

Dec 14, 2023 – 02:42 PM JST

PDB ID	:	8JB5
EMDB ID	:	EMD-36141
Title	:	The cryo-EM structure of Paeniclostridium sordellii lethal toxin (TcsL)
Authors	:	Zhan, X.; Tao, L.
Deposited on	:	2023-05-08
Resolution	:	2.90 Å(reported)

This is a Full wwPDB EM Validation 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/EMValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

:	0.0.1.dev70
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.36
	: : : : :

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 2.90 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	$egin{array}{c} { m Whole \ archive}\ (\#{ m Entries}) \end{array}$	$\mathop{{ m EM}}_{{ m (\#Entries)}}$				
Clashscore	158937	4297				
Ramachandran outliers	154571	4023				
Sidechain outliers	154315	3826				

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain					
			31%					
1	А	2372	70%	27%	••			



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19027 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 Cytotoxin-L.

Mol	Chain	Residues		At	AltConf	Trace			
1	А	2355	Total 19026	C 12183	N 3022	0 3774	S 47	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	2365	HIS	-	expression tag	UNP T0D3N5
А	2366	HIS	-	expression tag	UNP T0D3N5
А	2367	HIS	-	expression tag	UNP T0D3N5
А	2368	HIS	-	expression tag	UNP T0D3N5
А	2369	HIS	-	expression tag	UNP T0D3N5
А	2370	HIS	-	expression tag	UNP T0D3N5
А	2371	HIS	-	expression tag	UNP T0D3N5
A	2372	HIS	_	expression tag	UNP T0D3N5

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
2	А	1	Total Zn 1 1	0



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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Cytotoxin-L





