



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2023 – 10:35 PM EDT

PDB ID : 6WAT
Title : complex structure of PHF1
Authors : Dong, C.; Bountra, C.; Edwards, A.M.; Arrowsmith, C.H.; Min, J.R.; Structural Genomics Consortium (SGC)
Deposited on : 2020-03-26
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

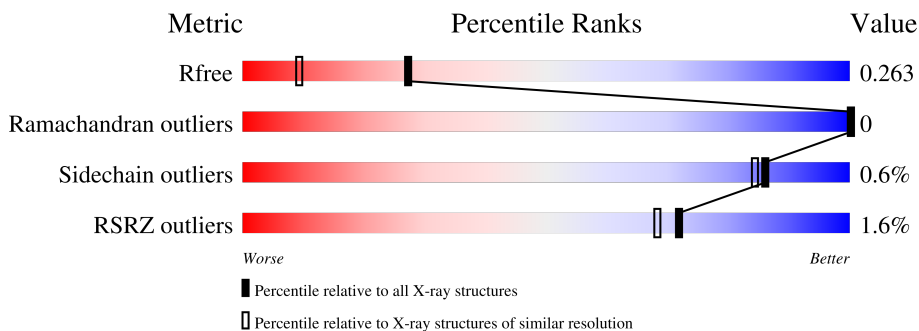
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	AA	61	98%
1	AC	61	97%
1	BA	61	98%
1	BC	61	98%
1	CA	61	98%
1	CC	61	2% 98%


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	DA	61	98%
1	DC	61	3% 98%
1	EA	61	98%
1	EC	61	97%
1	FA	61	2% 100%
1	FC	61	97%
1	GA	61	98%
1	GC	61	97%
1	HA	61	98%
1	HC	61	95%
1	IA	61	98%
1	IC	61	2% 97%
1	JA	61	98%
1	JC	61	2% 97%
1	KA	61	97%
1	KC	61	3% 97%
1	LA	61	100%
1	LC	61	2% 98%
1	MA	61	3% 98%
1	MC	61	95%
1	NA	61	5% 97%
1	NC	61	2% 97%
1	OA	61	7% 98%
1	OC	61	5% 97%
2	A	9	78% 11% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	9	 89% 11%
2	C	9	 78% 11% 11%
2	D	9	 78% 11% 11%
2	E	9	 11% 89% 11%
2	F	9	 89% 11%
2	G	9	 78% 11% 11%
2	H	9	 78% 11% 11%
2	I	9	 11% 89% 11%
2	J	9	 78% 11% 11%
2	K	9	 11% 89% 11%
2	L	9	 11% 89% 11%
2	M	9	 78% 11% 11%
2	N	9	 78% 11% 11%
2	O	9	 11% 89% 11%
2	P	9	 78% 11% 11%
2	Q	9	 78% 11% 11%
2	R	9	 78% 11% 11%
2	S	9	 89% 11%
2	T	9	 78% 11% 11%
2	V	9	 78% 11% 11%
2	Y	9	 78% 11% 11%
2	Z	9	 78% 11% 11%
2	a	9	 11% 78% 11% 11%
2	b	9	 11% 89% 11%
2	c	9	 67% 11% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	d	9	
2	e	9	
2	f	9	
2	g	9	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNX	AA	102	-	-	-	X
3	UNX	CA	102	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16435 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 PHD finger protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AA	60	470	307	74	88	1	0	1	0
1	AC	60	469	308	75	85	1	0	1	0
1	BA	60	475	310	76	88	1	0	2	0
1	BC	60	483	313	78	91	1	0	4	0
1	CA	60	472	308	73	90	1	0	1	0
1	CC	60	477	314	75	87	1	0	3	0
1	DA	60	468	304	75	88	1	0	1	0
1	DC	61	482	313	76	92	1	0	2	0
1	EA	60	467	305	73	88	1	0	1	0
1	EC	59	473	311	75	86	1	0	5	1
1	FA	61	478	313	74	90	1	0	3	0
1	FC	59	459	303	69	86	1	0	2	1
1	GA	60	474	309	74	90	1	0	1	0
1	GC	59	458	303	70	84	1	0	3	1
1	HA	60	468	306	73	88	1	0	1	0
1	HC	59	462	305	69	87	1	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	IA	60	464	302	73	88	1	0	1	0
1	IC	60	479	313	79	86	1	0	3	0
1	JA	60	466	304	73	88	1	0	1	0
1	JC	60	470	304	75	90	1	0	2	1
1	KA	59	445	291	71	82	1	0	0	1
1	KC	60	449	293	72	83	1	0	0	1
1	LA	61	458	300	72	85	1	0	0	1
1	LC	60	456	298	75	82	1	0	0	1
1	MA	60	449	292	72	84	1	0	0	0
1	MC	59	445	292	70	82	1	0	0	0
1	NA	60	452	293	75	83	1	0	0	1
1	NC	59	435	287	71	76	1	0	0	1
1	OA	60	445	288	72	84	1	0	0	1
1	OC	59	440	290	70	79	1	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	27	GLY	-	expression tag	UNP O43189
AC	27	GLY	-	expression tag	UNP O43189
BA	27	GLY	-	expression tag	UNP O43189
BC	27	GLY	-	expression tag	UNP O43189
CA	27	GLY	-	expression tag	UNP O43189
CC	27	GLY	-	expression tag	UNP O43189
DA	27	GLY	-	expression tag	UNP O43189
DC	27	GLY	-	expression tag	UNP O43189
EA	27	GLY	-	expression tag	UNP O43189
EC	27	GLY	-	expression tag	UNP O43189
FA	27	GLY	-	expression tag	UNP O43189

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
FC	27	GLY	-	expression tag	UNP O43189
GA	27	GLY	-	expression tag	UNP O43189
GC	27	GLY	-	expression tag	UNP O43189
HA	27	GLY	-	expression tag	UNP O43189
HC	27	GLY	-	expression tag	UNP O43189
IA	27	GLY	-	expression tag	UNP O43189
IC	27	GLY	-	expression tag	UNP O43189
JA	27	GLY	-	expression tag	UNP O43189
JC	27	GLY	-	expression tag	UNP O43189
KA	27	GLY	-	expression tag	UNP O43189
KC	27	GLY	-	expression tag	UNP O43189
LA	27	GLY	-	expression tag	UNP O43189
LC	27	GLY	-	expression tag	UNP O43189
MA	27	GLY	-	expression tag	UNP O43189
MC	27	GLY	-	expression tag	UNP O43189
NA	27	GLY	-	expression tag	UNP O43189
NC	27	GLY	-	expression tag	UNP O43189
OA	27	GLY	-	expression tag	UNP O43189
OC	27	GLY	-	expression tag	UNP O43189

- Molecule 2 is a protein called Histone H3.1t peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	8	Total	C	N	O	0	0	0
			64	41	13	10			
2	B	8	Total	C	N	O	0	0	0
			62	40	12	10			
2	C	8	Total	C	N	O	0	0	0
			64	41	13	10			
2	D	8	Total	C	N	O	0	0	0
			63	41	12	10			
2	E	9	Total	C	N	O	0	0	0
			68	44	13	11			
2	F	8	Total	C	N	O	0	0	0
			63	41	12	10			
2	G	8	Total	C	N	O	0	0	0
			63	41	12	10			
2	H	8	Total	C	N	O	0	0	0
			62	40	12	10			
2	I	9	Total	C	N	O	0	0	1
			66	42	14	10			
2	J	8	Total	C	N	O	0	0	0
			63	41	12	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	K	9	68	44	13	11	0	0	0
2	L	9	67	43	13	11	0	0	0
2	M	8	64	41	13	10	0	0	0
2	N	8	64	41	13	10	0	0	0
2	O	9	68	44	13	11	0	0	0
2	P	8	63	41	12	10	0	0	0
2	Q	8	58	39	10	9	0	0	0
2	R	8	63	41	12	10	0	0	0
2	S	9	64	41	13	10	0	0	1
2	T	8	59	38	12	9	0	0	1
2	V	8	55	36	10	9	0	0	1
2	Y	8	61	39	12	10	0	0	0
2	Z	8	64	41	13	10	0	0	0
2	a	8	59	38	12	9	0	0	1
2	b	8	55	37	9	9	0	0	0
2	c	7	55	37	10	8	0	0	0
2	d	8	57	38	9	10	0	0	0
2	e	7	55	36	11	8	0	0	0
2	f	8	54	36	9	9	0	0	1
2	g	8	62	40	12	10	0	0	0

