



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:13 AM UTC

PDB ID : 6YN1 / pdb_00006yn1
Title : Crystal structure of histone chaperone APLF acidic domain bound to the histone H2A-H2B-H3-H4 octamer
Authors : Corbeski, I.; Guo, X.; Van Ingen, H.; Sixma, T.K.
Deposited on : 2020-04-10
Resolution : 2.35 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	:	4-5-2 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

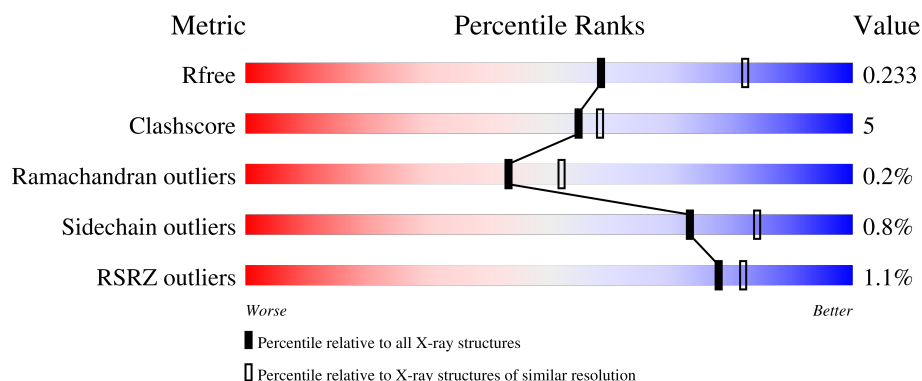
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

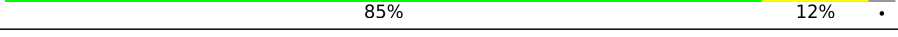
The reported resolution of this entry is 2.35 Å.

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.



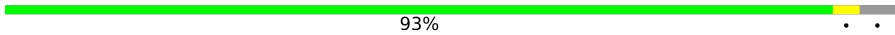
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	107	
1	F	107	
1	K	107	
1	P	107	
1	U	107	

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Mol	Chain	Length	Quality of chain
1	Z	107	
1	e	107	
1	j	107	
2	B	100	
2	G	100	
2	L	100	
2	Q	100	
2	V	100	
2	a	100	
2	f	100	
2	k	100	
3	C	99	
3	H	99	
3	M	99	
3	R	99	
3	W	99	
3	b	99	
3	g	99	
3	l	99	
4	D	84	
4	I	84	
4	N	84	
4	S	84	
4	X	84	
4	c	84	

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Mol	Chain	Length	Quality of chain
4	h	84	 2% 75% 14% 11%
4	m	84	 81% 8% 11%
5	E	43	 2% 51% 49%
5	J	43	 5% 60% 5% 33%
5	O	43	 2% 49% 51%
5	T	43	 2% 49% 49%
5	Y	43	 2% 42% 9% 49%
5	d	43	 2% 42% 5% 53%
5	i	43	 2% 44% 51%
5	n	43	 37% 9% 53%

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
6	GOL	c	201	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24986 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	0	0	0
			795	501	155	139			
1	F	103	Total	C	N	O	0	0	0
			795	501	155	139			
1	K	103	Total	C	N	O	0	0	0
			795	501	155	139			
1	P	104	Total	C	N	O	0	0	0
			804	507	157	140			
1	U	103	Total	C	N	O	0	0	0
			795	501	155	139			
1	Z	103	Total	C	N	O	0	0	0
			795	501	155	139			
1	e	102	Total	C	N	O	0	0	0
			786	495	153	138			
1	j	103	Total	C	N	O	0	0	0
			795	501	155	139			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP Q6AZJ8
F	12	MET	-	initiating methionine	UNP Q6AZJ8
K	12	MET	-	initiating methionine	UNP Q6AZJ8
P	12	MET	-	initiating methionine	UNP Q6AZJ8
U	12	MET	-	initiating methionine	UNP Q6AZJ8
Z	12	MET	-	initiating methionine	UNP Q6AZJ8
e	12	MET	-	initiating methionine	UNP Q6AZJ8
j	12	MET	-	initiating methionine	UNP Q6AZJ8

- Molecule 2 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	90	Total	C	N	O	S	0	1	0
			708	449	123	134	2			
2	G	88	Total	C	N	O	S	0	1	0
			697	442	122	131	2			
2	L	88	Total	C	N	O	S	0	0	0
			685	433	121	129	2			
2	Q	88	Total	C	N	O	S	0	0	0
			685	433	121	129	2			
2	V	89	Total	C	N	O	S	0	0	0
			694	438	122	132	2			
2	a	89	Total	C	N	O	S	0	1	0
			703	446	122	133	2			
2	f	88	Total	C	N	O	S	0	0	0
			685	433	121	129	2			
2	k	88	Total	C	N	O	S	0	0	0
			685	433	121	129	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	MET	-	initiating methionine	UNP A0A1L8FQA5
G	26	MET	-	initiating methionine	UNP A0A1L8FQA5
L	26	MET	-	initiating methionine	UNP A0A1L8FQA5
Q	26	MET	-	initiating methionine	UNP A0A1L8FQA5
V	26	MET	-	initiating methionine	UNP A0A1L8FQA5
a	26	MET	-	initiating methionine	UNP A0A1L8FQA5
f	26	MET	-	initiating methionine	UNP A0A1L8FQA5
k	26	MET	-	initiating methionine	UNP A0A1L8FQA5

