



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:48 AM GMT

PDB ID : 3JRO
Title : NUP84-NUP145C-SEC13 edge element of the NPC lattice
Authors : Brohawn, S.G.; Schwartz, T.U.
Deposited on : 2009-09-08
Resolution : 4.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

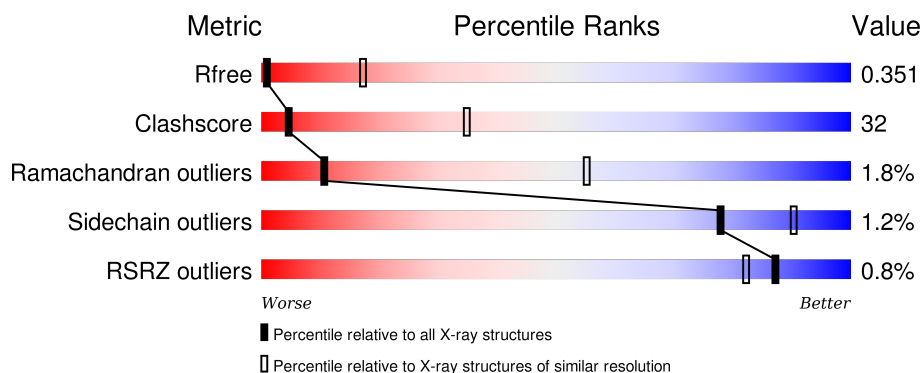
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 4.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	753	
2	C	426	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8671 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 Fusion Protein of Protein Transport Protein SEC13 and Nucleoporin NUP145.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	701	Total	C	N	O	S	Se	0	0	0
			5623	3598	943	1068	9	5			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1100	GLY	-	LINKER	UNP P49687
A	1101	GLY	-	LINKER	UNP P49687
A	1102	GLY	-	LINKER	UNP P49687
A	1103	GLY	-	LINKER	UNP P49687
A	1104	SER	-	LINKER	UNP P49687
A	1105	GLY	-	LINKER	UNP P49687
A	1106	GLY	-	LINKER	UNP P49687
A	1107	GLY	-	LINKER	UNP P49687
A	1108	GLY	-	LINKER	UNP P49687

- Molecule 2 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	379	Total	C	N	O	S	Se	0	0	0
			3048	1949	504	584	4	7			

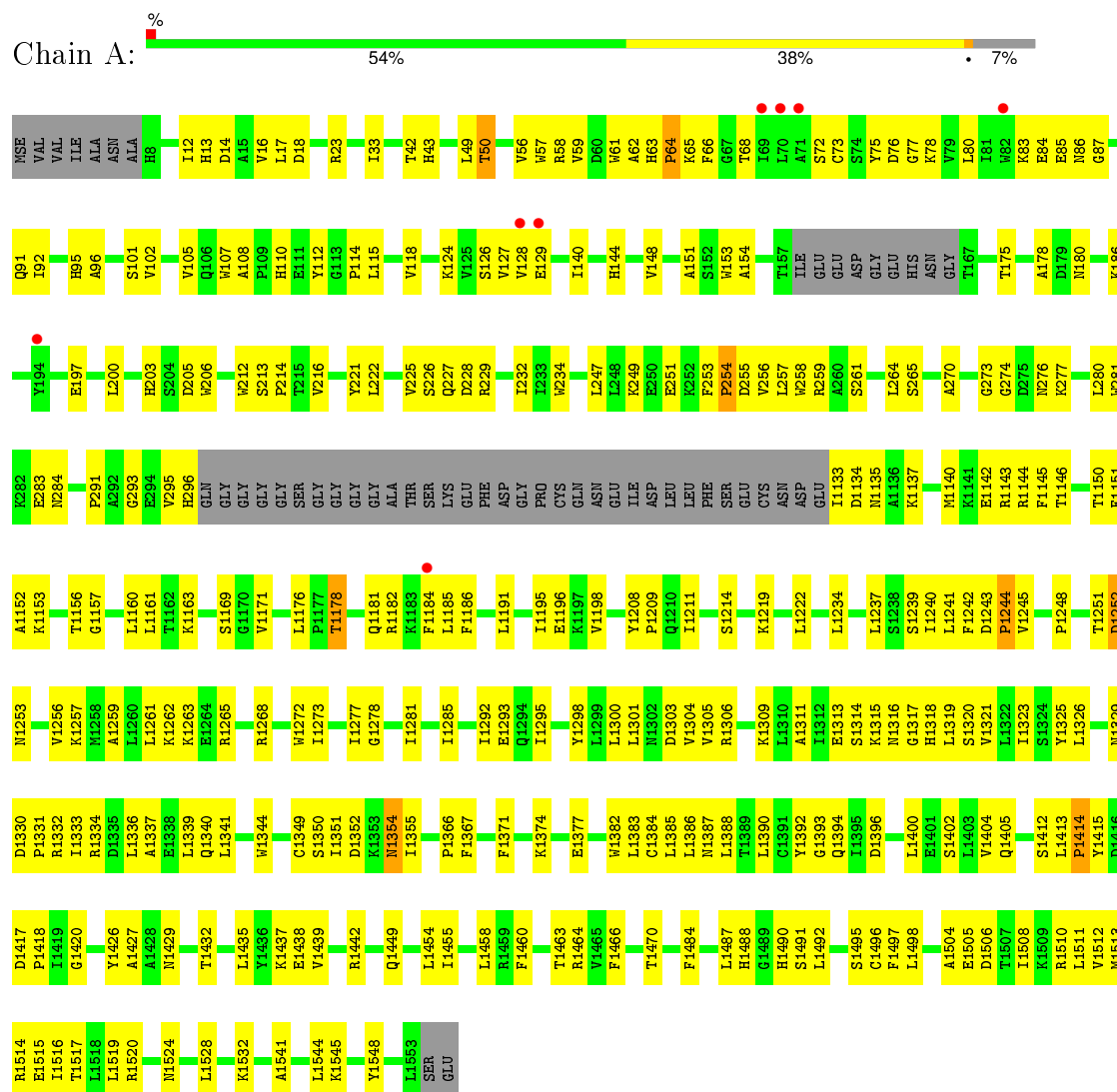
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP P52891
C	0	SER	-	EXPRESSION TAG	UNP P52891

