



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6G70 / pdb_00006g70
Title : Structure of murine Prpf39
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Deposited on : 2018-04-04
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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<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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

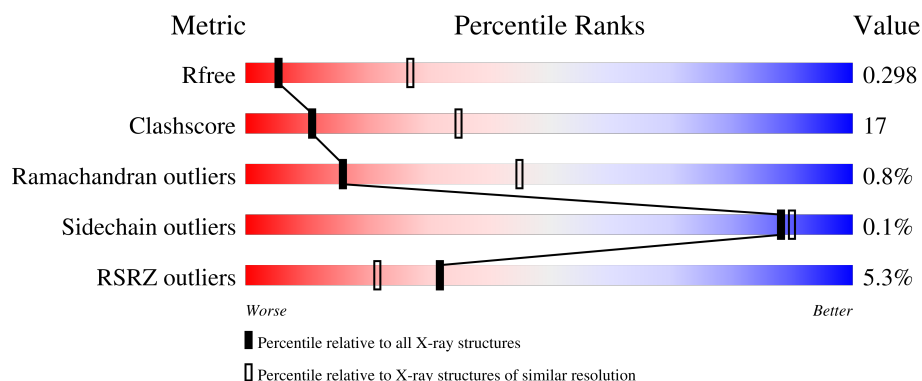
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	670	
1	B	670	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8592 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 Pre-mRNA-processing factor 39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4294	2747	747	781	19			
1	B	510	Total	C	N	O	S	0	0	0
			4298	2749	748	782	19			

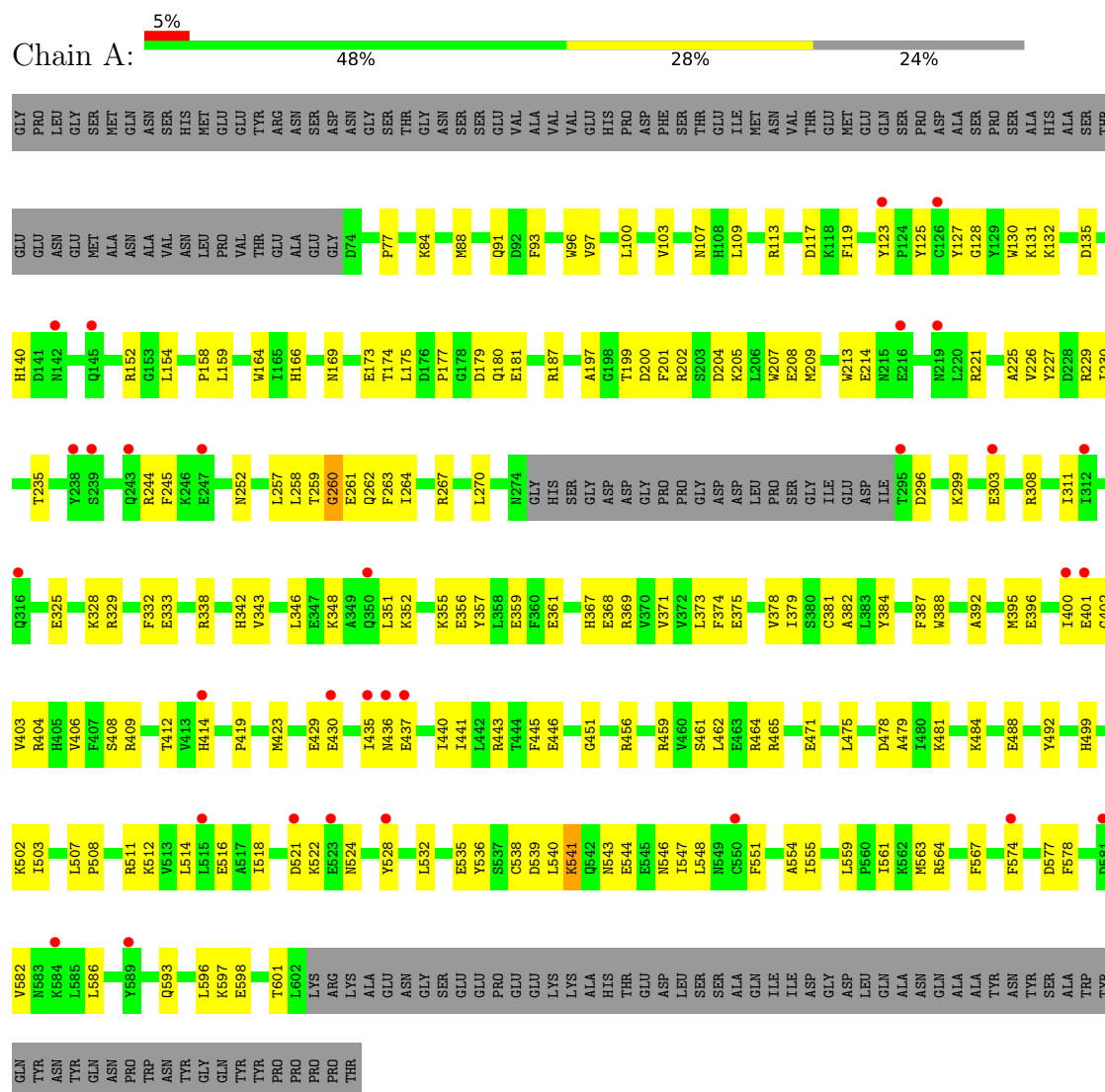
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP E9QJV4
A	-3	PRO	-	expression tag	UNP E9QJV4
A	-2	LEU	-	expression tag	UNP E9QJV4
A	-1	GLY	-	expression tag	UNP E9QJV4
A	0	SER	-	expression tag	UNP E9QJV4
B	-4	GLY	-	expression tag	UNP E9QJV4
B	-3	PRO	-	expression tag	UNP E9QJV4
B	-2	LEU	-	expression tag	UNP E9QJV4
B	-1	GLY	-	expression tag	UNP E9QJV4
B	0	SER	-	expression tag	UNP E9QJV4

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

• Molecule 1: Pre-mRNA-processing factor 39



• Molecule 1: Pre-mRNA-processing factor 39



GLN	ASN	PRO	TRP	ASN	TYR	GLY	GLN	TYR	GLN	TYR	PRO	PRO	PRO	THR
D577	F578	G579	S580	D581	V582	K597	E598	T601	L602	LYS	ARG	LYS	ALA	ASN
F491	Y492	K495	K502	I503	L507	P508	B511	K512	V513	L514	L515	ASN	GLY	SER
T412	V413	H414	K417	K418	P419	M423	L424	N425	A426	A427	E430	G433	A434	D437
F438	H439	R440	K441	K442	P443	M444	L445	N446	A447	A448	E449	G450	A451	D452
F453	H454	R455	K456	K457	P458	M459	L460	N461	A462	A463	E464	G465	A466	D467
F478	H479	R480	K481	K482	P483	M484	L485	N486	A487	A488	E489	G490	A491	D492
F497	H498	R499	K500	K501	P502	M503	L504	N505	A506	A507	E508	G509	A510	D511
F513	H514	R515	K516	K517	P518	M519	L520	N521	A522	A523	E524	G525	A526	D527
F538	H539	R540	K541	K542	P543	M544	L545	N546	A547	A548	E549	G550	A551	D552
F553	H554	R555	K556	K557	P558	M559	L560	N561	A562	A563	E564	G565	A566	D567
F573	H574	R575	K576	K577	P578	M579	L580	N581	A582	A583	E584	G585	A586	D587
F603	H604	R605	K606	K607	P608	M609	L610	N611	A612	A613	E614	G615	A616	D617
F628	H629	R630	K631	K632	P633	M634	L635	N636	A637	A638	E639	G640	A641	D642
F653	H654	R655	K656	K657	P658	M659	L660	N661	A662	A663	E664	G665	A666	D667
F678	H679	R680	K681	K682	P683	M684	L685	N686	A687	A688	E689	G690	A691	D692
F703	H704	R705	K706	K707	P708	M709	L710	N711	A712	A713	E714	G715	A716	D717
F728	H729	R730	K731	K732	P733	M734	L735	N736	A737	A738	E739	G740	A741	D742
F753	H754	R755	K756	K757	P758	M759	L760	N761	A762	A763	E764	G765	A766	D767
F778	H779	R780	K781	K782	P783	M784	L785	N786	A787	A788	E789	G790	A791	D792
F803	H804	R805	K806	K807	P808	M809	L810	N811	A812	A813	E814	G815	A816	D817
F828	H829	R830	K831	K832	P833	M834	L835	N836	A837	A838	E839	G840	A841	D842
F853	H854	R855	K856	K857	P858	M859	L860	N861	A862	A863	E864	G865	A866	D867