- Molecule 3 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	94	Total	C	N	O	S	0	0	0
			774	489	147	135	3			
3	H	94	Total	C	N	O	S	0	0	0
			774	489	147	135	3			
3	M	95	Total	C	N	O	S	0	0	0
			784	495	150	136	3			
3	R	94	Total	C	N	O	S	0	0	0
			774	489	147	135	3			
3	W	94	Total	C	N	O	S	0	0	0
			774	489	147	135	3			
3	b	96	Total	C	N	O	S	0	0	0
			790	498	152	137	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	g	94	Total	C	N	O	S	0	0	0
			774	489	147	135	3			
3	l	94	Total	C	N	O	S	0	0	0
			774	489	147	135	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	37	MET	-	initiating methionine	UNP A0A310TTQ1
H	37	MET	-	initiating methionine	UNP A0A310TTQ1
M	37	MET	-	initiating methionine	UNP A0A310TTQ1
R	37	MET	-	initiating methionine	UNP A0A310TTQ1
W	37	MET	-	initiating methionine	UNP A0A310TTQ1
b	37	MET	-	initiating methionine	UNP A0A310TTQ1
g	37	MET	-	initiating methionine	UNP A0A310TTQ1
l	37	MET	-	initiating methionine	UNP A0A310TTQ1

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	76	Total	C	N	O	S	0	0	0
			606	385	117	103	1			
4	I	76	Total	C	N	O	S	0	0	0
			606	385	117	103	1			
4	N	75	Total	C	N	O	S	0	0	0
			602	383	116	102	1			
4	S	77	Total	C	N	O	S	0	0	0
			614	389	119	105	1			
4	X	77	Total	C	N	O	S	0	0	0
			618	391	119	107	1			
4	c	76	Total	C	N	O	S	0	0	0
			610	387	118	104	1			
4	h	75	Total	C	N	O	S	0	0	0
			602	383	116	102	1			
4	m	75	Total	C	N	O	S	0	0	0
			598	379	116	102	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	19	MET	-	initiating methionine	UNP P62799
I	19	MET	-	initiating methionine	UNP P62799

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Chain	Residue	Modelled	Actual	Comment	Reference
N	19	MET	-	initiating methionine	UNP P62799
S	19	MET	-	initiating methionine	UNP P62799
X	19	MET	-	initiating methionine	UNP P62799
c	19	MET	-	initiating methionine	UNP P62799
h	19	MET	-	initiating methionine	UNP P62799
m	19	MET	-	initiating methionine	UNP P62799

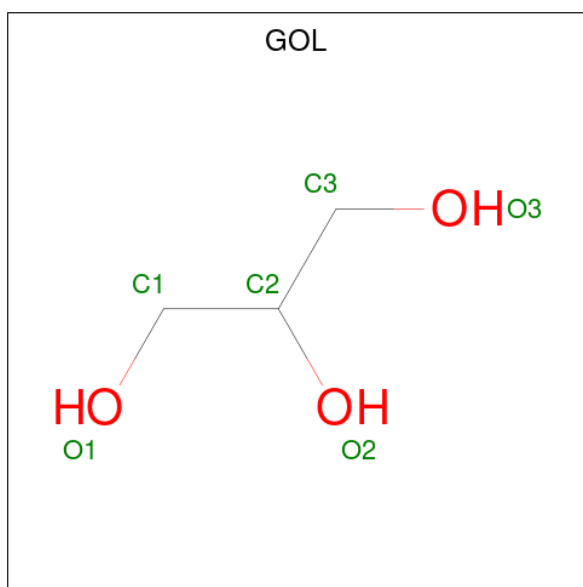
- Molecule 5 is a protein called Aprataxin and PNK-like factor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	22	Total	C	N	O	0	0	0
			188	114	25	49			
5	J	29	Total	C	N	O	0	0	0
			248	150	32	66			
5	O	21	Total	C	N	O	0	0	0
			179	109	24	46			
5	T	22	Total	C	N	O	0	0	0
			188	114	25	49			
5	Y	22	Total	C	N	O	0	0	0
			188	114	25	49			
5	d	20	Total	C	N	O	0	0	0
			170	104	23	43			
5	i	21	Total	C	N	O	0	0	0
			179	109	24	46			
5	n	20	Total	C	N	O	0	0	0
			170	104	24	42			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	448	GLY	-	expression tag	UNP Q8IW19
J	448	GLY	-	expression tag	UNP Q8IW19
O	448	GLY	-	expression tag	UNP Q8IW19
T	448	GLY	-	expression tag	UNP Q8IW19
Y	448	GLY	-	expression tag	UNP Q8IW19
d	448	GLY	-	expression tag	UNP Q8IW19
i	448	GLY	-	expression tag	UNP Q8IW19
n	448	GLY	-	expression tag	UNP Q8IW19

