



wwPDB X-ray Structure Validation Summary Report i

Nov 10, 2024 – 02:21 PM EST

PDB ID : 1LQL
Title : Crystal structure of OsmC like protein from Mycoplasma pneumoniae
Authors : Choi, I.-G.; Shin, D.H.; Brandsen, J.; Jancarik, J.; Kim, R.; Yokota, H.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2002-05-10
Resolution : 2.85 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

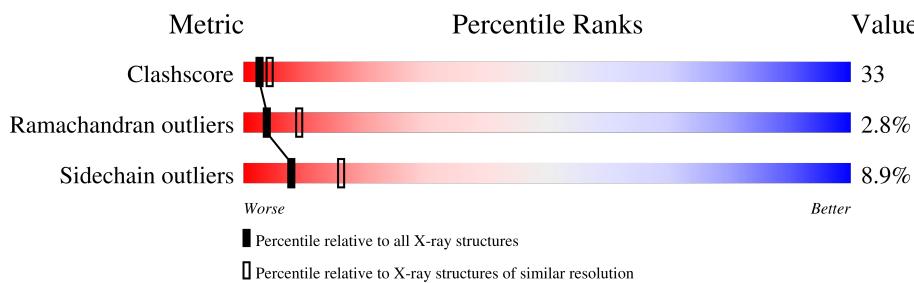
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

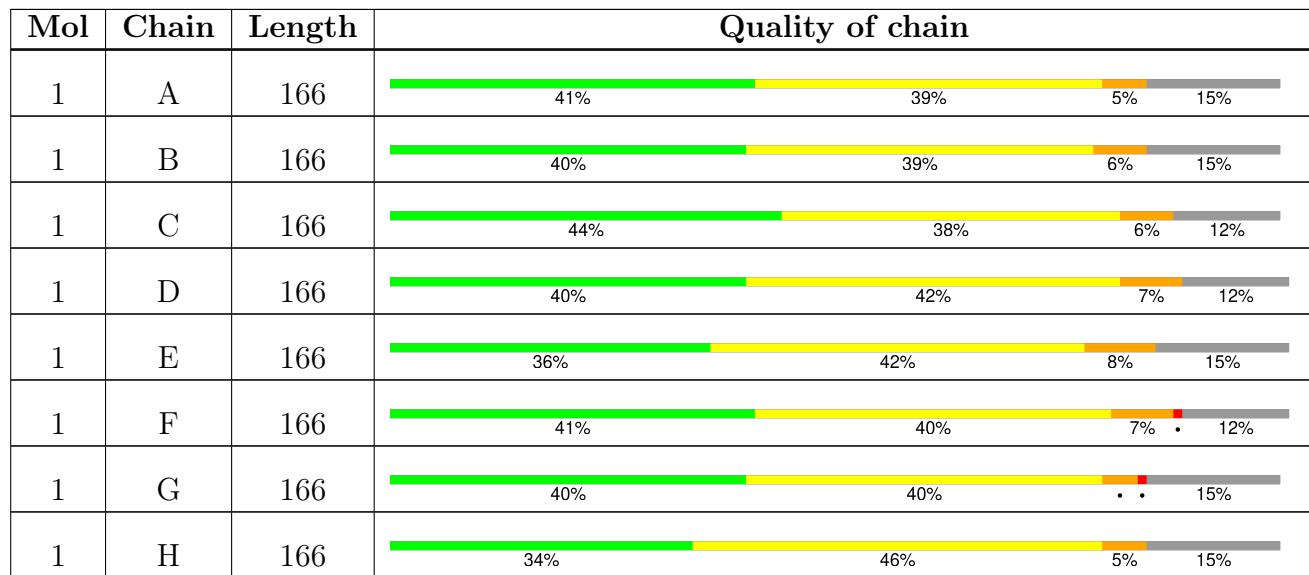
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.



