



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:10 PM GMT

PDB ID : 4KPN  
Title : Plant nucleoside hydrolase - PpNRh1 enzyme  
Authors : Morera, S.; Vigouroux, A.; Kopecny, D.  
Deposited on : 2013-05-14  
Resolution : 3.35 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

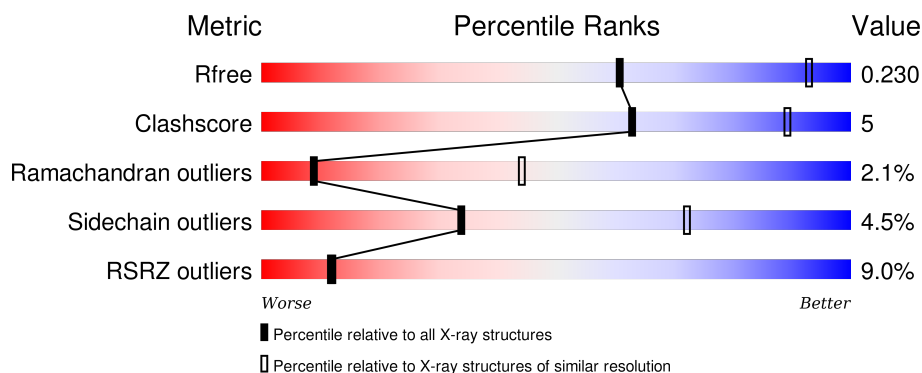
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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))
$R_{free}$	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	345	
1	B	345	
1	C	345	
1	D	345	
1	E	345	

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Mol	Chain	Length	Quality of chain
1	F	345	
1	G	345	
1	H	345	

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
2	CA	B	400	-	-	-	X
2	CA	D	400	-	-	-	X
2	CA	E	400	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19520 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 Nucleoside N-ribohydrolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2437	1561	405	464	7			
1	B	318	Total	C	N	O	S	0	0	0
			2437	1561	405	464	7			
1	C	318	Total	C	N	O	S	0	0	0
			2437	1561	405	464	7			
1	D	318	Total	C	N	O	S	0	0	0
			2437	1561	405	464	7			
1	E	318	Total	C	N	O	S	0	0	0
			2437	1561	405	464	7			
1	F	318	Total	C	N	O	S	0	0	0
			2437	1561	405	464	7			
1	G	318	Total	C	N	O	S	0	0	0
			2437	1561	405	464	7			
1	H	318	Total	C	N	O	S	0	0	0
			2437	1561	405	464	7			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP M1FQT3
A	-10	GLY	-	EXPRESSION TAG	UNP M1FQT3
A	-9	SER	-	EXPRESSION TAG	UNP M1FQT3
A	-8	SER	-	EXPRESSION TAG	UNP M1FQT3
A	-7	HIS	-	EXPRESSION TAG	UNP M1FQT3
A	-6	HIS	-	EXPRESSION TAG	UNP M1FQT3
A	-5	HIS	-	EXPRESSION TAG	UNP M1FQT3
A	-4	HIS	-	EXPRESSION TAG	UNP M1FQT3
A	-3	HIS	-	EXPRESSION TAG	UNP M1FQT3
A	-2	HIS	-	EXPRESSION TAG	UNP M1FQT3
A	-1	SER	-	EXPRESSION TAG	UNP M1FQT3
A	0	GLN	-	EXPRESSION TAG	UNP M1FQT3
A	1	ASP	-	EXPRESSION TAG	UNP M1FQT3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	PRO	-	EXPRESSION TAG	UNP M1FQT3
A	?	-	LYS	DELETION	UNP M1FQT3
B	-11	MET	-	EXPRESSION TAG	UNP M1FQT3
B	-10	GLY	-	EXPRESSION TAG	UNP M1FQT3
B	-9	SER	-	EXPRESSION TAG	UNP M1FQT3
B	-8	SER	-	EXPRESSION TAG	UNP M1FQT3
B	-7	HIS	-	EXPRESSION TAG	UNP M1FQT3
B	-6	HIS	-	EXPRESSION TAG	UNP M1FQT3
B	-5	HIS	-	EXPRESSION TAG	UNP M1FQT3
B	-4	HIS	-	EXPRESSION TAG	UNP M1FQT3
B	-3	HIS	-	EXPRESSION TAG	UNP M1FQT3
B	-2	HIS	-	EXPRESSION TAG	UNP M1FQT3
B	-1	SER	-	EXPRESSION TAG	UNP M1FQT3
B	0	GLN	-	EXPRESSION TAG	UNP M1FQT3
B	1	ASP	-	EXPRESSION TAG	UNP M1FQT3
B	2	PRO	-	EXPRESSION TAG	UNP M1FQT3
B	?	-	LYS	DELETION	UNP M1FQT3
C	-11	MET	-	EXPRESSION TAG	UNP M1FQT3
C	-10	GLY	-	EXPRESSION TAG	UNP M1FQT3
C	-9	SER	-	EXPRESSION TAG	UNP M1FQT3
C	-8	SER	-	EXPRESSION TAG	UNP M1FQT3
C	-7	HIS	-	EXPRESSION TAG	UNP M1FQT3
C	-6	HIS	-	EXPRESSION TAG	UNP M1FQT3
C	-5	HIS	-	EXPRESSION TAG	UNP M1FQT3
C	-4	HIS	-	EXPRESSION TAG	UNP M1FQT3
C	-3	HIS	-	EXPRESSION TAG	UNP M1FQT3
C	-2	HIS	-	EXPRESSION TAG	UNP M1FQT3
C	-1	SER	-	EXPRESSION TAG	UNP M1FQT3
C	0	GLN	-	EXPRESSION TAG	UNP M1FQT3
C	1	ASP	-	EXPRESSION TAG	UNP M1FQT3
C	2	PRO	-	EXPRESSION TAG	UNP M1FQT3
C	?	-	LYS	DELETION	UNP M1FQT3
D	-11	MET	-	EXPRESSION TAG	UNP M1FQT3
D	-10	GLY	-	EXPRESSION TAG	UNP M1FQT3
D	-9	SER	-	EXPRESSION TAG	UNP M1FQT3
D	-8	SER	-	EXPRESSION TAG	UNP M1FQT3
D	-7	HIS	-	EXPRESSION TAG	UNP M1FQT3
D	-6	HIS	-	EXPRESSION TAG	UNP M1FQT3
D	-5	HIS	-	EXPRESSION TAG	UNP M1FQT3
D	-4	HIS	-	EXPRESSION TAG	UNP M1FQT3
D	-3	HIS	-	EXPRESSION TAG	UNP M1FQT3
D	-2	HIS	-	EXPRESSION TAG	UNP M1FQT3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	SER	-	EXPRESSION TAG	UNP M1FQT3
D	0	GLN	-	EXPRESSION TAG	UNP M1FQT3
D	1	ASP	-	EXPRESSION TAG	UNP M1FQT3
D	2	PRO	-	EXPRESSION TAG	UNP M1FQT3
D	?	-	LYS	DELETION	UNP M1FQT3
E	-11	MET	-	EXPRESSION TAG	UNP M1FQT3
E	-10	GLY	-	EXPRESSION TAG	UNP M1FQT3
E	-9	SER	-	EXPRESSION TAG	UNP M1FQT3
E	-8	SER	-	EXPRESSION TAG	UNP M1FQT3
E	-7	HIS	-	EXPRESSION TAG	UNP M1FQT3
E	-6	HIS	-	EXPRESSION TAG	UNP M1FQT3
E	-5	HIS	-	EXPRESSION TAG	UNP M1FQT3
E	-4	HIS	-	EXPRESSION TAG	UNP M1FQT3
E	-3	HIS	-	EXPRESSION TAG	UNP M1FQT3
E	-2	HIS	-	EXPRESSION TAG	UNP M1FQT3
E	-1	SER	-	EXPRESSION TAG	UNP M1FQT3
E	0	GLN	-	EXPRESSION TAG	UNP M1FQT3
E	1	ASP	-	EXPRESSION TAG	UNP M1FQT3
E	2	PRO	-	EXPRESSION TAG	UNP M1FQT3
E	?	-	LYS	DELETION	UNP M1FQT3
F	-11	MET	-	EXPRESSION TAG	UNP M1FQT3
F	-10	GLY	-	EXPRESSION TAG	UNP M1FQT3
F	-9	SER	-	EXPRESSION TAG	UNP M1FQT3
F	-8	SER	-	EXPRESSION TAG	UNP M1FQT3
F	-7	HIS	-	EXPRESSION TAG	UNP M1FQT3
F	-6	HIS	-	EXPRESSION TAG	UNP M1FQT3
F	-5	HIS	-	EXPRESSION TAG	UNP M1FQT3
F	-4	HIS	-	EXPRESSION TAG	UNP M1FQT3
F	-3	HIS	-	EXPRESSION TAG	UNP M1FQT3
F	-2	HIS	-	EXPRESSION TAG	UNP M1FQT3
F	-1	SER	-	EXPRESSION TAG	UNP M1FQT3
F	0	GLN	-	EXPRESSION TAG	UNP M1FQT3
F	1	ASP	-	EXPRESSION TAG	UNP M1FQT3
F	2	PRO	-	EXPRESSION TAG	UNP M1FQT3
F	?	-	LYS	DELETION	UNP M1FQT3
G	-11	MET	-	EXPRESSION TAG	UNP M1FQT3
G	-10	GLY	-	EXPRESSION TAG	UNP M1FQT3
G	-9	SER	-	EXPRESSION TAG	UNP M1FQT3
G	-8	SER	-	EXPRESSION TAG	UNP M1FQT3
G	-7	HIS	-	EXPRESSION TAG	UNP M1FQT3
G	-6	HIS	-	EXPRESSION TAG	UNP M1FQT3
G	-5	HIS	-	EXPRESSION TAG	UNP M1FQT3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	HIS	-	EXPRESSION TAG	UNP M1FQT3
G	-3	HIS	-	EXPRESSION TAG	UNP M1FQT3
G	-2	HIS	-	EXPRESSION TAG	UNP M1FQT3
G	-1	SER	-	EXPRESSION TAG	UNP M1FQT3
G	0	GLN	-	EXPRESSION TAG	UNP M1FQT3
G	1	ASP	-	EXPRESSION TAG	UNP M1FQT3
G	2	PRO	-	EXPRESSION TAG	UNP M1FQT3
G	?	-	LYS	DELETION	UNP M1FQT3
H	-11	MET	-	EXPRESSION TAG	UNP M1FQT3
H	-10	GLY	-	EXPRESSION TAG	UNP M1FQT3
H	-9	SER	-	EXPRESSION TAG	UNP M1FQT3
H	-8	SER	-	EXPRESSION TAG	UNP M1FQT3
H	-7	HIS	-	EXPRESSION TAG	UNP M1FQT3
H	-6	HIS	-	EXPRESSION TAG	UNP M1FQT3
H	-5	HIS	-	EXPRESSION TAG	UNP M1FQT3
H	-4	HIS	-	EXPRESSION TAG	UNP M1FQT3
H	-3	HIS	-	EXPRESSION TAG	UNP M1FQT3
H	-2	HIS	-	EXPRESSION TAG	UNP M1FQT3
H	-1	SER	-	EXPRESSION TAG	UNP M1FQT3
H	0	GLN	-	EXPRESSION TAG	UNP M1FQT3
H	1	ASP	-	EXPRESSION TAG	UNP M1FQT3
H	2	PRO	-	EXPRESSION TAG	UNP M1FQT3
H	?	-	LYS	DELETION	UNP M1FQT3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is water.

