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PDB ID	:	8X2I
EMDB ID	:	EMD-38011
Title	:	Cryo-EM structure of the TcsL at pH 5.0 in its open conformation
Authors	:	Zhan, X.; Tao, L.
Deposited on	:	2023-11-09
Resolution	:	2.50 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:

EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	whole archive $(\#$ Entries)	$\mathop{\mathrm{EM}}\limits_{(\#\mathrm{Entries})}$
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		
			25%		
1	А	2372	65%	29% •	•



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18645 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	oms			AltConf	Trace
1	А	2303	Total 18644	C 11942	N 2959	O 3697	S 46	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





H1186 F1187	F1188	S1190	P1191	I1193	T1194	R1196	K1197	W1199	L1200	51201	11202 Y1203	D1204	V1205	L1206 N1207	11208	K1209 K1210	E1211	K1212 11213	D1214	F1215 S1216	K1217 D1218	L1219	V1221	N1224	A1225	P1226	R1228	V1229	G1231	Y1232	E1233 M1234	G1235	W1236	1123/ P1238	G1239	F1240	R1241	L1243	D1244	D1246		
G1247	K1249	L1251	D1252	11254	R1255	H1257	Y1258	G1260	Q1261	F1262	11263 W1264	R1265	Y1266	F1267	F1269	11270	A12/1 D1272	A1273	L1274	11275 T1276	K1277	L1278	P1280	R1281	Y1282	D1284	R1288	11289 N1290	L1291	G1293	N1294 T1295	R1296	11299	V1300	11303	T1304	E1306	q1307	11308 R1309	K1310		
N1311	S1313	F1 <mark>316</mark> Y1317	61318 81319	S1322	Y1323 S1324	L1325		M1332	N1333 11334	D1335 11236	N1337	L1338 V1339	E1340 N1 24 1	THOTN	V1345 I1346	D1347 V1348		V1351 V1352	K1353	11355 11355	T1356	E1358	S1359	D1360	11362	Q1363	E1 <mark>366</mark>	11368 11368	E1369	11371 11370	S1373	L1375	N1376	D1379	N1380							
11383 11383	L1 304 N1 385 N1 386	H1387	11389 N1390	F1391	D1394	11395 • N1396	E1397	06010	R1400	11402	S1403 L1404	T1405	S1407	11408	1 CTC	N1413 11414	11415 11416		L1420 V1421	S1422	K1423	Y1425	K1426 11427	S1430	G1431 N1432	K1435	L1436	11437 E1438	N1439 51440	S1441	D1442	Q1444	Q1445 K1446	11447 D1448								
H1449 I1450	G1451 F1452 M1452	01453 G1454	E1455 H1456	Q1457 K1458	Y1459 I1460	P1461	11402 S1463 V1/2/	11404 11465	D1466 N1467		Y1471	Y1477	K1479	K1480	F1484	E1 <mark>4</mark> 91	N1496	11497	P1500	N1503	N1504 L1505	C1E10	K1511	D1512 L1513	K1514 D1515	11516 R1517		D1523	N1530 Y1531	F1532 V1533	D1534	M1536	S1539									
L1540 S1541 F1543	D1546	11560	V1556	E1559	01564	11565			K1573 S1574	A1575	T1578	1.1582	M1583	L1586	E1587 S1588	I1589 M1500	11591	K1592 N1593	I1594	N1598	N1610	11613	S1614	81616 S1616	N1617 S1618	01621	11624		D1629	P1634	K1638	F1639 K1640										
I1641 K1642 F1643	E1043 T1644 S1645	Y1646	1651	N1652 R1653	01654 N1655		Y1662	S1667	01679		L1682 Y1683	G1684	R1687	11693	L1698	11706	P1707	K1710	P1711 N1712	Y1713	L1/14 C1715	P1716	D1722	11726	K1729	L1737	Y1741	S1748	D1749	11751	A1754	E1758										
N1770	F1772	D1779	81 <mark>782</mark>	V1791	K1795 11796	11797	F1800	S1801	S1806 D1807	G1808	Y1812		51818	Y1823	N1827	N1831	Y1838	D1 8/1	S1842	L1843	K1847	N1851	11 <mark>854</mark>	F1857	T1858	K1864	F1 <mark>867</mark>	<mark>S1872</mark>	S1876	11880	K1885	ц1 880										
L1895	V1899 11900	N1901	L1906 K1907	Y1908 F1909	A1910 P1911	A1912	L1 <mark>915</mark>	E1920	G1921 E1922	S1923	V1924 N1925	F1926 T1927	G1928	K1929 L1930	N1931	20011	11936 Y1937	Y1938	V1947	E1948 W1949	K1950 L1951	L1952	D1954	E1955 T1956	Y1957 Y1958	F1959 N1960	P1961	G1964	E1965 A1966	L1967	K1968 G1969	L1970 H1971	Q1972									
11973 G1974	D1975 N1976	K1977	Y1979 F1980	D1981 D1982	N1983 G1984	11985 M1086	01987 01987 11000	G1989	F1990	11991	11993	N1994	D1995		F1998	F2000	N2001	N2002	G2004	V2005		V2008	G2009	I2011	E2012	N2013	G2015	K2016	F2018	Y2019	G2021	K2022	N2023 G2024	E2025	R2026	ц2027 1.2028	G2029	V2030	F2031			
T2033	D2035	F2037	K2038	F2040	G2041 P2042	K2043	D2044 D2045	D2046	L2047	T2049	E2050	E2051	G2052	L2054	T2055	L2056	N2058	G2059	12060 L2061	N2062	F2063	G2065	K2066	12067	F2069	F2070	12072	S2073	N2074	A2076	V2077	G2079	W2080	G2081	12082 L2083	D2084	D2085	G2086	T2088	Y2089	F2091	D2092
D2093	T2095	E2097		I2100	G2101 L2102	T2103	V2104	N2106	D2107	C2108	Y2110	Y2111	F2112		N2115	G2116		Q2119	L2120	G2121 F2122	12123	T2124	N2126	D2127	N2128	F2130	Y2131	F2132 S2133	E2134	S2135	K2137	I2138	E2139 L2140	G2141	Y2142	Q2143	I2145	N2146	G2147	Y2149	F2150	12152
D2153	S2155		V2158	12160	G2161 V2162	F2163	D2164	P2166	D2167	G2168	K2170	Y2171	F2172	A2173	L2175	N2176	V2178	N2179	D2180	N2181	Y2183	G2184	42185	V2187	K2188	S2190	G2191	L2192 V2193	R2194	V2195	E2197	D2198	V2199 Y2200	Y2201	F2202	G2203	T2205	Y2206	K2207	E2209	12210 G2211	W2212