F878	H879	R880	K881	K882	P883	M884	L885	N886	A887	A888	E889	G890	A891	D892
F903	H904	R905	K906	K907	P908	M909	L910	N911	A912	A913	E914	G915	A916	D917
F928	H929	R930	K931	K932	P933	M934	L935	N936	A937	A938	E939	G940	A941	D942
F953	H954	R955	K956	K957	P958	M959	L960	N961	A962	A963	E964	G965	A966	D967
F978	H979	R980	K981	K982	P983	M984	L985	N986	A987	A988	E989	G990	A991	D992
F1003	H1004	R1005	K1006	K1007	P1008	M1009	L1010	N1011	A1012	A1013	E1014	G1015	A1016	D1017
F1028	H1029	R1030	K1031	K1032	P1033	M1034	L1035	N1036	A1037	A1038	E1039	G1040	A1041	D1042
F1053	H1054	R1055	K1056	K1057	P1058	M1059	L1060	N1061	A1062	A1063	E1064	G1065	A1066	D1067
F1078	H1079	R1080	K1081	K1082	P1083	M1084	L1085	N1086	A1087	A1088	E1089	G1090	A1091	D1092
F1103	H1104	R1105	K1106	K1107	P1108	M1109	L1110	N1111	A1112	A1113	E1114	G1115	A1116	D1117
F1128	H1129	R1130	K1131	K1132	P1133	M1134	L1135	N1136	A1137	A1138	E1139	G1140	A1141	D1142
F1153	H1154	R1155	K1156	K1157	P1158	M1159	L1160	N1161	A1162	A1163	E1164	G1165	A1166	D1167
F1178	H1179	R1180	K1181	K1182	P1183	M1184	L1185	N1186	A1187	A1188	E1189	G1190	A1191	D1192
F1203	H1204	R1205	K1206	K1207	P1208	M1209	L1210	N1211	A1212	A1213	E1214	G1215	A1216	D1217
F1228	H1229	R1230	K1231	K1232	P1233	M1234	L1235	N1236	A1237	A1238	E1239	G1240	A1241	D1242
F1253	H1254	R1255	K1256	K1257	P1258	M1259	L1260	N1261	A1262	A1263	E1264	G1265	A1266	D1267
F1278	H1279	R1280	K1281	K1282	P1283	M1284	L1285	N1286	A1287	A1288	E1289	G1290	A1291	D1292
F1303	H1304	R1305	K1306	K1307	P1308	M1309	L1310	N1311	A1312	A1313	E1314	G1315	A1316	D1317
F1328	H1329	R1330	K1331	K1332	P1333	M1334	L1335	N1336	A1337	A1338	E1339	G1340	A1341	D1342
F1353	H1354	R1355	K1356	K1357	P1358	M1359	L1360	N1361	A1362	A1363	E1364	G1365	A1366	D1367
F1378	H1379	R1380	K1381	K1382	P1383	M1384	L1385	N1386	A1387	A1388	E1389	G1390	A1391	D1392
F1403	H1404	R1405	K1406	K1407	P1408	M1409	L1410	N1411	A1412	A1413	E1414	G1415	A1416	D1417
F1428	H1429	R1430	K1431	K1432	P1433	M1434	L1435	N1436	A1437	A1438	E1439	G1440	A1441	D1442
F1453	H1454	R1455	K1456	K1457	P1458	M1459	L1460	N1461	A1462	A1463	E1464	G1465	A1466	D1467
F1478	H1479	R1480	K1481	K1482	P1483	M1484	L1485	N1486	A1487	A1488	E1489	G1490	A1491	D1492
F1503	H1504	R1505	K1506	K1507	P1508	M1509	L1510	N1511	A1512	A1513	E1514	G1515	A1516	D1517
F1528	H1529	R1530	K1531	K1532	P1533	M1534	L1535	N1536	A1537	A1538	E1539	G1540	A1541	D1542
F1553	H1554	R1555	K1556	K1557	P1558	M1559	L1560	N1561	A1562	A1563	E1564	G1565	A1566	D1567
F1578	H1579	R1580	K1581	K1582	P1583	M1584	L1585	N1586	A1587	A1588	E1589	G1590	A1591	D1592
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F1628	H1629	R1630	K1631	K1632	P1633	M1634	L1635	N1636	A1637	A1638	E1639	G1640	A1641	D1642
F1653	H1654	R1655	K1656	K1657	P1658	M1659	L1660	N1661	A1662	A1663	E1664	G1665	A1666	D1667
F1678	H1679	R1680	K1681	K1682	P1683	M1684	L1685	N1686	A1687	A1688	E1689	G1690	A1691	D1692
F1703	H1704	R1705	K1706	K1707	P1708	M1709	L1710	N1711	A1712	A1713	E1714	G1715	A1716	D1717
F1728	H1729	R1730	K1731	K1732	P1733	M1734	L1735	N1736	A1737	A1738	E1739	G1740	A1741	D1742