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Mol	Chain	Length	Quality of chain				
1	I	166	31%	51%	6%	•	12%
1	J	166	36%	45%	5%		14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11257 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called osmotically inducible protein C like family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1084	682	187	208	7	0	0	0
1	B	141	1084	682	187	208	7	0	0	0
1	C	146	1130	713	195	215	7	0	0	0
1	D	146	1130	713	195	215	7	0	0	0
1	E	141	1084	682	187	208	7	0	0	0
1	F	146	1130	713	195	215	7	0	0	0
1	G	141	1084	682	187	208	7	0	0	0
1	H	141	1084	682	187	208	7	0	0	0
1	I	146	1130	713	195	215	7	0	0	0
1	J	143	1098	690	191	210	7	0	0	0

There are 250 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	expression tag	UNP P75170
A	-23	GLY	-	expression tag	UNP P75170
A	-22	SER	-	expression tag	UNP P75170
A	-21	SER	-	expression tag	UNP P75170
A	-20	HIS	-	expression tag	UNP P75170
A	-19	HIS	-	expression tag	UNP P75170
A	-18	HIS	-	expression tag	UNP P75170
A	-17	HIS	-	expression tag	UNP P75170
A	-16	HIS	-	expression tag	UNP P75170

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP P75170
A	-14	ASP	-	expression tag	UNP P75170
A	-13	TYR	-	expression tag	UNP P75170
A	-12	ASP	-	expression tag	UNP P75170
A	-11	ILE	-	expression tag	UNP P75170
A	-10	PRO	-	expression tag	UNP P75170
A	-9	THR	-	expression tag	UNP P75170
A	-8	THR	-	expression tag	UNP P75170
A	-7	GLU	-	expression tag	UNP P75170
A	-6	ASN	-	expression tag	UNP P75170
A	-5	LEU	-	expression tag	UNP P75170
A	-4	TYR	-	expression tag	UNP P75170
A	-3	PHE	-	expression tag	UNP P75170
A	-2	GLN	-	expression tag	UNP P75170
A	-1	GLY	-	expression tag	UNP P75170
A	0	HIS	-	expression tag	UNP P75170
B	176	MET	-	expression tag	UNP P75170
B	177	GLY	-	expression tag	UNP P75170
B	178	SER	-	expression tag	UNP P75170
B	179	SER	-	expression tag	UNP P75170
B	180	HIS	-	expression tag	UNP P75170
B	181	HIS	-	expression tag	UNP P75170
B	182	HIS	-	expression tag	UNP P75170
B	183	HIS	-	expression tag	UNP P75170
B	184	HIS	-	expression tag	UNP P75170
B	185	HIS	-	expression tag	UNP P75170
B	186	ASP	-	expression tag	UNP P75170
B	187	TYR	-	expression tag	UNP P75170
B	188	ASP	-	expression tag	UNP P75170
B	189	ILE	-	expression tag	UNP P75170
B	190	PRO	-	expression tag	UNP P75170
B	191	THR	-	expression tag	UNP P75170
B	192	THR	-	expression tag	UNP P75170
B	193	GLU	-	expression tag	UNP P75170
B	194	ASN	-	expression tag	UNP P75170
B	195	LEU	-	expression tag	UNP P75170
B	196	TYR	-	expression tag	UNP P75170
B	197	PHE	-	expression tag	UNP P75170
B	198	GLN	-	expression tag	UNP P75170
B	199	GLY	-	expression tag	UNP P75170
B	300	HIS	-	expression tag	UNP P75170
C	376	MET	-	expression tag	UNP P75170

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Chain	Residue	Modelled	Actual	Comment	Reference
C	377	GLY	-	expression tag	UNP P75170
C	378	SER	-	expression tag	UNP P75170
C	379	SER	-	expression tag	UNP P75170
C	380	HIS	-	expression tag	UNP P75170
C	381	HIS	-	expression tag	UNP P75170
C	382	HIS	-	expression tag	UNP P75170
C	383	HIS	-	expression tag	UNP P75170
C	384	HIS	-	expression tag	UNP P75170
C	385	HIS	-	expression tag	UNP P75170
C	386	ASP	-	expression tag	UNP P75170
C	387	TYR	-	expression tag	UNP P75170
C	388	ASP	-	expression tag	UNP P75170
C	389	ILE	-	expression tag	UNP P75170
C	390	PRO	-	expression tag	UNP P75170
C	391	THR	-	expression tag	UNP P75170
C	392	THR	-	expression tag	UNP P75170
C	393	GLU	-	expression tag	UNP P75170
C	394	ASN	-	expression tag	UNP P75170
C	395	LEU	-	expression tag	UNP P75170
C	396	TYR	-	expression tag	UNP P75170
C	397	PHE	-	expression tag	UNP P75170
C	398	GLN	-	expression tag	UNP P75170
C	399	GLY	-	expression tag	UNP P75170
C	400	HIS	-	expression tag	UNP P75170
D	576	MET	-	expression tag	UNP P75170
D	577	GLY	-	expression tag	UNP P75170
D	578	SER	-	expression tag	UNP P75170
D	579	SER	-	expression tag	UNP P75170
D	580	HIS	-	expression tag	UNP P75170
D	581	HIS	-	expression tag	UNP P75170
D	582	HIS	-	expression tag	UNP P75170
D	583	HIS	-	expression tag	UNP P75170
D	584	HIS	-	expression tag	UNP P75170
D	585	HIS	-	expression tag	UNP P75170
D	586	ASP	-	expression tag	UNP P75170
D	587	TYR	-	expression tag	UNP P75170
D	588	ASP	-	expression tag	UNP P75170
D	589	ILE	-	expression tag	UNP P75170
D	590	PRO	-	expression tag	UNP P75170
D	591	THR	-	expression tag	UNP P75170
D	592	THR	-	expression tag	UNP P75170
D	593	GLU	-	expression tag	UNP P75170