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S1189	S1190 51101	F1191 S1192	I1193 T1194	Y1195 R1196	K1197 P1198	W1199	L1200 S1201	11202 Y1203	D1204	V1205 L1206	N1207 11208	K1209	61211 E1211	K1212 11213	D1214 F1215	S1216 V1017	01210 D1218	L1219 M1220	V1221 L1222	P1223 N1224	A1225	P1226 N1227	R1228 V1229	F1230	Y1232	E1233 M1234	G1235	W1236 T1237	P1238	G1239 F1240	R1241	S1242 L1243	D1244 N1245	D1246 G1247	T1248
K1249	L1250	D1252	R1253	R1255	H1257	E1259	G1260 Q1261	F1262	W1264	R1265	F1267	F1269	A1271	D1272	L1274	T1276	L1278	K1279 P1280	R1281 Y1282	E1283	T1285	N1286 V1287	R1288 11289	N1290	D1292	61293 N1294	T1295 R1296	S1297	r 1230 I 1299	V1302	I1303	T1304 T1305	E1306	11308 11309	
1310	1311	1313	1314	1316 1317	1319	1320	1322 1323 1324	1325	1326 1327	1328 🕈	1330	1332	1333 1334	1335 1336	1337	1339 1340	1344	1345 1348 1348	1349	1350	1352	1354	1356	1357	1359	1361	1362	1364	1365	1367	1368 1369	1370	1372		
K												W .					M							н ш _									- 1		
S1373	K1374	N1376	11377 E1378	D1379 N1380	K1381 11382 11382	L1384	N1385 N1386	H1387 T1386	11389 N1390	F1391	G1393 D1394	E1397	R1400	F1401 11402	S1403 L1404	T140E F1406	11407 11408	L1405 E1410	D1411 11412	N1413 11414	11415 11416	E1417	D1410 D1410 L1420	V1421	S1424 Y1425	K1426	C1 435		L1436 11437	E1438 N1439	S1440				
S1441	D1442	Q1445 K1446	11447 D1448	H1449 I1450	<mark>G1451</mark> F1452	N1453 G1454	E1455 H1456	Q1457 K1458	Y1459 I1460	P1461 Y1462	S1463 Y1464	11465 D1466	N1467 E1468	T1469 K1470	R1495 N1406	11497 Y1498	M1499 P1500	D1501 81502	N1503 N1504	L1505 F1506	11507	L1513 K1514	D1515 11516 11516	K1521	G1522 D1523	L1527	K1533	D1534 D1535							
S1539 1.1540	S1541	F1542 T1543	D1546 T1547	N1548	I1550 K1551	L1552 N1553	Y1556 L1557	G1561	K1573	S1574 A1575	L1576	T1578	L1582	F1585	S1588	L1591	L1599	N1602 11603	E1604 F1605	D1608 T1609	N1610 F1611	I1612	E1623 L1624 T1625	C1626 D1627	K1628 D1629	P1634	Y1635 F1636								
V1640	V1650	G1651 N1652 N1652	R1653	Y1662	H1663 L1664 D1665	G1668	N1669 11670	S1671	D1686 R1687	V1692	L1698 V1600	11719	D1722	11726	L1737	V1742	N1745	81756	Q1761 P1762	q1763	R1767			D1787	V1791	K1795 11796	I1797								
798	800	801	804	312	60 4	0 -			5 1	2	50								•	10	œ	<mark>ور</mark> م			•	••									
		- N		<u></u>	6 8	83 (<mark>8</mark>	8	1 <mark>840</mark>	84 84	87	876	88	1 <mark>89</mark>	006	906 000	1926	1927 1928	1929	1933	1936 93	6	194 194	1947 1948	1950 1950 951	1952	1953 1954	1955 1956								
Y1957				Y18	E181	D1820	N183	N1840	5184 S184	S187	S1876	11880	L189E	11900		F1926	11927	K1929	D1933	11936 11936	Y193	A194	E1948	K1950	L1952	D1953	E1955								
	F1959	01960	G1964 E1965	L1967 L1967 K1968	G1969 F181 F181	H1971 D1820 D1820 N1820	[1973 G1974 ↔ N183	D1975	K1977 D184 Y1978 S184	Y1979 F1980	D1981 D1982	N1983 11880 G1984	11985 M1986	q1987 T1988	(1989 F1990 ♦ F1000	11991 11992 F1926	I1993 (1927 N1994 (1928)	D1995 + K1929 K1996	V1997	Y1999 F2000 Y1937	N2001 N2002	D2003 A A194 G2004 A194	V2005 V1947 M2006 E1948	Q2007 W1343 V2008 ♦ 11950		12011 D1953	E2012 C E1955 V2013 C T1956	N2014	G2015 K2016	Y2017 F2018					
Y2019	F2020	42022 ♦ N1960	N2023 G1964 G2024 E1965	E2025 A A1960 L1967 R2026 K1968	Q2027 Q1969 E181 L2028 L1970	G2029 H1971 D1820 M1872 M1872	F2031 01974 01183	N2032 D1975 N1840 T2033 N1976 N1840	P2034 ♦ K1977 V D184 D184 × 1978 × 2184	C2036 11979 S187	F2037 D1981 S187(K2038 D1982 C	F2039 ↔ N1983 11880 F2040 G1984	C2041	K2043 1988 1988 1988	D2045	D2046 11991 11203 11902 11902	G2048 ■ I1993 ■ I1927 T2049 ● N1994 ● G1928	E2050 E2050 K1995 K1926 L1930 K1996 L1930	G2052 C1997 F1008	L2054 Y1999 11936	L2056 N2001 Y193	Y2057 ♥ D2003 ● A194 N2058 ● G2004 A194	G2059 ♦ V2005 V1947 12060 ♦ M2006 ♦ E1948	L2061 Q 2007 ML245 L2061 V2008 Q 11950	F2063 C2009 L1952	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	K2066 + E2012 + E1955 V2013 + T1956	12067 • N2014 • N2068 • N2014	F2069 C2016 K2016	F2070 Y Y2017 D2071 E F2018	12072	S2073	T2075		
G2079 Y2019	W2080 F2020 F1958		[2083 ♦ N2023 ♦ G1964 D2084 ♦ G2024 E1965	D2085 E2025 11967 C2086 R2026 11967	22087 ♦ q2027 ♦ G1969 F181 T2088 ♦ L2028 ♦ L1970	Y2089 C2029 H1971 D1820 V2029 Q1972 N1822	Y2090 ♥ ×2000 11973 ■ 11973 ■ 11973 ■ 11973	D2092 N2032 D1975 N1840	N2094 P2034 K1977 D184	12096 G2036 1979 1979 8187	E2097 E2097 F2037 K2038 K2038 K2038 F2037	C2099 F2039 F2040	12100 G2041 A 11985 L1895 G2101 P2042 M1986	L2102 X2043 T2103 T2103 T2103 T2103 T2103 T2103 T2103 T2103 T2103 T2103 T2102 T2102 T2102 T2002	V2104 V2104 C1906 L1906 V2105 V2105 V21045 V21045 V21045 V20045 V20055 V20045 V20055 V20045 V20045 V20045 V20045 V20055 V20045 V20055 V	N2106 D2046 11991 T1992 F1903	D2 201 G2048 I1993 I1927 C2108 T2049 N1994 G1928	K2109 ← E2050 ← D1995 ← K1929 Y2110 ← E2061 ← K1996	Y2111 • G2052 • V1997 • D1933 F2112 • E2053 • F1008 •	D2113 L2054 Y1999 11936 D314 Table Table Table Table	N2115 L2056 N2001 Y195	G2115 Y2057 N2063 A194 12117 N2058 G2004 A194	R2118 G2059 V12005 V1947 Q2119 I2060 M2006 H1000	L2120 L2061 Q Q2007 M1345 N1134 V2008 V1061	42111 N2062 G2009 11952 F2122 F2122 F2063 € V2046	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	I2125 K2066 K2066 I2012 I2013 I1956	N2126 12067 N2014	N2128 F2069 K2016 K2016	$\begin{array}{cccccccccccccccccccccccccccccccccccc$		F2132 ♥ S2073 ♥ S2133 ♦ N2074 ●	E2134 T2075	C2136 ↓ V2077 K2137 ◆ V2078	12138
(2139 🔶 G2079 🄶 Y2019 🔶	2140 W2080 F2020 F1958	2141 0202 0201 02021 01960	2143 ♦ L2083 ♦ N2023 ♦ G1964 2144 ♦ D2084 ♦ G2024 E1965	(2145 ♦ D2085 ♦ E2025 ♦ A1967 2146 ♦ C2086 ♦ R2026 ♦ K1967 ♦ 718	2147 ♦ 22087 ♦ q2027 ♦ 1969 19148 ● 79088 ● L2028 ● L1970	(2149 ♦ Y2089 ♦ G2029 ♦ H1971 D1820 N1822 N1822	2150 Y 2000 Y 2000 11973	[2152 ♥ D2092 ● N2032 ● D1975 ● N1840 [2153 ● D2093 ● T2033 ● N1976 ● N1840	12154 N2094 P2034 K1977 D184	22155 12095 2200 11079 12156 12095 22036 12096 2187	2157 E2097 E2037 11981 2187 2158 A2098 K2038 11982 2187	12159 C2099 F2039 V1983 1186 F2040 C2099 F2040 C1984	12100 ↓ 12100 62041 ♦ 11985 14895 14895 14895 14895 14895	(2162 ♦ 12102 ♦ K2043 ♦ 41987 11900 2163 ♦ T2103 ♦ T2044 ● T1888 ●	2164 V2104 D2045 11968 11968 11968 11968 11968 11996 P165 P1006 P1	22166 N12106 L2047 11991 71992 12926	22101 22108 22048 11993 11927 22168 22108 12049 11994 01928	2100 K2109 E2050 ↔ D1995 ↔ K1929 2170 Y2110 € E2051 ↔ K1996 L1930	(2171 ♦ Y2111 ♦ G2062 ♦ V1997 ♦ D1933 2172 ♦ F2112 ♦ E2063 FH048 ●	12173 D2113 L2054 11995 1>174 1	1275 N2115 L2056 N2001 Y195	121/5 12117 12117 12117 12117 12117 12117 12117	(2178 ♦ R2118 ♦ C2059 ♦ V2005 V1347 (2179 ♦ Q2119 ♦ I2060 ♦ M2006 ● U4000	22180 ♦ L2120 ♦ L2061 ♦ Q2007 N1393 M1911 ♦ M1911 ♦ L2061 ♦ 12068 ♦ 11961	2182 • F2122 • F2063 • C2009 • L1952	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	12125 4 12125 4 K2066 4 E2012 7 E1966 12125 12125 121966 121966 12196	12186 • N2126 • I2067 • N2014 • 12187 • N20127 • Y2068 • N2014	2188 A N2128 F2069 C2015 C2005 C2005 C2000	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		2192 F F2132 S2073 F 12193 S2133 N2074 S2133 S2133 S2074	2134 E2134 T2075		12198 • I2138 • I2138
9 🔶 E2139 🌪 G2079 🌪 Y2019	0 ♦ L2140 ♦ W2080 ♦ F2020 ♦ 11959 Contract ♦ Contract ♦ F1959	2 Y2142 Y2082 K2022	3	$5 \leftrightarrow 12145 \leftrightarrow 22085 \leftrightarrow 22026 \leftrightarrow 12067$ $5 \leftrightarrow N2146 \leftrightarrow 22086 \leftrightarrow R2026 \leftrightarrow 1267$	7 ♦ C2147 ♦ S2087 ♦ Q2027 ♦ G1699 E181 3 ♦ N2148 ♦ T2088 ♦ L2028 ♦ L1970	9 Y2149 Y2089 62029 H1971 D1820 1182 1182 1182 1182 1182 1182 1182	C ← F2150 ← Y2090 ← 2000 − 11973 − 11	2	4 • E2154 • N2094 • P2034 • K1977 · D164	SZI55 12095 2200 Y1979 S187 G2156 A2096 62036 F1980 S187	7 + L2157 + E2097 + F2037 101981 3 • V2158 • A2098 • K2038 • D1982 • S187	9 C 12159 C 2099 F 72039 11860 11983 11860 12984 11860 12984	1210 1210 22041 11985 11385 c2161 c2101 p2042 M1986 1385	2	4 D2164 V2104 D2004 L1906 L1906 7 77165 17105 0.0045 F1990 P1000	5 P2166 N2046 11991 11091 5 P2166 N2166 L2047 11992 12926	b 2 10 / b 2 10	Y2169 K2109 E2050 D1995 K1929 K2170 Y2110 E2051 K1996 L1930	1 • Y2171 • Y2111 • G2052 • Y1997 • D1933 2 • F2172 • F2112 • E2053 • F1946 • D1933	a A2173 D2113 L2054 T1999 T1939 1 P1174 D1114 monce F2000 T1933	C 12175 N2115 12005 N2001 V195 N2175 N2115 12005 N2002 N2002	N21/0 G210 Y2057 D2003 A194 1 12177 12117 N2058 G2004 A194	8	D D D2180 L2120 L2061 Q 02007 N1243 N1101 D 12120 L2061 V2008 11961	2 C 12182 C 22009 11462	3 ♦ Y2183 ♦ I2123 ♥ N2064 ♦ I2011 01953 1 ♦ C2184 ♦ T2124 ♦ C2065 ♦ I2011 01954	5 4 Q2185 12125 4 K2066 12012 12156 11956 11956	6	K2188 N12128 S F2069 K2016 K2016	$0 \qquad \qquad 12129 \qquad 12129 \qquad 12129 \qquad 12070 \qquad 12077 $		2 12192 12193 12193 12133 12133 12133 12133 12133	4 ♦ R2194 ♦ E2134 ♦ T2075 ♦ V195 ♦ S135 ♦ •••72	s ♦ N196 ♦ C2136 ♦ V2077	







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	229156	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	0.204	Depositor
Minimum map value	-0.099	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	321.752, 321.752, 321.752	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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: ZN

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).

Mal	Chain	Bond	lengths	Bond angles				
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5			
1	А	0.41	0/19409	0.51	5/26261~(0.0%)			

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	А	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	416	PRO	CA-N-CD	-12.75	93.65	111.50
1	А	1535	ASP	CB-CG-OD2	5.24	123.02	118.30
1	А	1982	ASP	CB-CG-OD2	5.22	123.00	118.30
1	А	669	ASP	CB-CG-OD2	5.21	122.99	118.30
1	А	1394	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	1028	GLY	Peptide
1	А	1452	PHE	Peptide



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	А	19026	0	18584	525	0
2	А	1	0	0	0	0
All	All	19027	0	18584	525	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 14.