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	K	1	Total	C	O	0	0
			6	3	3		
6	N	1	Total	C	O	0	0
			6	3	3		
6	P	1	Total	C	O	0	0
			6	3	3		
6	S	1	Total	C	O	0	0
			6	3	3		
6	U	1	Total	C	O	0	0
			6	3	3		
6	b	1	Total	C	O	0	0
			6	3	3		
6	c	1	Total	C	O	0	0
			6	3	3		
6	e	1	Total	C	O	0	0
			6	3	3		
6	h	1	Total	C	O	0	0
			6	3	3		
6	j	1	Total	C	O	0	0
			6	3	3		
6	j	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	1	Total Cl 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	16	Total O 16 16	0	0
8	B	10	Total O 10 10	0	0
8	C	14	Total O 14 14	0	0
8	D	13	Total O 13 13	0	0
8	E	1	Total O 1 1	0	0
8	F	17	Total O 17 17	0	0
8	G	7	Total O 7 7	0	0
8	H	19	Total O 19 19	0	0
8	I	13	Total O 13 13	0	0
8	J	4	Total O 4 4	0	0
8	K	10	Total O 10 10	0	0
8	L	10	Total O 10 10	0	0
8	M	23	Total O 23 23	0	0
8	N	6	Total O 6 6	0	0
8	O	1	Total O 1 1	0	0
8	P	10	Total O 10 10	0	0
8	Q	5	Total O 5 5	0	0
8	R	19	Total O 19 19	0	0

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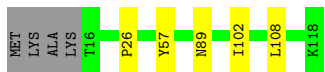
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	S	7	Total 7	O 7	0	0
8	U	16	Total 16	O 16	0	0
8	V	6	Total 6	O 6	0	0
8	W	19	Total 19	O 19	0	0
8	X	13	Total 13	O 13	0	0
8	Y	2	Total 2	O 2	0	0
8	Z	9	Total 9	O 9	0	0
8	a	6	Total 6	O 6	0	0
8	b	25	Total 25	O 25	0	0
8	c	7	Total 7	O 7	0	0
8	d	2	Total 2	O 2	0	0
8	e	8	Total 8	O 8	0	0
8	f	3	Total 3	O 3	0	0
8	g	25	Total 25	O 25	0	0
8	h	9	Total 9	O 9	0	0
8	i	1	Total 1	O 1	0	0
8	j	15	Total 15	O 15	0	0
8	k	8	Total 8	O 8	0	0
8	l	18	Total 18	O 18	0	0
8	m	18	Total 18	O 18	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.

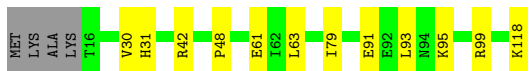
- Molecule 1: Histone H2A

Chain A:  92% 5% .



- Molecule 1: Histone H2A

Chain F:  85% 11% .



- Molecule 1: Histone H2A

Chain K:  90% 7% .



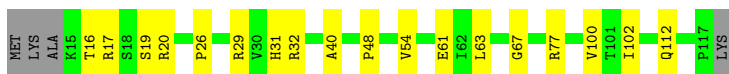
- Molecule 1: Histone H2A

Chain P:  85% 12% .



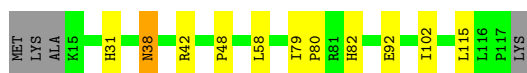
- Molecule 1: Histone H2A

Chain U:  79% 17% .



- Molecule 1: Histone H2A

Chain Z:  86% 9% . .



- Molecule 1: Histone H2A

Chain e: 82% 13% 5%



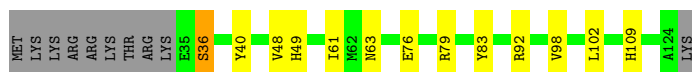
- Molecule 1: Histone H2A

Chain j: 93% . .



