



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:17 am GMT

PDB ID : 4YD9
Title : Crystal structure of squid hemocyanin
Authors : Matsuno, A.; Gai, Z.; Kato, K.; Tanaka, Y.; Yao, M.
Deposited on : 2015-02-21
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28972

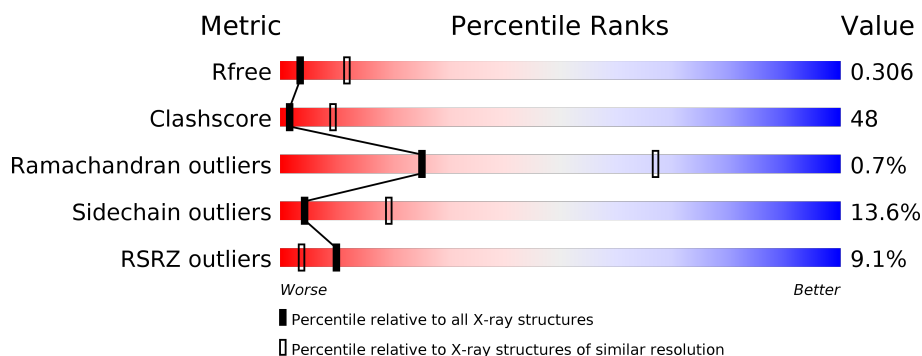
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 ≥ 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	2000	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>27%</div> <div>•</div> <div>17%</div> </div> </div>
1	D	2000	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div>29%</div> <div>5%</div> <div>17%</div> </div> </div>
1	G	2000	<div> <div>%</div> <div> <div></div> <div>48%</div> <div>29%</div> <div>5%</div> <div>17%</div> </div> </div>
1	J	2000	<div> <div>2%</div> <div> <div></div> <div>48%</div> <div>30%</div> <div>5%</div> <div>17%</div> </div> </div>
1	M	2000	<div> <div>%</div> <div> <div></div> <div>52%</div> <div>27%</div> <div>•</div> <div>17%</div> </div> </div>
1	P	2000	<div> <div>%</div> <div> <div></div> <div>50%</div> <div>28%</div> <div>5%</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	S	2000	
1	V	2000	
1	Y	2000	
1	b	2000	
2	B	920	
2	E	920	
2	H	920	
2	K	920	
2	N	920	
2	Q	920	
2	T	920	
2	W	920	
2	Z	920	
2	c	920	
3	C	394	
3	F	394	
3	I	394	
3	L	394	
3	O	394	
3	R	394	
3	U	394	
3	X	394	
3	a	394	
3	d	394	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CUO	A	5001	-	-	X	-
4	CUO	C	3401[A]	-	-	X	-
4	CUO	C	3401[B]	-	-	X	-
4	CUO	C	3402[A]	-	-	X	-
4	CUO	C	3402[B]	-	-	X	-
4	CUO	F	3401[B]	-	-	X	-
4	CUO	F	3402[A]	-	-	X	-
4	CUO	I	3401[A]	-	-	X	-
4	CUO	I	3402[A]	-	-	X	-
4	CUO	M	2105	-	-	X	-
4	CUO	O	3401[A]	-	-	X	-
4	CUO	O	3401[B]	-	-	X	-
4	CUO	S	2104	-	-	X	-
4	CUO	U	3401[A]	-	-	X	-
4	CUO	U	3401[B]	-	-	X	-
4	CUO	X	3401[A]	-	-	X	X
4	CUO	X	3401[B]	-	-	X	X
4	CUO	d	3401[A]	-	-	-	X
4	CUO	d	3401[B]	-	-	-	X
5	NAG	D	5014	-	-	X	-
5	NAG	G	2111	-	-	X	-
5	NAG	G	2112	-	-	X	X
5	NAG	M	2115	-	-	X	-
5	NAG	V	5015	-	-	X	-
5	NAG	V	5016	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 261470 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 hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	D	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	G	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	J	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	M	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	P	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	S	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	V	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	Y	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	b	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			

- Molecule 2 is a protein called hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	E	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	H	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	K	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			

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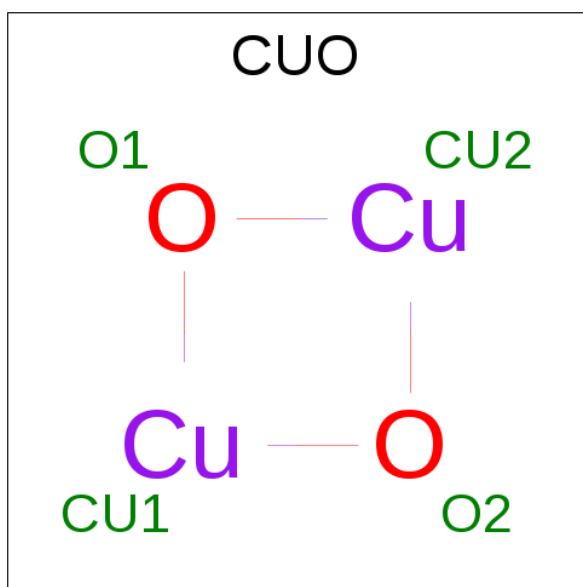
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	Q	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	T	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	W	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	Z	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	c	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			

- Molecule 3 is a protein called hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	F	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	I	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	L	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	O	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	R	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	U	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	X	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	a	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	d	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			

- Molecule 4 is CU2-O2 CLUSTER (three-letter code: CUO) (formula: Cu₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Cu	O	0	0
			4	2	2		
4	A	1	Total	Cu	O	0	0
			4	2	2		
4	A	1	Total	Cu	O	0	0
			4	2	2		
4	A	1	Total	Cu	O	0	0
			4	2	2		
4	A	1	Total	Cu	O	0	1
			8	4	4		
4	B	1	Total	Cu	O	0	0
			4	2	2		
4	B	1	Total	Cu	O	0	0
			4	2	2		
4	C	1	Total	Cu	O	0	1
			8	4	4		
4	C	1	Total	Cu	O	0	1
			8	4	4		
4	D	1	Total	Cu	O	0	0
			4	2	2		
4	D	1	Total	Cu	O	0	0
			4	2	2		
4	D	1	Total	Cu	O	0	0
			4	2	2		
4	D	1	Total	Cu	O	0	0
			4	2	2		
4	D	1	Total	Cu	O	0	1
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total 4	Cu 2	O 2	0	0
4	E	1	Total 4	Cu 2	O 2	0	0
4	F	1	Total 8	Cu 4	O 4	0	1
4	F	1	Total 8	Cu 4	O 4	0	1
4	G	1	Total 8	Cu 4	O 4	0	1
4	G	1	Total 4	Cu 2	O 2	0	0
4	G	1	Total 4	Cu 2	O 2	0	0
4	G	1	Total 4	Cu 2	O 2	0	0
4	G	1	Total 4	Cu 2	O 2	0	0
4	H	1	Total 4	Cu 2	O 2	0	0
4	H	1	Total 4	Cu 2	O 2	0	0
4	I	1	Total 8	Cu 4	O 4	0	1
4	I	1	Total 8	Cu 4	O 4	0	1
4	J	1	Total 4	Cu 2	O 2	0	0
4	J	1	Total 4	Cu 2	O 2	0	0
4	J	1	Total 4	Cu 2	O 2	0	0
4	J	1	Total 4	Cu 2	O 2	0	0
4	J	1	Total 8	Cu 4	O 4	0	1
4	K	1	Total 4	Cu 2	O 2	0	0
4	K	1	Total 4	Cu 2	O 2	0	0
4	M	1	Total 8	Cu 4	O 4	0	1

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	1	Total 4	Cu 2	O 2	0	0
4	M	1	Total 4	Cu 2	O 2	0	0
4	M	1	Total 4	Cu 2	O 2	0	0
4	M	1	Total 4	Cu 2	O 2	0	0
4	N	1	Total 4	Cu 2	O 2	0	0
4	N	1	Total 4	Cu 2	O 2	0	0
4	O	1	Total 8	Cu 4	O 4	0	1
4	P	1	Total 4	Cu 2	O 2	0	0
4	P	1	Total 4	Cu 2	O 2	0	0
4	P	1	Total 4	Cu 2	O 2	0	0
4	P	1	Total 4	Cu 2	O 2	0	0
4	P	1	Total 8	Cu 4	O 4	0	1
4	Q	1	Total 4	Cu 2	O 2	0	0
4	Q	1	Total 4	Cu 2	O 2	0	0
4	S	1	Total 8	Cu 4	O 4	0	1
4	S	1	Total 4	Cu 2	O 2	0	0
4	S	1	Total 4	Cu 2	O 2	0	0
4	S	1	Total 4	Cu 2	O 2	0	0
4	S	1	Total 4	Cu 2	O 2	0	0
4	T	1	Total 4	Cu 2	O 2	0	0
4	T	1	Total 4	Cu 2	O 2	0	0

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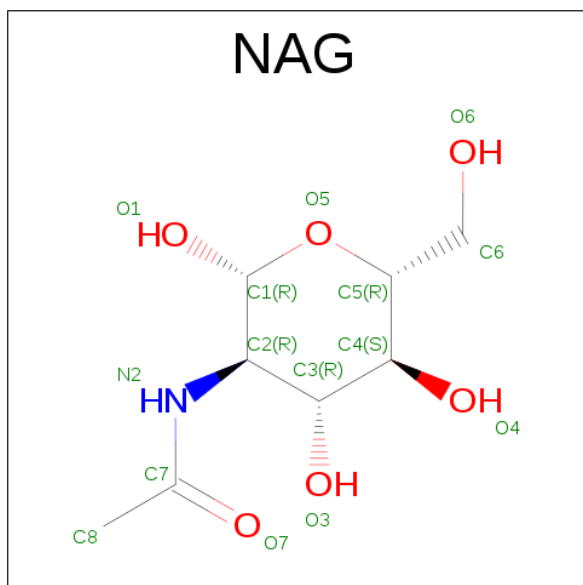
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	U	1	Total 8	Cu 4	O 4	0	1
4	V	1	Total 4	Cu 2	O 2	0	0
4	V	1	Total 4	Cu 2	O 2	0	0
4	V	1	Total 4	Cu 2	O 2	0	0
4	V	1	Total 4	Cu 2	O 2	0	0
4	V	1	Total 8	Cu 4	O 4	0	1
4	W	1	Total 4	Cu 2	O 2	0	0
4	W	1	Total 4	Cu 2	O 2	0	0
4	X	1	Total 8	Cu 4	O 4	0	1
4	Y	1	Total 8	Cu 4	O 4	0	1
4	Y	1	Total 4	Cu 2	O 2	0	0
4	Y	1	Total 4	Cu 2	O 2	0	0
4	Y	1	Total 4	Cu 2	O 2	0	0
4	Y	1	Total 4	Cu 2	O 2	0	0
4	Z	1	Total 4	Cu 2	O 2	0	0
4	Z	1	Total 4	Cu 2	O 2	0	0
4	b	1	Total 8	Cu 4	O 4	0	1
4	b	1	Total 4	Cu 2	O 2	0	0
4	b	1	Total 4	Cu 2	O 2	0	0
4	b	1	Total 4	Cu 2	O 2	0	0
4	b	1	Total 4	Cu 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	c	1	Total	Cu	O	0	0
			4	2	2		
4	c	1	Total	Cu	O	0	0
			4	2	2		
4	d	1	Total	Cu	O	0	1
			8	4	4		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	N	1	Total	C	N	O	0	0
			14	8	1	5		
5	N	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	Q	1	Total	C	N	O	0	0
			14	8	1	5		
5	Q	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	T	1	Total	C	N	O	0	0
			14	8	1	5		
5	T	1	Total	C	N	O	0	0
			14	8	1	5		
5	V	1	Total	C	N	O	0	0
			14	8	1	5		

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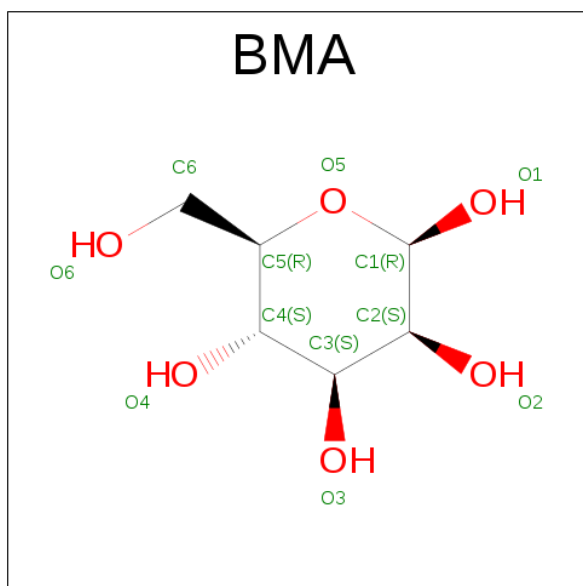
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	V	1	Total	C	N	O	0	0
			14	8	1	5		
5	V	1	Total	C	N	O	0	0
			14	8	1	5		
5	V	1	Total	C	N	O	0	0
			14	8	1	5		
5	V	1	Total	C	N	O	0	0
			14	8	1	5		
5	V	1	Total	C	N	O	0	0
			14	8	1	5		
5	V	1	Total	C	N	O	0	0
			14	8	1	5		
5	V	1	Total	C	N	O	0	0
			14	8	1	5		
5	W	1	Total	C	N	O	0	0
			14	8	1	5		
5	W	1	Total	C	N	O	0	0
			14	8	1	5		
5	Y	1	Total	C	N	O	0	0
			14	8	1	5		
5	Y	1	Total	C	N	O	0	0
			14	8	1	5		
5	Y	1	Total	C	N	O	0	0
			14	8	1	5		
5	Y	1	Total	C	N	O	0	0
			14	8	1	5		
5	Y	1	Total	C	N	O	0	0
			14	8	1	5		
5	Y	1	Total	C	N	O	0	0
			14	8	1	5		
5	Y	1	Total	C	N	O	0	0
			14	8	1	5		
5	Z	1	Total	C	N	O	0	0
			14	8	1	5		
5	Z	1	Total	C	N	O	0	0
			14	8	1	5		
5	b	1	Total	C	N	O	0	0
			14	8	1	5		
5	b	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	b	1	Total	C	N	O	0	0
			14	8	1	5		
5	b	1	Total	C	N	O	0	0
			14	8	1	5		
5	b	1	Total	C	N	O	0	0
			14	8	1	5		
5	b	1	Total	C	N	O	0	0
			14	8	1	5		
5	b	1	Total	C	N	O	0	0
			14	8	1	5		
5	c	1	Total	C	N	O	0	0
			14	8	1	5		
5	c	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



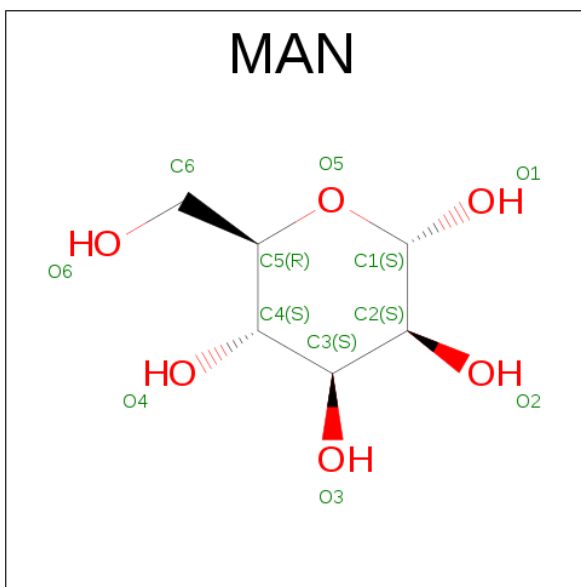
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	J	1	Total	C	O	0	0
			11	6	5		
6	M	1	Total	C	O	0	0
			11	6	5		
6	M	1	Total	C	O	0	0
			11	6	5		
6	M	1	Total	C	O	0	0
			11	6	5		
6	P	1	Total	C	O	0	0
			11	6	5		
6	P	1	Total	C	O	0	0
			11	6	5		
6	S	1	Total	C	O	0	0
			11	6	5		
6	T	1	Total	C	O	0	0
			11	6	5		
6	V	1	Total	C	O	0	0
			11	6	5		
6	V	1	Total	C	O	0	0
			11	6	5		
6	V	1	Total	C	O	0	0
			11	6	5		
6	V	1	Total	C	O	0	0
			11	6	5		
6	Y	1	Total	C	O	0	0
			11	6	5		
6	Y	1	Total	C	O	0	0
			11	6	5		
6	b	1	Total	C	O	0	0
			11	6	5		
6	b	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).

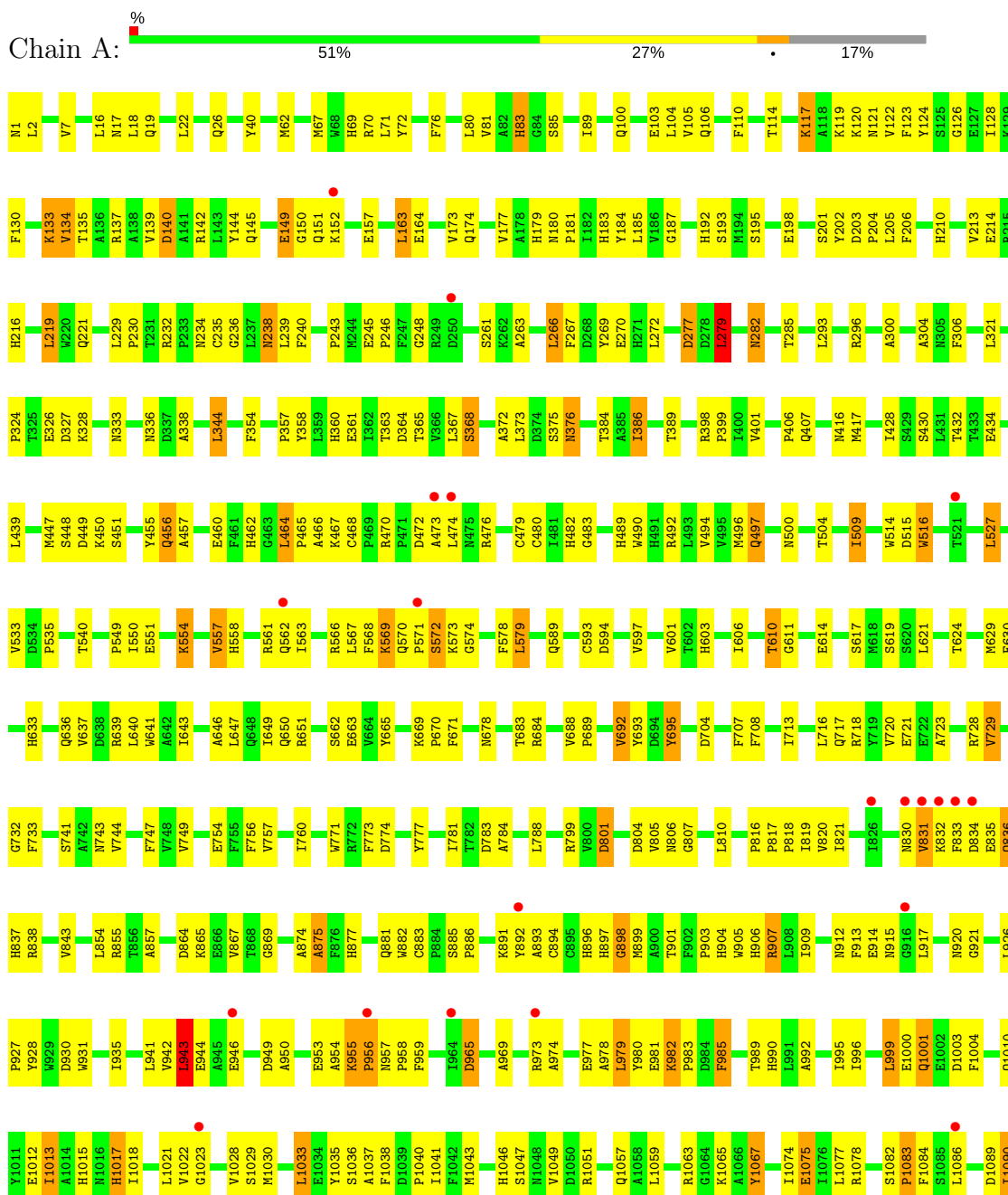


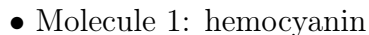
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	M	1	Total	C	O	0	0
			11	6	5		
7	M	1	Total	C	O	0	0
			11	6	5		
7	M	1	Total	C	O	0	0
			11	6	5		
7	S	1	Total	C	O	0	0
			11	6	5		
7	V	1	Total	C	O	0	0
			11	6	5		
7	Y	1	Total	C	O	0	0
			11	6	5		
7	b	1	Total	C	O	0	0
			11	6	5		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: hemocyanin