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1045888	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 x 4k)	Depositor
Maximum map value	12.371	Depositor
Minimum map value	-8.281	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	434.80002, 434.80002, 434.80002	wwPDB
Map dimensions	400, 400, 400	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	Bo	nd lengths	Bo	ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.45	2/19023~(0.0%)	0.56	2/25734~(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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	284	TYR	CD1-CE1	-5.46	1.31	1.39
1	А	284	TYR	CD2-CE2	-5.22	1.31	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	1505	LEU	CA-CB-CG	6.18	129.52	115.30
1	А	1982	ASP	CB-CG-OD2	5.10	122.89	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	1511	LYS	Peptide
1	А	364	ASP	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	18644	0	18175	508	0
2	А	1	0	0	0	0
All	All	18645	0	18175	508	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 (508) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	\mathbf{Clash}
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1956:THR:HG23	1:A:1986:MET:N	1.21	1.51
1:A:1956:THR:CG2	1:A:1986:MET:N	1.86	1.38
1:A:1956:THR:HG21	1:A:1986:MET:CA	1.71	1.19
1:A:1956:THR:HG21	1:A:1986:MET:CB	1.74	1.18
1:A:1956:THR:CG2	1:A:1986:MET:CB	2.34	1.05
1:A:1956:THR:CG2	1:A:1986:MET:H	1.50	1.04
1:A:1956:THR:HG22	1:A:1985:ILE:HG22	1.40	1.03
1:A:1956:THR:HG21	1:A:1986:MET:HB3	1.32	1.03
1:A:1956:THR:CG2	1:A:1986:MET:CA	2.32	1.03
1:A:699:ASN:H	1:A:741:GLN:HE21	1.12	0.95
1:A:1956:THR:CG2	1:A:1986:MET:HB3	1.96	0.94
1:A:1356:THR:HG23	1:A:1363:GLN:HB3	1.59	0.84
1:A:1956:THR:HG21	1:A:1986:MET:C	1.99	0.83
1:A:1591:ILE:HG22	1:A:1592:LYS:HD2	1.64	0.79
1:A:1154:GLU:HG3	1:A:1163:THR:HG22	1.65	0.79
1:A:1573:LYS:HA	1:A:1687:ARG:HH12	1.47	0.78
1:A:1956:THR:OG1	1:A:1986:MET:HB2	1.83	0.77
1:A:1956:THR:OG1	1:A:1986:MET:CB	2.33	0.77
1:A:1326:SER:HA	1:A:1347:ASP:HB3	1.65	0.76
1:A:1082:ALA:HB1	1:A:1405:THR:HG21	1.68	0.76
1:A:957:ASN:HA	1:A:960:ASN:HB2	1.68	0.76
1:A:2194:ARG:HG2	1:A:2199:VAL:HG12	1.67	0.75
1:A:1628:LYS:H	1:A:1628:LYS:HD2	1.51	0.74
1:A:2128:ASN:HB3	1:A:2157:LEU:HD22	1.70	0.73
1:A:499:ARG:NH1	1:A:502:GLU:OE1	2.22	0.73



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:1827:ASN:ND2	1:A:1831:ASN:O	2.22	0.72
1:A:1956:THR:HG21	1:A:1986:MET:O	1.88	0.72
1:A:1956:THR:CB	1:A:1986:MET:HB3	2.18	0.72
1:A:1956:THR:O	1:A:1985:ILE:HA	1.90	0.71
1:A:2088:THR:HG21	1:A:2118:ARG:HH21	1.54	0.71
1:A:1791:VAL:HG13	1:A:1795:LYS:HD2	1.72	0.71
1:A:1570:ASN:O	1:A:1687:ARG:NH2	2.24	0.70
1:A:1464:TYR:HB3	1:A:1471:TYR:HB2	1.71	0.70
1:A:1334:ILE:HB	1:A:1389:ILE:HG23	1.75	0.69
1:A:1427:ILE:HD13	1:A:1452:PHE:HE2	1.57	0.69
1:A:1345:VAL:HA	1:A:1403:SER:O	1.93	0.69
1:A:1233:GLU:HB3	1:A:1277:LYS:HB2	1.74	0.68
1:A:2123:ILE:O	1:A:2130:PHE:HB2	1.92	0.68
1:A:1952:LEU:HD12	1:A:1952:LEU:N	2.09	0.68
1:A:1427:ILE:O	1:A:1457:GLN:NE2	2.19	0.67
1:A:924:HIS:O	1:A:928:GLU:HG3	1.93	0.67
1:A:2017:TYR:HB2	1:A:2054:LEU:HD22	1.76	0.67
1:A:1128:SER:HB2	1:A:1250:LEU:HG	1.77	0.67
1:A:1371:ILE:HG23	1:A:1372:LEU:HD22	1.74	0.67
1:A:2119:GLN:HG3	1:A:2123:ILE:HG13	1.76	0.67
1:A:1353:LYS:HA	1:A:1367:LEU:HA	1.76	0.66
1:A:1348:VAL:HG21	1:A:1404:LEU:HD13	1.77	0.66
1:A:1956:THR:O	1:A:1985:ILE:HG23	1.95	0.65
1:A:2118:ARG:NH1	1:A:2135:SER:O	2.30	0.65
1:A:1307:GLN:O	1:A:1311:ASN:ND2	2.22	0.64
1:A:2253:LEU:HG	1:A:2260:ASN:HD21	1.61	0.64
1:A:294:GLN:NE2	1:A:357:SER:O	2.30	0.64
1:A:1899:VAL:HG11	1:A:1937:TYR:CE1	2.32	0.64
1:A:295:PRO:O	1:A:299:LYS:HE3	1.98	0.64
1:A:2111:TYR:HE1	1:A:2123:ILE:HB	1.61	0.64
1:A:1096:LEU:HD11	1:A:1357:ILE:HD11	1.79	0.63
1:A:1184:ILE:HD12	1:A:1265:ARG:HB3	1.79	0.63
1:A:2174:PRO:O	1:A:2181:ASN:ND2	2.31	0.63
1:A:921:TYR:CZ	1:A:925:ILE:HG21	2.33	0.63
1:A:1827:ASN:HD21	1:A:1831:ASN:HB2	1.63	0.63
1:A:1218:ASP:HB2	1:A:1296:ARG:HA	1.80	0.63
1:A:1737:LEU:HD13	1:A:1872:SER:HB2	1.82	0.62
1:A:2244:ASP:HB3	1:A:2250:ARG:CZ	2.29	0.62
1:A:1290:ASN:HA	1:A:1317:TYR:HB3	1.82	0.62
1:A:559:LYS:O	1:A:563:SER:OG	2.14	0.62
1:A:1960:ASN:HB3	1:A:1964:GLY:H	1.65	0.62



