



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:02 PM BST

PDB ID : 4BED
EMDB ID: : EMD-1569
Title : Keyhole limpet hemocyanin (KLH): 9A cryoEM structure and molecular model of the KLH1 didecamer reveal the interfaces and intricate topology of the 160 functional units
Authors : Gatsogiannis, C.; Markl, J.
Deposited on : 2013-03-08
Resolution : 9.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
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) : trunk27241

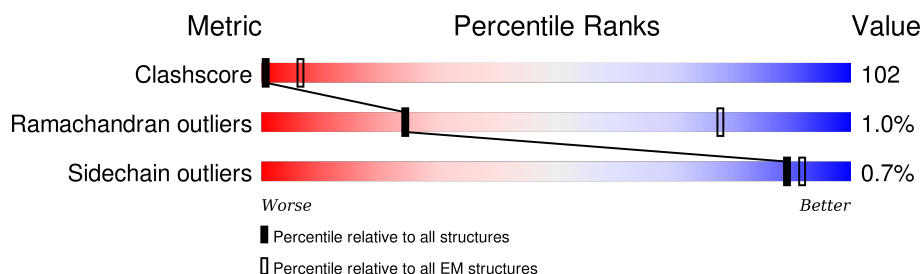
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1664	28% 72% .
1	C	1664	27% 72% .
2	B	1734	28% 69% .
2	D	1734	28% 69% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CUO	B	9008	-	-	X	-
3	CUO	D	9008	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 55292 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 KLH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1664	Total	C	N	O	S	0	0
			13530	8611	2347	2515	57		
1	C	1664	Total	C	N	O	S	0	0
			13530	8611	2347	2515	57		

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ASP	GLY	CONFLICT	UNP Q53IP9
A	139	VAL	ALA	CONFLICT	UNP Q53IP9
A	162	ALA	PRO	CONFLICT	UNP Q53IP9
A	178	ALA	PRO	CONFLICT	UNP Q53IP9
A	259	ASN	-	INSERTION	UNP Q53IP9
A	260	GLU	-	INSERTION	UNP Q53IP9
A	261	HIS	-	INSERTION	UNP Q53IP9
A	262	SER	-	INSERTION	UNP Q53IP9
A	263	THR	-	INSERTION	UNP Q53IP9
A	264	PRO	-	INSERTION	UNP Q53IP9
A	265	ALA	-	INSERTION	UNP Q53IP9
A	266	ASP	-	INSERTION	UNP Q53IP9
A	267	LEU	-	INSERTION	UNP Q53IP9
A	268	PHE	-	INSERTION	UNP Q53IP9
A	269	ASP	-	INSERTION	UNP Q53IP9
A	270	TYR	-	INSERTION	UNP Q53IP9
A	271	CYS	-	INSERTION	UNP Q53IP9
A	272	GLU	-	INSERTION	UNP Q53IP9
A	273	LEU	-	INSERTION	UNP Q53IP9
A	274	HIS	-	INSERTION	UNP Q53IP9
A	275	TYR	ASN	CONFLICT	UNP Q53IP9
A	.	-	TYR	DELETION	UNP Q53IP9
A	.	-	TRP	DELETION	UNP Q53IP9
A	.	-	GLY	DELETION	UNP Q53IP9
A	.	-	LEU	DELETION	UNP Q53IP9
A	.	-	PRO	DELETION	UNP Q53IP9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	.	-	GLY	DELETION	UNP Q53IP9
A	.	-	LYS	DELETION	UNP Q53IP9
A	.	-	LEU	DELETION	UNP Q53IP9
A	.	-	ASN	DELETION	UNP Q53IP9
A	.	-	ARG	DELETION	UNP Q53IP9
C	129	ASP	GLY	CONFLICT	UNP Q53IP9
C	139	VAL	ALA	CONFLICT	UNP Q53IP9
C	162	ALA	PRO	CONFLICT	UNP Q53IP9
C	178	ALA	PRO	CONFLICT	UNP Q53IP9
C	259	ASN	-	INSERTION	UNP Q53IP9
C	260	GLU	-	INSERTION	UNP Q53IP9
C	261	HIS	-	INSERTION	UNP Q53IP9
C	262	SER	-	INSERTION	UNP Q53IP9
C	263	THR	-	INSERTION	UNP Q53IP9
C	264	PRO	-	INSERTION	UNP Q53IP9
C	265	ALA	-	INSERTION	UNP Q53IP9
C	266	ASP	-	INSERTION	UNP Q53IP9
C	267	LEU	-	INSERTION	UNP Q53IP9
C	268	PHE	-	INSERTION	UNP Q53IP9
C	269	ASP	-	INSERTION	UNP Q53IP9
C	270	TYR	-	INSERTION	UNP Q53IP9
C	271	CYS	-	INSERTION	UNP Q53IP9
C	272	GLU	-	INSERTION	UNP Q53IP9
C	273	LEU	-	INSERTION	UNP Q53IP9
C	274	HIS	-	INSERTION	UNP Q53IP9
C	275	TYR	ASN	CONFLICT	UNP Q53IP9
C	.	-	TYR	DELETION	UNP Q53IP9
C	.	-	TRP	DELETION	UNP Q53IP9
C	.	-	GLY	DELETION	UNP Q53IP9
C	.	-	LEU	DELETION	UNP Q53IP9
C	.	-	PRO	DELETION	UNP Q53IP9
C	.	-	GLY	DELETION	UNP Q53IP9
C	.	-	LYS	DELETION	UNP Q53IP9
C	.	-	LEU	DELETION	UNP Q53IP9
C	.	-	ASN	DELETION	UNP Q53IP9
C	.	-	ARG	DELETION	UNP Q53IP9

- Molecule 2 is a protein called HEMOCYANIN KLH1.

