



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:40 am GMT

PDB ID : 1HC1  
Title : CRYSTAL STRUCTURE OF HEXAMERIC HAEMOCYANIN FROM PAN-  
ULIRUS INTERRUPTUS REFINED AT 3.2 ANGSTROMS RESOLUTION  
Authors : Volbeda, A.; Hol, W.G.J.  
Deposited on : 1991-05-15  
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

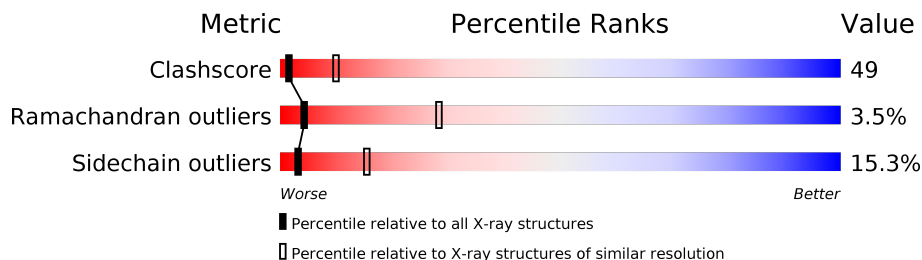
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	657	
1	B	657	
1	C	657	
1	D	657	
1	E	657	
1	F	657	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32166 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 ARTHROPODAN HEMOCYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	B	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	C	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	D	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	E	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	F	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ASP	GLU	CONFLICT	UNP P04254
A	163	PRO	GLN	CONFLICT	UNP P04254
A	458	ASN	LYS	CONFLICT	UNP P04254
A	514	SER	LYS	CONFLICT	UNP P04254
B	32	ASP	GLU	CONFLICT	UNP P04254
B	163	PRO	GLN	CONFLICT	UNP P04254
B	458	ASN	LYS	CONFLICT	UNP P04254
B	514	SER	LYS	CONFLICT	UNP P04254
C	32	ASP	GLU	CONFLICT	UNP P04254
C	163	PRO	GLN	CONFLICT	UNP P04254
C	458	ASN	LYS	CONFLICT	UNP P04254
C	514	SER	LYS	CONFLICT	UNP P04254
D	32	ASP	GLU	CONFLICT	UNP P04254
D	163	PRO	GLN	CONFLICT	UNP P04254
D	458	ASN	LYS	CONFLICT	UNP P04254
D	514	SER	LYS	CONFLICT	UNP P04254
E	32	ASP	GLU	CONFLICT	UNP P04254

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Chain	Residue	Modelled	Actual	Comment	Reference
E	163	PRO	GLN	CONFLICT	UNP P04254
E	458	ASN	LYS	CONFLICT	UNP P04254
E	514	SER	LYS	CONFLICT	UNP P04254
F	32	ASP	GLU	CONFLICT	UNP P04254
F	163	PRO	GLN	CONFLICT	UNP P04254
F	458	ASN	LYS	CONFLICT	UNP P04254
F	514	SER	LYS	CONFLICT	UNP P04254

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Cu 2 2	0	0
2	E	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0
2	A	2	Total Cu 2 2	0	0
2	F	2	Total Cu 2 2	0	0

- Molecule 3 is water.