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 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: Fusion Protein of Protein Transport Protein SEC13 and Nucleoporin NUP145



- Molecule 2: Nucleoporin NUP84



K421	R344	V345	P347	I351	L355	P356	I359	H360	V363	V370	LYS	GLY	THR	GLU	ALA	SER	ASN	ASP	ILE	ILE	D381	R387	I388	V389	H390	I391	A392	A393	I394	C395	L396	D397	I398	I399	M400	P401	V404	E405	E406	V407	D408	K411	L412	L413	T414	T415	Y416	L417	S418	L419	L420	R421	S422	L423	V424	P425	S426	E427	H428	I429	P430	L431	S432	E433	H434	P435	S436	E437	H438	I439	P440	S441	E442	H443	P444	S445	E446	H447	P448	S449	E450	H451	P452	S453	E454	H455	P456	S457	E458	H459	P460	S461	E462	H463	P464	S465	E466	H467	P468	S469	E470	H471	P472	S473	E474	H475	P476	S477	E478	H479	P480	S481	E482	H483	P484	S485	E486	H487	P488	S489	E490	H491	P492	S493	E494	H495	P496	S497	E498	H499	P500	S501	E502	H503	P504	S505	E506	H507	P508	S509	E510	H511	P512	S513	E514	H515	P516	S517	E518	H519	P520	S521	E522	H523	P524	S525	E526	H527	P528	S529	E530	H531	P532	S533	E534	H535	P536	S537	E538	H539	P540	S541	E542	H543	P544	S545	E546	H547	P548	S549	E550	H551	P552	S553	E554	H555	P556	S557	E558	H559	P560	S561	E562	H563	P564	S565	E566	H567	P568	S569	E570	H571	P572	S573	E574	H575	P576	S577	E578	H579	P580	S581	E582	H583	P584	S585	E586	H587	P588	S589	E590	H591	P592	S593	E594	H595	P596	S597	E598	H599	P600	S601	E602	H603	P604	S605	E606	H607	P608	S609	E610	H611	P612	S613	E614	H615	P616	S617	E618	H619	P620	S621	E622	H623	P624	S625	E626	H627	P628	S629	E630	H631	P632	S633	E634	H635	P636	S637	E638	H639	P640	S641	E642	H643	P644	S645	E646	H647	P648	S649	E650	H651	P652	S653	E654	H655	P656	S657	E658	H659	P660	S661	E662	H663	P664	S665	E666	H667	P668	S669	E670	H671	P672	S673	E674	H675	P676	S677	E678	H679	P680	S681	E682	H683	P684	S685	E686	H687	P688	S689	E690	H691	P692	S693	E694	H695	P696	S697	E698	H699	P700	S701	E702	H703	P704	S705	E706	H707	P708	S709	E710	H711	P712	S713	E714	H715	P716	S717	E718	H719	P720	S721	E722	H723	P724	S725	E726	H727	P728	S729	E730	H731	P732	S733	E734	H735	P736	S737	E738	H739	P740	S741	E742	H743	P744	S745	E746	H747	P748	S749	E750	H751	P752	S753	E754	H755	P756	S757	E758	H759	P760	S761	E762	H763	P764	S765	E766	H767	P768	S769	E770	H771	P772	S773	E774	H775	P776	S777	E778	H779	P780	S781	E782	H783	P784	S785	E786	H787	P788	S789	E790	H791	P792	S793	E794	H795	P796	S797	E798	H799	P800	S801	E802	H803	P804	S805	E806	H807	P808	S809	E810	H811	P812	S813	E814	H815	P816	S817	E818	H819	P820	S821	E822	H823	P824	S825	E826	H827	P828	S829	E830	H831	P832	S833	E834	H835	P836	S837	E838	H839	P840	S841	E842	H843	P844	S845	E846	H847	P848	S849	E850	H851	P852	S853	E854	H855	P856	S857	E858	H859	P860	S861	E862	H863	P864	S865	E866	H867	P868	S869	E870	H871	P872	S873	E874	H875	P876	S877	E878	H879	P880	S881	E882	H883	P884	S885	E886	H887	P888	S889	E890	H891	P892	S893	E894	H895	P896	S897	E898	H899	P900	S901	E902	H903	P904	S905	E906	H907	P908	S909	E910	H911	P912	S913	E914	H915	P916	S917	E918	H919	P920	S921	