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AA	7	Total X 7 7	0	0
3	AC	3	Total X 3 3	0	0
3	BA	7	Total X 7 7	0	0
3	BC	3	Total X 3 3	0	0
3	CA	7	Total X 7 7	0	0
3	CC	5	Total X 5 5	0	0
3	DA	5	Total X 5 5	0	0
3	DC	3	Total X 3 3	0	0
3	EA	6	Total X 6 6	0	0
3	EC	8	Total X 8 8	0	0
3	FA	3	Total X 3 3	0	0
3	FC	7	Total X 7 7	0	0
3	GA	3	Total X 3 3	0	0
3	GC	1	Total X 1 1	0	0
3	HA	5	Total X 5 5	0	0
3	HC	8	Total X 8 8	0	0
3	IA	3	Total X 3 3	0	0
3	IC	1	Total X 1 1	0	0
3	JA	6	Total X 6 6	0	0
3	JC	2	Total X 2 2	0	0
3	KA	1	Total X 1 1	0	0
3	KC	1	Total X 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	LA	2	Total X 2 2	0	0
3	LC	1	Total X 1 1	0	0
3	MA	1	Total X 1 1	0	0
3	MC	1	Total X 1 1	0	0
3	NA	3	Total X 3 3	0	0
3	NC	1	Total X 1 1	0	0
3	OA	2	Total X 2 2	0	0
3	OC	1	Total X 1 1	0	0
3	A	1	Total X 1 1	0	0
3	B	1	Total X 1 1	0	0
3	D	1	Total X 1 1	0	0
3	F	3	Total X 3 3	0	0
3	G	1	Total X 1 1	0	0
3	H	2	Total X 2 2	0	0
3	I	1	Total X 1 1	0	0
3	J	3	Total X 3 3	0	0
3	K	1	Total X 1 1	0	0
3	L	1	Total X 1 1	0	0
3	M	2	Total X 2 2	0	0
3	N	2	Total X 2 2	0	0
3	O	2	Total X 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	2	Total	X	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AA	34	Total	O	0	0
			34	34		
4	AC	27	Total	O	0	0
			27	27		
4	BA	29	Total	O	0	0
			29	29		
4	BC	29	Total	O	0	0
			29	29		
4	CA	28	Total	O	0	0
			28	28		
4	CC	22	Total	O	0	0
			22	22		
4	DA	16	Total	O	0	0
			16	16		
4	DC	32	Total	O	0	0
			32	32		
4	EA	24	Total	O	0	0
			24	24		
4	EC	18	Total	O	0	0
			18	18		
4	FA	32	Total	O	0	0
			32	32		
4	FC	23	Total	O	0	0
			23	23		
4	GA	34	Total	O	0	0
			34	34		
4	GC	19	Total	O	0	0
			19	19		
4	HA	27	Total	O	0	0
			27	27		
4	HC	20	Total	O	0	0
			20	20		
4	IA	12	Total	O	0	0
			12	12		
4	IC	19	Total	O	0	0
			19	19		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	JA	25	Total O 25 25	0	0
4	JC	10	Total O 10 10	0	0
4	KA	1	Total O 1 1	0	0
4	KC	3	Total O 3 3	0	0
4	LA	7	Total O 7 7	0	0
4	LC	3	Total O 3 3	0	0
4	MC	1	Total O 1 1	0	0
4	A	1	Total O 1 1	0	0
4	B	7	Total O 7 7	0	0
4	C	2	Total O 2 2	0	0
4	D	4	Total O 4 4	0	0
4	E	2	Total O 2 2	0	0
4	F	4	Total O 4 4	0	0
4	G	4	Total O 4 4	0	0
4	H	4	Total O 4 4	0	0
4	I	2	Total O 2 2	0	0
4	J	4	Total O 4 4	0	0
4	K	4	Total O 4 4	0	0
4	L	6	Total O 6 6	0	0
4	M	3	Total O 3 3	0	0
4	N	5	Total O 5 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	2	Total O 2 2	0	0
4	P	5	Total O 5 5	0	0
4	Q	2	Total O 2 2	0	0
4	R	3	Total O 3 3	0	0
4	S	2	Total O 2 2	0	0
4	T	2	Total O 2 2	0	0
4	Z	1	Total O 1 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: PHD finger protein 1

Chain AA:  98%



- Molecule 1: PHD finger protein 1

Chain AC:  97%



- Molecule 1: PHD finger protein 1

Chain BA:  98%



- Molecule 1: PHD finger protein 1

Chain BC:  98%



- Molecule 1: PHD finger protein 1

Chain CA:  98%



- Molecule 1: PHD finger protein 1

Chain CC:  98%



- Molecule 1: PHD finger protein 1

Chain DA:  98%



- Molecule 1: PHD finger protein 1

Chain DC:  98%



- Molecule 1: PHD finger protein 1

Chain EA:  98%



- Molecule 1: PHD finger protein 1

Chain EC:  97%



- Molecule 1: PHD finger protein 1

Chain FA:  100%



- Molecule 1: PHD finger protein 1

Chain FC:  97%



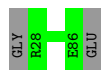
- Molecule 1: PHD finger protein 1

Chain GA:  98%



- Molecule 1: PHD finger protein 1

Chain GC: 97%



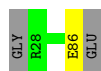
- Molecule 1: PHD finger protein 1

Chain HA: 98%



- Molecule 1: PHD finger protein 1

Chain HC: 95%



- Molecule 1: PHD finger protein 1

Chain IA: 98%



- Molecule 1: PHD finger protein 1

Chain IC: 97%



- Molecule 1: PHD finger protein 1

Chain JA: 98%



- Molecule 1: PHD finger protein 1

Chain JC: 97%



- Molecule 1: PHD finger protein 1

Chain KA: 97%



- Molecule 1: PHD finger protein 1

Chain KC: 97%



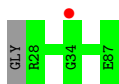
- Molecule 1: PHD finger protein 1

Chain LA: 100%

There are no outlier residues recorded for this chain.