F1753	H1754	R1755	K1756	K1757	P1758	M1759	L1760	N1761	A1762	A1763	E1764	G1765	A1766	D1767
F1778	H1779	R1780	K1781	K1782	P1783	M1784	L1785	N1786	A1787	A1788	E1789	G1790	A1791	D1792
F1803	H1804	R1805	K1806	K1807	P1808	M1809	L1810	N1811	A1812	A1813	E1814	G1815	A1816	D1817
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F1853	H1854	R1855	K1856	K1857	P1858	M1859	L1860	N1861	A1862	A1863	E1864	G1865	A1866	D1867
F1878	H1879	R1880	K1881	K1882	P1883	M1884	L1885	N1886	A1887	A1888	E1889	G1890	A1891	D1892
F1903	H1904	R1905	K1906	K1907	P1908	M1909	L1910	N1911	A1912	A1913	E1914	G1915	A1916	D1917
F1928	H1929	R1930	K1931	K1932	P1933	M1934	L1935	N1936	A1937	A1938	E1939	G1940	A1941	D1942
F1953	H1954	R1955	K1956	K1957	P1958	M1959	L1960	N1961	A1962	A1963	E1964	G1965	A1966	D1967
F1978	H1979	R1980	K1981	K1982	P1983	M1984	L1985	N1986	A1987	A1988	E1989	G1990	A1991	D1992
F2003	H2004	R2005	K2006	K2007	P2008	M2009	L2010	N2011	A2012	A2013	E2014	G2015	A2016	D2017
F2028	H2029	R2030	K2031	K2032	P2033	M2034	L2035	N2036	A2037	A2038	E2039	G2040	A2041	D2042
F2053	H2054	R2055	K2056	K2057	P2058	M2059	L2060	N2061	A2062	A2063	E2064	G2065	A2066	D2067
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F2128	H2129	R2130	K2131	K2132	P2133	M2134	L2135	N2136	A2137	A2138	E2139	G2140	A2141	D2142
F2153	H2154	R2155	K2156	K2157	P2158	M2159	L2160	N2161	A2162	A2163	E2164	G2165	A2166	D2167
F2178	H2179	R2180	K2181	K2182	P2183	M2184	L2185	N2186	A2187	A2188	E2189	G2190	A2191	D2192
F2203	H2204	R2205	K2206	K2207	P2208	M2209	L2210	N2211	A2212	A2213	E2214	G2215	A2216	D2217
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F2378	H2379	R2380	K2381	K2382	P2383	M2384	L2385	N2386	A2387	A2388	E2389	G2390	A2391	D2392
F2403	H2404	R2405	K2406	K2407	P2408	M2409	L2410	N2411	A2412	A2413	E2414	G2415	A2416	D2417
F2428	H2429	R2430	K2431	K2432	P2433	M2434	L2435	N2436	A2437	A2438	E2439	G2440	A2441	D2442
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F2503	H2504	R2505	K2506	K2507	P2508	M2509	L2510	N2511	A2512	A2513	E2514	G2515	A2516	D2517
F2528	H2529	R2530	K2531	K2532	P2533	M2534	L2535	N2536	A2537	A2538	E2539	G2540	A2541	D2542
F2553	H2554	R2555	K2556	K2557	P2558	M2559	L2560	N2561	A2562	A2563	E2564	G2565	A2566	D2567
F2578	H2579	R2580	K2581	K2582	P2583	M2584	L2585	N2586	A2587	A2588	E25			

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	189.49Å 72.76Å 207.10Å 90.00° 112.46° 90.00°	Depositor
Resolution (Å)	47.85 – 3.30 47.85 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.85-3.30) 98.5 (47.85-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.247 , 0.295 0.251 , 0.298	Depositor DCC
R_{free} test set	3056 reflections (7.68%)	wwPDB-VP
Wilson B-factor (Å ²)	120.3	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 107.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8592	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.21	0/4399	0.48	0/5934
1	B	0.21	0/4403	0.47	0/5939
All	All	0.21	0/8802	0.48	0/11873

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4294	0	4203	139	0
1	B	4298	0	4204	152	0
All	All	8592	0	8407	281	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 17.