- Molecule 2: Histone H2B

Chain B: 77% 12% . 10%



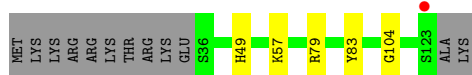
- Molecule 2: Histone H2B

Chain G: 72% 16% 12%



- Molecule 2: Histone H2B

Chain L: 83% 5% 12%



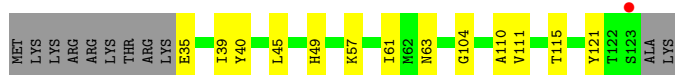
- Molecule 2: Histone H2B

Chain Q: 78% 10% 12%

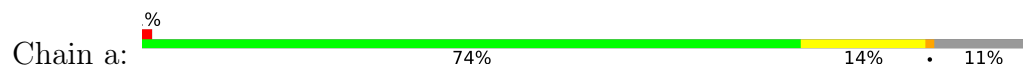


- Molecule 2: Histone H2B

Chain V: 76% 13% 11%



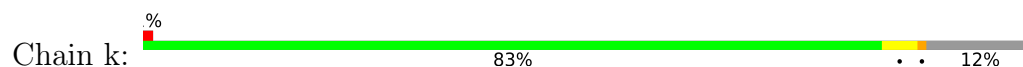
• Molecule 2: Histone H2B



• Molecule 2: Histone H2B



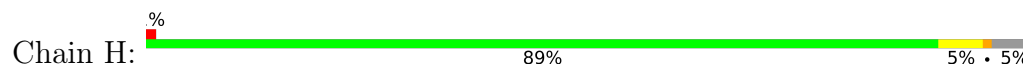
• Molecule 2: Histone H2B



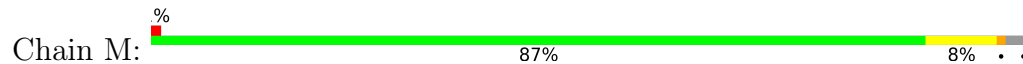
• Molecule 3: Histone H3



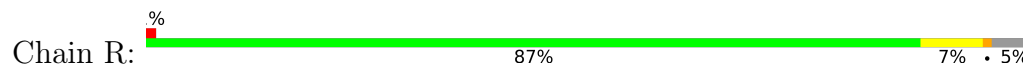
• Molecule 3: Histone H3



• Molecule 3: Histone H3



• Molecule 3: Histone H3





• Molecule 3: Histone H3

Chain W: 88% 7% 5%



• Molecule 3: Histone H3

Chain b: 84% 10% 6%



• Molecule 3: Histone H3

Chain g: 86% 9% 5%



• Molecule 3: Histone H3

Chain l: 84% 11% 5%



• Molecule 4: Histone H4

Chain D: 79% 12% 10%



• Molecule 4: Histone H4

Chain I: 81% 10% 10%



• Molecule 4: Histone H4

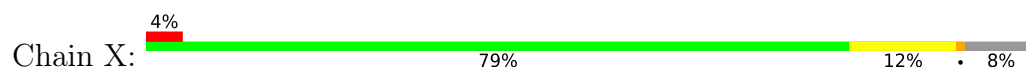
Chain N: 85% 5% 11%



- Molecule 4: Histone H4



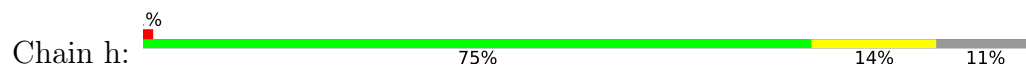
- Molecule 4: Histone H4



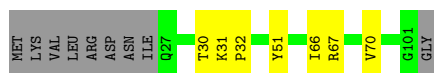
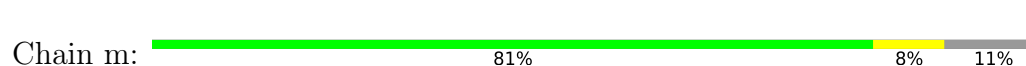
- Molecule 4: Histone H4



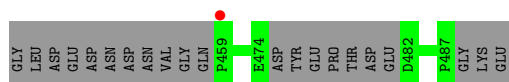
- Molecule 4: Histone H4



- Molecule 4: Histone H4

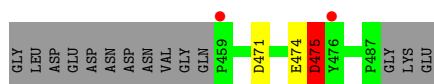


- Molecule 5: Aprataxin and PNK-like factor

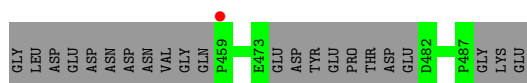


- Molecule 5: Aprataxin and PNK-like factor





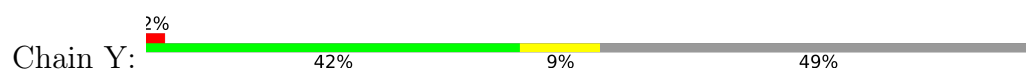
- Molecule 5: Aprataxin and PNK-like factor



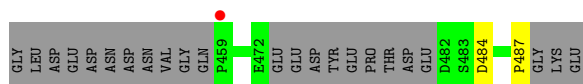
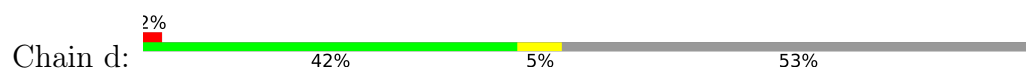
- Molecule 5: Aprataxin and PNK-like factor



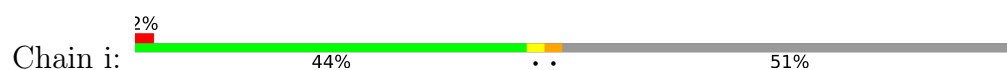
- Molecule 5: Aprataxin and PNK-like factor



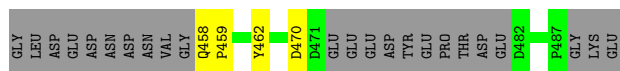
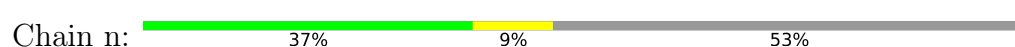
- Molecule 5: Aprataxin and PNK-like factor



- Molecule 5: Aprataxin and PNK-like factor



- Molecule 5: Aprataxin and PNK-like factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.22Å 189.69Å 204.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.35 19.99 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.35) 99.8 (19.99-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.19Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.177 , 0.233 0.177 , 0.233	Depositor DCC
R_{free} test set	10078 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.6	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	0.97	EDS
Total number of atoms	24986	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: CL, GOL