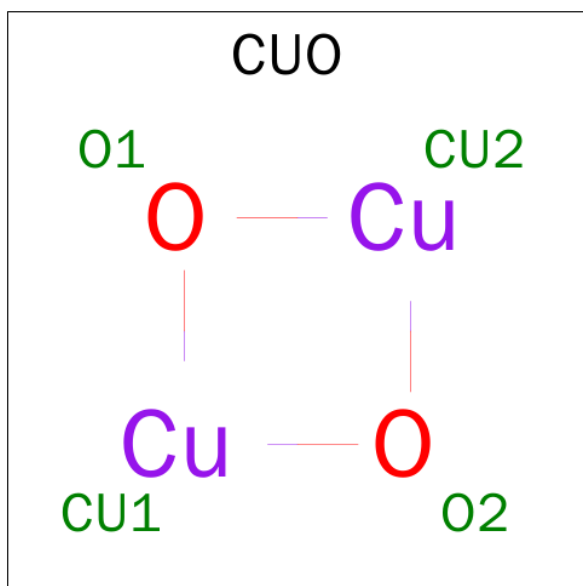
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1734	Total	C	N	O	S	0	0
			14084	8985	2438	2594	67		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	1734	Total	C	N	O	S	0	0
			14084	8985	2438	2594	67		

- Molecule 3 is CU2-O2 CLUSTER (three-letter code: CUO) (formula: Cu₂O₂).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	Cu	O	0
			16	8	8	
3	A	1	Total	Cu	O	0
			16	8	8	
3	A	1	Total	Cu	O	0
			16	8	8	
3	A	1	Total	Cu	O	0
			16	8	8	
3	B	1	Total	Cu	O	0
			16	8	8	
3	B	1	Total	Cu	O	0
			16	8	8	
3	B	1	Total	Cu	O	0
			16	8	8	
3	B	1	Total	Cu	O	0
			16	8	8	
3	C	1	Total	Cu	O	0
			16	8	8	
3	C	1	Total	Cu	O	0
			16	8	8	

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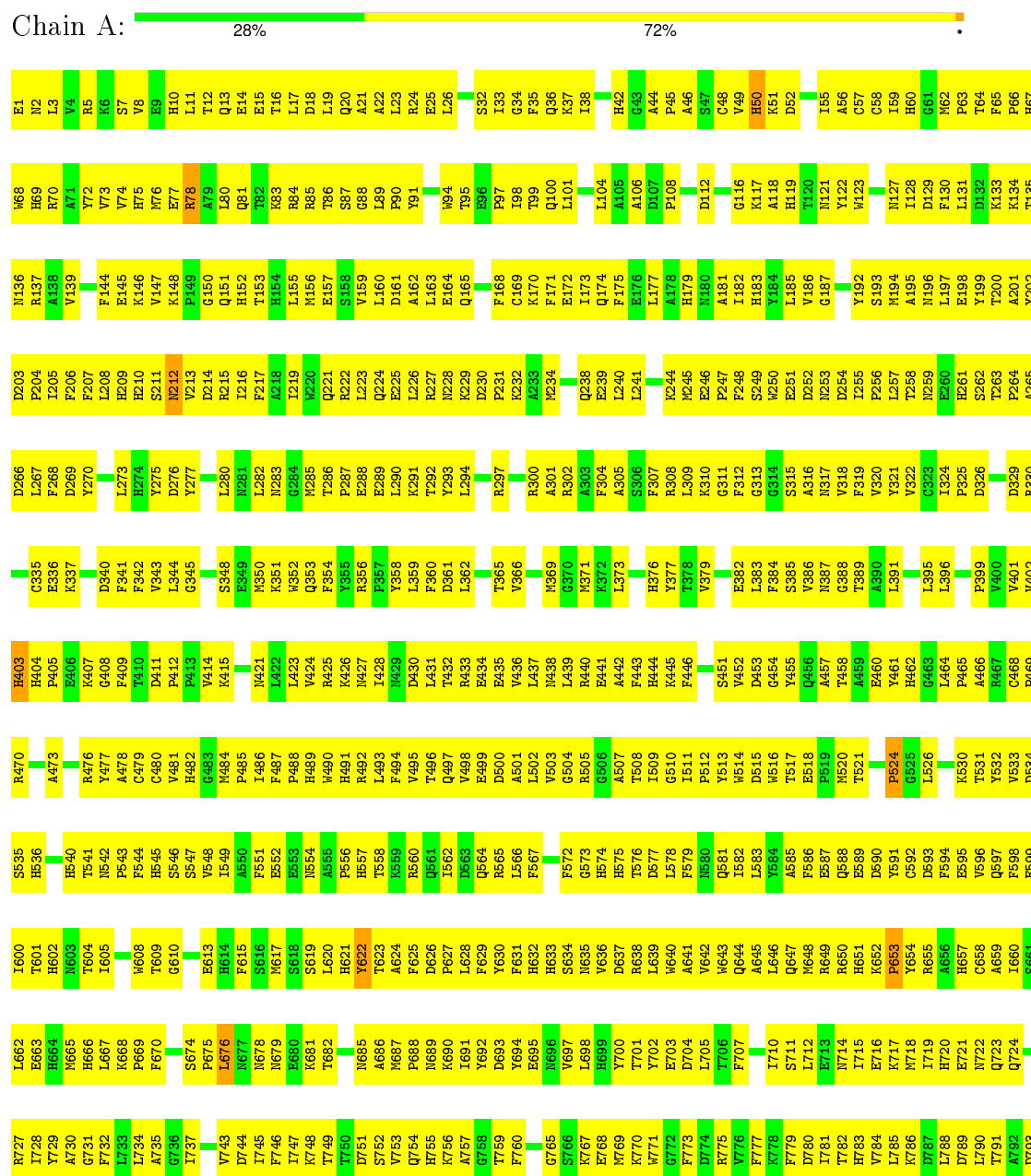
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Mol	Chain	Residues	Atoms			AltConf
3	C	1	Total 16	Cu 8	O 8	0
3	C	1	Total 16	Cu 8	O 8	0
3	D	1	Total 16	Cu 8	O 8	0
3	D	1	Total 16	Cu 8	O 8	0
3	D	1	Total 16	Cu 8	O 8	0
3	D	1	Total 16	Cu 8	O 8	0

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. 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.

