



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2021 – 04:02 PM EDT

PDB ID : 3GR9  
Title : Crystal structure of ColD H188K S187N  
Authors : Holden, H.M.; Cook, P.D.; Kubiak, R.L.; Toomey, D.P.  
Deposited on : 2009-03-25  
Resolution : 2.20 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

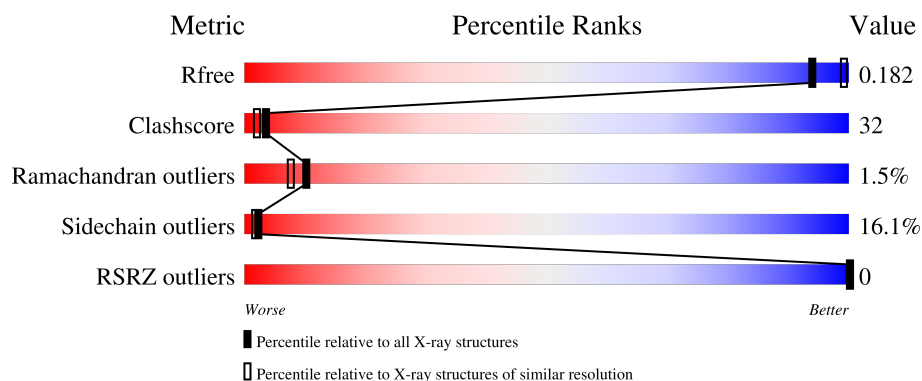
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.




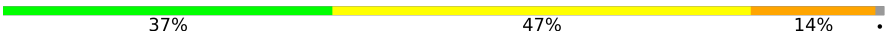

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	390	
1	B	390	
1	C	390	
1	D	390	
1	E	390	

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Mol	Chain	Length	Quality of chain
1	F	390	
1	G	390	
1	H	390	

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	AKG	B	402	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25205 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 ColD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	P	S	0	1	0
			3092	1983	505	589	1	14			
1	B	385	Total	C	N	O	P	S	0	1	0
			3104	1992	506	591	1	14			
1	C	388	Total	C	N	O	P	S	0	1	0
			3128	2007	510	595	1	15			
1	D	381	Total	C	N	O	P	S	0	1	0
			3072	1969	502	586	1	14			
1	E	383	Total	C	N	O	P	S	0	1	0
			3082	1977	503	587	1	14			
1	F	386	Total	C	N	O	P	S	0	1	0
			3112	1996	508	593	1	14			
1	G	387	Total	C	N	O	P	S	0	1	0
			3120	2002	509	594	1	14			
1	H	381	Total	C	N	O	P	S	0	1	0
			3072	1969	502	586	1	14			

There are 32 discrepancies between the modelled and reference sequences:

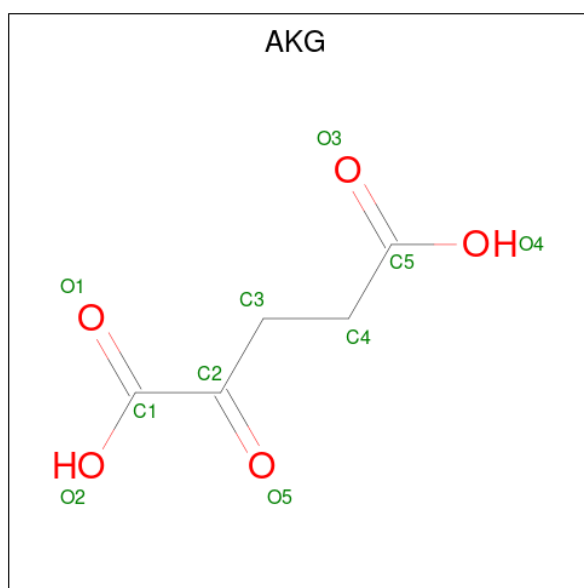
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9F118
A	0	HIS	-	expression tag	UNP Q9F118
A	187	ASN	SER	engineered mutation	UNP Q9F118
A	188	LLP	HIS	engineered mutation	UNP Q9F118
B	-1	GLY	-	expression tag	UNP Q9F118
B	0	HIS	-	expression tag	UNP Q9F118
B	187	ASN	SER	engineered mutation	UNP Q9F118
B	188	LLP	HIS	engineered mutation	UNP Q9F118
C	-1	GLY	-	expression tag	UNP Q9F118
C	0	HIS	-	expression tag	UNP Q9F118
C	187	ASN	SER	engineered mutation	UNP Q9F118
C	188	LLP	HIS	engineered mutation	UNP Q9F118
D	-1	GLY	-	expression tag	UNP Q9F118

