



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 07:37 pm BST

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

<https://www.wwpdb.org/validation/2017/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
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

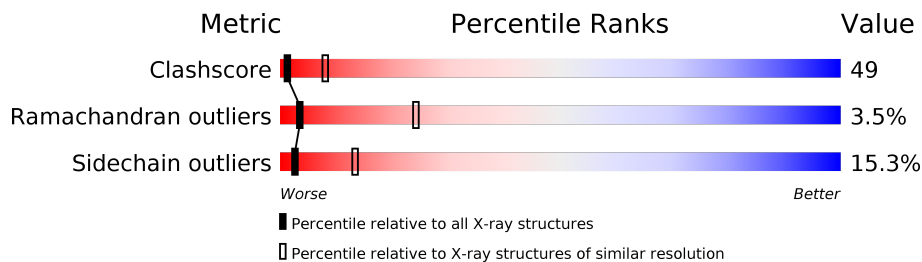
1 Overall quality at a glance

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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	657	8% 29% 46% 14% .
1	B	657	7% 32% 42% 16% .
1	C	657	35% 49% 11% . .
1	D	657	31% 50% 13% . .
1	E	657	34% 47% 13% . .
1	F	657	32% 50% 13% . .

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	634	5173	3283	892	977	21	0	0	0
1	B	634	5173	3283	892	977	21	0	0	0
1	C	634	5173	3283	892	977	21	0	0	0
1	D	634	5173	3283	892	977	21	0	0	0
1	E	634	5173	3283	892	977	21	0	0	0
1	F	634	5173	3283	892	977	21	0	0	0

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.

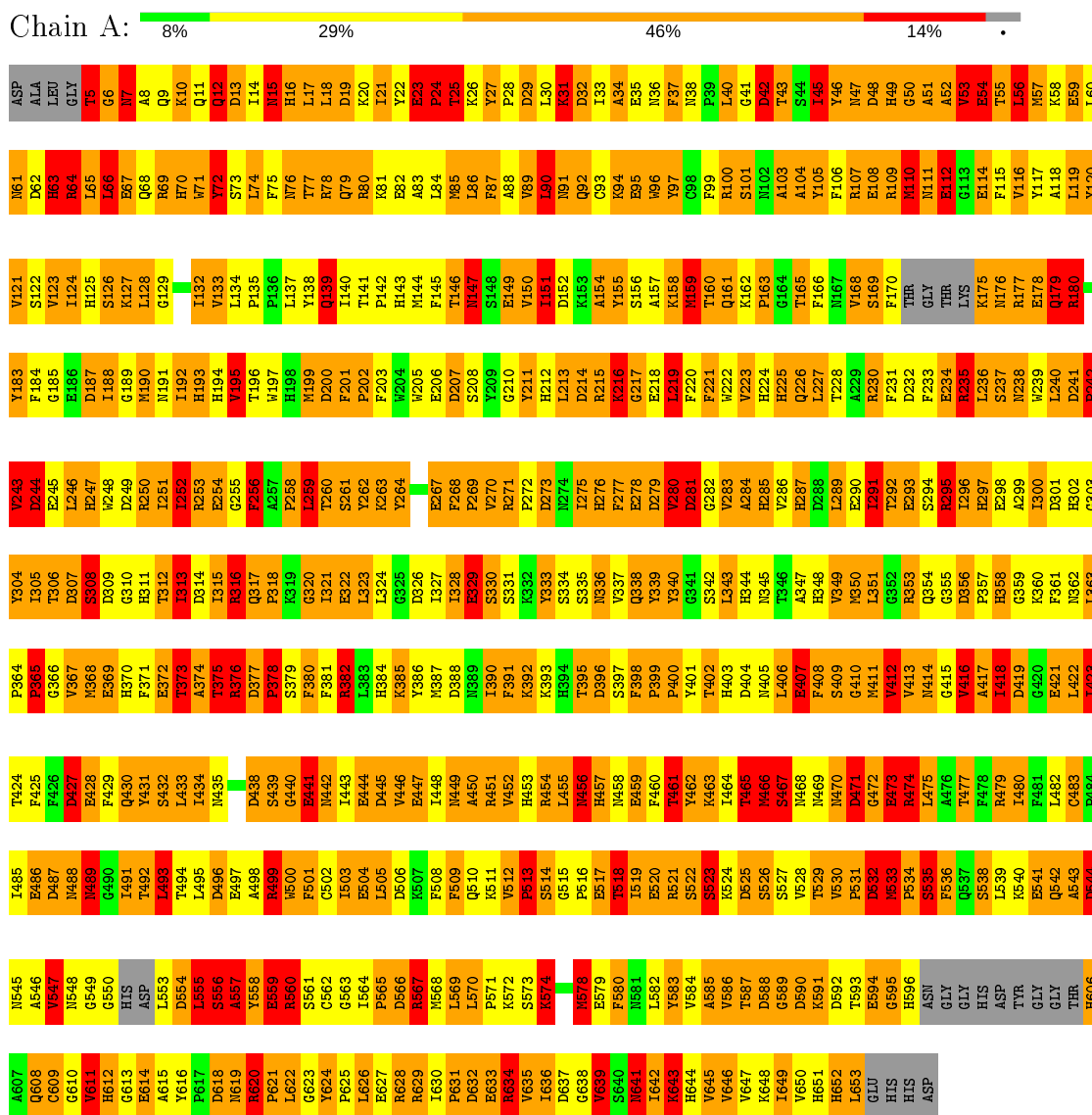
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	186	Total O 186 186	0	0
3	B	186	Total O 186 186	0	0
3	C	186	Total O 186 186	0	0
3	D	186	Total O 186 186	0	0
3	E	186	Total O 186 186	0	0
3	F	186	Total O 186 186	0	0