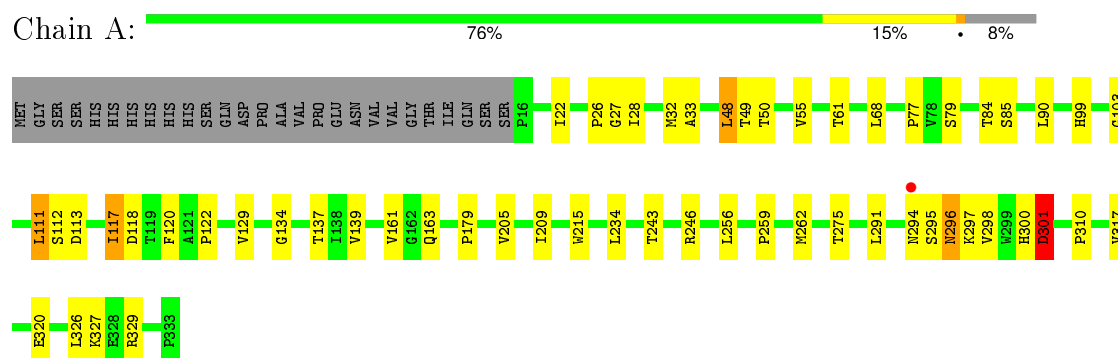
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	O 4	0	0
3	B	4	Total 4	O 4	0	0
3	C	2	Total 2	O 2	0	0
3	D	2	Total 2	O 2	0	0
3	E	3	Total 3	O 3	0	0
3	G	1	Total 1	O 1	0	0



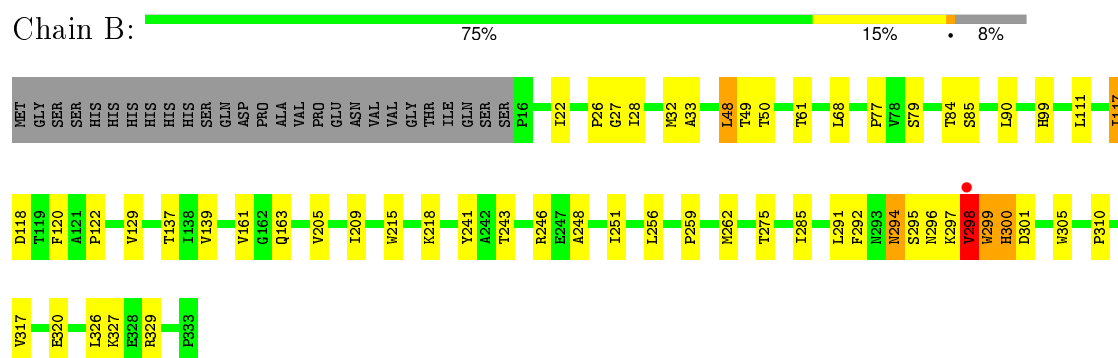
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