All (525) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1023:PRO:HG3	1:A:1649:TYR:CZ	1.49	1.48
1:A:1956:THR:HG23	1:A:1986:MET:N	1.21	1.45
1:A:1956:THR:CG2	1:A:1986:MET:N	1.86	1.38
1:A:1023:PRO:CG	1:A:1649:TYR:CZ	2.18	1.26
1:A:1180:LEU:HD21	1:A:1185:ASP:OD1	1.34	1.22
1:A:1956:THR:HG21	1:A:1986:MET:CA	1.72	1.20
1:A:1022:LEU:HD22	1:A:1023:PRO:CD	1.72	1.20
1:A:1180:LEU:CD2	1:A:1185:ASP:HA	1.70	1.19
1:A:1956:THR:HG21	1:A:1986:MET:CB	1.74	1.18
1:A:1022:LEU:CD2	1:A:1023:PRO:HD3	1.74	1.17
1:A:1023:PRO:HG2	1:A:1649:TYR:CE2	1.79	1.17
1:A:1023:PRO:CG	1:A:1649:TYR:OH	1.93	1.16
1:A:1023:PRO:HG3	1:A:1649:TYR:OH	0.96	1.12
1:A:1956:THR:CG2	1:A:1986:MET:H	1.50	1.10
1:A:1956:THR:HG21	1:A:1986:MET:HB3	1.32	1.07
1:A:1023:PRO:CG	1:A:1649:TYR:CE2	2.37	1.05
1:A:1022:LEU:HD22	1:A:1023:PRO:HD3	1.07	1.05
1:A:1036:ILE:HG21	1:A:1521:LYS:HG2	1.35	1.05
1:A:1956:THR:CG2	1:A:1986:MET:CA	2.32	1.04
1:A:1956:THR:CG2	1:A:1986:MET:CB	2.34	1.04
1:A:1956:THR:HG22	1:A:1985:ILE:HG22	1.40	1.02
1:A:1180:LEU:HD23	1:A:1185:ASP:CA	1.90	1.01
1:A:1180:LEU:CD2	1:A:1185:ASP:CA	2.44	0.95
1:A:1956:THR:CG2	1:A:1986:MET:HB3	1.96	0.94
1:A:1180:LEU:HD23	1:A:1185:ASP:HA	0.97	0.94



	Jus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1180:LEU:CD2	1:A:1185:ASP:OD1	2.16	0.93
1:A:1023:PRO:HG3	1:A:1649:TYR:HH	1.24	0.92
1:A:1180:LEU:HD21	1:A:1185:ASP:CG	1.90	0.90
1:A:1295:THR:HA	1:A:1322:SER:O	1.71	0.90
1:A:1505:LEU:O	1:A:1599:LEU:HD11	1.73	0.89
1:A:744:VAL:HG22	1:A:754:ILE:HG22	1.55	0.88
1:A:1534:ASP:O	1:A:1535:ASP:OD1	1.96	0.84
1:A:1025:LEU:HB3	1:A:1033:ALA:HB1	1.60	0.83
1:A:1956:THR:HG21	1:A:1986:MET:C	1.99	0.83
1:A:589:ILE:HD13	1:A:757:HIS:HA	1.64	0.80
1:A:622:SER:HA	1:A:639:GLN:HE22	1.48	0.79
1:A:1956:THR:OG1	1:A:1986:MET:HB2	1.83	0.78
1:A:577:TYR:HB3	1:A:645:LYS:HB2	1.65	0.78
1:A:1036:ILE:HG21	1:A:1521:LYS:CG	2.14	0.77
1:A:1550:ILE:HG21	1:A:1605:PHE:HE1	1.47	0.77
1:A:1956:THR:OG1	1:A:1986:MET:CB	2.33	0.77
1:A:1507:ILE:O	1:A:1598:ASN:OD1	2.03	0.76
1:A:1795:LYS:O	1:A:1799:THR:OG1	2.03	0.76
1:A:754:ILE:HD12	1:A:754:ILE:O	1.86	0.76
1:A:1180:LEU:CD2	1:A:1185:ASP:CG	2.54	0.76
1:A:2194:ARG:HG2	1:A:2199:VAL:HG12	1.67	0.75
1:A:1069:VAL:HG23	1:A:1461:PRO:HB3	1.69	0.75
1:A:1956:THR:CB	1:A:1986:MET:HB3	2.18	0.74
1:A:1956:THR:HG21	1:A:1986:MET:O	1.88	0.74
1:A:1041:LEU:HD23	1:A:1041:LEU:N	2.02	0.74
1:A:2128:ASN:HB3	1:A:2157:LEU:HD22	1.71	0.73
1:A:941:ASN:HD22	1:A:1056:LEU:HD13	1.54	0.73
1:A:1146:PRO:HD2	1:A:1221:VAL:HB	1.71	0.73
1:A:1956:THR:O	1:A:1985:ILE:HA	1.90	0.72
1:A:2088:THR:HG21	1:A:2118:ARG:HH21	1.55	0.72
1:A:589:ILE:CD1	1:A:757:HIS:HA	2.19	0.71
1:A:1031:ILE:HG22	1:A:1046:LYS:HD3	1.73	0.71
1:A:960:ASN:OD1	1:A:1652:ASN:ND2	2.20	0.70
1:A:1550:ILE:HB	1:A:1605:PHE:CD1	2.26	0.70
1:A:1737:LEU:HD13	1:A:1872:SER:HB2	1.74	0.69
1:A:1113:LEU:HG	1:A:1114:GLN:HG2	1.72	0.69
1:A:5:ASN:ND2	1:A:8:GLN:OE1	2.25	0.69
1:A:1022:LEU:HD22	1:A:1023:PRO:HD2	1.73	0.69
1:A:1772:PHE:HE1	1:A:1797:ILE:HD11	1.58	0.69
1:A:1025:LEU:HG	1:A:1612:ILE:HD13	1.75	0.68
1:A:1025:LEU:HD21	1:A:1635:TYR:CE1	2.28	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:708:GLU:HG3	1:A:787:ILE:HD12	1.76	0.68
1:A:1425:TYR:OH	1:A:1453:ASN:ND2	2.23	0.68
1:A:2123:ILE:O	1:A:2130:PHE:HB2	1.92	0.68
1:A:413:ASN:HD22	1:A:413:ASN:H	1.40	0.68
1:A:889:ILE:HG12	1:A:898:ILE:HG12	1.76	0.67
1:A:1180:LEU:CD2	1:A:1185:ASP:CB	2.72	0.67
1:A:2119:GLN:HG3	1:A:2123:ILE:HG13	1.76	0.67
1:A:1180:LEU:HD21	1:A:1185:ASP:CB	2.24	0.67
1:A:1952:LEU:HD12	1:A:1952:LEU:N	2.09	0.67
1:A:1408:ILE:HB	1:A:1446:LYS:HD2	1.76	0.67
1:A:1325:LEU:HD21	1:A:1334:ILE:HD12	1.77	0.67
1:A:792:LYS:HB2	1:A:835:GLN:HG3	1.77	0.66
1:A:1550:ILE:HG21	1:A:1605:PHE:CE1	2.30	0.66
1:A:1956:THR:O	1:A:1985:ILE:HG23	1.96	0.66
1:A:373:VAL:HG23	1:A:395:CYS:HB3	1.77	0.66
1:A:2017:TYR:HB2	1:A:2054:LEU:HD22	1.76	0.66
1:A:1025:LEU:HB3	1:A:1033:ALA:CB	2.26	0.66
1:A:2253:LEU:HG	1:A:2260:ASN:HD21	1.61	0.65
1:A:73:LYS:HD2	1:A:1726:ILE:HG23	1.78	0.65
1:A:2118:ARG:NH1	1:A:2135:SER:O	2.30	0.65
1:A:1089:PHE:HA	1:A:1092:LEU:HG	1.76	0.65
1:A:2111:TYR:HE1	1:A:2123:ILE:HB	1.61	0.65
1:A:1280:PRO:HB2	1:A:1282:TYR:HE1	1.61	0.64
1:A:879:ASP:N	1:A:879:ASP:OD1	2.31	0.64
1:A:577:TYR:HB3	1:A:645:LYS:CB	2.28	0.64
1:A:2244:ASP:HB3	1:A:2250:ARG:CZ	2.29	0.63
1:A:1111:LEU:H	1:A:1281:ARG:HH12	1.46	0.63
1:A:2174:PRO:O	1:A:2181:ASN:ND2	2.31	0.63
1:A:1197:LYS:NZ	1:A:1261:GLN:OE1	2.29	0.63
1:A:1368:ILE:HG23	1:A:1371:ILE:HB	1.80	0.62
1:A:956:VAL:HG21	1:A:1653:ARG:NE	2.14	0.62
1:A:1003:ASP:HB3	1:A:1006:LYS:HE2	1.82	0.62
1:A:94:VAL:HG22	1:A:368:VAL:HG22	1.81	0.62
1:A:644:ARG:NH1	1:A:687:SER:O	2.32	0.62
1:A:754:ILE:HG23	1:A:768:ILE:HG12	1.79	0.62
1:A:361:LEU:HD12	1:A:362:PRO:HD2	1.82	0.62
1:A:623:VAL:H	1:A:639:GLN:HE22	1.47	0.62
1:A:1550:ILE:HB	1:A:1605:PHE:CE1	2.34	0.62
1:A:1960:ASN:HB3	1:A:1964:GLY:H	1.65	0.62
1:A:754:ILE:CG2	1:A:768:ILE:HG12	2.29	0.62
1:A:1022:LEU:CD2	1:A:1023:PRO:CD	2.53	0.62