All (281) 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:561:ILE:N	1:B:564:ARG:HD3	1.62	1.13
1:B:561:ILE:H	1:B:564:ARG:HD3	0.93	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ILE:HG22	1:B:402:GLY:H	1.36	0.88
1:A:400:ILE:HG22	1:A:402:GLY:H	1.48	0.79
1:B:417:LYS:NZ	1:B:448:CYS:SG	2.58	0.76
1:B:552:ASP:OD1	1:B:571:LYS:NZ	2.18	0.75
1:B:221:ARG:NH1	1:B:258:LEU:O	2.18	0.75
1:B:329:ARG:NH1	1:B:361:GLU:OE2	2.20	0.75
1:A:446:GLU:OE1	1:A:459:ARG:NH1	2.20	0.74
1:A:329:ARG:NH2	1:A:361:GLU:OE2	2.21	0.74
1:A:456:ARG:NH2	1:A:478:ASP:OD1	2.21	0.73
1:A:555:ILE:O	1:A:564:ARG:NH2	2.21	0.73
1:A:577:ASP:O	1:B:464:ARG:NH1	2.22	0.73
1:A:117:ASP:OD1	1:A:152:ARG:NH1	2.22	0.73
1:A:329:ARG:HH22	1:A:369:ARG:HE	1.36	0.72
1:B:514:LEU:O	1:B:518:ILE:HG12	1.91	0.71
1:A:187:ARG:NH1	1:A:214:GLU:OE2	2.21	0.71
1:B:456:ARG:NH1	1:B:475:LEU:O	2.24	0.70
1:A:296:ASP:HB3	1:A:299:LYS:HB2	1.73	0.70
1:A:352:LYS:O	1:A:356:GLU:HG2	1.91	0.70
1:A:514:LEU:O	1:A:518:ILE:HG12	1.91	0.70
1:B:183:ASN:O	1:B:187:ARG:HG3	1.92	0.70
1:B:258:LEU:HB3	1:B:262:GLN:HB2	1.73	0.69
1:A:543:ASN:HA	1:A:546:ASN:HB2	1.75	0.69
1:B:561:ILE:N	1:B:564:ARG:CD	2.49	0.69
1:A:446:GLU:OE1	1:A:456:ARG:NH1	2.26	0.69
1:A:536:TYR:O	1:B:502:LYS:NZ	2.19	0.68
1:A:325:GLU:HA	1:A:328:LYS:HE2	1.76	0.67
1:A:461:SER:HB2	1:A:465:ARG:HH12	1.59	0.67
1:B:456:ARG:NH2	1:B:478:ASP:OD2	2.19	0.66
1:A:561:ILE:HG22	1:A:563:MET:H	1.60	0.65
1:B:252:ASN:O	1:B:308:ARG:NH2	2.24	0.65
1:A:93:PHE:HA	1:A:96:TRP:HD1	1.62	0.65
1:A:201:PHE:CD2	1:A:333:GLU:HG2	2.32	0.65
1:B:187:ARG:NH1	1:B:214:GLU:OE1	2.27	0.64
1:B:227:TYR:CD1	1:B:245:PHE:HB2	2.32	0.64
1:A:127:TYR:HA	1:A:130:TRP:HD1	1.61	0.64
1:A:107:ASN:OD1	1:A:140:HIS:NE2	2.22	0.64
1:A:258:LEU:HB3	1:A:262:GLN:HB2	1.80	0.64
1:A:440:ILE:HD12	1:A:443:ARG:HH21	1.61	0.64
1:B:346:LEU:HD12	1:B:381:CYS:HB3	1.80	0.64
1:B:511:ARG:NH2	1:B:543:ASN:OD1	2.31	0.64
1:A:252:ASN:O	1:A:308:ARG:NH2	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:TYR:HA	1:B:130:TRP:HD1	1.64	0.63
1:A:518:ILE:O	1:A:522:LYS:N	2.32	0.63
1:A:539:ASP:OD1	1:A:540:LEU:N	2.32	0.63
1:B:329:ARG:HH12	1:B:369:ARG:HD3	1.64	0.62
1:B:358:LEU:HD21	1:B:374:PHE:CE1	2.34	0.62
1:A:208:GLU:HG3	1:A:244:ARG:HH12	1.64	0.61
1:A:538:CYS:HB3	1:A:543:ASN:ND2	2.15	0.61
1:B:437:GLU:O	1:B:441:ILE:HG13	2.01	0.60
1:A:169:ASN:O	1:A:173:GLU:HG3	2.01	0.60
1:A:403:VAL:O	1:A:406:VAL:HG22	2.01	0.59
1:A:462:LEU:HD12	1:A:465:ARG:HH21	1.67	0.59
1:A:367:HIS:HE1	1:A:395:MET:HE1	1.66	0.59
1:B:204:ASP:OD1	1:B:235:THR:HB	2.01	0.59
1:B:538:CYS:HB3	1:B:543:ASN:HD22	1.67	0.59
1:B:518:ILE:HD12	1:B:528:TYR:CE1	2.37	0.59
1:A:538:CYS:HB3	1:A:543:ASN:HD22	1.67	0.59
1:B:561:ILE:HG22	1:B:563:MET:H	1.67	0.59
1:A:100:LEU:HA	1:A:103:VAL:HG12	1.84	0.59
1:A:131:LYS:NZ	1:A:135:ASP:OD2	2.35	0.58
1:A:207:TRP:CD1	1:A:230:ILE:HD13	2.39	0.58
1:A:329:ARG:NH2	1:A:369:ARG:HE	2.00	0.58