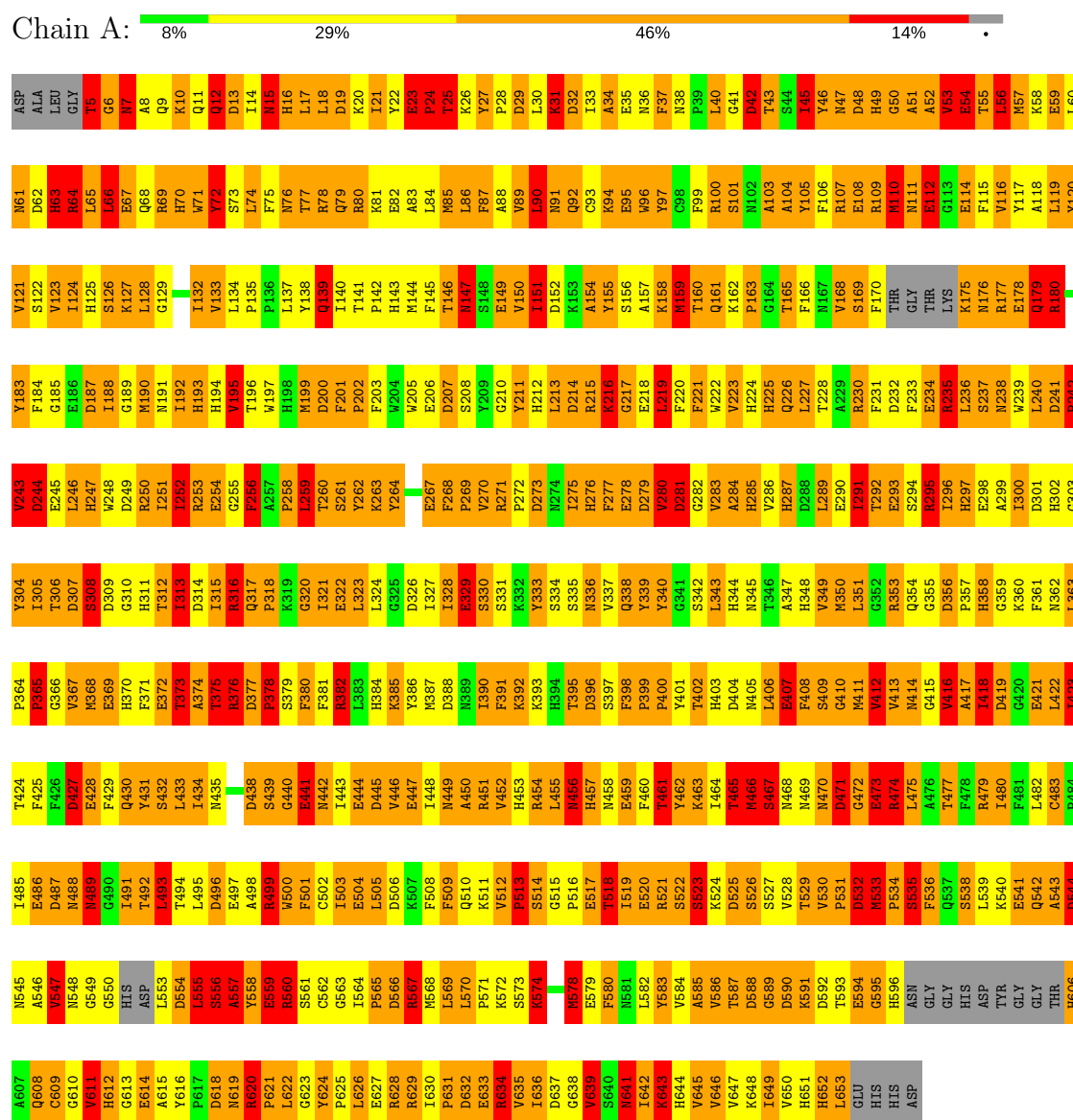
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	186	Total O 186 186	0	0
3	E	186	Total O 186 186	0	0
3	D	186	Total O 186 186	0	0
3	C	186	Total O 186 186	0	0
3	B	186	Total O 186 186	0	0
3	A	186	Total O 186 186	0	0

### 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.

Note EDS was not executed.