	h h	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1550:ILE:CG2	1:A:1605:PHE:CE1	2.82	0.62
1:A:1505:LEU:O	1:A:1599:LEU:CD1	2.45	0.61
1:A:1314:TYR:HB2	1:A:1334:ILE:HD13	1.82	0.61
1:A:173:ARG:NH2	1:A:823:GLU:OE2	2.28	0.61
1:A:873:LYS:NZ	1:A:882:HIS:O	2.33	0.61
1:A:2043:LYS:H	1:A:2051:GLU:HG2	1.65	0.61
1:A:1197:LYS:HG2	1:A:1198:PRO:HD2	1.83	0.60
1:A:57:ASP:OD1	1:A:76:LYS:NZ	2.33	0.60
1:A:1384:LEU:O	1:A:1387:HIS:HB2	2.01	0.60
1:A:1807:ASP:HB2	1:A:1812:TYR:HE2	1.67	0.60
1:A:243:LEU:HB3	1:A:245:LYS:HG2	1.84	0.60
1:A:1025:LEU:CD2	1:A:1635:TYR:CE1	2.85	0.60
1:A:1025:LEU:N	1:A:1025:LEU:HD22	2.16	0.60
1:A:1947:VAL:O	1:A:1959:PHE:HB2	2.01	0.60
1:A:1956:THR:CG2	1:A:1985:ILE:HG22	2.26	0.60
1:A:1968:LYS:O	1:A:1971:HIS:NE2	2.33	0.60
1:A:1955:GLU:HG2	1:A:1985:ILE:HD13	1.84	0.60
1:A:1575:ALA:HA	1:A:1578:THR:HG22	1.84	0.59
1:A:1495:ARG:HG2	1:A:1507:ILE:HG23	1.84	0.59
1:A:1239:GLY:H	1:A:1241:ARG:HH12	1.51	0.59
1:A:413:ASN:HD22	1:A:413:ASN:N	2.00	0.59
1:A:1956:THR:OG1	1:A:1986:MET:HB3	2.01	0.58
1:A:1354:ASN:O	1:A:1365:GLY:N	2.32	0.58
1:A:1296:ARG:HB2	1:A:1323:TYR:HD1	1.66	0.58
1:A:2273:TYR:HE2	1:A:2280:MET:HB3	1.68	0.58
1:A:1550:ILE:CG2	1:A:1605:PHE:HE1	2.17	0.58
1:A:1970:LEU:HD21	1:A:1977:LYS:HD3	1.84	0.58
1:A:1624:LEU:HD23	1:A:1634:PRO:HA	1.85	0.58
1:A:1128:SER:HB3	1:A:1250:LEU:HD22	1.84	0.58
1:A:540:GLU:OE2	1:A:540:GLU:HA	2.03	0.57
1:A:566:ILE:HD13	1:A:602:PRO:HB3	1.86	0.57
1:A:1447:ILE:O	1:A:1450:ILE:HG12	2.03	0.57
1:A:1400:ARG:HA	1:A:1420:LEU:HD12	1.87	0.57
1:A:270:ASP:OD2	1:A:384:ASN:ND2	2.37	0.57
1:A:587:ASP:OD1	1:A:653:HIS:NE2	2.35	0.57
1:A:1113:LEU:HB2	1:A:1280:PRO:HD3	1.87	0.57
1:A:1956:THR:HG23	1:A:1986:MET:H	0.58	0.57
1:A:1956:THR:CB	1:A:1986:MET:CB	2.78	0.57
1:A:2188:LYS:HB3	1:A:2206:TYR:CD2	2.40	0.57
1:A:1144:ILE:HD11	1:A:1217:LYS:HB2	1.86	0.57
1:A:1327:LEU:HD23	1:A:1351:VAL:HG21	1.87	0.57



	Jus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:2244:ASP:HB3	1:A:2250:ARG:NE	2.19	0.57
1:A:1598:ASN:OD1	1:A:1598:ASN:N	2.33	0.56
1:A:451:THR:OG1	1:A:826:ILE:HD13	2.05	0.56
1:A:622:SER:HA	1:A:639:GLN:NE2	2.17	0.56
1:A:1348:VAL:HB	1:A:1351:VAL:HB	1.87	0.56
1:A:1139:LEU:HD23	1:A:1143:ILE:HD12	1.88	0.56
1:A:133:SER:OG	1:A:239:ASP:OD2	2.17	0.56
1:A:704:SER:HB3	1:A:776:GLU:OE2	2.06	0.56
1:A:1023:PRO:HG3	1:A:1649:TYR:CE2	2.12	0.56
1:A:1787:ASP:N	1:A:1787:ASP:OD1	2.37	0.56
1:A:1433:CYS:O	1:A:1437:ILE:HG12	2.06	0.56
1:A:1022:LEU:HD23	1:A:1023:PRO:HD3	1.82	0.56
1:A:1218:ASP:HA	1:A:1296:ARG:HH11	1.71	0.56
1:A:1329:PRO:HB3	1:A:1355:ILE:HG13	1.88	0.56
1:A:2320:TYR:HE1	1:A:2324:LEU:HB2	1.69	0.56
1:A:1168:GLU:HB3	1:A:1199:TRP:HB3	1.88	0.55
1:A:1334:ILE:HB	1:A:1389:ILE:HD12	1.87	0.55
1:A:1929:LYS:HE3	1:A:1936:ILE:HG23	1.87	0.55
1:A:1949:TRP:CZ2	1:A:1973:ILE:HG21	2.40	0.55
1:A:1104:PRO:HG2	1:A:1305:THR:HG21	1.87	0.55
1:A:2293:VAL:HG12	1:A:2300:PHE:HD2	1.72	0.55
1:A:1356:THR:HG22	1:A:1363:GLN:HB3	1.88	0.55
1:A:1956:THR:CG2	1:A:1986:MET:O	2.54	0.55
1:A:420:GLU:O	1:A:420:GLU:HG3	2.07	0.55
1:A:688:PRO:HG2	1:A:730:ILE:HD11	1.89	0.55
1:A:589:ILE:HD11	1:A:757:HIS:O	2.05	0.55
1:A:791:SER:HA	1:A:838:GLU:OE2	2.05	0.55
1:A:1258:TYR:HB3	1:A:1261:GLN:HB2	1.87	0.55
1:A:2276:ILE:HG22	1:A:2277:LYS:HG2	1.88	0.55
1:A:2043:LYS:HE2	1:A:2050:GLU:HA	1.88	0.55
1:A:1656:LEU:HD23	1:A:1692:VAL:HG13	1.88	0.54
1:A:998:LEU:HD12	1:A:1001:ILE:HD12	1.88	0.54
1:A:1375:LEU:HB2	1:A:1384:LEU:HD13	1.89	0.54
1:A:1381:LYS:NZ	1:A:1383:ILE:HD11	2.22	0.54
1:A:1719:ILE:HG12	1:A:1767:ARG:HD2	1.89	0.54
1:A:2300:PHE:HB3	1:A:2339:ALA:HB3	1.88	0.54
1:A:2011:ILE:HD12	1:A:2020:PHE:HD2	1.72	0.54
1:A:2190:SER:HA	1:A:2202:PHE:HB2	1.90	0.54
1:A:954:HIS:O	1:A:954:HIS:ND1	2.40	0.54
1:A:995:SER:OG	1:A:996:THR:N	2.40	0.54
1:A:308:THR:HA	1:A:785:ASN:HD22	1.73	0.54



		Interstomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:145:ILE:HD12	1:A:263:TRP:HH2	1.73	0.54
1:A:1045:ILE:HG12	1:A:1066:ILE:HD13	1.91	0.53
1:A:1876:SER:HB3	1:A:1880:ILE:HG13	1.90	0.53
1:A:258:GLU:OE1	1:A:407:TYR:OH	2.16	0.53
1:A:1030:PRO:HB2	1:A:1556:TYR:CZ	2.43	0.53
1:A:1291:LEU:HD21	1:A:1316:PHE:HD1	1.73	0.53
1:A:447:MET:O	1:A:451:THR:HG23	2.08	0.53
1:A:1989:GLY:H	1:A:2000:PHE:HB2	1.74	0.53
1:A:1251:LEU:HA	1:A:1254:ILE:HD12	1.90	0.53
1:A:963:PHE:HD2	1:A:1022:LEU:HD11	1.72	0.53
1:A:1371:ILE:HA	1:A:1374:LYS:NZ	2.24	0.53
1:A:610:LYS:HE3	1:A:674:GLU:OE2	2.09	0.52
1:A:711:TYR:HB3	1:A:712:PRO:HD3	1.91	0.52
1:A:733:ASP:OD1	1:A:733:ASP:N	2.38	0.52
1:A:2244:ASP:CB	1:A:2250:ARG:CZ	2.87	0.52
1:A:2336:GLU:HG3	1:A:2338:ILE:HG22	1.91	0.52
1:A:1072:THR:HG22	1:A:1073:ALA:H	1.74	0.52
1:A:1171:ARG:HE	1:A:1261:GLN:HG2	1.74	0.52
1:A:2160:ILE:HA	1:A:2172:PHE:O	2.10	0.52
1:A:2244:ASP:CB	1:A:2250:ARG:NH2	2.73	0.52
1:A:968:LEU:HD12	1:A:978:LEU:HD21	1.92	0.52
1:A:1324:SER:HB3	1:A:1345:VAL:HG23	1.91	0.52
1:A:1024:THR:HG22	1:A:1636:PHE:CD1	2.45	0.52
1:A:1061:GLU:O	1:A:1065:GLY:N	2.43	0.52
1:A:1249:LYS:NZ	1:A:1253:ARG:HE	2.09	0.51
1:A:1366:GLU:OE2	1:A:1449:HIS:NE2	2.43	0.51
1:A:1383:ILE:HA	1:A:1387:HIS:O	2.11	0.51
1:A:1996:LYS:HB3	1:A:2025:GLU:HG2	1.91	0.51
1:A:2223:ASP:HB2	1:A:2230:TYR:HE2	1.73	0.51
1:A:1377:ILE:HD11	1:A:1420:LEU:HD23	1.92	0.51
1:A:578:ILE:HD11	1:A:640:ILE:O	2.11	0.51
1:A:703:TYR:CD2	1:A:710:THR:HG21	2.45	0.51
1:A:756:ASP:HB2	1:A:762:ILE:HD12	1.93	0.51
1:A:438:ILE:O	1:A:438:ILE:HG13	2.10	0.51
1:A:1505:LEU:HG	1:A:1507:ILE:HD11	1.93	0.51
1:A:1540:LEU:HG	1:A:1542:PHE:HD1	1.75	0.51
1:A:1981:ASP:OD1	1:A:1985:ILE:N	2.41	0.51
1:A:2208:ILE:HD13	1:A:2227:LYS:HG2	1.93	0.51
1:A:623:VAL:H	1:A:639:GLN:NE2	2.06	0.51
1:A:1550:ILE:CB	1:A:1605:PHE:CE1	2.94	0.51
1:A:2177:THR:OG1	1:A:2181:ASN:ND2	2.31	0.51



	Jus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1022:LEU:CB	1:A:1023:PRO:CD	2.89	0.51
1:A:2049:THR:HG22	1:A:2053:GLU:HB3	1.92	0.51
1:A:2242:TYR:HB2	1:A:2263:PHE:CZ	2.46	0.51
1:A:1968:LYS:HE2	1:A:1982:ASP:O	2.11	0.51
1:A:1976:ASN:HB3	1:A:2005:VAL:HG13	1.93	0.51
1:A:672:SER:OG	1:A:719:ILE:HG22	2.11	0.51
1:A:1383:ILE:HG12	1:A:1388:THR:HG22	1.93	0.51
1:A:1440:SER:HB3	1:A:1499:MET:SD	2.50	0.51
1:A:1957:TYR:HE1	1:A:1983:ASN:O	1.93	0.51
1:A:1154:GLU:HG2	1:A:1288:ARG:HB2	1.91	0.51
1:A:1981:ASP:OD1	1:A:1981:ASP:N	2.44	0.51
1:A:1367:LEU:HD21	1:A:1408:ILE:HG22	1.92	0.50
1:A:1354:ASN:N	1:A:1366:GLU:O	2.44	0.50
1:A:2277:LYS:HZ1	1:A:2313:PHE:HE1	1.60	0.50
1:A:2264:ASN:OD1	1:A:2267:GLY:N	2.44	0.50
1:A:1495:ARG:HG2	1:A:1507:ILE:HD12	1.93	0.50
1:A:878:LEU:HD11	1:A:911:ILE:HD11	1.93	0.50
1:A:1628:LYS:HG3	1:A:1629:ASP:OD1	2.12	0.50
1:A:1906:LEU:HB2	1:A:1945:ALA:HB3	1.93	0.50
1:A:1025:LEU:CD2	1:A:1025:LEU:N	2.75	0.50
1:A:1036:ILE:HB	1:A:1041:LEU:HD21	1.94	0.50
1:A:145:ILE:HD12	1:A:263:TRP:CH2	2.47	0.50
1:A:413:ASN:N	1:A:413:ASN:ND2	2.60	0.50
1:A:2011:ILE:HD12	1:A:2020:PHE:CD2	2.47	0.50
1:A:2058:ASN:HD21	1:A:2072:ILE:HA	1.77	0.50
1:A:383:ILE:HG12	1:A:385:GLN:HG3	1.93	0.49
1:A:513:GLU:O	1:A:517:THR:HG23	2.12	0.49
1:A:1151:VAL:HG12	1:A:1165:GLY:HA3	1.94	0.49
1:A:1171:ARG:HH21	1:A:1261:GLN:HG2	1.77	0.49
1:A:275:SER:O	1:A:279:GLU:HG2	2.12	0.49
1:A:368:VAL:HG23	1:A:390:LEU:HG	1.94	0.49
1:A:956:VAL:HG23	1:A:957:ASN:N	2.28	0.49
1:A:1085:ILE:HG13	1:A:1086:ALA:N	2.28	0.49
1:A:1375:LEU:HD12	1:A:1384:LEU:HB2	1.94	0.49
1:A:1956:THR:HG22	1:A:1985:ILE:CG2	2.26	0.49
1:A:1239:GLY:H	1:A:1241:ARG:NH1	2.09	0.49
1:A:2230:TYR:HD1	1:A:2234:ASN:HB3	1.78	0.49
1:A:708:GLU:H	1:A:708:GLU:CD	2.13	0.49
1:A:2244:ASP:HB2	1:A:2250:ARG:NH2	2.27	0.49
1:A:21:GLU:HG2	1:A:63:TYR:CZ	2.48	0.49
1:A:1216:SER:O	1:A:1216:SER:OG	2.29	0.49