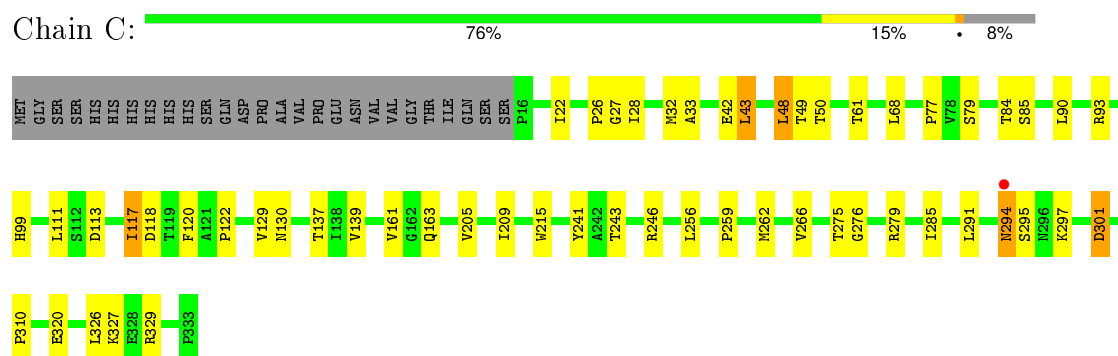
#### • Molecule 1: Nucleoside N-ribohydrolase 1



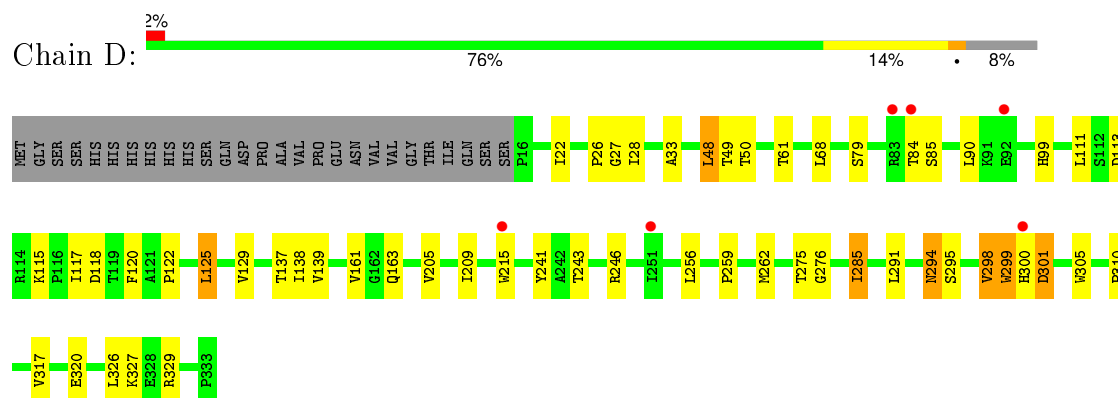
#### • Molecule 1: Nucleoside N-ribohydrolase 1



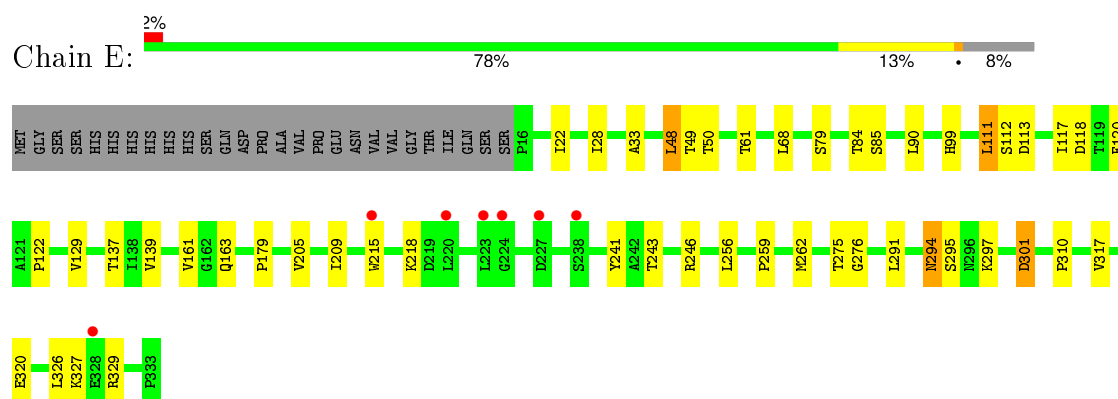
#### • Molecule 1: Nucleoside N-ribohydrolase 1



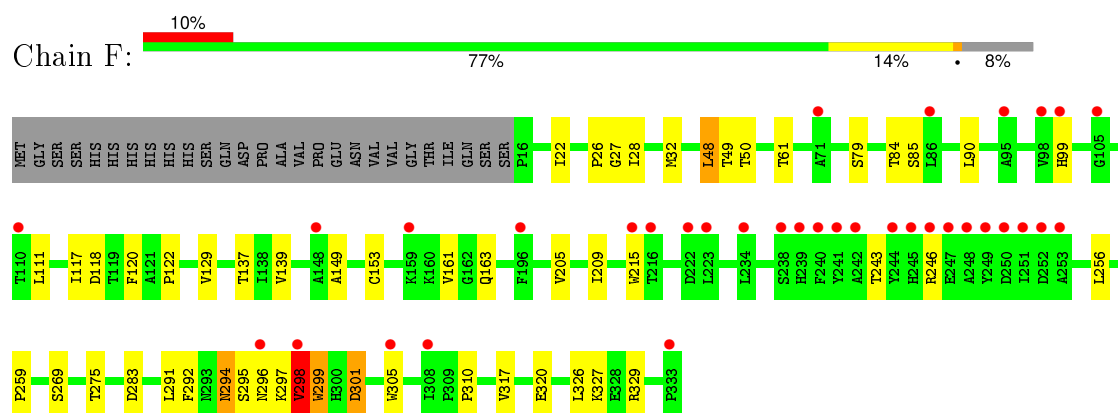
- Molecule 1: Nucleoside N-ribohydrolase 1



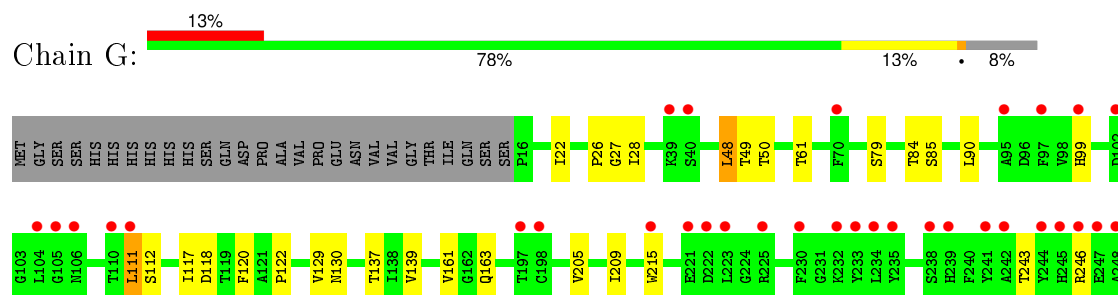
- Molecule 1: Nucleoside N-ribohydrolase 1