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. 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. 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



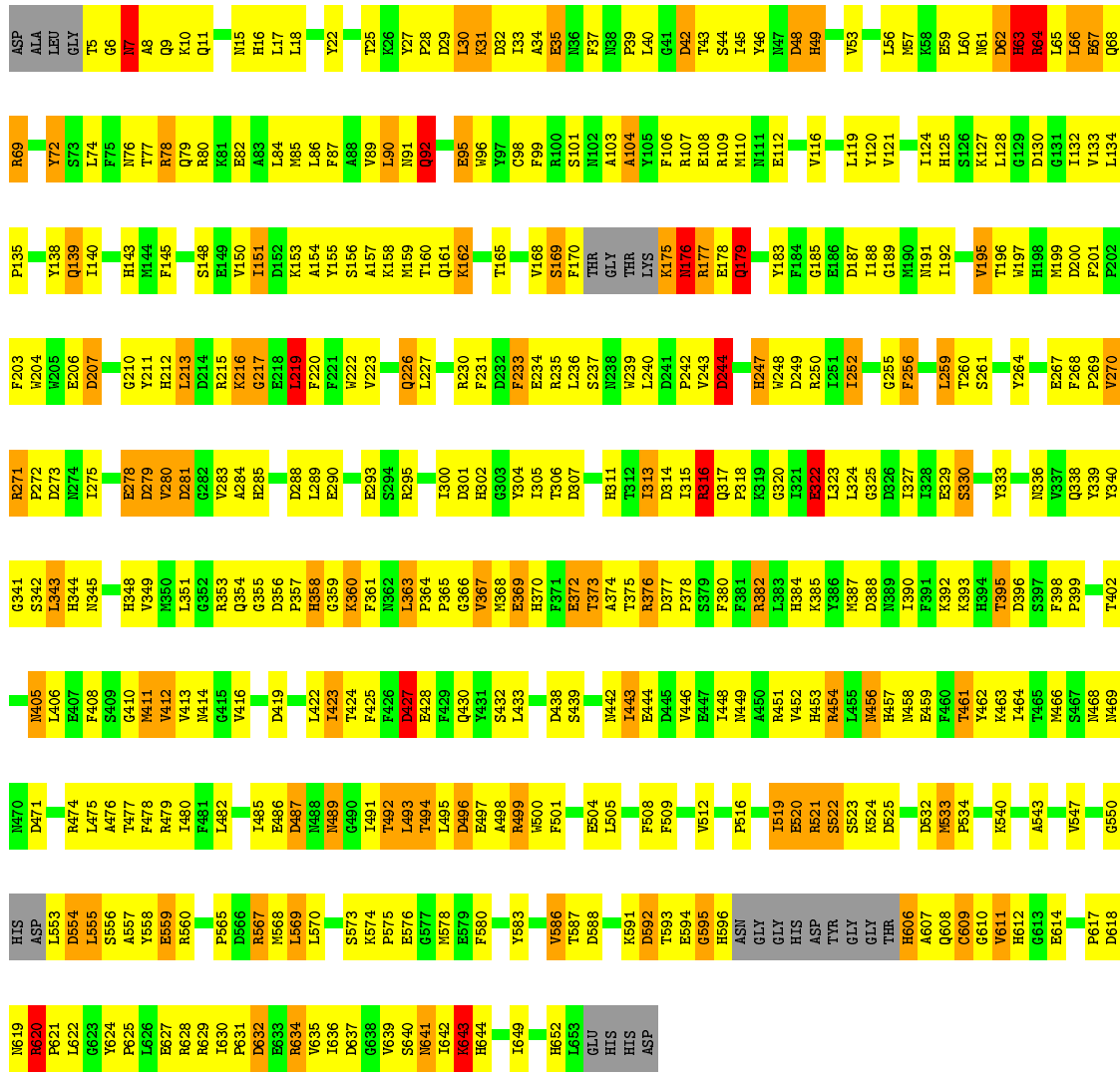
- Molecule 1: ARTHROPODAN HEMOCYANIN



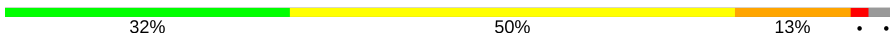
Y340	Y349	Y350	Y351	Y352	Y353	Y354	Y355	Y356	Y357	Y358	Y359	Y360	Y361	Y362	Y363	Y364	Y365	Y366	Y367	Y368	Y369	Y370	Y371	Y372	Y373	Y374	Y375	Y376	Y377	Y378	Y379	Y380	Y381	Y382	Y383	Y384	Y385	Y386	Y387	Y388	Y389	Y390	Y391	Y392	Y393	Y394	Y395	Y396	Y397	Y398	Y399	Y400	Y401	Y402	Y403																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
M404	M405	M406	M407	M408	M409	M410	M411	M412	M413	M414	M415	M416	M417	M418	M419	M420	M421	M422	M423	M424	M425	M426	M427	M428	M429	M430	M431	M432	M433	M434	M435	M436	M437	M438	M439	M440	M441	M442	M443	M444	M445	M446	M447	M448	M449	M450	M451	M452	M453	M454	M455	M456	M457	M458	M459	M460	M461	M462	M463	M464	M465	M466	M467	M468	M469	M470	M471	M472	M473	M474	M475	M476	M477	M478	M479	M480	M481	M482	M483	M484	M485	M486	M487	M488	M489	M490	M491	M492	M493	M494	M495	M496	M497	M498	M499	M500	M501	M502	M503	M504	M505	M506	M507	M508	M509	M510	M511	M512	M513	M514	M515	M516	M517	M518	M519	M520	M521	M522	M523	M524	M525	M526	M527	M528	M529	M530	M531	M532	M533	M534	M535	M536	M537	M538	M539	M540	M541	M542	M543	M544	M545	M546	M547	M548	M549	M550	M551	M552	M553	M554	M555	M556	M557	M558	M559	M560	M561	M562	M563	M564	M565	M566	M567	M568	M569	M570	M571	M572	M573	M574	M575	M576	M577	M578	M579	M580	M581	M582	M583	M584	M585	M586	M587	M588	M589	M590	M591	M592	M593	M594	M595	M596	M597	M598	M599	M600	M601	M602	M603	M604	M605	M606	M607	M608	M609	M610	M611	M612	M613	M614	M615	M616	M617	M618	M619	M620	M621	M622	M623	M624	M625	M626	M627	M628	M629	M630	M631	M632	M633	M634	M635	M636	M637	M638	M639	M640	M641	M642	M643	M644	M645	M646	M647	M648	M649	M650	M651	M652	M653	M654	M655	M656	M657	M658	M659	M660	M661	M662	M663	M664	M665	M666	M667	M668	M669	M670	M671	