#### • Molecule 1: ARTHROPODAN HEMOCYANIN



#### • Molecule 1: ARTHROPODAN HEMOCYANIN

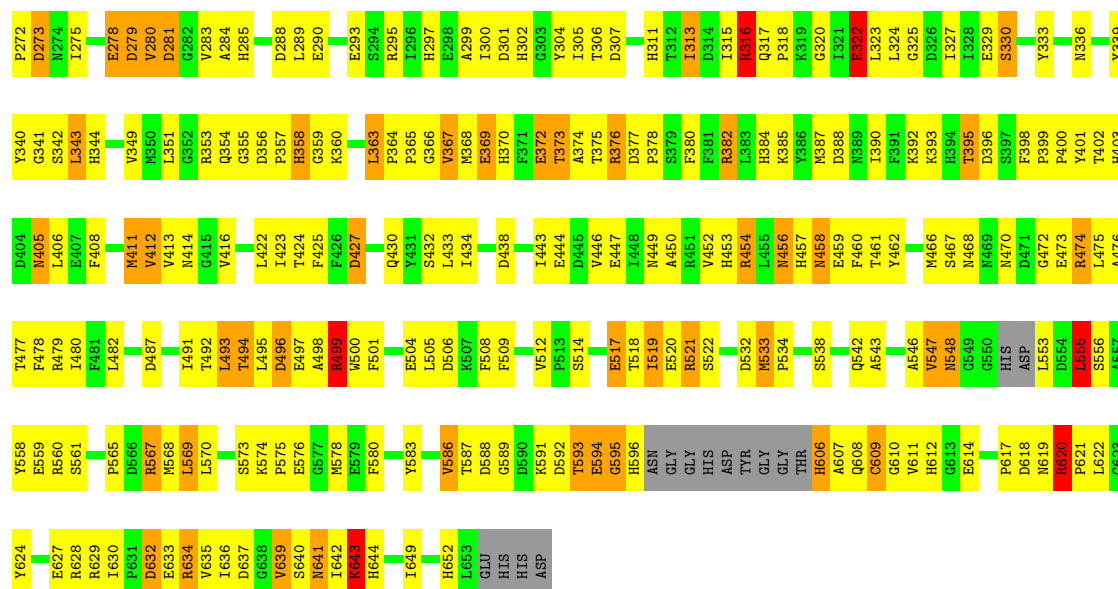
Chain B:  7% 32% 42% 16%

ASP	N61	V121	A182	P242	H302	N362	L422	L482	Q542	Tyr
ALA	D62	S122	Y183	V243	G303	L363	I423	C483	A543	GLY
LEU	H63	V123	F184	D244	Y304	P364	I424	C484	D544	GLY
GLY	R64	I124	G185	L245	I305	P365	F425	L485	N545	THR
T5	L66	S126	E186	L246	T306	G366	F426	E486	A546	H606
G6	L67	K127	D187	L247	S308	V367	D427	D487	V547	A607
H7	Q68	L128	I188	V248	D309	N368	E428	N488	N548	Q608
A8	Q69	G129	M189	D249	G310	E369	F429	G489	G549	C609
Q9	R69	H130	M190	R250	H311	H370	Q431	L491	HIS	H611
K10	H70	D131	N191	L251	T312	F371	S432	T492	ASP	G610
Q11	W71	G131	I192	L252	H313	E372	S433	L493	L553	H612
D12	Y72	I132	H193	R253	I314	A373	I434	T494	D554	G613
D13	S73	V133	H194	G254	I315	T374	N435	L495	L555	E614
I14	L74	L134	V195	G255	R316	R375	A436	D496	S556	A615
M15	F75	P135	T196	F256	R317	R376	A437	E497	L557	Y616
H16	N76	G137	H197	A257	D318	P378	D438	A498	Y558	P617
L17	T77	Y138	H198	R258	K319	S379	S439	N499	E559	D618
L18	R78	Y139	M199	L259	K320	F380	G440	V500	R560	N619
D19	Q79	Q139	D200	T260	I321	F381	E441	F501	S561	R620
K20	R80	I140	F201	S261	E322	R382	N442	C502	C562	P621
I21	A81	T141	P202	Y262	L323	L383	I443	L503	G563	L622
E22	E82	P142	W204	Y263	L324	H384	E444	E504	I564	G623
E23	A83	H143	W205	G264	K325	K385	I445	L505	P565	Y624
P24	L84	M144	E206	G265	D326	Y386	D446	D506	D566	P625
T25	N85	F145	E207	E267	I327	R387	E447	Y507	R567	L626
K26	L86	T146	D207	F268	I328	D388	I448	F508	M568	E627
Y27	F87	N147	S208	P269	E329	N389	N449	F509	R569	R628
P28	A88	Y209	Y209	Y270	S330	I390	A450	Q510	L570	R629