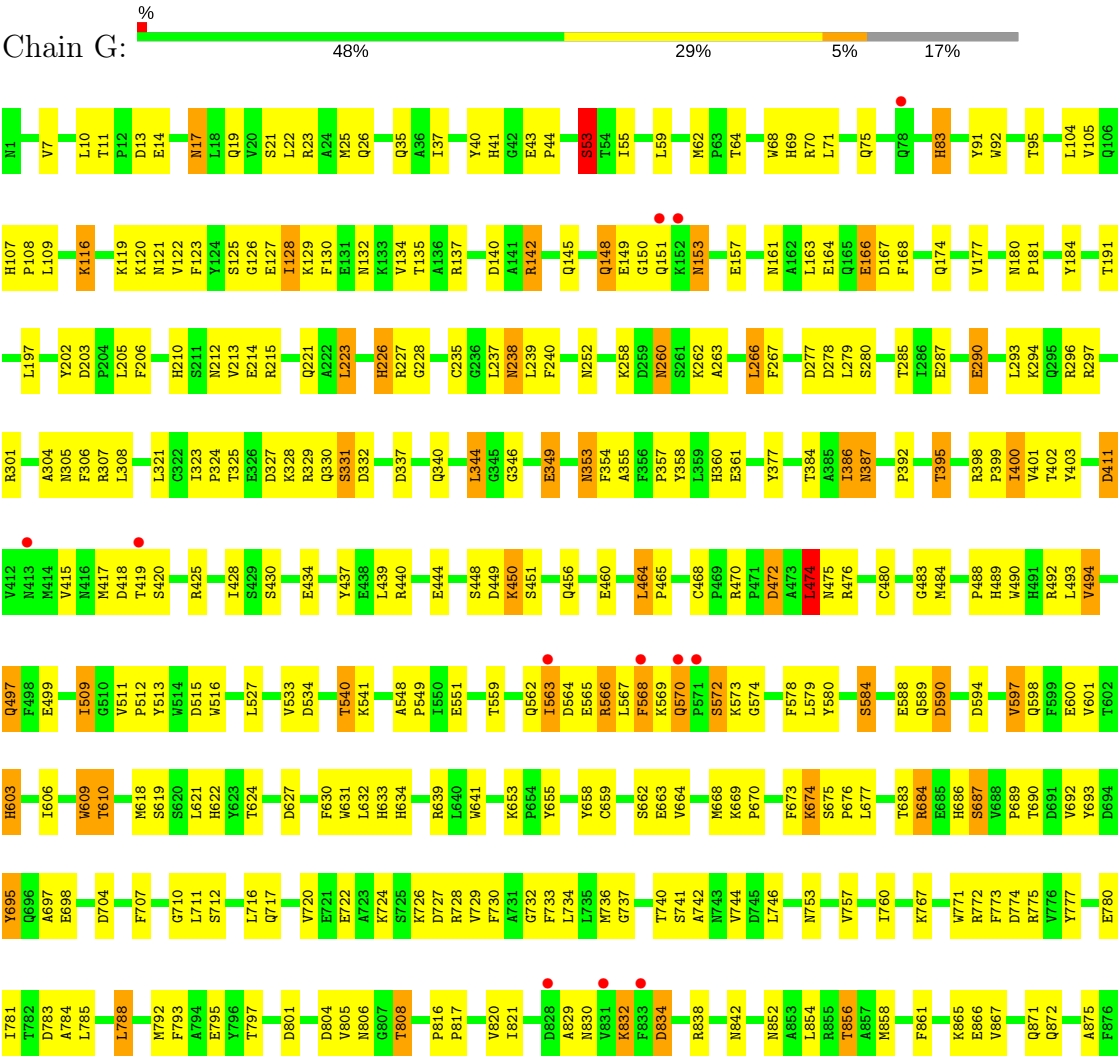




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R1605	L1506	T1407	M1307	Y1211	L1129	E1034	P959	V970	G758	K669	K573	G483	P399	T285
K1616	T1507	H1408	V1308	I1217	I1133	Y1035	P960	Y870	S759	P670	G574	M494	V401	L289
K1617	F1508	F1409	T1310	I1217	M1140	A1037	S961	H877	G962	F671	F578	P488	Q407	R296
M1621	S1511	V1410	C1311	T1221	V1144	I1041	A963	T880	S766	F673	L579	H489	G408	R296
Q1622	V1516	F1411	G1312	L1228	V1144	F1042	D965	Q881	K767	S675	L583	W490	D411	R301
R1627	Y1519	T1414	H1314	K1229	V1144	H1045	S966	C883	W771	P676	F587	V494	N416	A304
E1628	Q1520	T1414	L1148	L1149	E1149	H1045	S970	C883	W771	L677	E588	V494	N305	F306
M1630	Y1525	E1420	M1316	V1231	E1149	H1045	S970	C883	W771	L677	E588	V494	N305	F306
E1631	Y1526	H1422	P1317	V1232	K1152	N1047	T971	S885	Y777	M678	Q589	Q497	M417	F306
L1632	K1527	H1422	F1319	V1234	K1153	N1047	S972	S885	Y777	M678	Q589	Q497	M417	F306
E1633	Y1528	H1422	F1319	V1234	K1153	N1047	S972	S885	Y777	M678	Q589	Q497	M417	F306
L1634	T1529	H1425	F1320	V1236	S1154	D1050	P975	K891	E780	K682	C593	E499	T419	N316
V1635	D1530	H1427	H1321	Y1236	L1156	R1051	L979	Y892	I781	T683	D594	S507	S420	R317
N1636	L1530	H1427	H1321	Y1236	L1156	R1051	L979	Y892	I781	T683	D594	S507	S420	R317
G1637	T1537	H1433	S1328	G1241	F1160	Q1057	P983	C895	L788	P689	T602	V511	T432	T325
S1638	P1538	L1434	L1329	N1242	I1161	L1059	D984	H896	E795	V692	H603	Y513	T433	E326
K1639	Q1539	G1435	L1329	G1244	T1166	Q1060	P985	H897	E795	V692	H603	Y513	T433	E326
T1641	R1542	G1436	D1332	G1244	T1166	Q1060	P985	H897	E795	V692	H603	Y513	T433	E326
I1644	T1543	R1437	E1333	R1247	D1167	R1063	Y988	A900	R799	Y703	W609	D516	L439	R329
M1647	N1547	D1438	E1333	R1247	D1167	R1063	Y988	A900	R799	Y703	W609	D516	L439	R329
I1650	R1550	D1446	E1333	R1247	D1167	R1063	Y988	A900	R799	Y703	W609	D516	L439	R329
D1651	D1551	Y1447	E1333	R1247	D1167	R1063	Y988	A900	R799	Y703	W609	D516	L439	R329
F1652	R1552	Y1447	E1333	R1247	D1167	R1063	Y988	A900	R799	Y703	W609	D516	L439	R329
D1656	T1562	D1451	E1361	R1260	E1174	I1076	S997	H906	N806	G807	L621	L527	F446	Q340
VAL	K1563	H1457	T1363	F1266	F1175	L1077	A998	L908	N806	G807	L621	L527	F446	Q340
PHE	A1564	D1462	S1367	M1271	Y1177	R1078	E1000	N915	T813	L711	P627	D534	M447	M350
GLU	V1568	D1462	S1367	M1271	Y1177	R1078	E1000	N915	T813	L711	P627	D534	M447	M350
ASP	C1573	E1470	N1372	R1275	W1186	S1082	Q1001	L926	P816	P817	P627	D534	M447	M350
THR	V1574	Q1472	K1187	N1276	F1188	F1083	Q1001	L926	P816	P817	P627	D534	M447	M350
TRP	P1575	R1473	K1279	N1276	F1188	F1083	Q1001	L926	P816	P817	P627	D534	M447	M350
ARG	T1576	Y1474	Q1280	N1281	D1189	P1092	I1013	W929	N830	W831	Q636	A548	Q456	E361
ASP	G1577	R1475	Q1280	N1281	D1189	P1092	I1013	W929	N830	W831	Q636	A548	Q456	E361
VAL	I1578	K1476	A1282	D1283	F1191	T1096	H1015	I935	D834	R833	D638	F549	E460	T363
VAL	G1579	L1477	A1282	D1283	F1191	T1096	H1015	I935	D834	R833	D638	F549	E460	T363
THR	E1581	S1478	F1378	F1378	F1378	T1096	H1015	I935	D834	R833	D638	F549	E460	T363
SER	N1582	Y1479	F1384	E1385	D1196	Y1099	H1018	I942	R838	G732	T643	S560	P465	L371
ALA	C1583	Y1479	F1384	E1385	D1196	Y1099	H1018	I942	R838	G732	T643	S560	P465	L371
ASN	G1584	G1484	D1390	R1391	T1197	F1112	A1020	E946	K841	W736	Q662	R561	A466	V383
ARG	N1585	A1485	D1390	R1391	T1197	F1112	A1020	E946	K841	W736	Q662	R561	A466	V383
ARG	P1492	P1492	D1392	Y1296	V1199	H1113	I1021	T948	N842	G737	L647	I563	K467	T384
ARG	G1595	M1493	T1393	Q1299	M1200	D1023	G1023	D949	V843	V843	R651	D564	C468	A385
ASN	E1596	C1494	Q1394	P1301	M1203	D1117	G1024	A950	V843	V843	R651	D564	C468	A385
LEU	T1597	R1494	P1395	P1301	M1203	D1117	G1024	A950	V843	V843	R651	D564	C468	A385
LYS	E1598	S1497	E1396	S1302	L1205	T1118	T1025	E953	R855	T748	V658	R566	P471	T389
ASP	N1498	S1498	L1397	D1303	H1206	L1121	V1028	A954	F861	W748	V658	R566	P471	T389
LEU	S1499	S1499	L1397	D1303	H1206	L1121	V1028	A954	F861	W748	V658	R566	P471	T389
SER	W1601	T1500	G1305	G1305	D1209	I1126	M1030	P956	K865	E966	S662	K569	C480	Q394
														T395
														I396
														P397

LYS	SER	VAL	ALA	PHE
GLU	LEU	THR	ALA	THR
ASP	VAL	VAL	TYR	THR
MET	GLU	ARG	ASP	ASN
PHE	ASN	PRO	PRO	ARG
SER	GLU	PRO	ILE	ASN
LEU	LEU	ARG	PHE	ASP
ARG	LEU	ASP	PHE	ASP
ALA	ALA	GLN	LEU	VAL
ALA	ARG	LEU	HIS	VAL
PHE	GLY	PHE	HIS	THR
LYS	SER	ASN	SER	GLN
ARG	ASP	ASN	THR	ASN
LYS	ASP	VAL	VAL	ASN
MET	MET	ARG	THR	ASP
THR	THR	TYR	ASP	SER
ASP	VAL	LEU	ARG	LEU
ASP	PRO	TYR	LEU	TYR
GLY	TRP	GLU	TRP	ALA
TYR	ASP	HIS	ILE	ASP
GLU	TRP	LEU	TRP	ASP
ILE	ILE	PHE	GLN	ASP
ILE	GLU	ALA	ASP	ALA
ALA	PRO	PHE	GLN	ALA
ALA	LEU	GLU	ARG	ALA
PHE	ASP	HIS	ARG	ALA
PHE	ASP	THR	TYR	ALA
HIS	SER	THR	GLY	ALA
GLY	LEU	ASP	LEU	ALA
LEU	PRO	PHE	LYS	ALA
PRO	GLY	ILE	ILE	ALA
ALA	LEU	CYS	LEU	ALA
ALA	LEU	ASP	ASP	ALA
GLN	ILE	PHE	TYR	ALA
CYS	SER	GLU	ASN	ALA
PRO	ASN	LEU	LEU	ALA
THR	ILE	ASN	LEU	ALA
HIS	LYS	THR	LEU	ALA
THR	ASN	ILE	ASN	ALA
CYS	GLU	ASP	ASP	ALA
CYS	ASP	SER	PRO	ALA
LEU	ILE	TRP	MET	ALA
HIS	GLU	TRP	ARG	ALA
GLY	ASN	ALA	PRO	ALA
MET	PRO	GLY	PHE	ALA
PRO	PHE	ASN	ASN	ALA
THR	HIS	THR	ASN	ALA
PHE	HIS	PRO	LYS	ALA
THR	GLY	THR	THR	ALA
PRO	LYS	ALA	ALA	ALA
HIS	ILE	SER	ILE	ALA
TRP	TRP	MET	ASN	ALA
HIS	SER	SER	GLN	ALA
ARG	SER	SER	ASP	ALA
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TYR	ASP	ASP	ALA	ALA
LEU	ALA	THR	THR	ALA

● Molecule 1: hemocyanin



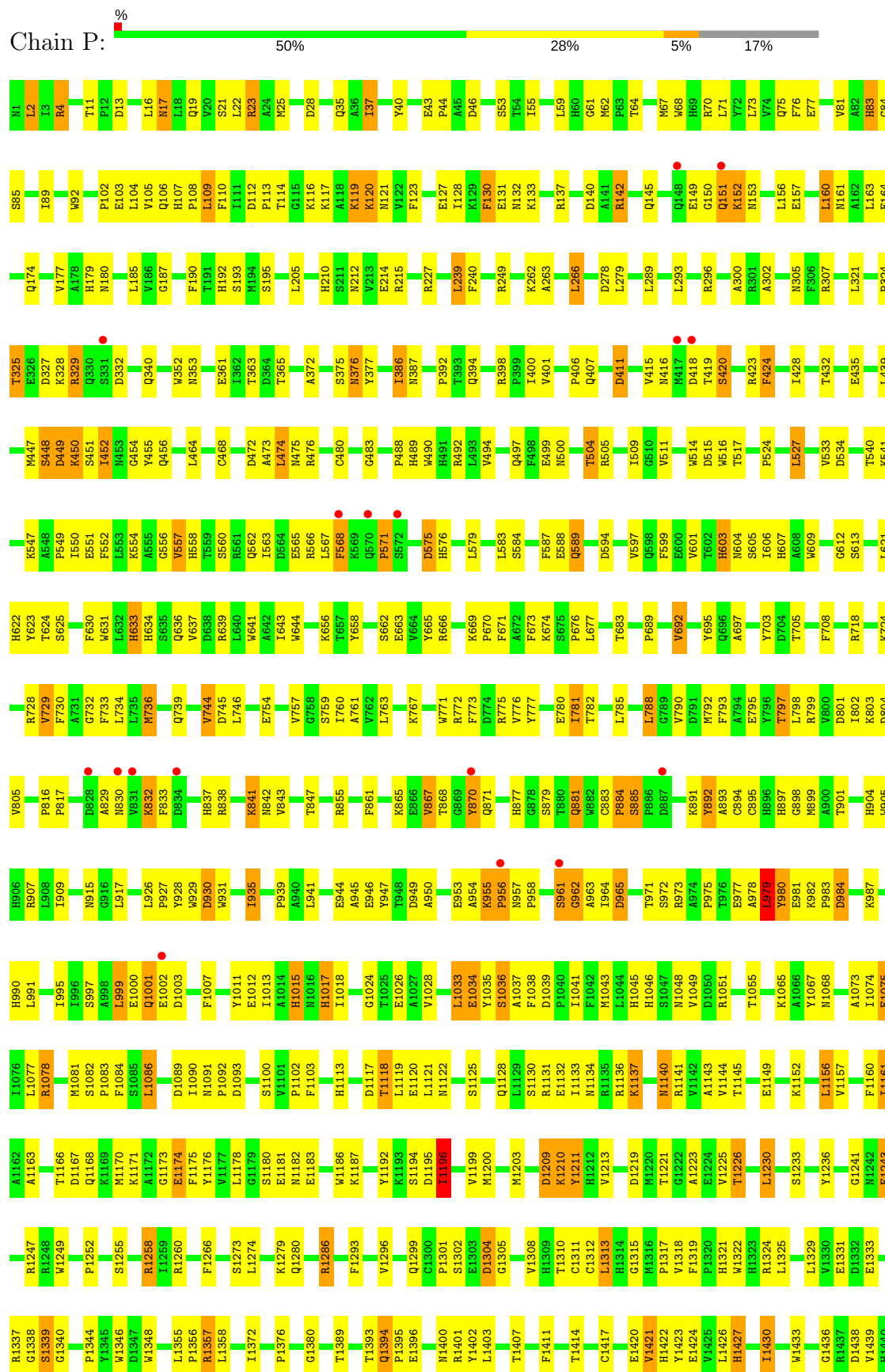








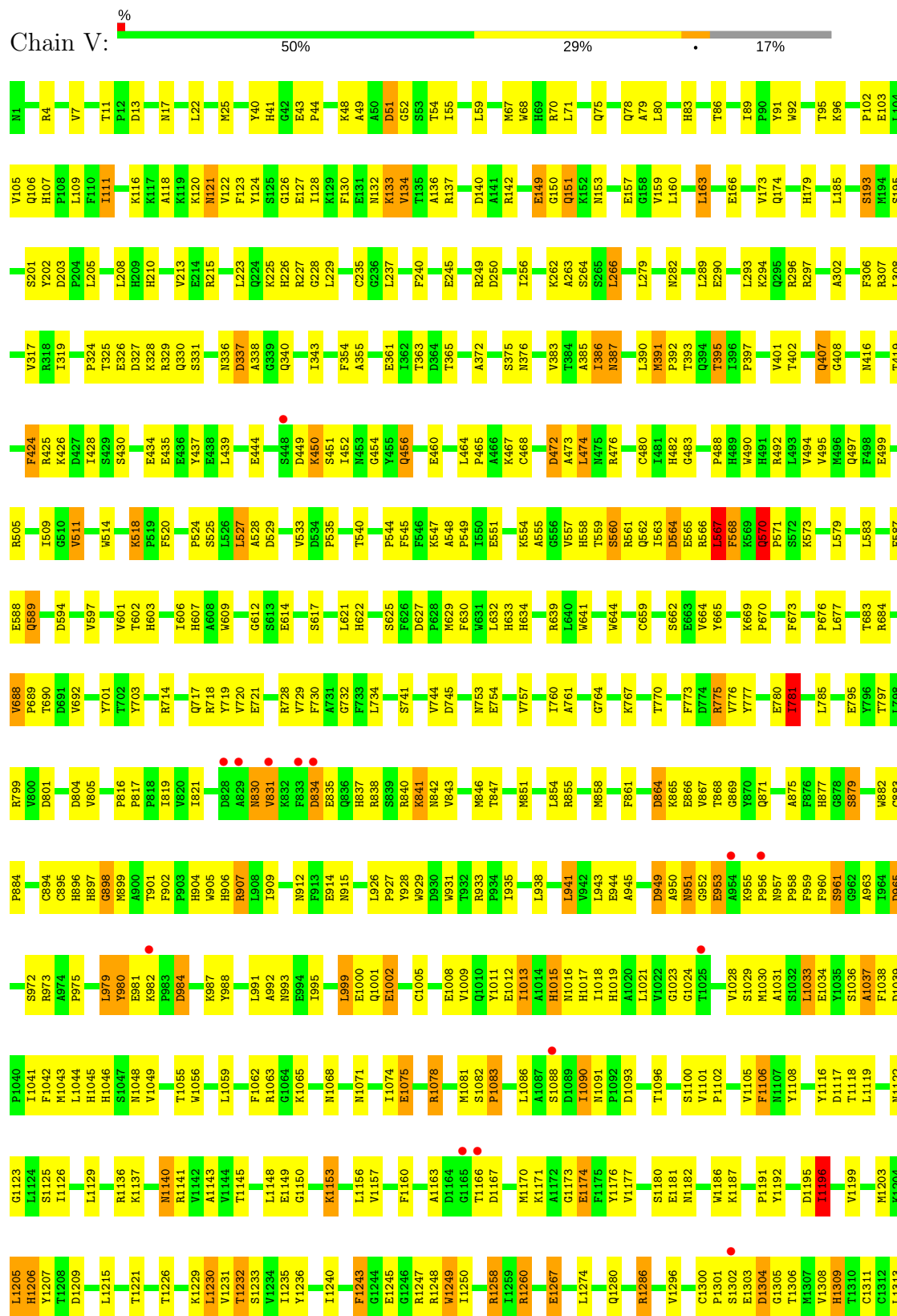
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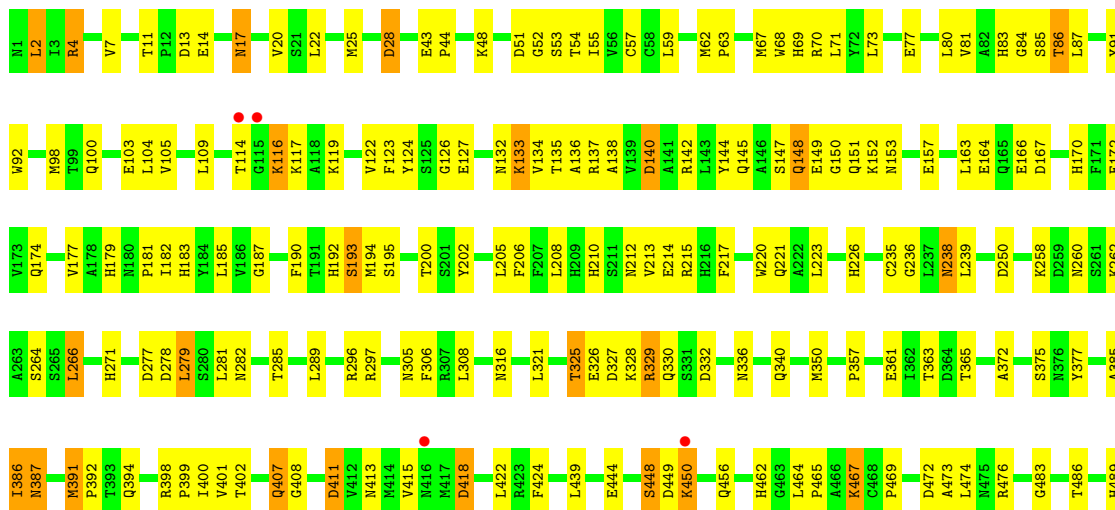