M672	M673	M674	M675	M676	M677	M678	M679	M680	M681	M682	M683	M684	M685	M686	M687	M688	M689	M690	M691	M692	M693	M694	M695	M696	M697	M698	M699	M700	M701	M702	M703	M704	M705	M706	M707	M708	M709	M710	M711	M712	M713	M714	M715	M716	M717	M718	M719	M720	M721	M722	M723	M724	M725	M726	M727	M728	M729	M730	M731	M732	M733	M734	M735	M736	M737	M738	M739	M740	M741	M742	M743	M744	M745	M746	M747	M748	M749	M750	M751	M752	M753	M754	M755	M756	M757	M758	M759	M760	M761	M762	M763	M764	M765	M766	M767	M768	M769	M770	M771	M772	M773	M774	M775	M776	M777	M778	M779	M780	M781	M782	M783	M784	M785	M786	M787	M788	M789	M790	M791	M792	M793	M794	M795	M796	M797	M798	M799	M800	M801	M802	M803	M804	M805	M806	M807	M808	M809	M810	M811	M812	M813	M814	M815	M816	M817	M818	M819	M820	M821	M822	M823	M824	M825	M826	M827	M828	M829	M830	M831	M832	M833	M834	M835	M836	M837	M838	M839	M840	M841	M842	M843	M844	M845	M846	M847	M848	M849	M850	M851	M852	M853	M854	M855	M856	M857	M858	M859	M860	M861	M862	M863	M864	M865	M866	M867	M868	M869	M870	M871	M872	M873	M874	M875	M876	M877	M878	M879	M880	M881	M882	M883	M884	M885	M886	M887	M888	M889	M890	M891	M892	M893	M894	M895	M896	M897	M898	M899	M900	M901	M902	M903	M904	M905	M906	M907	M908	M909	M910	M911	M912	M913	M914	M915	M916	M917	M918	M919	M920	M921	M922	M923	M924	M925	M926	M927	M928	M929	M930	M931	M932	M933	M934	M935	M936	M937	M938	M939	M940	M941	M942	M943	M944	M945	M946	M947	M948	M949	M950	M951	M952	M953	M954	M955	M956	M957	M958	M959	M960	M961	M962	M963	M964	M965	M966	M967	M968	M969	M970	M971	M972	M973	M974	M975	M976	M977	M978	M979	M980	M981	M982	M983	M984	M985	M986	M987	M988	M989	M990	M991	M992	M993	M994	M995	M996	M997	M998	M999	M1000	M1001	M1002	M1003	M1004	M1005	M1006	M1007	M1008	M1009	M1010	M1011	M1012	M1013	M1014	M1015	M1016	M1017	M1018	M1019	M1020	M1021	M1022	M1023	M1024	M1025	M1026	M1027	M1028	M1029	M1030	M1031	M1032	M1033	M1034	M1035	M1036	M1037	M1038	M1039	M1040	M1041	M1042	M1043	M1044	M1045	M1046	M1047	M1048	M1049	M1050	M1051	M1052	M1053	M1054	M1055	M1056	