	Juo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1369:GLU:OE1	1:A:1370:ASN:HB2	2.12	0.49
1:A:1124:PHE:HA	1:A:1127:ILE:HG12	1.95	0.49
1:A:707:ALA:O	1:A:710:THR:OG1	2.24	0.49
1:A:1048:LEU:HD22	1:A:1066:ILE:HD11	1.94	0.49
1:A:1381:LYS:HD3	1:A:1390:ASN:HD22	1.77	0.48
1:A:1791:VAL:HG13	1:A:1795:LYS:HD2	1.94	0.48
1:A:21:GLU:OE2	1:A:68:ARG:NH2	2.37	0.48
1:A:1041:LEU:HD12	1:A:1045:ILE:HD11	1.94	0.48
1:A:1255:ARG:HH22	1:A:1259:GLU:HG2	1.79	0.48
1:A:2172:PHE:CE2	1:A:2186:ALA:HB2	2.48	0.48
1:A:549:LEU:HD11	1:A:589:ILE:HD12	1.96	0.48
1:A:925:ILE:HG13	1:A:926:SER:N	2.28	0.48
1:A:1238:PRO:HG3	1:A:1271:ALA:HB1	1.94	0.48
1:A:1745:ASN:N	1:A:1745:ASN:OD1	2.46	0.48
1:A:2341:THR:O	1:A:2353:PHE:HB2	2.14	0.48
1:A:754:ILE:HD12	1:A:754:ILE:C	2.33	0.48
1:A:1030:PRO:HB2	1:A:1556:TYR:OH	2.14	0.48
1:A:1303:ILE:O	1:A:1309:ARG:HD2	2.14	0.48
1:A:1385:ASN:O	1:A:1387:HIS:ND1	2.44	0.48
1:A:1041:LEU:HD23	1:A:1041:LEU:H	1.75	0.47
1:A:703:TYR:CD2	1:A:703:TYR:N	2.82	0.47
1:A:2317:SER:O	1:A:2317:SER:OG	2.32	0.47
1:A:940:VAL:HG21	1:A:1060:ILE:HA	1.96	0.47
1:A:974:THR:HG21	1:A:1664:LEU:H	1.80	0.47
1:A:1973:ILE:HD13	1:A:1978:TYR:HD2	1.79	0.47
1:A:155:GLU:OE2	1:A:538:TYR:OH	2.28	0.47
1:A:1464:TYR:CE1	1:A:1466:ASP:HB2	2.50	0.47
1:A:1977:LYS:HD2	1:A:2006:MET:SD	2.55	0.47
1:A:1024:THR:HG22	1:A:1636:PHE:CE1	2.50	0.47
1:A:1967:LEU:HB3	1:A:1971:HIS:CD2	2.50	0.47
1:A:1195:TYR:HD2	1:A:1196:ARG:HD3	1.79	0.47
1:A:1502:SER:O	1:A:1505:LEU:HB2	2.15	0.47
1:A:1345:VAL:HG12	1:A:1403:SER:HB2	1.97	0.47
1:A:2243:PHE:CE2	1:A:2249:MET:HG3	2.50	0.47
1:A:1550:ILE:HD12	1:A:1605:PHE:CZ	2.50	0.47
1:A:140:THR:O	1:A:144:THR:OG1	2.29	0.47
1:A:1168:GLU:O	1:A:1230:PHE:HB2	2.15	0.47
1:A:1170:TRP:CE2	1:A:1195:TYR:HB3	2.50	0.47
1:A:1427:ILE:HG13	1:A:1452:PHE:CE2	2.49	0.47
1:A:375:ILE:HG12	1:A:383:ILE:O	2.15	0.46
1:A:905:THR:HG23	1:A:907:ASN:H	1.79	0.46



	Juo puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:1947:VAL:O	1:A:1948:GLU:O	2.33	0.46
1:A:2264:ASN:HD21	1:A:2266:ASP:HB3	1.80	0.46
1:A:1205:VAL:HG13	1:A:1257:HIS:CD2	2.50	0.46
1:A:2129:ILE:O	1:A:2157:LEU:HA	2.15	0.46
1:A:2223:ASP:HB2	1:A:2230:TYR:CE2	2.49	0.46
1:A:2360:LEU:HG	1:A:2362:VAL:HG13	1.97	0.46
1:A:882:HIS:HA	1:A:901:ILE:O	2.16	0.46
1:A:1955:GLU:CG	1:A:1985:ILE:HD13	2.45	0.46
1:A:779:SER:OG	1:A:780:PHE:N	2.48	0.46
1:A:1307:GLN:O	1:A:1311:ASN:ND2	2.31	0.46
1:A:1738:SER:O	1:A:1840:ASN:ND2	2.43	0.46
1:A:1402:ILE:CG2	1:A:1418:ILE:HB	2.46	0.46
1:A:1452:PHE:HZ	1:A:1457:GLN:HB3	1.81	0.46
1:A:2177:THR:N	1:A:2181:ASN:OD1	2.43	0.46
1:A:2215:ASN:O	1:A:2217:THR:N	2.37	0.46
1:A:1543:THR:HG23	1:A:1551:LYS:HB3	1.96	0.46
1:A:1756:SER:HB2	1:A:1763:GLN:HB2	1.98	0.46
1:A:1988:THR:HG21	1:A:2002:ASN:HA	1.98	0.46
1:A:2151:TYR:HB2	1:A:2172:PHE:CZ	2.51	0.46
1:A:2242:TYR:HE1	1:A:2256:PHE:HB2	1.81	0.46
1:A:1036:ILE:CG2	1:A:1521:LYS:HG2	2.26	0.46
1:A:384:ASN:OD1	1:A:384:ASN:N	2.48	0.46
1:A:669:ASP:OD1	1:A:718:LYS:HE2	2.16	0.46
1:A:1125:LYS:HD3	1:A:1246:ASP:HB3	1.97	0.46
1:A:2050:GLU:N	1:A:2053:GLU:OE2	2.48	0.46
1:A:324:LYS:HE3	1:A:359:ILE:HD11	1.98	0.45
1:A:646:ILE:CG2	1:A:691:ILE:HG13	2.46	0.45
1:A:1546:ASP:OD2	1:A:1549:THR:OG1	2.27	0.45
1:A:1437:ILE:HD12	1:A:1497:ILE:HD12	1.98	0.45
1:A:2113:ASP:OD2	1:A:2117:ILE:HB	2.16	0.45
1:A:2090:TYR:O	1:A:2099:CYS:N	2.50	0.45
1:A:610:LYS:HE3	1:A:674:GLU:CD	2.37	0.45
1:A:1761:GLN:O	1:A:1763:GLN:N	2.46	0.45
1:A:1179:THR:O	1:A:1180:LEU:HD23	2.17	0.45
1:A:229:LEU:O	1:A:233:THR:OG1	2.30	0.45
1:A:573:ARG:HD2	1:A:1804:ALA:O	2.17	0.45
1:A:1557:LEU:HB3	1:A:1561:GLY:HA3	1.98	0.45
1:A:1629:ASP:OD1	1:A:1629:ASP:N	2.50	0.45
1:A:1997:VAL:HB	1:A:2026:ARG:HB3	1.98	0.45
1:A:2170:LYS:HE3	1:A:2186:ALA:HB1	1.98	0.45
1:A:1009:GLU:O	1:A:1013:THR:OG1	2.35	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:2353:PHE:CZ	1:A:2360:LEU:HB2	2.51	0.45
1:A:623:VAL:N	1:A:639:GLN:HE22	2.12	0.45
1:A:1035:ILE:HB	1:A:1610:ASN:HD22	1.82	0.45
1:A:1533:LYS:O	1:A:1535:ASP:N	2.42	0.45
1:A:1957:TYR:CE1	1:A:1983:ASN:O	2.70	0.45
1:A:1352:VAL:O	1:A:1368:ILE:HG22	2.16	0.44
1:A:1979:TYR:HD1	1:A:1987:GLN:HB2	1.81	0.44
1:A:2092:ASP:N	1:A:2092:ASP:OD1	2.50	0.44
1:A:580:TYR:OH	1:A:634:TYR:HA	2.18	0.44
1:A:2299:GLY:HA3	1:A:2338:ILE:HD12	1.99	0.44
1:A:966:GLN:HE21	1:A:970:GLU:HG3	1.83	0.44
1:A:1036:ILE:HG21	1:A:1521:LYS:HE2	1.99	0.44
1:A:1081:SER:O	1:A:1085:ILE:HG23	2.17	0.44
1:A:876:ASN:N	1:A:876:ASN:HD22	2.16	0.44
1:A:1255:ARG:HA	1:A:1262:PHE:HB3	2.00	0.44
1:A:2354:ASP:OD1	1:A:2355:PRO:HD2	2.17	0.44
1:A:332:SER:O	1:A:335:PHE:N	2.50	0.44
1:A:1025:LEU:CD2	1:A:1025:LEU:H	2.30	0.44
1:A:1047:GLU:O	1:A:1051:THR:OG1	2.29	0.44
1:A:1344:TRP:O	1:A:1402:ILE:HD12	2.17	0.44
1:A:1400:ARG:NH2	1:A:1421:VAL:HB	2.32	0.44
1:A:1959:PHE:HE1	1:A:1966:ALA:HB2	1.82	0.44
1:A:321:MET:SD	1:A:326:TYR:HB2	2.58	0.44
1:A:1025:LEU:HD23	1:A:1623:GLU:OE2	2.17	0.44
1:A:589:ILE:HD11	1:A:757:HIS:HA	1.99	0.44
1:A:1353:LYS:HA	1:A:1367:LEU:HA	2.00	0.44
1:A:2095:THR:HG23	1:A:2097:GLU:HG3	1.99	0.44
1:A:955:GLU:O	1:A:959:LEU:HG	2.17	0.44
1:A:1123:TYR:O	1:A:1127:ILE:HG23	2.17	0.44
1:A:1585:PHE:O	1:A:1588:SER:OG	2.22	0.44
1:A:1993:ILE:O	1:A:1996:LYS:HB2	2.17	0.44
1:A:2195:VAL:HG12	1:A:2196:ASN:N	2.32	0.44
1:A:2230:TYR:CD1	1:A:2234:ASN:HB3	2.53	0.44
1:A:1376:ASN:ND2	1:A:1378:GLU:OE2	2.51	0.44
1:A:1686:ASP:OD1	1:A:1686:ASP:N	2.51	0.44
1:A:2254:ILE:HB	1:A:2263:PHE:HE2	1.82	0.44
1:A:2285:LYS:HA	1:A:2285:LYS:HD3	1.72	0.44
1:A:674:GLU:O	1:A:678:ILE:HG13	2.18	0.43
1:A:1154:GLU:O	1:A:1155:ILE:HD13	2.18	0.43
1:A:1507:ILE:CG2	1:A:1598:ASN:HD21	2.31	0.43
1:A:1949:TRP:CE3	1:A:1958:TYR:HB2	2.53	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:1951:LEU:CD2	1:A:1956:THR:HA	2.48	0.43
1:A:377:PHE:CD2	1:A:502:GLU:HG3	2.53	0.43
1:A:1253:ARG:HD2	1:A:1257:HIS:HE1	1.83	0.43
1:A:2013:VAL:O	1:A:2016:LYS:HE2	2.18	0.43
1:A:2142:TYR:CD2	1:A:2166:PRO:HD2	2.53	0.43
1:A:2329:LYS:HE3	1:A:2360:LEU:H	1.82	0.43
1:A:308:THR:HA	1:A:785:ASN:ND2	2.34	0.43
1:A:1030:PRO:CB	1:A:1556:TYR:OH	2.66	0.43
1:A:1306:GLU:O	1:A:1310:LYS:HE2	2.19	0.43
1:A:1466:ASP:O	1:A:1469:THR:HB	2.18	0.43
1:A:1498:TYR:HB3	1:A:1501:ASP:O	2.19	0.43
1:A:1959:PHE:CE1	1:A:1966:ALA:HB2	2.53	0.43
1:A:2304:ALA:O	1:A:2315:GLY:N	2.52	0.43
1:A:414:LEU:HG	1:A:418:ILE:CD1	2.48	0.43
1:A:1022:LEU:HB3	1:A:1023:PRO:CD	2.48	0.43
1:A:1381:LYS:HZ2	1:A:1383:ILE:HD11	1.84	0.43
1:A:2185:GLN:NE2	1:A:2186:ALA:O	2.51	0.43
1:A:2235:VAL:HG22	1:A:2240:LYS:HG3	2.00	0.43
1:A:1123:TYR:OH	1:A:1228:ARG:NH2	2.52	0.43
1:A:1371:ILE:HG23	1:A:1372:LEU:HD22	2.00	0.43
1:A:1498:TYR:CE2	1:A:1500:PRO:HD2	2.54	0.43
1:A:577:TYR:HB2	1:A:645:LYS:O	2.18	0.43
1:A:1167:CYS:SG	1:A:1202:ILE:HD12	2.59	0.43
1:A:1515:ASP:OD1	1:A:1515:ASP:N	2.49	0.43
1:A:1155:ILE:HB	1:A:1289:ILE:HD12	2.00	0.43
1:A:1427:ILE:HG13	1:A:1452:PHE:HE2	1.84	0.43
1:A:1459:TYR:OH	1:A:1522:GLY:O	2.25	0.43
1:A:1900:ILE:HD12	1:A:1909:PHE:CD2	2.54	0.43
1:A:1973:ILE:HB	1:A:1978:TYR:CE2	2.53	0.43
1:A:2219:LYS:HE3	1:A:2249:MET:HB3	2.00	0.43
1:A:535:LYS:HB3	1:A:535:LYS:HE3	1.81	0.43
1:A:937:PHE:CD2	1:A:947:LYS:HB2	2.54	0.43
1:A:958:THR:OG1	1:A:959:LEU:N	2.51	0.43
1:A:1041:LEU:N	1:A:1041:LEU:CD2	2.73	0.43
1:A:968:LEU:HD12	1:A:968:LEU:HA	1.83	0.43
1:A:1212:LYS:HA	1:A:1212:LYS:HD3	1.76	0.43
1:A:1251:LEU:HD22	1:A:1264:TRP:CG	2.54	0.43
1:A:2178:VAL:HG21	1:A:2189:TYR:HB2	2.00	0.43
1:A:708:GLU:OE2	1:A:708:GLU:N	2.29	0.42
1:A:1116:LYS:NZ	1:A:1276:THR:OG1	2.42	0.42
1:A:1370:ASN:OD1	1:A:1373:SER:OG	2.24	0.42