	, as page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1405:THR:HG22	1:A:1415:ILE:HG12	1.81	0.62
1:A:421:GLY:O	1:A:426:THR:HB	2.00	0.62
1:A:1324:SER:HB2	1:A:1345:VAL:HG23	1.82	0.62
1:A:1143:ILE:HG23	1:A:1219:LEU:HG	1.82	0.61
1:A:622:SER:HA	1:A:639:GLN:HE22	1.64	0.61
1:A:1295:THR:HA	1:A:1322:SER:O	2.00	0.61
1:A:1003:ASP:HB3	1:A:1006:LYS:HB2	1.80	0.61
1:A:2043:LYS:H	1:A:2051:GLU:HG2	1.65	0.61
1:A:744:VAL:HG22	1:A:754:ILE:HG22	1.82	0.61
1:A:1170:TRP:O	1:A:1232:TYR:OH	2.12	0.60
1:A:769:ILE:HG21	1:A:824:CYS:HB3	1.82	0.60
1:A:1181:THR:O	1:A:1184:ILE:HG22	2.01	0.60
1:A:1316:PHE:HE2	1:A:1334:ILE:HG23	1.65	0.60
1:A:250:ASP:HB3	1:A:404:LYS:HE2	1.83	0.60
1:A:324:LYS:O	1:A:325:GLU:HG2	2.02	0.60
1:A:1001:ILE:HD12	1:A:1010:LEU:HD13	1.84	0.60
1:A:1956:THR:CB	1:A:1986:MET:CB	2.78	0.60
1:A:1722:ASP:OD1	1:A:1722:ASP:N	2.25	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	0.59
1:A:1956:THR:OG1	1:A:1986:MET:HB3	2.01	0.59
1:A:1587:GLU:HA	1:A:1592:LYS:HD3	1.84	0.59
1:A:1818:SER:HB2	1:A:1823:TYR:CE1	2.37	0.59
1:A:1970:LEU:HD21	1:A:1977:LYS:HD3	1.84	0.58
1:A:854:TYR:CE1	1:A:960:ASN:HB3	2.37	0.58
1:A:1947:VAL:O	1:A:1959:PHE:HB2	2.01	0.58
1:A:959:LEU:HB2	1:A:1651:GLY:HA3	1.85	0.58
1:A:1772:PHE:CE1	1:A:1797:ILE:HD11	2.39	0.58
1:A:1915:LEU:CD2	1:A:1925:ASN:O	2.51	0.58
1:A:158:ARG:HG3	1:A:539:PHE:HE1	1.68	0.58
1:A:637:PRO:HD2	1:A:640:ILE:HD11	1.84	0.58
1:A:966:GLN:O	1:A:970:GLU:HB3	2.03	0.58
1:A:1153:SER:HB2	1:A:1163:THR:HG23	1.85	0.58
1:A:1496:ASN:O	1:A:1505:LEU:HA	2.03	0.58
1:A:979:SER:HA	1:A:982:SER:HB3	1.85	0.58
1:A:2244:ASP:HB3	1:A:2250:ARG:NE	2.19	0.58
1:A:631:ILE:HD12	1:A:637:PRO:HG3	1.86	0.58
1:A:2320:TYR:HE1	1:A:2324:LEU:HB2	1.69	0.57
1:A:1858:THR:HB	1:A:1867:PHE:HE2	1.70	0.57
1:A:1956:THR:HG23	1:A:1986:MET:H	0.58	0.57
1:A:2273:TYR:HE2	1:A:2280:MET:HB3	1.68	0.57



	juo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1640:LYS:HE2	1:A:1643:GLU:HA	1.86	0.57
1:A:2188:LYS:HB3	1:A:2206:TYR:CD2	2.40	0.57
1:A:173:ARG:NH2	1:A:823:GLU:OE2	2.34	0.57
1:A:528:LYS:NZ	1:A:545:GLU:OE2	2.33	0.57
1:A:577:TYR:HB3	1:A:645:LYS:HB2	1.87	0.57
1:A:1748:SER:HB2	1:A:1770:ASN:HA	1.86	0.57
1:A:1929:LYS:HE3	1:A:1936:ILE:HG23	1.87	0.57
1:A:196:GLU:HG3	1:A:197:ASN:N	2.20	0.57
1:A:540:GLU:HG2	1:A:541:GLY:H	1.70	0.57
1:A:702:SER:HB3	1:A:776:GLU:HB2	1.86	0.57
1:A:529:SER:O	1:A:533:GLU:HG3	2.04	0.56
1:A:1511:LYS:HG2	1:A:1512:ASP:OD1	2.05	0.56
1:A:1908:TYR:O	1:A:1923:SER:HA	2.05	0.56
1:A:1908:TYR:CE2	1:A:1930:LEU:HD21	2.40	0.56
1:A:1348:VAL:HG23	1:A:1406:PHE:HB3	1.86	0.56
1:A:921:TYR:CE1	1:A:925:ILE:HD13	2.40	0.56
1:A:1385:ASN:O	1:A:1387:HIS:ND1	2.34	0.56
1:A:2300:PHE:HB3	1:A:2339:ALA:HB3	1.88	0.56
1:A:60:LEU:HD13	1:A:73:LYS:HE2	1.87	0.56
1:A:1437:ILE:HD12	1:A:1497:ILE:HD12	1.87	0.56
1:A:1899:VAL:HG11	1:A:1937:TYR:CZ	2.40	0.56
1:A:1956:THR:CG2	1:A:1985:ILE:HG22	2.26	0.56
1:A:1292:ASP:OD1	1:A:1296:ARG:NH1	2.26	0.56
1:A:1949:TRP:CZ2	1:A:1973:ILE:HG21	2.40	0.56
1:A:1864:LYS:HE3	1:A:1895:LEU:HD13	1.87	0.56
1:A:1956:THR:CG2	1:A:1986:MET:O	2.54	0.56
1:A:310:THR:HG23	1:A:511:LEU:HD13	1.87	0.56
1:A:1154:GLU:HA	1:A:1288:ARG:O	2.06	0.56
1:A:1345:VAL:HG12	1:A:1403:SER:HB3	1.87	0.55
1:A:1586:LEU:HD21	1:A:1613:ILE:HD11	1.88	0.55
1:A:2276:ILE:HG22	1:A:2277:LYS:HG2	1.88	0.55
1:A:1303:ILE:HB	1:A:1309:ARG:HG2	1.88	0.55
1:A:1151:VAL:HG12	1:A:1165:GLY:HA3	1.88	0.55
1:A:545:GLU:HB2	1:A:757:HIS:CD2	2.41	0.55
1:A:1346:ILE:HG22	1:A:1348:VAL:HG13	1.87	0.55
1:A:1515:ASP:HB3	1:A:1530:ASN:ND2	2.22	0.55
1:A:562:VAL:O	1:A:566:ILE:HG13	2.07	0.55
1:A:2293:VAL:HG12	1:A:2300:PHE:HD2	1.72	0.55
1:A:955:GLU:O	1:A:959:LEU:HG	2.07	0.55
1:A:2011:ILE:HD12	1:A:2020:PHE:HD2	1.72	0.55
1:A:1316:PHE:HB2	1:A:1336:LEU:HD23	1.89	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:2043:LYS:HE2	1:A:2050:GLU:HA	1.88	0.54
1:A:708:GLU:HG3	1:A:787:ILE:HD12	1.89	0.54
1:A:814:ASP:OD2	1:A:814:ASP:N	2.37	0.54
1:A:968:LEU:HG	1:A:985:MET:HG3	1.90	0.54
1:A:1185:ASP:HB2	1:A:1265:ARG:O	2.07	0.54
1:A:1425:TYR:O	1:A:1456:HIS:NE2	2.36	0.54
1:A:1166:LYS:HD2	1:A:1227:ASN:HB3	1.90	0.54
1:A:2190:SER:HA	1:A:2202:PHE:HB2	1.90	0.54
1:A:559:LYS:NZ	1:A:628:ILE:O	2.35	0.53
1:A:1168:GLU:HB2	1:A:1229:VAL:HA	1.90	0.53
1:A:1432:ASN:OD1	1:A:1435:LYS:N	2.30	0.53
1:A:420:GLU:HG3	1:A:430:ILE:HD13	1.91	0.53
1:A:226:GLU:OE1	1:A:230:ASN:ND2	2.39	0.53
1:A:1514:LYS:N	1:A:1530:ASN:O	2.39	0.53
1:A:1638:LYS:HG3	1:A:1647:THR:HG23	1.90	0.53
1:A:1714:ILE:HG13	1:A:1716:PRO:HD3	1.89	0.53
1:A:1512:ASP:OD1	1:A:1512:ASP:N	2.41	0.53
1:A:2223:ASP:HB2	1:A:2230:TYR:HE2	1.73	0.53
1:A:1316:PHE:CE2	1:A:1334:ILE:HG23	2.43	0.53
1:A:1448:ASP:OD1	1:A:1477:TYR:OH	2.25	0.53
1:A:692:GLU:HG2	1:A:736:THR:HB	1.90	0.53
1:A:719:ILE:HA	1:A:722:ARG:HE	1.73	0.53
1:A:1125:LYS:HG3	1:A:1247:GLY:HA3	1.91	0.53
1:A:1698:LEU:HD12	1:A:1726:ILE:HG13	1.89	0.53
1:A:1334:ILE:HB	1:A:1389:ILE:HD12	1.91	0.53
1:A:672:SER:HB3	1:A:722:ARG:NH2	2.24	0.53
1:A:1264:TRP:HE1	1:A:1265:ARG:HH21	1.56	0.53
1:A:1996:LYS:HB3	1:A:2025:GLU:HG2	1.91	0.53
1:A:1989:GLY:H	1:A:2000:PHE:HB2	1.73	0.53
1:A:980:ASN:N	1:A:980:ASN:OD1	2.41	0.52
1:A:373:VAL:HG23	1:A:395:CYS:HB3	1.91	0.52
1:A:1624:LEU:HD23	1:A:1634:PRO:HA	1.91	0.52
1:A:573:ARG:HG2	1:A:1806:SER:O	2.09	0.52
1:A:633:LYS:HE2	1:A:634:TYR:CE1	2.44	0.52
1:A:1340:GLU:HB2	1:A:1396:ASN:HD21	1.74	0.52
1:A:175:ARG:O	1:A:179:ILE:HG13	2.09	0.52
1:A:1533:LYS:HE2	1:A:1536:MET:HE3	1.92	0.52
1:A:1847:LYS:O	1:A:1851:ASN:N	2.39	0.52
1:A:1336:LEU:HD12	1:A:1338:LEU:HD23	1.92	0.52
1:A:1221:VAL:HG22	1:A:1299:ILE:HG23	1.90	0.52
1:A:2160:ILE:HA	1:A:2172:PHE:O	2.10	0.52



