



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 11, 2024 – 09:04 PM EDT

PDB ID : 1XWO  
Title : crystal structrue of goose delta crystallin  
Authors : Lee, H.J.; Lai, Y.H.; Wu, S.Y.; Chang, G.G.  
Deposited on : 2004-11-02  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 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) : 2.36.2

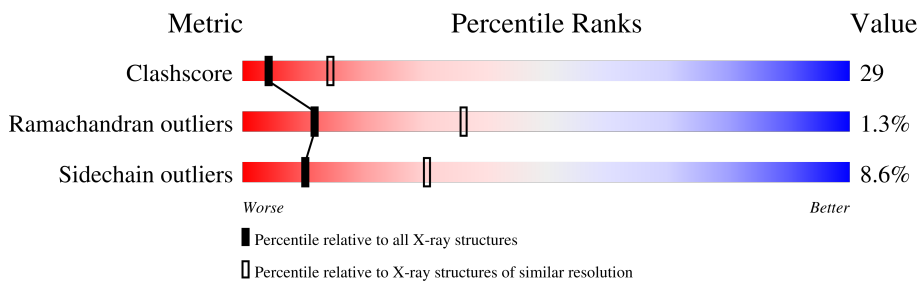
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	465	<div> <div>50%</div> <div>42%</div> <div>• •</div> </div>
1	B	465	<div> <div>45%</div> <div>48%</div> <div>• •</div> </div>
1	C	465	<div> <div>53%</div> <div>38%</div> <div>5% •</div> </div>
1	D	465	<div> <div>46%</div> <div>45%</div> <div>5% •</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14142 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 Delta crystallin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3474	2193	588	678	15			
1	B	448	Total	C	N	O	S	0	0	0
			3471	2191	588	677	15			
1	C	449	Total	C	N	O	S	0	0	0
			3480	2196	589	680	15			
1	D	449	Total	C	N	O	S	0	0	0
			3483	2198	590	680	15			

- Molecule 2 is water.

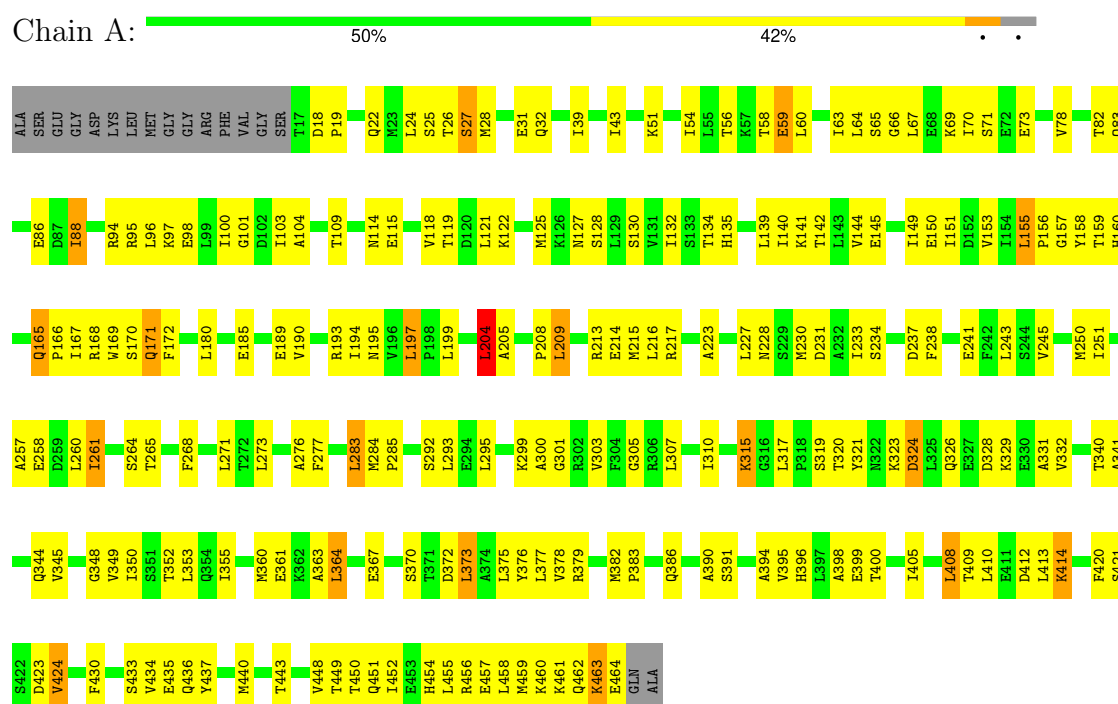
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	82	Total	O	0	0
			82	82		
2	B	53	Total	O	0	0
			53	53		
2	C	59	Total	O	0	0
			59	59		
2	D	40	Total	O	0	0
			40	40		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Delta crystallin