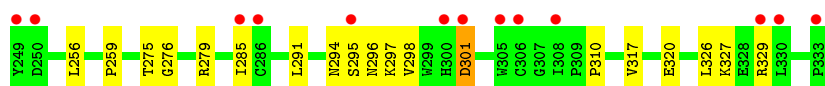


- Molecule 1: Nucleoside N-ribohydrolase 1

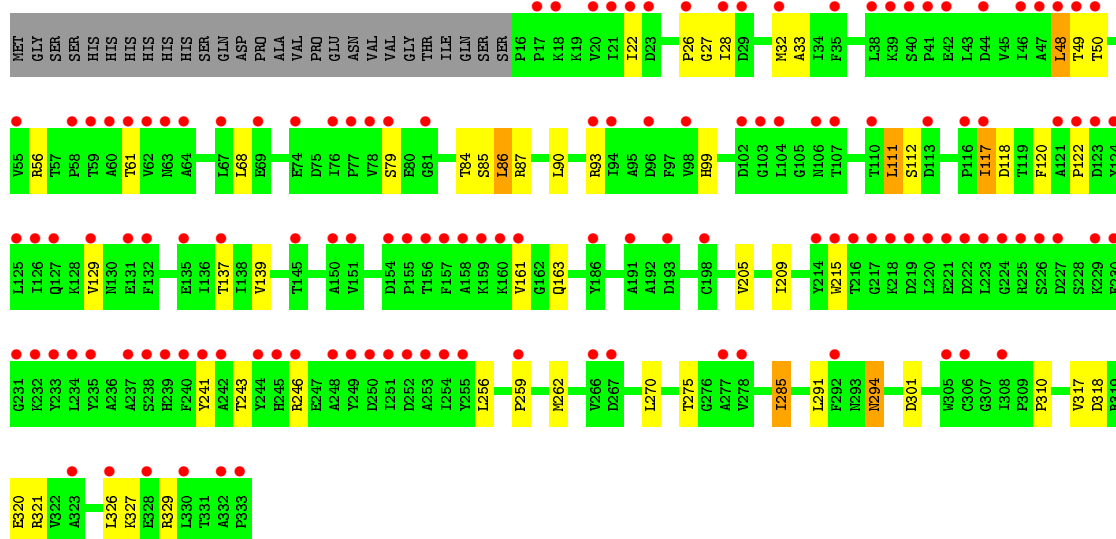
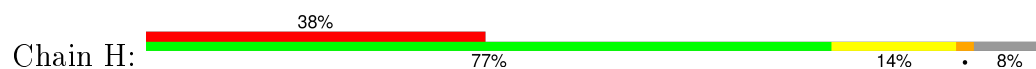


- Molecule 1: Nucleoside N-ribohydrolase 1





● Molecule 1: Nucleoside N-ribohydrolase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.85Å 126.08Å 253.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.68 – 3.35 44.67 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.68-3.35) 99.5 (44.67-3.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.203 , 0.213 0.218 , 0.230	Depositor DCC
$R_{free}$ test set	2927 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.6	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 59.8	EDS
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 58554 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	19520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CA

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	0.38	0/2494	0.69	2/3405 (0.1%)
1	B	0.38	0/2494	0.68	1/3405 (0.0%)
1	C	0.38	0/2494	0.66	0/3405
1	D	0.39	0/2494	0.68	0/3405
1	E	0.38	0/2494	0.68	1/3405 (0.0%)
1	F	0.39	0/2494	0.69	2/3405 (0.1%)
1	G	0.39	0/2494	0.69	2/3405 (0.1%)
1	H	0.39	0/2494	0.68	1/3405 (0.0%)
All	All	0.38	0/19952	0.68	9/27240 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	111	LEU	C-N-CA	8.95	144.08	121.70
1	A	111	LEU	C-N-CA	8.93	144.02	121.70
1	H	111	LEU	C-N-CA	8.90	143.96	121.70
1	G	111	LEU	C-N-CA	8.89	143.93	121.70
1	F	298	VAL	C-N-CA	8.66	143.36	121.70
1	B	298	VAL	C-N-CA	8.52	142.99	121.70
1	F	48	LEU	N-CA-CB	5.11	120.61	110.40
1	G	48	LEU	N-CA-CB	5.09	120.58	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ASN	C-N-CA	5.09	134.42	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	283	ASP	Mainchain

## 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	2437	0	2418	28	0
1	B	2437	0	2418	32	0
1	C	2437	0	2418	34	0
1	D	2437	0	2418	25	0
1	E	2437	0	2418	23	0
1	F	2437	0	2418	28	0
1	G	2437	0	2418	24	0
1	H	2437	0	2418	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	1	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	G	1	0	0	0	0
All	All	19520	0	19344	204	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 5.