1:B:267:ARG:HA	1:B:270:LEU:HD12	1.84	0.58
1:B:401:GLU:O	1:B:404:ARG:HB3	2.04	0.57
1:A:93:PHE:CG	1:A:343:VAL:HG11	2.39	0.57
1:B:208:GLU:CG	1:B:244:ARG:HH12	2.17	0.57
1:B:532:LEU:HD11	1:B:551:PHE:CZ	2.39	0.57
1:B:539:ASP:OD1	1:B:540:LEU:N	2.36	0.57
1:B:107:ASN:OD1	1:B:140:HIS:NE2	2.29	0.57
1:B:484:LYS:N	1:B:488:GLU:OE2	2.32	0.57
1:A:159:LEU:HA	1:A:197:ALA:HB2	1.85	0.57
1:A:375:GLU:OE2	1:A:409:ARG:NH1	2.34	0.56
1:A:511:ARG:NH1	1:A:535:GLU:OE2	2.38	0.56
1:B:136:LEU:HD12	1:B:139:ARG:HE	1.71	0.56
1:B:259:THR:O	1:B:262:GLN:N	2.39	0.56
1:B:119:PHE:CE1	1:B:123:TYR:HB2	2.41	0.56
1:A:175:LEU:O	1:A:177:PRO:HD3	2.06	0.56
1:B:91:GLN:N	1:B:91:GLN:OE1	2.39	0.56
1:B:457:LEU:O	1:B:461:SER:OG	2.20	0.56
1:A:538:CYS:SG	1:A:539:ASP:N	2.79	0.55
1:B:131:LYS:NZ	1:B:135:ASP:OD2	2.39	0.55
1:B:348:LYS:HA	1:B:351:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LYS:O	1:A:88:MET:N	2.39	0.54
1:A:430:GLU:OE1	1:B:582:VAL:HG21	2.06	0.54
1:A:259:THR:O	1:A:262:GLN:N	2.40	0.54
1:B:200:ASP:OD1	1:B:202:ARG:N	2.32	0.54
1:A:119:PHE:CE1	1:A:123:TYR:HB2	2.42	0.54
1:B:375:GLU:OE2	1:B:409:ARG:NH2	2.40	0.54
1:A:267:ARG:HA	1:A:270:LEU:HD12	1.90	0.54
1:A:518:ILE:HD12	1:A:528:TYR:CE1	2.43	0.54
1:B:561:ILE:O	1:B:564:ARG:HG2	2.07	0.54
1:B:329:ARG:NH1	1:B:369:ARG:HD3	2.22	0.53
1:B:100:LEU:HA	1:B:103:VAL:HG22	1.89	0.53
1:B:518:ILE:O	1:B:522:LYS:N	2.41	0.53
1:A:204:ASP:OD1	1:A:235:THR:HB	2.07	0.53
1:A:554:ALA:HB1	1:A:567:PHE:CD2	2.43	0.53
1:B:128:GLY:O	1:B:132:LYS:HG3	2.08	0.53
1:A:227:TYR:CD2	1:A:245:PHE:HB2	2.43	0.53
1:A:348:LYS:HA	1:A:351:LEU:HD12	1.90	0.53
1:B:358:LEU:HD11	1:B:374:PHE:CG	2.43	0.53
1:B:174:THR:O	1:B:174:THR:OG1	2.27	0.52
1:A:559:LEU:HB3	1:A:561:ILE:HG13	1.91	0.52
1:B:359:GLU:OE2	1:B:390:LYS:NZ	2.39	0.52
1:A:154:LEU:HD22	1:A:164:TRP:CE2	2.43	0.52
1:B:131:LYS:HE3	1:B:166:HIS:ND1	2.25	0.52
1:A:346:LEU:HD12	1:A:381:CYS:HB3	1.92	0.52
1:A:479:ALA:HB1	1:A:492:TYR:CD2	2.44	0.52
1:A:484:LYS:N	1:A:488:GLU:OE1	2.36	0.52
1:A:392:ALA:O	1:A:396:GLU:HG3	2.10	0.52
1:A:464:ARG:NE	1:B:577:ASP:O	2.43	0.52
1:B:93:PHE:HA	1:B:96:TRP:HD1	1.75	0.52
1:B:179:ASP:OD1	1:B:181:GLU:N	2.36	0.52
1:B:207:TRP:CD1	1:B:230:ILE:HD13	2.45	0.52
1:B:446:GLU:HG3	1:B:451:GLY:HA2	1.92	0.52
1:B:392:ALA:O	1:B:396:GLU:HG3	2.10	0.51
1:A:91:GLN:N	1:A:91:GLN:OE1	2.43	0.51
1:B:511:ARG:NH2	1:B:535:GLU:OE2	2.40	0.51
1:A:125:TYR:CD2	1:A:379:ILE:HA	2.45	0.51
1:A:437:GLU:O	1:A:441:ILE:HG12	2.10	0.51
1:B:462:LEU:HD12	1:B:463:GLU:HG2	1.93	0.51
1:A:208:GLU:OE2	1:A:244:ARG:NH2	2.43	0.51
1:A:179:ASP:OD1	1:A:181:GLU:N	2.28	0.51
1:B:564:ARG:HG2	1:B:565:ILE:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:TYR:CD2	1:B:379:ILE:HA	2.46	0.51
1:B:374:PHE:O	1:B:378:VAL:HG23	2.12	0.50
1:A:355:LYS:O	1:A:359:GLU:HG3	2.11	0.50
1:B:267:ARG:NE	1:B:303:GLU:OE2	2.39	0.50
1:B:358:LEU:HD11	1:B:374:PHE:CD2	2.46	0.50
1:B:419:PRO:HA	1:B:445:PHE:HE2	1.74	0.50