E922	H923	P924	S925	E926	H927	P928	S929	E930	H931	P932	S933	E934	H935	P936	S937	E938	H939	P940	S941	E942	H943	P944	S945	E946	H947	P948	S949	E950	H951	P952	S953	E954	H955	P956	S957	E958	H959	P960	S961	E962	H963	P964	S965	E966	H967	P968	S969	E970	H971	P972	S973	E974	H975	P976	S977	E978	H979	P980	S981	E982	H983	P984	S985	E986	H987	P988	S989	E990	H991	P992	S993	E994	H995	P996	S997	E998	H999	P1000	S1001	E1002	H1003	P1004	S1005	E1006	H1007	P1008	S1009	E1010	H1011	P1012	S1013	E1014	H1015	P1016	S1017	E1018	H1019	P1020	S1021	E1022	H1023	P1024	S1025	E1026	H1027	P1028	S1029	E1030	H1031	P1032	S1033	E1034	H1035	P1036	S1037	E1038	H1039	P1040	S1041	E1042	H1043	P1044	S1045	E1046	H1047	P1048	S1049	E1050	H1051	P1052	S1053	E1054	H1055	P1056	S1057	E1058	H1059	P1060	S1061	E1062	H1063	P1064	S1065	E1066	H1067	P1068	S1069	E1070	H1071	P1072	S1073	E1074	H1075	P1076	S1077	E1078	H1079	P1080	S1081	E1082	H1083	P1084	S1085	E1086	H1087	P1088	S1089	E1090	H1091	P1092	S1093	E1094	H1095	P1096	S1097	E1098	H1099	P1100	S1101	E1102	H1103	P1104	S1105	E1106	H1107	P1108	S1109	E1110	H1111	P1112	S1113	E1114	H1115	P1116	S1117	E1118	H1119	P1120	S1121	E1122	H1123	P1124	S1125	E1126	H1127	P1128	S1129	E1130	H1131	P1132	S1133	E1134	H1135	P1136	S1137	E1138	H1139	P1140	S1141	E1142	H1143	P1144	S1145	E1146	H1147	P1148	S1149	E1150	H1151	P1152	S1153	E1154	H1155	P1156	S1157	E1158	H1159	P1160	S1161	E1162	H1163	P1164	S1165	E1166	H1167	P1168	S1169	E1170	H1171	P1172	S1173	E1174	H1175	P1176	S1177	E1178	H1179	P1180	S1181	E1182	H1183	P1184	S1185	E1186	H1187	P1188	S1189	E1190	H1191	P1192	S1193	E1194	H1195	P1196	S1197	E1198	H1199	P1200	S1201	E1202	H1203	P1204	S1205	E1206	H1207	P1208	S1209	E1210	H1211	P1212	S1213	E1214	H1215	P1216	S1217	E1218	H1219	P1220	S1221	E1222	H1223	P1224	S1225	E1226	H1227	P1228	S1229	E1230	H1231	P1232	S1233	E1234	H1235	P1236	S1237	E1238	H1239	P1240	S1241	E1242	H1243	P1244	S1245	E1246	H1247	P1248	S1249	E1250	H1251	P1252	S1253	E1254	H1255	P1256	S1257	E1258	H1259	P1260	S1261	E1262	H1263	P1264	S1265	E1266	H1267	P1268	S1269	E1270	H1271	P1272	S1273	E1274	H1275	P1276	S1277	E1278	H1279	P1280	S1281	E1282	H1283	P1284	S1285	E1286	H1287	P1288	S1289	E1290	H1291	P1292	S1293	E1294	H1295	P1296	S1297	E1298	H1299	P1300	S1301	E1302	H1303	P1304	S1305	E1306	H1307	P1308	S1309	E1310	H1311	P1312	S1313	E1314	H1315	P1316	S1317	E1318	H1319	P1320	S1321	E1322	H1323	P1324	S1325	E1326	H1327	P1328	S1329	E1330	H1331	P1332	S1333	E1334	H1335	P1336	S1337	E1338	H1339	P1340	S1341	E1342	H1343	P1344	S1345	E1346	H1347	P1348	S1349	E1350	H1351	P1352	S1353	E1354	H1355	P1356	S1357	E1358	H1359	P1360	S1361	E1362	H1363	P1364	S1365	E1366	H1367	P1368	S1369	E1370	H1371	P1372	S1373	E1374	H1375	P1376	S1377	E1378	H1379	P1380	S1381	E1382	H1383	P1384	S1385	E1386	H1387	P1388	S1389	E1390	H1391	P1392	S1393	E1394	H1395	P1396	S1397	E1398	H1399	P1400	S1401	E1402	H1403	P1404	S1405	E1406	H1407	P1408	S1409	E1410	H1411	P1412	S1413	E1414	H1415	P1416	S1417	E1418	H1419	P1420	S1421	E1422	H1423	P1424	S1425	E1426	H1427	P1428	S1429	E1430	