M1057	M1058	M1059	M1060	M1061	M1062	M1063	M1064	M1065	M1066	M1067	M1068	M1069	M1070	M1071	M1072	M1073	M1074	M1075	M1076	M1077	M1078	M1079	M1080	M1081	M1082	M1083	M1084	M1085	M1086	M1087	M1088	M1089	M1090	M1091	M1092	M1093	M1094	M1095	M1096	M1097	M1098	M1099	M1100	M1101	M1102	M1103	M1104	M1105	M1106	M1107	M1108	M1109	M1110	M1111	M1112	M1113	M1114	M1115	M1116	M1117	M1118	M1119	M1120	M1121	M1122	M1123	M1124	M1125	M1126	M1127	M1128	M1129	M1130	M1131	M1132	M1133	M1134	M1135	M1136	M1137	M1138	M1139	M1140	M1141	M1142	M1143	M1144	M1145	M1146	M1147	M1148	M1149	M1150	M1151	M1152	M1153	M1154	M1155	M1156	M1157	M1158	M1159	M1160	M1161	M1162	M1163	M1164	M1165	M1166	M1167	M1168	M1169	M1170	M1171	M1172	M1173	M1174	M1175	M1176	M1177	M1178	M1179	M1180	M1181	M1182	M1183	M1184	M1185	M1186	M1187	M1188	M1189	M1190	M1191	M1192	M1193	M1194	M1195	M1196	M1197	M1198	M1199	M1200	M1201	M1202	M1203	M1204	M1205	M1206	M1207	M1208	M1209	M1210	M1211	M1212	M1213	M1214	M1215	M1216	M1217	M1218	M1219	M1220	M1221	M1222	M1223	M1224	M1225	M1226	M1227	M1228	M1229	M1230	M1231	M1232	M1233	M1234	M1235	M1236	M1237	M1238	M1239	M1240	M1241	M1242	M1243	M1244	M1245	M1246	M1247	M1248	M1249	M1250	M1251	M1252	M1253	M1254	M1255	M1256	M1257	M1258	M1259	M1260	M1261	M1262	M1263	M1264	M1265	M1266	M1267	M1268	M1269	M1270	M1271	M1272	M1273	M1274	M1275	M1276	M1277	M1278	M1279	M1280	M1281	M1282	M1283	M1284	M1285	M1286	M1287	M1288	M1289	M1290	M1291	M1292	M1293	M1294	M1295	M1296	M1297	M1298	M1299	M1300	M1301	M1302	M1303	M1304	M1305	M1306	M1307	M1308	M1309	M1310	M1311	M1312	M1313	M1314	M1315	M1316	M1317	M1318	M1319	M1320	M1321	M1322	M1323	M1324	M1325	M1326	M1327	M1328	M1329	M1330	M1331	M1332	M1333	M1334	M1335	M1336	M1337	M1338	M1339	M1340	M1341	M1342	M1343	M1344	M1345	M1346	M1347	M1348	M1349	M1350	M1351	M1352	M1353	M1354	M1355	M1356	M1357	M1358	M1359	M1360	M1361	M1362	M1363	M1364	M1365	M1366	M1367	M1368	M1369	M1370	M1371	M1372	M1373	M1374	M1375	M1376	M1377	M1378	M1379	M1380	M1381	M1382	M1383	M1384	M1385	