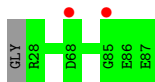
- Molecule 1: PHD finger protein 1

Chain LC: 98%



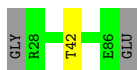
- Molecule 1: PHD finger protein 1

Chain MA: 98%



- Molecule 1: PHD finger protein 1

Chain MC: 95%

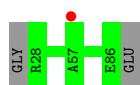


- Molecule 1: PHD finger protein 1

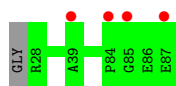
Chain NA: 97%



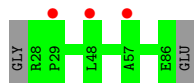
- Molecule 1: PHD finger protein 1



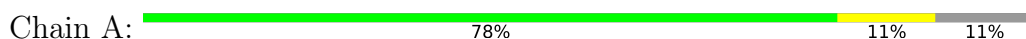
- Molecule 1: PHD finger protein 1



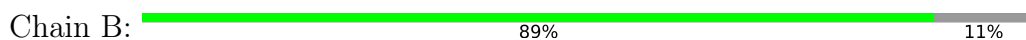
- Molecule 1: PHD finger protein 1



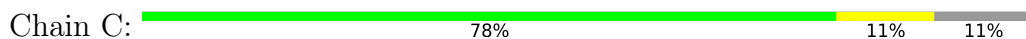
- Molecule 2: Histone H3.1t peptide



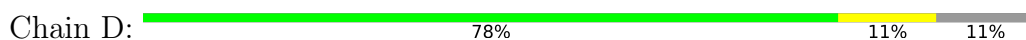
- Molecule 2: Histone H3.1t peptide



- Molecule 2: Histone H3.1t peptide

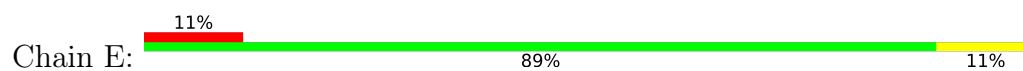


- Molecule 2: Histone H3.1t peptide

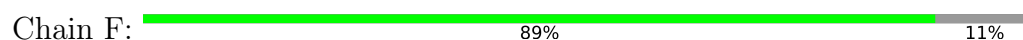




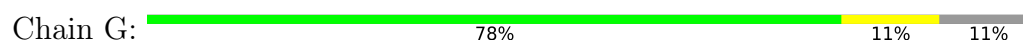
- Molecule 2: Histone H3.1t peptide



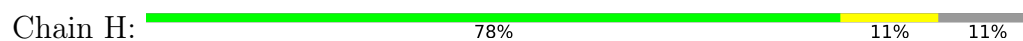
- Molecule 2: Histone H3.1t peptide



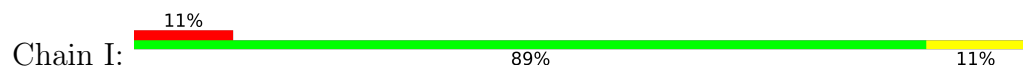
- Molecule 2: Histone H3.1t peptide



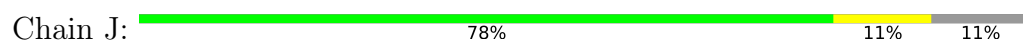
- Molecule 2: Histone H3.1t peptide



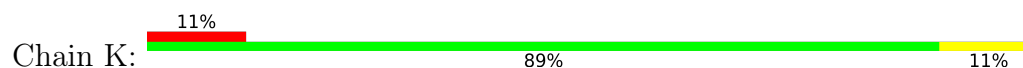
- Molecule 2: Histone H3.1t peptide



- Molecule 2: Histone H3.1t peptide

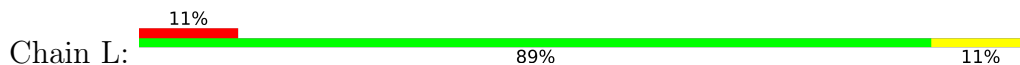


- Molecule 2: Histone H3.1t peptide

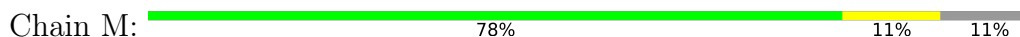




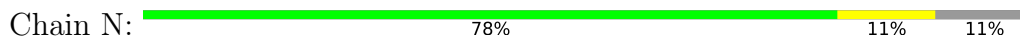
- Molecule 2: Histone H3.1t peptide



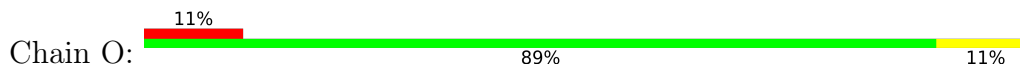
- Molecule 2: Histone H3.1t peptide



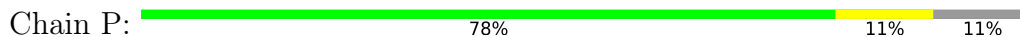
- Molecule 2: Histone H3.1t peptide



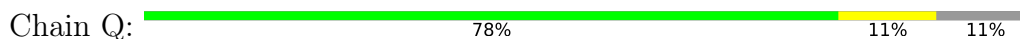
- Molecule 2: Histone H3.1t peptide



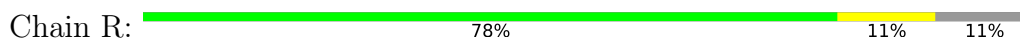
- Molecule 2: Histone H3.1t peptide



- Molecule 2: Histone H3.1t peptide

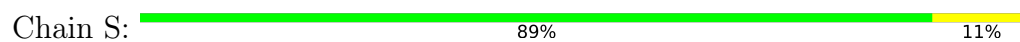


- Molecule 2: Histone H3.1t peptide

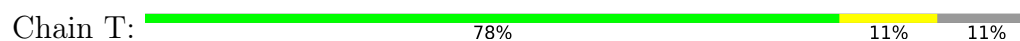




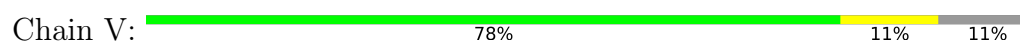
- Molecule 2: Histone H3.1t peptide



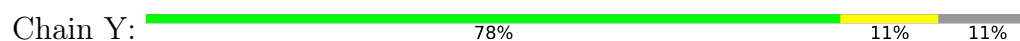
- Molecule 2: Histone H3.1t peptide



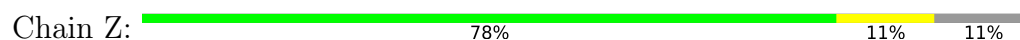
- Molecule 2: Histone H3.1t peptide



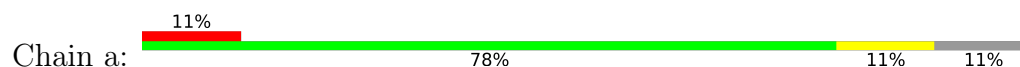
- Molecule 2: Histone H3.1t peptide



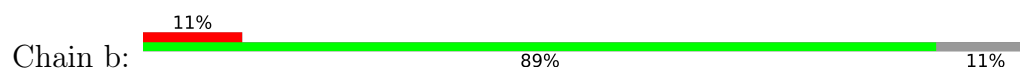
- Molecule 2: Histone H3.1t peptide



- Molecule 2: Histone H3.1t peptide

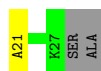


- Molecule 2: Histone H3.1t peptide

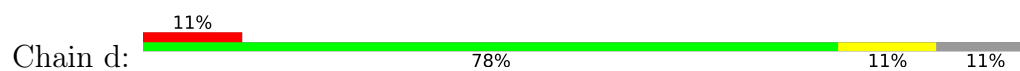




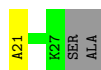
- Molecule 2: Histone H3.1t peptide



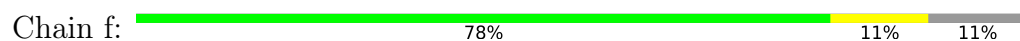
- Molecule 2: Histone H3.1t peptide



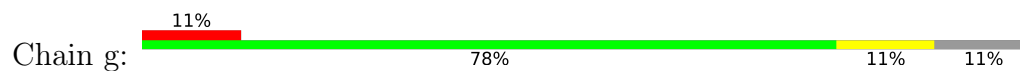
- Molecule 2: Histone H3.1t peptide



- Molecule 2: Histone H3.1t peptide



- Molecule 2: Histone H3.1t peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	32.75Å 286.81Å 123.54Å 90.00° 90.72° 90.00°	Depositor
Resolution (Å)	40.76 – 1.80 47.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.9 (40.76-1.80) 99.3 (47.80-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.79Å)	Xtrriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.234 , 0.268 0.228 , 0.263	Depositor DCC
R_{free} test set	10495 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtrriage
Anisotropy	0.312	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.63$, $\langle L^2 \rangle = 0.49$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16435	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3774e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AYA, UNX, M3L

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	AA	0.41	0/484	0.56	0/660
1	AC	0.37	0/483	0.55	0/661
1	BA	0.38	0/492	0.55	0/671
1	BC	0.37	0/509	0.55	0/695
1	CA	0.40	0/486	0.56	0/663
1	CC	0.36	0/497	0.54	0/680
1	DA	0.38	0/482	0.55	0/660
1	DC	0.41	0/499	0.60	0/681
1	EA	0.35	0/481	0.54	0/657
1	EC	0.35	0/499	0.53	0/684
1	FA	0.39	0/498	0.55	0/680
1	FC	0.35	0/476	0.55	0/651
1	GA	0.37	0/488	0.56	0/665
1	GC	0.33	0/475	0.54	0/650
1	HA	0.39	0/482	0.54	0/658
1	HC	0.35	0/479	0.54	0/656
1	IA	0.32	0/478	0.53	0/654
1	IC	0.32	0/501	0.52	0/684
1	JA	0.35	0/480	0.53	0/656
1	JC	0.33	0/487	0.54	0/667
1	KA	0.26	0/456	0.48	0/626
1	KC	0.29	0/460	0.48	0/632
1	LA	0.32	0/469	0.51	0/642
1	LC	0.28	0/467	0.50	0/639
1	MA	0.28	0/460	0.47	0/631
1	MC	0.27	0/456	0.49	0/624
1	NA	0.28	0/463	0.48	0/636
1	NC	0.26	0/446	0.47	0/613
1	OA	0.27	0/456	0.47	0/626
1	OC	0.26	0/451	0.48	0/619
2	A	0.34	0/43	0.66	0/56
2	B	0.34	0/41	0.60	0/54