#### • Molecule 1: Delta crystallin





L220	D221	A308	S309	I310	L311	S224	I225	N228	S229	M230	D231	S234	E235	R236	D237	F238	V239	L243	L249	H252	L253	S254	K255	M256	A257	L260	I261	I262	T265	S266	E267	F268	L271	I272	D275	S282	K287	K288	L293	F294	L295	I296	R297	S298	K299	V303	R306	L307																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
G392	I393	L394	M395	N396	O397	P398	Q399	R400	S401	T402	U403	V404	W405	X406	Y407	Z408	A409	B410	C411	D412	E413	F414	G415	H416	I417	J418	K419	L420	M421	N422	O423	P424	Q425	R426	S427	T428	U429	V430	W431	X432	Y433	Z434	A435	B436	C437	D438	E439	F440	G441	H442	I443	J444	K445	L446	M447	N448	O449	P450	Q451	R452	S453	T454	U455	V456	W457	X458	Y459	Z460	A461	B462	C463	D464	E465	F466	G467	H468	I469	J470	K471	L472	M473	N474	O475	P476	Q477	R478	S479	T480	U481	V482	W483	X484	Y485	Z486	A487	B488	C489	D490	E491	F492	G493	H494	I495	J496	K497	L498	M499	N500	O501	P502	Q503	R504	S505	T506	U507	V508	W509	X510	Y511	Z512	A513	B514	C515	D516	E517	F518	G519	H520	I521	J522	K523	L524	M525	N526	O527	P528	Q529	R530	S531	T532	U533	V534	W535	X536	Y537	Z538	A539	B540	C541	D542	E543	F544	G545	H546	I547	J548	K549	L550	M551	N552	O553	P554	Q555	R556	S557	T558	U559	V560	W561	X562	Y563	Z564	A565	B566	C567	D568	E569	F570	G571	H572	I573	J574	K575	L576	M577	N578	O579	P580	Q581	R582	S583	T584	U585	V586	W587	X588	Y589	Z590	A591	B592	C593	D594	E595	F596	G597	H598	I599	J600	K601	L602	M603	N604	O605	P606	Q607	R608	S609	T610	U611	V612	W613	X614	Y615	Z616	A617	B618	C619	D620	E621	F622	G623	H624	I625	J626	K627	L628	M629	N630	O631	P632	Q633	R634	S635	T636	U637	V638	W639	X640	Y641	Z642	A643	B644	C645	D646	E647	F648	G649	H650	I651	J652	K653	L654	M655	N656	O657	P658	Q659	R660	S661	T662	U663	V664	W665	X666	Y667	Z668	A669	B670	C671	D672	E673	F674	G675	H676	I677	J678	K679	L680	M681	N682	O683	P684	Q685	R686	S687	T688	U689	V690	W691	X692	Y693	Z694	A695	B696	C697	D698	E699	F700	G701	H702	I703	J704	K705	L706	M707	N708	O709	P710	Q711	R712	S713	T714	U715	V716	W717	X718	Y719	Z720	A721	B722	C723	D724	E725	F726	G727	H728	I729	J730	K731	L732	M733	N734	O735	P736	Q737	R738	S739	T740	U741	V742	W743	X744	Y745	Z746	A747	B748	C749	D750	E751	F752	G753	H754	I755	J756	K757	L758	M759	N760	O761	P762	Q763	R764	S765	T766	U767	V768	W769	X770	Y771	Z772	A773	B774	C775	D776	E777	F778	G779	H780	I781	J782	K783	L784	M785	N786	O787	P788	Q789	R790	S791	T792	U793	V794	W795	X796	Y797	Z798	A799	B800	C801	D802	E803	F804	G805	H806	I807	J808	K809	L810	M811	N812	O813	P814	Q815	R816	S817	T818	U819	V820	W821	X822	Y823	Z824	A825	B826	C827	D828	E829	F830	G831	H832	I833	J834	K835	L836	M837	N838	O839	P840	Q841	R842	S843	T844	U845	V846	W847	X848	Y849	Z850	