D29	V89	G210	G210	R271	S331	F391	A451	K511	P571	T630
L30	R90	V150	Y211	R272	K332	K392	V452	V512	K572	D631
K31	N91	I151	H212	D273	Y333	K393	H453	P513	S573	E632
D32	Q92	D152	L213	D274	S334	H394	R454	S514	K574	F633
I33	C93	D214	R215	L275	N335	D395	L455	Q515	P575	R634
A34	K94	R216	G217	H276	N336	T396	N456	P516	E576	V635
E35	E95	A157	G218	F277	Y337	F397	H457	E517	G577	L636
N36	Y96	K158	E218	E278	Q338	N398	N458	T518	M578	D637
F37	Y97	C98	L219	D279	Y339	P399	E459	T519	E579	G638
N38	C98	F99	F220	Y280	Y340	F400	F460	E520	F580	V639
P39	R100	Q161	F221	D281	G341	Y401	T461	R521	N581	G640
L40	L40	P162	Y222	G282	L342	T402	Y462	S522	L582	N641
G41	G41	P163	Y223	P283	H343	H403	K463	S523	Y583	T642
N101	N101	G164	H224	A284	H344	D404	I464	K524	V584	K643
T43	T43	T165	H225	H285	N345	N405	T465	D525	A585	H644
S44	S44	F166	Q226	V286	T346	L406	M466	S526	V586	V645
I45	I45	M167	L227	H287	A347	E407	S467	S527	T587	T646
Y46	Y46	V168	T228	D288	H348	F408	N468	V528	D588	V649
N47	N47	S169	A229	L289	V349	S409	N469	T529	G589	V650
D48	D48	F170	R230	E290	M350	Q410	N470	V530	G590	H651
H49	H49	THR	F231	T291	L351	N411	D471	P531	K591	H652
G50	G50	GLY	D232	T292	G352	V412	G472	D532	D592	L653
A51	A51	THR	F233	E293	R353	V413	E473	R533	R593	GLU
A52	A52	LYS	E234	S294	Q354	N414	R474	P534	E594	HIS
V53	V53	K175	R235	R295	G355	O415	L475	S535	G595	ASP
E54	E54	N176	L236	L296	D356	V416	A476	F536	H596	
T55	T55	R177	S237	H297	P357	A417	T477	Q537	ASN	
L56	L56	E178	N238	E298	H358	T418	F478	S538	GLY	
M57	M57	Q179	N239	A299	G359	D419	R479	L539	GLY	
E58	E58	L119	W239	L240	K360	L420	I480	K540	HIS	
E59	E59	V181	D241	D301	F361	E421	F481	E541	ASP	