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1575:ALA:HA	1:A:1578:THR:HG22	1.91	0.52
1:A:1796:ILE:O	1:A:1800:PHE:HB2	2.10	0.52
1:A:2244:ASP:CB	1:A:2250:ARG:CZ	2.87	0.52
1:A:2049:THR:HG22	1:A:2053:GLU:HB3	1.92	0.51
1:A:1510:SER:OG	1:A:1511:LYS:O	2.27	0.51
1:A:1540:LEU:HD11	1:A:1552:LEU:HD22	1.92	0.51
1:A:1957:TYR:HE1	1:A:1983:ASN:O	1.93	0.51
1:A:196:GLU:HG3	1:A:197:ASN:H	1.74	0.51
1:A:2336:GLU:HG3	1:A:2338:ILE:HG22	1.91	0.51
1:A:975:LYS:O	1:A:976:GLU:HG2	2.11	0.51
1:A:1120:VAL:HG13	1:A:1278:LEU:HD11	1.92	0.51
1:A:2242:TYR:HB2	1:A:2263:PHE:CZ	2.46	0.51
1:A:513:GLU:O	1:A:517:THR:HG23	2.09	0.51
1:A:549:LEU:HD11	1:A:589:ILE:HD12	1.92	0.51
1:A:621:TYR:HD2	1:A:628:ILE:HG13	1.76	0.51
1:A:1976:ASN:HB3	1:A:2005:VAL:HG13	1.93	0.51
1:A:2244:ASP:CB	1:A:2250:ARG:NH2	2.73	0.51
1:A:13:ALA:O	1:A:68:ARG:NH1	2.44	0.51
1:A:1444:GLN:HA	1:A:1447:ILE:HG22	1.93	0.51
1:A:1968:LYS:HE2	1:A:1982:ASP:O	2.11	0.51
1:A:1116:LYS:O	1:A:1120:VAL:HG23	2.11	0.51
1:A:1559:GLU:OE1	1:A:1618:SER:OG	2.27	0.51
1:A:576:GLU:HB2	1:A:577:TYR:CD1	2.46	0.51
1:A:979:SER:O	1:A:983:VAL:HG22	2.11	0.51
1:A:1117:ALA:O	1:A:1121:ILE:HD12	2.10	0.51
1:A:966:GLN:HE21	1:A:970:GLU:HB2	1.76	0.50
1:A:2177:THR:OG1	1:A:2181:ASN:ND2	2.31	0.50
1:A:1586:LEU:O	1:A:1591:ILE:HB	2.11	0.50
1:A:1400:ARG:NH2	1:A:1421:VAL:HB	2.26	0.50
1:A:2011:ILE:HD12	1:A:2020:PHE:CD2	2.47	0.50
1:A:1497:ILE:HG12	1:A:1505:LEU:HB2	1.93	0.50
1:A:1291:LEU:O	1:A:1319:SER:OG	2.22	0.50
1:A:2177:THR:N	1:A:2181:ASN:OD1	2.43	0.50
1:A:340:GLU:O	1:A:344:ARG:HG2	2.12	0.50
1:A:1251:LEU:HD13	1:A:1264:TRP:CZ2	2.46	0.50
1:A:1352:VAL:HG13	1:A:1371:ILE:HG12	1.93	0.50
1:A:2244:ASP:HB2	1:A:2250:ARG:NH2	2.27	0.50
1:A:1981:ASP:N	1:A:1981:ASP:OD1	2.44	0.49
1:A:190:TYR:O	1:A:194:ILE:HG13	2.12	0.49
1:A:700:MET:HB3	1:A:739:ALA:HB1	1.94	0.49
1:A:2264:ASN:OD1	1:A:2267:GLY:N	2.45	0.49