● Molecule 1: hemocyanin





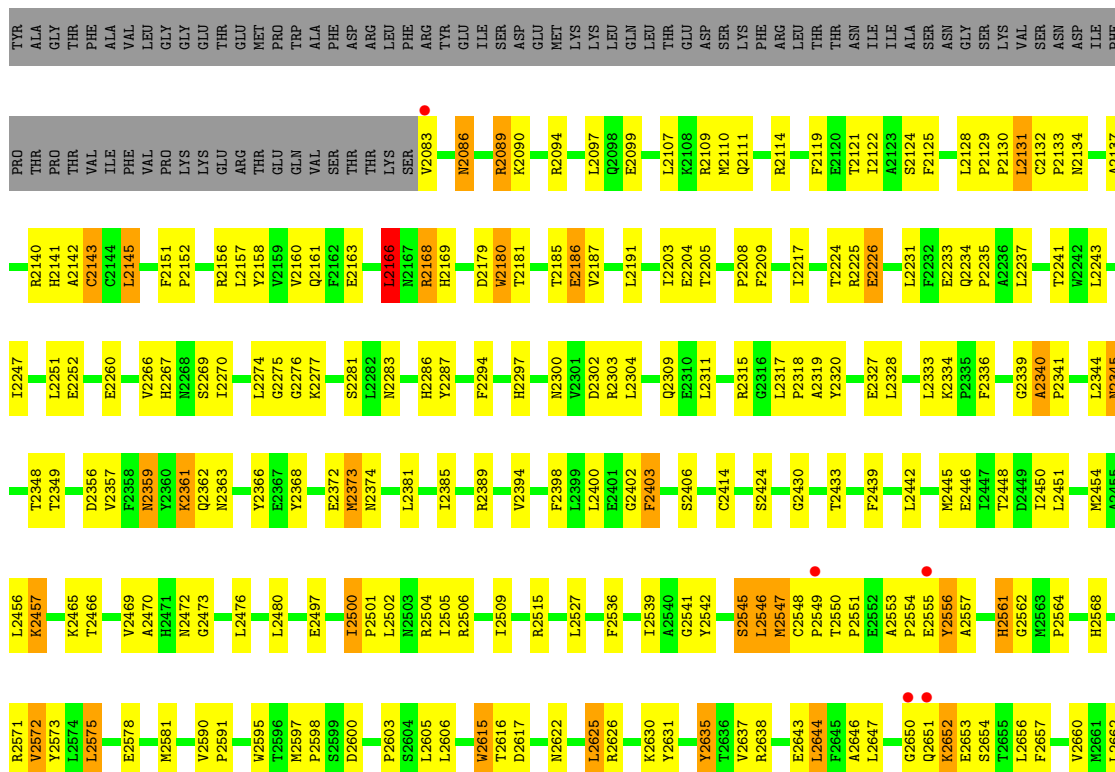
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ASN	THR	TRP	THR	V1568	L1456	L1457	S1047	E1149	W1346	R1258	E1149	H1047	S1047	P958	Q882	W882	Q883	T683	Q589	H491
HIS	THR	ARG	ARG	C1573	H1457	H1458	N1048	S1154	D1347	R1259	E1155	N1049	F960	P959	C883	W883	L1493	R684	Q593	L493
SER	CYS	ASP	VAL	V1574	H1459	S1459	W1050	L1155	V1348	R1260	L1156	D1050	V1049	S961	S885	P884	V494	S687	D594	V494
TRP	LEU	VAL	THR	P1575	S1459	S1459	R1051	L1156	V1349	L1263	L1157	R1051	D1051	P964	P886	Q497	Q497	V597	F498	Q497
ILE	HIS	THR	THR	T1576	N1460	N1461	T1055	V1157	P1356	E1284	V1158	T1055	W1056	D965	D887	P888	F499	T602	F499	F499
GLY	ASN	GLY	SER	G1577	N1461	N1461	W1056	V1158	R1357	E1285	V1159	T1056	W1056	S966	A888	P889	F499	T603	T602	T603
PRO	PRO	MET	ALA	I1578	N1462	N1462	F1160	V1159	R1358	G1286	V1160	W1056	W1056	P967	A889	D891	F499	T604	T603	T604
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ASN	THR	THR	ARG	E1580	E1470	E1470	L1063	I1162	Y1365	I1290	I1162	L1063	L1063	S972	K893	X803	G510	Q696	Q696	G510
PRO	HIS	PHE	ILE	E1581	L1471	L1471	R1064	A1163	N1366	I1291	A1163	R1064	R1064	S972	C894	D804	V511	Q696	Q696	V511
HIS	GLY	PRO	ARG	N1582	Q1472	Q1472	G1065	D1164	N1366	F1293	G1165	G1065	G1065	P975	C895	W609	W514	Y703	Y703	W514
ASN	GLY	TRP	ASN	C1584	R1473	R1473	T1065	G1165	T1369	F1293	G1165	G1065	G1065	P976	C895	W609	W514	Y703	Y703	W514
MET	ILE	TRP	ASN	G1584	R1473	R1473	T1065	G1165	T1369	F1293	G1165	G1065	G1065	P976	C895	W609	W514	Y703	Y703	W514
SER	SER	SER	LEU	G1594	R1474	R1474	Y1067	T1166	T1369	F1293	G1165	G1065	G1065	P976	C895	W609	W514	Y703	Y703	W514
SER	SER	SER	LEU	G1595	R1475	R1475	Y1067	T1166	T1369	F1293	G1165	G1065	G1065	P976	C895	W609	W514	Y703	Y703	W514
LEU	ALA	ASP	ASP	E1596	K1476	K1476	A1070	O1168	D1392	Q1299	O1168	A1070	A1070	P976	C895	W609	W514	Y703	Y703	W514
ASP	ASP	LEU	LEU	T1597	L1477	L1477	C1300	O1168	D1392	Q1299	O1168	A1070	A1070	P976	C895	W609	W514	Y703	Y703	W514
ASP	ASP	LEU	LEU	E1598	Y1478	Y1478	S1302	K1170	I1382	C1300	M1170	A1070	A1070	P976	C895	W609	W514	Y703	Y703	W514
ALA	VAL	SER	GLY	M1599	Y1479	Y1479	E1303	K1171	I1382	C1300	M1170	A1070	A1070	P976	C895	W609	W514	Y703	Y703	W514
TYR	VAL	VAL	ASP	P1600	M1488	M1488	D1304	G1173	A1387	E1303	A1172	E1075	E1075	K987	H904	W905	Y533	H622	H622	Y533
ASP	ARG	GLY	MET	W1601	M1489	M1489	G1305	E1174	A1387	E1303	A1172	E1075	E1075	K987	H904	W905	Y533	H622	H622	Y533
PRO	LYS	LYS	PHE	W1601	M1489	M1489	G1305	E1174	A1387	E1303	A1172	E1075	E1075	K987	H904	W905	Y533	H622	H622	Y533
ILE	PRO	ARG	SER	D1604	P1492	P1492	M1307	F1175	D1392	T1596	F1175	P1083	P1083	L991	R907	H906	D534	T624	T624	D534
PHE	PHE	ARG	SER	R1605	M1493	M1493	M1307	F1175	D1392	T1596	F1175	P1083	P1083	L991	R907	H906	D534	T624	T624	D534
LEU	LEU	LEU	LEU	F1607	R1494	R1494	M1307	F1175	D1392	T1596	F1175	P1083	P1083	L991	R907	H906	D534	T624	T624	D534
ALA	ALA	ALA	ALA	R1608	S1497	S1497	M1307	F1175	D1392	T1596	F1175	P1083	P1083	L991	R907	H906	D534	T624	T624	D534
GLY	ARG	GLY	ALA	N1621	S1497	S1497	M1307	F1175	D1392	T1596	F1175	P1083	P1083	L991	R907	H906	D534	T624	T624	D534
SER	ASN	SER	LYS	Q1622	R1505	R1505	L1403	Y1404	T1407	H1316	Y1404	T1407	H1316	L991	R907	H906	D534	T624	T624	D534
THR	ASN	ASN	ASP	H1625	L1506	L1506	G1315	Y1404	T1407	H1316	Y1404	T1407	H1316	L991	R907	H906	D534	T624	T624	D534
VAL	ASN	ASN	VAL	F1626	T1507	T1507	M1316	Y1404	T1407	H1316	Y1404	T1407	H1316	L991	R907	H906	D534	T624	T624	D534
ASP	TYR	ALA	THR	R1627	F1508	F1508	P1317	Y1404	T1407	H1316	Y1404	T1407	H1316	L991	R907	H906	D534	T624	T624	D534
ARG	LEU	VAL	ASP	V1628	S1511	S1511	P1317	Y1404	T1407	H1316	Y1404	T1407	H1316	L991	R907	H906	D534	T624	T624	D534
LEU	LEU	VAL	ASP	E1629	R1513	R1513	F1319	Y1404	T1407	H1316	Y1404	T1407	H1316	L991	R907	H906	D534	T624	T624	D534
TRP	GLY	PRO	GLY	V1629	F1513	F1513	F1319	Y1404	T1407	H1316	Y1404	T1407	H1316	L991	R907	H906	D534	T624	T624	D534
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ILE	ALA	ASP	TYR	E1631	D1515	D1515	H1321	Y1404	T1407	H1316	Y1404	T1407	H1316	L991	R907	H906	D534	T624	T624	D534
GLN	LEU	LEU	GLU	L1632	V1516	V1516	H1321	Y1404	T1407	H1316	Y1404	T1407	H1316	L991	R907	H906	D534	T624	T624	D534
ASP	PHE	ALA	ILE	L1632	V1516	V1516	H1321	Y1404	T1407	H1316	Y1404	T1407	H1316	L991	R907	H906	D534	T624	T624	D534
LEU	PHE	PHE	ALA	M1636	L1530	L1530	L1325	C1417	C1417	L1325	C1417	C1417	C1417	L991	R907	H906	D534	T624	T624	D534
GLN	GLY	ALA	ALA	G1637	S1536	S1536	Y1421	Y1421	Y1421	L1325	C1417	C1417	C1417	L991	R907	H906	D534	T624	T624	D534
ARG	ASN	PHE	PHE	K1639	H1422	H1422	Y1421	Y1421	Y1421	L1325	C1417	C1417	C1417	L991	R907	H906	D534	T624	T624	D534
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LYS	ASP	PRO	GLY	N1647	L1426	L1426	Y1421	Y1421	Y1421	L1325	C1417	C1417	C1417	L991	R907	H906	D534	T624	T624	D534
LEU	CYS	PRO	LEU	P1648	L1426	L1426	Y1421	Y1421	Y1421	L1325	C1417	C1417	C1417	L991	R907	H906	D534	T624	T624	D534
ASP	ASP	LEU	ALA	D1656	L1426	L1426	Y1421	Y1421	Y1421	L1325	C1417	C1417	C1417	L991	R907	H906	D534	T624	T624	D534
TYR	PHE	ILE	GLN	VAL	L1426	L1426	Y1421	Y1421	Y1421	L1325	C1417	C1417	C1417	L991	R907	H906	D534	T624	T624	D534
ASN	ASN	GLY	CYS	VAL	L1426	L1426	Y1421	Y1421	Y1421	L1325	C1417	C1417	C1417	L991	R907	H906	D534	T624	T624	D534
ALA	ASN	GLY	ASN	VAL	L1426	L1426	Y1421	Y1421	Y1421	L1325	C1417	C1417	C1417	L991	R907	H906	D534	T624	T624	D534
ASN	ASN	GLY	ASN	VAL	L1426	L1426	Y1421	Y1421	Y1421	L1325	C1417	C1417	C1417	L991	R907	H906	D534	T624	T624	D534
CYS	CYS	THR	ASP	GLU	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
ALA	ASN	THR	ALA	GLU	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
GLY	GLY	THR	GLY	PHE	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
ALA	ALA	LYS	GLY	GLU	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
LEU	LEU	LEU	SER	GLU	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
LEU	LEU	LEU	SER	GLU	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
LEU	LEU	LEU	SER	GLU	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
LEU	LEU	LEU	SER	GLU	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
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LEU	LEU	LEU	SER	GLU	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
LEU	LEU	LEU	SER	GLU	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
LEU	LEU	LEU	SER	GLU	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
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LEU	LEU	LEU	SER	GLU	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
LEU	LEU	LEU	SER	GLU	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
LEU	LEU	LEU	SER	GLU	G1556	G1556	W1433	W1433	W1433	G1556	G1556	W1433	W1433	L991	R907	H906	D534	T624	T624	D534
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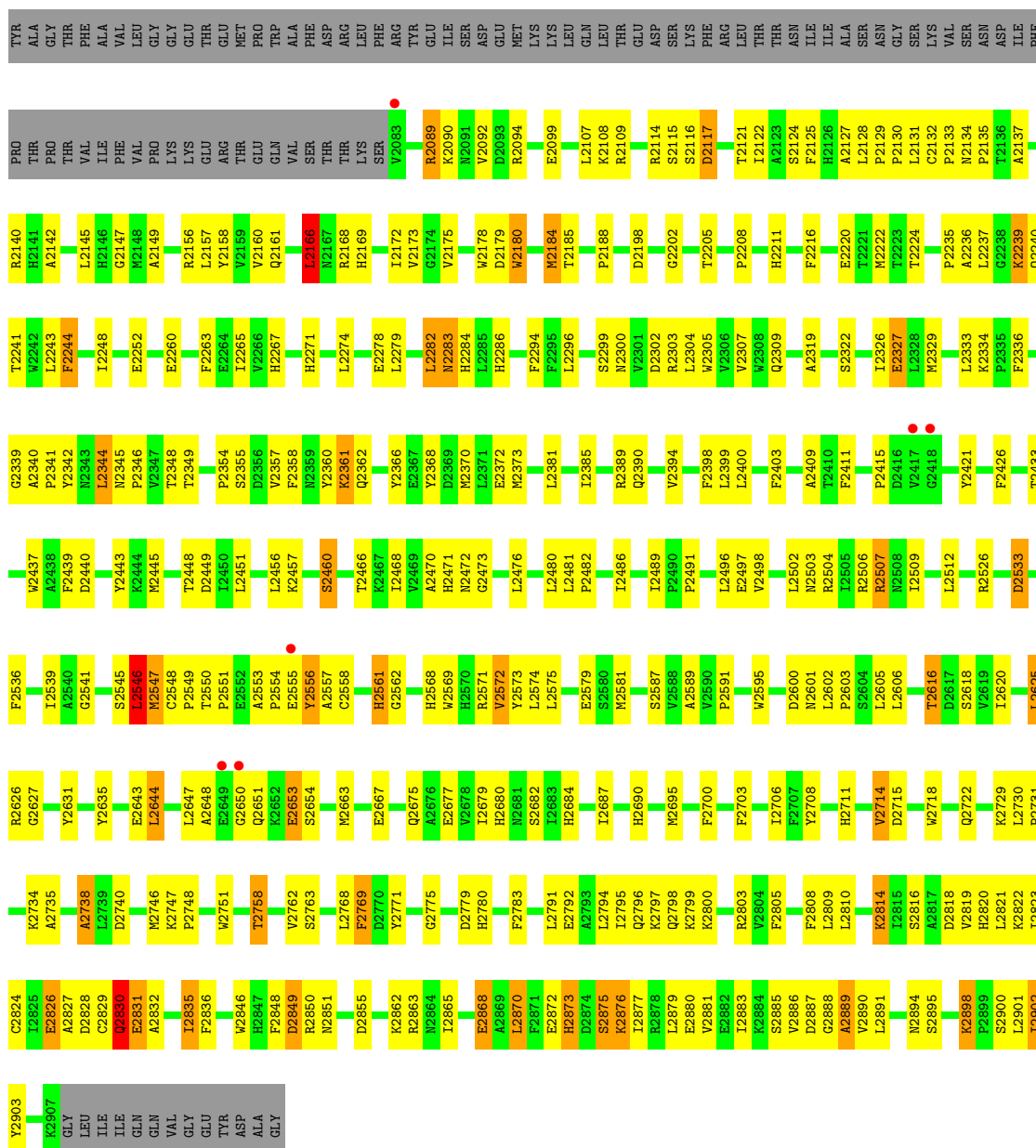
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GLY	PRO	A2142	W2242	K2361	R2507	D2610	K2722	I2825	ILE
THR	THR	C2143	N2246	Q2362	I2509	E2808	K2726	E2826	GLN
PHE	VAL	L2145	E2246	Y2368	R2515	T2616	K2727	A2827	GLN
VAL	PHE	M2148	E2252	M2373	D2516	D2617	R2728	D2828	VAL
LEU	VAL	A2149	E2260	E2382	S2522	F2624	K2729	C2829	GLY
GLY	LYS	H2155	F2263	E2382	R2526	L2625	L2730	Q2830	TYR
GLY	LYS	L2157	F2267	E2385	R2527	R2626	C2737	G2833	ASP
THR	GLU	Y2158	H2267	R2385	K2528	G2627	A2738	G2840	ALA
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PRO	THR	V2159	H2271	R2393	I2539	R2638	A2743	M2844	
TRP	GLN	Q2161	L2274	V2394	A2540	E2643	P2744	F2848	
ALA	VAL	F2162	L2274	G2404	G2541	L2644	P2745	D2849	
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ARG	THR	N2167	N2283	F2411	E2551	E2648	E2751	D2854	
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ILE	ILE		Y2287		T2550				
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MET	GLU	T2181	Y2290		A2553			I2865	
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SER	LYS		D2302				Y2778	I2883	
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LEU	THR	S2116	K2313		R2570	H2695	N2782	V2886	
THR	THR		Y2320		Y2572		K2786	D2887	
THR	ASN	T2121	G2312		E2578	M2699		G2888	
ASN	ILE	I2122	H2313		E2578		L2791	A2889	
ILE	ILE	A2123	I2214		R2582	S2702	K2799	V2890	
ALA	ALA	F2125	F2216			F2703		L2891	
ALA	SER	H2126	I2217		W2595	I2706	D2802	V2894	
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ASN	GLY	L2128	T2221		M2597		F2805	L2901	
GLY	LYS	P2129			P2598	H2711		I2902	
SER	LYS	L2130	R2225		S2599			Y2903	
VAL	VAL	L2131	E2226		D2600	V2714	L2809	A2904	
SER	SER	L2132	S2237		N2601	D2715		P2905	
ASN	ASN	P2133	Y2342		L2602	L2716	K2814	A2906	
ASP	ASP	N2134	N2943		P2603	I2717		K2907	
ILE	ILE	L2237	L2344		S2604				
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● Molecule 2: hemocyanin

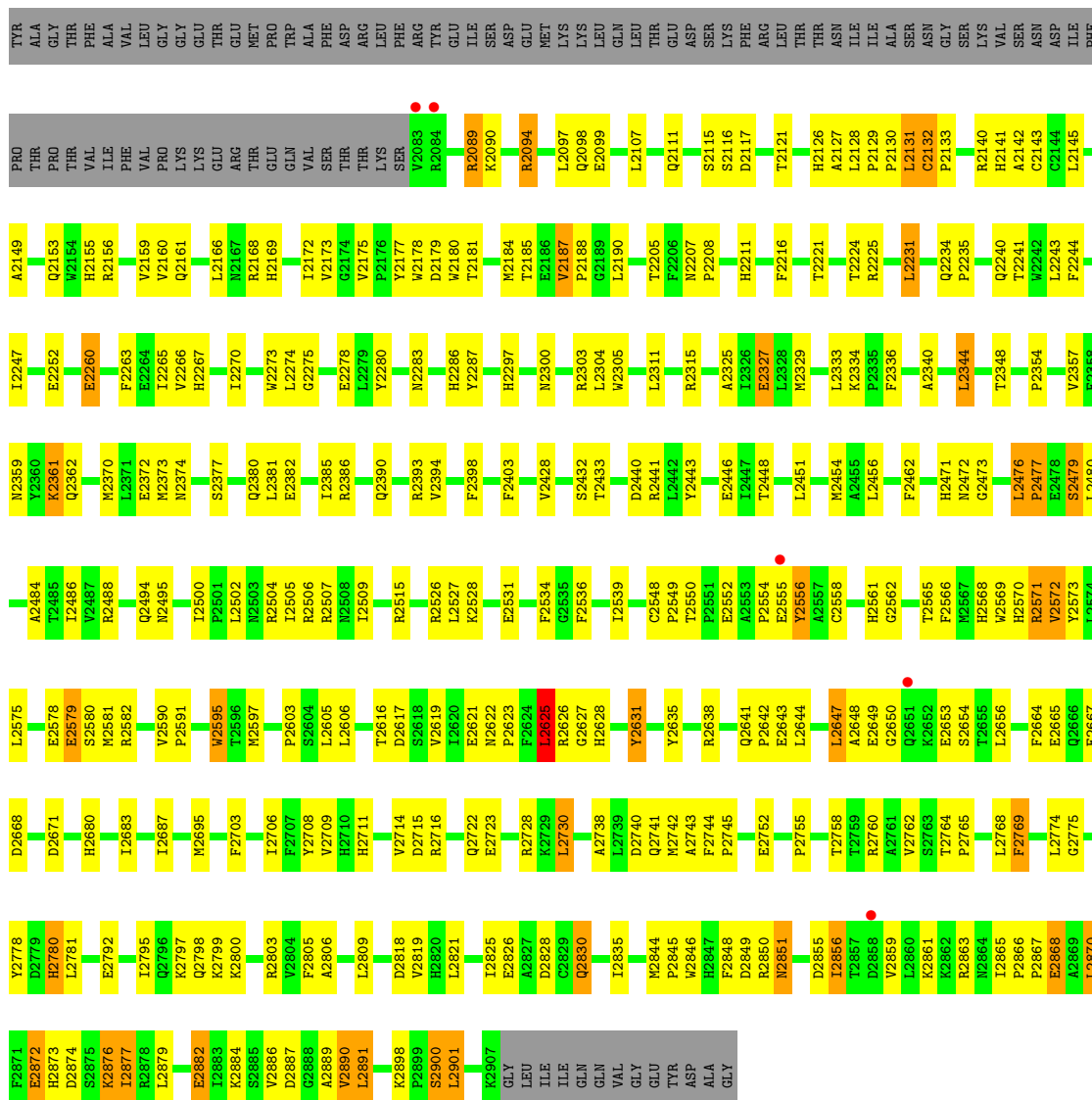


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GLY	PRO	T2221	E2220		GLY	PRO	T2221	E2220	
THR	THR	R2140	M2222		THR	THR	R2140	M2222	
PHE	VAL	H2141	T2223		PHE	VAL	H2141	T2223	
VAL	ALA	A2142	T2224		VAL	ALA	A2142	T2224	
LEU	VAL	C2143	R2225		LEU	VAL	C2143	R2225	
GLY	PRO	G2144			GLY	PRO	G2144		
GLY	LYS	H2145	E2233		GLY	LYS	H2145	E2233	
ASP	GLU	G2147	Q2234		ASP	GLU	G2147	Q2234	
ALA	THR	M2148	P2235		ALA	THR	M2148	P2235	
GLY	MET	A2149	L2237		GLY	MET	A2149	L2237	
	PRO	W2154	G2238			PRO	W2154	G2238	
	GLN	R2155	K2239			GLN	R2155	K2239	
	VAL	L2157	Q2240			VAL	L2157	Q2240	
	SER	Y2158	T2241			SER	Y2158	T2241	
	THR	V2159	W2242			THR	V2159	W2242	
	LYS	F2162	L2243			LYS	F2162	L2243	
	SER	Q2161	N2245			SER	Q2161	N2245	
	TYR	E2163	N2246			TYR	E2163	N2246	
	GLU	H2164	I2247			GLU	H2164	I2247	
	ILE	S2165	E2252			ILE	S2165	E2252	
	SER	L2166	Q2253			SER	L2166	Q2253	
	ASP	N2167	T2254			ASP	N2167	T2254	
	GLU	R2168				GLU	R2168		
	MET	H2169	C2257			MET	H2169	C2257	
	LYS					LYS			
	LYS		E2260			LYS		E2260	
	LEU	I2172	V2261			LEU	I2172	V2261	
	GLN	G2173	Q2262			GLN	G2173	Q2262	
	THR	V2175	F2263			THR	V2175	F2263	
	GLU	P2176	E2264			GLU	P2176	E2264	
	ASP	Y2177	I2265			ASP	Y2177	I2265	
	SER	W2178	V2266			SER	W2178	V2266	
	LYS	D2179	H2267			LYS	D2179	H2267	
	LEU	T2180				LEU	T2180		
	GLN	T2181	I2270			GLN	T2181	I2270	
	THR	M2184	S2271			THR	M2184	S2271	
	ASP	L2191	Q2272			ASP	L2191	Q2272	
	SER	Y2196	G2273			SER	Y2196	G2273	
	LYS	T2205	L2274			LYS	T2205	L2274	
	ASN	P2208	G2275			ASN	P2208	G2275	
	GLY	N2209	E2276			GLY	N2209	E2276	
	SER	H2210	D2277			SER	H2210	D2277	
	LYS	G2212	E2278			LYS	G2212	E2278	
	VAL	H2213				VAL	H2213		
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	ASN	I2217				ASN	I2217		
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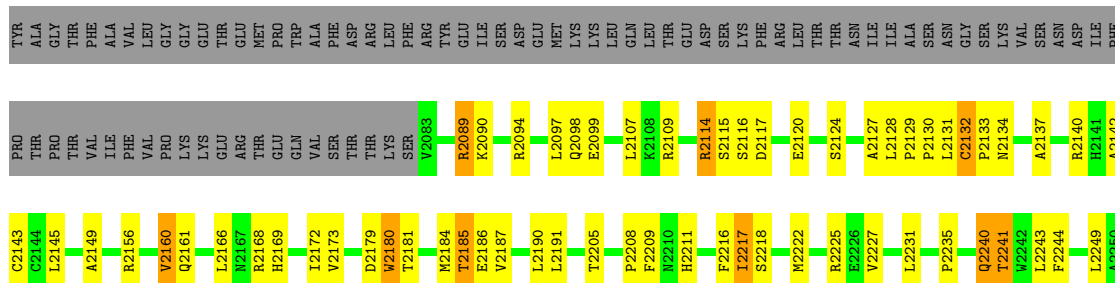