M1386	M1387	M1388	M1389	M1390	M1391	M1392	M1393	M1394	M1395	M1396	M1397	M1398	M1399	M1400	M1401	M1402	M1403	M1404	M1405	M1406	M1407	M1408	M1409	M1410	M1411	M1412	M1413	M1414	M1415	M1416	M1417	M1418	M1419	M1420	M1421	M1422	M1423	M1424	M1425	M1426	M1427	M1428	M1429	M1430	M1431	M1432	M1433	M1434	M1435	M1436	M1437	M1438	M1439	M1440	M1441	M1442	M1443	M1444	M1445	M1446	M1447	M1448	M1449	M1450	M1451	M1452	M1453	M1454	M1455	M1456	M1457	M1458	M1459	M1460	M1461	M1462	M1463	M1464	M1465	M1466	M1467	M1468	M1469	M1470	M1471	M1472	M1473	M1474	M1475	M1476	M1477	M1478	M1479	M1480	M1481	M1482	M1483	M1484	M1485	M1486	M1487	M1488	M1489	M1490	M1491	M1492	M1493	M1494	M1495	M1496	M1497	M1498	M1499	M1500	M1501	M1502	M1503	M1504	M1505	M1506	M1507	M1508	M1509	M1510	M1511	M1512	M1513	M1514	M1515	M1516	M1517	M1518	M1519	M1520	M1521	M1522	M1523	M1524	M1525	M1526	M1527	M1528	M1529	M1530	M1531	M1532	M1533	M1534	M1535	M1536	M1537	M1538	M1539	M1540	M1541	M1542	M1543	M1544	M1545	M1546	M1547	M1548	M1549	M1550	M1551	M1552	M1553	M1554	M1555	M1556	M1557	M1558	M1559	M1560	M1561	M1562	M1563	M1564	M1565	M1566	M1567	M1568	M1569	M1570	M1571	M1572	M1573	M1574	M1575	M1576	M1577	M1578	M1579	M1580	M1581	M1582	M1583	M1584	M1585	M1586	M1587	M1588	M1589	M1590	M1591	M1592	M1593	M1594	M1595	M1596	M1597	M1598	M1599	M1600	M1601	M1602	M1603	M1604	M1605	M1606	M1607	M1608	M1609	M1610	M1611	M1612	M1613	M1614	M1615	M1616	M1617	M1618	M1619	M1620	M1621	M1622	M1623	M1624	M1625	M1626	M1627	M1628	M1629	M1630	M1631	M1632	M1633	M1634	M1635	M1636	M1637	M1638	M1639	M1640	M1641	M1642	M1643	M1644	M1645	M1646	M1647	M1648	M1649	M1650	M1651	M1652	M1653	M1654	M1655	M1656	M1657	M1658	M1659	M1660	M1661	M1662	M1663	M1664	M1665	M1666	M1667	M1668	M1669	M1670	M1671	M1672	M1673	M1674	M1675	M1676	M1677	M1678	M1679	M1680	M1681	M1682	M1683	M1684	M1685	M1686	M1687	M1688	M1689	M1690	M1691	M1692	M1693	M1694	M1695	M1696	M1697	M1698	M1699	M1700	M1701	M1702	M1703	M1704	M1705	M1706	M1707	M1708	M1709	M1710	M1711	M1712	M1713	M1714	M1715

