



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:49 PM 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
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

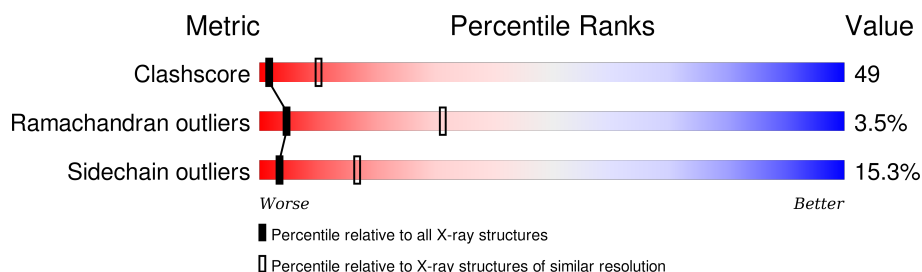
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (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 ≥ 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.

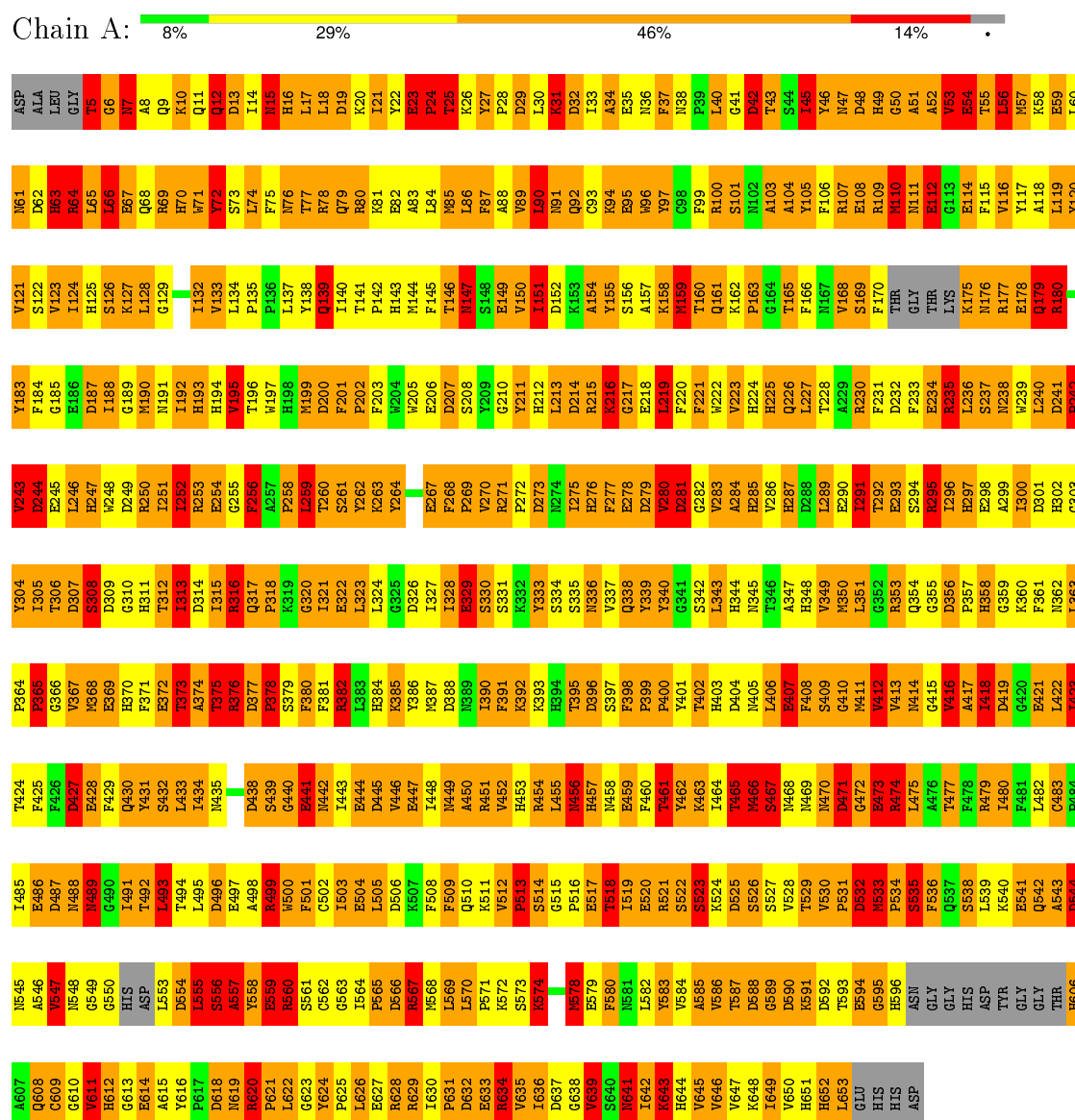
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	186	Total O 186 186	0	0
3	E	186	Total O 186 186	0	0
3	D	186	Total O 186 186	0	0
3	C	186	Total O 186 186	0	0
3	B	186	Total O 186 186	0	0
3	A	186	Total O 186 186	0	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: ARTHROPODAN HEMOCYANIN



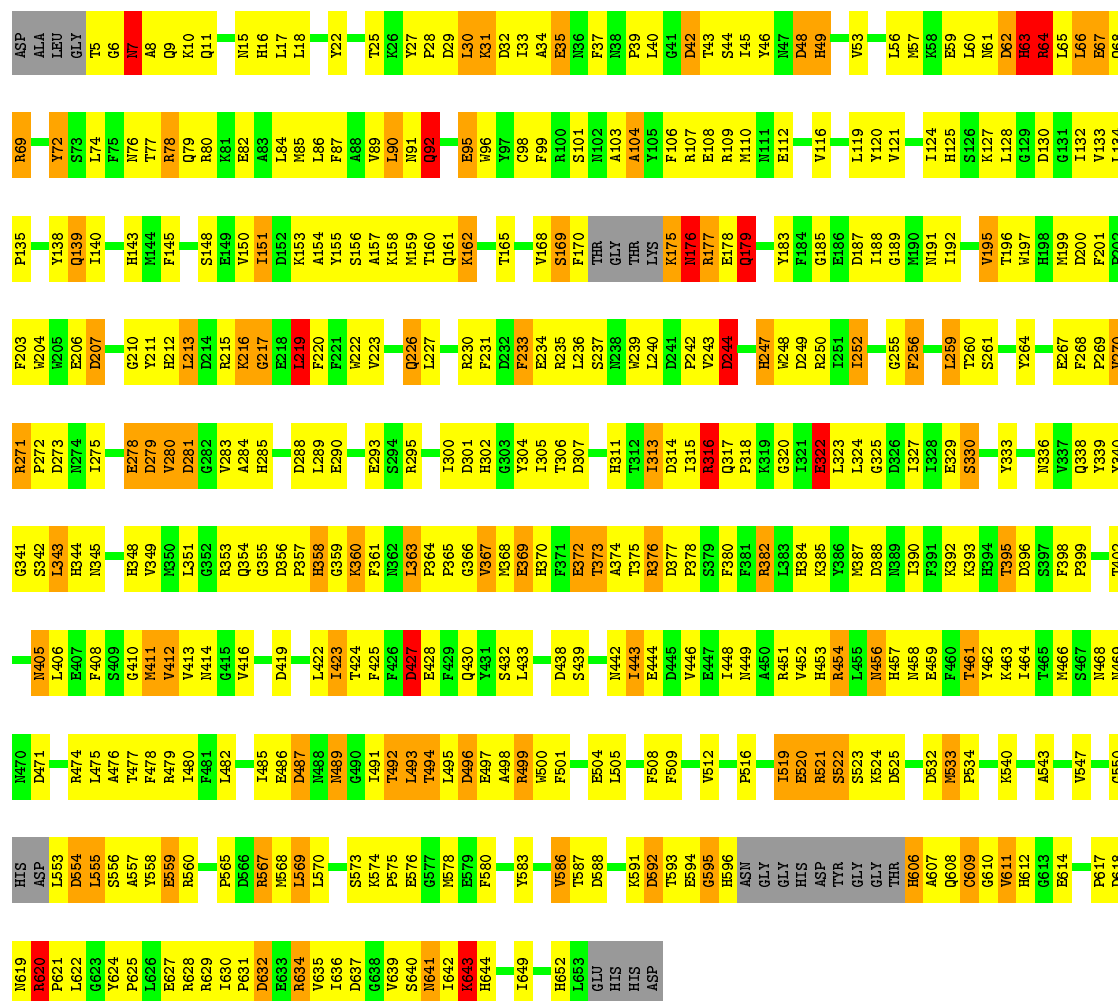
• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain B: 

ASP	ALA	LEU	GLY	TS	G6	H7	A8	Q9	H10	Q11	D12	D13	I14	M15	H16	H17	H18	L19	D20	I21	Y22	E23	A24	T25	T26	T27	T28	V29	W30	W31	W32	W33	W34	W35	W36	W37	W38	W39	W40	W41	W42	W43	W44	W45	W46	W47	W48	W49	W50	W51	W52	W53	W54	W55	W56	W57	W58	W59	W60	W61	W62	W63	W64	W65	W66	W67	W68	W69	W70	W71	W72	W73	W74	W75	W76	W77	W78	W79	W80	W81	W82	W83	W84	W85	W86	W87	W88	W89	W90	W91	W92	W93	W94	W95	W96	W97	W98	W99	W100	W101	W102	W103	W104	W105	W106	W107	W108	W109	W110	W111	W112	W113	W114	W115	W116	W117	W118	W119	W120	W121	W122	W123	W124	W125	W126	W127	W128	W129	W130	W131	W132	W133	W134	W135	W136	W137	W138	W139	W140	W141	W142	W143	W144	W145	W146	W147	W148	W149	W150	W151	W152	W153	W154	W155	W156	W157	W158	W159	W160	W161	W162	W163	W164	W165	W166	W167	W168	W169	W170	W171	W172	W173	W174	W175	W176	W177	W178	W179	W180	W181	W182	W183	W184	W185	W186	W187	W188	W189	W190	W191	W192	W193	W194	W195	W196	W197	W198	W199	W200	W201	W202	