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	C	0.30	0/43	0.59	0/56
2	D	0.35	0/42	0.62	0/55
2	E	0.41	0/47	0.62	0/62
2	F	0.44	0/42	0.63	0/55
2	G	0.44	0/42	0.58	0/55
2	H	0.30	0/41	0.55	0/54
2	I	0.45	0/45	0.57	0/59
2	J	0.31	0/42	0.50	0/55
2	K	0.37	0/47	0.58	0/62
2	L	0.31	0/46	0.62	0/61
2	M	0.32	0/43	0.55	0/56
2	N	0.33	0/43	0.53	0/56
2	O	0.36	0/47	0.56	0/62
2	P	0.33	0/42	0.63	0/55
2	Q	0.29	0/39	0.48	0/51
2	R	0.35	0/42	0.47	0/55
2	S	0.42	0/43	0.49	0/57
2	T	0.37	0/38	0.55	0/50
2	V	0.27	0/34	0.52	0/45
2	Y	0.28	0/40	0.52	0/53
2	Z	0.30	0/43	0.45	0/56
2	a	0.35	0/38	0.63	0/50
2	b	0.29	0/37	0.60	0/49
2	c	0.32	0/36	0.56	0/46
2	d	0.25	0/36	0.65	0/48
2	e	0.26	0/36	0.55	0/47
2	f	0.27	0/33	0.58	0/44
2	g	0.29	0/41	0.53	0/54
All	All	0.34	0/15572	0.53	0/21239

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	AA	59/61 (97%)	59 (100%)	0	0	100	100
1	AC	59/61 (97%)	59 (100%)	0	0	100	100
1	BA	60/61 (98%)	60 (100%)	0	0	100	100
1	BC	62/61 (102%)	62 (100%)	0	0	100	100
1	CA	59/61 (97%)	59 (100%)	0	0	100	100
1	CC	61/61 (100%)	61 (100%)	0	0	100	100
1	DA	59/61 (97%)	59 (100%)	0	0	100	100
1	DC	61/61 (100%)	61 (100%)	0	0	100	100
1	EA	59/61 (97%)	59 (100%)	0	0	100	100
1	EC	62/61 (102%)	62 (100%)	0	0	100	100
1	FA	62/61 (102%)	62 (100%)	0	0	100	100
1	FC	59/61 (97%)	59 (100%)	0	0	100	100
1	GA	59/61 (97%)	59 (100%)	0	0	100	100
1	GC	59/61 (97%)	59 (100%)	0	0	100	100
1	HA	59/61 (97%)	59 (100%)	0	0	100	100
1	HC	59/61 (97%)	59 (100%)	0	0	100	100
1	IA	59/61 (97%)	59 (100%)	0	0	100	100
1	IC	61/61 (100%)	61 (100%)	0	0	100	100
1	JA	59/61 (97%)	59 (100%)	0	0	100	100
1	JC	60/61 (98%)	59 (98%)	1 (2%)	0	100	100
1	KA	57/61 (93%)	57 (100%)	0	0	100	100
1	KC	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
1	LA	59/61 (97%)	59 (100%)	0	0	100	100
1	LC	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
1	MA	58/61 (95%)	58 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	MC	57/61 (93%)	55 (96%)	2 (4%)	0	100	100
1	NA	58/61 (95%)	58 (100%)	0	0	100	100
1	NC	57/61 (93%)	57 (100%)	0	0	100	100
1	OA	58/61 (95%)	58 (100%)	0	0	100	100
1	OC	57/61 (93%)	57 (100%)	0	0	100	100
2	A	5/9 (56%)	5 (100%)	0	0	100	100
2	B	5/9 (56%)	5 (100%)	0	0	100	100
2	C	5/9 (56%)	5 (100%)	0	0	100	100
2	D	5/9 (56%)	5 (100%)	0	0	100	100
2	E	6/9 (67%)	6 (100%)	0	0	100	100
2	F	5/9 (56%)	5 (100%)	0	0	100	100
2	G	5/9 (56%)	5 (100%)	0	0	100	100
2	H	5/9 (56%)	5 (100%)	0	0	100	100
2	I	6/9 (67%)	5 (83%)	1 (17%)	0	100	100
2	J	5/9 (56%)	5 (100%)	0	0	100	100
2	K	6/9 (67%)	6 (100%)	0	0	100	100
2	L	6/9 (67%)	6 (100%)	0	0	100	100
2	M	5/9 (56%)	5 (100%)	0	0	100	100
2	N	5/9 (56%)	5 (100%)	0	0	100	100
2	O	6/9 (67%)	6 (100%)	0	0	100	100
2	P	5/9 (56%)	5 (100%)	0	0	100	100
2	Q	5/9 (56%)	5 (100%)	0	0	100	100
2	R	5/9 (56%)	5 (100%)	0	0	100	100
2	S	6/9 (67%)	6 (100%)	0	0	100	100
2	T	5/9 (56%)	5 (100%)	0	0	100	100
2	V	5/9 (56%)	5 (100%)	0	0	100	100
2	Y	5/9 (56%)	5 (100%)	0	0	100	100
2	Z	5/9 (56%)	4 (80%)	1 (20%)	0	100	100
2	a	5/9 (56%)	5 (100%)	0	0	100	100
2	b	5/9 (56%)	5 (100%)	0	0	100	100
2	c	5/9 (56%)	5 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	d	5/9 (56%)	5 (100%)	0	0	100	100
2	e	5/9 (56%)	4 (80%)	1 (20%)	0	100	100
2	f	5/9 (56%)	5 (100%)	0	0	100	100
2	g	5/9 (56%)	5 (100%)	0	0	100	100
All	All	1930/2100 (92%)	1921 (100%)	9 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	AA	48/52 (92%)	48 (100%)	0	100	100
1	AC	46/52 (88%)	45 (98%)	1 (2%)	52	39
1	BA	48/52 (92%)	48 (100%)	0	100	100
1	BC	50/52 (96%)	50 (100%)	0	100	100
1	CA	48/52 (92%)	48 (100%)	0	100	100
1	CC	48/52 (92%)	48 (100%)	0	100	100
1	DA	47/52 (90%)	47 (100%)	0	100	100
1	DC	50/52 (96%)	49 (98%)	1 (2%)	55	44
1	EA	47/52 (90%)	47 (100%)	0	100	100
1	EC	49/52 (94%)	49 (100%)	0	100	100
1	FA	49/52 (94%)	49 (100%)	0	100	100
1	FC	47/52 (90%)	47 (100%)	0	100	100
1	GA	49/52 (94%)	49 (100%)	0	100	100
1	GC	46/52 (88%)	46 (100%)	0	100	100
1	HA	47/52 (90%)	47 (100%)	0	100	100
1	HC	47/52 (90%)	46 (98%)	1 (2%)	53	42
1	IA	46/52 (88%)	46 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IC	49/52 (94%)	48 (98%)	1 (2%)	55	44
1	JA	47/52 (90%)	47 (100%)	0	100	100
1	JC	49/52 (94%)	48 (98%)	1 (2%)	55	44
1	KA	43/52 (83%)	43 (100%)	0	100	100
1	KC	43/52 (83%)	42 (98%)	1 (2%)	50	37
1	LA	44/52 (85%)	44 (100%)	0	100	100
1	LC	44/52 (85%)	44 (100%)	0	100	100
1	MA	42/52 (81%)	42 (100%)	0	100	100
1	MC	42/52 (81%)	41 (98%)	1 (2%)	49	36
1	NA	44/52 (85%)	43 (98%)	1 (2%)	50	37
1	NC	39/52 (75%)	39 (100%)	0	100	100
1	OA	41/52 (79%)	41 (100%)	0	100	100
1	OC	40/52 (77%)	40 (100%)	0	100	100
2	A	4/5 (80%)	4 (100%)	0	100	100
2	B	3/5 (60%)	3 (100%)	0	100	100
2	C	4/5 (80%)	4 (100%)	0	100	100
2	D	3/5 (60%)	3 (100%)	0	100	100
2	E	3/5 (60%)	3 (100%)	0	100	100
2	F	3/5 (60%)	3 (100%)	0	100	100
2	G	3/5 (60%)	3 (100%)	0	100	100
2	H	3/5 (60%)	3 (100%)	0	100	100
2	I	4/5 (80%)	4 (100%)	0	100	100
2	J	3/5 (60%)	3 (100%)	0	100	100
2	K	3/5 (60%)	3 (100%)	0	100	100
2	L	3/5 (60%)	3 (100%)	0	100	100
2	M	4/5 (80%)	4 (100%)	0	100	100
2	N	4/5 (80%)	4 (100%)	0	100	100
2	O	3/5 (60%)	3 (100%)	0	100	100
2	P	3/5 (60%)	3 (100%)	0	100	100
2	Q	2/5 (40%)	2 (100%)	0	100	100
2	R	3/5 (60%)	3 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	3/5 (60%)	3 (100%)	0	100	100
2	T	3/5 (60%)	3 (100%)	0	100	100
2	V	3/5 (60%)	3 (100%)	0	100	100
2	Y	3/5 (60%)	3 (100%)	0	100	100
2	Z	4/5 (80%)	4 (100%)	0	100	100
2	a	3/5 (60%)	3 (100%)	0	100	100
2	b	2/5 (40%)	2 (100%)	0	100	100
2	c	4/5 (80%)	4 (100%)	0	100	100
2	d	2/5 (40%)	2 (100%)	0	100	100
2	e	3/5 (60%)	3 (100%)	0	100	100
2	f	2/5 (40%)	2 (100%)	0	100	100
2	g	3/5 (60%)	3 (100%)	0	100	100
All	All	1472/1710 (86%)	1464 (100%)	8 (0%)	86	87