• Molecule 1: HEMOCYANIN KLH1



H1661	L1589	S1518	L1453	F1374	T1306	H1243	D1479	Y1116	T1055	A992	A924	K864	G794
T1662	G1590	F1519	H1464	L1379	S1307	E1244	E1182	L1119	W1056	A993	L925	S865	D795
E1663	G1591	H1465	H1466	T1380	C1308	G1245	M1183	E1120	Q1057	Q994	P926	S866	F796
	E1594	Y1521	T1457	L1381	V1310	E1246	F1121	F1121	A1058	Y995	Y927	K867	E797
	M1595	Y1522	T1458	E1382	G1312	Y1248	W1185	N1122	L1059	L996	D928	F869	T799
	D1596	H1524	D1459	L1388	G1313	Q1249	A1186	G1123	K1061	L997	Y930	K870	W800
	M1525	M1526	H1460	L1388	H1314	A1250	Y1187	L1124	T1062	A998	T931	K871	W801
	L1526	L1527	H1461	D1392	T1315	E1251	D1188	S1125	R1063	L999	T932	L872	D802
	F1599	T1528	A1462	L1393	F1316	Y1252	V1190	S1127	K1065	Q1001	P933	G873	T803
	M1529	L1532	H1463	L1394	H1317	Y1253	F1191	K1128	A874	L934	L934	A874	E804
	H1602	H1603	Y1465	F1395	H1318	S1254	K1192	L1129	P1066	D1002	H936	F875	W805
	Y1603	Y1531	Q1466	H1396	W1319	R1257	Y1193	M1130	M1068	D1006	L937	G877	D806
	S1632	S1633	D1467	S1397	H1320	L1258	D1194	K1131	V1069	F1007	L940	E878	T808
	L1533	L1534	H1468	L1398	R1321	L1259	L1195	K1132	T1009	E1008	R809	R879	R808
	Q1534	Q1535	Q1469	Y1399	L1322	N1260	L1196	L1133	Q1010	Y1010	L941	K880	L810
	L1536	L1537	R1470	F1400	Y1323	N1261	E1197	E1134	Y1011	Y1011	H943	W881	A811
			F1471	Y1401	V1324	I1262	K1198	A1135	E1073	E1012	F944	C882	
			R1472	E1402	V1325	E1263	L1199	I1136	T1075	I1013	K945	S883	L814
			K1473	Q1403	V1326	N1264	H1200	K1137	S1076	A1014	T946	S884	L815
			L1474	V1404	V1327	L1265	D1201	S1138	R1077	H1015		P885	P816
			P1475	L1405	E1328		L1202	Q1139	R1078	M1016	D951	E886	H817
			Y1476	Y1406	N1329	G1268	K1203	D1140	E1079	Y1017	G952	A887	A818
			R1477	A1407	A1330	E1269	L1204	R1141	P1080	I1018	Y953	S888	S819
			E1478	L1408	L1331	L1270	H1205	F1142	L1081	H1019	E954	K889	W820
				E1409	L1332	S1272	A1207	A1144	Q1082	A1020	K955	K890	L821
			Q1484	F1413	K1333	S1273	E1207	G1145	P1083	L1021	H956	R891	R822
			L1485	F1414	K1334	L1273	F1210	F1146	F1084	V1022	P957	A892	E823
			M1486	D1415	V1338	R1274	F1211	L1147	G1085	K893	K959	C894	R826
			H1487	D1416	A1339	A1276	I1212	L1148	S1087	P1026	P960	V895	W827
			P1489	Q1419	A1340	L1277	D1213	S1149	A1088	P1027	D961	H896	K828
			L1490	L1420	P1341	L1278	Y1214	G1150	N1039	Y1028	G962	G897	F829
			Q1491	E1421	Y1342	E1279	F1215	F1151	G1029	H963	H963	M898	D830
			F1492	E1422	D1343	I1280	V1216	K1152	N1091	I964	I964	S899	K831
			D1494	L1423	W1345	E1281	F1217	S1154	T1092	A1031	D965	W900	
			K1495	L1424		N1282	D1218	S1155	D1093	S1032	T966	P901	R836
				M1425	T1349	D1283	L1219	L1156	H1094	S1033	P967	P902	L837
			N1498	L1427	E1350	G1284	K1220	L1157	T1095	R1034	D968	H903	T838
			D1500	L1426	H1351	T1285		K1158	T1096	Y1035	K969	W904	R839
			E1501	L1430	L1352	E1287	G1225	F1159	K1097	T1036	T970	H905	K840
			A1502	L1431	P1353	S1288	K1226	N1160	E1098	A1037	T971	R906	W841
			H1503	K1436	T1356	L1289	D1227	L1161	H1099	F1038	T972	L907	W842
			T1504	Y1437	S1357	A1290	L1228	C1162	V1101	D1039	R973	L908	D843
			T1505	Y1437	T1357	K1291	F1229	T1163	P1040	S974	T909	T909	R844
			H1506	L1442	Y1361	A1291	Q1231	D1164	L1041	Y975	Q911	W910	L845
			A1507	D1443	Y1362	H1293	P1232	C1168	Y1043	Y1043	N977	S912	E848
			T1508	Y1444	M1363	H1294	S1233	H1169	H1045	H1045	P980	E913	F849
			P1509	L1445	S1364	P1296	V1234	P1170	D1107	H1046	E981	A915	H850
			H1510	A1446	R1365		I1235	A1171	Y1108	Q982	E981	L916	E852
			D1511	F1447	Q1366	C1299	H1236	G1172	K1109	N1048	P983	R917	L853
			G1512	F1447	H1367	Q1300	E1237	E1173	T1110	T1049	E984	R918	R854
			F1513	D1448	H1368	L1301	P1238	F1174	T1111	D1050	F985	H919	
			E1514	P1449	H1369	N1302	N1239	Y1175	F1112	R1051		G920	L857
			Y1515	V1450	T1371	G1303	L1240	L1176	N1113	I1052	T989	Y921	L860
			W1517	F1452	M1372	P1305	G1241	L1177	F1114	W1053	S990	D922	L861
					P1373		H1242	G1178	E1115	A1054	Y991	G923	