## • Molecule 1: ARTHROPODAN HEMOCYANIN

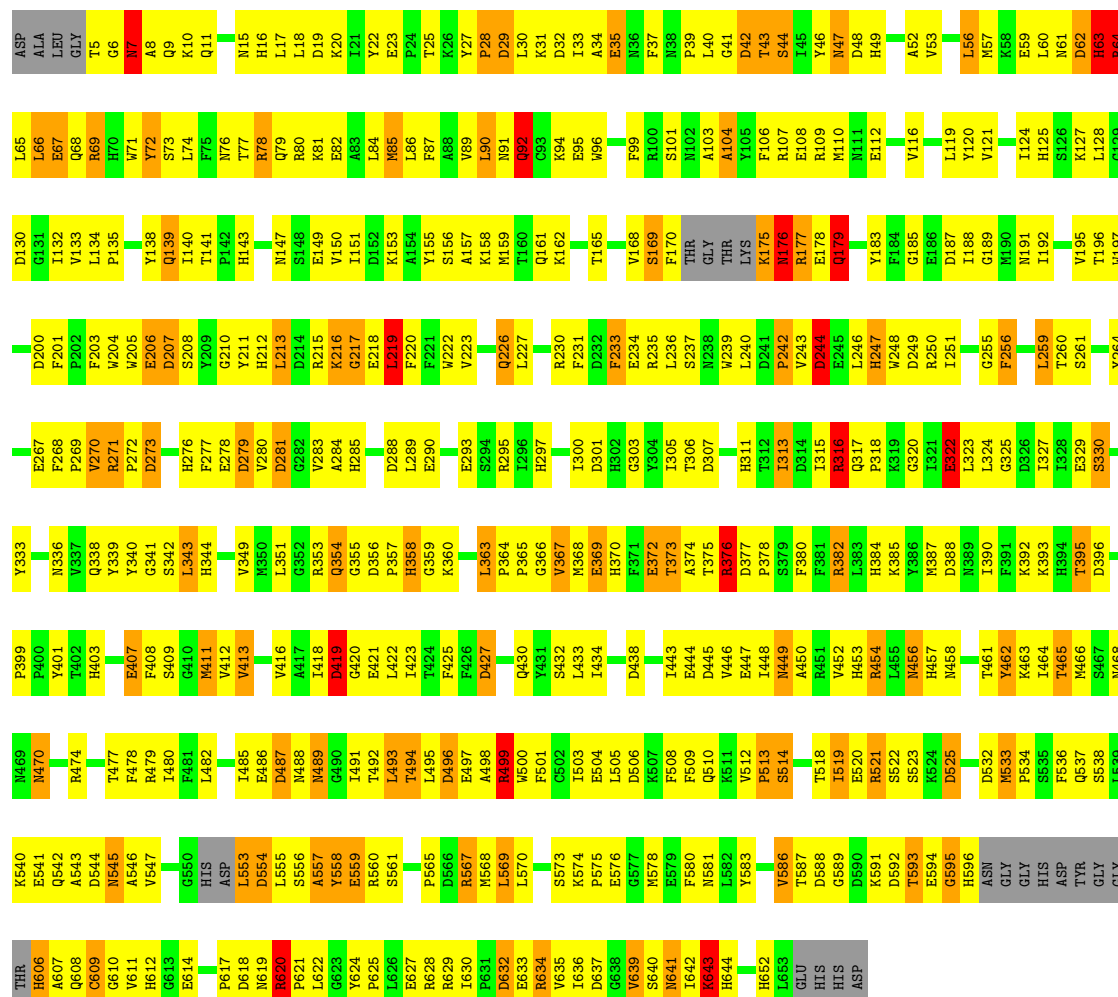
Chain C:  35% 49% 11%

ASP	L66	V133	W204	G210	T146	V150	V133	W204	G210	T146
ALA	E67	L134	W205	Q139	V151	V151	L134	W205	Q139	V151
LEU	R69	P135	D207	Y71	D152	D152	P135	D207	Y71	D152
GLY	H70	S136	E208	H72	K153	K153	H70	S136	E208	H72
T5	W71	Y138	D209	Y73	A154	A154	W71	Y138	D209	Y73
G6	H72	Q139	D210	Y74	Y155	Y155	G6	H72	Q139	D210
H7	Y73	T141	D211	Y75	S156	S156	H7	Y73	T141	D211
A8	S73	H143	D212	Y76	A157	A157	A8	S73	H143	D212
Q9	L74	H144	D213	Y77	H16	H16	Q9	L74	H144	D213
K10	F75	H145	D214	T77	H17	H17	K10	F75	H145	D214
Q11	G76	H146	D215	T78	H18	H18	Q11	G76	H146	D215
M15	Q79	V150	D216	T79	H19	H19	M15	Q79	V150	D216
H16	Q80	V151	D217	T80	H20	H20	H16	Q80	V151	D217
L17	R80	V152	D218	T81	H21	H21	L17	R80	V152	D218
D18	E81	K153	D219	T82	A154	A154	D18	E81	K153	D219
D19	E82	K154	D220	T83	Y155	Y155	D19	E82	K154	D220
K20	N83	Y156	D221	T84	S156	S156	K20	N83	Y156	D221
E21	L84	Y157	D222	T85	A157	A157	E21	L84	Y157	D222
Y22	H85	S158	D223	T86	H16	H16	Y22	H85	S158	D223
E23	R86	A159	D224	T87	H17	H17	E23	R86	A159	D224
P24	T87	M159	D225	T88	H18	H18	P24	T87	M159	D225
T25	A88	T160	D226	T89	H19	H19	T25	A88	T160	D226
K26	Y89	Q161	D227	T90	H20	H20	K26	Y89	Q161	D227
Y27	L90	Q162	D228	T91	H21	H21	Y27	L90	Q162	D228
E28	N91	Q163	D229	T92	H22	H22	E28	N91	Q163	D229
P29	Q92	Q164	D230	T93	H23	H23	P29	Q92	Q164	D230