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	NA	83	LEU
1	MC	42	THR
1	JC	86	GLU
1	IC	79	SER
1	KC	79	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	AC	70	GLN
1	NA	70	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

60 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	AYA	D	21	2	6,7,8	0.96	0	5,8,10	1.19	1 (20%)
2	AYA	Y	21	2	6,7,8	1.43	1 (16%)	5,8,10	1.38	1 (20%)
2	M3L	Z	27	2	10,11,12	0.57	0	9,14,16	0.42	0
2	AYA	R	21	2	6,7,8	1.19	0	5,8,10	1.68	2 (40%)
2	AYA	V	21	2	6,7,8	1.46	1 (16%)	5,8,10	1.36	1 (20%)
2	AYA	G	21	2	6,7,8	1.24	1 (16%)	5,8,10	2.00	1 (20%)
2	M3L	A	27	2	10,11,12	0.49	0	9,14,16	0.59	0
2	AYA	d	21	2	6,7,8	1.38	1 (16%)	5,8,10	1.40	1 (20%)
2	AYA	A	21	2	6,7,8	1.12	0	5,8,10	1.66	1 (20%)
2	M3L	R	27	2	10,11,12	0.47	0	9,14,16	0.49	0
2	M3L	K	27	2	10,11,12	0.50	0	9,14,16	0.47	0
2	AYA	f	21	2	6,7,8	1.43	1 (16%)	5,8,10	1.45	1 (20%)
2	AYA	b	21	2	3,4,8	0.93	0	2,4,10	0.63	0
2	AYA	e	21	2	4,5,8	1.73	1 (25%)	1,5,10	1.20	0
2	M3L	G	27	2	10,11,12	0.43	0	9,14,16	0.50	0
2	M3L	L	27	2	10,11,12	0.51	0	9,14,16	0.55	0
2	M3L	D	27	2	10,11,12	0.43	0	9,14,16	0.32	0
2	M3L	V	27	2	10,11,12	0.52	0	9,14,16	0.54	0
2	AYA	Z	21	2	6,7,8	1.18	1 (16%)	5,8,10	1.41	1 (20%)
2	M3L	g	27	2	10,11,12	0.57	0	9,14,16	0.44	0
2	M3L	Y	27	2	10,11,12	0.54	0	9,14,16	0.45	0
2	M3L	f	27	2	10,11,12	0.56	0	9,14,16	0.49	0
2	M3L	b	27	2	10,11,12	0.57	0	9,14,16	0.42	0
2	AYA	O	21	2	6,7,8	1.32	1 (16%)	5,8,10	0.92	0
2	M3L	e	27	2	10,11,12	0.57	0	9,14,16	0.47	0
2	M3L	B	27	2	10,11,12	0.51	0	9,14,16	0.49	0
2	M3L	I	27	2	10,11,12	0.47	0	9,14,16	0.48	0
2	AYA	L	21	2	6,7,8	1.12	0	5,8,10	1.30	1 (20%)
2	AYA	P	21	2	6,7,8	1.14	1 (16%)	5,8,10	1.30	1 (20%)
2	AYA	N	21	2	6,7,8	1.10	1 (16%)	5,8,10	1.28	1 (20%)
2	M3L	S	27	2	10,11,12	0.53	0	9,14,16	0.49	0
2	M3L	N	27	2	10,11,12	0.51	0	9,14,16	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AYA	g	21	2	6,7,8	1.15	0	5,8,10	1.32	1 (20%)
2	AYA	Q	21	2	4,5,8	1.65	1 (25%)	1,5,10	1.47	0
2	AYA	K	21	2	6,7,8	1.22	1 (16%)	5,8,10	1.18	1 (20%)
2	M3L	c	27	2	10,11,12	0.52	0	9,14,16	0.48	0
2	AYA	C	21	2	6,7,8	1.24	0	5,8,10	2.11	1 (20%)
2	M3L	H	27	2	10,11,12	0.43	0	9,14,16	0.55	0
2	AYA	M	21	2	6,7,8	1.10	0	5,8,10	1.73	1 (20%)
2	AYA	T	21	2	6,7,8	1.44	1 (16%)	5,8,10	1.35	1 (20%)
2	AYA	a	21	2	6,7,8	1.43	1 (16%)	5,8,10	1.26	1 (20%)
2	M3L	P	27	2	10,11,12	0.48	0	9,14,16	0.51	0
2	AYA	J	21	2	6,7,8	1.26	1 (16%)	5,8,10	1.26	1 (20%)
2	AYA	c	21	2	4,5,8	1.76	1 (25%)	1,5,10	1.11	0
2	M3L	a	27	2	10,11,12	0.48	0	9,14,16	0.51	0
2	AYA	E	21	2	6,7,8	0.97	0	5,8,10	1.67	1 (20%)
2	M3L	Q	27	2	10,11,12	0.44	0	9,14,16	0.46	0
2	AYA	I	21	2	6,7,8	1.11	0	5,8,10	1.44	1 (20%)
2	AYA	H	21	2	6,7,8	1.33	1 (16%)	5,8,10	0.99	0
2	M3L	C	27	2	10,11,12	0.54	0	9,14,16	0.53	0
2	M3L	F	27	2	10,11,12	0.49	0	9,14,16	0.54	0
2	M3L	M	27	2	10,11,12	0.52	0	9,14,16	0.56	0
2	AYA	F	21	2	6,7,8	0.98	0	5,8,10	0.80	0
2	M3L	T	27	2	10,11,12	0.52	0	9,14,16	0.53	0
2	M3L	E	27	2	10,11,12	0.49	0	9,14,16	0.59	0
2	AYA	B	21	2	6,7,8	0.98	0	5,8,10	0.86	0
2	M3L	d	27	2	10,11,12	0.55	0	9,14,16	0.49	0
2	M3L	J	27	2	10,11,12	0.54	0	9,14,16	0.52	0
2	AYA	S	21	2	6,7,8	1.23	1 (16%)	5,8,10	1.78	1 (20%)
2	M3L	O	27	2	10,11,12	0.53	0	9,14,16	0.45	0