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP Q9F118
D	187	ASN	SER	engineered mutation	UNP Q9F118
D	188	LLP	HIS	engineered mutation	UNP Q9F118
E	-1	GLY	-	expression tag	UNP Q9F118
E	0	HIS	-	expression tag	UNP Q9F118
E	187	ASN	SER	engineered mutation	UNP Q9F118
E	188	LLP	HIS	engineered mutation	UNP Q9F118
F	-1	GLY	-	expression tag	UNP Q9F118
F	0	HIS	-	expression tag	UNP Q9F118
F	187	ASN	SER	engineered mutation	UNP Q9F118
F	188	LLP	HIS	engineered mutation	UNP Q9F118
G	-1	GLY	-	expression tag	UNP Q9F118
G	0	HIS	-	expression tag	UNP Q9F118
G	187	ASN	SER	engineered mutation	UNP Q9F118
G	188	LLP	HIS	engineered mutation	UNP Q9F118
H	-1	GLY	-	expression tag	UNP Q9F118
H	0	HIS	-	expression tag	UNP Q9F118
H	187	ASN	SER	engineered mutation	UNP Q9F118
H	188	LLP	HIS	engineered mutation	UNP Q9F118

- Molecule 2 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula:  $C_5H_6O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	1	Total	C	O	0	0
			10	5	5		
2	F	1	Total	C	O	0	0
			10	5	5		
2	H	1	Total	C	O	0	0
			10	5	5		

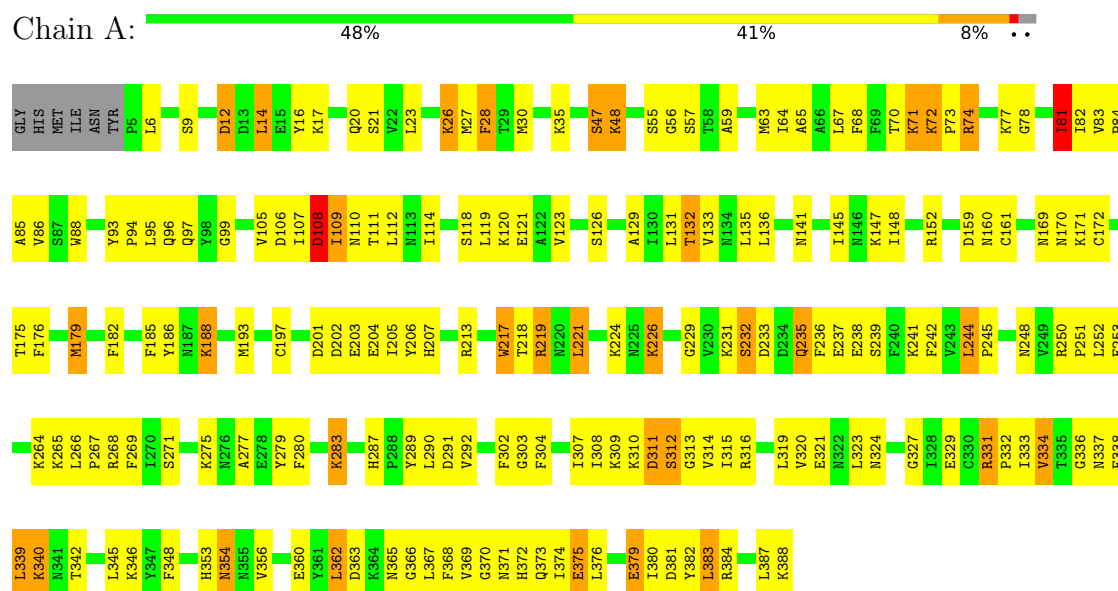
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	52	Total	O	0	0
			52	52		
3	C	50	Total	O	0	0
			50	50		
3	D	55	Total	O	0	0
			55	55		
3	E	37	Total	O	0	0
			37	37		
3	F	43	Total	O	0	0
			43	43		
3	G	41	Total	O	0	0
			41	41		
3	H	43	Total	O	0	0
			43	43		