I33	R93	Q165	D231	T94	H24	H24	I33	R93	Q165	D231
A34	S101	Q166	D232	T95	H25	H25	A34	S101	Q166	D232
E35	N102	Q167	D233	T96	H26	H26	E35	N102	Q167	D233
N36	A103	Q168	D234	T97	H27	H27	N36	A103	Q168	D234
F37	L104	Q169	D235	T98	H28	H28	F37	L104	Q169	D235
N38	Y105	Q170	D236	T99	H29	H29	N38	Y105	Q170	D236
P39	A106	Q171	D237	T100	H30	H30	P39	A106	Q171	D237
L40	F106	Q172	D238	T101	H31	H31	L40	F106	Q172	D238
G41	R107	Q173	D239	T102	H32	H32	G41	R107	Q173	D239
D42	E108	Q174	D240	T103	H33	H33	D42	E108	Q174	D240
T43	R109	Q175	D241	T104	H34	H34	T43	R109	Q175	D241
S44	M110	Q176	D242	T105	H35	H35	S44	M110	Q176	D242
I45	N111	Q177	D243	T106	H36	H36	I45	N111	Q177	D243
Y46	E112	Q178	D244	T107	H37	H37	Y46	E112	Q178	D244
N47	V116	Q179	D245	T108	H38	H38	N47	V116	Q179	D245
D48	L119	Q180	D246	T109	H39	H39	D48	L119	Q180	D246
H49	Y120	Q181	D247	T110	H40	H40	H49	Y120	Q181	D247
V53	V121	Q182	D248	T111	H41	H41	V53	V121	Q182	D248
L56	T124	Q183	D249	T112	H42	H42	L56	T124	Q183	D249
M57	H125	Q184	D250	T113	H43	H43	M57	H125	Q184	D250
K58	S126	Q185	D251	T114	H44	H44	K58	S126	Q185	D251
E59	K127	Q186	D252	T115	H45	H45	E59	K127	Q186	D252
L60	L128	Q187	D253	T116	H46	H46	L60	L128	Q187	D253
N61	G129	Q188	D254	T117	H47	H47	N61	G129	Q188	D254
D62	D130	Q189	D255	T118	H48	H48	D62	D130	Q189	D255
H63	G131	Q190	D256	T119	H49	H49	H63	G131	Q190	D256
R64	T132	Q191	D257	T120	H50	H50	R64	T132	Q191	D257
L65		Q192	D258	T121	H51	H51	L65		Q192	D258