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	AYA	D	21	2	-	0/4/6/8	-
2	AYA	Y	21	2	-	0/4/6/8	-
2	M3L	Z	27	2	-	0/9/10/12	-
2	AYA	R	21	2	-	0/4/6/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AYA	V	21	2	-	2/4/6/8	-
2	AYA	G	21	2	-	0/4/6/8	-
2	M3L	A	27	2	-	0/9/10/12	-
2	AYA	d	21	2	-	0/4/6/8	-
2	AYA	A	21	2	-	0/4/6/8	-
2	M3L	R	27	2	-	1/9/10/12	-
2	M3L	K	27	2	-	0/9/10/12	-
2	AYA	f	21	2	-	0/4/6/8	-
2	AYA	b	21	2	-	0/0/2/8	-
2	AYA	e	21	2	-	0/1/4/8	-
2	M3L	G	27	2	-	0/9/10/12	-
2	M3L	L	27	2	-	1/9/10/12	-
2	M3L	D	27	2	-	1/9/10/12	-
2	M3L	V	27	2	-	5/9/10/12	-
2	AYA	Z	21	2	-	0/4/6/8	-
2	M3L	g	27	2	-	0/9/10/12	-
2	M3L	Y	27	2	-	0/9/10/12	-
2	M3L	f	27	2	-	1/9/10/12	-
2	M3L	b	27	2	-	2/9/10/12	-
2	AYA	O	21	2	-	0/4/6/8	-
2	M3L	e	27	2	-	1/9/10/12	-
2	M3L	B	27	2	-	0/9/10/12	-
2	M3L	I	27	2	-	0/9/10/12	-
2	AYA	L	21	2	-	0/4/6/8	-
2	AYA	P	21	2	-	0/4/6/8	-
2	AYA	N	21	2	-	0/4/6/8	-
2	M3L	S	27	2	-	0/9/10/12	-
2	M3L	N	27	2	-	1/9/10/12	-
2	AYA	g	21	2	-	1/4/6/8	-
2	AYA	Q	21	2	-	0/1/4/8	-
2	AYA	K	21	2	-	0/4/6/8	-
2	M3L	c	27	2	-	0/9/10/12	-
2	AYA	C	21	2	-	0/4/6/8	-
2	M3L	H	27	2	-	1/9/10/12	-
2	AYA	M	21	2	-	0/4/6/8	-
2	AYA	T	21	2	-	0/4/6/8	-
2	AYA	a	21	2	-	0/4/6/8	-
2	M3L	P	27	2	-	1/9/10/12	-
2	AYA	J	21	2	-	0/4/6/8	-
2	AYA	c	21	2	-	1/1/4/8	-
2	M3L	a	27	2	-	1/9/10/12	-
2	AYA	E	21	2	-	0/4/6/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M3L	Q	27	2	-	0/9/10/12	-
2	AYA	I	21	2	-	0/4/6/8	-
2	AYA	H	21	2	-	0/4/6/8	-
2	M3L	C	27	2	-	0/9/10/12	-
2	M3L	F	27	2	-	0/9/10/12	-
2	M3L	M	27	2	-	0/9/10/12	-
2	AYA	F	21	2	-	0/4/6/8	-
2	M3L	T	27	2	-	1/9/10/12	-
2	M3L	E	27	2	-	0/9/10/12	-
2	AYA	B	21	2	-	0/4/6/8	-
2	M3L	d	27	2	-	0/9/10/12	-
2	M3L	J	27	2	-	0/9/10/12	-
2	AYA	S	21	2	-	0/4/6/8	-
2	M3L	O	27	2	-	0/9/10/12	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	21	AYA	CA-N	-2.97	1.43	1.46
2	T	21	AYA	CA-N	-2.91	1.43	1.46
2	f	21	AYA	CA-N	-2.90	1.43	1.46
2	c	21	AYA	CT-N	-2.85	1.39	1.46
2	e	21	AYA	CT-N	-2.85	1.39	1.46

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	21	AYA	CB-CA-N	4.24	114.32	109.61
2	G	21	AYA	CB-CA-N	4.14	114.21	109.61
2	S	21	AYA	CB-CA-N	3.63	113.64	109.61
2	M	21	AYA	CB-CA-N	3.34	113.33	109.61
2	A	21	AYA	CB-CA-N	3.30	113.28	109.61

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	27	M3L	O-C-CA-CB
2	H	27	M3L	O-C-CA-CB
2	L	27	M3L	O-C-CA-CB
2	N	27	M3L	O-C-CA-CB
2	P	27	M3L	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 130 ligands modelled in this entry, 130 are unknown - 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	AA	60/61 (98%)	-0.36	0 100 100	13, 19, 32, 49	0
1	AC	60/61 (98%)	-0.23	0 100 100	14, 22, 41, 48	0
1	BA	60/61 (98%)	-0.35	0 100 100	14, 20, 39, 52	0
1	BC	60/61 (98%)	-0.26	0 100 100	15, 23, 43, 48	0
1	CA	60/61 (98%)	-0.30	0 100 100	14, 19, 33, 50	0
1	CC	60/61 (98%)	-0.13	1 (1%) 70 66	15, 22, 40, 56	0
1	DA	60/61 (98%)	-0.12	0 100 100	14, 22, 46, 52	0
1	DC	61/61 (100%)	-0.09	2 (3%) 46 40	14, 20, 41, 53	0
1	EA	60/61 (98%)	-0.42	0 100 100	15, 20, 36, 49	0
1	EC	59/61 (96%)	-0.32	0 100 100	16, 23, 38, 46	0
1	FA	61/61 (100%)	-0.33	1 (1%) 72 68	15, 20, 33, 47	0
1	FC	59/61 (96%)	-0.30	0 100 100	16, 22, 37, 44	0
1	GA	60/61 (98%)	-0.36	0 100 100	16, 22, 36, 50	0
1	GC	59/61 (96%)	-0.29	0 100 100	16, 23, 37, 45	0
1	HA	60/61 (98%)	-0.39	0 100 100	15, 21, 34, 47	0
1	HC	59/61 (96%)	-0.24	0 100 100	17, 24, 40, 46	0
1	IA	60/61 (98%)	-0.23	0 100 100	22, 31, 43, 58	0
1	IC	60/61 (98%)	-0.19	1 (1%) 70 66	21, 29, 51, 54	0
1	JA	60/61 (98%)	-0.38	0 100 100	19, 23, 36, 51	0
1	JC	60/61 (98%)	-0.04	1 (1%) 70 66	21, 32, 51, 58	0
1	KA	59/61 (96%)	0.46	0 100 100	39, 50, 60, 69	0
1	KC	60/61 (98%)	0.18	2 (3%) 46 40	31, 46, 58, 61	0
1	LA	61/61 (100%)	-0.04	0 100 100	30, 37, 51, 59	0
1	LC	60/61 (98%)	0.06	1 (1%) 70 66	34, 41, 55, 64	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	MA	60/61 (98%)	0.23	2 (3%) 46 40	38, 43, 60, 67	0
1	MC	59/61 (96%)	0.27	0 100 100	38, 46, 59, 64	0
1	NA	60/61 (98%)	0.53	3 (5%) 28 23	42, 48, 68, 69	0
1	NC	59/61 (96%)	0.46	1 (1%) 70 66	43, 50, 59, 61	0
1	OA	60/61 (98%)	0.68	4 (6%) 17 14	44, 50, 62, 76	0
1	OC	59/61 (96%)	0.69	3 (5%) 28 22	45, 54, 63, 65	0
2	A	6/9 (66%)	-0.11	0 100 100	17, 21, 28, 45	0
2	B	6/9 (66%)	-0.26	0 100 100	15, 16, 26, 39	0
2	C	6/9 (66%)	-0.26	0 100 100	17, 21, 29, 45	0
2	D	6/9 (66%)	-0.41	0 100 100	17, 17, 28, 42	0
2	E	7/9 (77%)	0.19	1 (14%) 2 1	16, 22, 47, 62	0
2	F	6/9 (66%)	-0.13	0 100 100	15, 17, 26, 39	0
2	G	6/9 (66%)	-0.65	0 100 100	16, 22, 26, 43	0
2	H	6/9 (66%)	-0.02	0 100 100	17, 19, 28, 45	0
2	I	7/9 (77%)	0.27	1 (14%) 2 1	18, 24, 45, 58	0
2	J	6/9 (66%)	0.00	0 100 100	18, 19, 28, 41	0
2	K	7/9 (77%)	0.11	1 (14%) 2 1	17, 22, 46, 54	0
2	L	7/9 (77%)	0.61	1 (14%) 2 1	16, 18, 41, 60	0
2	M	6/9 (66%)	-0.28	0 100 100	19, 22, 33, 43	0
2	N	6/9 (66%)	-0.37	0 100 100	17, 18, 31, 41	0
2	O	7/9 (77%)	0.13	1 (14%) 2 1	17, 23, 44, 55	0
2	P	6/9 (66%)	-0.36	0 100 100	16, 19, 31, 44	0
2	Q	6/9 (66%)	-0.21	0 100 100	26, 31, 34, 48	0
2	R	6/9 (66%)	-0.40	0 100 100	21, 24, 35, 44	0
2	S	7/9 (77%)	-0.02	0 100 100	22, 28, 44, 48	0
2	T	6/9 (66%)	-0.20	0 100 100	22, 26, 42, 45	0
2	V	6/9 (66%)	0.67	0 100 100	50, 53, 54, 56	0
2	Y	6/9 (66%)	0.18	0 100 100	33, 36, 48, 54	0
2	Z	6/9 (66%)	0.38	0 100 100	33, 38, 51, 53	0
2	a	6/9 (66%)	0.76	1 (16%) 1 1	36, 40, 48, 57	0
2	b	6/9 (66%)	0.31	1 (16%) 1 1	40, 44, 48, 60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	c	5/9 (55%)	0.25	0 100 100	45, 46, 51, 52	0
2	d	6/9 (66%)	0.21	1 (16%) 1 1	47, 49, 53, 67	0
2	e	5/9 (55%)	0.59	0 100 100	48, 49, 53, 60	0
2	f	6/9 (66%)	0.35	0 100 100	49, 54, 57, 58	0
2	g	6/9 (66%)	0.82	1 (16%) 1 1	46, 51, 59, 71	0
All	All	1979/2100 (94%)	-0.05	31 (1%) 72 68	13, 29, 56, 76	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DC	27	GLY	4.8
2	L	29	ALA	4.6
1	MA	85	GLY	4.6
2	a	28	SER	4.1
1	NA	83	LEU	3.7