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Chain	Residue	Modelled	Actual	Comment	Reference
D	594	ASN	-	expression tag	UNP P75170
D	595	LEU	-	expression tag	UNP P75170
D	596	TYR	-	expression tag	UNP P75170
D	597	PHE	-	expression tag	UNP P75170
D	598	GLN	-	expression tag	UNP P75170
D	599	GLY	-	expression tag	UNP P75170
D	600	HIS	-	expression tag	UNP P75170
E	776	MET	-	expression tag	UNP P75170
E	777	GLY	-	expression tag	UNP P75170
E	778	SER	-	expression tag	UNP P75170
E	779	SER	-	expression tag	UNP P75170
E	780	HIS	-	expression tag	UNP P75170
E	781	HIS	-	expression tag	UNP P75170
E	782	HIS	-	expression tag	UNP P75170
E	783	HIS	-	expression tag	UNP P75170
E	784	HIS	-	expression tag	UNP P75170
E	785	HIS	-	expression tag	UNP P75170
E	786	ASP	-	expression tag	UNP P75170
E	787	TYR	-	expression tag	UNP P75170
E	788	ASP	-	expression tag	UNP P75170
E	789	ILE	-	expression tag	UNP P75170
E	790	PRO	-	expression tag	UNP P75170
E	791	THR	-	expression tag	UNP P75170
E	792	THR	-	expression tag	UNP P75170
E	793	GLU	-	expression tag	UNP P75170
E	794	ASN	-	expression tag	UNP P75170
E	795	LEU	-	expression tag	UNP P75170
E	796	TYR	-	expression tag	UNP P75170
E	797	PHE	-	expression tag	UNP P75170
E	798	GLN	-	expression tag	UNP P75170
E	799	GLY	-	expression tag	UNP P75170
E	800	HIS	-	expression tag	UNP P75170
F	976	MET	-	expression tag	UNP P75170
F	977	GLY	-	expression tag	UNP P75170
F	978	SER	-	expression tag	UNP P75170
F	979	SER	-	expression tag	UNP P75170
F	980	HIS	-	expression tag	UNP P75170
F	981	HIS	-	expression tag	UNP P75170
F	982	HIS	-	expression tag	UNP P75170
F	983	HIS	-	expression tag	UNP P75170
F	984	HIS	-	expression tag	UNP P75170
F	985	HIS	-	expression tag	UNP P75170