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	0.58	0/805	0.63	0/1088
1	F	0.35	0/805	0.53	0/1088
1	K	0.42	0/805	0.55	0/1088
1	P	0.38	0/814	0.56	0/1099
1	U	0.35	0/805	0.48	0/1088
1	Z	0.35	0/805	0.52	0/1088
1	e	0.40	0/796	0.51	0/1077
1	j	0.40	0/805	0.53	0/1088
2	B	0.58	0/723	0.63	1/976 (0.1%)
2	G	0.58	0/709	0.50	0/957
2	L	0.67	0/696	0.60	0/939
2	Q	0.54	0/696	0.54	0/939
2	V	0.45	0/705	0.55	0/951
2	a	0.61	0/718	0.60	0/969
2	f	0.66	0/696	0.57	0/939
2	k	0.55	0/696	0.68	0/939
3	C	0.38	0/784	0.58	0/1052
3	H	0.40	0/784	0.62	0/1052
3	M	0.38	0/795	0.55	0/1067
3	R	0.37	0/784	0.62	0/1052
3	W	0.36	0/784	0.58	0/1052
3	b	0.43	0/800	0.60	0/1073
3	g	0.37	0/784	0.56	0/1052
3	l	0.36	0/784	0.57	0/1052
4	D	0.38	0/613	0.55	0/821
4	I	0.39	0/613	0.51	0/821
4	N	0.34	0/609	0.53	0/816
4	S	0.42	0/621	0.59	0/832
4	X	0.41	0/625	0.64	0/838
4	c	0.37	0/617	0.55	0/827
4	h	0.40	0/609	0.54	0/816
4	m	0.35	0/605	0.52	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	E	0.28	0/192	0.40	0/260
5	J	0.71	0/255	0.77	1/349 (0.3%)
5	O	0.27	0/183	0.38	0/248
5	T	0.57	0/192	0.51	0/260
5	Y	0.31	0/192	0.53	0/260
5	d	0.63	0/174	0.65	0/236
5	i	0.71	0/183	0.69	1/248 (0.4%)
5	n	0.78	0/174	0.88	0/237
All	All	0.46	0/24835	0.57	3/33444 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	i	472	GLU	N-CA-C	-6.08	105.99	113.41
5	J	475	ASP	N-CA-C	-5.96	104.14	112.12
2	B	36	SER	N-CA-C	5.57	117.71	108.13

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	795	0	846	4	0
1	F	795	0	846	10	0
1	K	795	0	846	5	0
1	P	804	0	859	11	0
1	U	795	0	846	16	1
1	Z	795	0	846	10	0
1	e	786	0	833	12	0
1	j	795	0	846	2	0
2	B	708	0	723	12	0
2	G	697	0	711	13	0
2	L	685	0	703	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	685	0	703	6	0
2	V	694	0	709	11	0
2	a	703	0	718	14	0
2	f	685	0	703	14	0
2	k	685	0	703	5	0
3	C	774	0	813	9	0
3	H	774	0	813	7	0
3	M	784	0	820	7	0
3	R	774	0	813	10	0
3	W	774	0	813	6	0
3	b	790	0	831	14	0
3	g	774	0	813	10	0
3	l	774	0	813	11	1
4	D	606	0	650	12	0
4	I	606	0	650	7	0
4	N	602	0	647	5	0
4	S	614	0	656	13	0
4	X	618	0	657	12	0
4	c	610	0	653	16	0
4	h	602	0	647	10	0
4	m	598	0	639	5	0
5	E	188	0	139	0	0
5	J	248	0	183	3	0
5	O	179	0	133	0	0
5	T	188	0	139	3	0
5	Y	188	0	139	3	0
5	d	170	0	127	2	0
5	i	179	0	133	1	0
5	n	170	0	128	4	0
6	A	6	0	8	0	0
6	D	6	0	8	0	0
6	H	6	0	8	0	0
6	K	6	0	8	1	0
6	N	6	0	8	2	0
6	P	6	0	8	0	0
6	S	6	0	8	1	0
6	U	6	0	8	2	0
6	b	6	0	8	0	0
6	c	6	0	8	4	0
6	e	6	0	8	1	0
6	h	6	0	8	3	0
6	j	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	1	0	0	0	0
8	A	16	0	0	0	0
8	B	10	0	0	0	0
8	C	14	0	0	0	0
8	D	13	0	0	0	0
8	E	1	0	0	0	0
8	F	17	0	0	0	0
8	G	7	0	0	0	0
8	H	19	0	0	0	0
8	I	13	0	0	0	0
8	J	4	0	0	0	0
8	K	10	0	0	0	0
8	L	10	0	0	0	0
8	M	23	0	0	0	0
8	N	6	0	0	0	0
8	O	1	0	0	0	0
8	P	10	0	0	0	0
8	Q	5	0	0	0	0
8	R	19	0	0	0	0
8	S	7	0	0	0	0
8	U	16	0	0	0	0
8	V	6	0	0	0	0
8	W	19	0	0	0	0
8	X	13	0	0	0	0
8	Y	2	0	0	0	0
8	Z	9	0	0	0	0
8	a	6	0	0	0	0
8	b	25	0	0	1	0
8	c	7	0	0	0	0
8	d	2	0	0	0	0
8	e	8	0	0	0	0
8	f	3	0	0	0	0
8	g	25	0	0	2	0
8	h	9	0	0	0	0
8	i	1	0	0	0	0
8	j	15	0	0	0	0
8	k	8	0	0	0	0
8	l	18	0	0	0	0
8	m	18	0	0	0	0
All	All	24986	0	25402	239	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 239 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)
4:D:84:MET:CE	4:D:101:GLY:HA3	1.88	1.02
2:k:86:ARG:HG2	2:k:86:ARG:HH21	1.27	0.98
4:X:26:ILE:CD1	4:X:59:LYS:HB2	2.06	0.85
4:D:84:MET:HE2	4:D:101:GLY:HA3	1.59	0.83
1:F:118:LYS:N	1:F:118:LYS:HD3	1.97	0.79