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	AYA	g	21	8/9	0.77	0.37	58,62,66,70	0
2	M3L	g	27	12/13	0.80	0.18	55,59,68,69	0
2	M3L	V	27	12/13	0.82	0.17	52,57,59,63	0
2	M3L	e	27	12/13	0.82	0.21	55,60,68,70	0
2	M3L	f	27	12/13	0.83	0.16	53,56,61,61	0
2	AYA	Y	21	8/9	0.83	0.28	46,52,56,57	0
2	AYA	Q	21	6/9	0.83	0.15	37,43,44,50	0
2	M3L	c	27	12/13	0.84	0.18	53,56,63,70	0
2	AYA	a	21	8/9	0.85	0.16	42,46,57,57	0
2	AYA	e	21	6/9	0.88	0.14	58,61,62,65	0
2	AYA	V	21	8/9	0.89	0.26	53,57,64,65	0
2	M3L	a	27	12/13	0.89	0.13	42,47,50,50	0
2	M3L	d	27	12/13	0.90	0.14	50,54,57,58	0
2	M3L	Z	27	12/13	0.90	0.11	33,39,50,51	0
2	M3L	A	27	12/13	0.91	0.12	16,21,35,35	0
2	M3L	Y	27	12/13	0.91	0.14	35,41,47,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AYA	b	21	5/9	0.92	0.16	47,50,53,56	0
2	AYA	c	21	6/9	0.92	0.11	51,55,58,61	0
2	M3L	E	27	12/13	0.92	0.12	17,21,33,34	0
2	AYA	d	21	8/9	0.92	0.19	52,57,63,64	0
2	AYA	O	21	8/9	0.92	0.10	25,28,33,36	0
2	AYA	C	21	8/9	0.92	0.11	25,28,32,34	0
2	AYA	Z	21	8/9	0.92	0.15	41,48,51,53	0
2	AYA	f	21	8/9	0.92	0.18	49,56,61,62	0
2	AYA	R	21	8/9	0.92	0.12	25,30,39,40	0
2	M3L	T	27	12/13	0.92	0.10	29,34,37,39	0
2	M3L	C	27	12/13	0.92	0.10	20,22,32,42	0
2	M3L	R	27	12/13	0.93	0.12	22,23,31,34	0
2	M3L	b	27	12/13	0.93	0.11	46,48,54,55	0
2	M3L	H	27	12/13	0.93	0.09	18,21,27,36	0
2	M3L	O	27	12/13	0.93	0.12	18,22,30,34	0
2	AYA	M	21	8/9	0.93	0.14	26,28,32,33	0
2	M3L	M	27	12/13	0.93	0.10	21,24,30,34	0
2	M3L	G	27	12/13	0.94	0.10	19,21,26,28	0
2	M3L	N	27	12/13	0.94	0.10	17,22,27,28	0
2	AYA	A	21	8/9	0.94	0.10	20,26,30,31	0
2	AYA	I	21	8/9	0.94	0.09	25,27,33,34	0
2	M3L	P	27	12/13	0.94	0.09	21,23,28,29	0
2	M3L	I	27	12/13	0.94	0.09	18,23,29,33	0
2	M3L	J	27	12/13	0.94	0.10	19,22,28,31	0
2	AYA	K	21	8/9	0.94	0.11	21,25,32,34	0
2	M3L	S	27	12/13	0.94	0.11	21,25,35,35	0
2	AYA	G	21	8/9	0.94	0.10	26,31,34,40	0
2	AYA	E	21	8/9	0.95	0.11	21,27,32,35	0
2	M3L	K	27	12/13	0.95	0.11	20,22,32,36	0
2	M3L	L	27	12/13	0.95	0.10	19,21,26,27	0
2	M3L	D	27	12/13	0.95	0.09	18,21,26,26	0
2	M3L	F	27	12/13	0.95	0.10	17,20,26,28	0
2	M3L	Q	27	12/13	0.95	0.09	31,33,38,39	0
2	M3L	B	27	12/13	0.96	0.10	18,20,26,26	0
2	AYA	S	21	8/9	0.96	0.11	29,33,39,40	0
2	AYA	N	21	8/9	0.96	0.09	17,21,24,27	0
2	AYA	H	21	8/9	0.96	0.09	18,20,23,25	0
2	AYA	L	21	8/9	0.97	0.08	16,19,22,22	0
2	AYA	B	21	8/9	0.97	0.12	16,19,21,22	0
2	AYA	D	21	8/9	0.97	0.08	17,20,23,26	0
2	AYA	J	21	8/9	0.97	0.09	16,18,19,21	0
2	AYA	P	21	8/9	0.98	0.08	17,19,20,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AYA	F	21	8/9	0.98	0.11	17,17,19,20	0
2	AYA	T	21	8/9	0.98	0.07	20,24,26,27	0