1:A:464:ARG:NH1	1:A:499:HIS:HD2	2.10	0.50
1:B:93:PHE:CG	1:B:343:VAL:HG21	2.47	0.50
1:A:521:ASP:OD1	1:A:524:ASN:N	2.43	0.50
1:B:159:LEU:HA	1:B:197:ALA:HB2	1.93	0.50
1:B:208:GLU:HG3	1:B:244:ARG:HH12	1.76	0.50
1:B:521:ASP:CG	1:B:524:ASN:HD22	2.20	0.50
1:B:359:GLU:HA	1:B:362:ILE:HD12	1.94	0.49
1:B:398:HIS:O	1:B:400:ILE:HG13	2.12	0.49
1:B:154:LEU:HD22	1:B:164:TRP:CE2	2.46	0.49
1:B:561:ILE:O	1:B:564:ARG:CG	2.60	0.49
1:B:597:LYS:O	1:B:601:THR:HG23	2.13	0.49
1:A:461:SER:HB2	1:A:465:ARG:NH1	2.25	0.49
1:B:260:GLY:O	1:B:264:ILE:HG13	2.13	0.49
1:B:521:ASP:OD1	1:B:524:ASN:N	2.32	0.49
1:A:502:LYS:HE2	1:B:536:TYR:CE1	2.47	0.49
1:A:174:THR:O	1:A:174:THR:OG1	2.28	0.49
1:A:402:GLY:O	1:A:406:VAL:HG13	2.13	0.49
1:B:538:CYS:SG	1:B:539:ASP:N	2.85	0.49
1:A:544:GLU:O	1:A:548:LEU:HG	2.13	0.48
1:B:442:LEU:HD11	1:B:462:LEU:HD21	1.94	0.48
1:B:563:MET:O	1:B:566:THR:OG1	2.25	0.48
1:A:260:GLY:O	1:A:264:ILE:HG13	2.14	0.48
1:A:512:LYS:O	1:A:516:GLU:HG3	2.14	0.48
1:B:382:ALA:O	1:B:388:TRP:NE1	2.45	0.48
1:B:226:VAL:O	1:B:230:ILE:HG22	2.13	0.48
1:B:393:LYS:O	1:B:396:GLU:HB2	2.14	0.48
1:B:518:ILE:HD13	1:B:527:LEU:HD13	1.96	0.48
1:B:446:GLU:OE2	1:B:456:ARG:NE	2.46	0.48
1:B:477:GLN:O	1:B:480:ILE:HG13	2.14	0.48
1:A:419:PRO:O	1:A:423:MET:HG2	2.14	0.47
1:A:507:LEU:N	1:A:508:PRO:HD2	2.29	0.47
1:A:367:HIS:O	1:A:371:VAL:HG23	2.14	0.47
1:A:598:GLU:O	1:A:601:THR:OG1	2.26	0.47
1:A:200:ASP:OD1	1:A:202:ARG:N	2.32	0.47
1:A:361:GLU:HG3	1:A:373:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:SER:HB3	1:B:576:GLU:O	2.14	0.47
1:A:267:ARG:NE	1:A:303:GLU:OE2	2.35	0.47
1:A:131:LYS:HE3	1:A:166:HIS:ND1	2.30	0.47
1:A:226:VAL:O	1:A:230:ILE:HG22	2.14	0.47
1:A:597:LYS:O	1:A:601:THR:HG23	2.14	0.47
1:B:181:GLU:O	1:B:185:THR:HG23	2.15	0.47
1:B:337:LYS:HD2	1:B:350:GLN:NE2	2.29	0.47
1:A:199:THR:HG22	1:A:369:ARG:NH1	2.30	0.47
1:A:199:THR:HG22	1:A:369:ARG:HH11	1.78	0.47
1:B:109:LEU:HD21	1:B:113:ARG:CZ	2.45	0.47
1:B:187:ARG:NH2	1:B:219:ASN:HD22	2.13	0.47
1:A:368:GLU:H	1:A:368:GLU:CD	2.23	0.47
1:A:464:ARG:HH22	1:A:499:HIS:HB2	1.79	0.47
1:A:471:GLU:O	1:A:475:LEU:HG	2.15	0.47
1:B:175:LEU:O	1:B:177:PRO:HD3	2.15	0.47
1:B:346:LEU:CD1	1:B:381:CYS:HB3	2.44	0.47
1:B:446:GLU:OE1	1:B:459:ARG:NH1	2.47	0.47
1:B:269:GLU:OE1	1:B:310:ARG:NH2	2.43	0.46
1:B:143:ILE:O	1:B:146:SER:N	2.48	0.46
1:B:213:TRP:HD1	1:B:214:GLU:HG2	1.79	0.46
1:B:543:ASN:HA	1:B:546:ASN:HB2	1.97	0.46
1:A:478:ASP:HA	1:A:481:LYS:HD2	1.96	0.46
1:B:119:PHE:HE1	1:B:123:TYR:HB2	1.81	0.46
1:B:561:ILE:O	1:B:564:ARG:CD	2.63	0.46
1:A:586:LEU:HD11	1:B:427:ALA:HB1	1.98	0.46
1:A:559:LEU:O	1:A:564:ARG:NE	2.47	0.46
1:A:128:GLY:O	1:A:132:LYS:HG3	2.15	0.46
1:A:374:PHE:O	1:A:378:VAL:HG23	2.16	0.46
1:B:479:ALA:HB1	1:B:492:TYR:CD2	2.51	0.46
1:B:296:ASP:HB3	1:B:299:LYS:HB2	1.97	0.46
1:A:532:LEU:HD11	1:A:551:PHE:CZ	2.50	0.46
1:B:419:PRO:HA	1:B:445:PHE:CE2	2.50	0.46