	jae page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1327:LEU:HD13	1:A:1346:ILE:HG23	1.94	0.49
1:A:1807:ASP:HB2	1:A:1812:TYR:HE2	1.77	0.49
1:A:1104:PRO:HA	1:A:1112:ILE:O	2.13	0.49
1:A:886:PHE:HB2	1:A:988:GLN:HE22	1.77	0.49
1:A:1238:PRO:HG3	1:A:1271:ALA:HB1	1.94	0.49
1:A:1582:LEU:O	1:A:1586:LEU:HG	2.13	0.49
1:A:722:ARG:HA	1:A:725:GLU:HG2	1.94	0.49
1:A:1169:ILE:HG23	1:A:1232:TYR:HE2	1.77	0.49
1:A:2208:ILE:HD13	1:A:2227:LYS:HG2	1.93	0.49
1:A:557:LEU:HD22	1:A:607:LEU:HD23	1.95	0.49
1:A:2172:PHE:CE2	1:A:2186:ALA:HB2	2.48	0.49
1:A:2215:ASN:O	1:A:2217:THR:N	2.37	0.49
1:A:106:GLN:NE2	1:A:231:LYS:HD3	2.28	0.48
1:A:1956:THR:HG22	1:A:1985:ILE:CG2	2.26	0.48
1:A:2058:ASN:HD21	1:A:2072:ILE:HA	1.77	0.48
1:A:2230:TYR:HD1	1:A:2234:ASN:HB3	1.77	0.48
1:A:1144:ILE:HD11	1:A:1217:LYS:HD2	1.95	0.48
1:A:1113:LEU:HB2	1:A:1280:PRO:HD3	1.94	0.48
1:A:1352:VAL:HG13	1:A:1371:ILE:HG21	1.95	0.48
1:A:1981:ASP:OD1	1:A:1985:ILE:N	2.41	0.48
1:A:1348:VAL:HB	1:A:1351:VAL:HB	1.96	0.48
1:A:1437:ILE:HD11	1:A:1484:PHE:CE2	2.47	0.48
1:A:959:LEU:HB2	1:A:1651:GLY:CA	2.43	0.48
1:A:1076:THR:O	1:A:1080:THR:HG23	2.13	0.48
1:A:921:TYR:O	1:A:925:ILE:HG12	2.14	0.48
1:A:1901:ASN:HA	1:A:1906:LEU:HA	1.96	0.48
1:A:635:ARG:NH2	1:A:685:ASP:OD1	2.47	0.47
1:A:1154:GLU:HG3	1:A:1163:THR:CG2	2.39	0.47
1:A:2341:THR:O	1:A:2353:PHE:HB2	2.14	0.47
1:A:838:GLU:HA	1:A:838:GLU:OE1	2.13	0.47
1:A:956:VAL:HG23	1:A:957:ASN:H	1.79	0.47
1:A:1439:ASN:OD1	1:A:1442:ASP:HB3	2.14	0.47
1:A:1542:PHE:HB3	1:A:1552:LEU:HD23	1.94	0.47
1:A:1967:LEU:HB3	1:A:1971:HIS:CD2	2.50	0.47
1:A:2317:SER:O	1:A:2317:SER:OG	2.32	0.47
1:A:41:SER:O	1:A:45:LYS:HG3	2.13	0.47
1:A:1610:ASN:OD1	1:A:1610:ASN:N	2.47	0.47
1:A:1634:PRO:HD2	1:A:1654:GLN:NE2	2.30	0.47
1:A:2129:ILE:O	1:A:2157:LEU:HA	2.15	0.47
1:A:1292:ASP:OD1	1:A:1292:ASP:N	2.46	0.47
1:A:1409:LEU:HD11	1:A:1446:LYS:HG3	1.97	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:801:LEU:HD13	1:A:828:VAL:HB	1.97	0.47
1:A:1169:ILE:HD12	1:A:1202:ILE:HD11	1.97	0.47
1:A:1327:LEU:HD22	1:A:1348:VAL:HG12	1.96	0.47
1:A:1439:ASN:O	1:A:1443:ILE:HG13	2.15	0.47
1:A:1977:LYS:HD2	1:A:2006:MET:SD	2.55	0.47
1:A:2243:PHE:CE2	1:A:2249:MET:HG3	2.50	0.47
1:A:1156:ASP:OD1	1:A:1290:ASN:ND2	2.48	0.47
1:A:1167:CYS:HB2	1:A:1203:TYR:CD2	2.50	0.47
1:A:1458:LYS:HE3	1:A:1458:LYS:HB3	1.55	0.47
1:A:1973:ILE:HD13	1:A:1978:TYR:HD2	1.79	0.47
1:A:689:LYS:HD3	1:A:729:SER:HB2	1.97	0.47
1:A:1480:LYS:HG3	1:A:1500:PRO:HD3	1.97	0.47
1:A:1838:TYR:CE1	1:A:1843:LEU:HB2	2.50	0.47
1:A:270:ASP:HB3	1:A:469:SER:HB2	1.96	0.46
1:A:2242:TYR:HE1	1:A:2256:PHE:HB2	1.81	0.46
1:A:2264:ASN:HD21	1:A:2266:ASP:HB3	1.80	0.46
1:A:754:ILE:HG23	1:A:768:ILE:HG12	1.97	0.46
1:A:1354:ASN:N	1:A:1366:GLU:O	2.44	0.46
1:A:1371:ILE:HG22	1:A:1450:ILE:HD12	1.96	0.46
1:A:2113:ASP:OD2	1:A:2117:ILE:HB	2.16	0.46
1:A:2151:TYR:HB2	1:A:2172:PHE:CZ	2.51	0.46
1:A:587:ASP:OD2	1:A:590:SER:OG	2.21	0.46
1:A:822:THR:O	1:A:826:ILE:HD12	2.15	0.46
1:A:1380:ASN:HB3	1:A:1391:PHE:O	2.16	0.46
1:A:201:ILE:HD11	1:A:203:ASP:HB2	1.97	0.46
1:A:960:ASN:ND2	1:A:1652:ASN:HA	2.31	0.46
1:A:2360:LEU:HG	1:A:2362:VAL:HG13	1.97	0.46
1:A:1947:VAL:O	1:A:1948:GLU:O	2.33	0.46
1:A:278:LYS:HD3	1:A:279:GLU:OE1	2.16	0.46
1:A:935:THR:O	1:A:947:LYS:HB3	2.16	0.46
1:A:2170:LYS:HE3	1:A:2186:ALA:HB1	1.98	0.46
1:A:1997:VAL:HB	1:A:2026:ARG:HB3	1.98	0.45
1:A:1310:LYS:HE2	1:A:1310:LYS:HB2	1.68	0.45
1:A:1396:ASN:N	1:A:1399:ASN:OD1	2.31	0.45
1:A:1979:TYR:HD1	1:A:1987:GLN:HB2	1.81	0.45
1:A:243:LEU:HB3	1:A:245:LYS:H	1.81	0.45
1:A:262:ARG:HA	1:A:262:ARG:HD3	1.77	0.45
1:A:1452:PHE:HE1	1:A:1460:ILE:HD11	1.81	0.45
1:A:1741:TYR:CE1	1:A:1754:ALA:HB2	2.50	0.45
1:A:1750:LEU:HD12	1:A:1751:ILE:H	1.82	0.45
1:A:2142:TYR:OH	1:A:2167:ASP:OD2	2.21	0.45