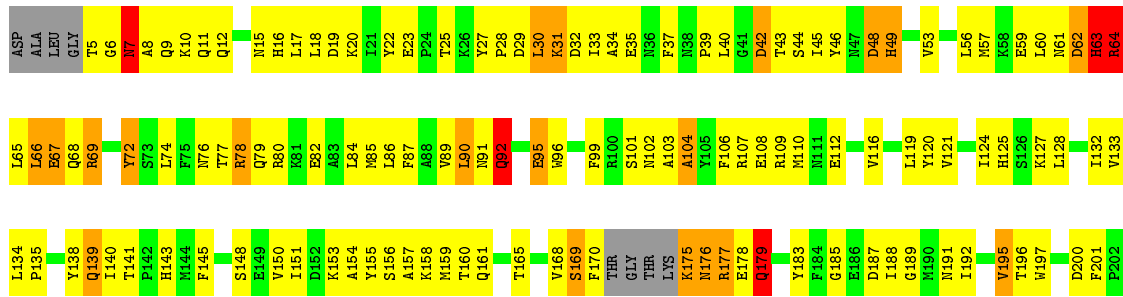
• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain E: 



• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain F: 



G610	N548	M470	Q338	V270	F203
V611	G549	D471	I339	R271	W204
G613	G550	G472	Y340	P272	W205
E614	HIS	E473	G341	D273	E206
	ASP	R474	S342	N274	D207
	L553	L475	L343	L275	
F617	D554	A476	H344		G210
D618	L555	S409	N345		Y211
M619	S956	G410		E278	H212
R620	A557	F478	H348	D279	L213
P621	Y558	R479	V280	V280	L214
L622	E559	I480	M411	D281	R215
G623	R560	F481	M350	G282	K216
Y624	S561	L482	L351	V283	G217
P625	G562	G415	G352	A284	
L626	E485	V416	R353	H285	E218
E627	E486		Q354		L219
R628	I564	L422	G355	D288	F220
R629	P565	I423	G356	D289	F221
I630	D566	T424	D357	E290	W222
	R567	F425	H358		V223
P631	M568	F426	G359	E293	
D632	L569	D427	K360	S294	Q226
E633	L570	E428		R295	L227
R634		F429	L363	I296	
V635	S573	Q430	P364	H297	R230
I636	K574	F431	P365		F231
D637	P575	S432	G366	I300	D232
G638	E576	L433	G367	D301	F233
V639	G577	I434	M368	H302	E234
S640	M578	D438	E369	G303	R235
M641	P579	S439	H370	Y304	L236
I642	F580		E371	I305	S237
K643	M581	E504	E372	I306	W238
H644	L582	L505	T373	D307	W239
	Y583	F508	A374		L240
V650	V584	F509	T375	H311	D241
H651	A585	D445	R376	T312	P242
H652	V586	V446	D377	I313	V243
L653	T587	E447	P378	D314	D244
GLU	D588	I448	S379	I315	
HIS		M449	F380	R316	H247
ASP	K591	A450	F381	W248	D249
	D592	R451	R382	D249	R250
	T593	Y452	I383	E251	I261
	E594	H453	H384	I262	
	G595	E520	K385	I321	R253
	H596	R454	Y386	E322	E254
	ASN	S522	M455	L323	G255
	GLY	D532	H457	L324	F256
	GLY	M533	M458	L327	
	HIS	E459	R389	D326	L259
	ASP	F460	I390	I327	T260
	TYR	P534	K392	I328	S261
	GLY	S535	K393	E329	
	GLY	F536	H394	S330	Y264
	GLY	K463	T395		Y264
	THR	A543	D396	Y333	
H606	D544	M466	D396		E267
A607	M545	S467	S397	M336	F268
Q608	A546	N468	F398		P269
C609	V547	N469	P399	V337	

4 Data and refinement statistics

Xtrriage (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, 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.	Xtrriage
Total number of atoms	32166	wwPDB-VP
Average B, all atoms (Å ²)	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	626/657 (95%)	501 (80%)	97 (16%)	28 (4%)	2	18
1	B	626/657 (95%)	506 (81%)	89 (14%)	31 (5%)	2	16
1	C	626/657 (95%)	517 (83%)	95 (15%)	14 (2%)	6	35
1	D	626/657 (95%)	516 (82%)	91 (14%)	19 (3%)	4	28
1	E	626/657 (95%)	512 (82%)	95 (15%)	19 (3%)	4	28
1	F	626/657 (95%)	503 (80%)	102 (16%)	21 (3%)	3	24
All	All	3756/3942 (95%)	3055 (81%)	569 (15%)	132 (4%)	3	24

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	564/580 (97%)	438 (78%)	126 (22%)	1 4
1	B	564/580 (97%)	450 (80%)	114 (20%)	1 6
1	C	564/580 (97%)	494 (88%)	70 (12%)	4 21
1	D	564/580 (97%)	489 (87%)	75 (13%)	4 18
1	E	564/580 (97%)	498 (88%)	66 (12%)	5 23
1	F	564/580 (97%)	498 (88%)	66 (12%)	5 23
All	All	3384/3480 (97%)	2867 (85%)	517 (15%)	2 13

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 [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.