H1431	P1432	S1433	E1434	H1435	P1436	S1437	E1438	H1439	P1440	S1441	E1442	H1443	P1444	S1445	E1446	H1447	P1448	S1449	E1450	H1451	P1452	S1453	E1454	H1455	P1456	S1457	E1458	H1459	P1460	S1461	E1462	H1463	P1464	S1465	E1466	H1467	P1468	S1469	E1470	H1471	P1472	S1473	E1474	H1475	P1476	S1477	E1478	H1479	P1480	S1481	E1482	H1483	P1484	S1485	E1486	H1487	P1488	S1489	E1490	H1491	P1492	S1493	E1494	H1495	P1496	S1497	E1498	H1499	P1500	S1501	E1502	H1503	P1504	S1505	E1506	H1507	P1508	S1509	E1510	H1511	P1512	S1513	E1514	H1515	P1516	S1517	E1518	H1519	P1520	S1521	E1522	H1523	P1524	S1525	E1526	H1527	P1528	S1529	E1530	H1531	P1532	S1533	E1534	H1535	P1536	S1537	E1538	H1539	P1540	S1541	E1542	H1543	P1544	S1545	E1546	H1547	P1548	S1549	E1550	H1551	P1552	S1553	E1554	H1555	P1556	S1557	E1558	H1559	P1560	S1561	E1562	H1563	P1564	S1565	E1566	H1567	P1568	S1569	E1570	H1571	P1572	S1573	E1574	H1575	P1576	S1577	E1578	H1579	P1580	S1581	E1582	H1583	P1584	S1585	E1586	H1587	P1588	S1589	E1590	H1591	P1592	S1593	E1594	H1595	P1596	S1597	E1598	H1599	P1600	S1601	E1602	H1603	P1604	S1605	E1606	H1607	P1608	S1609	E1610	H1611	P1612	S1613	E1614	H1615	P1616	S1617	E1618	H1619	P1620	S1621	E1622	H1623	P1624	S1625	E1626	H1627	P1628	S1629	E1630	H1631	P1632	S1633	E1634	H1635	P1636	S1637	E1638	H1639	P1640	S1641	E1642	H1643	P1644	S1645	E1646	H1647	P1648	S1649	E1650	H1651	P1652	S1653	E1654	H1655	P1656	S1657	E1658	H1659	P1660	S1661	E1662	H1663	P1664	S1665	E1666	H1667	P1668	S1669	E1670	H1671	P1672	S1673	E1674	H1675	P1676	S1677	E1678	H1679	P1680	S1681	E1682	H1683	P1684	S1685	E1686	H1687	P1688	S1689	E1690	H1691	P1692	S1693	E1694	H1695	P1696	S1697	E1698	H1699	P1700	S1701	E1702	H1703	P1704	S1705	E1706	H1707	P1708	S1709	E1710	H1711	P1712	S1713	E1714	H1715	P1716	S1717	E1718	H1719	P1720	S1721	E1722	H1723	P1724	S1725	E1726	H1727	P1728	S1729	E1730	H1731	P1732	S1733	E1734	H1735	P1736	S1737	E1738	H1739	P1740	S1741	E1742	H1743	P1744	S1745	E1746	H1747	P1748	S1749	E1750	H1751	P1752	S1753	E1754	H1755	P1756	S1757	E1758	H1759	P1760	S1761	E1762	H1763	P1764	S1765	E1766	H1767	P1768	S1769	E1770	H1771	P1772	S1773	E1774	H1775	P1776	S1777	E1778	H1779	P1780	S1781	E1782	H1783	P1784	S1785	E1786	H1787	P1788	S1789	E1790	H1791	P1792	S1793	E1794	H1795	P1796	S1797	E1798	H1799	P1800	S1
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4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.47Å 170.47Å 270.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.89 – 4.00 49.89 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.89-4.00) 99.9 (49.89-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.282 , 0.329 0.292 , 0.351	Depositor DCC
R_{free} test set	1586 reflections (8.50%)	DCC
Wilson B-factor (Å ²)	133.7	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 124.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 20246 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8671	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.24	0/5744	0.41	0/7776
2	C	0.28	0/3101	0.49	0/4202
All	All	0.25	0/8845	0.44	0/11978