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:61:GLU:OE1	3:l:42:ARG:NH1[2_555]	1.80	0.40

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	A	101/107 (94%)	100 (99%)	1 (1%)	0	100	100
1	F	101/107 (94%)	99 (98%)	2 (2%)	0	100	100
1	K	101/107 (94%)	99 (98%)	2 (2%)	0	100	100
1	P	102/107 (95%)	100 (98%)	2 (2%)	0	100	100
1	U	101/107 (94%)	99 (98%)	2 (2%)	0	100	100
1	Z	101/107 (94%)	97 (96%)	4 (4%)	0	100	100
1	e	100/107 (94%)	96 (96%)	4 (4%)	0	100	100
1	j	101/107 (94%)	99 (98%)	2 (2%)	0	100	100
2	B	89/100 (89%)	88 (99%)	1 (1%)	0	100	100
2	G	87/100 (87%)	86 (99%)	0	1 (1%)	11	11
2	L	86/100 (86%)	84 (98%)	1 (1%)	1 (1%)	10	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	86/100 (86%)	85 (99%)	0	1 (1%)	10	9
2	V	87/100 (87%)	85 (98%)	1 (1%)	1 (1%)	11	11
2	a	88/100 (88%)	87 (99%)	0	1 (1%)	11	11
2	f	86/100 (86%)	84 (98%)	1 (1%)	1 (1%)	10	9
2	k	86/100 (86%)	85 (99%)	0	1 (1%)	10	9
3	C	92/99 (93%)	92 (100%)	0	0	100	100
3	H	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
3	M	93/99 (94%)	93 (100%)	0	0	100	100
3	R	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
3	W	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
3	b	94/99 (95%)	93 (99%)	1 (1%)	0	100	100
3	g	92/99 (93%)	92 (100%)	0	0	100	100
3	l	92/99 (93%)	92 (100%)	0	0	100	100
4	D	74/84 (88%)	73 (99%)	1 (1%)	0	100	100
4	I	74/84 (88%)	72 (97%)	2 (3%)	0	100	100
4	N	73/84 (87%)	70 (96%)	3 (4%)	0	100	100
4	S	75/84 (89%)	72 (96%)	3 (4%)	0	100	100
4	X	75/84 (89%)	74 (99%)	1 (1%)	0	100	100
4	c	74/84 (88%)	73 (99%)	1 (1%)	0	100	100
4	h	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
4	m	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
5	E	18/43 (42%)	18 (100%)	0	0	100	100
5	J	27/43 (63%)	24 (89%)	3 (11%)	0	100	100
5	O	17/43 (40%)	16 (94%)	1 (6%)	0	100	100
5	T	18/43 (42%)	18 (100%)	0	0	100	100
5	Y	18/43 (42%)	18 (100%)	0	0	100	100
5	d	16/43 (37%)	15 (94%)	1 (6%)	0	100	100
5	i	17/43 (40%)	17 (100%)	0	0	100	100
5	n	16/43 (37%)	15 (94%)	1 (6%)	0	100	100
All	All	2980/3464 (86%)	2925 (98%)	48 (2%)	7 (0%)	43	52