● Molecule 1: HEMOCYANIN KLH1

Chain C:  27% 72%

E1	L1589	S1518	L1453	F1374	T1306	H1243	D1479	Y1116	T1055	A992	A924	K864	G794
N2	G1590	F1519	H1464	L1379	S1307	E1244	E1182	L1119	W1056	A993	L925	S865	D795
L3	G1591	H1465	H1466	T1380	C1308	G1245	M1183	E1120	Q1057	Q994	P926	S866	F796
V4	E1594	Y1521	T1457	L1381	V1310	E1246	F1121	F1121	A1058	Y995	Y927	K867	E797
R5	M1595	Y1522	T1458	E1382	G1312	Y1248	W1185	N1122	L1059	L996	D928	F869	T799
K6	Y1523	T1459	D1459	L1388	H1314	Q1249	A1186	G1123	K1061	L997	Y930	K870	W800
S7	D1596	H1524	D1460	L1388	G1313	A1250	Y1187	L1124	T1062	A998	T931	K871	W801
V8	M1525	M1526	H1461	D1392	T1315	E1251	D1188	S1125	R1063	L999	T932	L872	D802
E9	L1526	L1527	H1462	L1393	F1316	Y1252	V1190	S1127	K1065	Q1001	P933	G873	T803
H10	F1599	T1528	A1463	L1394	H1317	Y1253	F1191	K1128	A874	L934	L934	A874	E804
L11	M1529	L1532	H1464	F1395	H1318	S1254	K1192	L1129	P1066	D1002	H936	F875	W805
T12	H1602	H1603	Y1465	F1396	W1319	R1257	Y1193	M1130	M1068	D1006	L937	G877	D806
Q13	Y1603	Y1531	Q1466	H1396	H1320	L1258	D1194	K1131	V1069	F1007	L940	E878	T808
E14	S1632	S1633	D1467	S1397	R1321	L1259	L1195	K1132	T1009	E1008	R809	R879	R808
E15	L1533	L1534	H1468	L1398	L1322	N1260	L1196	L1133	Q1010	Y1010	L941	K880	L810
T16	Q1534	Q1535	Q1469	Y1399	Y1323	N1261	E1197	E1134	Y1011	Y1011	H943	W881	A811
L17	L1536	L1537	R1470	F1400	V1324	I1262	K1198	A1135	E1073	E1012	F944	C882	
D18			F1471	Y1401	V1325	E1263	L1199	I1136	T1075	I1013	K945	S883	L814
L19			R1472	E1402	V1326	N1264	H1200	K1137	S1076	A1014	T946	S884	L815
Q20			K1473	Q1403	V1327	L1265	D1201	S1138	R1077	H1015		P885	P816
A21			L1474	V1404	E1328		L1202	Q1139	R1078	M1016	D951	E886	H817
A22			Y1476	Y1406	N1329	G1268	K1203	D1140	E1079	Y1017	G952	A887	A818
L23			R1477	A1407	A1330	E1269	L1204	R1141	P1080	I1018	Y953	S888	S819
R24			E1478	L1408	L1331	L1270	H1205	F1142	L1081	H1019	E954	K889	W820
E25				E1409	L1332	S1272	A1207	A1144	Q1082	A1020	K955	K890	L821
L26			Q1484	F1413	K1333	S1273	E1207	G1145	P1083	L1021	H956	R891	R822
			L1485	F1414	K1334	L1273	F1210	F1146	F1084	V1022	P957	A892	E823
			M1486	D1415	V1338	R1274	F1211	L1147	G1085	K893	K959	C894	R826
			H1487	D1416	A1339	A1276	I1212	L1148	S1087	P1026	P960	V895	W827
			P1489	Q1419	A1340	L1277	D1213	S1149	A1088	P1027	D961	H896	K828
			L1490	L1420	P1341	L1278	Y1214	G1150	N1039	Y1028	G962	G897	F829
			Q1491	E1421	Y1342	E1279	F1215	F1151	G1029	H963	H963	M898	D830
			F1492	E1422	D1343	I1280	V1216	K1152	N1091	I964	I964	S899	K831
			D1494	L1423	W1345	E1281	F1217	S1154	T1092	A1031	D965	W900	
			K1495	L1424		N1282	D1218	S1155	D1093	S1032	T966	P901	R836
				M1425	T1349	D1283	L1219	L1156	H1094	S1033	P967	P902	L837
			N1498	L1427	E1350	G1284	K1220	L1157	T1095	R1034	D968	H903	T838
			D1500	L1426	H1351	T1285		K1158	T1096	Y1035	K969	W904	R839
			E1501	L1430	L1352	E1287	G1225	F1159	K1097	T1036	T970	H905	K840
			A1502	L1431	P1353	S1288	K1226	N1160	E1098	A1037	T971	R906	W841
			H1503	K1436	T1356	L1289	D1227	L1161	H1099	F1038	T972	L907	W842
			T1504	Y1437	S1357	A1290	L1228	C1162	V1101	D1039	R973	L908	D843
			T1505	Y1437	T1357	K1291	F1229	T1163	P1040	S974	T909	T909	R844
			H1506	L1442	Y1361	A1291	Q1231	D1164	L1041	Y975	Q911	W910	L845
			A1507	D1443	Y1362	H1293	P1232	C1168	Y1043	Y1043	N977	S912	E848
			T1508	Y1444	M1363	H1294	S1233	H1169	H1045	H1045	P980	E913	F849
			P1509	L1445	S1364	P1296	V1234	P1170	D1107	H1046	E981	A915	H850