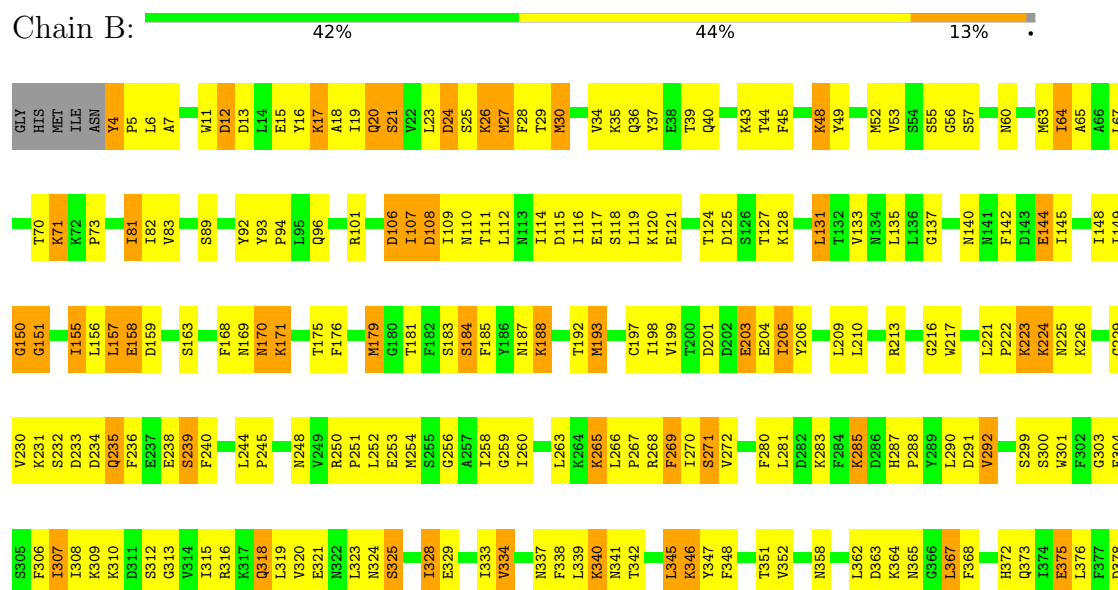
### 3 Residue-property plots

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: Cold



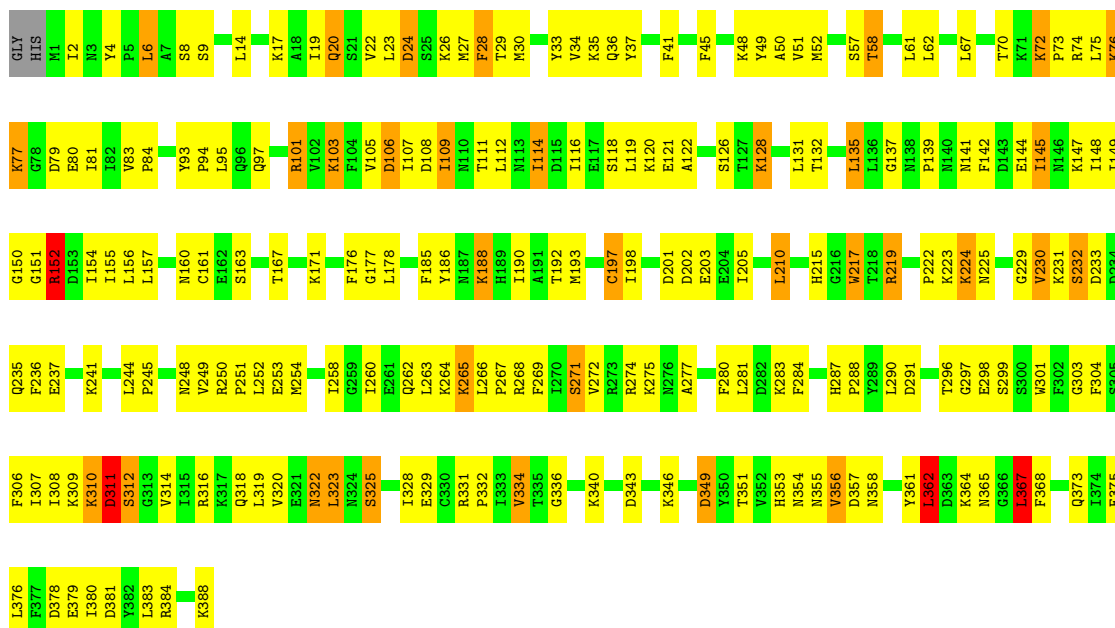
