D	502	10/10	0.97	0.05	17,20,26,38	0
5	OGA	G	502	10/10	0.98	0.04	28,30,32,33	0
5	OGA	A	502	10/10	0.98	0.04	20,23,25,26	0
4	MN	J	501	1/1	0.99	0.02	37,37,37,37	0
4	MN	G	501	1/1	1.00	0.01	33,33,33,33	0
4	MN	A	501	1/1	1.00	0.01	23,23,23,23	0
4	MN	D	501	1/1	1.00	0.03	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.