Y1114	H1053	S990	H919	L857	D789	Q724	L662	I600	S535	R470	V402	D266	D203	M136	H68
E1115	A1054	I991	G920	L857	L790	Q724	E663	T601	H536	A473	H403	L267	P204	R137	H69
Y1116	I1055	A992	Y921	L860	T791	R727	E664	H602	H560	A473	H404	F268	I205	A138	R70
L1119	H1056	K993	Q923	L861	D793	I728	H665	H603	T541	R476	H405	D269	F206	V139	A71
E1120	A1058	I994	G924	K861	D794	Q729	H666	H604	H542	Y477	H406	Y270	L208	F144	V72
F1121	I1059	L996	L925	K864	D795	Q731	H668	I605	H543	A478	G408	L273	L207	E145	V74
M1122	Q1060	A998	F926	S865	F796	G732	H669	H608	H544	C479	D411	H210	H209	E146	H75
G1123	I1062	L999	W928	A866	F797	L733	H670	G610	H545	C480	P413	Y275	S211	V147	H76
S1125	R1063	E1000	W929	F869	F798	L734	A671	G610	S546	H482	P413	D276	N212	K148	E77
L1126	K1064	I1001	W930	G870	W800	G736	S673	E613	V548	H483	V414	Y277	Y213	P149	R78
T1127	K1065	D1002	T931	Q871	D801	I737	S674	H614	H549	H484	K415	L280	D214	G150	A79
Q1128	P1066	D1006	S932	L872	I802		F675	F615	A550	P485		N281	R215	Q151	L80
L1129	Y1067	F1007	F933	G873	T803	V743	L676	S616	F551	L486	N421	L282	I216	H152	Q81
M1130	N1068	A1074	L934	A874	E804	D744	H677	H617	E552	L486	L422	N283	F217	T153	T82
V1069	V1069	E1008	R934	F875	D805	I745	H678	S618	E553	P488	L423	H284	I219	H155	R83
K1132	K1131	I1009	H945	H876	D806	F746	H679	S619	H554	H489	V424	G285	L223	M156	R84
L1133	A1070	L940	Y946	G877	D807	I747	H680	L620	A555	H490	R425	T286	Q221	E157	T86
E1134	A1073	Y1011	H943	E878	R808	K748	K681	H621	F556	H491	K426	P287	R222	S158	S87
A1135	Y1074	E1012	E944	R879	T809	T749	T682	Y622	H557	R492	N427	E288	L223	V159	G88
T1136	T1075	I1013	K945	K880	L810	T750	H683	A624	F558	L493	I428	E289	Q224	L160	L89
K1137	S1076	A1014	W881	W881	A811	T751	H684	T623	T559	F494	N429	L290	E225	D161	P90
L1138	M1077	H1015	C882	C882	A811	S752	H685	H625	H560	V495	D430	K291	R226	A162	P91
Q1139	K1078	H1016	D951	P883	L814	S753	H686	D626	H561	T496	L431	T292	L226	E163	
E1140	E1079	Y1017	G952	S884	I815	Q754	H687	D627	H562	Q497	T432	R227	R227	E164	
L1141	P1080	I1018	V953	P885	R816	H755	H688	L628	H563	V498	R433	E293	K228	E164	
F1142	L1081	H1019	E954	E886	H817	K756	H689	F629	H564	H499	R434	L294	D230	Q165	
F1143	Q1082	A1020	K955	H887	A818	G757	H691	H630	H565	D500	E435	P231	K232	F168	
A1144	P1083	H1021	H956	S888	S819	H758	H692	H631	H566	A501	V436	R297	K233	K170	P97
G1145	F1084	V1022	H957	K889	W820	D760	H693	H632	F567	L502	L437	R300	N234	K171	T99
F1146	G1085	G1023	P958	K890	I821	T760	H694	H633	F572	V503	N438	A301	K234	E171	Q100
L1086	L1086	Q1026	W959	F891	R822	A761	E695	S634	G573	G504	N439	A302	H234	E172	L101
S1087	S1087	P1027	F960	A892	E823	L762	H696	H635	H574	R505	R440	A303	Q238	I173	
L1148	A1088	G1028	D961	C893	E823	G763	H697	H636	H575	G506	R441	A304	Q239	Q174	L104
G1150	H1089	H1029	Q962	C894	R826	G764	H698	H637	H576	A507	A442	A305	L240	F175	A105
F1151	I1090	K1030	H963	H895	W827	G765	H699	H638	T576	T508	F443	S306	L241	E176	A106
K1152	I1091	M1030	I964	H896	K828	S766	H700	L639	D577	L509	H444	F307		L177	D107
K1153	T1092	A1031	T965	G897	F829	K767	T701	H640	L578	G510	K445	A308	K244	A178	P108
S1154	D1093	S1032	T966	M898	D830	E768	T702	A641	F579	P512	F446	L309	N245	H179	
L1156	H1094	R1034	V967	S899	K831	K769	E703	H642	H580	P513		K310	E246	N180	D112
V1095	V1095	R1035	K968	V900	R836	K770	L705	H643	H581	H514	S451	G311	P247	A181	G116
T1096	T1096	Y1035	K969	F901	L837	G772	T706	H644	L583	D515	V452	F312	E247	I182	K117
K1097	K1097	T1037	T970	P902	L838	F773	F707	A645	H584	H516	G454	G313	S249	H183	
F1159	E1098	A1037	T971	H903	R839	D774		L646	A585	T517	Y455	G314	W250	E184	A118
M1160	H1099	F1038	T972	H904	R840	R775		H648	F586	T518	Q456	S315	E251	L185	H119
T1161	S1100	D1039	R973	H905	K841	R776	S711	H649	E587	E518	H457	A316	D252	V186	T120
C1162	V1101	P1040	S974	R906	H841	V776	S712	H650	E587	P519	T458	N317	D253	G187	N121
T1163	P1102	L1041	Y975	L907	W842	F777	L712	H651	Q588	H520	T459	V318	D254	Y122	Y122
D1164	F1103	F1042	Q976	L908	D843	K778	E713	H651	E589	T521	A459	F319	T255	H123	
	M1104	Y1043	N977	T909	R844	F779	H714	K652	D590		E460	V320	P256	Y192	
C1168	V1105	L1044		V910	L845	D780	I715	P653	H591	P524	Y461	Y321	L257	S193	N127
H1169	F1106	H1045	F980	Q911	T781	I781	E716	G525	C592	G525	H462	Y322	T258	N194	I128
P1170	D1107	H1046	E981	S912	T782	K717	H655	L526	D593	L526	G463	C323	N259	A195	I128
Y1171	Y1108	E913	E913	E913	E849	H718	H656		F594		L464	I324	E260	N196	D129
G1172	K1109	N914	H850	N914	W784	I719	H657	H657	E595	K530	P465	P325	E261	L197	F130
E1173	T1110	T1049	E984	A915	L785	L785	H657	C658	V596	T531	A466	D326	S262	Y199	I131
F1174	M1111	D1050	E985	L916	K786	K786	H659	A659	Q597	V532	R467	P399	S263	T200	K133
Y1175	F1112	L853	W722	R917	D787	D787	E721	L660	F598	Y533	R467	D329	F264	A201	K134
L1176	M1113	I1052	T989	R918	R854	L788	Q723	S661	E599	D534	P469	R330	A265	Y202	T135