#### • Molecule 1: Cold





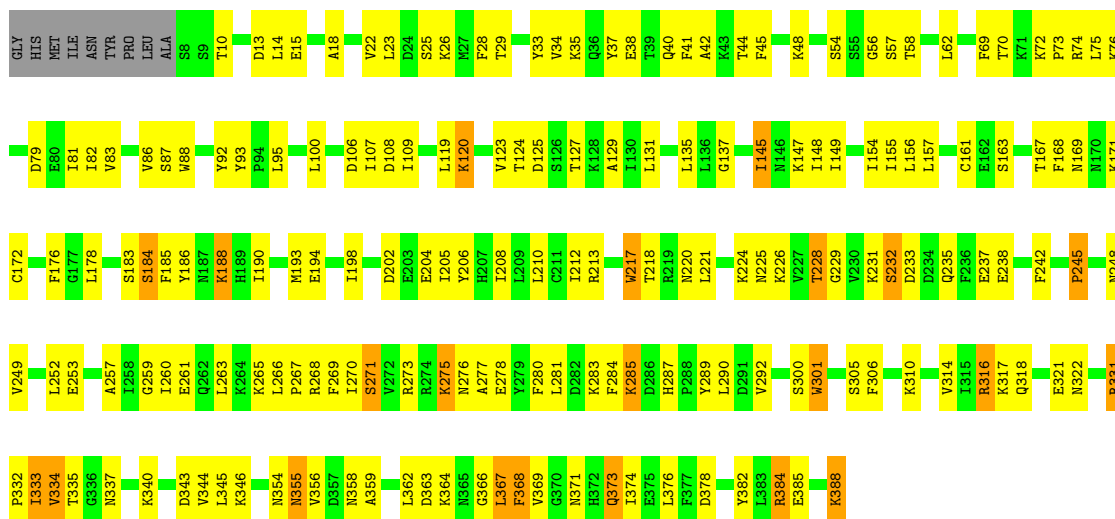
• Molecule 1: Cold

Chain C: 45% 44% 9% ..



• Molecule 1: Cold

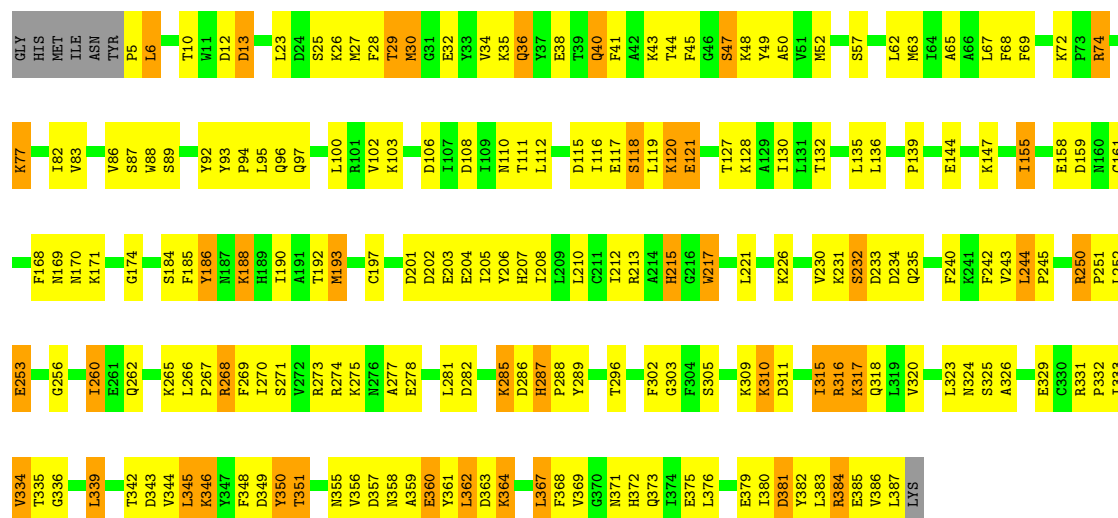
Chain D: 51% 41% 6% .