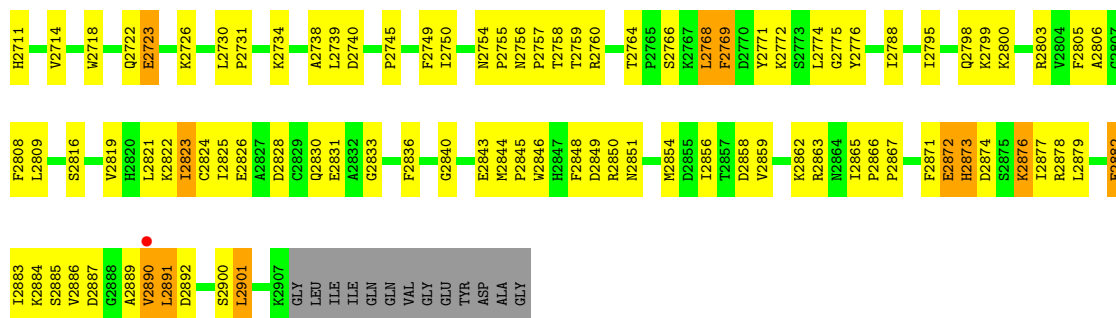


Chain N: %



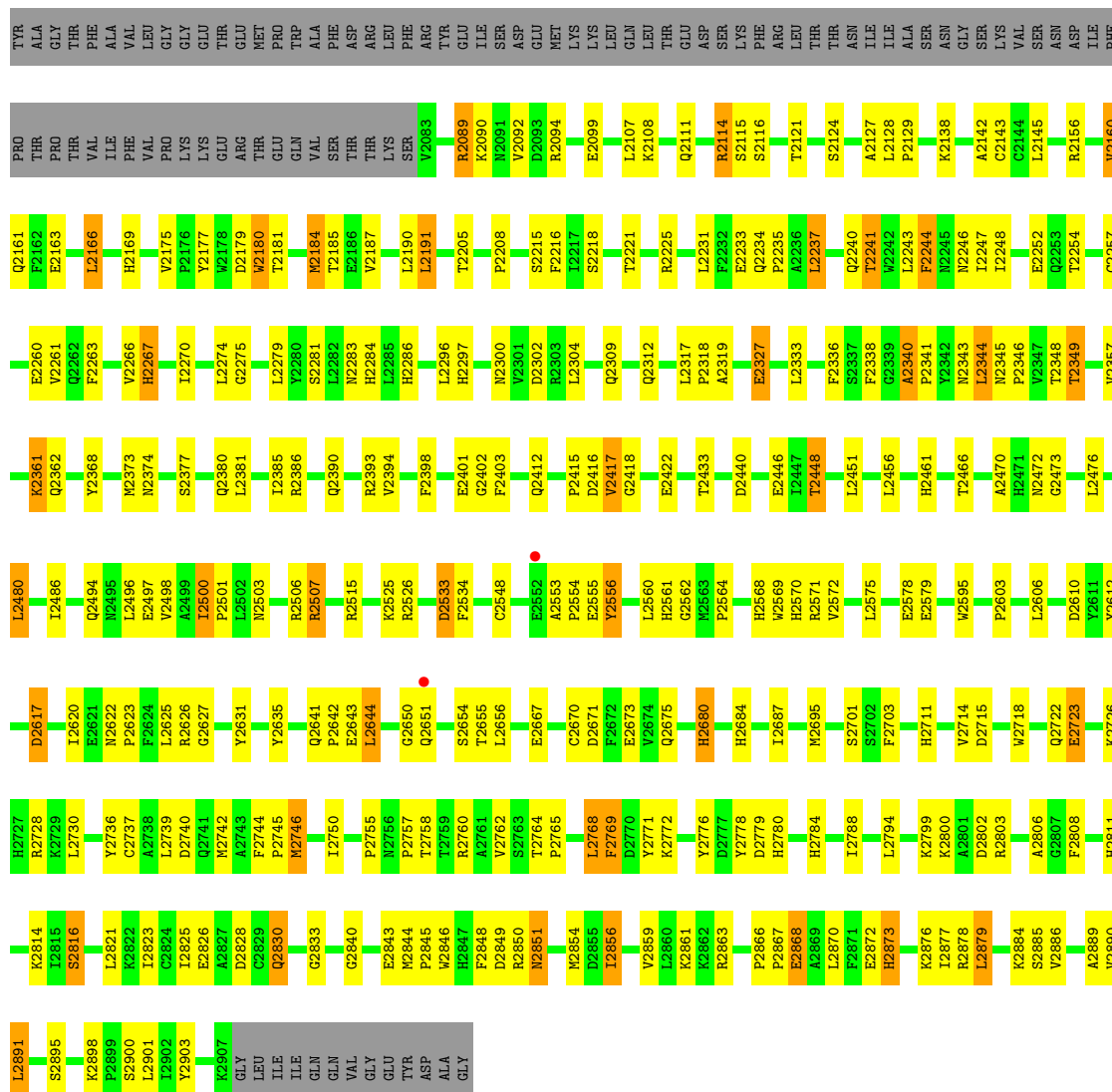
Chain Q: 58% 27% 5% 10%





• Molecule 2: hemocyanin

Chain W: 59% 27% 10%

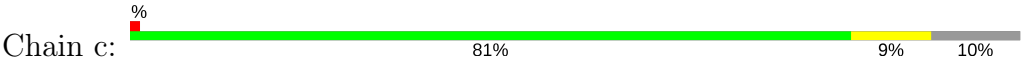


• Molecule 2: hemocyanin

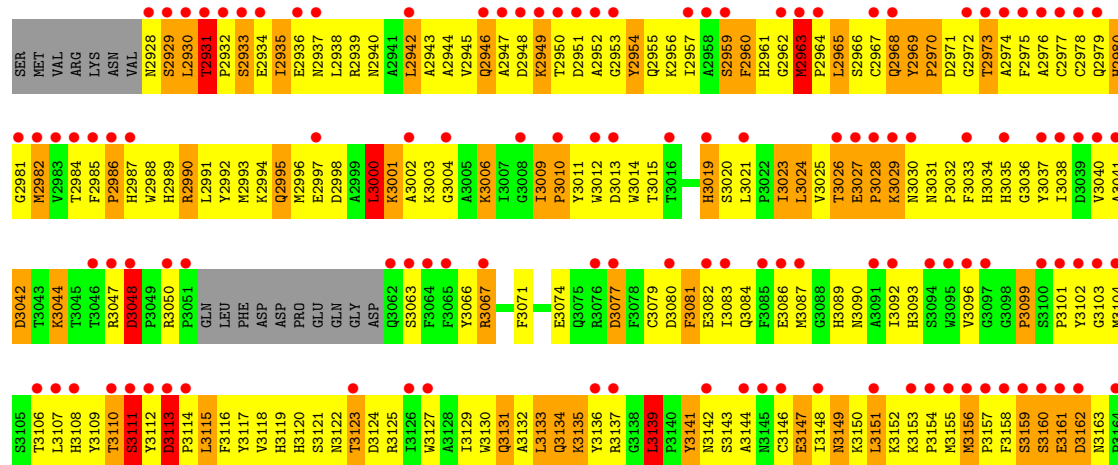
Chain Z: 57% 29% 10%

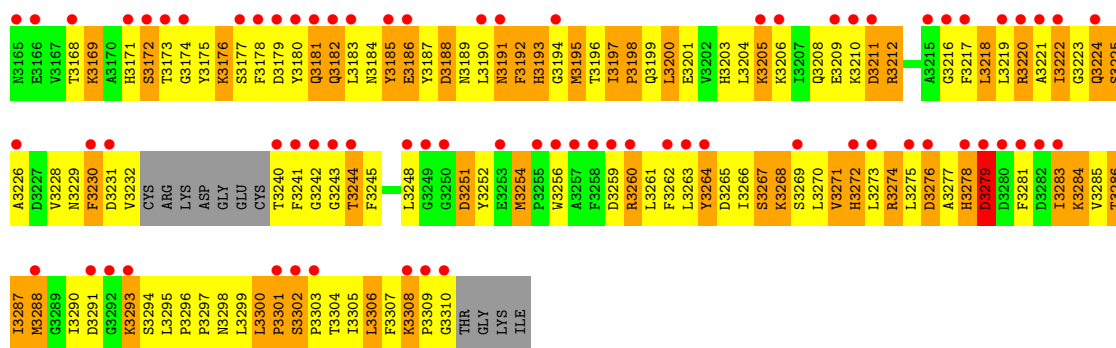
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PRO	THR	PRO	THR	VAL	PHE	VAL	LEU	GLY	GLY	THR	GLU	GLU	ARG	THR	GLU	GLN	VAL	SER	THR	THR	LYS	SER	R2083	R2084	R2089	R2090	R2091	R2092	E2099	L2107	R2109	R2110	S2116	D2117	T2121	T2122	A2123	S2124	F2125	H2126	A2127	L2128	P2129	L2237	P2130	L2131	C2132	P2133	N2134	P2135	T2136	A2137	R2140	H2141					
C2257	D2258	F2259	E2260	L2265	V2266	H2267	W2273	L2274	W2275	V2159	V2160	Q2161	L2166	L2172	V2173	Y2177	Q2178	D2179	V2180	T2181	M2184	G2189	L2190	L2191	T2192	P2208	H2211	T2221	T2224	R2225	E2226	E2233	Q2234	P2235	L2128	A2236	L2237	G2238	K2239	Q2240	T2241	V2242	L2243	F2244	L2249														
C2257	D2258	F2259	E2260	L2265	V2266	H2267	W2273	L2274	W2275	V2159	V2160	Q2161	L2166	L2172	V2173	Y2177	Q2178	D2179	V2180	T2181	M2184	G2189	L2190	L2191	T2192	P2208	H2211	T2221	T2224	R2225	E2226	E2233	Q2234	P2235	L2128	A2236	L2237	G2238	K2239	Q2240	T2241	V2242	L2243	F2244	L2249														
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● Molecule 2: hemocyanin

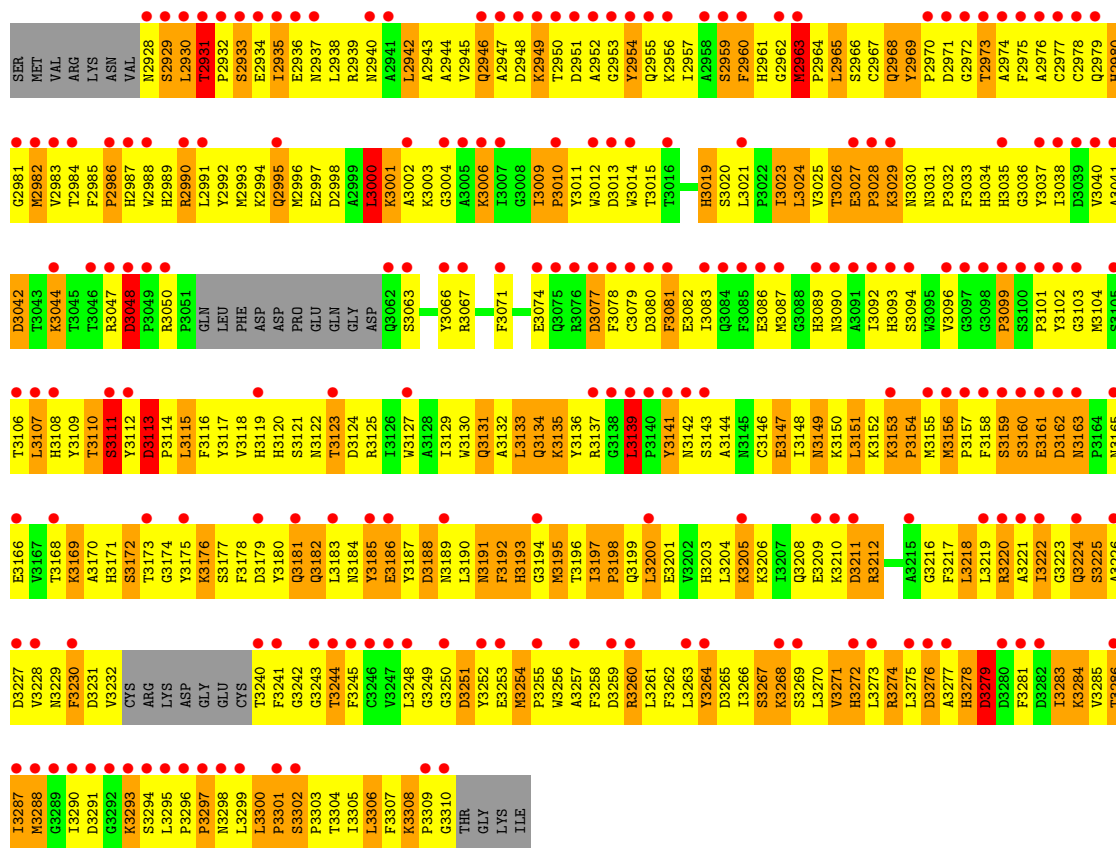
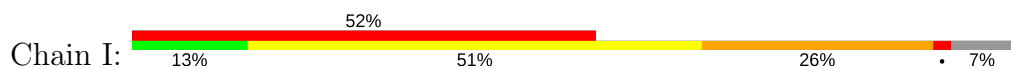


TYR	ALA	GLY	THR	PHE	ALA	VAL	LEU	GLY	GLY	THR	GLU	GLU	MET	PRO	TRP	ALA	PHE	ASP	ARG	LEU	PHE	ARG	TYR	GLU	ILE	SER	ASP	GLU	MET	LYS	LYS	LEU	GLN	LEU	THR	GLU	ASP	SER	LYS	PHE	ARG	LEU	THR	THR	ASN	ILE	ALA	SER	ASN	GLY	LYS	LYS	VAL	SER	ASN	ASP	ILE	PHE
PRO	THR	PRO	THR	VAL	ILE	PHE	VAL	PRO	LYS	LYS	GLU	THR	ARG	GLU	GLN	VAL	SER	THR	THR	THR	SER	ARG	GLU	R2083	R2084	R2089	A2127	L2131	C2132	L2145	V2160	L2166	W2178	D2179	W2180	T2185	I2203	T2221	E2226	Q2234	T2241	L2249	D2255	H2267														
L2270	I2326	E2327	L2333	L2344	K2361	M2373	Q2404	S2405	S2406	Q2452	H2461	H2471	L2480	M2495	L2496	E2497	I2500	R2507	L2546	M2547	C2548	P2549	E2552	Y2556	H2561	T2565	V2572	L2575	E2579	S2580	M2581	W2596	L2597	D2608																								
T2616	K2630	Y2631	L2640	E2649	Q2650	K2652	E2653	H2680	L2683	D2733	M2742	T2750	T2758	S2763	F2769	D2779	M2782	F2783	H2784	M2785	M2786	L2809	T2823	D2828	C2829	Q2830	E2831	E2841	F2848	D2849	R2850	D2855	L2860	L2870	D2874																							

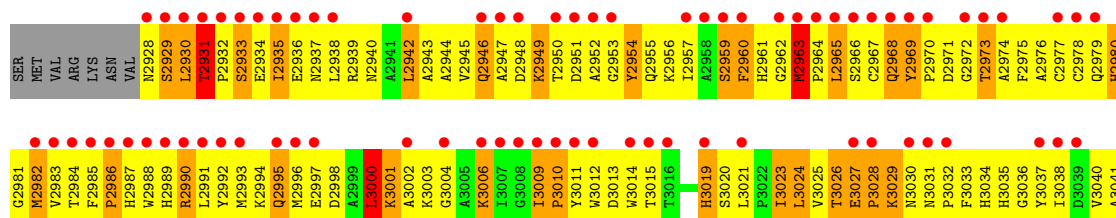
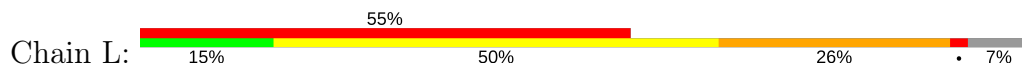


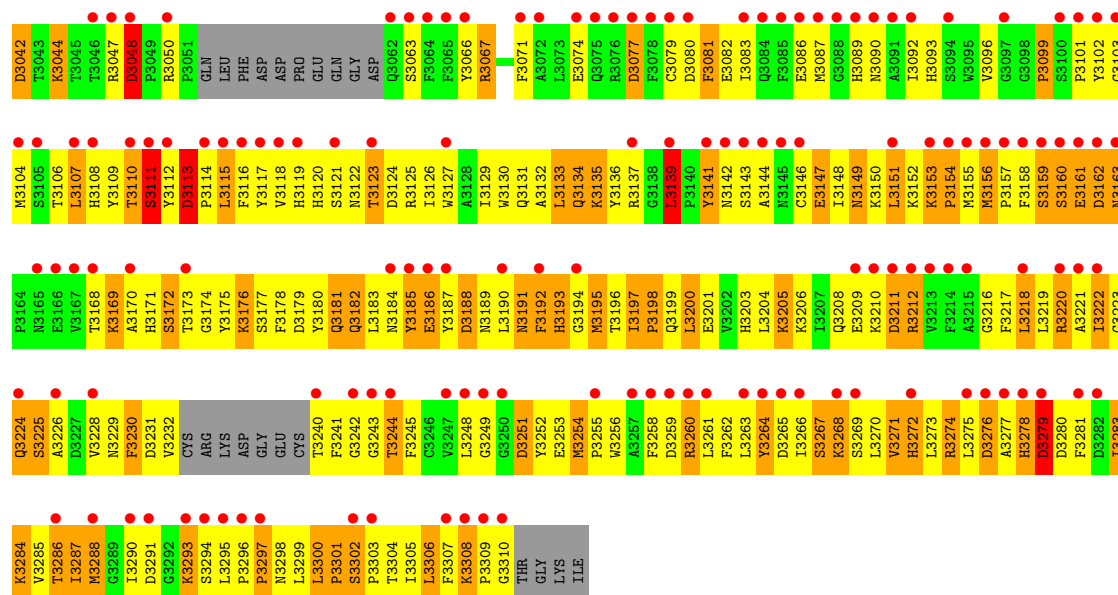


• Molecule 3: hemocyanin

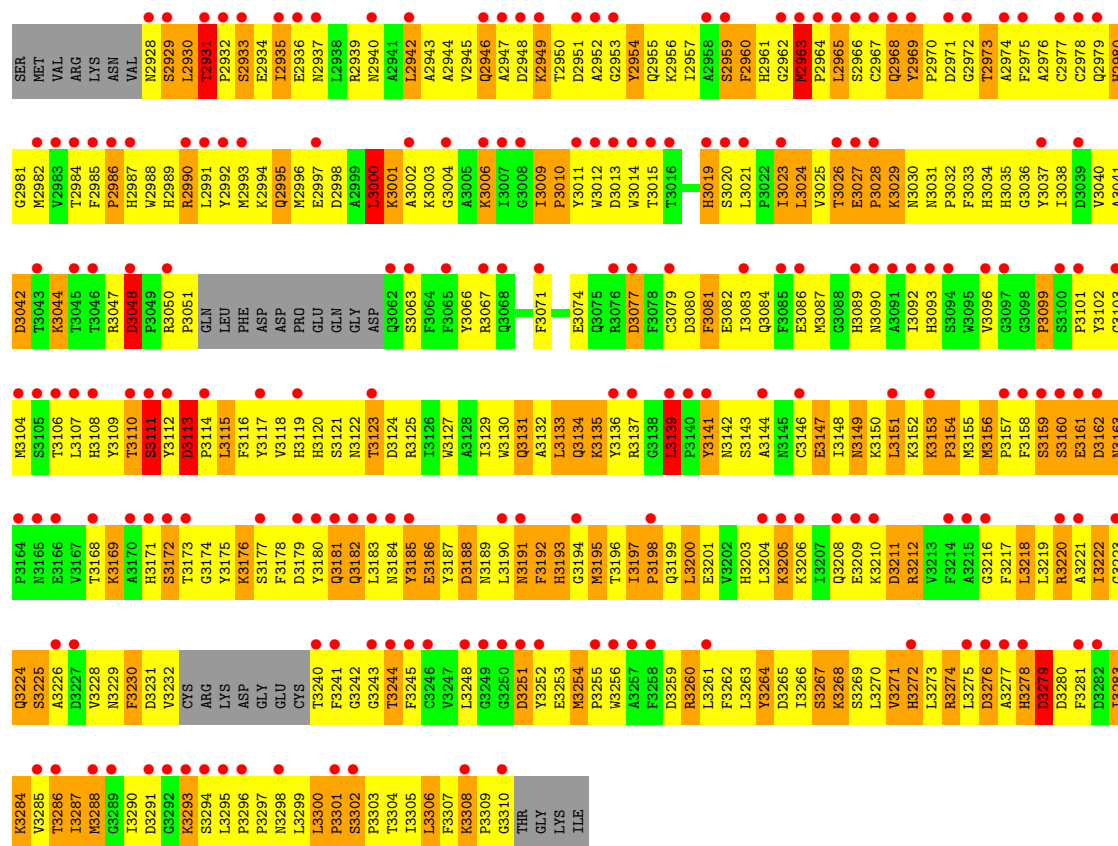
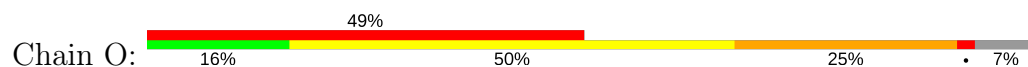


