



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:24 PM UTC

PDB ID : 1GGY / pdb_00001ggy
Title : HUMAN FACTOR XIII WITH YTTERBIUM BOUND IN THE ION SITE
Authors : Fox, B.A.; Yee, V.C.; Pederson, L.C.; Trong, I.L.; Bishop, P.D.; Stenkamp, R.E.; Teller, D.C.
Deposited on : 1998-07-23
Resolution : 2.50 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

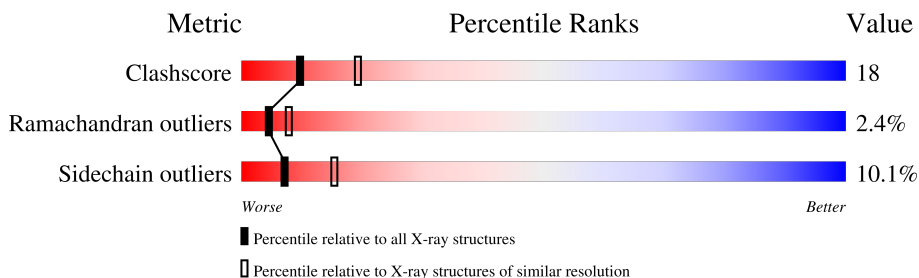
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 ≥ 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	731	
1	B	731	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11569 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 PROTEIN (COAGULATION FACTOR XIII).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	702	Total	C	N	O	S	0	0	0
			5637	3577	968	1066	26			
1	B	705	Total	C	N	O	S	0	0	0
			5659	3589	973	1071	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	651	GLU	GLN	conflict	UNP P00488
B	651	GLU	GLN	conflict	UNP P00488

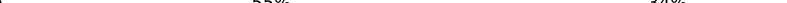
- Molecule 2 is YTTERBIUM (III) ION (CCD ID: YB) (formula: Yb).

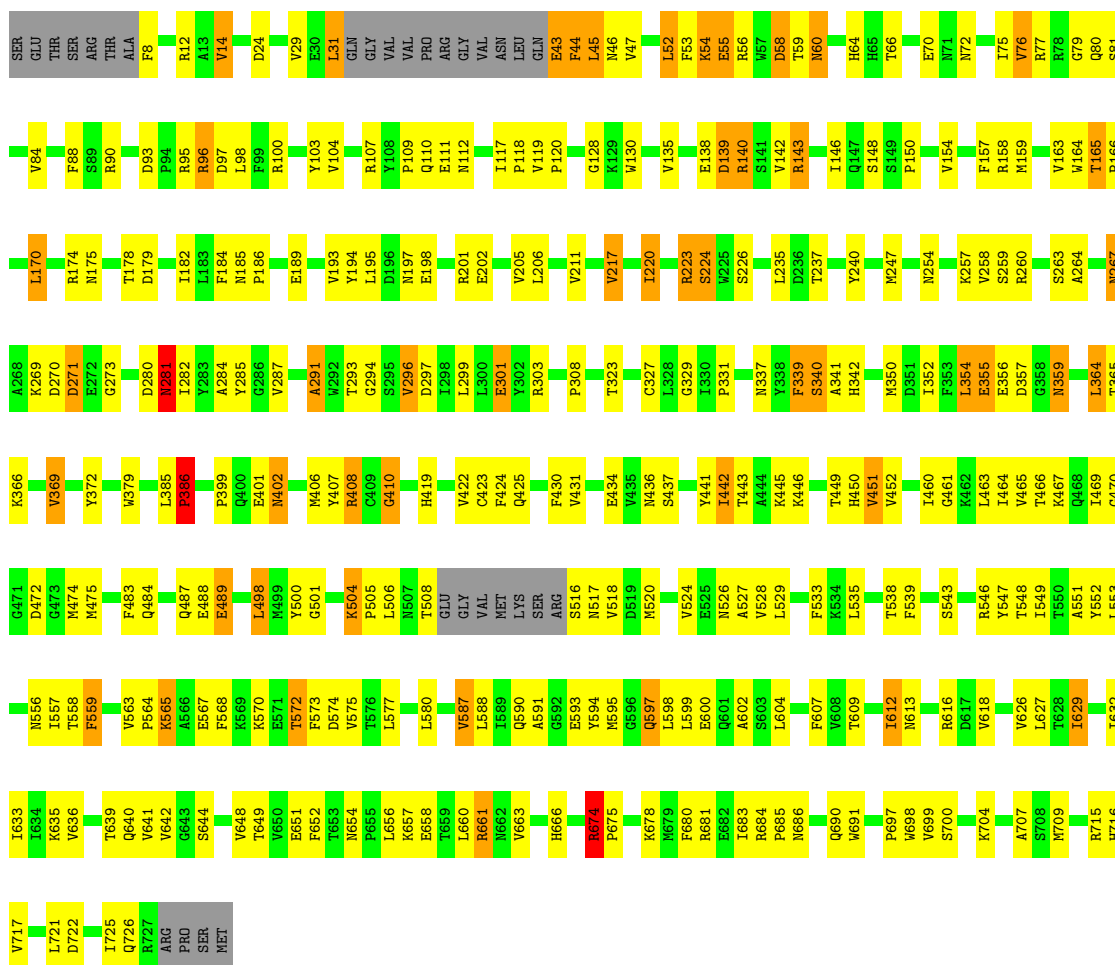
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Yb	0	0
			5	5		
2	B	3	Total	Yb	0	0
			3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total	O	0	0
			139	139		
3	B	126	Total	O	0	0
			126	126		

Note EDS was not executed.