• Molecule 1: Cold

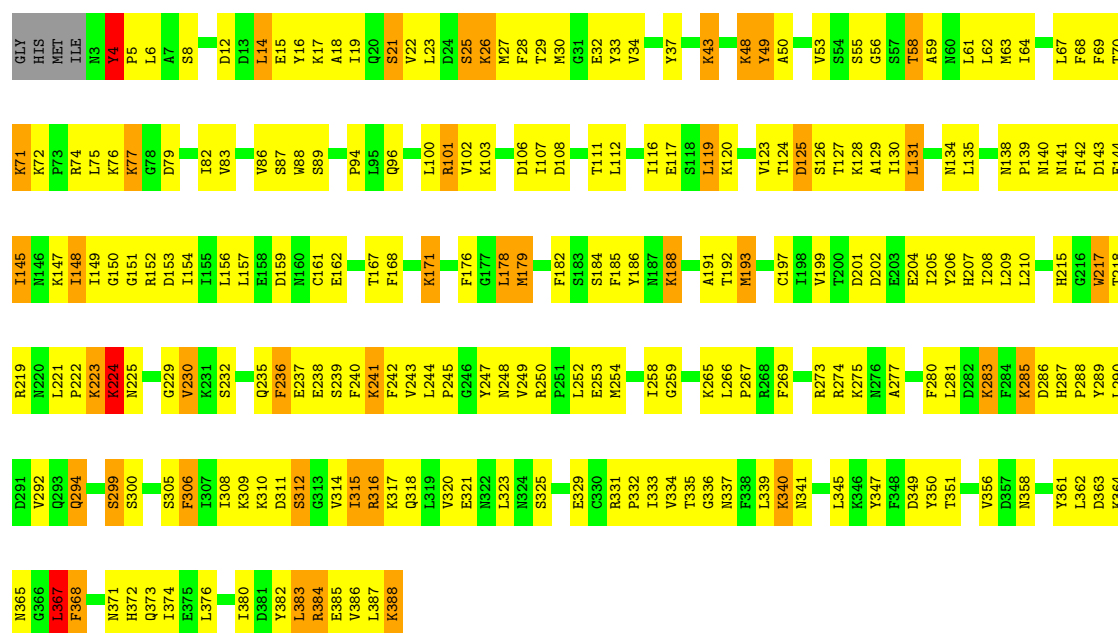
Chain E: 46% 41% 11% .





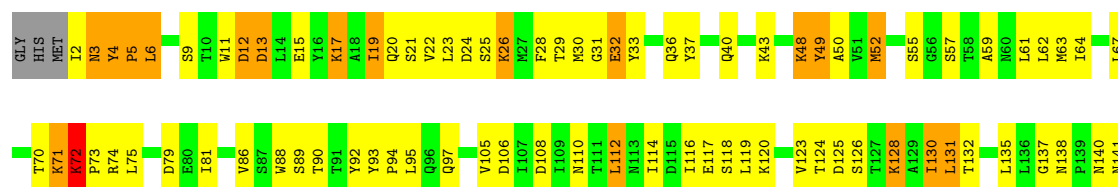
### • Molecule 1: Cold

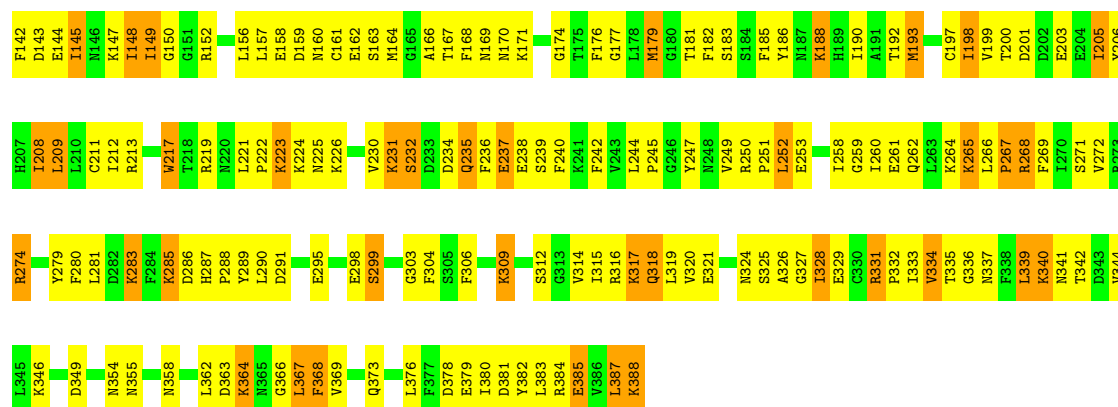
Chain F: 39% 49% 10% ..