W203	W204	W205	W206	W207	W208	W209	W210	W211	W212	W213	W214	W215	W216	W217	W218	W219	W220	W221	W222	W223	W224	W225	W226	W227	W228	W229	W230	W231	W232	W233	W234	W235	W236	W237	W238	W239	W240	W241	W242	W243	W244	W245	W246	W247	W248	W249	W250	W251	W252	W253	W254	W255	W256	W257	W258	W259	W260	W261	W262	W263	W264	W265	W266	W267	W268	W269	W270	W271	W272	W273	W274	W275	W276	W277	W278	W279	W280	W281	W282	W283	W284	W285	W286	W287	W288	W289	W290	W291	W292	W293	W294	W295	W296	W297	W298	W299	W300	W301	W302	W303	W304	W305	W306	W307	W308	W309	W310	W311	W312	W313	W314	W315	W316	W317	W318	W319	W320	W321	W322	W323	W324	W325	W326	W327	W328	W329	W330	W331	W332	W333	W334	W335	W336	W337	W338	W339	W340	W341	W342	W343	W344	W345	W346	W347	W348	W349	W350	W351	W352	W353	W354	W355	W356	W357	W358	W359	W360	W361	W362	W363	W364	W365	W366	W367	W368	W369	W370	W371	W372	W373	W374	W375	W376	W377	W378	W379	W380	W381	W382	W383	W384	W385	W386	W387	W388	W389	W390	W391	W392	W393	W394	W395	W396	W397	W398	W399	W400	W401	W402	W403	W404	W405	W406	W407	W408	W409	W410	W411	W412	W413	W414	W415	W416	W417	W418	W419	W420	W421	W422	W423	W424	W425	W426	W427	W428	W429	W430	W431	W432	W433	W434	W435	W436	W437	W438	W439	W440	W441	W442	W443	W444	W445	W446	W447	W448	W449	W450	W451	W452	W453	W454	W455	W456	W457	W458	W459	W460	W461	W462	W463	W464	W465	W466	W467	W468	W469	W470	W471	W472	W473	W474	W475	W476	W477	W478	W479	W480	W481	W482	W483	W484	W485	W486	W487	W488	W489	W490	W491	W492	W493	W494	W495	W496	W497	W498	W499	W500	W501	W502	W503	W504	W505	W506	W507	W508	W509	W510	W511	W512	W513	W514	W515	W516	W517	W518	W519	W520	W521	W522	W523	W524	W525	W526	W527	W528	W529	W530	W531	W532	W533	W534	W535	W536	W537	W538	W539	W540	W541	W542	W543	W544	W545	W546	W547	