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
3	UNX	IC	101	1/1	0.15	0.39	38,38,38,38	0
3	UNX	CA	102	1/1	0.41	0.49	41,41,41,41	0
3	UNX	AA	102	1/1	0.52	0.42	41,41,41,41	0
3	UNX	EA	103	1/1	0.64	0.17	38,38,38,38	0
3	UNX	HC	101	1/1	0.65	0.30	32,32,32,32	0
3	UNX	JA	103	1/1	0.68	0.22	34,34,34,34	0
3	UNX	D	101	1/1	0.68	0.31	46,46,46,46	0
3	UNX	NA	102	1/1	0.73	0.26	44,44,44,44	0
3	UNX	CA	101	1/1	0.73	0.20	43,43,43,43	0
3	UNX	O	101	1/1	0.73	0.26	31,31,31,31	0
3	UNX	M	101	1/1	0.74	0.23	34,34,34,34	0
3	UNX	FC	107	1/1	0.74	0.28	31,31,31,31	0
3	UNX	EC	104	1/1	0.76	0.21	30,30,30,30	0
3	UNX	EA	104	1/1	0.76	0.22	27,27,27,27	0
3	UNX	OA	101	1/1	0.76	0.27	40,40,40,40	0
3	UNX	HA	101	1/1	0.77	0.16	31,31,31,31	0
3	UNX	F	102	1/1	0.77	0.11	32,32,32,32	0
3	UNX	BA	107	1/1	0.78	0.16	28,28,28,28	0
3	UNX	JC	101	1/1	0.78	0.19	33,33,33,33	0
3	UNX	DC	103	1/1	0.79	0.14	29,29,29,29	0
3	UNX	NA	101	1/1	0.79	0.17	43,43,43,43	0
3	UNX	AA	104	1/1	0.79	0.20	37,37,37,37	0
3	UNX	CC	103	1/1	0.79	0.23	39,39,39,39	0
3	UNX	S	101	1/1	0.79	0.18	35,35,35,35	0
3	UNX	AA	103	1/1	0.81	0.16	21,21,21,21	0
3	UNX	BC	103	1/1	0.81	0.11	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UNX	B	101	1/1	0.81	0.29	27,27,27,27	0
3	UNX	CA	105	1/1	0.81	0.12	20,20,20,20	0
3	UNX	BA	106	1/1	0.82	0.11	31,31,31,31	0
3	UNX	M	102	1/1	0.82	0.27	31,31,31,31	0
3	UNX	HA	105	1/1	0.82	0.13	33,33,33,33	0
3	UNX	O	102	1/1	0.82	0.12	34,34,34,34	0
3	UNX	GA	103	1/1	0.82	0.15	30,30,30,30	0
3	UNX	HC	102	1/1	0.83	0.13	34,34,34,34	0
3	UNX	A	101	1/1	0.83	0.12	30,30,30,30	0
3	UNX	KA	101	1/1	0.83	0.13	36,36,36,36	0
3	UNX	FC	104	1/1	0.83	0.15	36,36,36,36	0
3	UNX	FC	102	1/1	0.83	0.16	32,32,32,32	0
3	UNX	NC	101	1/1	0.84	0.24	46,46,46,46	0
3	UNX	FC	101	1/1	0.84	0.13	35,35,35,35	0
3	UNX	OC	101	1/1	0.84	0.19	47,47,47,47	0
3	UNX	AC	102	1/1	0.84	0.13	33,33,33,33	0
3	UNX	FC	103	1/1	0.84	0.14	24,24,24,24	0
3	UNX	DC	102	1/1	0.84	0.14	32,32,32,32	0
3	UNX	J	101	1/1	0.85	0.18	27,27,27,27	0
3	UNX	S	102	1/1	0.85	0.24	35,35,35,35	0
3	UNX	AA	106	1/1	0.86	0.10	36,36,36,36	0
3	UNX	AC	103	1/1	0.86	0.12	35,35,35,35	0
3	UNX	HC	107	1/1	0.86	0.13	30,30,30,30	0
3	UNX	CA	103	1/1	0.86	0.12	24,24,24,24	0
3	UNX	EA	102	1/1	0.86	0.19	32,32,32,32	0
3	UNX	HA	102	1/1	0.86	0.12	35,35,35,35	0
3	UNX	BA	101	1/1	0.86	0.13	24,24,24,24	0
3	UNX	LA	102	1/1	0.86	0.17	32,32,32,32	0
3	UNX	CC	102	1/1	0.87	0.20	35,35,35,35	0
3	UNX	BA	102	1/1	0.87	0.11	23,23,23,23	0
3	UNX	DA	104	1/1	0.87	0.19	33,33,33,33	0
3	UNX	CC	101	1/1	0.88	0.12	34,34,34,34	0
3	UNX	DA	105	1/1	0.88	0.17	32,32,32,32	0
3	UNX	FA	103	1/1	0.88	0.18	23,23,23,23	0
3	UNX	K	101	1/1	0.88	0.19	30,30,30,30	0
3	UNX	IA	102	1/1	0.88	0.19	33,33,33,33	0
3	UNX	HC	104	1/1	0.89	0.18	38,38,38,38	0
3	UNX	CA	106	1/1	0.89	0.14	30,30,30,30	0
3	UNX	EC	101	1/1	0.89	0.15	39,39,39,39	0
3	UNX	EC	103	1/1	0.89	0.12	33,33,33,33	0
3	UNX	BC	102	1/1	0.89	0.22	35,35,35,35	0
3	UNX	EA	105	1/1	0.90	0.11	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UNX	MA	101	1/1	0.90	0.24	38,38,38,38	0
3	UNX	FC	105	1/1	0.90	0.23	27,27,27,27	0
3	UNX	CA	107	1/1	0.90	0.14	33,33,33,33	0
3	UNX	NA	103	1/1	0.90	0.13	37,37,37,37	0
3	UNX	JA	102	1/1	0.90	0.17	34,34,34,34	0
3	UNX	N	102	1/1	0.90	0.14	29,29,29,29	0
3	UNX	DA	101	1/1	0.90	0.22	27,27,27,27	0
3	UNX	JA	106	1/1	0.90	0.16	27,27,27,27	0
3	UNX	EA	101	1/1	0.90	0.20	29,29,29,29	0
3	UNX	HC	105	1/1	0.90	0.30	30,30,30,30	0
3	UNX	BA	105	1/1	0.91	0.16	31,31,31,31	0
3	UNX	OA	102	1/1	0.91	0.17	45,45,45,45	0
3	UNX	H	102	1/1	0.91	0.20	28,28,28,28	0
3	UNX	EC	102	1/1	0.91	0.18	27,27,27,27	0
3	UNX	JA	104	1/1	0.91	0.20	33,33,33,33	0
3	UNX	EC	108	1/1	0.91	0.18	32,32,32,32	0
3	UNX	J	102	1/1	0.92	0.16	31,31,31,31	0
3	UNX	BA	103	1/1	0.92	0.14	25,25,25,25	0
3	UNX	CA	104	1/1	0.92	0.10	24,24,24,24	0
3	UNX	JA	101	1/1	0.92	0.15	27,27,27,27	0
3	UNX	GA	101	1/1	0.92	0.18	25,25,25,25	0
3	UNX	F	101	1/1	0.92	0.12	29,29,29,29	0
3	UNX	LA	101	1/1	0.92	0.38	38,38,38,38	0
3	UNX	IA	101	1/1	0.92	0.20	28,28,28,28	0
3	UNX	LC	101	1/1	0.92	0.22	37,37,37,37	0
3	UNX	H	101	1/1	0.93	0.11	17,17,17,17	0
3	UNX	BA	104	1/1	0.93	0.08	28,28,28,28	0
3	UNX	HA	104	1/1	0.93	0.09	23,23,23,23	0
3	UNX	MC	101	1/1	0.93	0.12	40,40,40,40	0
3	UNX	DC	101	1/1	0.93	0.10	21,21,21,21	0
3	UNX	AA	105	1/1	0.93	0.15	29,29,29,29	0
3	UNX	EA	106	1/1	0.94	0.08	24,24,24,24	0
3	UNX	GC	101	1/1	0.94	0.11	22,22,22,22	0
3	UNX	FA	101	1/1	0.94	0.09	28,28,28,28	0
3	UNX	L	101	1/1	0.94	0.15	20,20,20,20	0
3	UNX	EC	105	1/1	0.94	0.09	22,22,22,22	0
3	UNX	HC	108	1/1	0.94	0.15	24,24,24,24	0
3	UNX	N	101	1/1	0.94	0.19	30,30,30,30	0
3	UNX	EC	106	1/1	0.94	0.11	28,28,28,28	0
3	UNX	JC	102	1/1	0.94	0.21	24,24,24,24	0
3	UNX	F	103	1/1	0.94	0.18	26,26,26,26	0
3	UNX	EC	107	1/1	0.94	0.10	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UNX	GA	102	1/1	0.94	0.09	32,32,32,32	0
3	UNX	AC	101	1/1	0.95	0.10	21,21,21,21	0
3	UNX	HC	103	1/1	0.95	0.16	30,30,30,30	0
3	UNX	IA	103	1/1	0.95	0.07	31,31,31,31	0
3	UNX	KC	101	1/1	0.95	0.19	43,43,43,43	0
3	UNX	AA	107	1/1	0.96	0.10	27,27,27,27	0
3	UNX	J	103	1/1	0.96	0.15	19,19,19,19	0
3	UNX	DA	103	1/1	0.96	0.13	16,16,16,16	0
3	UNX	BC	101	1/1	0.96	0.25	12,12,12,12	0
3	UNX	JA	105	1/1	0.97	0.14	26,26,26,26	0
3	UNX	FA	102	1/1	0.97	0.17	14,14,14,14	0
3	UNX	G	101	1/1	0.97	0.16	18,18,18,18	0
3	UNX	I	101	1/1	0.98	0.13	14,14,14,14	0
3	UNX	CC	104	1/1	0.98	0.17	15,15,15,15	0
3	UNX	HA	103	1/1	0.98	0.10	19,19,19,19	0
3	UNX	FC	106	1/1	0.98	0.14	13,13,13,13	0
3	UNX	AA	101	1/1	0.98	0.23	10,10,10,10	0
3	UNX	HC	106	1/1	0.98	0.08	19,19,19,19	0
3	UNX	DA	102	1/1	0.98	0.19	14,14,14,14	0
3	UNX	CC	105	1/1	0.99	0.08	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.