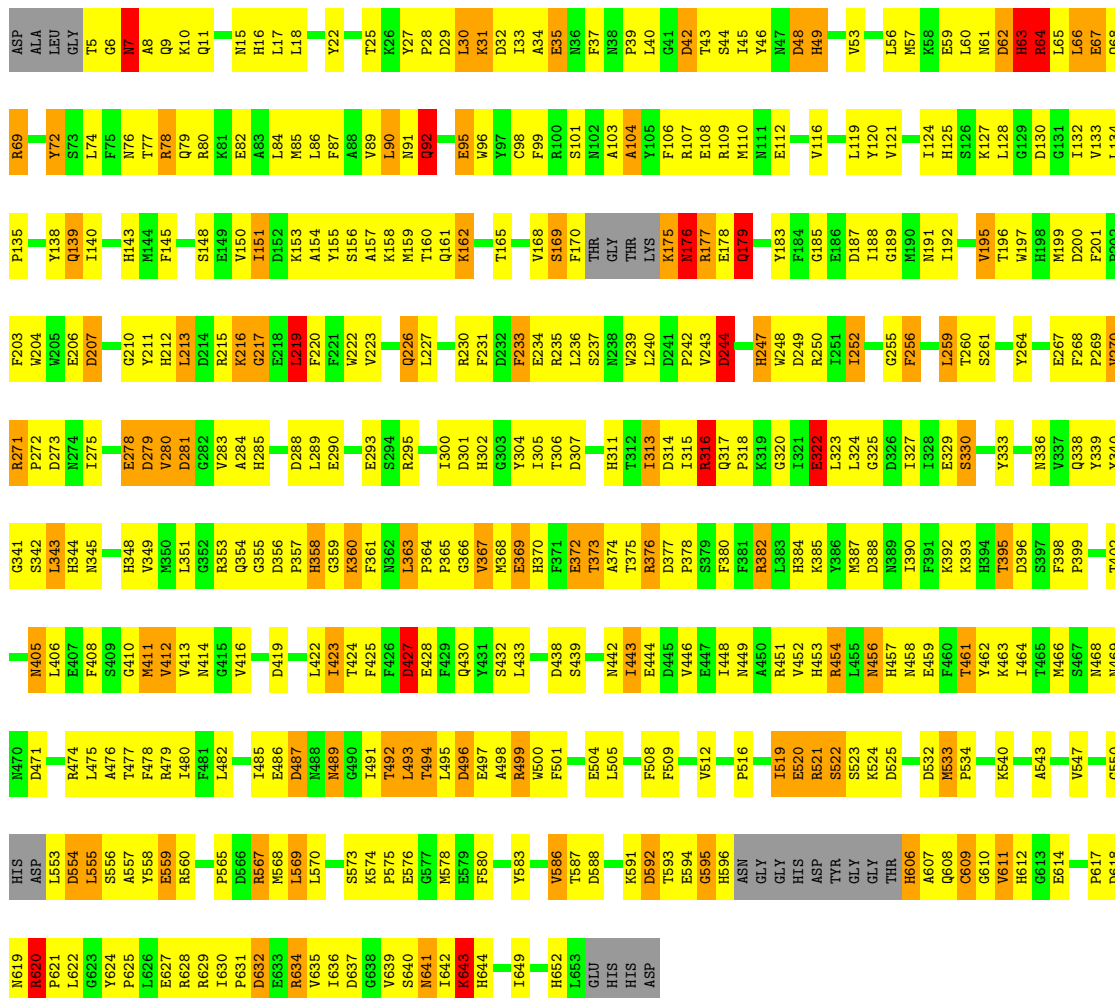
# Molecule 1: ARTHROPODAN HEMOCYANIN

Chain D: 31% 50% 13%



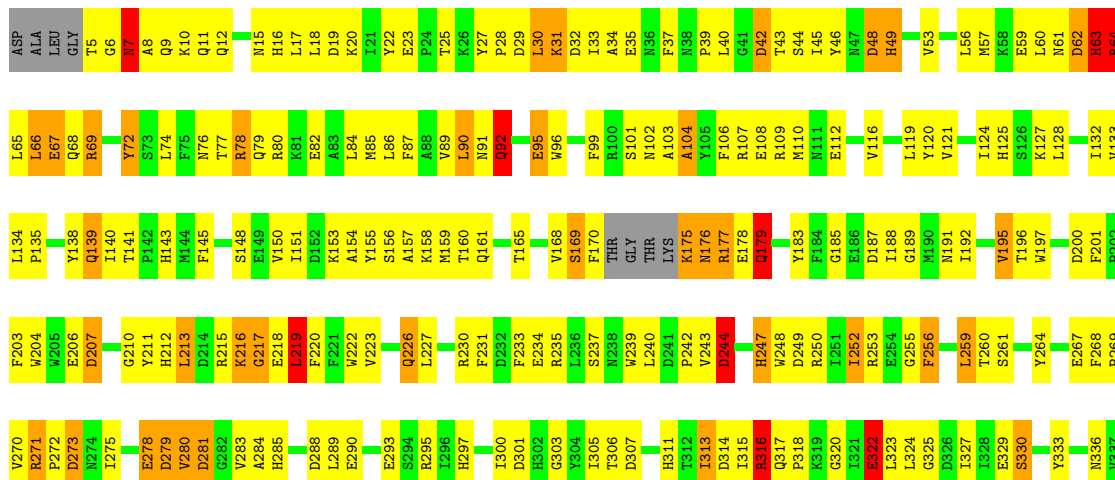
• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain E: 



• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain F: 







## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.80Å 193.10Å 122.20Å 90.00° 118.10° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.201 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32166	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
CU