W548	W549	W550	W551	W552	W553	W554	W555	W556	W557	W558	W559	W560	W561	W562	W563	W564	W565	W566	W567	W568	W569	W570	W571	W572	W573	W574	W575	W576	W577	W578	W579	W580	W581	W582	W583	W584	W585	W586	W587	W588	W589	W590	W591	W592	W593	W594	W595	W596	W597	W598	W599	W600	W601	W602	W603	W604	W605	W606	W607	W608	W609	W610	W611	W612	W613	W614	W615	W616	W617	W618	W619	W620	W621	W622	W623	W624	W625	W626	W627	W628	W629	W630	W631	W632	W633	W634	W635	W636	W637	W638	W639	W640	W641	W642	W643	W644	W645	W646	W647	W648	W649	W650	W651	W652	W653	W654	W655	W656	W657	W658	W659	W660	W661	W662	W663	W664	W665	W666	W667	W668	W669	W670	W671	W672	W673	W674	W675	W676	W677	W678	W679	W680	W681	W682	W683	W684	W685	W686	W687	W688	W689	W690	W691	W692	W693	W694	W695	W696	W697	W698	W699	W700	W701	W702	W703	W704	W705	W706	W707	W708	W709	W710	W711	W712	W713	W714	W715	W716	W717	W718	W719	W720	W721	W722	W723	W724	W725	W726	W727	W728	W729	W730	W731	W732	W733	W734	W735	W736	W737	W738	W739	W740	W741	W742	W743	W744	W745	W746	W747	W748	W749	W750	W751	W752	W753	W754	W755	W756	W757	W758	W759	W760	W761	W762	W763	W764	W765	W766	W767	W768	W769	W770	W771	W772	W773	W774	W775	W776	W777	W778	W779	W780	W781	W782	W783	W784	W785	W786	W787	W788	W789	W790	W791	W792	W793	W794	W795	W796	W797	W798	W799	W800	W801	W802	W803	W804	W805	W806	W807	W808	W809	W810	W811	W812	W813	W814	W815	W816	W817	W818	W819	W820	W821	W822	W823	W824	W825	W826	W827	W828	W829	W830	W831	W832	W833	W834	W835	W836	W837	W838	W839	W840	W841	W842	W843	W844	W845	W846	W847	W848	W849	W850	W851	W852	W853	W854	W855	W856	W857	W858	W859	W860	W861	W862	W863	W864	W865	W866	W867	W868	W869	W870	W871	W872	W873	W874	W875	W876	W877	W878	W879	W880	W881	W882	W883	W884	W885	W886	W887	W888	W889	W890	W891	W892	W893	