A851	B852	C853	D854	E855	F856	G857	H858	I859	J860	K861	L862	M863	N864	O865	P866	Q867	R868	S869	T870	U871	V872	W873	X874	Y875	Z876	A877	B878	C879	D880	E881	F882	G883	H884	I885	J886	K887	L888	M889	N890	O891	P892	Q893	R894	S895	T896	U897	V898	W899	X900	Y901	Z902	A903	B904	C905	D906	E907	F908	G909	H910	I911	J912	K913	L914	M915	N916	O917	P918	Q919	R920	S921	T922	U923	V924	W925	X926	Y927	Z928	A929	B930	C931	D932	E933	F934	G935	H936	I937	J938	K939	L940	M941	N942	O943	P944	Q945	R946	S947	T948	U949	V950	W951	X952	Y953	Z954	A955	B956	C957	D958	E959	F960	G961	H962	I963	J964	K965	L966	M967	N968	O969	P970	Q971	R972	S973	T974	U975	V976	W977	X978	Y979	Z980	A981	B982	C983	D984	E985	F986	G987	H988	I989	J990	K991	L992	M993	N994	O995	P996	Q997	R998	S999	T1000	U1001	V1002	W1003	X1004	Y1005	Z1006	A1007	B1008	C1009	D1010	E1011	F1012	G1013	H1014	I1015	J1016	K1017	L1018	M1019	N1020	O1021	P1022	Q1023	R1024	S1025	T1026	U1027	V1028	W1029	X1030	Y1031	Z1032	A1033	B1034	C1035	D1036	E1037	F1038	G1039	H1040	I1041	J1042	K1043	L1044	M1045	N1046	O1047	P1048	Q1049	R1050	S1051	T1052	U1053	V1054	W1055	X1056	Y1057	Z1058	A1059	B1060	C1061	D1062	E1063	F1064	G1065	H1066	I1067	J1068	K1069	L1070	M1071	N1072	O1073	P1074	Q1075	R1076	S1077	T1078	U1079	V1080	W1081	X1082	Y1083	Z1084	A1085	B1086	C1087	D1088	E1089	F1090	G1091	H1092	I1093	J1094	K1095	L1096	M1097	N1098	O1099	P1100	Q1101	R1102	S1103	T1104	U1105	V1106	W1107	X1108	Y1109	Z1110	A1111	B1112	C1113	D1114	E1115	F1116	G1117	H1118	I1119	J1120	K1121	L1122	M1123	N1124	O1125	P1126	Q1127	R1128	S1129	T1130	U1131	V1132	W1133	X1134	Y1135	Z1136	A1137	B1138	C1139	D1140	E1141	F1142	G1143	H1144	I1145	J1146	K1147	L1148	M1149	N1150	O1151	P1152	Q1153	R1154	S1155	T1156	U1157	V1158	W1159	X1160	Y1161	Z1162	A1163	B1164	C1165	D1166	E1167	F1168	G1169	H1170	I1171	J1172	K1173	L1174	M1175	N1176	O1177	P1178	Q1179	R1180	S1181	T1182	U1183	V1184	W1185	X1186	Y1187	Z1188	A1189	B1190	C1191	D1192	E1193	F1194	G1195	H1196	I1197	J1198	K1199	L1200	M1201	N1202	O1203	P1204	Q1205	R1206	S1207	T1208	U1209	V1210	W1211	X1212	Y1213	Z1214	A1215	B1216	C1217	D1218	E1219	F1220	G1221	H1222	I1223	J1224	K1225	L1226	M1227	N1228	O1229	P1230	Q1231	R1232	S1233	T1234	U1235	V1236	W1237	X1238	Y1239	Z1240	A1241	B1242	C1243	D1244	E1245	F1246	G1247	H1248	I1249	J1250	K1251	L1252	M1253	N1254	O1255	P1256	Q1257	R1258	S1259	T1260	U1261	V1262	W1263	X1264	Y1265	Z1266	A1267	B1268	C1269	D1270	E1271	F1272	G1273	H1274	I1275	J1276	K1277	L1278	M1279	N1280	O1281	P1282	Q1283	R1284	S1285	T1286	U1287	V1288	W1289	X1290	Y1291	Z1292	A1293	B1294	C1295	D1296	E1297	F1298	G1299	H1300	I1301	J1302	K1303	L1304	M1305	N1306	O1307	P1308	Q1309	R1310	S1311	T1312	U1313	V1314	W1315	X1316	