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	1.41	11/5316 (0.2%)	4.13	1053/7205 (14.6%)
1	B	1.40	14/5316 (0.3%)	3.74	1016/7205 (14.1%)
1	C	0.75	0/5316	1.64	87/7205 (1.2%)
1	D	0.77	1/5316 (0.0%)	1.66	94/7205 (1.3%)
1	E	0.76	2/5316 (0.0%)	1.64	87/7205 (1.2%)
1	F	0.75	0/5316	1.65	94/7205 (1.3%)
All	All	1.02	28/31896 (0.1%)	2.64	2431/43230 (5.6%)

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	1
1	B	0	2
All	All	0	3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	550	GLY	C-O	7.84	1.36	1.23
1	B	208	SER	CB-OG	7.79	1.52	1.42
1	A	441	GLU	CB-CG	7.42	1.66	1.52
1	A	526	SER	CB-OG	6.86	1.51	1.42
1	B	267	GLU	CD-OE2	-6.23	1.18	1.25

The worst 5 of 2431 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ARG	NE-CZ-NH2	89.27	164.93	120.30
1	A	207	ASP	CB-CG-OD1	43.98	157.88	118.30
1	B	271	ARG	NE-CZ-NH1	43.24	141.92	120.30
1	A	273	ASP	CB-CG-OD1	40.24	154.52	118.30
1	B	273	ASP	CB-CG-OD1	39.23	153.61	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	521	ARG	Sidechain

## 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	5173	0	4880	687	0
1	B	5173	0	4883	651	1
1	C	5173	0	4888	416	3
1	D	5173	0	4888	472	1
1	E	5173	0	4888	428	0
1	F	5173	0	4888	416	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	186	0	0	39	0
3	B	186	0	0	15	0
3	C	186	0	0	11	0
3	D	186	0	0	11	0
3	E	186	0	0	10	0
3	F	186	0	0	9	0
All	All	32166	0	29315	2986	3

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 49.

The worst 5 of 2986 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLN:OE1	1:B:443:ILE:HD13	1.28	1.29
1:A:422:LEU:CD2	1:A:570:LEU:HD21	1.66	1.23
1:A:316:ARG:HD3	3:A:829:HOH:O	1.41	1.19
1:A:165:THR:CG2	1:A:449:ASN:HB2	1.73	1.17
1:B:456:ASN:HD22	1:B:457:HIS:N	1.42	1.17

All (3) 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:B:309:ASP:OD1	1:C:49:HIS:CD2[2_647]	1.85	0.35
1:C:594:GLU:OE1	1:F:471:ASP:CB[2_657]	2.13	0.07
1:C:474:ARG:NH2	1:D:41:GLY:O[2_656]	2.17	0.03

## 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	626/657 (95%)	501 (80%)	97 (16%)	28 (4%)	3	21
1	B	626/657 (95%)	506 (81%)	89 (14%)	31 (5%)	2	19
1	C	626/657 (95%)	517 (83%)	95 (15%)	14 (2%)	8	41
1	D	626/657 (95%)	516 (82%)	91 (14%)	19 (3%)	5	32
1	E	626/657 (95%)	512 (82%)	95 (15%)	19 (3%)	5	32
1	F	626/657 (95%)	503 (80%)	102 (16%)	21 (3%)	4	28
All	All	3756/3942 (95%)	3055 (81%)	569 (15%)	132 (4%)	4	28

5 of 132 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	147	ASN
1	A	176	ASN
1	A	441	GLU
1	A	471	ASP

### 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	564/580 (97%)	438 (78%)	126 (22%)	1	5
1	B	564/580 (97%)	450 (80%)	114 (20%)	1	7
1	C	564/580 (97%)	494 (88%)	70 (12%)	5	24
1	D	564/580 (97%)	489 (87%)	75 (13%)	4	21
1	E	564/580 (97%)	498 (88%)	66 (12%)	6	27
1	F	564/580 (97%)	498 (88%)	66 (12%)	6	27
All	All	3384/3480 (97%)	2867 (85%)	517 (15%)	3	15

5 of 517 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	596	HIS
1	C	461	THR
1	F	313	ILE
1	C	23	GLU
1	C	279	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 158 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	405	ASN
1	D	147	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	338	GLN
1	C	435	ASN
1	D	11	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.