### • Molecule 1: Cold

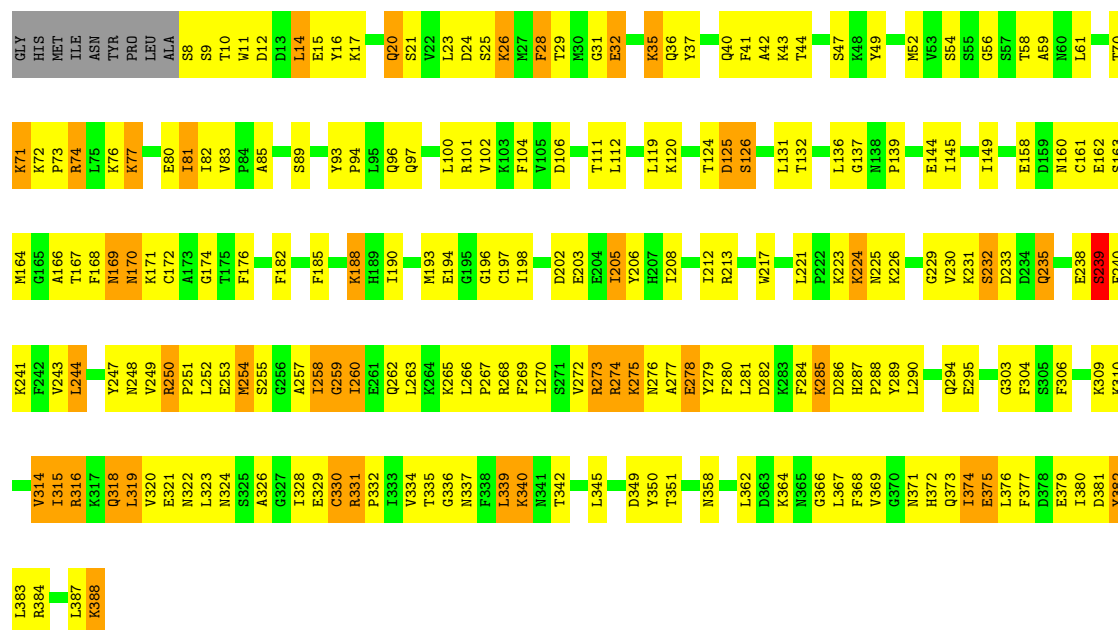
Chain G: 37% 47% 14% .





• Molecule 1: Cold

Chain H: 42% 44% 11% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.73Å 114.66Å 114.57Å 78.98° 76.23° 76.33°	Depositor
Resolution (Å)	50.00 – 2.20 49.10 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.8 (50.00-2.20) 90.4 (49.10-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.62 (at 2.20Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.177 , 0.272 0.182 , 0.182	Depositor DCC
$R_{free}$ test set	15300 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 69.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.289 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	25205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.91 % 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 5.4201e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 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: LLP, AKG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.73	0/3134	1.10	7/4230 (0.2%)
1	B	0.74	0/3147	1.09	6/4249 (0.1%)
1	C	0.72	0/3171	1.08	7/4281 (0.2%)
1	D	0.74	0/3113	1.09	6/4201 (0.1%)
1	E	0.70	0/3124	1.06	7/4219 (0.2%)
1	F	0.70	0/3155	1.07	6/4260 (0.1%)
1	G	0.70	1/3163 (0.0%)	1.07	6/4271 (0.1%)
1	H	0.68	0/3113	1.07	6/4201 (0.1%)
All	All	0.71	1/25120 (0.0%)	1.08	51/33912 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	231	LYS	CB-CG	6.07	1.69	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	G	339	LEU	CA-CB-CG	-7.37	98.35	115.30
1	C	323	LEU	CA-CB-CG	-7.13	98.90	115.30
1	A	213	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	E	381	ASP	CB-CG-OD1	-7.00	112.00	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3092	0	3062	171	0
1	B	3104	0	3070	201	0
1	C	3128	0	3099	195	0
1	D	3072	0	3038	141	0
1	E	3082	0	3050	187	0
1	F	3112	0	3076	251	0
1	G	3120	0	3088	256	0
1	H	3072	0	3039	205	0
2	A	10	0	4	1	0
2	B	10	0	4	5	0
2	C	10	0	4	1	0
2	D	10	0	4	2	0
2	F	10	0	4	3	0
2	H	10	0	4	0	0
3	A	42	0	0	4	0
3	B	52	0	0	4	0
3	C	50	0	0	4	0
3	D	55	0	0	7	0
3	E	37	0	0	4	0
3	F	43	0	0	4	0
3	G	41	0	0	6	0
3	H	43	0	0	6	0
All	All	25205	0	24546	1569	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 32.