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Chain	Residue	Modelled	Actual	Comment	Reference
F	986	ASP	-	expression tag	UNP P75170
F	987	TYR	-	expression tag	UNP P75170
F	988	ASP	-	expression tag	UNP P75170
F	989	ILE	-	expression tag	UNP P75170
F	990	PRO	-	expression tag	UNP P75170
F	991	THR	-	expression tag	UNP P75170
F	992	THR	-	expression tag	UNP P75170
F	993	GLU	-	expression tag	UNP P75170
F	994	ASN	-	expression tag	UNP P75170
F	995	LEU	-	expression tag	UNP P75170
F	996	TYR	-	expression tag	UNP P75170
F	997	PHE	-	expression tag	UNP P75170
F	998	GLN	-	expression tag	UNP P75170
F	999	GLY	-	expression tag	UNP P75170
F	1000	HIS	-	expression tag	UNP P75170
G	1176	MET	-	expression tag	UNP P75170
G	1177	GLY	-	expression tag	UNP P75170
G	1178	SER	-	expression tag	UNP P75170
G	1179	SER	-	expression tag	UNP P75170
G	1180	HIS	-	expression tag	UNP P75170
G	1181	HIS	-	expression tag	UNP P75170
G	1182	HIS	-	expression tag	UNP P75170
G	1183	HIS	-	expression tag	UNP P75170
G	1184	HIS	-	expression tag	UNP P75170
G	1185	HIS	-	expression tag	UNP P75170
G	1186	ASP	-	expression tag	UNP P75170
G	1187	TYR	-	expression tag	UNP P75170
G	1188	ASP	-	expression tag	UNP P75170
G	1189	ILE	-	expression tag	UNP P75170
G	1190	PRO	-	expression tag	UNP P75170
G	1191	THR	-	expression tag	UNP P75170
G	1192	THR	-	expression tag	UNP P75170
G	1193	GLU	-	expression tag	UNP P75170
G	1194	ASN	-	expression tag	UNP P75170
G	1195	LEU	-	expression tag	UNP P75170
G	1196	TYR	-	expression tag	UNP P75170
G	1197	PHE	-	expression tag	UNP P75170
G	1198	GLN	-	expression tag	UNP P75170
G	1199	GLY	-	expression tag	UNP P75170
G	1200	HIS	-	expression tag	UNP P75170
H	1376	MET	-	expression tag	UNP P75170
H	1377	GLY	-	expression tag	UNP P75170

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1378	SER	-	expression tag	UNP P75170
H	1379	SER	-	expression tag	UNP P75170
H	1380	HIS	-	expression tag	UNP P75170
H	1381	HIS	-	expression tag	UNP P75170
H	1382	HIS	-	expression tag	UNP P75170
H	1383	HIS	-	expression tag	UNP P75170
H	1384	HIS	-	expression tag	UNP P75170
H	1385	HIS	-	expression tag	UNP P75170
H	1386	ASP	-	expression tag	UNP P75170
H	1387	TYR	-	expression tag	UNP P75170
H	1388	ASP	-	expression tag	UNP P75170
H	1389	ILE	-	expression tag	UNP P75170
H	1390	PRO	-	expression tag	UNP P75170
H	1391	THR	-	expression tag	UNP P75170
H	1392	THR	-	expression tag	UNP P75170
H	1393	GLU	-	expression tag	UNP P75170
H	1394	ASN	-	expression tag	UNP P75170
H	1395	LEU	-	expression tag	UNP P75170
H	1396	TYR	-	expression tag	UNP P75170
H	1397	PHE	-	expression tag	UNP P75170
H	1398	GLN	-	expression tag	UNP P75170
H	1399	GLY	-	expression tag	UNP P75170
H	1400	HIS	-	expression tag	UNP P75170
I	1576	MET	-	expression tag	UNP P75170
I	1577	GLY	-	expression tag	UNP P75170
I	1578	SER	-	expression tag	UNP P75170
I	1579	SER	-	expression tag	UNP P75170
I	1580	HIS	-	expression tag	UNP P75170
I	1581	HIS	-	expression tag	UNP P75170
I	1582	HIS	-	expression tag	UNP P75170
I	1583	HIS	-	expression tag	UNP P75170
I	1584	HIS	-	expression tag	UNP P75170
I	1585	HIS	-	expression tag	UNP P75170
I	1586	ASP	-	expression tag	UNP P75170
I	1587	TYR	-	expression tag	UNP P75170
I	1588	ASP	-	expression tag	UNP P75170
I	1589	ILE	-	expression tag	UNP P75170
I	1590	PRO	-	expression tag	UNP P75170
I	1591	THR	-	expression tag	UNP P75170
I	1592	THR	-	expression tag	UNP P75170
I	1593	GLU	-	expression tag	UNP P75170
I	1594	ASN	-	expression tag	UNP P75170