All (204) 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:B:292:PHE:CE2	1:B:294:ASN:HB3	1.94	1.02
1:C:43:LEU:HD11	1:C:266:VAL:HG22	1.55	0.88
1:C:130:ASN:HB3	1:G:130:ASN:ND2	1.93	0.83
1:F:298:VAL:HA	1:F:299:TRP:CD1	2.15	0.81
1:F:292:PHE:CE2	1:F:294:ASN:HB3	2.16	0.80
1:B:22:ILE:HG22	1:B:139:VAL:HB	1.66	0.78
1:F:22:ILE:HG22	1:F:139:VAL:HB	1.66	0.78
1:E:22:ILE:HG22	1:E:139:VAL:HB	1.66	0.78
1:H:22:ILE:HG22	1:H:139:VAL:HB	1.66	0.77
1:A:22:ILE:HG22	1:A:139:VAL:HB	1.67	0.77
1:D:22:ILE:HG22	1:D:139:VAL:HB	1.67	0.77
1:B:298:VAL:HA	1:B:299:TRP:CD1	2.19	0.76
1:G:22:ILE:HG22	1:G:139:VAL:HB	1.66	0.76
1:C:22:ILE:HG22	1:C:139:VAL:HB	1.66	0.76
1:F:205:VAL:HG13	1:F:209:ILE:HD11	1.73	0.71
1:D:205:VAL:HG13	1:D:209:ILE:HD11	1.73	0.70
1:G:205:VAL:HG13	1:G:209:ILE:HD11	1.74	0.70
1:H:205:VAL:HG13	1:H:209:ILE:HD11	1.74	0.69
1:A:205:VAL:HG13	1:A:209:ILE:HD11	1.74	0.69
1:B:205:VAL:HG13	1:B:209:ILE:HD11	1.74	0.69
1:A:215:TRP:HZ2	1:A:326:LEU:O	1.77	0.68
1:C:205:VAL:HG13	1:C:209:ILE:HD11	1.75	0.68
1:B:251:ILE:HD11	3:B:501:HOH:O	1.94	0.68
1:D:215:TRP:HZ2	1:D:326:LEU:O	1.77	0.67
1:E:205:VAL:HG13	1:E:209:ILE:HD11	1.75	0.67
1:B:215:TRP:HZ2	1:B:326:LEU:O	1.77	0.67
1:E:215:TRP:HZ2	1:E:326:LEU:O	1.78	0.67
1:H:215:TRP:HZ2	1:H:326:LEU:O	1.77	0.67
1:F:215:TRP:HZ2	1:F:326:LEU:O	1.77	0.67
1:C:215:TRP:HZ2	1:C:326:LEU:O	1.77	0.66
1:E:179:PRO:HD2	1:F:305:TRP:CE3	2.30	0.66
1:G:215:TRP:HZ2	1:G:326:LEU:O	1.78	0.66
1:E:256:LEU:HB3	1:E:259:PRO:HG2	1.81	0.62
1:F:122:PRO:HB2	1:G:90:LEU:HD21	1.81	0.62
1:C:256:LEU:HB3	1:C:259:PRO:HG2	1.81	0.62
1:F:256:LEU:HB3	1:F:259:PRO:HG2	1.81	0.62
1:A:256:LEU:HB3	1:A:259:PRO:HG2	1.82	0.62
1:H:256:LEU:HB3	1:H:259:PRO:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:LEU:HB3	1:G:259:PRO:HG2	1.82	0.62
1:B:256:LEU:HB3	1:B:259:PRO:HG2	1.82	0.62
1:D:256:LEU:HB3	1:D:259:PRO:HG2	1.82	0.61
1:H:86:LEU:HD12	1:H:87:ARG:NH1	2.16	0.60
1:C:43:LEU:CD1	1:C:266:VAL:HG22	2.29	0.59
1:D:28:ILE:H	1:D:99:HIS:CD2	2.22	0.57
1:F:292:PHE:CE2	1:F:294:ASN:CB	2.87	0.57
1:E:129:VAL:HG11	1:E:161:VAL:HG12	1.86	0.57
1:B:28:ILE:H	1:B:99:HIS:CD2	2.22	0.57
1:C:28:ILE:H	1:C:99:HIS:CD2	2.22	0.56
1:E:28:ILE:H	1:E:99:HIS:CD2	2.23	0.56
1:C:49:THR:HG22	1:C:79:SER:HB3	1.87	0.56
1:A:129:VAL:HG11	1:A:161:VAL:HG12	1.87	0.56
1:H:129:VAL:HG11	1:H:161:VAL:HG12	1.87	0.56
1:F:28:ILE:H	1:F:99:HIS:CD2	2.23	0.56
1:E:49:THR:HG22	1:E:79:SER:HB3	1.87	0.56
1:A:28:ILE:H	1:A:99:HIS:CD2	2.23	0.56
1:B:292:PHE:HE2	1:B:294:ASN:HB3	1.62	0.56
1:F:298:VAL:HA	1:F:299:TRP:CG	2.40	0.55
1:F:49:THR:HG22	1:F:79:SER:HB3	1.88	0.55
1:G:28:ILE:H	1:G:99:HIS:CD2	2.24	0.55
1:G:49:THR:HG22	1:G:79:SER:HB3	1.87	0.55
1:B:122:PRO:HB2	1:C:90:LEU:HD21	1.88	0.55
1:C:130:ASN:CB	1:G:130:ASN:ND2	2.68	0.55
1:H:28:ILE:H	1:H:99:HIS:CD2	2.24	0.55
1:H:49:THR:HG22	1:H:79:SER:HB3	1.88	0.55
1:A:49:THR:HG22	1:A:79:SER:HB3	1.88	0.55
1:B:49:THR:HG22	1:B:79:SER:HB3	1.88	0.55
1:D:49:THR:HG22	1:D:79:SER:HB3	1.88	0.55
1:B:298:VAL:HA	1:B:299:TRP:CG	2.41	0.54
1:D:28:ILE:H	1:D:99:HIS:HD2	1.56	0.54
1:C:28:ILE:H	1:C:99:HIS:HD2	1.56	0.54
1:E:28:ILE:H	1:E:99:HIS:HD2	1.56	0.53
1:F:153:CYS:HB2	1:G:90:LEU:HD13	1.89	0.53
1:F:28:ILE:H	1:F:99:HIS:HD2	1.57	0.53
1:H:270:LEU:HB3	1:H:318:ASP:OD2	2.09	0.53
1:F:215:TRP:CZ2	1:F:326:LEU:O	2.62	0.52
1:B:215:TRP:CZ2	1:B:326:LEU:O	2.62	0.52
1:B:28:ILE:H	1:B:99:HIS:HD2	1.56	0.52
1:D:22:ILE:HG13	1:D:48:LEU:HG	1.92	0.52
1:A:28:ILE:H	1:A:99:HIS:HD2	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:ILE:H	1:G:99:HIS:HD2	1.58	0.52
1:A:22:ILE:HG13	1:A:48:LEU:HG	1.92	0.51
1:E:22:ILE:HG13	1:E:48:LEU:HG	1.92	0.51
1:C:22:ILE:HG13	1:C:48:LEU:HG	1.92	0.51
1:C:130:ASN:HB3	1:G:130:ASN:HD22	1.73	0.51
1:B:22:ILE:HG13	1:B:48:LEU:HG	1.92	0.51
1:H:22:ILE:HG13	1:H:48:LEU:HG	1.92	0.50
1:A:50:THR:HG21	1:A:61:THR:HA	1.93	0.50
1:G:137:THR:HG23	1:G:163:GLN:HB3	1.93	0.50
1:C:43:LEU:HD12	1:C:43:LEU:N	2.26	0.50
1:A:215:TRP:CZ2	1:A:326:LEU:O	2.62	0.50
1:F:137:THR:HG23	1:F:163:GLN:HB3	1.93	0.50
1:H:28:ILE:H	1:H:99:HIS:HD2	1.57	0.50
1:D:137:THR:HG23	1:D:163:GLN:HB3	1.92	0.50
1:C:42:GLU:HG2	1:C:43:LEU:HD12	1.92	0.50
1:B:32:MET:HE2	1:B:259:PRO:HG3	1.94	0.50
1:E:137:THR:HG23	1:E:163:GLN:HB3	1.94	0.50
1:B:50:THR:HG21	1:B:61:THR:HA	1.94	0.50
1:C:50:THR:HG21	1:C:61:THR:HA	1.94	0.50
1:C:137:THR:HG23	1:C:163:GLN:HB3	1.94	0.50
1:C:32:MET:HE2	1:C:259:PRO:HG3	1.93	0.50
1:D:215:TRP:CZ2	1:D:326:LEU:O	2.62	0.49
1:C:215:TRP:CZ2	1:C:326:LEU:O	2.62	0.49
1:B:137:THR:HG23	1:B:163:GLN:HB3	1.94	0.49
1:B:243:THR:HG22	1:B:246:ARG:HH22	1.76	0.49
1:H:137:THR:HG23	1:H:163:GLN:HB3	1.93	0.49
1:H:50:THR:HG21	1:H:61:THR:HA	1.94	0.49
1:A:137:THR:HG23	1:A:163:GLN:HB3	1.93	0.49
1:A:243:THR:HG22	1:A:246:ARG:HH22	1.78	0.49