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	104	GLY
2	G	104	GLY
2	f	104	GLY
2	a	104	GLY
2	V	104	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	82/85 (96%)	82 (100%)	0	100	100
1	F	82/85 (96%)	82 (100%)	0	100	100
1	K	82/85 (96%)	82 (100%)	0	100	100
1	P	83/85 (98%)	82 (99%)	1 (1%)	63	77
1	U	82/85 (96%)	82 (100%)	0	100	100
1	Z	82/85 (96%)	81 (99%)	1 (1%)	63	77
1	e	81/85 (95%)	80 (99%)	1 (1%)	63	77
1	j	82/85 (96%)	82 (100%)	0	100	100
2	B	77/86 (90%)	77 (100%)	0	100	100
2	G	76/86 (88%)	76 (100%)	0	100	100
2	L	75/86 (87%)	75 (100%)	0	100	100
2	Q	75/86 (87%)	75 (100%)	0	100	100
2	V	76/86 (88%)	76 (100%)	0	100	100
2	a	77/86 (90%)	75 (97%)	2 (3%)	40	54
2	f	75/86 (87%)	74 (99%)	1 (1%)	61	76
2	k	75/86 (87%)	74 (99%)	1 (1%)	61	76
3	C	82/86 (95%)	82 (100%)	0	100	100
3	H	82/86 (95%)	81 (99%)	1 (1%)	63	77
3	M	83/86 (96%)	82 (99%)	1 (1%)	63	77
3	R	82/86 (95%)	81 (99%)	1 (1%)	63	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	W	82/86 (95%)	82 (100%)	0	100	100
3	b	83/86 (96%)	80 (96%)	3 (4%)	31	41
3	g	82/86 (95%)	82 (100%)	0	100	100
3	l	82/86 (95%)	82 (100%)	0	100	100
4	D	62/69 (90%)	62 (100%)	0	100	100
4	I	62/69 (90%)	62 (100%)	0	100	100
4	N	62/69 (90%)	62 (100%)	0	100	100
4	S	63/69 (91%)	61 (97%)	2 (3%)	34	46
4	X	64/69 (93%)	62 (97%)	2 (3%)	35	47
4	c	63/69 (91%)	61 (97%)	2 (3%)	34	46
4	h	62/69 (90%)	62 (100%)	0	100	100
4	m	61/69 (88%)	61 (100%)	0	100	100
5	E	22/40 (55%)	22 (100%)	0	100	100
5	J	29/40 (72%)	28 (97%)	1 (3%)	32	43
5	O	21/40 (52%)	21 (100%)	0	100	100
5	T	22/40 (55%)	22 (100%)	0	100	100
5	Y	22/40 (55%)	22 (100%)	0	100	100
5	d	20/40 (50%)	20 (100%)	0	100	100
5	i	21/40 (52%)	20 (95%)	1 (5%)	23	29
5	n	20/40 (50%)	20 (100%)	0	100	100
All	All	2596/2928 (89%)	2575 (99%)	21 (1%)	73	84