• Molecule 3: hemocyanin



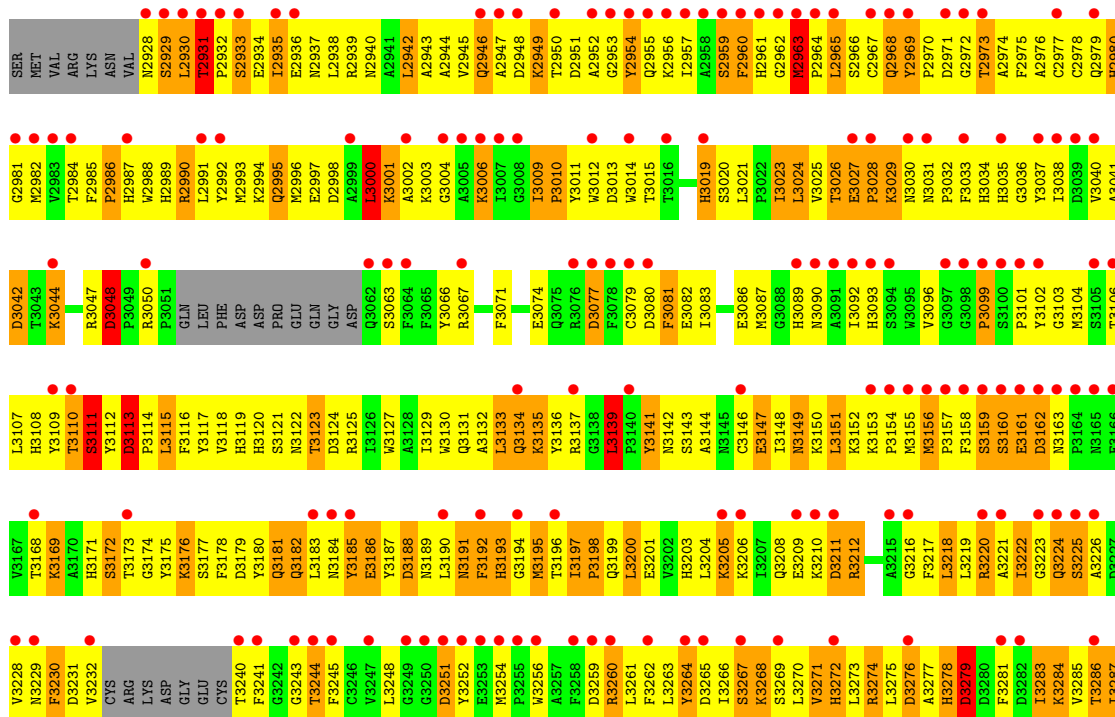
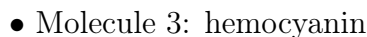


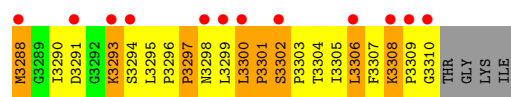
• Molecule 3: hemocyanin



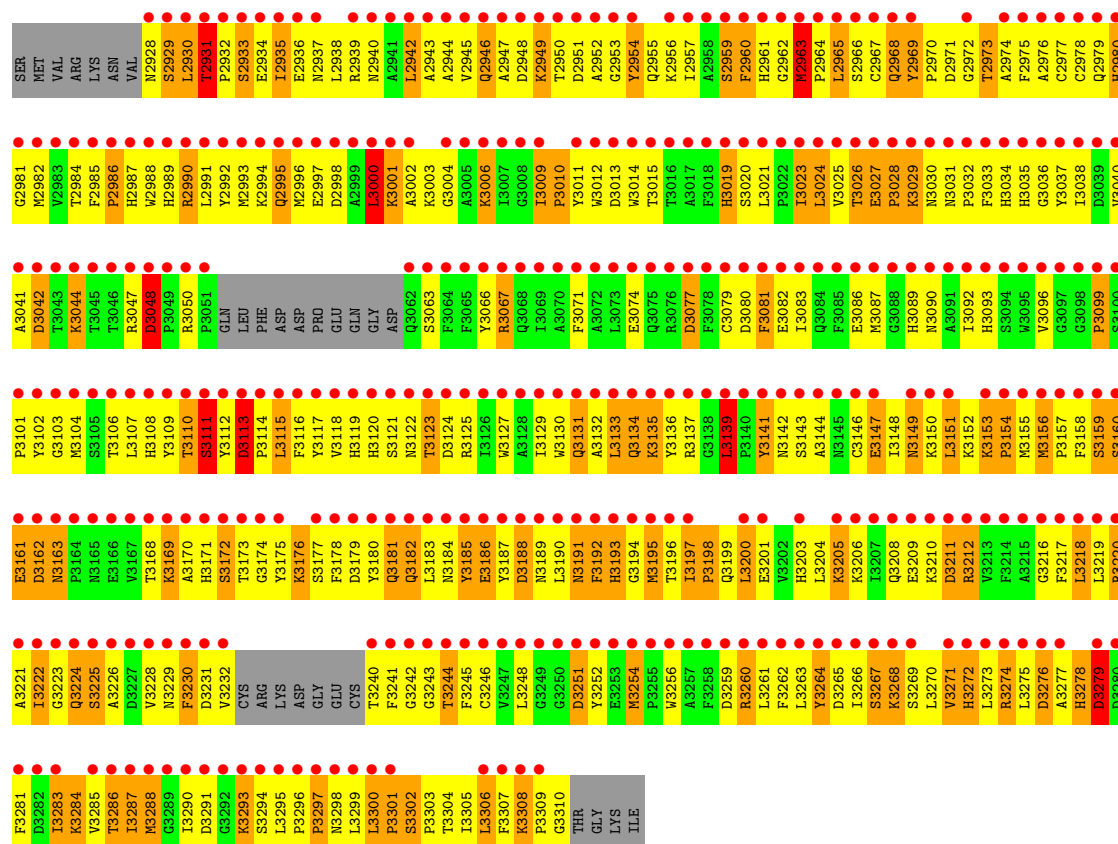
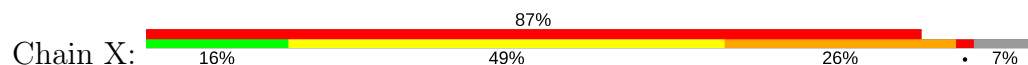
• Molecule 3: hemocyanin



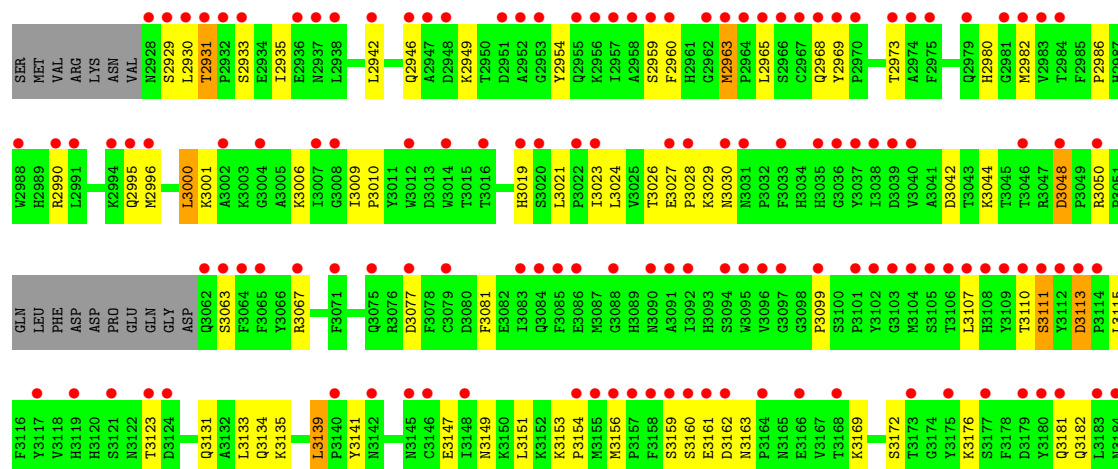


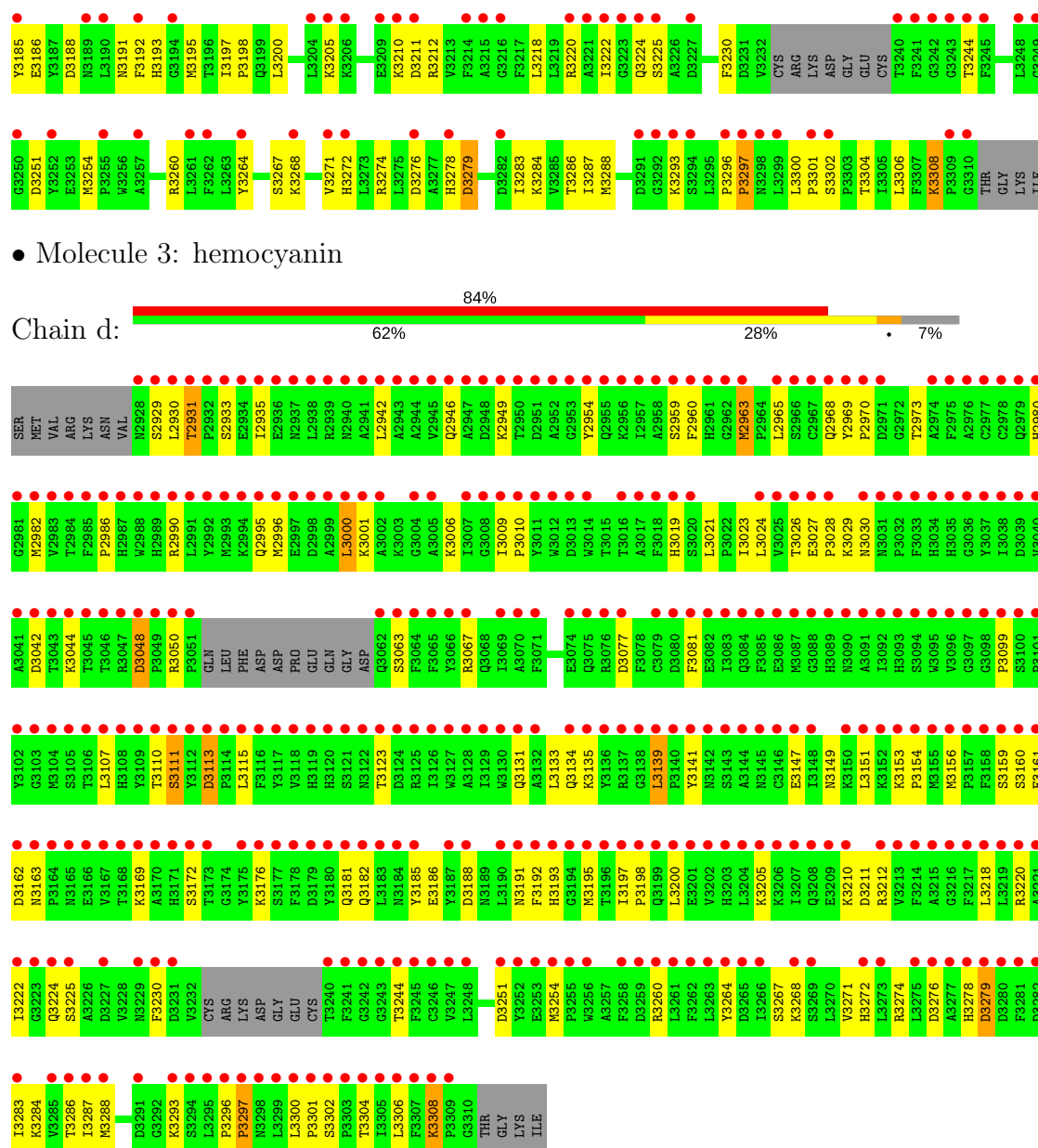


• Molecule 3: hemocyanin

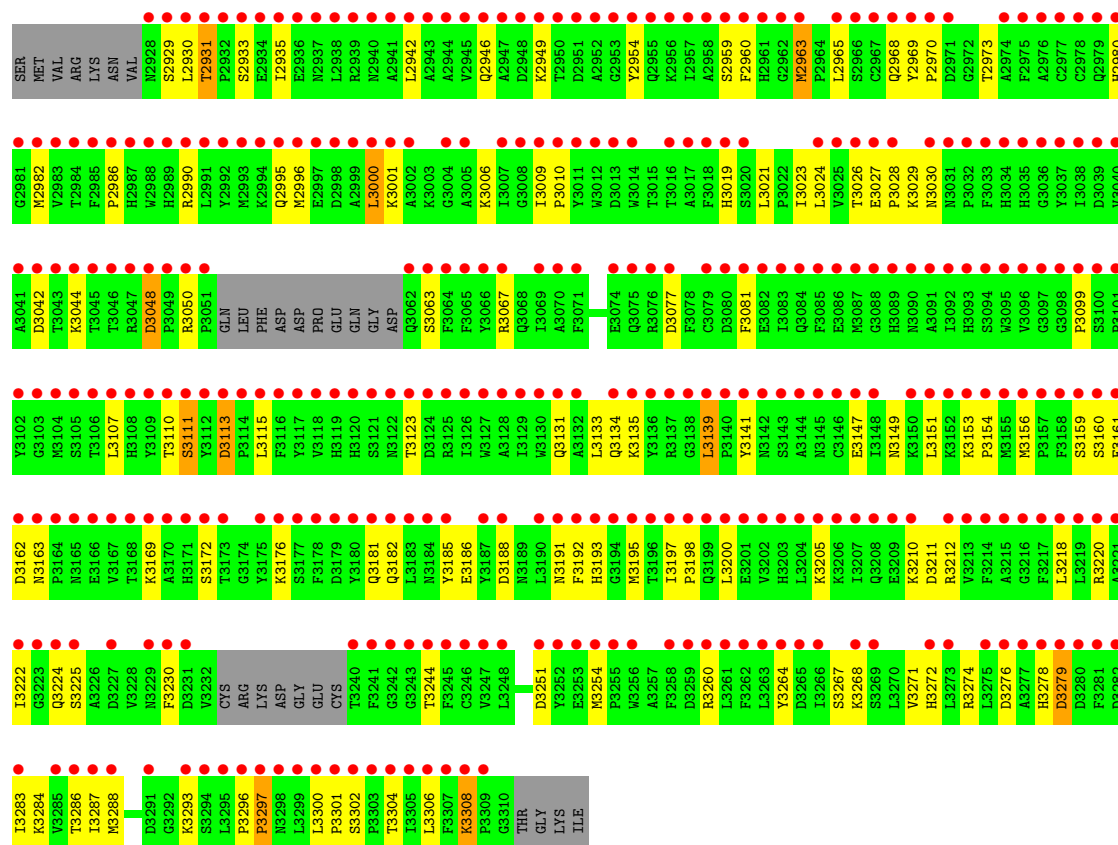
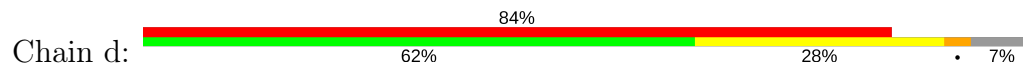


• Molecule 3: hemocyanin





● Molecule 3: hemocyanin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	171.37Å 538.66Å 310.92Å 90.00° 104.09° 90.00°	Depositor
Resolution (Å)	49.10 – 3.00 49.10 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.10-3.00) 89.6 (49.10-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.274 , 0.303 0.280 , 0.306	Depositor DCC
R_{free} test set	53588 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 11.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	261470	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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: CUO, BMA, NAG, MAN

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	0.29	0/13698	0.54	4/18607 (0.0%)
1	D	0.29	0/13698	0.54	4/18607 (0.0%)
1	G	0.28	0/13698	0.53	3/18607 (0.0%)
1	J	0.29	0/13698	0.53	2/18607 (0.0%)
1	M	0.28	0/13698	0.52	2/18607 (0.0%)
1	P	0.28	0/13698	0.53	3/18607 (0.0%)
1	S	0.27	0/13698	0.52	4/18607 (0.0%)
1	V	0.28	0/13698	0.52	4/18607 (0.0%)
1	Y	0.27	0/13698	0.51	3/18607 (0.0%)
1	b	0.27	0/13698	0.52	3/18607 (0.0%)
2	B	0.27	0/6909	0.51	2/9383 (0.0%)
2	E	0.28	0/6909	0.52	1/9383 (0.0%)
2	H	0.28	0/6909	0.51	2/9383 (0.0%)
2	K	0.28	0/6909	0.52	2/9383 (0.0%)
2	N	0.28	0/6909	0.50	1/9383 (0.0%)
2	Q	0.27	0/6909	0.50	0/9383
2	T	0.27	0/6909	0.50	2/9383 (0.0%)
2	W	0.26	0/6909	0.49	1/9383 (0.0%)
2	Z	0.27	0/6909	0.49	1/9383 (0.0%)
2	c	0.27	0/6909	0.49	0/9383
3	C	0.80	12/6100 (0.2%)	0.90	34/8282 (0.4%)
3	F	0.80	12/6100 (0.2%)	0.90	34/8282 (0.4%)
3	I	0.80	12/6100 (0.2%)	0.90	34/8282 (0.4%)
3	L	0.80	12/6100 (0.2%)	0.91	34/8282 (0.4%)
3	O	0.80	12/6100 (0.2%)	0.90	34/8282 (0.4%)
3	R	0.80	14/6100 (0.2%)	0.90	34/8282 (0.4%)
3	U	0.80	12/6100 (0.2%)	0.91	34/8282 (0.4%)
3	X	0.80	12/6100 (0.2%)	0.90	34/8282 (0.4%)
3	a	0.80	12/6100 (0.2%)	0.90	34/8282 (0.4%)
3	d	0.80	14/6100 (0.2%)	0.90	34/8282 (0.4%)
All	All	0.45	124/267070 (0.0%)	0.63	384/362720 (0.1%)

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	A	0	2
1	D	0	3
1	G	0	1
1	J	0	2
1	M	0	1
1	S	0	3
1	Y	0	1
1	b	0	2
2	B	0	1
2	K	0	3
2	N	0	1
2	Q	0	1
2	T	0	2
2	W	0	1
2	Z	0	2
2	c	0	1
3	C	0	4
3	F	0	4
3	I	0	4
3	L	0	4
3	O	0	4
3	R	0	4
3	U	0	4
3	X	0	4
3	a	0	4
3	d	0	4
All	All	0	67

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3154[A]	PRO	N-CD	5.36	1.55	1.47
3	C	3154[B]	PRO	N-CD	5.36	1.55	1.47
3	X	3154[A]	PRO	N-CD	5.25	1.55	1.47
3	X	3154[B]	PRO	N-CD	5.25	1.55	1.47
3	O	3154[A]	PRO	N-CD	5.24	1.55	1.47

The worst 5 of 384 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	979	LEU	CA-CB-CG	7.97	133.62	115.30
1	V	567	LEU	CA-CB-CG	7.90	133.47	115.30
1	A	279	LEU	CA-CB-CG	7.27	132.02	115.30
2	K	2546	LEU	CA-CB-CG	6.93	131.25	115.30
1	M	1230	LEU	CA-CB-CG	6.68	130.67	115.30

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	464	LEU	Peptide
1	A	982	LYS	Peptide
2	B	2127	ALA	Peptide
3	C	3113[A]	ASP	Mainchain
3	C	3113[B]	ASP	Mainchain

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	13318	0	12755	443	1
1	D	13318	0	12755	467	0
1	G	13318	0	12754	485	0
1	J	13318	0	12755	493	0
1	M	13318	0	12755	427	0
1	P	13318	0	12755	438	0
1	S	13318	0	12755	437	0
1	V	13318	0	12755	434	0
1	Y	13318	0	12744	397	0
1	b	13318	0	12754	0	1
2	B	6704	0	6445	199	0
2	E	6704	0	6445	232	0
2	H	6704	0	6445	232	0
2	K	6704	0	6445	209	0
2	N	6704	0	6445	192	0
2	Q	6704	0	6445	207	0
2	T	6704	0	6445	214	0
2	W	6704	0	6445	214	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	6704	0	6444	181	0
2	c	6704	0	6445	0	0
3	C	5912	0	5607	2272	0
3	F	5912	0	5599	1400	0
3	I	5912	0	5601	2391	0
3	L	5912	0	5604	2283	0
3	O	5912	0	5604	1994	0
3	R	5912	0	5597	2373	0
3	U	5912	0	5612	1410	0
3	X	5912	0	5598	1993	0
3	a	5912	0	5594	0	0
3	d	5912	0	5607	0	0
4	A	24	0	0	2	0
4	B	8	0	0	0	0
4	C	16	0	0	14	0
4	D	24	0	0	2	0
4	E	8	0	0	0	0
4	F	16	0	0	7	0
4	G	24	0	0	1	0
4	H	8	0	0	0	0
4	I	16	0	0	12	0
4	J	24	0	0	2	0
4	K	8	0	0	0	0
4	M	24	0	0	3	0
4	N	8	0	0	0	0
4	O	8	0	0	10	0
4	P	24	0	0	0	0
4	Q	8	0	0	0	0
4	S	24	0	0	3	0
4	T	8	0	0	1	0
4	U	8	0	0	10	0
4	V	24	0	0	2	0
4	W	8	0	0	1	0
4	X	8	0	0	10	0
4	Y	24	0	0	3	0
4	Z	8	0	0	0	0
4	b	24	0	0	0	0
4	c	8	0	0	0	0
4	d	8	0	0	0	0
5	A	112	0	98	3	0
5	B	28	0	25	3	0
5	D	112	0	98	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	28	0	25	1	0
5	G	112	0	99	18	0
5	H	28	0	25	2	0
5	J	112	0	99	11	0
5	K	28	0	25	0	0
5	M	112	0	97	9	0
5	N	28	0	25	1	0
5	P	112	0	98	6	0
5	Q	28	0	25	6	0
5	S	112	0	99	8	0
5	T	28	0	24	3	0
5	V	112	0	96	13	0
5	W	28	0	25	6	0
5	Y	112	0	98	8	0
5	Z	28	0	25	8	0
5	b	112	0	98	0	0
5	c	28	0	25	0	0
6	A	22	0	19	0	0
6	D	22	0	19	1	0
6	G	11	0	10	0	0
6	J	11	0	10	0	0
6	M	33	0	27	3	0
6	P	22	0	20	1	0
6	S	11	0	9	0	0
6	T	11	0	10	0	0
6	V	44	0	39	3	0
6	Y	22	0	19	1	0
6	b	22	0	19	0	0
7	A	11	0	10	0	0
7	D	11	0	10	1	0
7	M	33	0	30	2	0
7	S	11	0	10	0	0
7	V	11	0	10	1	0
7	Y	11	0	10	0	0
7	b	11	0	10	0	0
All	All	261470	0	249529	19352	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 48.