1:A:32:MET:HE2	1:A:259:PRO:HG3	1.93	0.49
1:G:279:ARG:HB3	1:H:285:ILE:HD13	1.95	0.49
1:A:90:LEU:HD21	1:E:122:PRO:HB2	1.94	0.49
1:E:243:THR:HG22	1:E:246:ARG:HH22	1.77	0.49
1:D:50:THR:HG21	1:D:61:THR:HA	1.94	0.49
1:F:50:THR:HG21	1:F:61:THR:HA	1.94	0.48
1:F:32:MET:HE2	1:F:259:PRO:HG3	1.95	0.48
1:F:243:THR:HG22	1:F:246:ARG:HH22	1.78	0.48
1:G:50:THR:HG21	1:G:61:THR:HA	1.94	0.48
1:D:243:THR:HG22	1:D:246:ARG:HH22	1.77	0.48
1:G:243:THR:HG22	1:G:246:ARG:HH22	1.78	0.48
1:G:215:TRP:CZ2	1:G:326:LEU:O	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:THR:HG21	1:E:61:THR:HA	1.94	0.48
1:E:215:TRP:CZ2	1:E:326:LEU:O	2.62	0.48
1:C:243:THR:HG22	1:C:246:ARG:HH22	1.78	0.48
1:H:32:MET:HE2	1:H:259:PRO:HG3	1.94	0.48
1:H:243:THR:HG22	1:H:246:ARG:HH22	1.79	0.47
1:H:215:TRP:CZ2	1:H:326:LEU:O	2.62	0.47
1:A:134:GLY:HA3	1:H:56:ARG:HH21	1.79	0.47
1:C:26:PRO:HA	1:C:27:GLY:HA3	1.78	0.47
1:D:125:LEU:HD22	1:D:138:ILE:HD13	1.98	0.46
1:G:129:VAL:HG21	1:G:161:VAL:HG12	1.98	0.46
1:F:295:SER:C	1:F:297:LYS:H	2.20	0.46
1:D:26:PRO:HA	1:D:27:GLY:HA3	1.78	0.46
1:C:84:THR:HG22	1:C:90:LEU:HA	1.98	0.45
1:A:84:THR:HG22	1:A:90:LEU:HA	1.98	0.45
1:D:129:VAL:HG21	1:D:161:VAL:HG12	1.98	0.45
1:E:179:PRO:HG2	1:F:305:TRP:HB2	1.99	0.45
1:C:129:VAL:HG21	1:C:161:VAL:HG12	1.97	0.45
1:F:84:THR:HG22	1:F:90:LEU:HA	1.98	0.45
1:F:292:PHE:HE2	1:F:294:ASN:HB3	1.77	0.44
1:C:279:ARG:HB3	1:D:285:ILE:HD13	1.99	0.44
1:B:129:VAL:HG21	1:B:161:VAL:HG12	1.99	0.44
1:B:84:THR:HG22	1:B:90:LEU:HA	1.99	0.44
1:E:84:THR:HG22	1:E:90:LEU:HA	1.98	0.44
1:F:129:VAL:HG21	1:F:161:VAL:HG12	1.98	0.44
1:H:48:LEU:HD13	1:H:68:LEU:HD11	1.99	0.44
1:A:48:LEU:HD13	1:A:68:LEU:HD11	1.99	0.44
1:D:48:LEU:HD13	1:D:68:LEU:HD11	1.99	0.44
1:C:48:LEU:HD13	1:C:68:LEU:HD11	2.00	0.44
1:D:84:THR:HG22	1:D:90:LEU:HA	1.99	0.44
1:B:275:THR:HG22	1:B:310:PRO:HB2	1.99	0.44
1:H:84:THR:HG22	1:H:90:LEU:HA	1.99	0.44
1:B:48:LEU:HD13	1:B:68:LEU:HD11	2.00	0.43
1:E:48:LEU:HD13	1:E:68:LEU:HD11	1.99	0.43
1:G:84:THR:HG22	1:G:90:LEU:HA	1.99	0.43
1:B:295:SER:C	1:B:297:LYS:H	2.21	0.43
1:D:275:THR:HG22	1:D:310:PRO:HB2	1.99	0.43
1:B:77:PRO:HB2	1:B:117:ILE:HG12	2.00	0.43
1:H:26:PRO:HA	1:H:27:GLY:HA3	1.79	0.43
1:E:275:THR:HG22	1:E:310:PRO:HB2	2.00	0.43
1:D:298:VAL:HG13	1:D:299:TRP:H	1.84	0.43
1:C:285:ILE:HG22	1:D:305:TRP:CH2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:THR:HG22	1:A:310:PRO:HB2	2.00	0.43
1:H:275:THR:HG22	1:H:310:PRO:HB2	2.01	0.43
1:A:77:PRO:HB2	1:A:117:ILE:HG12	2.00	0.43
1:C:120:PHE:CD2	1:C:122:PRO:HD2	2.54	0.43
1:A:26:PRO:HA	1:A:27:GLY:HA3	1.79	0.43
1:F:26:PRO:HA	1:F:27:GLY:HA3	1.78	0.42
1:A:179:PRO:HD2	1:B:305:TRP:CE3	2.54	0.42
1:D:120:PHE:CD2	1:D:122:PRO:HD2	2.54	0.42
1:F:275:THR:HG22	1:F:310:PRO:HB2	2.01	0.42
1:D:33:ALA:HB1	1:D:262:MET:HE2	2.02	0.42
1:B:26:PRO:HA	1:B:27:GLY:HA3	1.79	0.42
1:C:43:LEU:HD11	1:C:266:VAL:CG2	2.37	0.42
1:A:120:PHE:CD2	1:A:122:PRO:HD2	2.54	0.42
1:G:276:GLY:HA2	1:G:295:SER:HB2	2.02	0.42
1:H:120:PHE:CD2	1:H:122:PRO:HD2	2.55	0.42
1:C:275:THR:HG22	1:C:310:PRO:HB2	2.01	0.42
1:G:26:PRO:HA	1:G:27:GLY:HA3	1.80	0.42
1:C:77:PRO:HB2	1:C:117:ILE:HG12	2.01	0.42
1:B:120:PHE:CD2	1:B:122:PRO:HD2	2.54	0.41
1:B:33:ALA:HB1	1:B:262:MET:HE2	2.01	0.41
1:G:120:PHE:CD2	1:G:122:PRO:HD2	2.55	0.41
1:F:120:PHE:CD2	1:F:122:PRO:HD2	2.55	0.41
1:G:275:THR:HG22	1:G:310:PRO:HB2	2.01	0.41
1:E:120:PHE:CD2	1:E:122:PRO:HD2	2.54	0.41
1:E:33:ALA:HB1	1:E:262:MET:HE2	2.02	0.41
1:A:32:MET:HG2	1:A:234:LEU:HD13	2.03	0.41
1:C:276:GLY:HA2	1:C:295:SER:HB2	2.03	0.41
1:E:276:GLY:HA2	1:E:295:SER:HB2	2.02	0.41
1:E:28:ILE:HD13	1:E:241:TYR:HB2	2.03	0.41
1:A:55:VAL:HG11	1:A:103:GLY:HA3	2.02	0.41
1:H:33:ALA:HB1	1:H:262:MET:HE2	2.03	0.41
1:D:276:GLY:HA2	1:D:295:SER:HB2	2.03	0.41
1:A:300:HIS:O	1:A:301:ASP:HB2	2.21	0.40
1:D:28:ILE:HD13	1:D:241:TYR:HB2	2.03	0.40
1:B:28:ILE:HD13	1:B:241:TYR:HB2	2.03	0.40
1:A:298:VAL:HG13	1:B:248:ALA:O	2.21	0.40
1:C:28:ILE:HD13	1:C:241:TYR:HB2	2.03	0.40
1:H:270:LEU:HD13	1:H:321:ARG:HB3	2.04	0.40
1:B:294:ASN:CG	1:B:294:ASN:O	2.59	0.40
1:F:149:ALA:HB1	1:G:90:LEU:HD11	2.03	0.40
1:C:33:ALA:HB1	1:C:262:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:28:ILE:HD13	1:H:241:TYR:HB2	2.03	0.40
1:A:33:ALA:HB1	1:A:262:MET:HE2	2.02	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	316/345 (92%)	289 (92%)	19 (6%)	8 (2%)	7	40
1	B	316/345 (92%)	290 (92%)	19 (6%)	7 (2%)	8	43
1	C	316/345 (92%)	291 (92%)	20 (6%)	5 (2%)	12	49
1	D	316/345 (92%)	286 (90%)	21 (7%)	9 (3%)	6	37
1	E	316/345 (92%)	291 (92%)	19 (6%)	6 (2%)	10	46
1	F	316/345 (92%)	289 (92%)	20 (6%)	7 (2%)	8	43
1	G	316/345 (92%)	291 (92%)	19 (6%)	6 (2%)	10	46
1	H	316/345 (92%)	291 (92%)	20 (6%)	5 (2%)	12	49
All	All	2528/2760 (92%)	2318 (92%)	157 (6%)	53 (2%)	9	44