W894	W895	W896	W897	W898	W899	W900	W901	W902	W903	W904	W905	W906	W907	W908	W909	W910	W911	W912	W913	W914	W915	W916	W917	W918	W919	W920	W921	W922	W923	W924	W925	W926	W927	W928	W929	W930	W931	W932	W933	W934	W935	W936	W937	W938	W939	W940	W941	W942	W943	W944	W945	W946	W947	W948	W949	W950	W951	W952	W953	W954	W955	W956	W957	W958	W959	W960	W961	W962	W963	W964	W965	W966	W967	W968	W969	W970	W971	W972	W973	W974	W975	W976	W977	W978	W979	W980	W981	W982	W983	W984	W985	W986	W987	W988	W989	W990	W991	W992	W993	W994	W995	W996	W997	W998	W999	W1000	W1001	W1002	W1003	W1004	W1005	W1006	W1007	W1008	W1009	W1010	W1011	W1012	W1013	W1014	W1015	W1016	W1017	W1018	W1019	W1020	W1021	W1022	W1023	W1024	W1025	W1026	W1027	W1028	W1029	W1030	W1031	W1032	W1033	W1034	W1035	W1036	W1037	W1038	W1039	W1040	W1041	W1042	W1043	W1044	W1045	W1046	W1047	W1048	W1049	W1050	W1051	W1052	W1053	W1054	W1055	W1056	W1057	W1058	W1059	W1060	W1061	W1062	W1063	W1064	W1065	W1066	W1067	W1068	W1069	W1070	W1071	W1072	W1073	W1074	W1075	W1076	W1077	W1078	W1079	W1080	W1081	W1082	W1083	W1084	W1085	W1086	W1087	W1088	W1089	W1090	W1091	W1092	W1093	W1094	W1095	W1096	W1097	W1098	W1099	W1100	W1101	W1102	W1103	W1104	W1105	W1106	W1107	W1108	W1109	W1110	W1111	W1112	W1113	W1114	W1115	W1116	W1117	W1118	W1119	W1120	W1121	W1122	W1123	W1124	W1125	W1126	W1127	W1128	W1129	W1130	W1131	W1132	W1133	W1134	W1135	W1136	W1137	W1138	W1139	W1140	W1141	W1142	W1143	W1144	W1145	W1146	W1147	W1148	W1149	W1150	W1151	W1152	W1153	W1154	W1155	W1156	W1157	W1158	W1159	W1160	W1161	W1162	W1163	W1164	W1165	W1166	W1167	W1168	W1169	W1170	W1171	W1172	W1173	W1174	W1175	W1176	W1177	W1178	W1179	W1180	W1181	W1182	W1183	W1184	W1185	W1186	W1187	W1188	W1189	W1190	W1191	W1192	W1193	W1194	W1195	W1196	W1197	W1198	