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	5623	0	5577	286	0
2	C	3048	0	3033	306	0
All	All	8671	0	8610	555	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 32.

The worst 5 of 555 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:C:104:LEU:HA	2:C:219:LEU:HD12	1.19	1.09
2:C:215:ILE:HG21	2:C:267:LEU:HD13	1.31	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:HIS:HB2	2:C:160:PHE:HB2	1.44	0.99
2:C:412:LEU:HB3	2:C:416:TYR:HE2	1.32	0.94
1:A:1251:THR:H	1:A:1257:LYS:HE2	1.35	0.91

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	695/753 (92%)	608 (88%)	78 (11%)	9 (1%)	15	60
2	C	373/426 (88%)	297 (80%)	66 (18%)	10 (3%)	6	47
All	All	1068/1179 (91%)	905 (85%)	144 (14%)	19 (2%)	11	55

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	218	TYR
2	C	281	ASP
2	C	55	ASN
2	C	171	VAL
2	C	222	VAL

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	621/655 (95%)	618 (100%)	3 (0%)	92	96
2	C	345/384 (90%)	336 (97%)	9 (3%)	54	81
All	All	966/1039 (93%)	954 (99%)	12 (1%)	78	90

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	163	ARG
2	C	170	ASP
2	C	301	TYR
2	C	99	TYR
2	C	280	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	234	GLN
2	C	360	HIS
2	C	273	ASN
2	C	118	GLN
2	C	240	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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	696/753 (92%)	-0.19	8 (1%)	82 75	159, 188, 244, 325	0
2	C	372/426 (87%)	-0.34	1 (0%)	94 92	134, 171, 248, 370	0
All	All	1068/1179 (90%)	-0.24	9 (0%)	87 82	134, 183, 246, 370	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	LEU	3.2
1	A	71	ALA	2.9
1	A	194	TYR	2.9
1	A	82	TRP	2.8
1	A	69	ILE	2.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.