1:B:507:LEU:N	1:B:508:PRO:HD2	2.31	0.45
1:B:563:MET:O	1:B:567:PHE:HD1	1.99	0.45
1:A:559:LEU:HB2	1:A:564:ARG:HD3	1.97	0.45
1:B:259:THR:O	1:B:260:GLY:C	2.60	0.45
1:B:263:PHE:O	1:B:266:LEU:HB3	2.17	0.45
1:A:208:GLU:CG	1:A:244:ARG:HH12	2.29	0.45
1:A:332:PHE:CD1	1:A:357:TYR:HB2	2.52	0.45
1:A:436:ASN:O	1:A:440:ILE:HG12	2.16	0.45
1:A:338:ARG:NH2	1:A:342:HIS:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:PRO:O	1:B:423:MET:HG2	2.17	0.45
1:B:439:ARG:O	1:B:443:ARG:HG3	2.17	0.45
1:A:578:PHE:CD1	1:B:503:ILE:HD11	2.52	0.45
1:B:442:LEU:CD1	1:B:462:LEU:HD21	2.47	0.45
1:B:120:PHE:HZ	1:B:129:TYR:C	2.24	0.45
1:A:409:ARG:O	1:A:414:HIS:ND1	2.45	0.44
1:B:344:LYS:HD2	1:B:344:LYS:HA	1.82	0.44
1:B:512:LYS:O	1:B:516:GLU:HG3	2.17	0.44
1:A:541:LYS:O	1:A:544:GLU:HB3	2.17	0.44
1:B:221:ARG:HA	1:B:257:LEU:O	2.18	0.44
1:A:404:ARG:NH1	1:A:429:GLU:OE2	2.51	0.44
1:B:338:ARG:NH1	1:B:342:HIS:HB3	2.32	0.44
1:A:259:THR:O	1:A:260:GLY:C	2.60	0.44
1:A:388:TRP:HH2	1:A:414:HIS:CE1	2.36	0.44
1:A:593:GLN:HA	1:A:596:LEU:HD12	2.00	0.44
1:A:574:PHE:CE1	1:A:578:PHE:HD2	2.35	0.43
1:A:351:LEU:HD21	1:A:384:TYR:CE2	2.53	0.43
1:B:263:PHE:CZ	1:B:307:MET:HE1	2.54	0.43
1:A:109:LEU:HD21	1:A:113:ARG:CZ	2.49	0.43
1:A:419:PRO:HA	1:A:445:PHE:CE2	2.53	0.43
1:B:208:GLU:CD	1:B:244:ARG:HH12	2.27	0.43
1:B:471:GLU:O	1:B:475:LEU:HG	2.18	0.43
1:B:408:SER:O	1:B:412:THR:N	2.48	0.43
1:B:560:PRO:C	1:B:564:ARG:HD3	2.38	0.43
1:A:179:ASP:OD1	1:A:180:GLN:N	2.52	0.43
1:B:491:PHE:O	1:B:495:LYS:HG2	2.18	0.43
1:A:435:ILE:HG23	1:A:436:ASN:H	1.84	0.43
1:A:419:PRO:HA	1:A:445:PHE:HE2	1.84	0.43
1:B:158:PRO:HD2	1:B:159:LEU:HD12	2.00	0.43
1:B:174:THR:O	1:B:175:LEU:HG	2.19	0.43
1:A:446:GLU:HG3	1:A:451:GLY:HA2	2.01	0.42
1:B:260:GLY:O	1:B:263:PHE:HB3	2.19	0.42
1:A:205:LYS:O	1:A:209:MET:HB2	2.19	0.42
1:A:351:LEU:HD22	1:A:387:PHE:HE2	1.83	0.42
1:B:116:PHE:HD1	1:B:120:PHE:CE2	2.37	0.42
1:B:298:ALA:O	1:B:302:THR:HG23	2.19	0.42
1:B:191:GLU:OE2	1:B:210:TYR:OH	2.34	0.42
1:B:433:GLY:O	1:B:435:ILE:HG12	2.19	0.42
1:B:445:PHE:CD1	1:B:445:PHE:C	2.98	0.42
1:B:299:LYS:O	1:B:302:THR:OG1	2.30	0.42
1:B:401:GLU:H	1:B:401:GLU:HG2	1.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TYR:CE2	1:A:379:ILE:HA	2.55	0.42
1:A:582:VAL:HG12	1:A:586:LEU:HG	2.01	0.42
1:A:259:THR:O	1:A:261:GLU:N	2.53	0.42
1:B:598:GLU:O	1:B:601:THR:OG1	2.32	0.42
1:A:536:TYR:CE1	1:B:502:LYS:HE3	2.54	0.42
1:A:464:ARG:NH1	1:A:503:ILE:HG13	2.35	0.41
1:B:355:LYS:O	1:B:359:GLU:HG3	2.20	0.41
1:B:458:ARG:HE	1:B:458:ARG:HB2	1.70	0.41
1:B:386:GLU:H	1:B:386:GLU:HG3	1.58	0.41
1:A:225:ALA:O	1:A:229:ARG:HG3	2.20	0.41
1:A:260:GLY:O	1:A:263:PHE:HB3	2.20	0.41
1:B:191:GLU:OE1	1:B:229:ARG:NH1	2.51	0.41
1:A:367:HIS:CE1	1:A:395:MET:HE1	2.52	0.41
1:A:401:GLU:O	1:A:404:ARG:HB3	2.20	0.41
1:B:93:PHE:HD1	1:B:123:TYR:CD2	2.37	0.41
1:A:93:PHE:O	1:A:97:VAL:HG23	2.19	0.41