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	A	118	ASP
1	A	297	LYS
1	A	301	ASP
1	B	118	ASP
1	B	298	VAL
1	C	118	ASP
1	C	294	ASN

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Mol	Chain	Res	Type
1	C	301	ASP
1	D	118	ASP
1	D	294	ASN
1	D	301	ASP
1	E	112	SER
1	E	294	ASN
1	E	301	ASP
1	F	118	ASP
1	F	298	VAL
1	F	301	ASP
1	G	112	SER
1	G	118	ASP
1	G	294	ASN
1	G	301	ASP
1	H	112	SER
1	H	118	ASP
1	H	294	ASN
1	A	117	ILE
1	A	294	ASN
1	A	327	LYS
1	B	117	ILE
1	B	299	TRP
1	B	327	LYS
1	C	117	ILE
1	C	327	LYS
1	D	117	ILE
1	D	298	VAL
1	D	300	HIS
1	D	327	LYS
1	E	117	ILE
1	E	118	ASP
1	E	327	LYS
1	F	117	ILE
1	F	299	TRP
1	F	327	LYS
1	G	117	ILE
1	G	327	LYS
1	H	117	ILE
1	H	327	LYS
1	A	295	SER
1	B	300	HIS
1	D	299	TRP

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Mol	Chain	Res	Type
1	D	115	LYS
1	F	296	ASN
1	B	296	ASN

### 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	259/283 (92%)	249 (96%)	10 (4%)	39	75
1	B	259/283 (92%)	247 (95%)	12 (5%)	33	71
1	C	259/283 (92%)	247 (95%)	12 (5%)	33	71
1	D	259/283 (92%)	247 (95%)	12 (5%)	33	71
1	E	259/283 (92%)	247 (95%)	12 (5%)	33	71
1	F	259/283 (92%)	249 (96%)	10 (4%)	39	75
1	G	259/283 (92%)	247 (95%)	12 (5%)	33	71
1	H	259/283 (92%)	246 (95%)	13 (5%)	30	68
All	All	2072/2264 (92%)	1979 (96%)	93 (4%)	34	72

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	85	SER
1	A	111	LEU
1	A	113	ASP
1	A	291	LEU
1	A	296	ASN
1	A	301	ASP
1	A	317	VAL
1	A	320	GLU
1	A	329	ARG
1	B	48	LEU
1	B	85	SER

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Mol	Chain	Res	Type
1	B	111	LEU
1	B	218	LYS
1	B	285	ILE
1	B	291	LEU
1	B	294	ASN
1	B	300	HIS
1	B	301	ASP
1	B	317	VAL
1	B	320	GLU
1	B	329	ARG
1	C	43	LEU
1	C	48	LEU
1	C	85	SER
1	C	93	ARG
1	C	111	LEU
1	C	113	ASP
1	C	291	LEU
1	C	294	ASN
1	C	297	LYS
1	C	301	ASP
1	C	320	GLU
1	C	329	ARG
1	D	48	LEU
1	D	85	SER
1	D	111	LEU
1	D	113	ASP
1	D	125	LEU
1	D	285	ILE
1	D	291	LEU
1	D	294	ASN
1	D	301	ASP
1	D	317	VAL
1	D	320	GLU
1	D	329	ARG
1	E	48	LEU
1	E	85	SER
1	E	111	LEU
1	E	113	ASP
1	E	218	LYS
1	E	291	LEU
1	E	294	ASN
1	E	297	LYS