The worst 5 of 19352 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)
3:C:3079[B]:CYS:CB	3:L:3161[B]:GLU:HG2	1.22	1.65
3:C:2982[B]:MET:SD	3:L:3156[B]:MET:HB2	1.37	1.64
3:C:2975[B]:PHE:CD1	3:L:3107[B]:LEU:HD11	1.28	1.63
3:I:3174[B]:GLY:CA	3:R:3154[B]:PRO:HB3	1.17	1.62
3:O:3153[B]:LYS:CD	3:X:3176[B]:LYS:HD3	1.31	1.60

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:A:1:ASN:N	1:b:887:ASP:OD1[1_455]	2.19	0.01

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	1654/2000 (83%)	1552 (94%)	89 (5%)	13 (1%)	22	64
1	D	1654/2000 (83%)	1541 (93%)	100 (6%)	13 (1%)	22	64
1	G	1654/2000 (83%)	1560 (94%)	78 (5%)	16 (1%)	18	59
1	J	1654/2000 (83%)	1537 (93%)	103 (6%)	14 (1%)	22	64
1	M	1654/2000 (83%)	1569 (95%)	73 (4%)	12 (1%)	25	67
1	P	1654/2000 (83%)	1562 (94%)	78 (5%)	14 (1%)	22	64
1	S	1654/2000 (83%)	1581 (96%)	64 (4%)	9 (0%)	32	74
1	V	1654/2000 (83%)	1570 (95%)	68 (4%)	16 (1%)	18	59
1	Y	1654/2000 (83%)	1580 (96%)	66 (4%)	8 (0%)	32	74
1	b	1654/2000 (83%)	1564 (95%)	80 (5%)	10 (1%)	28	70
2	B	823/920 (90%)	778 (94%)	40 (5%)	5 (1%)	28	70
2	E	823/920 (90%)	781 (95%)	34 (4%)	8 (1%)	18	59
2	H	823/920 (90%)	787 (96%)	33 (4%)	3 (0%)	38	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	823/920 (90%)	778 (94%)	37 (4%)	8 (1%)	18	59
2	N	823/920 (90%)	789 (96%)	32 (4%)	2 (0%)	51	86
2	Q	823/920 (90%)	787 (96%)	32 (4%)	4 (0%)	32	74
2	T	823/920 (90%)	794 (96%)	22 (3%)	7 (1%)	20	62
2	W	823/920 (90%)	791 (96%)	28 (3%)	4 (0%)	32	74
2	Z	823/920 (90%)	797 (97%)	23 (3%)	3 (0%)	38	78
2	c	823/920 (90%)	791 (96%)	29 (4%)	3 (0%)	38	78
3	C	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	22	64
3	F	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	22	64
3	I	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	22	64
3	L	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	22	64
3	O	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	22	64
3	R	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	22	64
3	U	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	22	64
3	X	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	22	64
3	a	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	22	64
3	d	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	22	64
All	All	31970/33140 (96%)	30149 (94%)	1589 (5%)	232 (1%)	25	67

5 of 232 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1196	ILE
1	D	695	TYR
1	D	1196	ILE
1	G	331	SER
1	G	1086	LEU

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	1429/1738 (82%)	1278 (89%)	151 (11%)	8	30
1	D	1429/1738 (82%)	1267 (89%)	162 (11%)	7	27
1	G	1429/1738 (82%)	1264 (88%)	165 (12%)	6	27
1	J	1429/1738 (82%)	1266 (89%)	163 (11%)	7	27
1	M	1429/1738 (82%)	1284 (90%)	145 (10%)	9	33
1	P	1429/1738 (82%)	1264 (88%)	165 (12%)	6	27
1	S	1429/1738 (82%)	1269 (89%)	160 (11%)	7	28
1	V	1429/1738 (82%)	1270 (89%)	159 (11%)	7	28
1	Y	1429/1738 (82%)	1261 (88%)	168 (12%)	6	25
1	b	1429/1738 (82%)	1277 (89%)	152 (11%)	8	30
2	B	731/814 (90%)	666 (91%)	65 (9%)	11	40
2	E	731/814 (90%)	655 (90%)	76 (10%)	8	31
2	H	731/814 (90%)	634 (87%)	97 (13%)	4	20
2	K	731/814 (90%)	656 (90%)	75 (10%)	8	31
2	N	731/814 (90%)	652 (89%)	79 (11%)	7	29
2	Q	731/814 (90%)	654 (90%)	77 (10%)	8	30
2	T	731/814 (90%)	660 (90%)	71 (10%)	9	35
2	W	731/814 (90%)	659 (90%)	72 (10%)	9	34
2	Z	731/814 (90%)	655 (90%)	76 (10%)	8	31
2	c	731/814 (90%)	652 (89%)	79 (11%)	7	29
3	C	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	F	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	I	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	L	636/343 (185%)	430 (68%)	206 (32%)	0	1
3	O	636/343 (185%)	430 (68%)	206 (32%)	0	1
3	R	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	U	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	X	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	a	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	d	636/343 (185%)	432 (68%)	204 (32%)	0	1
All	All	27960/28950 (97%)	23559 (84%)	4401 (16%)	4	14

5 of 4401 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	2887	ASP
3	R	2959[B]	SER
1	b	1053	TRP
3	O	3024[B]	LEU
1	P	376	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 300 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	192	HIS
1	P	679	ASN
1	b	779	HIS
1	M	881	GLN
2	N	2230	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

230 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
4	CUO	A	5001	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	A	5002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	A	5003	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	A	5004	1	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	A	5005	1,5	14,14,15	0.61	0	15,19,21	1.77	4 (26%)
5	NAG	A	5006	5	14,14,15	0.33	0	15,19,21	0.54	0
5	NAG	A	5007	1,5	14,14,15	0.94	1 (7%)	15,19,21	1.48	2 (13%)
5	NAG	A	5008	5	14,14,15	0.23	0	15,19,21	1.04	1 (6%)
5	NAG	A	5009	1,5	14,14,15	0.59	0	15,19,21	1.70	2 (13%)
5	NAG	A	5010	5,6	14,14,15	0.51	0	15,19,21	1.10	1 (6%)
6	BMA	A	5011	5,7	11,11,12	0.50	0	13,15,17	2.31	4 (30%)
7	MAN	A	5012	6	11,11,12	0.24	0	13,15,17	0.67	0
5	NAG	A	5013	1,5	14,14,15	0.63	0	15,19,21	1.07	1 (6%)
5	NAG	A	5014	5,6	14,14,15	0.56	0	15,19,21	1.25	1 (6%)
6	BMA	A	5015	5	11,11,12	0.26	0	13,15,17	1.11	2 (15%)
4	CUO	A	5016[C]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	A	5016[D]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	B	3001	2	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	B	3002	2	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	B	3003	2,5	14,14,15	1.12	1 (7%)	15,19,21	1.29	2 (13%)
5	NAG	B	3004	5	14,14,15	0.42	0	15,19,21	0.92	0
4	CUO	C	3401[A]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	C	3401[B]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	C	3402[A]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	C	3402[B]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	D	5001	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	D	5002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	D	5003	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	D	5004	1	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	D	5005	1,5	14,14,15	1.05	1 (7%)	15,19,21	1.74	2 (13%)
5	NAG	D	5006	5	14,14,15	0.48	0	15,19,21	1.32	3 (20%)
5	NAG	D	5007	1,5	14,14,15	0.82	1 (7%)	15,19,21	1.22	2 (13%)
5	NAG	D	5008	5,6	14,14,15	0.27	0	15,19,21	0.70	1 (6%)
6	BMA	D	5009	5	11,11,12	0.25	0	13,15,17	0.43	0
5	NAG	D	5010	1,5	14,14,15	0.67	0	15,19,21	1.24	1 (6%)
5	NAG	D	5011	5,6	14,14,15	0.26	0	15,19,21	0.63	0
6	BMA	D	5012	5,7	11,11,12	0.28	0	13,15,17	0.73	0
7	MAN	D	5013	6	11,11,12	0.27	0	13,15,17	0.97	1 (7%)
5	NAG	D	5014	1,5	14,14,15	0.39	0	15,19,21	0.99	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	5015	5	14,14,15	0.36	0	15,19,21	0.85	1 (6%)
4	CUO	D	5016[C]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	D	5016[D]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	E	3001	2	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	E	3002	2	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	E	3003	2,5	14,14,15	0.51	0	15,19,21	1.72	3 (20%)
5	NAG	E	3004	5	14,14,15	0.38	0	15,19,21	1.04	2 (13%)
4	CUO	F	3401[A]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	F	3401[B]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	F	3402[A]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	F	3402[B]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	G	2101[C]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	G	2101[D]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	G	2102	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	G	2103	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	G	2104	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	G	2105	1	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	G	2106	1,5	14,14,15	0.59	0	15,19,21	1.06	1 (6%)
5	NAG	G	2107	5	14,14,15	0.43	0	15,19,21	1.02	1 (6%)
5	NAG	G	2108	5	14,14,15	0.93	1 (7%)	15,19,21	2.04	3 (20%)
5	NAG	G	2109	5	14,14,15	0.30	0	15,19,21	0.66	0
5	NAG	G	2110	1,5	14,14,15	0.55	0	15,19,21	1.31	2 (13%)
5	NAG	G	2111	5	14,14,15	0.50	0	15,19,21	0.96	2 (13%)
5	NAG	G	2112	1,5	14,14,15	0.70	0	15,19,21	1.80	4 (26%)
5	NAG	G	2113	5,6	14,14,15	0.57	0	15,19,21	0.97	0
6	BMA	G	2114	5	11,11,12	0.23	0	13,15,17	0.53	0
4	CUO	H	3001	2	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	H	3002	2	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	H	3003	2,5	14,14,15	0.82	1 (7%)	15,19,21	1.26	2 (13%)
5	NAG	H	3004	5	14,14,15	0.33	0	15,19,21	0.81	1 (6%)
4	CUO	I	3401[A]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	I	3401[B]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	I	3402[A]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	I	3402[B]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	J	5001	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	J	5002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	J	5003	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	J	5004	1	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	J	5005	1,5	14,14,15	0.64	0	15,19,21	1.53	3 (20%)
5	NAG	J	5006	5	14,14,15	0.31	0	15,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	J	5007	1,5	14,14,15	0.86	1 (7%)	15,19,21	1.76	4 (26%)
5	NAG	J	5008	5	14,14,15	0.31	0	15,19,21	0.76	0
5	NAG	J	5009	1,5	14,14,15	0.57	0	15,19,21	1.17	2 (13%)
5	NAG	J	5010	5	14,14,15	0.35	0	15,19,21	0.99	1 (6%)
5	NAG	J	5011	1,5	14,14,15	0.72	1 (7%)	15,19,21	1.99	4 (26%)
5	NAG	J	5012	5,6	14,14,15	0.41	0	15,19,21	1.17	1 (6%)
6	BMA	J	5013	5	11,11,12	0.29	0	13,15,17	0.63	0
4	CUO	J	5014[C]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	J	5014[D]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	K	3001	2	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	K	3002	2	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	K	3003	2,5	14,14,15	0.48	0	15,19,21	1.00	0
5	NAG	K	3004	5	14,14,15	0.49	0	15,19,21	1.02	1 (6%)
4	CUO	M	2101[C]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	M	2101[D]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	M	2102	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	M	2103	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	M	2104	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	M	2105	1	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	M	2106	1,5	14,14,15	0.88	1 (7%)	15,19,21	1.25	2 (13%)
5	NAG	M	2107	5,6	14,14,15	0.35	0	15,19,21	2.01	3 (20%)
6	BMA	M	2108	5	11,11,12	0.23	0	13,15,17	1.23	2 (15%)
5	NAG	M	2109	1,5	14,14,15	1.12	1 (7%)	15,19,21	2.22	3 (20%)
5	NAG	M	2110	5,6	14,14,15	0.58	0	15,19,21	1.64	4 (26%)
6	BMA	M	2111	5,7	11,11,12	0.45	0	13,15,17	2.64	4 (30%)
7	MAN	M	2112	6	11,11,12	0.22	0	13,15,17	0.49	0
7	MAN	M	2113	6	11,11,12	0.42	0	13,15,17	2.06	4 (30%)
5	NAG	M	2114	1,5	14,14,15	0.73	1 (7%)	15,19,21	1.58	2 (13%)
5	NAG	M	2115	5,6	14,14,15	0.51	0	15,19,21	1.66	4 (26%)
6	BMA	M	2116	5,7	11,11,12	0.23	0	13,15,17	1.98	4 (30%)
7	MAN	M	2117	6	11,11,12	0.32	0	13,15,17	0.90	1 (7%)
5	NAG	M	2118	1,5	14,14,15	0.43	0	15,19,21	1.02	1 (6%)
5	NAG	M	2119	5	14,14,15	0.41	0	15,19,21	1.17	1 (6%)
4	CUO	N	3001	2	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	N	3002	2	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	N	3003	2,5	14,14,15	1.11	1 (7%)	15,19,21	1.47	2 (13%)
5	NAG	N	3004	5	14,14,15	0.31	0	15,19,21	0.70	0
4	CUO	O	3401[A]	3	0,4,4	0.00	-	0,4,4	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CUO	O	3401[B]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	P	5001	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	P	5002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	P	5003	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	P	5004	1	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	P	5005	1,5	14,14,15	1.01	1 (7%)	15,19,21	1.57	2 (13%)
5	NAG	P	5006	5,6	14,14,15	0.41	0	15,19,21	0.80	0
6	BMA	P	5007	5	11,11,12	0.25	0	13,15,17	0.60	0
5	NAG	P	5008	1,5	14,14,15	0.74	1 (7%)	15,19,21	1.40	2 (13%)
5	NAG	P	5009	5	14,14,15	0.40	0	15,19,21	1.06	2 (13%)
5	NAG	P	5010	1,5	14,14,15	0.72	0	15,19,21	1.33	1 (6%)
5	NAG	P	5011	5,6	14,14,15	0.30	0	15,19,21	1.16	1 (6%)
6	BMA	P	5012	5	11,11,12	0.28	0	13,15,17	1.39	2 (15%)
5	NAG	P	5013	1,5	14,14,15	0.94	1 (7%)	15,19,21	2.06	2 (13%)
5	NAG	P	5014	5	14,14,15	0.41	0	15,19,21	1.17	2 (13%)
4	CUO	P	5015[C]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	P	5015[D]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	Q	3001	2	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	Q	3002	2	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	Q	3003	2,5	14,14,15	0.83	1 (7%)	15,19,21	1.46	2 (13%)
5	NAG	Q	3004	5	14,14,15	0.42	0	15,19,21	1.14	3 (20%)
4	CUO	S	2101[C]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	S	2101[D]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	S	2102	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	S	2103	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	S	2104	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	S	2105	1	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	S	2106	1,5	14,14,15	0.96	1 (7%)	15,19,21	1.92	2 (13%)
5	NAG	S	2107	5	14,14,15	0.38	0	15,19,21	0.73	1 (6%)
5	NAG	S	2108	1,5	14,14,15	0.93	1 (7%)	15,19,21	1.15	2 (13%)
5	NAG	S	2109	5	14,14,15	0.27	0	15,19,21	0.81	1 (6%)
5	NAG	S	2110	1,5	14,14,15	0.66	0	15,19,21	1.24	3 (20%)
5	NAG	S	2111	5,6	14,14,15	0.41	0	15,19,21	1.02	1 (6%)
6	BMA	S	2112	5,7	11,11,12	0.29	0	13,15,17	2.05	3 (23%)
7	MAN	S	2113	6	11,11,12	0.24	0	13,15,17	0.47	0
5	NAG	S	2114	1,5	14,14,15	0.72	1 (7%)	15,19,21	1.36	3 (20%)
5	NAG	S	2115	5	14,14,15	0.55	0	15,19,21	1.08	1 (6%)
4	CUO	T	3001	2	0,4,4	0.00	-	0,4,4	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CUO	T	3002	2	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	T	3003	2,5	14,14,15	1.09	1 (7%)	15,19,21	1.61	1 (6%)
5	NAG	T	3004	5,6	14,14,15	0.33	0	15,19,21	0.99	1 (6%)
6	BMA	T	3005	5	11,11,12	0.22	0	13,15,17	0.53	0
4	CUO	U	3401[A]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	U	3401[B]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	V	5001	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	V	5002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	V	5003	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	V	5004	1	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	V	5005	1,5	14,14,15	0.77	1 (7%)	15,19,21	1.26	1 (6%)
5	NAG	V	5006	5,6	14,14,15	0.30	0	15,19,21	1.32	2 (13%)
6	BMA	V	5007	5	11,11,12	0.26	0	13,15,17	0.95	1 (7%)
5	NAG	V	5008	1,5	14,14,15	0.81	1 (7%)	15,19,21	1.49	2 (13%)
5	NAG	V	5009	5,6	14,14,15	0.36	0	15,19,21	2.23	3 (20%)
6	BMA	V	5010	5	11,11,12	0.23	0	13,15,17	0.79	0
5	NAG	V	5011	1,5	14,14,15	0.79	1 (7%)	15,19,21	1.51	2 (13%)
5	NAG	V	5012	5,6	14,14,15	0.49	0	15,19,21	0.97	1 (6%)
6	BMA	V	5013	5,7	11,11,12	0.62	0	13,15,17	1.42	2 (15%)
7	MAN	V	5014	6	11,11,12	0.22	0	13,15,17	1.34	2 (15%)
5	NAG	V	5015	1,5	14,14,15	0.72	0	15,19,21	1.36	1 (6%)
5	NAG	V	5016	5,6	14,14,15	0.41	0	15,19,21	1.17	2 (13%)
6	BMA	V	5017	5	11,11,12	0.31	0	13,15,17	0.95	1 (7%)
4	CUO	V	5018[C]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	V	5018[D]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	W	3001	2	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	W	3002	2	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	W	3003	2,5	14,14,15	0.69	0	15,19,21	1.17	1 (6%)
5	NAG	W	3004	5	14,14,15	0.29	0	15,19,21	0.60	0
4	CUO	X	3401[A]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	X	3401[B]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	Y	2101[C]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	Y	2101[D]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	Y	2102	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	Y	2103	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	Y	2104	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	Y	2105	1	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	Y	2106	1,5	14,14,15	0.81	1 (7%)	15,19,21	1.58	2 (13%)
5	NAG	Y	2107	5	14,14,15	0.53	0	15,19,21	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	Y	2108	1,5	14,14,15	0.83	1 (7%)	15,19,21	1.20	1 (6%)
5	NAG	Y	2109	5	14,14,15	0.34	0	15,19,21	0.80	0
5	NAG	Y	2110	1,5	14,14,15	0.72	0	15,19,21	2.02	5 (33%)
5	NAG	Y	2111	5,6	14,14,15	0.37	0	15,19,21	1.37	2 (13%)
6	BMA	Y	2112	5,7	11,11,12	0.29	0	13,15,17	1.47	1 (7%)
7	MAN	Y	2113	6	11,11,12	0.42	0	13,15,17	2.00	3 (23%)
5	NAG	Y	2114	1,5	14,14,15	1.03	1 (7%)	15,19,21	2.46	4 (26%)
5	NAG	Y	2115	5,6	14,14,15	0.44	0	15,19,21	1.20	2 (13%)
6	BMA	Y	2116	5	11,11,12	0.22	0	13,15,17	0.52	0
4	CUO	Z	3001	2	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	Z	3002	2	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	Z	3003	2,5	14,14,15	1.02	1 (7%)	15,19,21	2.51	4 (26%)
5	NAG	Z	3004	5	14,14,15	0.32	0	15,19,21	1.69	3 (20%)
4	CUO	b	2101[C]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	b	2101[D]	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	b	2102	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	b	2103	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	b	2104	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	b	2105	1	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	b	2106	1,5	14,14,15	0.74	1 (7%)	15,19,21	1.11	1 (6%)
5	NAG	b	2107	5,6	14,14,15	0.36	0	15,19,21	0.89	0
6	BMA	b	2108	5	11,11,12	0.25	0	13,15,17	0.90	1 (7%)
5	NAG	b	2109	1,5	14,14,15	1.24	1 (7%)	15,19,21	1.69	2 (13%)
5	NAG	b	2110	5	14,14,15	0.54	0	15,19,21	1.13	1 (6%)
5	NAG	b	2111	1,5	14,14,15	0.64	0	15,19,21	1.15	1 (6%)
5	NAG	b	2112	5,6	14,14,15	0.36	0	15,19,21	0.98	1 (6%)
6	BMA	b	2113	5,7	11,11,12	0.62	0	13,15,17	2.41	4 (30%)
7	MAN	b	2114	6	11,11,12	0.27	0	13,15,17	0.71	0
5	NAG	b	2115	1,5	14,14,15	0.55	0	15,19,21	2.32	3 (20%)
5	NAG	b	2116	5	14,14,15	0.24	0	15,19,21	0.73	0
4	CUO	c	3001	2	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	c	3002	2	0,4,4	0.00	-	0,4,4	0.00	-
5	NAG	c	3003	2,5	14,14,15	1.18	1 (7%)	15,19,21	2.25	4 (26%)
5	NAG	c	3004	5	14,14,15	0.44	0	15,19,21	0.79	0
4	CUO	d	3401[A]	3	0,4,4	0.00	-	0,4,4	0.00	-
4	CUO	d	3401[B]	3	0,4,4	0.00	-	0,4,4	0.00	-