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1595	LEU	-	expression tag	UNP P75170
I	1596	TYR	-	expression tag	UNP P75170
I	1597	PHE	-	expression tag	UNP P75170
I	1598	GLN	-	expression tag	UNP P75170
I	1599	GLY	-	expression tag	UNP P75170
I	1600	HIS	-	expression tag	UNP P75170
J	1776	MET	-	expression tag	UNP P75170
J	1777	GLY	-	expression tag	UNP P75170
J	1778	SER	-	expression tag	UNP P75170
J	1779	SER	-	expression tag	UNP P75170
J	1780	HIS	-	expression tag	UNP P75170
J	1781	HIS	-	expression tag	UNP P75170
J	1782	HIS	-	expression tag	UNP P75170
J	1783	HIS	-	expression tag	UNP P75170
J	1784	HIS	-	expression tag	UNP P75170
J	1785	HIS	-	expression tag	UNP P75170
J	1786	ASP	-	expression tag	UNP P75170
J	1787	TYR	-	expression tag	UNP P75170
J	1788	ASP	-	expression tag	UNP P75170
J	1789	ILE	-	expression tag	UNP P75170
J	1790	PRO	-	expression tag	UNP P75170
J	1791	THR	-	expression tag	UNP P75170
J	1792	THR	-	expression tag	UNP P75170
J	1793	GLU	-	expression tag	UNP P75170
J	1794	ASN	-	expression tag	UNP P75170
J	1795	LEU	-	expression tag	UNP P75170
J	1796	TYR	-	expression tag	UNP P75170
J	1797	PHE	-	expression tag	UNP P75170
J	1798	GLN	-	expression tag	UNP P75170
J	1799	GLY	-	expression tag	UNP P75170
J	1800	HIS	-	expression tag	UNP P75170

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	25	Total O 25 25	0	0
2	B	34	Total O 34 34	0	0
2	C	17	Total O 17 17	0	0
2	D	16	Total O 16 16	0	0

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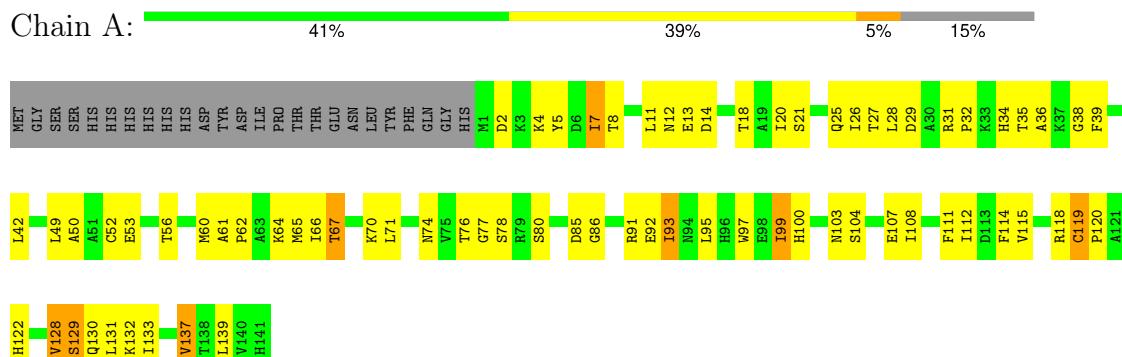
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	21	Total O 21 21	0	0
2	F	34	Total O 34 34	0	0
2	G	11	Total O 11 11	0	0
2	H	16	Total O 16 16	0	0
2	I	23	Total O 23 23	0	0
2	J	22	Total O 22 22	0	0

3 Residue-property plots

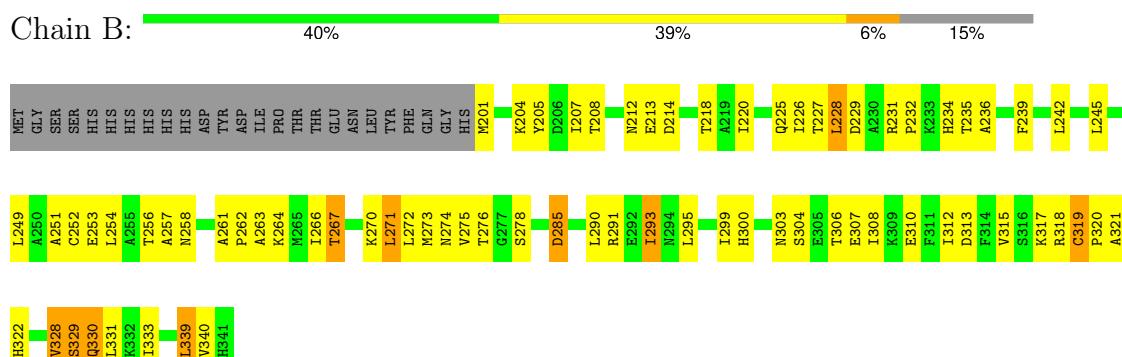
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