	juo pugo	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:1679:GLN:O	1:A:1712:ASN:ND2	2.47	0.45
1:A:2223:ASP:HB2	1:A:2230:TYR:CE2	2.49	0.45
1:A:294:GLN:HG3	1:A:358:GLU:O	2.16	0.45
1:A:899:ARG:HB2	1:A:910:PHE:CE1	2.52	0.45
1:A:2095:THR:HG23	1:A:2097:GLU:HG3	1.99	0.45
1:A:2354:ASP:OD1	1:A:2355:PRO:HD2	2.17	0.45
1:A:554:ASN:OD1	1:A:586:GLY:HA3	2.17	0.45
1:A:1372:LEU:HD23	1:A:1450:ILE:HG21	1.99	0.45
1:A:610:LYS:HE3	1:A:674:GLU:OE2	2.17	0.45
1:A:873:LYS:HG2	1:A:878:LEU:HB2	1.99	0.45
1:A:1171:ARG:HG3	1:A:1194:THR:HB	1.98	0.45
1:A:1264:TRP:HB2	1:A:1275:ILE:HG13	1.99	0.45
1:A:1640:LYS:HE3	1:A:1661:SER:CB	2.47	0.45
1:A:1895:LEU:HD21	1:A:1921:GLY:HA3	1.97	0.45
1:A:1988:THR:HG21	1:A:2002:ASN:HA	1.98	0.45
1:A:1374:LYS:HD2	1:A:1385:ASN:H	1.82	0.45
1:A:1408:ILE:HD12	1:A:1409:LEU:HD12	1.99	0.45
1:A:1908:TYR:HE2	1:A:1932:ILE:HD11	1.82	0.45
1:A:2254:ILE:HB	1:A:2263:PHE:HE2	1.82	0.45
1:A:70:LYS:HG3	1:A:1698:LEU:HD11	1.98	0.45
1:A:374:LYS:HB2	1:A:388:ILE:HB	1.99	0.45
1:A:1230:PHE:CE2	1:A:1280:PRO:HB3	2.51	0.45
1:A:1655:ASN:HB3	1:A:1693:ILE:CD1	2.47	0.45
1:A:1959:PHE:HE1	1:A:1966:ALA:HB2	1.82	0.45
1:A:1993:ILE:O	1:A:1996:LYS:HB2	2.17	0.45
1:A:936:ILE:HG13	1:A:946:LYS:HG3	1.99	0.44
1:A:1885:LYS:HE3	1:A:1922:GLU:OE2	2.17	0.44
1:A:1296:ARG:O	1:A:1323:TYR:HA	2.18	0.44
1:A:1400:ARG:O	1:A:1420:LEU:HG	2.17	0.44
1:A:1432:ASN:O	1:A:1436:LEU:N	2.51	0.44
1:A:2090:TYR:O	1:A:2099:CYS:N	2.50	0.44
1:A:587:ASP:OD2	1:A:587:ASP:N	2.45	0.44
1:A:406:ARG:HG2	1:A:446:PHE:CE2	2.52	0.44
1:A:93:PRO:HA	1:A:366:ILE:O	2.17	0.44
1:A:2299:GLY:HA3	1:A:2338:ILE:HD12	1.99	0.44
1:A:540:GLU:HG2	1:A:541:GLY:N	2.32	0.44
1:A:936:ILE:HG13	1:A:946:LYS:CD	2.47	0.44
1:A:2092:ASP:N	1:A:2092:ASP:OD1	2.50	0.44
1:A:2185:GLN:NE2	1:A:2186:ALA:O	2.51	0.44
1:A:2277:LYS:HZ1	1:A:2313:PHE:HE1	1.66	0.44



	jus page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1113:LEU:O	1:A:1114:GLN:NE2	2.51	0.44
1:A:1155:ILE:HB	1:A:1289:ILE:HG23	1.99	0.44
1:A:1400:ARG:HA	1:A:1420:LEU:HD12	1.99	0.44
1:A:1533:LYS:O	1:A:1535:ASP:N	2.44	0.44
1:A:505:LYS:HB2	1:A:505:LYS:HE2	1.60	0.44
1:A:978:LEU:HD23	1:A:982:SER:HB2	2.00	0.44
1:A:1001:ILE:HG22	1:A:1007:VAL:HG23	1.99	0.44
1:A:1955:GLU:CG	1:A:1985:ILE:HD13	2.45	0.44
1:A:2195:VAL:HG12	1:A:2196:ASN:N	2.32	0.44
1:A:2329:LYS:HE3	1:A:2360:LEU:H	1.82	0.44
1:A:1164:LEU:HG	1:A:1203:TYR:CD2	2.53	0.44
1:A:1291:LEU:HD23	1:A:1323:TYR:CG	2.52	0.44
1:A:1513:LEU:HA	1:A:1513:LEU:HD12	1.72	0.44
1:A:1959:PHE:CE1	1:A:1966:ALA:HB2	2.53	0.44
1:A:2235:VAL:HG22	1:A:2240:LYS:HG3	2.00	0.44
1:A:1218:ASP:O	1:A:1296:ARG:HG3	2.18	0.43
1:A:1296:ARG:NH1	1:A:1296:ARG:HB2	2.33	0.43
1:A:1531:TYR:CD1	1:A:1594:ILE:HD13	2.53	0.43
1:A:1706:THR:HA	1:A:1707:PRO:HD3	1.83	0.43
1:A:2285:LYS:HD3	1:A:2285:LYS:HA	1.72	0.43
1:A:429:LYS:HA	1:A:429:LYS:HD2	1.81	0.43
1:A:622:SER:O	1:A:626:ALA:N	2.51	0.43
1:A:1405:THR:HG22	1:A:1415:ILE:HG23	1.99	0.43
1:A:2178:VAL:HG21	1:A:2189:TYR:HB2	2.00	0.43
1:A:2219:LYS:HE3	1:A:2249:MET:HB3	2.01	0.43
1:A:936:ILE:HG13	1:A:946:LYS:HD2	2.00	0.43
1:A:1089:PHE:HD2	1:A:1299:ILE:HD13	1.83	0.43
1:A:1316:PHE:N	1:A:1335:ASP:O	2.47	0.43
1:A:1949:TRP:CE3	1:A:1958:TYR:HB2	2.53	0.43
1:A:1957:TYR:CE1	1:A:1983:ASN:O	2.70	0.43
1:A:2050:GLU:N	1:A:2053:GLU:OE2	2.48	0.43
1:A:1973:ILE:HB	1:A:1978:TYR:CE2	2.53	0.43
1:A:2142:TYR:CD2	1:A:2166:PRO:HD2	2.53	0.43
1:A:2226:THR:HG22	1:A:2228:LYS:HD3	2.00	0.43
1:A:2304:ALA:O	1:A:2315:GLY:N	2.52	0.43
1:A:1951:LEU:CD2	1:A:1956:THR:HA	2.48	0.43
1:A:2013:VAL:O	1:A:2016:LYS:HE2	2.18	0.43
1:A:277:LEU:HD23	1:A:277:LEU:HA	1.76	0.43
1:A:1171:ARG:NH1	1:A:1197:LYS:HD3	2.33	0.43
1:A:1413:ASN:OD1	1:A:1430:SER:HB2	2.18	0.43
1:A:87:LYS:HB3	1:A:87:LYS:HE3	1.75	0.43