The worst 5 of 1569 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:C:52:MET:SD	1:C:52:MET:CE	2.03	1.46
1:F:188:LLP:H4'1	2:F:405:AKG:O5	1.36	1.25
1:B:124:THR:HG22	1:B:125:ASP:H	1.11	1.15
1:C:152:ARG:CG	1:C:152:ARG:HH21	1.59	1.12
1:F:222:PRO:HG2	1:F:225:ASN:HB3	1.26	1.09

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	382/390 (98%)	352 (92%)	25 (6%)	5 (1%)	12	9
1	B	383/390 (98%)	342 (89%)	35 (9%)	6 (2%)	9	7
1	C	386/390 (99%)	336 (87%)	43 (11%)	7 (2%)	8	5
1	D	379/390 (97%)	354 (93%)	22 (6%)	3 (1%)	19	19
1	E	381/390 (98%)	337 (88%)	37 (10%)	7 (2%)	8	5
1	F	384/390 (98%)	338 (88%)	41 (11%)	5 (1%)	12	9
1	G	385/390 (99%)	339 (88%)	40 (10%)	6 (2%)	9	7
1	H	379/390 (97%)	327 (86%)	46 (12%)	6 (2%)	9	7
All	All	3059/3120 (98%)	2725 (89%)	289 (9%)	45 (2%)	10	8

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	SER
1	C	152	ARG
1	G	354	ASN
1	A	311	ASP
1	B	150	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/344 (99%)	287 (84%)	53 (16%)	2	2
1	B	341/344 (99%)	284 (83%)	57 (17%)	2	1
1	C	344/344 (100%)	291 (85%)	53 (15%)	2	2
1	D	338/344 (98%)	293 (87%)	45 (13%)	4	3
1	E	339/344 (98%)	292 (86%)	47 (14%)	3	3
1	F	342/344 (99%)	285 (83%)	57 (17%)	2	1
1	G	343/344 (100%)	282 (82%)	61 (18%)	2	1
1	H	338/344 (98%)	269 (80%)	69 (20%)	1	1
All	All	2725/2752 (99%)	2283 (84%)	442 (16%)	2	2

5 of 442 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	260	ILE
1	F	217	TRP
1	H	374	ILE
1	H	170	ASN
1	E	316	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	170	ASN
1	H	322	ASN
1	D	322	ASN
1	D	235	GLN
1	H	324	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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
1	LLP	D	188	1	23,24,25	1.23	2 (8%)	25,32,34	1.03	2 (8%)
1	LLP	E	188	1	23,24,25	1.30	4 (17%)	25,32,34	1.16	1 (4%)
1	LLP	F	188	1	23,24,25	1.03	2 (8%)	25,32,34	1.14	1 (4%)
1	LLP	C	188	1	23,24,25	1.11	1 (4%)	25,32,34	0.98	2 (8%)
1	LLP	B	188	1	23,24,25	1.09	2 (8%)	25,32,34	1.15	1 (4%)
1	LLP	H	188	1	23,24,25	1.40	4 (17%)	25,32,34	1.16	2 (8%)
1	LLP	G	188	1	23,24,25	1.25	1 (4%)	25,32,34	1.18	2 (8%)
1	LLP	A	188	1	23,24,25	1.47	4 (17%)	25,32,34	1.29	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	D	188	1	-	5/16/17/19	0/1/1/1
1	LLP	E	188	1	-	3/16/17/19	0/1/1/1
1	LLP	F	188	1	-	8/16/17/19	0/1/1/1
1	LLP	C	188	1	-	9/16/17/19	0/1/1/1
1	LLP	B	188	1	-	5/16/17/19	0/1/1/1
1	LLP	H	188	1	-	5/16/17/19	0/1/1/1
1	LLP	G	188	1	-	6/16/17/19	0/1/1/1
1	LLP	A	188	1	-	9/16/17/19	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	188	LLP	P-OP1	4.34	1.64	1.50
1	D	188	LLP	P-OP1	4.28	1.64	1.50
1	G	188	LLP	P-OP1	4.25	1.64	1.50
1	A	188	LLP	P-OP1	4.22	1.64	1.50
1	E	188	LLP	P-OP1	3.91	1.63	1.50

The worst 5 of 14 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	188	LLP	C4-C3-C2	-3.71	117.89	120.19
1	H	188	LLP	C4-C3-C2	-3.68	117.91	120.19
1	B	188	LLP	OP2-P-OP4	3.00	114.72	106.73
1	A	188	LLP	OP4-C5'-C5	-2.89	103.84	109.35
1	F	188	LLP	C5-C6-N1	-2.45	119.74	123.82

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	188	LLP	C5'-OP4-P-OP3
1	A	188	LLP	N-CA-CB-CG
1	A	188	LLP	O-C-CA-CB
1	B	188	LLP	N-CA-CB-CG
1	B	188	LLP	O-C-CA-CB

There are no ring outliers.