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
4	CUO	A	5001	1	-	0/0/4/4	0/1/1/1
4	CUO	A	5002	1	-	0/0/4/4	0/1/1/1
4	CUO	A	5003	1	-	0/0/4/4	0/1/1/1
4	CUO	A	5004	1	-	0/0/4/4	0/1/1/1
5	NAG	A	5005	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	5006	5	-	0/6/23/26	0/1/1/1
5	NAG	A	5007	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	5008	5	-	0/6/23/26	0/1/1/1
5	NAG	A	5009	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	5010	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	5011	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	5012	6	-	0/2/19/22	0/1/1/1
5	NAG	A	5013	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	5014	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	5015	5	-	0/2/19/22	0/1/1/1
4	CUO	A	5016[C]	-	-	0/0/4/4	0/1/1/1
4	CUO	A	5016[D]	-	-	0/0/4/4	0/1/1/1
4	CUO	B	3001	2	-	0/0/4/4	0/1/1/1
4	CUO	B	3002	2	-	0/0/4/4	0/1/1/1
5	NAG	B	3003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	3004	5	-	0/6/23/26	0/1/1/1
4	CUO	C	3401[A]	3	-	0/0/4/4	0/1/1/1
4	CUO	C	3401[B]	3	-	0/0/4/4	0/1/1/1
4	CUO	C	3402[A]	3	-	0/0/4/4	0/1/1/1
4	CUO	C	3402[B]	3	-	0/0/4/4	0/1/1/1
4	CUO	D	5001	1	-	0/0/4/4	0/1/1/1
4	CUO	D	5002	1	-	0/0/4/4	0/1/1/1
4	CUO	D	5003	1	-	0/0/4/4	0/1/1/1
4	CUO	D	5004	1	-	0/0/4/4	0/1/1/1
5	NAG	D	5005	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	5006	5	-	0/6/23/26	0/1/1/1
5	NAG	D	5007	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	5008	5,6	-	0/6/23/26	0/1/1/1
6	BMA	D	5009	5	-	0/2/19/22	0/1/1/1
5	NAG	D	5010	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	5011	5,6	-	0/6/23/26	0/1/1/1
6	BMA	D	5012	5,7	-	0/2/19/22	0/1/1/1
7	MAN	D	5013	6	-	0/2/19/22	0/1/1/1
5	NAG	D	5014	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	5015	5	-	0/6/23/26	0/1/1/1
4	CUO	D	5016[C]	-	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CUO	D	5016[D]	-	-	0/0/4/4	0/1/1/1
4	CUO	E	3001	2	-	0/0/4/4	0/1/1/1
4	CUO	E	3002	2	-	0/0/4/4	0/1/1/1
5	NAG	E	3003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	E	3004	5	-	0/6/23/26	0/1/1/1
4	CUO	F	3401[A]	3	-	0/0/4/4	0/1/1/1
4	CUO	F	3401[B]	3	-	0/0/4/4	0/1/1/1
4	CUO	F	3402[A]	3	-	0/0/4/4	0/1/1/1
4	CUO	F	3402[B]	3	-	0/0/4/4	0/1/1/1
4	CUO	G	2101[C]	-	-	0/0/4/4	0/1/1/1
4	CUO	G	2101[D]	-	-	0/0/4/4	0/1/1/1
4	CUO	G	2102	1	-	0/0/4/4	0/1/1/1
4	CUO	G	2103	1	-	0/0/4/4	0/1/1/1
4	CUO	G	2104	1	-	0/0/4/4	0/1/1/1
4	CUO	G	2105	1	-	0/0/4/4	0/1/1/1
5	NAG	G	2106	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2107	5	-	0/6/23/26	0/1/1/1
5	NAG	G	2108	5	-	0/6/23/26	0/1/1/1
5	NAG	G	2109	5	-	0/6/23/26	0/1/1/1
5	NAG	G	2110	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2111	5	-	0/6/23/26	0/1/1/1
5	NAG	G	2112	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2113	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	2114	5	-	0/2/19/22	0/1/1/1
4	CUO	H	3001	2	-	0/0/4/4	0/1/1/1
4	CUO	H	3002	2	-	0/0/4/4	0/1/1/1
5	NAG	H	3003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	H	3004	5	-	0/6/23/26	0/1/1/1
4	CUO	I	3401[A]	3	-	0/0/4/4	0/1/1/1
4	CUO	I	3401[B]	3	-	0/0/4/4	0/1/1/1
4	CUO	I	3402[A]	3	-	0/0/4/4	0/1/1/1
4	CUO	I	3402[B]	3	-	0/0/4/4	0/1/1/1
4	CUO	J	5001	1	-	0/0/4/4	0/1/1/1
4	CUO	J	5002	1	-	0/0/4/4	0/1/1/1
4	CUO	J	5003	1	-	0/0/4/4	0/1/1/1
4	CUO	J	5004	1	-	0/0/4/4	0/1/1/1
5	NAG	J	5005	1,5	-	0/6/23/26	0/1/1/1
5	NAG	J	5006	5	-	0/6/23/26	0/1/1/1
5	NAG	J	5007	1,5	-	0/6/23/26	0/1/1/1
5	NAG	J	5008	5	-	0/6/23/26	0/1/1/1
5	NAG	J	5009	1,5	-	0/6/23/26	0/1/1/1
5	NAG	J	5010	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	5011	1,5	-	0/6/23/26	0/1/1/1
5	NAG	J	5012	5,6	-	0/6/23/26	0/1/1/1
6	BMA	J	5013	5	-	0/2/19/22	0/1/1/1
4	CUO	J	5014[C]	-	-	0/0/4/4	0/1/1/1
4	CUO	J	5014[D]	-	-	0/0/4/4	0/1/1/1
4	CUO	K	3001	2	-	0/0/4/4	0/1/1/1
4	CUO	K	3002	2	-	0/0/4/4	0/1/1/1
5	NAG	K	3003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	K	3004	5	-	0/6/23/26	0/1/1/1
4	CUO	M	2101[C]	-	-	0/0/4/4	0/1/1/1
4	CUO	M	2101[D]	-	-	0/0/4/4	0/1/1/1
4	CUO	M	2102	1	-	0/0/4/4	0/1/1/1
4	CUO	M	2103	1	-	0/0/4/4	0/1/1/1
4	CUO	M	2104	1	-	0/0/4/4	0/1/1/1
4	CUO	M	2105	1	-	0/0/4/4	0/1/1/1
5	NAG	M	2106	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2107	5,6	-	0/6/23/26	0/1/1/1
6	BMA	M	2108	5	-	0/2/19/22	0/1/1/1
5	NAG	M	2109	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2110	5,6	-	0/6/23/26	0/1/1/1
6	BMA	M	2111	5,7	-	0/2/19/22	0/1/1/1
7	MAN	M	2112	6	-	0/2/19/22	0/1/1/1
7	MAN	M	2113	6	-	0/2/19/22	0/1/1/1
5	NAG	M	2114	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2115	5,6	-	0/6/23/26	0/1/1/1
6	BMA	M	2116	5,7	-	0/2/19/22	0/1/1/1
7	MAN	M	2117	6	-	0/2/19/22	0/1/1/1
5	NAG	M	2118	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2119	5	-	0/6/23/26	0/1/1/1
4	CUO	N	3001	2	-	0/0/4/4	0/1/1/1
4	CUO	N	3002	2	-	0/0/4/4	0/1/1/1
5	NAG	N	3003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	N	3004	5	-	0/6/23/26	0/1/1/1
4	CUO	O	3401[A]	3	-	0/0/4/4	0/1/1/1
4	CUO	O	3401[B]	3	-	0/0/4/4	0/1/1/1
4	CUO	P	5001	1	-	0/0/4/4	0/1/1/1
4	CUO	P	5002	1	-	0/0/4/4	0/1/1/1
4	CUO	P	5003	1	-	0/0/4/4	0/1/1/1
4	CUO	P	5004	1	-	0/0/4/4	0/1/1/1
5	NAG	P	5005	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	5006	5,6	-	0/6/23/26	0/1/1/1
6	BMA	P	5007	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	P	5008	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	5009	5	-	0/6/23/26	0/1/1/1
5	NAG	P	5010	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	5011	5,6	-	0/6/23/26	0/1/1/1
6	BMA	P	5012	5	-	0/2/19/22	0/1/1/1
5	NAG	P	5013	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	5014	5	-	0/6/23/26	0/1/1/1
4	CUO	P	5015[C]	-	-	0/0/4/4	0/1/1/1
4	CUO	P	5015[D]	-	-	0/0/4/4	0/1/1/1
4	CUO	Q	3001	2	-	0/0/4/4	0/1/1/1
4	CUO	Q	3002	2	-	0/0/4/4	0/1/1/1
5	NAG	Q	3003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	3004	5	-	0/6/23/26	0/1/1/1
4	CUO	S	2101[C]	-	-	0/0/4/4	0/1/1/1
4	CUO	S	2101[D]	-	-	0/0/4/4	0/1/1/1
4	CUO	S	2102	1	-	0/0/4/4	0/1/1/1
4	CUO	S	2103	1	-	0/0/4/4	0/1/1/1
4	CUO	S	2104	1	-	0/0/4/4	0/1/1/1
4	CUO	S	2105	1	-	0/0/4/4	0/1/1/1
5	NAG	S	2106	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2107	5	-	0/6/23/26	0/1/1/1
5	NAG	S	2108	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2109	5	-	0/6/23/26	0/1/1/1
5	NAG	S	2110	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2111	5,6	-	0/6/23/26	0/1/1/1
6	BMA	S	2112	5,7	-	0/2/19/22	0/1/1/1
7	MAN	S	2113	6	-	0/2/19/22	0/1/1/1
5	NAG	S	2114	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2115	5	-	0/6/23/26	0/1/1/1
4	CUO	T	3001	2	-	0/0/4/4	0/1/1/1
4	CUO	T	3002	2	-	0/0/4/4	0/1/1/1
5	NAG	T	3003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	T	3004	5,6	-	0/6/23/26	0/1/1/1
6	BMA	T	3005	5	-	0/2/19/22	0/1/1/1
4	CUO	U	3401[A]	3	-	0/0/4/4	0/1/1/1
4	CUO	U	3401[B]	3	-	0/0/4/4	0/1/1/1
4	CUO	V	5001	1	-	0/0/4/4	0/1/1/1
4	CUO	V	5002	1	-	0/0/4/4	0/1/1/1
4	CUO	V	5003	1	-	0/0/4/4	0/1/1/1
4	CUO	V	5004	1	-	0/0/4/4	0/1/1/1
5	NAG	V	5005	1,5	-	0/6/23/26	0/1/1/1
5	NAG	V	5006	5,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	V	5007	5	-	0/2/19/22	0/1/1/1
5	NAG	V	5008	1,5	-	0/6/23/26	0/1/1/1
5	NAG	V	5009	5,6	-	0/6/23/26	0/1/1/1
6	BMA	V	5010	5	-	0/2/19/22	0/1/1/1
5	NAG	V	5011	1,5	-	0/6/23/26	0/1/1/1
5	NAG	V	5012	5,6	-	0/6/23/26	0/1/1/1
6	BMA	V	5013	5,7	-	0/2/19/22	0/1/1/1
7	MAN	V	5014	6	-	0/2/19/22	0/1/1/1
5	NAG	V	5015	1,5	-	0/6/23/26	0/1/1/1
5	NAG	V	5016	5,6	-	0/6/23/26	0/1/1/1
6	BMA	V	5017	5	-	0/2/19/22	0/1/1/1
4	CUO	V	5018[C]	-	-	0/0/4/4	0/1/1/1
4	CUO	V	5018[D]	-	-	0/0/4/4	0/1/1/1
4	CUO	W	3001	2	-	0/0/4/4	0/1/1/1
4	CUO	W	3002	2	-	0/0/4/4	0/1/1/1
5	NAG	W	3003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	W	3004	5	-	0/6/23/26	0/1/1/1
4	CUO	X	3401[A]	3	-	0/0/4/4	0/1/1/1
4	CUO	X	3401[B]	3	-	0/0/4/4	0/1/1/1
4	CUO	Y	2101[C]	-	-	0/0/4/4	0/1/1/1
4	CUO	Y	2101[D]	-	-	0/0/4/4	0/1/1/1
4	CUO	Y	2102	1	-	0/0/4/4	0/1/1/1
4	CUO	Y	2103	1	-	0/0/4/4	0/1/1/1
4	CUO	Y	2104	1	-	0/0/4/4	0/1/1/1
4	CUO	Y	2105	1	-	0/0/4/4	0/1/1/1
5	NAG	Y	2106	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2107	5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2108	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2109	5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2110	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2111	5,6	-	0/6/23/26	0/1/1/1
6	BMA	Y	2112	5,7	-	0/2/19/22	0/1/1/1
7	MAN	Y	2113	6	-	0/2/19/22	0/1/1/1
5	NAG	Y	2114	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2115	5,6	-	0/6/23/26	0/1/1/1
6	BMA	Y	2116	5	-	0/2/19/22	0/1/1/1
4	CUO	Z	3001	2	-	0/0/4/4	0/1/1/1
4	CUO	Z	3002	2	-	0/0/4/4	0/1/1/1
5	NAG	Z	3003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	Z	3004	5	-	0/6/23/26	0/1/1/1
4	CUO	b	2101[C]	-	-	0/0/4/4	0/1/1/1
4	CUO	b	2101[D]	-	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CUO	b	2102	1	-	0/0/4/4	0/1/1/1
4	CUO	b	2103	1	-	0/0/4/4	0/1/1/1
4	CUO	b	2104	1	-	0/0/4/4	0/1/1/1
4	CUO	b	2105	1	-	0/0/4/4	0/1/1/1
5	NAG	b	2106	1,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2107	5,6	-	0/6/23/26	0/1/1/1
6	BMA	b	2108	5	-	0/2/19/22	0/1/1/1
5	NAG	b	2109	1,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2110	5	-	0/6/23/26	0/1/1/1
5	NAG	b	2111	1,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2112	5,6	-	0/6/23/26	0/1/1/1
6	BMA	b	2113	5,7	-	0/2/19/22	0/1/1/1
7	MAN	b	2114	6	-	0/2/19/22	0/1/1/1
5	NAG	b	2115	1,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2116	5	-	0/6/23/26	0/1/1/1
4	CUO	c	3001	2	-	0/0/4/4	0/1/1/1
4	CUO	c	3002	2	-	0/0/4/4	0/1/1/1
5	NAG	c	3003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	c	3004	5	-	0/6/23/26	0/1/1/1
4	CUO	d	3401[A]	3	-	0/0/4/4	0/1/1/1
4	CUO	d	3401[B]	3	-	0/0/4/4	0/1/1/1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	2114	NAG	C1-C2	2.02	1.55	1.52
5	Y	2108	NAG	C1-C2	2.11	1.55	1.52
5	M	2114	NAG	C1-C2	2.15	1.55	1.52
5	V	5005	NAG	C1-C2	2.15	1.55	1.52
5	J	5011	NAG	C1-C2	2.21	1.55	1.52

The worst 5 of 211 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	2115	NAG	C2-N2-C7	-7.18	112.46	122.94
6	M	2111	BMA	C2-C3-C4	-5.20	101.81	110.88
5	M	2107	NAG	O4-C4-C3	-5.15	99.14	110.36
5	V	5009	NAG	O4-C4-C3	-4.86	99.78	110.36
5	A	5009	NAG	O5-C1-C2	-4.48	105.23	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

102 monomers are involved in 211 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5001	CUO	2	0
5	A	5007	NAG	2	0
5	A	5014	NAG	1	0
5	B	3003	NAG	3	0
5	B	3004	NAG	1	0
4	C	3401[A]	CUO	5	0
4	C	3401[B]	CUO	2	0
4	C	3402[A]	CUO	5	0
4	C	3402[B]	CUO	2	0
4	D	5001	CUO	1	0
4	D	5004	CUO	1	0
5	D	5005	NAG	4	0
5	D	5006	NAG	3	0
5	D	5007	NAG	4	0
5	D	5008	NAG	1	0
5	D	5010	NAG	1	0
5	D	5011	NAG	1	0
6	D	5012	BMA	1	0
7	D	5013	MAN	1	0
5	D	5014	NAG	9	0
5	D	5015	NAG	4	0
5	E	3003	NAG	1	0
5	E	3004	NAG	1	0
4	F	3401[B]	CUO	2	0
4	F	3402[A]	CUO	5	0
4	G	2104	CUO	1	0
5	G	2106	NAG	3	0
5	G	2110	NAG	3	0
5	G	2111	NAG	7	0
5	G	2112	NAG	8	0
5	G	2113	NAG	3	0
5	H	3003	NAG	2	0
4	I	3401[A]	CUO	5	0
4	I	3401[B]	CUO	1	0
4	I	3402[A]	CUO	5	0
4	I	3402[B]	CUO	1	0
4	J	5001	CUO	1	0
4	J	5002	CUO	1	0
5	J	5005	NAG	1	0
5	J	5007	NAG	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	5009	NAG	1	0
5	J	5010	NAG	2	0
5	J	5011	NAG	2	0
4	M	2104	CUO	1	0
4	M	2105	CUO	2	0
6	M	2111	BMA	2	0
7	M	2113	MAN	2	0
5	M	2114	NAG	6	0
5	M	2115	NAG	8	0
6	M	2116	BMA	1	0
5	M	2118	NAG	1	0
5	N	3003	NAG	1	0
4	O	3401[A]	CUO	5	0
4	O	3401[B]	CUO	5	0
5	P	5005	NAG	3	0
5	P	5006	NAG	1	0
5	P	5010	NAG	1	0
5	P	5011	NAG	2	0
6	P	5012	BMA	1	0
5	P	5013	NAG	1	0
5	Q	3003	NAG	6	0
5	Q	3004	NAG	6	0
4	S	2102	CUO	1	0
4	S	2104	CUO	2	0
5	S	2108	NAG	2	0
5	S	2109	NAG	1	0
5	S	2110	NAG	1	0
5	S	2114	NAG	3	0
5	S	2115	NAG	3	0
4	T	3002	CUO	1	0
5	T	3003	NAG	2	0
5	T	3004	NAG	3	0
4	U	3401[A]	CUO	5	0
4	U	3401[B]	CUO	5	0
4	V	5003	CUO	1	0
4	V	5004	CUO	1	0
5	V	5005	NAG	2	0
5	V	5006	NAG	2	0
5	V	5008	NAG	1	0
5	V	5011	NAG	1	0
5	V	5012	NAG	1	0
6	V	5013	BMA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	V	5014	MAN	1	0
5	V	5015	NAG	7	0
5	V	5016	NAG	9	0
6	V	5017	BMA	2	0
4	W	3002	CUO	1	0
5	W	3003	NAG	4	0
5	W	3004	NAG	2	0
4	X	3401[A]	CUO	5	0
4	X	3401[B]	CUO	5	0
4	Y	2102	CUO	1	0
4	Y	2104	CUO	1	0
4	Y	2105	CUO	1	0
5	Y	2108	NAG	2	0
5	Y	2109	NAG	1	0
5	Y	2110	NAG	1	0
5	Y	2114	NAG	3	0
5	Y	2115	NAG	5	0
6	Y	2116	BMA	1	0
5	Z	3003	NAG	6	0
5	Z	3004	NAG	5	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	1656/2000 (82%)	-0.30	28 (1%) 70 42	36, 70, 118, 164	0
1	D	1656/2000 (82%)	-0.30	34 (2%) 64 34	37, 67, 114, 176	0
1	G	1656/2000 (82%)	-0.33	24 (1%) 75 49	31, 68, 109, 152	0
1	J	1656/2000 (82%)	-0.30	31 (1%) 67 37	30, 64, 119, 162	0
1	M	1656/2000 (82%)	-0.40	21 (1%) 77 51	29, 56, 109, 157	0
1	P	1656/2000 (82%)	-0.44	19 (1%) 80 55	27, 53, 97, 176	0
1	S	1656/2000 (82%)	-0.40	32 (1%) 67 37	31, 60, 108, 164	0
1	V	1656/2000 (82%)	-0.46	15 (0%) 84 61	26, 55, 105, 154	0
1	Y	1656/2000 (82%)	-0.36	17 (1%) 82 58	31, 66, 112, 160	0
1	b	1656/2000 (82%)	-0.41	17 (1%) 82 58	30, 60, 105, 161	0
2	B	825/920 (89%)	-0.52	4 (0%) 90 74	32, 57, 101, 140	0
2	E	825/920 (89%)	-0.48	8 (0%) 82 58	30, 59, 106, 137	0
2	H	825/920 (89%)	-0.42	10 (1%) 79 53	31, 63, 112, 147	0
2	K	825/920 (89%)	-0.43	6 (0%) 87 67	34, 60, 101, 158	0
2	N	825/920 (89%)	-0.54	5 (0%) 89 71	21, 46, 92, 135	0
2	Q	825/920 (89%)	-0.54	3 (0%) 92 77	26, 49, 100, 134	0
2	T	825/920 (89%)	-0.51	3 (0%) 92 77	30, 53, 93, 137	0
2	W	825/920 (89%)	-0.54	2 (0%) 94 85	25, 53, 99, 129	0
2	Z	825/920 (89%)	-0.51	5 (0%) 89 71	25, 52, 95, 130	0
2	c	825/920 (89%)	-0.52	6 (0%) 87 67	26, 55, 103, 135	0
3	C	366/394 (92%)	2.75	232 (63%) 0 0	68, 90, 99, 110	0
3	F	366/394 (92%)	2.44	196 (53%) 0 0	56, 78, 88, 107	0
3	I	366/394 (92%)	2.52	204 (55%) 0 0	57, 79, 91, 111	0
3	L	366/394 (92%)	2.61	215 (58%) 0 0	64, 89, 99, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
3	O	366/394 (92%)	2.37	192 (52%)	0	0	52, 75, 95, 107	0
3	R	366/394 (92%)	2.52	215 (58%)	0	0	59, 79, 90, 109	0
3	U	366/394 (92%)	2.28	171 (46%)	0	0	52, 74, 93, 103	0
3	X	366/394 (92%)	4.89	344 (93%)	0	0	79, 102, 111, 116	0
3	a	366/394 (92%)	2.40	190 (51%)	0	0	54, 76, 88, 96	0
3	d	366/394 (92%)	4.58	331 (90%)	0	0	81, 99, 107, 111	0
All	All	28470/33140 (85%)	0.02	2580 (9%)	10	4	21, 63, 107, 176	0