- Chain A:  55% 34% 7% .



- Chain B: 55% 35% 6% . .

L714	R715	H716	V717	L721	D722	V723	T724	T725	Q726	R727	ARG	PRO	SER	MET
A610	R611	I612	I613	R616	A620	K623	K624	K625	K626	K627	K628	K629	K630	K631
F539	R540	N541	N542	S543	H544	N545	T548	T549	T550	A551	Y552	L553	S554	A555
V563	K565	A566	E567	F568	K569	F573	P574	V575	T576	L577	E578	P579	L580	S581
F582	K583	K584	L588	T589	Q590	A591	Y594	Q597	L598	L599	E600	L604	H605	F606
P607	V608	T609	R684	P685	P687	S700	G701	H702	R703	L704	L705	I706	A707	S708
M646	T647	V648	T649	V650	E651	L656	T659	V672	T673	R674	P675	H676	K677	K678
M679	R684	P685	P687	S700	G701	H702	R703	L704	L705	I706	A707	S708	M709	S713
T458	K462	L463	K467	Q468	I469	G470	G473	M474	I477	E485	A486	Q487	E490	R491
L492	L498	G501	A502	K503	K504	T508	GLU	GLY	VAL	MET	LYS	SER	ARG	S516
N517	V518	M520	D521	F522	E525	N526	A527	V528	L529	G530	K531	D532	F533	F534
L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549
L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564
L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579
L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594
L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609
L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624
L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639
L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654
L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669
L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684
L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699
L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714
L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729
L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744
L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759
L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774
L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789
L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804
L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819
L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834
L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849
L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864
L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879
L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894
L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909
L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924
L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939
L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954
L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969
L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984
L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999
L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014
L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029
L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044
L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059
L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074
L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089
L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104
L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119
L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134
L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149
L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164
L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179
L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194
L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209
L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224
L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239
L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254
L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269
L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284
L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299
L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314
L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329
L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344
L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359
L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374
L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389
L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404
L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419
L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434
L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449
L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464
L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479
L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494
L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509
L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524
L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539
L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554
L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569
L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584
L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599
L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614
L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629
L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644
L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659
L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674
L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689
L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704
L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719
L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734
L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749
L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764
L1765	L1766													

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, α , β , γ	101.06Å 72.39Å 135.99Å 90.00° 106.09° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	75.9 (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.188 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11569	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: YB

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	0.69	0/5770	1.10	38/7830 (0.5%)
1	B	0.67	0/5792	1.11	43/7859 (0.5%)
All	All	0.68	0/11562	1.10	81/15689 (0.5%)

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	B	0	1

There are no bond length outliers.

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ILE	CA-C-N	10.80	130.21	118.97
1	B	117	ILE	C-N-CA	10.80	130.21	118.97
1	A	52	LEU	N-CA-C	-8.24	97.64	110.42
1	A	269	LYS	N-CA-C	-7.58	96.20	108.41
1	B	382	ARG	CA-C-N	7.37	127.07	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	181	TYR	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	5637	0	5489	206	0
1	B	5659	0	5508	195	0
2	A	5	0	0	0	0
2	B	3	0	0	0	0
3	A	139	0	0	7	0
3	B	126	0	0	8	0
All	All	11569	0	10997	395	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 18.

The worst 5 of 395 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:B:575:VAL:HG13	1:B:583:LYS:HD3	1.43	1.01
1:B:220:ILE:HD13	1:B:474:MET:HE1	1.41	0.99
1:B:356:GLU:HG3	1:B:446:LYS:HD2	1.48	0.96
1:A:331:PRO:HG2	1:A:379:TRP:HB3	1.46	0.96
1:B:211:VAL:HG22	1:B:467:LYS:HD2	1.49	0.93

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	696/731 (95%)	617 (89%)	60 (9%)	19 (3%)	4 6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	699/731 (96%)	620 (89%)	65 (9%)	14 (2%)	6	10
All	All	1395/1462 (95%)	1237 (89%)	125 (9%)	33 (2%)	4	8

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	139	ASP
1	B	45	LEU
1	B	55	GLU
1	B	600	GLU

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	619/644 (96%)	562 (91%)	57 (9%)	8	19
1	B	621/644 (96%)	553 (89%)	68 (11%)	6	13
All	All	1240/1288 (96%)	1115 (90%)	125 (10%)	7	15

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	12	ARG
1	B	540	ARG
1	B	119	VAL
1	B	535	LEU
1	B	639	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	112	ASN
1	B	421	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	267	ASN
1	B	605	HIS
1	A	373	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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.