L1177	G1241	H1304	P1449	F1513	H1581	E1649	L1177	G1241	H1304	P1449	F1513	H1581	E1649
G1178	H1242	P1305	V1450	E1514	E1582	H1656	F1730	H1242	P1305	V1450	E1514	E1582	H1656
D1179	H1243	I1306	F1451	E1515	A1583	H1657	P1731	H1243	I1306	F1451	E1515	A1583	H1657
	E1244	S1307	F1452	F1516	G1584	T1657	Q1732	E1244	S1307	F1452	F1516	G1584	T1657
E1182	G1245	C1308	H1453	S1517	M1585	D1658	H1733	G1245	C1308	H1453	S1517	M1585	D1658
M1183	E1246	C1309	H1454	F1519	I1588	D1659	R1735	M1183	C1309	H1454	F1519	I1588	D1659
P1184	V1247	V1310	H1455	G1520	L1589	G1660	L1736	P1184	V1310	H1455	G1520	L1589	G1660
W1185	Y1248	H1311	A1456	Y1521	L1590	H1661	Y1737	W1185	H1311	A1456	Y1521	L1590	H1661
A1186	Q1249	M1313	T1457	A1522	G1591	E1663	T1738	A1186	M1313	T1457	A1522	G1591	E1663
Y1187	A1250	P1314	D1459	A1523	G1591	P1664	Y1739	Y1187	P1314	D1459	A1523	G1591	P1664
D1188	Y1251	T1315	T1460	Y1524	E1594		Y1740	D1188	T1315	T1460	Y1524	E1594	
R1189	V1252	F1316	W1461	N1525	M1595		Q1741	R1189	F1316	W1461	N1525	M1595	
V1190	T1253	P1317	W1462	L1526	S1596		Q1742	V1190	P1317	W1462	L1526	S1596	
F1191	S1254	H1318	A1463	E1527	F1597		D1743	F1191	H1318	A1463	E1527	F1597	
K1192		W1319	L1464	L1528	V1598		Y1744	K1192	W1319	L1464	L1528	V1598	
Y1193		H1320	F1465	N1529	F1599		H1746	Y1193	H1320	F1465	N1529	F1599	
D1194		R1321	Q1466	H1530	D1600		K1747	D1194	R1321	Q1466	H1530	D1600	
I1195		R1322	D1467	Y1531	R1601		H1748	I1195	R1322	D1467	Y1531	R1601	
T1196		L1322	S1397	S1532	L1602		G1749	T1196	L1322	S1397	S1532	L1602	
E1197		Y1323	D1398	I1533	K1604		A1750	E1197	Y1323	D1398	I1533	K1604	
K1198		V1324	F1399	F1534	K1604			K1198	V1324	F1399	F1534	K1604	
L1198		V1325	F1400	Q1535	L1605			L1198	V1325	F1400	Q1535	L1605	
H1200		N1264	F1471	L1536	D1606			H1200	N1264	F1471	L1536	D1606	
D1201		L1265	E1402	D1537	L1607			D1201	L1265	E1402	D1537	L1607	
L1202			Q1403	H1538	T1608			L1202		Q1403	H1538	T1608	
K1203			V1404	M1539	K1609			K1203		V1404	M1539	K1609	
L1204			L1405	L1540	A1610			L1204		L1405	L1540	A1610	
H1205			Y1406	Q1541	L1611			H1205		Y1406	Q1541	L1611	
A1206			L1407	E1542	K1612			A1206		L1407	E1542	K1612	
E1207			E1408	R1543	L1613			E1207		E1408	R1543	L1613	
F1210			E1409	F1544	M1614			F1210		E1409	F1544	M1614	
I1211			F1413	Q1484	G1615			I1211		F1413	Q1484	G1615	
I1212			C1414	L1485	H1616			I1212		C1414	L1485	H1616	
D1213			D1415	M1486	H1617			D1213		D1415	M1486	H1617	
Y1214			F1416	H1487	L1618			Y1214		F1416	H1487	L1618	
E1215			T1488	V1549				E1215		T1488	V1549		
V1216			F1489	F1550				V1216		F1489	F1550		
F1217			L1490	A1551				F1217		L1490	A1551		
D1218			E1421	G1552				D1218		E1421	G1552		
L1219			I1422	F1553				L1219		I1422	F1553		
G1224			L1423	L1554				G1224		L1423	L1554		
G1225			H1424	L1555				G1225		H1424	L1555		
K1226			K1495	H1556				K1226		K1495	H1556		
D1227			M1498	N1557				D1227		M1498	N1557		
L1228			T1560					L1228		T1560			
F1229			S1561					F1229		S1561			
K1230			E1501					K1230		E1501			
Q1231			L1431					Q1231		L1431			
P1232			K1436					P1232		K1436			
S1233			Y1437					S1233		Y1437			
V1234			T1503					V1234		T1503			
I1235			K1504					I1235		K1504			
H1236			H1505					H1236		H1505			
E1237			L1442					E1237		L1442			
P1238			D1443					P1238		D1443			
R1239			Y1444					R1239		Y1444			
G1300			Q1366					G1300		Q1366			
L1301			H1367					L1301		H1367			
N1302			H1368					N1302		H1368			
G1303			F1446					G1303		F1446			
			D1447							D1447			
			D1448							D1448			