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Mol	Chain	Res	Type
1	E	301	ASP
1	E	317	VAL
1	E	320	GLU
1	E	329	ARG
1	F	48	LEU
1	F	85	SER
1	F	111	LEU
1	F	269	SER
1	F	291	LEU
1	F	294	ASN
1	F	301	ASP
1	F	317	VAL
1	F	320	GLU
1	F	329	ARG
1	G	48	LEU
1	G	85	SER
1	G	111	LEU
1	G	285	ILE
1	G	291	LEU
1	G	296	ASN
1	G	297	LYS
1	G	298	VAL
1	G	301	ASP
1	G	317	VAL
1	G	320	GLU
1	G	329	ARG
1	H	48	LEU
1	H	85	SER
1	H	86	LEU
1	H	93	ARG
1	H	111	LEU
1	H	117	ILE
1	H	285	ILE
1	H	291	LEU
1	H	294	ASN
1	H	301	ASP
1	H	317	VAL
1	H	320	GLU
1	H	329	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	99	HIS
1	A	174	ASN
1	A	208	ASN
1	B	99	HIS
1	B	172	GLN
1	B	174	ASN
1	B	208	ASN
1	C	99	HIS
1	C	174	ASN
1	C	208	ASN
1	D	99	HIS
1	D	172	GLN
1	D	174	ASN
1	D	208	ASN
1	E	99	HIS
1	E	172	GLN
1	E	174	ASN
1	E	208	ASN
1	F	99	HIS
1	F	172	GLN
1	F	208	ASN
1	G	99	HIS
1	G	172	GLN
1	G	208	ASN
1	G	294	ASN
1	H	99	HIS
1	H	174	ASN
1	H	208	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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	318/345 (92%)	-0.08	1 (0%) 94 95	52, 68, 91, 126	0
1	B	318/345 (92%)	-0.07	1 (0%) 94 95	48, 69, 94, 111	0
1	C	318/345 (92%)	-0.11	1 (0%) 94 95	50, 69, 99, 124	0
1	D	318/345 (92%)	0.17	6 (1%) 70 70	56, 84, 112, 128	0
1	E	318/345 (92%)	0.11	7 (2%) 65 65	51, 79, 113, 140	0
1	F	318/345 (92%)	0.65	35 (11%) 7 7	64, 104, 154, 175	0
1	G	318/345 (92%)	0.64	46 (14%) 3 3	81, 102, 138, 172	0
1	H	318/345 (92%)	1.92	131 (41%) 0 1	111, 173, 210, 225	0
All	All	2544/2760 (92%)	0.40	228 (8%) 12 12	48, 86, 180, 225	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	47	ALA	11.5
1	H	158	ALA	9.0
1	H	224	GLY	7.1
1	H	241	TYR	7.0
1	H	29	ASP	6.7
1	F	244	TYR	6.6
1	H	223	LEU	6.4
1	H	79	SER	6.3
1	H	76	ILE	5.9
1	H	222	ASP	5.8
1	H	48	LEU	5.7
1	H	77	PRO	5.6
1	H	32	MET	5.5
1	H	28	ILE	5.4
1	G	248	ALA	5.3
1	H	220	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	F	238	SER	5.2
1	H	49	THR	5.2
1	H	326	LEU	5.2
1	F	249	TYR	5.2
1	F	99	HIS	5.1
1	H	64	ALA	5.0
1	H	125	LEU	4.9
1	G	245	HIS	4.8
1	H	245	HIS	4.7
1	H	216	THR	4.7
1	H	124	TYR	4.7
1	H	215	TRP	4.7
1	H	107	THR	4.7
1	H	267	ASP	4.7
1	H	238	SER	4.7
1	F	245	HIS	4.6
1	H	127	GLN	4.6
1	F	250	ASP	4.5
1	H	62	VAL	4.4
1	G	244	TYR	4.4
1	H	20	VAL	4.4
1	H	218	LYS	4.3
1	H	96	ASP	4.2
1	H	214	TYR	4.2
1	H	266	VAL	4.2
1	H	157	PHE	4.2
1	H	333	PRO	4.2
1	F	305	TRP	4.2
1	F	240	PHE	4.2
1	H	154	ASP	4.2
1	H	60	ALA	4.1
1	H	103	GLY	4.1
1	F	241	TYR	4.1
1	H	102	ASP	4.1
1	H	234	LEU	4.1
1	H	156	THR	4.0
1	G	241	TYR	4.0
1	H	235	TYR	4.0
1	H	113	ASP	3.9
1	H	78	VAL	3.9
1	H	225	ARG	3.9
1	D	92	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	93	ARG	3.8
1	H	104	LEU	3.8
1	H	246	ARG	3.8
1	H	67	LEU	3.7
1	H	129	VAL	3.6
1	F	248	ALA	3.6
1	H	231	GLY	3.6
1	H	277	ALA	3.5
1	G	249	TYR	3.5
1	H	330	LEU	3.5
1	H	132	PHE	3.4
1	H	217	GLY	3.4
1	G	333	PRO	3.4
1	H	230	PHE	3.4
1	H	69	GLU	3.4
1	H	35	PHE	3.4
1	H	248	ALA	3.4
1	G	250	ASP	3.3
1	H	219	ASP	3.3
1	H	221	GLU	3.3
1	H	137	THR	3.3
1	F	333	PRO	3.3
1	H	38	LEU	3.3
1	H	155	PRO	3.3
1	H	227	ASP	3.2
1	F	251	ILE	3.2
1	G	300	HIS	3.2
1	H	253	ALA	3.2
1	H	198	CYS	3.2
1	H	22	ILE	3.2
1	F	215	TRP	3.2
1	H	232	LYS	3.1
1	H	233	TYR	3.1
1	H	328	GLU	3.1
1	H	242	ALA	3.0
1	G	301	ASP	3.0
1	H	159	LYS	3.0
1	F	247	GLU	3.0
1	G	102	ASP	3.0
1	H	251	ILE	3.0
1	H	63	ASN	3.0
1	H	135	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	286	CYS	2.9
1	H	252	ASP	2.9
1	H	131	GLU	2.9
1	H	254	ILE	2.9
1	H	308	ILE	2.9
1	F	252	ASP	2.9
1	G	222	ASP	2.9
1	F	216	THR	2.9
1	H	332	ALA	2.8
1	H	255	TYR	2.8
1	H	26	PRO	2.8
1	G	105	GLY	2.8
1	F	242	ALA	2.8
1	G	215	TRP	2.8
1	H	122	PRO	2.8
1	H	46	ILE	2.8
1	H	39	LYS	2.8
1	G	247	GLU	2.8
1	F	71	ALA	2.8
1	H	110	THR	2.8
1	F	234	LEU	2.8
1	C	294	ASN	2.8
1	H	21	ILE	2.7
1	F	98	VAL	2.7
1	H	123	ASP	2.7
1	H	244	TYR	2.7
1	H	106	ASN	2.7
1	E	227	ASP	2.7
1	E	215	TRP	2.7
1	F	253	ALA	2.6
1	G	40	SER	2.6
1	F	296	ASN	2.6
1	H	41	PRO	2.6
1	F	95	ALA	2.6
1	H	117	ILE	2.6
1	G	223	LEU	2.6
1	H	249	TYR	2.6
1	H	121	ALA	2.6
1	D	84	THR	2.6
1	G	235	TYR	2.6
1	F	223	LEU	2.5
1	G	97	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	305	TRP	2.5
1	G	225	ARG	2.5
1	H	226	SER	2.5
1	H	23	ASP	2.5
1	H	193	ASP	2.5
1	G	329	ARG	2.5
1	G	221	GLU	2.5
1	D	251	ILE	2.5
1	H	145	THR	2.5
1	F	222	ASP	2.5
1	H	305	TRP	2.5
1	D	300	HIS	2.5
1	H	40	SER	2.5
1	G	239	HIS	2.4
1	G	111	LEU	2.4
1	G	70	PHE	2.4
1	E	238	SER	2.4
1	G	285	ILE	2.4
1	G	238	SER	2.4
1	H	18	LYS	2.4
1	H	186	TYR	2.4
1	H	229	LYS	2.4
1	H	81	GLY	2.4
1	D	83	ARG	2.4
1	F	298	VAL	2.4
1	H	44	ASP	2.4
1	H	237	ALA	2.4
1	G	99	HIS	2.4
1	G	246	ARG	2.3
1	H	42	GLU	2.3
1	H	58	PRO	2.3
1	F	246	ARG	2.3
1	G	197	THR	2.3
1	B	298	VAL	2.3
1	G	230	PHE	2.3
1	H	292	PHE	2.3
1	F	110	THR	2.3
1	G	242	ALA	2.2
1	H	74	GLU	2.2
1	G	234	LEU	2.2
1	H	17	PRO	2.2
1	H	161	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	233	TYR	2.2
1	H	250	ASP	2.2
1	G	306	CYS	2.2
1	G	95	ALA	2.2
1	H	239	HIS	2.2
1	H	306	CYS	2.2
1	G	104	LEU	2.2
1	H	50	THR	2.2
1	H	240	PHE	2.2
1	H	160	LYS	2.2
1	E	224	GLY	2.2
1	E	223	LEU	2.2
1	F	148	ALA	2.2
1	G	39	LYS	2.2
1	F	196	PHE	2.2
1	F	308	ILE	2.2
1	E	328	GLU	2.1
1	H	323	ALA	2.1
1	H	278	VAL	2.1
1	H	94	ILE	2.1
1	H	116	PRO	2.1
1	G	330	LEU	2.1
1	H	55	VAL	2.1
1	H	150	ALA	2.1
1	G	198	CYS	2.1
1	F	159	LYS	2.1
1	G	308	ILE	2.1
1	A	294	ASN	2.1
1	F	105	GLY	2.1
1	H	259	PRO	2.1
1	H	151	VAL	2.1
1	G	106	ASN	2.1
1	F	239	HIS	2.0
1	H	98	VAL	2.1
1	G	110	THR	2.0
1	H	59	THR	2.0
1	H	126	ILE	2.0
1	H	191	ALA	2.0
1	G	232	LYS	2.0
1	F	86	LEU	2.0
1	D	215	TRP	2.0
1	G	295	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	61	THR	2.0
1	E	220	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	B	400	1/1	0.97	0.32	5.66	65,65,65,65	0
2	CA	E	400	1/1	0.92	0.24	2.67	77,77,77,77	0
2	CA	D	400	1/1	0.94	0.27	2.62	64,64,64,64	0
2	CA	C	400	1/1	0.95	0.24	1.69	62,62,62,62	0
2	CA	A	400	1/1	0.95	0.20	-0.04	62,62,62,62	0
2	CA	G	400	1/1	0.95	0.13	-0.94	86,86,86,86	0
2	CA	H	400	1/1	0.68	0.10	-1.00	146,146,146,146	0
2	CA	F	400	1/1	0.96	0.09	-2.30	85,85,85,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.