	t i -	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:333:LYS:H	1:A:333:LYS:HD2	1.84	0.43
1:A:569:SER:O	1:A:571:LYS:HD2	2.19	0.43
1:A:1166:LYS:HD3	1:A:1228:ARG:O	2.19	0.43
1:A:1368:ILE:HG13	1:A:1371:ILE:HB	2.00	0.43
1:A:1908:TYR:CE1	1:A:1910:ALA:HB2	2.54	0.43
1:A:2182:ILE:HB	1:A:2185:GLN:HB2	2.01	0.43
1:A:209:TYR:CZ	1:A:213:GLU:HG3	2.54	0.43
1:A:333:LYS:O	1:A:337:MET:HG3	2.19	0.43
1:A:794:LEU:HA	1:A:794:LEU:HD23	1.86	0.43
1:A:1025:LEU:HD23	1:A:1621:GLN:OE1	2.18	0.43
1:A:640:ILE:H	1:A:640:ILE:HG12	1.62	0.43
1:A:2177:THR:HG1	1:A:2181:ASN:HD21	1.61	0.43
1:A:1416:ILE:HD12	1:A:1427:ILE:HG13	2.01	0.43
1:A:1512:ASP:HA	1:A:1514:LYS:HZ2	1.83	0.43
1:A:1652:ASN:OD1	1:A:1652:ASN:N	2.52	0.43
1:A:706:SER:HB3	1:A:709:GLU:CG	2.49	0.42
1:A:1533:LYS:HG3	1:A:1590:ASN:HB2	2.01	0.42
1:A:1432:ASN:HA	1:A:1464:TYR:CE2	2.55	0.42
1:A:1679:GLN:O	1:A:1682:LEU:HB2	2.19	0.42
1:A:1952:LEU:N	1:A:1952:LEU:CD1	2.80	0.42
1:A:1909:PHE:HB3	1:A:1921:GLY:O	2.19	0.42
1:A:860:LYS:HA	1:A:860:LYS:HD3	1.69	0.42
1:A:2230:TYR:CD1	1:A:2234:ASN:HB3	2.53	0.42
1:A:2273:TYR:CE2	1:A:2280:MET:HB3	2.52	0.42
1:A:209:TYR:CE2	1:A:213:GLU:HG3	2.54	0.42
1:A:971:TYR:HH	1:A:1662:TYR:HD1	1.68	0.42
1:A:1299:ILE:HG13	1:A:1300:VAL:N	2.35	0.42
1:A:339:ASP:O	1:A:343:GLN:HG3	2.19	0.42
1:A:886:PHE:HB2	1:A:988:GLN:NE2	2.34	0.42
1:A:972:ASN:ND2	1:A:986:LYS:HD3	2.34	0.42
1:A:1515:ASP:HB3	1:A:1530:ASN:HD21	1.83	0.42
1:A:1729:LYS:HB2	1:A:1729:LYS:HE2	1.73	0.42
1:A:2259:ASN:HB2	1:A:2261:TYR:CE2	2.55	0.42
1:A:548:ASN:OD1	1:A:548:ASN:N	2.53	0.42
1:A:1376:ASN:HB2	1:A:1383:ILE:HB	2.01	0.42
1:A:1415:ILE:O	1:A:1416:ILE:HD13	2.19	0.42
1:A:1912:ALA:N	1:A:1920:GLU:HB3	2.34	0.42
1:A:2243:PHE:HE2	1:A:2249:MET:HG3	1.85	0.42
1:A:1234:MET:H	1:A:1234:MET:HG2	1.62	0.42
1:A:1369:GLU:OE2	1:A:1370:ASN:HB2	2.20	0.42
1:A:1432:ASN:ND2	1:A:1464:TYR:OH	2.39	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1253:ARG:HH11	1:A:1253:ARG:HG3	1.83	0.42
1:A:601:ASP:OD2	1:A:604:SER:OG	2.38	0.42
1:A:1383:ILE:HA	1:A:1387:HIS:O	2.20	0.42
1:A:2174:PRO:HG2	1:A:2177:THR:HG21	2.02	0.42
1:A:2229:ALA:O	1:A:2231:LYS:HD2	2.20	0.42
1:A:566:ILE:HG23	1:A:571:LYS:NZ	2.35	0.41
1:A:905:THR:HG23	1:A:907:ASN:H	1.84	0.41
1:A:1025:LEU:HD12	1:A:1556:TYR:HE2	1.84	0.41
1:A:1224:ASN:N	1:A:1224:ASN:OD1	2.52	0.41
1:A:1230:PHE:HE2	1:A:1280:PRO:HB3	1.83	0.41
1:A:1352:VAL:HG21	1:A:1406:PHE:CD2	2.55	0.41
1:A:1876:SER:HB2	1:A:1880:ILE:HG13	2.00	0.41
1:A:1889:PHE:CE1	1:A:1895:LEU:HB2	2.55	0.41
1:A:711:TYR:HB3	1:A:712:PRO:HD3	2.02	0.41
1:A:1407:SER:HA	1:A:1413:ASN:HA	2.03	0.41
1:A:1536:MET:HE2	1:A:1564:GLN:HG3	2.02	0.41
1:A:6:LYS:HE3	1:A:28:LEU:HB3	2.02	0.41
1:A:970:GLU:C	1:A:972:ASN:H	2.23	0.41
1:A:157:PHE:CD2	1:A:166:PHE:CE2	3.08	0.41
1:A:2242:TYR:HB2	1:A:2263:PHE:CE1	2.56	0.41
1:A:2342:GLY:HA2	1:A:2353:PHE:O	2.20	0.41
1:A:1200:LEU:HD22	1:A:1258:TYR:CD1	2.56	0.41
1:A:1228:ARG:HB3	1:A:1282:TYR:CE1	2.55	0.41
1:A:2235:VAL:HG13	1:A:2240:LYS:HG3	2.02	0.41
1:A:2309:LEU:HD12	1:A:2309:LEU:HA	1.87	0.41
1:A:339:ASP:HB2	1:A:342:VAL:HG22	2.03	0.41
1:A:557:LEU:HD23	1:A:619:TYR:CD1	2.56	0.41
1:A:1335:ASP:HA	1:A:1390:ASN:O	2.19	0.41
1:A:1991:ILE:HD12	1:A:2000:PHE:CD2	2.56	0.41
1:A:2276:ILE:HB	1:A:2281:PHE:CE2	2.54	0.41
1:A:2340:ALA:HB3	1:A:2353:PHE:CG	2.55	0.41
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.90	0.41
1:A:1556:TYR:OH	1:A:1616:SER:OG	2.30	0.41
1:A:1642:LYS:O	1:A:1643:GLU:HB2	2.20	0.41
1:A:1926:PHE:HE1	1:A:1930:LEU:HB2	1.86	0.41
1:A:98:LEU:HD21	1:A:363:LEU:HD11	2.02	0.41
1:A:1212:LYS:HD2	1:A:1212:LYS:HA	1.69	0.41
1:A:1423:LYS:HD3	1:A:1423:LYS:HA	1.87	0.41
1:A:1566:LEU:HD22	1:A:1684:GLY:HA3	2.02	0.41
1:A:1854:ILE:HD13	1:A:1854:ILE:HA	1.93	0.41
1:A:1999:TYR:CE1	1:A:2011:ILE:HG21	2.56	0.41



	juo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:333:LYS:HD2	1:A:333:LYS:N	2.36	0.41
1:A:1102:GLY:HA3	1:A:1114:GLN:HE22	1.85	0.41
1:A:1241:ARG:HD3	1:A:1267:PHE:HZ	1.86	0.41
1:A:1316:PHE:CE2	1:A:1334:ILE:HD12	2.56	0.41
1:A:1464:TYR:CZ	1:A:1466:ASP:HB2	2.56	0.41
1:A:1491:GLU:HG2	1:A:1511:LYS:HA	2.03	0.41
1:A:2198:ASP:OD1	1:A:2198:ASP:N	2.48	0.41
1:A:921:TYR:O	1:A:925:ILE:HG23	2.21	0.41
1:A:324:LYS:C	1:A:325:GLU:HG2	2.42	0.40
1:A:589:ILE:HD11	1:A:757:HIS:HA	2.04	0.40
1:A:925:ILE:HG13	1:A:926:SER:N	2.35	0.40
1:A:1241:ARG:HE	1:A:1241:ARG:HB2	1.68	0.40
1:A:1296:ARG:HB2	1:A:1296:ARG:CZ	2.52	0.40
1:A:2090:TYR:CZ	1:A:2105:ILE:HG12	2.57	0.40
1:A:470:GLY:O	1:A:473:VAL:HG22	2.21	0.40
1:A:950:LEU:H	1:A:950:LEU:HD22	1.85	0.40
1:A:1973:ILE:HB	1:A:1978:TYR:HE2	1.86	0.40
1:A:331:THR:HB	1:A:333:LYS:HD2	2.03	0.40
1:A:435:LEU:HD23	1:A:435:LEU:HA	1.83	0.40
1:A:671:LEU:O	1:A:675:ILE:HG13	2.22	0.40
1:A:1184:ILE:HG12	1:A:1267:PHE:CD1	2.56	0.40
1:A:1353:LYS:HB3	1:A:1353:LYS:HE2	1.87	0.40
1:A:113:ASN:ND2	1:A:328:PRO:HD2	2.37	0.40
1:A:1143:ILE:HG12	1:A:1219:LEU:HD23	2.03	0.40
1:A:1938:TYR:CE2	1:A:1952:LEU:HD23	2.56	0.40
1:A:2291:ILE:HA	1:A:2303:PHE:O	2.21	0.40
1:A:925:ILE:O	1:A:929:ILE:HG13	2.22	0.40
1:A:955:GLU:O	1:A:958:THR:HB	2.21	0.40
1:A:1089:PHE:CE2	1:A:1299:ILE:HB	2.57	0.40
1:A:1196:ARG:H	1:A:1196:ARG:HG2	1.74	0.40
1:A:1958:TYR:HD1	1:A:1967:LEU:HD13	1.85	0.40
1:A:2008:VAL:HG23	1:A:2021:GLY:O	2.21	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	Percentiles
1	А	2295/2372~(97%)	2163 (94%)	128 (6%)	4 (0%)	47 68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	1948	GLU
1	А	633	LYS
1	А	2342	GLY
1	А	422	THR