	ius puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1543:THR:HG22	1:A:1553:ASN:HD21	1.84	0.42
1:A:1722:ASP:OD1	1:A:1722:ASP:N	2.49	0.42
1:A:1742:VAL:HG12	1:A:1801:SER:HB2	2.00	0.42
1:A:2182:ILE:HB	1:A:2185:GLN:HB2	2.01	0.42
1:A:375:ILE:HG13	1:A:387:LEU:HD23	2.01	0.42
1:A:571:LYS:HA	1:A:600:LYS:O	2.19	0.42
1:A:1662:TYR:HD2	1:A:1670:ILE:HG23	1.85	0.42
1:A:224:TYR:O	1:A:228:SER:OG	2.33	0.42
1:A:250:ASP:HB2	1:A:404:LYS:HE2	2.02	0.42
1:A:1200:LEU:HD22	1:A:1258:TYR:CG	2.54	0.42
1:A:1513:LEU:HD23	1:A:1516:ILE:HD11	2.00	0.42
1:A:1650:VAL:HG12	1:A:1650:VAL:O	2.18	0.42
1:A:646:ILE:HG23	1:A:691:ILE:HG13	2.00	0.42
1:A:1306:GLU:HA	1:A:1309:ARG:HG3	2.02	0.42
1:A:1384:LEU:HD22	1:A:1404:LEU:HD21	2.01	0.42
1:A:2309:LEU:HD12	1:A:2309:LEU:HA	1.87	0.42
1:A:1036:ILE:CG2	1:A:1521:LYS:HE2	2.49	0.42
1:A:981:LEU:HA	1:A:981:LEU:HD12	1.78	0.42
1:A:1354:ASN:HB3	1:A:1365:GLY:HA3	2.00	0.42
1:A:1512:ASP:O	1:A:1514:LYS:HG3	2.19	0.42
1:A:1664:LEU:HD23	1:A:1669:ASN:O	2.20	0.42
1:A:2276:ILE:HB	1:A:2281:PHE:CE2	2.54	0.42
1:A:18:ARG:NH1	1:A:1668:GLY:O	2.53	0.42
1:A:578:ILE:HG12	1:A:640:ILE:HB	2.02	0.42
1:A:1169:ILE:HA	1:A:1230:PHE:HB2	2.02	0.42
1:A:312:TRP:HA	1:A:312:TRP:CE3	2.55	0.42
1:A:902:ASN:CG	1:A:905:THR:HG22	2.39	0.42
1:A:1114:GLN:OE1	1:A:1119:LYS:HB3	2.20	0.42
1:A:1236:TRP:CZ3	1:A:1273:ALA:HB2	2.55	0.42
1:A:911:ILE:HG22	1:A:912:GLU:O	2.20	0.41
1:A:1041:LEU:HD12	1:A:1045:ILE:CD1	2.50	0.41
1:A:1958:TYR:HD1	1:A:1967:LEU:HD13	1.85	0.41
1:A:2226:THR:HG22	1:A:2228:LYS:HD3	2.00	0.41
1:A:1022:LEU:HB3	1:A:1023:PRO:HD2	2.02	0.41
1:A:1371:ILE:HA	1:A:1374:LYS:HZ3	1.84	0.41
1:A:2142:TYR:OH	1:A:2167:ASP:OD2	2.21	0.41
1:A:2243:PHE:HE2	1:A:2249:MET:HG3	1.85	0.41
1:A:2259:ASN:HB2	1:A:2261:TYR:CE2	2.55	0.41
1:A:2342:GLY:HA2	1:A:2353:PHE:O	2.20	0.41
1:A:1264:TRP:CE2	1:A:1265:ARG:HD2	2.55	0.41
1:A:937:PHE:CE2	1:A:947:LYS:HB2	2.55	0.41



		Interstomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:A:977:SER:HG	1:A:1699:TYR:HE2	1.68	0.41	
1:A:1086:ALA:HB2	1:A:1405:THR:OG1	2.20	0.41	
1:A:1121:ILE:HD13	1:A:1248:THR:HG22	2.02	0.41	
1:A:2229:ALA:O	1:A:2231:LYS:HD2	2.20	0.41	
1:A:416:PRO:HB2	1:A:434:LYS:HE2	2.03	0.41	
1:A:1573:LYS:HD3	1:A:1687:ARG:HH22	1.84	0.41	
1:A:1999:TYR:CE1	1:A:2011:ILE:HG21	2.56	0.41	
1:A:2340:ALA:HB3	1:A:2353:PHE:CG	2.56	0.41	
1:A:970:GLU:C	1:A:972:ASN:H	2.24	0.41	
1:A:1582:LEU:HD21	1:A:1611:PHE:CD1	2.54	0.41	
1:A:1608:ASP:OD1	1:A:1609:THR:N	2.52	0.41	
1:A:2235:VAL:HG13	1:A:2240:LYS:HG3	2.02	0.41	
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.85	0.41	
1:A:1086:ALA:O	1:A:1090:SER:OG	2.20	0.41	
1:A:2162:VAL:HG11	1:A:2200:TYR:HD2	1.85	0.41	
1:A:280:ASP:N	1:A:280:ASP:OD1	2.54	0.41	
1:A:340:GLU:O	1:A:344:ARG:HG3	2.21	0.41	
1:A:493:LEU:HD22	1:A:497:GLU:OE1	2.20	0.41	
1:A:1452:PHE:CZ	1:A:1457:GLN:HB3	2.56	0.41	
1:A:72:LEU:HA	1:A:72:LEU:HD23	1.73	0.41	
1:A:93:PRO:HA	1:A:366:ILE:O	2.21	0.41	
1:A:445:MET:CE	1:A:449:LYS:HE3	2.50	0.41	
1:A:1406:PHE:CE1	1:A:1414:ILE:HB	2.56	0.41	
1:A:1539:SER:HB2	1:A:1556:TYR:HB3	2.02	0.41	
1:A:603:TYR:CD1	1:A:623:VAL:HG22	2.56	0.41	
1:A:622:SER:CA	1:A:639:GLN:HE22	2.26	0.41	
1:A:1253:ARG:HH11	1:A:1257:HIS:HE1	1.69	0.41	
1:A:1550:ILE:HD12	1:A:1603:ILE:HG21	2.02	0.41	
1:A:1973:ILE:HB	1:A:1978:TYR:HE2	1.85	0.41	
1:A:1991:ILE:HD12	1:A:2000:PHE:CD2	2.56	0.41	
1:A:2223:ASP:O	1:A:2227:LYS:HA	2.21	0.41	
1:A:2242:TYR:HB2	1:A:2263:PHE:CE1	2.56	0.41	
1:A:566:ILE:CD1	1:A:602:PRO:HB3	2.48	0.40	
1:A:1938:TYR:CE2	1:A:1952:LEU:HD23	2.56	0.40	
1:A:2281:PHE:HD1	1:A:2289:MET:SD	2.45	0.40	
1:A:72:LEU:O	1:A:75:PHE:HB3	2.22	0.40	
1:A:1031:ILE:CG2	1:A:1046:LYS:HD3	2.48	0.40	
1:A:1160:ASN:HA	1:A:1215:PHE:CE2	2.56	0.40	
1:A:1195:TYR:CD2	1:A:1196:ARG:HD3	2.56	0.40	
1:A:1286:ASN:OD1	1:A:1313:SER:HB2	2.21	0.40	
1:A:1470:LYS:HE3	1:A:1470:LYS:HB2	1.99	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2008:VAL:HG23	1:A:2021:GLY:O	2.21	0.40
1:A:363:LEU:HD22	1:A:366:ILE:HD11	2.02	0.40
1:A:1663:HIS:H	1:A:1671:SER:HG	1.70	0.40
1:A:1926:PHE:HE1	1:A:1930:LEU:HB2	1.86	0.40
1:A:1111:LEU:N	1:A:1281:ARG:HH12	2.13	0.40
1:A:2130:PHE:CD2	1:A:2132:PHE:HE2	2.40	0.40
1:A:1409:LEU:HB2	1:A:1412:ILE:HB	2.03	0.40
1:A:2174:PRO:HG2	1:A:2177:THR:HG21	2.02	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 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	Perce	ntiles
1	А	2351/2372~(99%)	2210 (94%)	135 (6%)	6~(0%)	41	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	707	ALA
1	А	1948	GLU
1	А	1029	LEU
1	А	1762	PRO
1	А	2342	GLY
1	А	1023	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	А	2130/2146~(99%)	2033~(95%)	97~(5%)	27	60

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	92	THR
1	А	192	SER
1	А	200	PHE
1	А	228	SER
1	А	238	ASN
1	А	244	GLU
1	А	272	LEU
1	А	280	ASP
1	А	288	ASP
1	А	339	ASP
1	А	395	CYS
1	А	413	ASN
1	А	417	SER
1	А	419	ASN
1	А	469	SER
1	А	485	LYS
1	А	492	HIS
1	А	529	SER
1	А	535	LYS
1	А	574	ASN
1	А	644	ARG
1	А	646	ILE
1	А	656	SER
1	А	685	ASP
1	А	702	SER
1	А	703	TYR
1	А	757	HIS
1	А	863	GLU
1	А	865	ILE
1	А	879	ASP
1	А	881	SER
1	А	897	ARG
1	А	914	GLU
1	А	937	PHE
1	А	946	LYS



Mol	Chain	Res	Type
1	А	958	THR
1	А	968	LEU
1	А	971	TYR
1	А	1010	LEU
1	А	1013	THR
1	А	1019	ILE
1	А	1040	SER
1	А	1041	LEU
1	А	1055	LEU
1	А	1058	GLN
1	А	1072	THR
1	А	1116	LYS
1	А	1167	CYS
1	А	1230	PHE
1	А	1285	THR
1	A	1297	SER
1	А	1305	THR
1	А	1307	GLN
1	А	1310	LYS
1	А	1332	MET
1	А	1340	GLU
1	А	1392	TYR
1	А	1433	CYS
1	А	1462	TYR
1	А	1527	LEU
1	А	1534	ASP
1	А	1543	THR
1	А	1547	THR
1	A	1576	LEU
1	А	1591	ILE
1	А	1598	ASN
1	A	1602	ASN
1	A	1626	CYS
1	A	1629	ASP
1	A	1662	TYR
1	A	1665	ASP
1	A	1698	LEU
1	A	1775	ASP
1	A	1776	THR
1	A	1795	LYS
1	A	1801	SER
1	А	1814	PHE



Mol	Chain	Res	Type
1	А	1820	ASP
1	А	1821	ASN
1	А	1831	ASN
1	А	1842	SER
1	А	1895	LEU
1	А	1927	ILE
1	A	1947	VAL
1	А	1955	GLU
1	А	1995	ASP
1	А	2032	ASN
1	А	2037	PHE
1	А	2051	GLU
1	А	2092	ASP
1	А	2131	TYR
1	A	2183	TYR
1	А	2212	TRP
1	А	2259	ASN
1	А	2320	TYR
1	А	2323	TRP
1	А	2362	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	5	ASN
1	А	8	GLN
1	А	106	GLN
1	А	236	ASN
1	А	413	ASN
1	А	419	ASN
1	А	639	GLN
1	А	732	GLN
1	А	741	GLN
1	А	785	ASN
1	А	876	ASN
1	А	941	ASN
1	А	949	ASN
1	А	988	GLN
1	А	1109	ASN
1	А	1390	ASN
1	А	1453	ASN
1	А	1520	ASN



Mol	Chain	Res	Type
1	А	1553	ASN
1	А	1593	ASN
1	А	1631	ASN
1	А	1763	GLN
1	А	2058	ASN
1	А	2143	GLN
1	А	2260	ASN
1	А	2319	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)

Of 1 ligands modelled in this entry, 1 is 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 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-36141. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



The images above show the map projected in three orthogonal directions.



6.2 Central slices (i)

6.2.1 Primary map



X Index: 148



Y Index: 148



Z Index: 148

6.2.2 Raw map



X Index: 148

Y Index: 148



The images above show central slices of the map in three orthogonal directions.



6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 159



Y Index: 130



Z Index: 135

6.3.2 Raw map



X Index: 159

Y Index: 130



The images above show the largest variance slices of the map in three orthogonal directions.



6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)



The volume at the recommended contour level is 100 $\rm nm^3;$ this corresponds to an approximate mass of 90 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.345 $\rm \AA^{-1}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.345 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{B}_{\mathbf{a}}$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.40	4.04	3.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.40 differs from the reported value 2.9 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-36141 and PDB model 8JB5. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).



9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6390	0.4770
A	0.6390	0.4770