8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	188	LLP	1	0
1	E	188	LLP	3	0
1	F	188	LLP	8	0
1	C	188	LLP	4	0
1	B	188	LLP	6	0
1	H	188	LLP	3	0
1	G	188	LLP	3	0
1	A	188	LLP	4	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands 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	AKG	A	401	-	3,9,9	0.38	0	4,11,11	1.16	1 (25%)
2	AKG	D	404	-	3,9,9	0.33	0	4,11,11	2.27	1 (25%)
2	AKG	H	406	-	3,9,9	1.09	0	4,11,11	2.95	3 (75%)
2	AKG	B	402	-	3,9,9	1.17	0	4,11,11	2.21	2 (50%)
2	AKG	F	405	-	3,9,9	0.27	0	4,11,11	1.80	1 (25%)
2	AKG	C	403	-	3,9,9	0.48	0	4,11,11	1.34	1 (25%)

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	AKG	A	401	-	-	2/3/9/9	-
2	AKG	D	404	-	-	2/3/9/9	-
2	AKG	H	406	-	-	2/3/9/9	-
2	AKG	B	402	-	-	0/3/9/9	-
2	AKG	F	405	-	-	2/3/9/9	-
2	AKG	C	403	-	-	2/3/9/9	-

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	406	AKG	C4-C3-C2	-3.99	104.53	113.14
2	D	404	AKG	C3-C4-C5	-3.85	106.20	112.67
2	H	406	AKG	C3-C4-C5	-3.55	106.72	112.67
2	F	405	AKG	C4-C3-C2	-3.37	105.86	113.14
2	B	402	AKG	C3-C4-C5	-3.24	107.24	112.67

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	403	AKG	O5-C2-C3-C4
2	F	405	AKG	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	C	403	AKG	C1-C2-C3-C4
2	D	404	AKG	O5-C2-C3-C4
2	D	404	AKG	C1-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	AKG	1	0
2	D	404	AKG	2	0
2	B	402	AKG	5	0
2	F	405	AKG	3	0
2	C	403	AKG	1	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 [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, 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	383/390 (98%)	-1.59	0 100 100	11, 37, 67, 96	0
1	B	384/390 (98%)	-1.59	0 100 100	14, 36, 70, 88	0
1	C	387/390 (99%)	-1.58	0 100 100	10, 38, 73, 89	0
1	D	380/390 (97%)	-1.59	0 100 100	11, 37, 66, 94	0
1	E	382/390 (97%)	-1.56	0 100 100	13, 42, 72, 94	0
1	F	385/390 (98%)	-1.57	0 100 100	13, 40, 73, 92	0
1	G	386/390 (98%)	-1.55	0 100 100	15, 45, 74, 98	0
1	H	380/390 (97%)	-1.54	0 100 100	14, 45, 77, 100	0
All	All	3067/3120 (98%)	-1.57	0 100 100	10, 40, 73, 100	0

There are no RSRZ outliers to report.

### 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	LLP	F	188	24/25	0.99	0.05	32,59,99,99	0
1	LLP	B	188	24/25	1.00	0.05	11,28,86,99	0
1	LLP	C	188	24/25	1.00	0.05	10,26,55,83	0
1	LLP	D	188	24/25	1.00	0.05	14,36,61,69	0
1	LLP	E	188	24/25	1.00	0.05	5,40,99,99	0
1	LLP	A	188	24/25	1.00	0.05	7,34,55,78	0
1	LLP	G	188	24/25	1.00	0.05	13,26,57,66	0
1	LLP	H	188	24/25	1.00	0.05	13,39,98,99	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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	AKG	A	401	10/10	0.99	0.07	34,66,99,99	0
2	AKG	B	402	10/10	0.99	0.05	16,32,70,79	0
2	AKG	C	403	10/10	0.99	0.04	16,32,99,99	0
2	AKG	D	404	10/10	0.99	0.05	23,42,99,99	0
2	AKG	F	405	10/10	0.99	0.06	43,62,99,99	0
2	AKG	H	406	10/10	0.99	0.04	15,37,99,99	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.