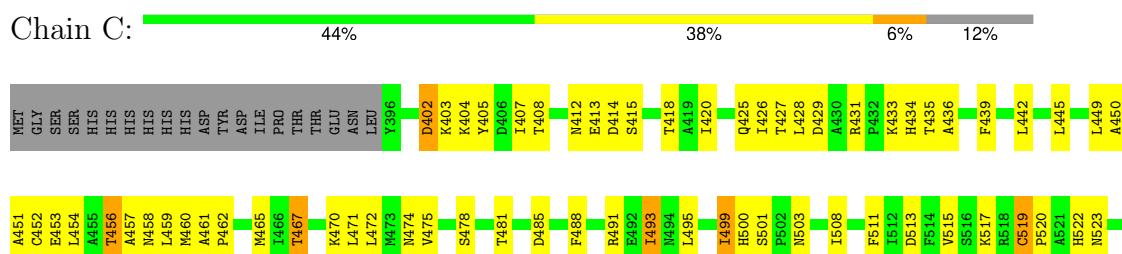
- Molecule 1: osmotically inducible protein C like family



- Molecule 1: osmotically inducible protein C like family



- Molecule 1: osmotically inducible protein C like family





- Molecule 1: osmotically inducible protein C like family

Chain D:



1649	A650	T656	M650	A651	C652	E653	P652	1656	T657	M651	A652	C653	E654	P653
1656	T657	M651	A652	C653	E654	P653	1663	T658	M652	A653	C654	E655	P654	1670
1663	T658	M652	A653	C654	E655	P654	1670	T659	M653	A654	C655	E656	P655	1676
1670	T659	M653	A654	C655	E656	P655	1676	T660	M654	A655	C656	E657	P656	1683
1676	T660	M654	A655	C656	E657	P656	1683	T661	M655	A656	C657	E658	P657	1689
1683	T661	M655	A656	C657	E658	P657	1689	T662	M656	A657	C658	E659	P658	1696
1689	T662	M656	A657	C658	E659	P658	1696	T663	M657	A658	C659	E660	P659	1703
1696	T663	M657	A658	C659	E660	P659	1703	T664	M658	A659	C660	E661	P660	1710
1703	T664	M658	A659	C660	E661	P660	1710	T665	M659	A660	C661	E662	P661	1717
1710	T665	M659	A660	C661	E662	P661	1717	T666	M660	A661	C662	E663	P662	1724
1717	T666	M660	A661	C662	E663	P662	1724	T667	M661	A662	C663	E664	P663	1731
1724	T667	M661	A662	C663	E664	P663	1731	T668	M662	A663	C664	E665	P664	1738
1731	T668	M662	A663	C664	E665	P664	1738	T669	M663	A664	C665	E666	P665	1745
1738	T669	M663	A664	C665	E666	P665	1745	T670	M664	A665	C666	E667	P666	1752
1745	T670	M664	A665	C666	E667	P666	1752	T671	M665	A666	C667	E668	P667	1759
1752	T671	M665	A666	C667	E668	P667	1759	T672	M666	A667	C668	E669	P668	1766
1759	T672	M666	A667	C668	E669	P668	1766	T673	M667	A668	C669	E670	P669	1773
1766	T673	M667	A668	C669	E670	P669	1773	T674	M668	A669	C670	E671	P670	1780
1773	T674	M668	A669	C670	E671	P670	1780	T675	M669	A670	C671	E672	P671	1787
1780	T675	M669	A670	C671	E672	P671	1787	T676	M670	A671	C672	E673	P672	1794
1787	T676	M670	A671	C672	E673	P672	1794	T677	M671	A672	C673	E674	P673	1801
1794	T677	M671	A672	C673	E674	P673	1801	T678	M672	A673	C674	E675	P674	1808
1801	T678	M672	A673	C674	E675	P674	1808	T679	M673	A674	C675	E676	P675	1815
1808	T679	M673	A674	C675	E676	P675	1815	T680	M674	A675	C676	E677	P676	1822
1815	T680	M674	A675	C676	E677	P676	1822	T681	M675	A676	C677	E678	P677	1829
1822	T681	M675	A676	C677	E678	P677	1829	T682	M676	A677	C678	E679	P678	1836
1829	T682	M676	A677	C678	E679	P678	1836	T683	M677	A678	C679	E680	P679	1843
1836	T683	M677	A678	C679	E680	P679	1843	T684	M678	A679	C680	E681	P680	1850
1843	T684	M678	A679	C680	E681	P680	1850	T685	M679	A680	C681	E682	P681	1857