• Molecule 2: HEMOCYANIN KLH1

Chain B: 28% 69%

V1665	T1729	I1793	K1857	A1920	V1988	T2062	V1665	T1729	I1793	K1857	A1920	V1988	T2062
M1666	F1730	E1794	E1858	P1921	D1989	P2063	M1666	F1730	E1794	E1858	P1921	D1989	P2063
I1667	P1731	F1795	P1859	Y1922	Q1990	S2064	I1667	P1731	F1795	P1859	Y1922	Q1990	S2064
R1668	Q1732	H1796	Y1860	N1923	F1991	T2065	R1668	Q1732	H1796	Y1860	N1923	F1991	T2065
K1669	H1733	G1797	G1861	L1924	V1992	T2066	K1669	H1733	G1797	G1861	L1924	V1992	T2066
D1670	R1735	E1798	I1862	N1925	K1993	T2067	D1670	R1735	E1798	I1862	N1925	K1993	T2067
L1671	L1736	H1799	G1863	D1926	R1994	T2068	L1671	L1736	H1799	G1863	D1926	R1994	T2068
Q1672	Y1737	R1800	H1864	H1927	T1995	A2070	Q1672	Y1737	R1800	H1864	H1927	T1995	A2070
T1673	T1738	L1801	L1866	T1928	K1999	H2071	T1673	T1738	L1801	L1866	T1928	K1999	H2071
L1674	Y1739	H1802	H1867	F1931	E2000	H2072	L1674	Y1739	H1802	H1867	F1931	E2000	H2072
D1675	Q1740	K1803	A1868	S1932	D2000	D2073	D1675	Q1740	K1803	A1868	S1932	D2000	D2073
K1676	F1741	R1804	S1869	K1933	D2001	T2074	K1676	F1741	R1804	S1869	K1933	D2001	T2074
Q1678	Q1742	D1805	Y1870	P1934	A2002		Q1678	Q1742	D1805	Y1870	P1934	A2002	
L1679	D1743	L1806	D1871	G2003			L1679	D1743	L1806	D1871	G2003		
P1680	S1744	N1807	P1872	V2004			P1680	S1744	N1807	P1872	V2004		
S1681	L1745	R1808	L1873	F2005			S1681	L1745	R1808	L1873	F2005		
L1682	R1746	D1809	F1874	T2006			L1682	R1746	D1809	F1874	T2006		
V1683	K1747	R1810	Y1875	V2007			V1683	K1747	R1810	Y1875	V2007		
K1684	H1748	L1811	L1876	D1939			K1684	H1748	L1811	L1876	D1939		
A1685	G1749	F1812	H1877	G2010			A1685	G1749	F1812	H1877	G2010		
L1686	A1750	S1815	H1878	E2011			L1686	A1750	S1815	H1878	E2011		
E1687		T1816	H1879	K2012			E1687		T1816	H1879	K2012		
S1688	L1754	K1817	S1879	F1943			S1688	L1754	K1817	S1879	F1943		
M1689	P1755	T1818	Q1880	G1944			M1689	P1755	T1818	Q1880	G1944		
K1690	Y1756	D1818	D1882	Y1946			K1690	Y1756	D1818	D1882	Y1946		
		H1819	R1883	Y1947					H1819	R1883	Y1947		
H1693	D1757	H1820	L1884	D1948			H1693	D1757	H1820	L1884	D1948		
S1694	Y1759	N1821	L1884	F1949			S1694	Y1759	N1821	L1884	F1949		
G1695	T1760	W1822	Q1888	L1950			G1695	T1760	W1822	Q1888	L1950		
D1696	L1761	F1823	V1888	E1951			D1696	L1761	F1823	V1888	E1951		
F1697	P1762	I1824	Q1889	F1952			F1697	P1762	I1824	Q1889	F1952		
F1698	R1763	E1825	Q1890	A1953			F1698	R1763	E1825	Q1890	A1953		
Q1699	S1764	Q1826	L1891	G1954			Q1699	S1764	Q1826	L1891	G1954		
A1700	E1765	A1827	Q1892	W1955			A1700	E1765	A1827	Q1892	W1955		
I1701	L1766	L1828	R1893	F1956			I1701	L1766	L1828	R1893	F1956		
F1704	P1767	L1829	F1894	I1957			F1704	P1767	L1829	F1894	I1957		
H1705	E1768	A1830	R1895	G1958			H1705	E1768	A1830	R1895	G1958		
L1706	L1769	Q1833	G1896	G1959			L1706	L1769	Q1833	G1896	G1959		
L1707	L1770		L1897	D1961			L1707	L1770		L1897	D1961		
P1708	T1771		S1898	H1962			P1708	T1771		S1898	H1962		
P1709	S1772	D1838	F1839	I1963			P1709	S1772	D1838	F1839	I1963		
L1710	H1773	P1733	E1840	V1964			L1710	H1773	P1733	E1840	V1964		
C1711	I1775	V1841	E1901	R1965			C1711	I1775	V1841	E1901	R1965		
P1712	H1776	Q1842	A1902	N1966			P1712	H1776	Q1842	A1902	N1966		
S1713	D1777	F1843	N1903	E1967			S1713	D1777	F1843	N1903	E1967		
P1714	E1778	E1844	V1906				P1714	E1778	E1844	V1906			
A1715	S1779	L1845	N1907				A1715	S1779	L1845	N1907			
A1716	T1780	M1846	L1908				A1716	T1780	M1846	L1908			
S1717	G1781	H1847	M1909				S1717	G1781	H1847	M1909			
K1718	R1782	N1848	K1910	F1977			K1718	R1782	N1848	K1910	F1977		
R1719	D1783	G1849	L1911	T2046			R1719	D1783	G1849	L1911	T2046		
F1720	L1784	V1850	P1912	L1979			F1720	L1784	V1850	P1912	L1979		
A1721	P1785	H1851	L1913	T2048			A1721	P1785	H1851	L1913	T2048		
C1722	P1786	L1852	K1914	S2049			C1722	P1786	L1852	K1914	S2049		
F1723	P1787	W1853	F1982				F1723	P1787	W1853	F1982			
V1724	F1788	K1853	S1985	E1986			V1724	F1788	K1853	S1985	E1986		
H1725	L1789	G1855	P1915				H1725	L1789	G1855	P1915			
	G1790	F1856	F1918					G1790	F1856	F1918			

A3133	E3072	L3006	A2943	F2862	Y2717	L2654	G2589	L2519	D2450	V2384	L3221	A2353	Y2192	H2132
I3136	I3073	P3007	G2944	I2863	R2718	E2655	Y2592	K2520	V2451	F3385	M3222	V2254	D2193	R2133
	L3074	T3008	F2945	F2864	G2719	Q2656	Y2593	D2521	F2452	A3386	T3232	Q2255	I2194	I2134
	L3075	F3009	H2946	H2865	T2794	T2657	Y2594	A2522		G2387	Q3234	F2256	I2195	E2135
V3139	E3077	F3010	G2947	R2658	F2795	D2658	G2594	M2523	E2456	F2388	I2325	E2257	R2196	V2136
P3140	I3078		Y2948	R2867	Y2722	F2659	G2595	V2526	P2457	L2389	M2326	V2258	I2197	A2137
L3141	V3078	I3016	P2949	I2868	D2723	C2660	T2596	M2527	F2458	L2390	R2327	M2259	R2198	C2138
H3142	H3017	R3017	N2950	I2869		Q2661		M2528	F2460		F2328	H2260	V2199	C2139
P3143	A3080	G3018	L2951	L2870	E2728	F2662	F2599	A2528	L2460	I2393	F3229	I2261	M2200	L2140
F3144	L3081	F3019	C2952	L2799	I2729	E2663	A2601	D2529	K2461	R2394	T2262	T2263	P2201	H2141
N3145	I3082	F3020	P2953	F2664		V2664	L2602	F2534	F2462	T2395	Y2331	T2263	I2202	G2142
Y3146	G3083	K3021	E2954	Q2665	K2732	Q2665	L2603	Y2535	S2463	S2396	E2332	H264	P2203	M2143
E3147	G3084		K2955	Q2667	R2734	E2667	T2604		V2464	A2397	I2333	Y2265	P2204	M2144
S3148	A3085	I3024	G2956	L2875	M2735	I2668	F2605		T2465	D2395	M2334	L2266	A2205	T2145
V3149	E3086	K3025	D2957	K2874	K2733	T2669	F2606		A2466	V2399	H2335	V2267	R2206	F2146
N3150	K3026	S3026	E2958	L2876	R2736	T2669	T2607		V2467	Q2400	Q2337	Q2268	G2207	T2147
N3151	K3027	I3027	K2959	E2670	R2737	H2670	D2608		I2468	F2401	Q2338	G2269	Y2208	H2148
D3152	S3089	N3028	Y2960	F2679	P2738		D2609			Q2402	T2339	P2270	V2209	I2149
	M3090	Q3039	P2961	L2680		I2673			V2471	I2403	K2340	Q2271	P2210	H2150
	S3091	D3036	C2962	L2681	D2742				L2472	C2404	K2341	V2272	S2211	L2151
	T3092	T3031	K2963	W2676	P2742		N2612		P2473	C2405	A2342	S2274	D2212	L2152
L3160	L3093	F3032	F2822	T2677	I2743	G2678	P2613		L2477	L2405	H2342	L2275	D2213	Y2153
P3161	E3094	R3033	G2824	G2678	N2744	G2679	F2614			T2406	A2343	L2274	T2214	Y2154
N3162	T2885	I3032	H2816	G2679		L2680	H2615		L2477	Q2407	V2344	S2276	Y2215	L2155
A3163	V2886	D2817		L2681					A2479	S2407	P2345	S2277	T2216	Q2156
V3164	E2887			T2681					P2480		M2346	L2278	V2217	F2157
V3165	H2888													I2158
L3166	G2892													Q2159
S3167	K2893													
H3168	E2896													A2160
R3169	E2900													L2161
F3170	E2905													R2162
M3171	D2906													R2163
Y3172	D2908													H2164
Y3173	D2909													G2165
Y3174	D2910													S2166
D3175	D2911													L2227
Y3176	D2912													T2228
	D2913													I2289
	D2914													H2290
	D2915													S2228
	D2916													H2291
	D2917													T2230
	D2918													E2232
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PER MICROGRAPH, Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163	Depositor