Y1317	Z1318	A1319	B1320	C1321	D1322	E1323	F1324	G1325	H1326	I1327	J1328	K1329	L1330	M1331	N1332	O1333	P1334	Q1335	R1336	S1337	T1338	U1339	V1340	W1341	X1342	Y1343	Z1344	A1345	B1346	C1347	D1348	E1349	F1350	G1351	H1352	I1353	J1354	K1355	L1356	M1357	N1358	O1359	P1360	Q1361	R1362	S1363	T1364	U1365	V1366	W1367	X1368	Y1369	Z1370	A1371	B1372	C1373	D1374	E1375	F1376	G1377	H1378	I1379	J1380	K1381	L1382	M1383	N1384	O1385	P1386	Q1387	R1388	S1389	T1390	U1391	V1392	W1393	X1394	Y1395	Z1396	A1397	B1398	C1399	D1400	E1401	F1402	G1403	H1404	I1405	J1406	K1407	L1408	M1409	N1410	O1411	P1412	Q1413	R1414	S1415	T1416	U1417	V1418	W1419	X1420	Y1421	Z1422	A1423	B1424	C1425	D1426	E1427	F1428	G1429	H1430	I1431	J1432	K1433	L1434	M1435	N1436	O1437	P1438	Q1439	R1440	S1441	T1442	U1443	V1444	W1445	X1446	Y1447	Z1448	A1449	B1450	C1451	D1452	E1453	F1454	G1455	H1456	I1457	J1458	K1459	L1460	M1461	N1462	O1463	P1464	Q1465	R1466	S1467	T1468	U1469	V1470	W1471	X1472	Y1473	Z1474	A1475	B1476	C1477	D1478	E1479	F1480	G1481	H1482	I1483	J1484	K1485	L1486	M1487	N1488	O1489	P1490	Q1491	R1492	S1493	T1494	U1495	V1496	W1497	X1498	Y1499	Z1500	A1501	B1502	C1503	D1504	E1505	F1506	G1507	H1508	I1509	J1510	K1511	L1512	M1513	N1514	O1515	P1516	Q1517	R1518	S1519	T1520	U1521	V1522	W1523	X1524	Y1525	Z1526	A1527	B1528	C1529	D1530	E1531	F1532	G1533	H1534	I1535	J1536	K1537	L1538	M1539	N1540	O1541	P1542	Q1543	R1544	S1545	T1546	U1547	V1548	W1549	X1550	Y1551	Z1552	A1553	B1554	C1555	D1556	E1557	F1558	G1559	H1560	I1561	J1562	K1563	L1564	M1565	N1566	O1567	P1568	Q1569	R1570	S1571	T1572	U1573	V1574	W1575	X1576	Y1577	Z1578	A1579	B1580	C1581	D1582	E1583	F1584	G1585	H1586	I1587	J1588	K1589	L1590	M1591	N1592	O1593	P1594	Q1595	R1596	S1597	T1598	U1599	V1600	W1601	X1602	Y1603	Z1604	A1605	B1606	C1607	D1608	E1609	F1610	G1611	H1612	I1613	J1614	K1615	L1616	M1617	N1618	O1619	P1620	Q1621	R1622	S1623	T1624	U1625	V1626	W1627	X1628	Y1629	Z1630	A1631	B1632	C1633	D1634	E1635	F1636	G1637	H1638	I1639	J1640	K1641	L1642	M1643	N1644	O1645	P1646	Q1647	R1648	S1649	T1650	U1651	V1652	W1653	X1654	Y1655	Z1656	A1657	B1658	C1659	D1660	E1661	F1662	G1663	H1664	I1665	J1666	K1667	L1668	M1669	N1670	O1671	P1672	Q1673	R1674	S1675	T1676	U1677	V1678	W1679	X1680	Y1681	Z1682	A1683	B1684	C1685	D1686	E1687	F1688	G1689	H1690	I1691	J1692	K1693	L1694	M1695	N1696	O1697	P1698	Q1699	R1700	S1701	T1702	U1703	V1704	W1705	X1706	Y1707	Z1708	A1709	B1710	C1711	D1712	E1713	F1714	G1715	H1716	I1717	J1718	K1719	L1720	M1721	N1722	O1723	P1724	Q1725	R1726	S1727	T1728	U1729	V1730	W1731	X1732	Y1733	Z1734	A1735	B1736	C1737	D1738	E1739	F1740	G1741	H1742	I1743	J1744	K1745	L1746	M1747	N1748	O1749	P1750	Q1751	R1752	S1753	T1754	U1755	V1756	W1757	X1758