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 PDB entries followed by that with respect to all EM entries.

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	Perce	entiles
1	А	2088/2146~(97%)	1919~(92%)	169 (8%)	11	23

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	41	SER
1	А	74	LYS
1	А	94	VAL
1	А	106	GLN
1	А	161	LEU
1	А	195	GLU
1	А	201	ILE
1	А	223	LYS
1	А	244	GLU
1	А	253	ARG
1	А	272	LEU
1	А	275	SER
1	А	276	MET



Mol	Chain	Res	Type
1	А	299	LYS
1	А	332	SER
1	А	333	LYS
1	А	340	GLU
1	А	342	VAL
1	А	345	SER
1	А	348	SER
1	А	366	ILE
1	А	368	VAL
1	А	385	GLN
1	А	405	ASN
1	А	408	LYS
1	А	439	SER
1	А	489	THR
1	А	508	ILE
1	А	517	THR
1	А	518	SER
1	А	519	LEU
1	А	520	TRP
1	А	529	SER
1	А	532	GLU
1	А	548	ASN
1	А	558	ASP
1	А	567	LEU
1	А	570	MET
1	А	573	ARG
1	А	576	GLU
1	А	577	TYR
1	А	590	SER
1	A	632	ASP
1	А	640	ILE
1	А	644	ARG
1	A	657	GLU
1	A	662	THR
1	A	667	ASP
1	A	670	SER
1	А	692	GLU
1	A	722	ARG
1	A	738	SER
1	A	756	ASP
1	A	757	HIS
1	А	774	SER



Mol	Chain	Res	Type
1	А	826	ILE
1	А	830	SER
1	А	865	ILE
1	А	866	SER
1	А	890	SER
1	А	903	LYS
1	А	911	ILE
1	А	920	GLU
1	А	937	PHE
1	А	945	VAL
1	А	946	LYS
1	А	947	LYS
1	А	950	LEU
1	A	968	LEU
1	А	970	GLU
1	A	971	TYR
1	А	972	ASN
1	А	978	LEU
1	А	1002	THR
1	А	1005	SER
1	А	1006	LYS
1	А	1072	THR
1	А	1129	LEU
1	А	1131	GLU
1	А	1138	LEU
1	А	1142	LYS
1	А	1149	ASP
1	А	1161	SER
1	А	1166	LYS
1	А	1167	CYS
1	А	1169	ILE
1	A	1178	HIS
1	A	1181	THR
1	A	1186	HIS
1	A	1210	LYS
1	A	1211	GLU
1	A	1212	LYS
1	A	1214	ASP
1	A	1228	ARG
1	A	1230	PHE
1	A	1251	LEU
1	A	1256	ASP



Mol	Chain	Res	Type
1	А	1269	PHE
1	А	1279	LYS
1	А	1284	ASP
1	А	1307	GLN
1	А	1323	TYR
1	А	1327	LEU
1	А	1332	MET
1	А	1341	ASN
1	А	1345	VAL
1	А	1356	THR
1	А	1397	GLU
1	А	1401	PHE
1	А	1403	SER
1	А	1407	SER
1	А	1409	LEU
1	A	1423	LYS
1	А	1435	LYS
1	А	1462	TYR
1	А	1465	ILE
1	А	1478	SER
1	А	1512	ASP
1	А	1516	ILE
1	А	1517	ARG
1	А	1539	SER
1	А	1541	SER
1	А	1546	ASP
1	А	1582	LEU
1	А	1583	MET
1	A	1588	SER
1	A	1591	ILE
1	А	1610	ASN
1	A	1614	SER
1	А	1616	SER
1	A	1628	LYS
1	A	1629	ASP
1	A	1641	ILE
1	А	1645	SER
1	A	1647	THR
1	A	1652	ASN
1	A	1653	ARG
1	А	1662	TYR
1	А	1667	SER



Mol	Chain	Res	Type
1	А	1682	LEU
1	А	1698	LEU
1	А	1710	LYS
1	А	1714	ILE
1	А	1722	ASP
1	А	1748	SER
1	А	1758	GLU
1	А	1779	ASP
1	А	1782	SER
1	А	1795	LYS
1	А	1801	SER
1	А	1841	ASP
1	А	1842	SER
1	А	1857	PHE
1	А	1885	LYS
1	А	1927	ILE
1	А	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	A	2131	TYR
1	А	2183	TYR
1	А	2212	TRP
1	А	2259	ASN
1	A	2320	TYR
1	А	2323	TRP
1	А	2362	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	2	ASN
1	А	106	GLN
1	А	302	ASN
1	А	419	ASN
1	А	639	GLN
1	А	694	ASN
1	А	741	GLN
1	А	757	HIS



Mol	Chain	Res	Type
1	А	924	HIS
1	А	988	GLN
1	А	1114	GLN
1	А	1178	HIS
1	А	1207	ASN
1	А	1257	HIS
1	А	1290	ASN
1	А	1333	ASN
1	А	1444	GLN
1	А	1449	HIS
1	А	1530	ASN
1	А	1548	ASN
1	А	1598	ASN
1	А	1654	GLN
1	А	1663	HIS
1	А	1690	ASN
1	А	1724	ASN
1	А	1727	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-38011. 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: 200



Y Index: 200



Z Index: 200

6.2.2 Raw map



X Index: 200

Y Index: 200

Z Index: 200 $\,$

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



6.3 Largest variance slices (i)

6.3.1 Primary map









Z Index: 226

6.3.2 Raw map



X Index: 204

Y Index: 182



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 0.25. 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 802 nm^3 ; this corresponds to an approximate mass of 724 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 0.400 ${\rm \AA^{-1}}$



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 0.400 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	2.80	2.51
Unmasked-calculated*	2.93	3.49	2.97

*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 2.93 differs from the reported value 2.5 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-38011 and PDB model 8X2I. 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 0.25 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 (0.25).



9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.4140
A	0.7210	0.4140