W1199	W1200	W1201	W1202	W1203	W1204	W1205	W1206	W1207	W1208	W1209	W1210	W1211	W1212	W1213	W1214	W1215	W1216	W1217	W1218	W1219	W1220	W1221	W1222	W1223	W1224	W1225	W1226	W1227	W1228	W1229	W1230	W1231	W1232	W1233	W1234	W1235	W1236	W1237	W1238	W1239	W1240	W1241	W1242	W1243	W1244	W1245	W1246	W1247	W1248	W1249	W1250	W1251	W1252	W1253	W1254	W1255	W1256	W1257	W1258	W1259	W1260	W1261	W1262	W1263	W1264	W1265	W1266	W1267	W1268	W1269	W1270	W1271	W1272	W1273	W1274	W1275	W1276	W1277	W1278	W1279	W1280	W1281	W1282	W1283	W1284	W1285	W1286	W1287	W1288	W1289	W1290	W1291	W1292	W1293	W1294	W1295	W1296	W1297	W1298	W1299	W1300	W1301	W1302	W1303	W1304	W1305	W1306	W1307	W1308	W1309	W1310	W1311	W1312	W1313	W1314	W1315	W1316	W1317	W1318	W1319	W1320	W1321	W1322	W1323	W1324	W1325	W1326	W1327	W1328	W1329
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● Molecule 1: ARTHROPODAN HEMOCYANIN

Chain E: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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:B:456:ASN:HD22	1:B:457:HIS:N	1.42	1.17
1:A:165:THR:CG2	1:A:449:ASN:HB2	1.73	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	24
1	B	626/657 (95%)	506 (81%)	89 (14%)	31 (5%)	3	21
1	C	626/657 (95%)	517 (83%)	95 (15%)	14 (2%)	8	45
1	D	626/657 (95%)	516 (82%)	91 (14%)	19 (3%)	5	35
1	E	626/657 (95%)	512 (82%)	95 (15%)	19 (3%)	5	35
1	F	626/657 (95%)	503 (80%)	102 (16%)	21 (3%)	5	31
All	All	3756/3942 (95%)	3055 (81%)	569 (15%)	132 (4%)	4	31

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%)	6	27
1	D	564/580 (97%)	489 (87%)	75 (13%)	5	23
1	E	564/580 (97%)	498 (88%)	66 (12%)	7	30
1	F	564/580 (97%)	498 (88%)	66 (12%)	7	30
All	All	3384/3480 (97%)	2867 (85%)	517 (15%)	3	17

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.