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: CUO

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.95	2/13940 (0.0%)	1.19	15/18926 (0.1%)
1	C	0.95	2/13938 (0.0%)	1.19	15/18923 (0.1%)
2	B	0.93	2/14526 (0.0%)	1.10	8/19734 (0.0%)
2	D	0.93	2/14526 (0.0%)	1.10	9/19734 (0.0%)
All	All	0.94	8/56930 (0.0%)	1.14	47/77317 (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	1
1	C	0	1
2	B	0	2
2	D	0	2
All	All	0	6

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	524	PRO	N-CD	16.06	1.70	1.47
1	A	524	PRO	N-CD	16.04	1.70	1.47
2	B	2457	PRO	N-CD	13.70	1.67	1.47
2	D	2457	PRO	N-CD	13.65	1.67	1.47
1	C	653	PRO	N-CD	8.88	1.60	1.47

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1632	ASN	CB-CG-OD1	-38.50	44.60	121.60
1	A	1632	ASN	CB-CG-OD1	-38.48	44.65	121.60
1	A	212	ASN	CB-CG-OD1	-38.25	45.10	121.60
1	C	212	ASN	CB-CG-OD1	-38.23	45.13	121.60
1	A	212	ASN	CB-CG-ND2	-9.73	93.35	116.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1150	GLY	Mainchain
2	B	2951	LEU	Peptide
2	B	3248	ARG	Sidechain
1	C	1150	GLY	Mainchain
2	D	2951	LEU	Peptide

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	13530	0	12792	2867	0
1	C	13530	0	12787	2893	0
2	B	14084	0	13309	2799	0
2	D	14084	0	13311	2767	0
3	A	16	0	0	1	0
3	B	16	0	0	3	0
3	C	16	0	0	1	0
3	D	16	0	0	3	0
All	All	55292	0	52199	10907	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 102.

The worst 5 of 10907 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)
2:D:2279:HIS:HE1	2:D:2280:TYR:CZ	1.08	1.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2279:HIS:CE1	2:D:2280:TYR:CE2	1.80	1.65
1:C:724:GLN:HE22	1:C:828:LYS:CE	1.10	1.63
2:B:2279:HIS:CE1	2:B:2280:TYR:CE2	1.80	1.63
2:B:2279:HIS:HE1	2:B:2280:TYR:CZ	1.08	1.63

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1662/1664 (100%)	1601 (96%)	56 (3%)	5 (0%)	46	83
1	C	1662/1664 (100%)	1599 (96%)	58 (4%)	5 (0%)	46	83
2	B	1732/1734 (100%)	1608 (93%)	94 (5%)	30 (2%)	11	55
2	D	1732/1734 (100%)	1608 (93%)	94 (5%)	30 (2%)	11	55
All	All	6788/6796 (100%)	6416 (94%)	302 (4%)	70 (1%)	24	65

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2960	TYR
2	B	3028	ASN
2	B	3050	SER
2	B	3148	SER
2	B	3225	SER

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 PDB entries followed by that with respect to all EM entries.

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	1457/1457 (100%)	1456 (100%)	1 (0%)	95	97
1	C	1456/1457 (100%)	1455 (100%)	1 (0%)	95	97
2	B	1522/1522 (100%)	1502 (99%)	20 (1%)	76	89
2	D	1522/1522 (100%)	1502 (99%)	20 (1%)	76	89
All	All	5957/5958 (100%)	5915 (99%)	42 (1%)	89	94

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	3305	GLU
2	D	2955	LYS
2	D	3297	ASN
2	B	3341	ASN
1	C	1365	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 230 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	3042	GLN
1	C	575	HIS
2	D	2977	HIS
2	B	3106	HIS
2	B	3359	HIS

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 ⓘ

16 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
3	CUO	A	9001	1	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	A	9002	1	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	A	9003	1	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	A	9004	1	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	B	9005	2	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	B	9006	2	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	B	9007	2	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	B	9008	2	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	C	9001	1	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	C	9002	1	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	C	9003	1	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	C	9004	1	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	D	9005	2	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	D	9006	2	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	D	9007	2	0,4,4	0.00	-	0,4,4	0.00	-
3	CUO	D	9008	2	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
3	CUO	A	9001	1	-	0/0/4/4	0/1/1/1
3	CUO	A	9002	1	-	0/0/4/4	0/1/1/1
3	CUO	A	9003	1	-	0/0/4/4	0/1/1/1
3	CUO	A	9004	1	-	0/0/4/4	0/1/1/1
3	CUO	B	9005	2	-	0/0/4/4	0/1/1/1
3	CUO	B	9006	2	-	0/0/4/4	0/1/1/1
3	CUO	B	9007	2	-	0/0/4/4	0/1/1/1
3	CUO	B	9008	2	-	0/0/4/4	0/1/1/1
3	CUO	C	9001	1	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CUO	C	9002	1	-	0/0/4/4	0/1/1/1
3	CUO	C	9003	1	-	0/0/4/4	0/1/1/1
3	CUO	C	9004	1	-	0/0/4/4	0/1/1/1
3	CUO	D	9005	2	-	0/0/4/4	0/1/1/1
3	CUO	D	9006	2	-	0/0/4/4	0/1/1/1
3	CUO	D	9007	2	-	0/0/4/4	0/1/1/1
3	CUO	D	9008	2	-	0/0/4/4	0/1/1/1

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.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9003	CUO	1	0
3	B	9008	CUO	3	0
3	C	9003	CUO	1	0
3	D	9008	CUO	3	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.