The worst 5 of 2580 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	d	2977[A]	CYS	16.0
3	d	3101[A]	PRO	15.1
3	X	2979[A]	GLN	14.3
3	a	3062[A]	GLN	13.4
3	O	3062[A]	GLN	12.9

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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	G	2112	14/15	0.87	0.25	2.18	79,88,107,112	0
5	NAG	G	2106	14/15	0.86	0.22	1.60	61,73,85,88	0
5	NAG	V	5015	14/15	0.89	0.28	1.24	79,97,106,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	M	2118	14/15	0.85	0.19	0.82	88,96,102,103	0
5	NAG	B	3003	14/15	0.89	0.19	0.74	59,68,91,95	0
4	CUO	Y	2103	4/4	0.93	0.18	0.69	58,65,82,85	0
5	NAG	b	2115	14/15	0.83	0.22	0.63	97,107,114,118	0
5	NAG	V	5005	14/15	0.92	0.17	0.59	50,66,77,82	0
5	NAG	D	5011	14/15	0.82	0.21	0.51	69,84,96,97	0
5	NAG	P	5005	14/15	0.86	0.19	0.50	46,67,81,90	0
5	NAG	D	5014	14/15	0.81	0.19	0.47	77,91,99,104	0
4	CUO	V	5001	4/4	0.96	0.15	0.37	39,39,64,66	0
5	NAG	c	3003	14/15	0.90	0.21	0.29	75,83,99,108	0
4	CUO	B	3001	4/4	0.91	0.15	0.26	49,55,75,88	0
5	NAG	J	5011	14/15	0.84	0.21	0.18	78,100,106,118	0
5	NAG	S	2106	14/15	0.90	0.16	0.15	57,62,72,81	0
5	NAG	H	3003	14/15	0.93	0.18	0.11	71,77,85,90	0
5	NAG	D	5007	14/15	0.88	0.15	0.09	71,83,92,99	0
5	NAG	Y	2106	14/15	0.91	0.15	0.03	51,66,83,92	0
5	NAG	J	5005	14/15	0.89	0.15	0.02	53,69,82,85	0
4	CUO	A	5002	4/4	0.91	0.17	0.01	55,75,89,91	0
5	NAG	G	2108	14/15	0.90	0.14	-0.05	47,61,75,75	0
4	CUO	c	3001	4/4	0.90	0.16	-0.09	48,56,77,80	0
5	NAG	T	3003	14/15	0.88	0.17	-0.23	59,71,83,91	0
5	NAG	D	5005	14/15	0.93	0.16	-0.26	59,67,76,76	0
5	NAG	Y	2114	14/15	0.81	0.21	-0.28	78,87,93,98	0
5	NAG	b	2111	14/15	0.91	0.19	-0.36	62,72,77,78	0
4	CUO	E	3001	4/4	0.89	0.13	-0.43	55,55,80,85	0
4	CUO	D	5001	4/4	0.92	0.14	-0.54	64,68,95,98	0
5	NAG	A	5005	14/15	0.90	0.11	-0.54	62,79,86,94	0
5	NAG	P	5013	14/15	0.89	0.19	-0.56	74,81,89,91	0
4	CUO	S	2103	4/4	0.96	0.13	-0.56	49,52,72,80	0
4	CUO	V	5002	4/4	0.92	0.14	-0.58	50,61,67,72	0
5	NAG	K	3003	14/15	0.84	0.15	-0.59	80,94,105,105	0
5	NAG	D	5010	14/15	0.92	0.15	-0.60	52,57,72,76	0
4	CUO	W	3001	4/4	0.95	0.13	-0.60	37,41,72,78	0
4	CUO	G	2103	4/4	0.93	0.14	-0.60	49,58,62,73	0
4	CUO	J	5002	4/4	0.94	0.13	-0.60	53,56,80,83	0
4	CUO	S	2102	4/4	0.94	0.13	-0.61	54,65,85,90	0
4	CUO	U	3401[B]	4/4	0.69	0.36	-0.65	81,81,81,81	4
4	CUO	U	3401[A]	4/4	0.69	0.36	-0.65	81,81,81,81	4
5	NAG	A	5013	14/15	0.89	0.14	-0.66	85,93,112,115	0
4	CUO	Q	3001	4/4	0.95	0.12	-0.67	37,43,64,70	0
5	NAG	A	5009	14/15	0.88	0.18	-0.69	57,79,95,97	0
4	CUO	D	5002	4/4	0.94	0.14	-0.71	51,60,82,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	W	3003	14/15	0.90	0.15	-0.72	56,63,83,93	0
5	NAG	M	2106	14/15	0.93	0.13	-0.72	52,67,74,75	0
4	CUO	P	5001	4/4	0.95	0.13	-0.74	36,38,56,71	0
5	NAG	P	5010	14/15	0.95	0.16	-0.74	52,60,70,76	0
5	NAG	b	2106	14/15	0.94	0.13	-0.74	56,62,71,72	0
5	NAG	M	2114	14/15	0.91	0.19	-0.75	60,67,72,81	0
5	NAG	S	2114	14/15	0.91	0.16	-0.76	80,84,96,97	0
5	NAG	V	5011	14/15	0.93	0.16	-0.81	49,68,77,78	0
5	NAG	S	2108	14/15	0.90	0.15	-0.86	87,95,100,108	0
4	CUO	B	3002	4/4	0.94	0.14	-0.88	57,58,80,91	0
4	CUO	b	2103	4/4	0.94	0.13	-0.92	55,59,71,73	0
4	CUO	A	5001	4/4	0.90	0.12	-0.94	70,73,87,92	0
4	CUO	V	5004	4/4	0.96	0.12	-0.95	44,50,62,65	0
4	CUO	N	3001	4/4	0.93	0.14	-0.96	36,39,74,80	0
4	CUO	T	3001	4/4	0.96	0.13	-0.98	44,59,84,85	0
4	CUO	X	3401[B]	4/4	0.39	0.56	-0.99	121,121,121,121	4
4	CUO	J	5014[D]	4/4	0.59	0.31	-1.00	98,98,98,98	4
4	CUO	K	3002	4/4	0.95	0.11	-1.02	52,69,75,79	0
4	CUO	G	2104	4/4	0.90	0.17	-1.07	58,85,92,97	0
4	CUO	P	5003	4/4	0.93	0.14	-1.07	45,54,76,83	0
4	CUO	T	3002	4/4	0.93	0.13	-1.08	52,69,74,84	0
5	NAG	Y	2110	14/15	0.96	0.13	-1.08	60,66,76,78	0
4	CUO	S	2105	4/4	0.94	0.13	-1.09	45,45,62,71	0
5	NAG	V	5008	14/15	0.93	0.15	-1.10	46,58,71,75	0
4	CUO	Y	2104	4/4	0.90	0.13	-1.14	69,75,80,100	0
4	CUO	Z	3001	4/4	0.96	0.12	-1.14	46,54,67,69	0
4	CUO	M	2102	4/4	0.97	0.11	-1.14	41,52,59,63	0
4	CUO	C	3402[A]	4/4	0.73	0.31	-1.17	100,100,100,100	4
4	CUO	F	3402[A]	4/4	0.74	0.28	-1.20	85,85,85,85	4
4	CUO	C	3402[B]	4/4	0.73	0.31	-1.20	100,100,100,100	4
4	CUO	F	3402[B]	4/4	0.74	0.28	-1.22	85,85,85,85	4
4	CUO	X	3401[A]	4/4	0.39	0.56	-1.22	121,121,121,121	4
4	CUO	C	3401[A]	4/4	0.71	0.28	-1.28	99,99,99,99	4
5	NAG	S	2110	14/15	0.95	0.14	-1.30	61,71,75,75	0
4	CUO	P	5004	4/4	0.95	0.13	-1.31	40,48,67,68	0
4	CUO	C	3401[B]	4/4	0.71	0.28	-1.33	99,99,99,99	4
5	NAG	G	2110	14/15	0.93	0.15	-1.38	56,67,78,80	0
4	CUO	G	2102	4/4	0.97	0.10	-1.40	57,62,65,70	0
4	CUO	O	3401[A]	4/4	0.67	0.32	-1.42	85,85,85,85	4
5	NAG	J	5009	14/15	0.91	0.19	-1.42	64,80,91,91	0
4	CUO	O	3401[B]	4/4	0.67	0.32	-1.42	85,85,85,85	4
4	CUO	J	5004	4/4	0.95	0.11	-1.43	49,58,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CUO	M	2101[D]	4/4	0.71	0.27	-1.43	103,103,103,103	4
4	CUO	M	2103	4/4	0.97	0.11	-1.44	50,59,66,68	0
4	CUO	N	3002	4/4	0.95	0.12	-1.47	48,51,70,74	0
4	CUO	J	5001	4/4	0.93	0.12	-1.49	49,52,60,69	0
4	CUO	Y	2101[D]	4/4	0.72	0.28	-1.49	99,99,99,99	4
4	CUO	V	5003	4/4	0.90	0.11	-1.51	66,79,89,90	0
4	CUO	V	5018[D]	4/4	0.52	0.36	-1.53	113,113,113,113	4
4	CUO	H	3001	4/4	0.95	0.11	-1.64	58,60,72,78	0
4	CUO	G	2101[D]	4/4	0.69	0.28	-1.64	104,104,104,104	4
4	CUO	M	2104	4/4	0.90	0.10	-1.65	58,70,74,76	0
4	CUO	P	5002	4/4	0.94	0.12	-1.68	56,59,75,82	0
4	CUO	D	5016[D]	4/4	0.59	0.30	-1.71	109,109,109,109	4
4	CUO	F	3401[B]	4/4	0.70	0.23	-1.71	86,86,86,86	4
4	CUO	S	2104	4/4	0.93	0.11	-1.71	74,79,82,87	0
4	CUO	d	3401[B]	4/4	0.60	0.43	-1.73	111,111,111,111	4
4	CUO	b	2102	4/4	0.95	0.10	-1.75	60,63,73,78	0
4	CUO	I	3401[A]	4/4	0.76	0.21	-1.76	84,84,84,84	4
4	CUO	A	5016[D]	4/4	0.62	0.20	-1.77	95,95,95,95	4
4	CUO	b	2104	4/4	0.91	0.13	-1.83	60,75,83,94	0
4	CUO	Z	3002	4/4	0.94	0.11	-1.84	48,68,69,72	0
4	CUO	Y	2102	4/4	0.95	0.10	-1.88	59,67,69,83	0
4	CUO	I	3402[B]	4/4	0.49	0.23	-2.02	84,84,84,84	4
4	CUO	b	2105	4/4	0.92	0.11	-2.14	54,57,68,74	0
4	CUO	I	3401[B]	4/4	0.76	0.21	-2.14	84,84,84,84	4
4	CUO	A	5004	4/4	0.96	0.11	-2.16	51,60,67,70	0
4	CUO	d	3401[A]	4/4	0.60	0.43	-2.20	111,111,111,111	4
4	CUO	Q	3002	4/4	0.94	0.10	-2.26	53,62,64,73	0
4	CUO	F	3401[A]	4/4	0.70	0.23	-2.39	86,86,86,86	4
4	CUO	W	3002	4/4	0.94	0.12	-2.44	58,62,70,77	0
4	CUO	c	3002	4/4	0.95	0.08	-2.48	70,71,79,80	0
4	CUO	D	5004	4/4	0.98	0.07	-2.63	52,54,59,62	0
4	CUO	I	3402[A]	4/4	0.49	0.23	-2.64	84,84,84,84	4
4	CUO	A	5003	4/4	0.94	0.07	-2.67	79,87,89,89	0
4	CUO	G	2105	4/4	0.96	0.08	-2.79	58,60,66,69	0
4	CUO	J	5003	4/4	0.94	0.09	-2.83	89,96,96,103	0
4	CUO	M	2105	4/4	0.95	0.12	-2.84	48,60,61,62	0
4	CUO	K	3001	4/4	0.96	0.08	-2.85	57,73,73,80	0
4	CUO	D	5003	4/4	0.94	0.08	-2.93	60,62,67,79	0
5	NAG	Z	3003	14/15	0.95	0.10	-3.10	69,77,85,86	0
4	CUO	H	3002	4/4	0.97	0.08	-3.13	67,79,83,84	0
4	CUO	Y	2105	4/4	0.96	0.10	-3.45	47,59,61,62	0
4	CUO	E	3002	4/4	0.98	0.06	-4.08	57,61,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	K	3004	14/15	0.62	0.23	-	104,115,125,125	0
5	NAG	P	5009	14/15	0.66	0.32	-	78,96,107,116	0
5	NAG	N	3004	14/15	0.92	0.20	-	53,71,87,100	0
6	BMA	P	5007	11/12	0.76	0.18	-	114,119,149,149	0
5	NAG	G	2109	14/15	0.87	0.14	-	54,72,84,88	0
5	NAG	A	5008	14/15	0.81	0.27	-	106,116,123,129	0
5	NAG	A	5010	14/15	0.80	0.29	-	99,105,109,109	0
6	BMA	A	5015	11/12	0.72	0.31	-	108,114,120,126	0
6	BMA	J	5013	11/12	0.83	0.30	-	107,110,117,128	0
5	NAG	E	3003	14/15	0.92	0.17	-	67,77,90,98	0
6	BMA	D	5012	11/12	0.75	0.26	-	98,113,119,128	0
5	NAG	W	3004	14/15	0.88	0.20	-	71,82,95,107	0
7	MAN	M	2117	11/12	0.78	0.20	-	94,114,123,126	0
4	CUO	D	5016[C]	4/4	0.59	0.30	-	109,109,109,109	4
6	BMA	M	2116	11/12	0.71	0.25	-	97,112,128,130	0
6	BMA	b	2113	11/12	0.86	0.17	-	96,97,104,125	0
6	BMA	V	5013	11/12	0.58	0.23	-	85,101,110,113	0
6	BMA	b	2108	11/12	0.74	0.49	-	102,117,134,138	0
6	BMA	G	2114	11/12	0.77	0.28	-	111,120,128,129	0
5	NAG	M	2107	14/15	0.94	0.22	-	65,83,94,109	0
5	NAG	G	2107	14/15	0.90	0.20	-	43,67,86,87	0
4	CUO	b	2101[C]	4/4	0.68	0.31	-	106,106,106,106	4
6	BMA	Y	2116	11/12	0.70	0.25	-	101,110,119,119	0
6	BMA	M	2108	11/12	0.76	0.30	-	102,116,123,123	0
5	NAG	S	2107	14/15	0.85	0.19	-	64,84,98,101	0
4	CUO	P	5015[D]	4/4	0.52	0.42	-	114,114,114,114	4
5	NAG	J	5006	14/15	0.76	0.25	-	50,90,102,103	0
4	CUO	b	2101[D]	4/4	0.68	0.31	-	106,106,106,106	4
6	BMA	S	2112	11/12	0.87	0.14	-	112,120,124,127	0
5	NAG	b	2112	14/15	0.86	0.15	-	72,80,89,91	0
5	NAG	b	2109	14/15	0.94	0.11	-	57,70,80,85	0
7	MAN	M	2113	11/12	0.60	0.44	-	135,140,150,154	0
4	CUO	P	5015[C]	4/4	0.52	0.42	-	114,114,114,114	4
5	NAG	G	2113	14/15	0.91	0.13	-	84,91,98,102	0
4	CUO	Y	2101[C]	4/4	0.72	0.28	-	99,99,99,99	4
5	NAG	b	2110	14/15	0.91	0.16	-	55,73,85,91	0
5	NAG	J	5008	14/15	0.84	0.22	-	86,100,114,132	0
4	CUO	J	5014[C]	4/4	0.59	0.31	-	98,98,98,98	4
4	CUO	S	2101[D]	4/4	0.65	0.27	-	94,94,94,94	4
6	BMA	V	5010	11/12	0.74	0.35	-	104,115,132,134	0
4	CUO	A	5016[C]	4/4	0.62	0.20	-	95,95,95,95	4
5	NAG	M	2119	14/15	0.76	0.26	-	91,104,121,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	BMA	T	3005	11/12	0.39	0.29	-	96,123,130,130	0
7	MAN	D	5013	11/12	0.72	0.21	-	114,118,122,128	0
5	NAG	Y	2107	14/15	0.88	0.15	-	75,89,96,100	0
5	NAG	V	5012	14/15	0.82	0.20	-	74,88,101,105	0
5	NAG	b	2107	14/15	0.91	0.23	-	61,80,101,112	0
5	NAG	V	5016	14/15	0.84	0.17	-	88,108,127,131	0
5	NAG	T	3004	14/15	0.82	0.30	-	88,97,115,124	0
6	BMA	M	2111	11/12	0.59	0.40	-	124,134,140,150	0
5	NAG	Q	3003	14/15	0.94	0.14	-	57,70,83,84	0
4	CUO	S	2101[C]	4/4	0.65	0.27	-	94,94,94,94	4
5	NAG	P	5008	14/15	0.95	0.08	-	57,70,74,80	0
5	NAG	A	5014	14/15	0.84	0.15	-	84,94,107,114	0
5	NAG	N	3003	14/15	0.90	0.14	-	41,56,75,80	0
5	NAG	E	3004	14/15	0.82	0.28	-	72,91,105,110	0
5	NAG	B	3004	14/15	0.84	0.26	-	84,92,107,111	0
5	NAG	D	5008	14/15	0.91	0.14	-	88,104,119,123	0
5	NAG	S	2109	14/15	0.83	0.25	-	73,97,113,113	0
5	NAG	G	2111	14/15	0.92	0.16	-	80,88,92,93	0
4	CUO	G	2101[C]	4/4	0.69	0.28	-	104,104,104,104	4
5	NAG	J	5007	14/15	0.90	0.22	-	73,78,87,92	0
5	NAG	J	5012	14/15	0.80	0.19	-	88,104,108,111	0
5	NAG	P	5006	14/15	0.89	0.16	-	61,82,96,102	0
7	MAN	S	2113	11/12	0.83	0.18	-	114,125,132,145	0
5	NAG	D	5006	14/15	0.94	0.19	-	49,57,73,79	0
6	BMA	V	5007	11/12	0.85	0.24	-	82,103,108,108	0
6	BMA	P	5012	11/12	0.68	0.19	-	98,114,124,127	0
5	NAG	V	5009	14/15	0.84	0.20	-	70,82,98,108	0
5	NAG	A	5006	14/15	0.83	0.23	-	69,83,96,102	0
5	NAG	H	3004	14/15	0.73	0.36	-	89,102,108,116	0
5	NAG	Q	3004	14/15	0.74	0.32	-	69,83,101,104	0
5	NAG	Y	2111	14/15	0.85	0.19	-	67,81,92,93	0
5	NAG	M	2109	14/15	0.86	0.16	-	79,85,93,96	0
5	NAG	M	2110	14/15	0.80	0.29	-	92,105,121,128	0
5	NAG	J	5010	14/15	0.85	0.19	-	82,97,104,106	0
6	BMA	Y	2112	11/12	0.85	0.26	-	79,99,114,127	0
5	NAG	V	5006	14/15	0.81	0.26	-	78,91,95,98	0
5	NAG	P	5014	14/15	0.88	0.21	-	49,73,85,91	0
7	MAN	A	5012	11/12	0.70	0.20	-	103,117,133,133	0
5	NAG	M	2115	14/15	0.86	0.16	-	58,78,82,90	0
5	NAG	P	5011	14/15	0.84	0.17	-	61,77,95,103	0
5	NAG	Z	3004	14/15	0.84	0.19	-	84,93,116,127	0
6	BMA	V	5017	11/12	0.64	0.29	-	130,136,142,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	S	2111	14/15	0.90	0.17	-	87,92,98,104	0
4	CUO	M	2101[C]	4/4	0.71	0.27	-	103,103,103,103	4
5	NAG	b	2116	14/15	0.81	0.16	-	97,115,121,125	0
7	MAN	b	2114	11/12	0.82	0.15	-	107,112,125,133	0
5	NAG	A	5007	14/15	0.91	0.13	-	88,95,105,109	0
5	NAG	c	3004	14/15	0.92	0.24	-	83,92,102,114	0
4	CUO	V	5018[C]	4/4	0.52	0.36	-	113,113,113,113	4
6	BMA	A	5011	11/12	0.88	0.17	-	110,124,133,139	0
7	MAN	Y	2113	11/12	0.70	0.32	-	87,103,122,135	0
5	NAG	D	5015	14/15	0.86	0.23	-	80,95,108,108	0
6	BMA	D	5009	11/12	0.81	0.23	-	110,119,126,133	0
5	NAG	Y	2108	14/15	0.88	0.19	-	70,80,88,90	0
7	MAN	M	2112	11/12	0.63	0.36	-	121,135,151,154	0
5	NAG	Y	2115	14/15	0.90	0.14	-	76,89,100,104	0
5	NAG	S	2115	14/15	0.79	0.19	-	62,82,95,101	0
5	NAG	Y	2109	14/15	0.86	0.21	-	82,92,100,100	0
7	MAN	V	5014	11/12	0.72	0.31	-	94,107,126,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.