## 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, $\alpha$ , $\beta$ , $\gamma$	93.70Å 99.00Å 106.50Å 90.00° 101.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.80)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.210 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

## 5 Model quality [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.48	0/3517	0.70	0/4746
1	B	0.48	0/3514	0.66	0/4742
1	C	0.51	2/3523 (0.1%)	0.70	1/4754 (0.0%)
1	D	0.46	0/3526	0.66	0/4758
All	All	0.48	2/14080 (0.0%)	0.68	1/19000 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	464	GLU	CG-CD	-7.96	1.40	1.51
1	C	464	GLU	CB-CG	-7.51	1.37	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	464	GLU	OE1-CD-OE2	5.80	130.26	123.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3474	0	3590	211	0
1	B	3471	0	3589	237	0
1	C	3480	0	3595	203	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3483	0	3598	246	0
2	A	82	0	0	9	0
2	B	53	0	0	5	0
2	C	59	0	0	8	0
2	D	40	0	0	4	0
All	All	14142	0	14372	826	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 29.

The worst 5 of 826 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:D:320:THR:HG22	1:D:321:TYR:H	1.16	1.09
1:D:194:ILE:HG12	2:D:498:HOH:O	1.52	1.08
1:A:310:ILE:HG12	2:A:531:HOH:O	1.54	1.06
1:C:283:LEU:H	1:C:283:LEU:HD22	1.19	1.02
1:C:243:LEU:HD11	1:C:310:ILE:HD12	1.37	1.02

There are no symmetry-related clashes.

## 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	446/465 (96%)	409 (92%)	33 (7%)	4 (1%)	17	46
1	B	446/465 (96%)	398 (89%)	44 (10%)	4 (1%)	17	46
1	C	447/465 (96%)	400 (90%)	42 (9%)	5 (1%)	14	41
1	D	447/465 (96%)	392 (88%)	45 (10%)	10 (2%)	6	22
All	All	1786/1860 (96%)	1599 (90%)	164 (9%)	23 (1%)	12	36

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	LEU
1	B	204	LEU
1	B	419	LEU
1	D	109	THR
1	A	462	GLN

### 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	394/405 (97%)	362 (92%)	32 (8%)	11	33
1	B	394/405 (97%)	366 (93%)	28 (7%)	14	39
1	C	395/405 (98%)	355 (90%)	40 (10%)	7	22
1	D	395/405 (98%)	360 (91%)	35 (9%)	9	28
All	All	1578/1620 (97%)	1443 (91%)	135 (9%)	10	30

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	171	GLN
1	D	215	MET
1	D	399	GLU
1	B	219	GLU
1	B	218	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	116	GLN
1	D	407	ASN
1	C	286	GLN
1	D	406	ASN
1	D	228	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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.