1:B:243:GLN:O	1:B:247:GLU:HG3	2.20	0.41
1:B:518:ILE:HD12	1:B:528:TYR:HE1	1.86	0.41
1:A:127:TYR:O	1:A:130:TRP:HB2	2.20	0.41
1:A:382:ALA:O	1:A:388:TRP:NE1	2.52	0.41
1:A:536:TYR:O	1:A:536:TYR:HD1	2.04	0.41
1:A:547:ILE:HG21	1:A:574:PHE:CE2	2.56	0.41
1:A:577:ASP:OD1	1:B:495:LYS:HE3	2.21	0.41
1:B:337:LYS:HD2	1:B:350:GLN:HE21	1.86	0.41
1:A:213:TRP:HD1	1:A:214:GLU:HG2	1.86	0.41
1:A:221:ARG:HA	1:A:257:LEU:O	2.21	0.41
1:A:408:SER:O	1:A:412:THR:N	2.50	0.41
1:B:358:LEU:HD21	1:B:374:PHE:CZ	2.56	0.41
1:A:392:ALA:HB1	1:A:403:VAL:HG13	2.03	0.40
1:B:225:ALA:O	1:B:229:ARG:HG3	2.21	0.40
1:B:445:PHE:C	1:B:445:PHE:HD1	2.29	0.40
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.84	0.40
1:B:351:LEU:HD22	1:B:387:PHE:HE2	1.86	0.40

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 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	505/670 (75%)	479 (95%)	22 (4%)	4 (1%)	16	45
1	B	506/670 (76%)	478 (94%)	24 (5%)	4 (1%)	16	45
All	All	1011/1340 (75%)	957 (95%)	46 (4%)	8 (1%)	16	45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	GLY
1	B	260	GLY
1	A	77	PRO
1	B	541	LYS
1	A	541	LYS
1	B	77	PRO
1	A	158	PRO
1	B	158	PRO

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	464/598 (78%)	463 (100%)	1 (0%)	87	88
1	B	464/598 (78%)	464 (100%)	0	100	100
All	All	928/1196 (78%)	927 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	311	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	353	ASN
1	B	183	ASN
1	B	219	ASN
1	B	241	HIS
1	B	350	GLN
1	B	431	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 oligosaccharides 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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	509/670 (75%)	0.61	31 (6%) 27 18	88, 153, 222, 286	0
1	B	510/670 (76%)	0.48	23 (4%) 38 25	86, 151, 209, 307	0
All	All	1019/1340 (76%)	0.55	54 (5%) 32 22	86, 152, 216, 307	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	581	ASP	4.5
1	B	361	GLU	4.4
1	A	528	TYR	4.3
1	A	243	GLN	4.1
1	A	295	THR	4.0
1	B	295	THR	3.9
1	A	145	GLN	3.9
1	A	414	HIS	3.7
1	A	142	ASN	3.4
1	B	142	ASN	3.4
1	A	437	GLU	3.3
1	B	123	TYR	3.1
1	A	247	GLU	3.1
1	B	126	CYS	3.1
1	B	430	GLU	3.0
1	B	243	GLN	2.9
1	A	123	TYR	2.8
1	B	414	HIS	2.7
1	B	259	THR	2.7
1	A	550	CYS	2.6
1	A	435	ILE	2.6
1	B	400	ILE	2.6
1	B	466	HIS	2.6
1	B	238	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	515	LEU	2.5
1	B	581	ASP	2.5
1	A	316	GLN	2.5
1	A	523	GLU	2.5
1	B	347	GLU	2.4
1	A	216	GLU	2.4
1	A	303	GLU	2.4
1	A	350	GLN	2.4
1	A	312	ILE	2.3
1	B	425	TRP	2.3
1	A	400	ILE	2.3
1	B	440	ILE	2.3
1	B	216	GLU	2.3
1	A	238	TYR	2.3
1	A	126	CYS	2.3
1	A	589	TYR	2.2
1	B	246	LYS	2.2
1	A	401	GLU	2.2
1	B	579	GLY	2.2
1	A	239	SER	2.2
1	B	554	ALA	2.2
1	B	83	TRP	2.2
1	A	584	LYS	2.1
1	A	521	ASP	2.1
1	B	541	LYS	2.1
1	A	430	GLU	2.1
1	A	574	PHE	2.1
1	A	219	ASN	2.0
1	A	436	ASN	2.0
1	B	457	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.