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	b	134	ARG
1	e	17	ARG
2	k	86	ARG
2	f	112	SER
4	c	26	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
5	T	465	ASN
1	j	24	GLN
1	U	112	GLN
1	j	110	ASN
1	e	38	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	$\# Z > 2$
6	GOL	A	201	-	5,5,5	0.09	0	5,5,5	0.31	0
6	GOL	h	201	-	5,5,5	0.10	0	5,5,5	0.30	0
6	GOL	N	201	-	5,5,5	0.08	0	5,5,5	0.29	0
6	GOL	S	201	-	5,5,5	0.08	0	5,5,5	0.32	0
6	GOL	b	201	-	5,5,5	0.08	0	5,5,5	0.31	0
6	GOL	j	201	-	5,5,5	0.08	0	5,5,5	0.31	0
6	GOL	U	201	-	5,5,5	0.09	0	5,5,5	0.32	0
6	GOL	P	201	-	5,5,5	0.09	0	5,5,5	0.32	0
6	GOL	D	201	-	5,5,5	0.09	0	5,5,5	0.31	0
6	GOL	K	201	-	5,5,5	0.09	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	H	201	-	5,5,5	0.09	0	5,5,5	0.31	0
6	GOL	e	201	-	5,5,5	0.09	0	5,5,5	0.32	0
6	GOL	j	202	-	5,5,5	0.07	0	5,5,5	0.32	0
6	GOL	c	201	-	5,5,5	0.09	0	5,5,5	0.31	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
6	GOL	A	201	-	-	1/4/4/4	-
6	GOL	h	201	-	-	0/4/4/4	-
6	GOL	N	201	-	-	2/4/4/4	-
6	GOL	S	201	-	-	3/4/4/4	-
6	GOL	b	201	-	-	2/4/4/4	-
6	GOL	j	201	-	-	2/4/4/4	-
6	GOL	U	201	-	-	1/4/4/4	-
6	GOL	P	201	-	-	2/4/4/4	-
6	GOL	D	201	-	-	1/4/4/4	-
6	GOL	K	201	-	-	2/4/4/4	-
6	GOL	H	201	-	-	1/4/4/4	-
6	GOL	e	201	-	-	2/4/4/4	-
6	GOL	j	202	-	-	2/4/4/4	-
6	GOL	c	201	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	201	GOL	O1-C1-C2-C3
6	P	201	GOL	O1-C1-C2-O2
6	b	201	GOL	O1-C1-C2-O2
6	b	201	GOL	O1-C1-C2-C3
6	P	201	GOL	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	h	201	GOL	3	0
6	N	201	GOL	2	0
6	S	201	GOL	1	0
6	U	201	GOL	2	0
6	K	201	GOL	1	0
6	e	201	GOL	1	0
6	j	202	GOL	1	0
6	c	201	GOL	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	103/107 (96%)	-0.53	0 100 100	39, 53, 80, 112	0
1	F	103/107 (96%)	-0.38	0 100 100	44, 64, 94, 105	0
1	K	103/107 (96%)	-0.46	1 (0%) 79 83	43, 57, 86, 110	0
1	P	104/107 (97%)	-0.41	2 (1%) 66 71	44, 58, 88, 125	0
1	U	103/107 (96%)	-0.40	0 100 100	44, 59, 93, 94	0
1	Z	103/107 (96%)	-0.47	0 100 100	45, 59, 86, 96	0
1	e	102/107 (95%)	-0.33	0 100 100	48, 63, 97, 105	0
1	j	103/107 (96%)	-0.38	0 100 100	46, 60, 88, 114	0
2	B	90/100 (90%)	-0.46	0 100 100	33, 55, 75, 113	1 (1%)
2	G	88/100 (88%)	-0.38	0 100 100	27, 61, 85, 99	1 (1%)
2	L	88/100 (88%)	-0.45	1 (1%) 78 82	45, 58, 84, 113	0
2	Q	88/100 (88%)	-0.52	0 100 100	45, 58, 80, 95	0
2	V	89/100 (89%)	-0.36	1 (1%) 78 82	47, 62, 82, 98	0
2	a	89/100 (89%)	-0.49	1 (1%) 78 82	33, 58, 76, 96	1 (1%)
2	f	88/100 (88%)	-0.31	2 (2%) 61 66	50, 65, 92, 103	0
2	k	88/100 (88%)	-0.42	1 (1%) 78 82	48, 61, 86, 104	0
3	C	94/99 (94%)	-0.59	0 100 100	39, 52, 78, 118	0
3	H	94/99 (94%)	-0.63	1 (1%) 78 82	38, 49, 78, 128	0
3	M	95/99 (95%)	-0.54	1 (1%) 78 82	41, 55, 85, 129	0
3	R	94/99 (94%)	-0.53	1 (1%) 78 82	40, 52, 83, 118	0
3	W	94/99 (94%)	-0.58	0 100 100	40, 55, 82, 104	0
3	b	96/99 (96%)	-0.53	2 (2%) 63 68	42, 53, 84, 146	0
3	g	94/99 (94%)	-0.62	1 (1%) 78 82	41, 53, 76, 126	0
3	l	94/99 (94%)	-0.52	1 (1%) 78 82	43, 54, 78, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
4	D	76/84 (90%)	-0.45	2 (2%) 57 63	42, 54, 83, 95	0
4	I	76/84 (90%)	-0.63	0 100 100	38, 50, 76, 102	0
4	N	75/84 (89%)	-0.53	0 100 100	43, 54, 83, 101	0
4	S	77/84 (91%)	-0.45	3 (3%) 43 49	41, 51, 86, 123	0
4	X	77/84 (91%)	-0.40	3 (3%) 43 49	44, 54, 92, 149	0
4	c	76/84 (90%)	-0.52	0 100 100	41, 52, 78, 114	0
4	h	75/84 (89%)	-0.47	1 (1%) 75 79	39, 53, 85, 108	0
4	m	75/84 (89%)	-0.50	0 100 100	42, 55, 79, 104	0
5	E	22/43 (51%)	0.09	1 (4%) 38 44	57, 81, 113, 133	0
5	J	29/43 (67%)	0.27	2 (6%) 23 26	56, 79, 127, 146	0
5	O	21/43 (48%)	0.12	1 (4%) 35 41	64, 80, 116, 121	0
5	T	22/43 (51%)	0.13	1 (4%) 38 44	53, 78, 109, 122	0
5	Y	22/43 (51%)	0.16	1 (4%) 38 44	54, 79, 119, 131	0
5	d	20/43 (46%)	0.25	1 (5%) 34 40	58, 79, 108, 113	0
5	i	21/43 (48%)	0.18	1 (4%) 35 41	50, 76, 105, 121	0
5	n	20/43 (46%)	0.29	0 100 100	61, 84, 126, 138	0
All	All	3071/3464 (88%)	-0.44	33 (1%) 78 82	27, 57, 92, 149	3 (0%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	b	135	ALA	5.5
4	h	26	ILE	4.6
3	H	41	TYR	3.6
4	D	101	GLY	3.6
5	T	459	PRO	3.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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
6	GOL	D	201	6/6	0.68	0.19	75,84,86,87	0
6	GOL	b	201	6/6	0.72	0.15	84,84,87,88	0
6	GOL	j	202	6/6	0.77	0.12	79,82,89,90	0
6	GOL	h	201	6/6	0.82	0.13	88,90,92,94	0
6	GOL	N	201	6/6	0.82	0.11	61,85,91,98	0
6	GOL	S	201	6/6	0.85	0.14	92,93,94,96	0
6	GOL	H	201	6/6	0.85	0.13	93,93,96,100	0
6	GOL	P	201	6/6	0.88	0.11	59,71,73,83	0
6	GOL	e	201	6/6	0.89	0.13	67,72,77,81	0
6	GOL	U	201	6/6	0.90	0.11	68,72,76,78	0
6	GOL	j	201	6/6	0.91	0.11	55,65,72,73	0
6	GOL	c	201	6/6	0.92	0.11	71,73,74,76	0
6	GOL	A	201	6/6	0.93	0.09	52,66,67,67	0
6	GOL	K	201	6/6	0.93	0.08	61,69,73,74	0
7	CL	J	501	1/1	0.96	0.06	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.