1850	T685	M679	A680	C681	E682	P681	1857	T686	M680	A681	C682	E683	P682	1864
1857	T686	M680	A681	C682	E683	P682	1864	T687	M681	A682	C683	E684	P683	1871
1864	T687	M681	A682	C683	E684	P683	1871	T688	M682	A683	C684	E685	P684	1878
1871	T688	M682	A683	C684	E685	P684	1878	T689	M683	A684	C685	E686	P685	1885
1878	T689	M683	A684	C685	E686	P685	1885	T690	M684	A685	C686	E687	P686	1892
1885	T690	M684	A685	C686	E687	P686	1892	T691	M685	A686	C687	E688	P687	1899
1892	T691	M685	A686	C687	E688	P687	1899	T692	M686	A687	C688	E689	P688	1906
1899	T692	M686	A687	C688	E689	P688	1906	T693	M687	A688	C689	E690	P689	1913
1906	T693	M687	A688	C689	E690	P689	1913	T694	M688	A689	C690	E691	P690	1920
1913	T694	M688	A689	C690	E691	P690	1920	T695	M689	A690	C691	E692	P691	1927
1920	T695	M689	A690	C691	E692	P691	1927	T696	M690	A691	C692	E693	P692	1934
1927	T696	M690	A691	C692	E693	P692	1934	T697	M691	A692	C693	E694	P693	1941
1934	T697	M691	A692	C693	E694	P693	1941	T698	M692	A693	C694	E695	P694	1948
1941	T698	M692	A693	C694	E695	P694	1948	T699	M693	A694	C695	E696	P695	1955
1948	T699	M693	A694	C695	E696	P695	1955	T700	M694	A695	C696	E697	P696	1962
1955	T700	M694	A695	C696	E697	P696	1962	T701	M695	A696	C697	E698	P697	1969
1962	T701	M695	A696	C697	E698	P697	1969	T702	M696	A697	C698	E699	P698	1976
1969	T702	M696	A697	C698	E699	P698	1976	T703	M697	A698	C699	E700	P699	1983
1976	T703	M697	A698	C699	E700	P699	1983	T704	M698	A699	C700	E701	P700	1990
1983	T704	M698	A699	C700	E701	P700	1990	T705	M699	A700	C701	E702	P701	1997
1990	T705	M699	A700	C701	E702	P701	1997	T706	M700	A701	C702	E703	P702	2004
1997	T706	M700	A701	C702	E703	P702	2004	T707	M701	A702	C703	E704	P703	2011
2004	T707	M701	A702	C703	E704	P703	2011	T708	M702	A703	C704	E705	P704	2018
2011	T708	M702	A703	C704	E705	P704	2018	T709	M703	A704	C705	E706	P705	2025
2018	T709	M703	A704	C705	E706	P705	2025	T710	M704	A705	C706	E707	P706	2032
2025	T710	M704	A705	C706	E707	P706	2032	T711	M705	A706	C707	E708	P707	2039
2032	T711	M705	A706	C707	E708	P707	2039	T712	M706	A707	C708	E709	P708	2046
2039	T712	M706	A707	C708	E709	P708	2046	T713	M707	A708	C709	E710	P709	2053
2046	T713	M707	A708	C709	E710	P709	2053	T714	M708	A709	C710	E711	P710	2060
2053	T714	M708	A709	C710	E711	P710	2060	T715	M709	A710	C711	E712	P711	2067
2060	T715	M709	A710	C711	E712	P711	2067	T716	M710	A711	C712	E713	P712	2074
2067	T716	M710	A711	C712	E713	P712	2074	T717	M711	A712	C713	E714	P713	2081
2074	T717	M711	A712	C713	E714	P713	2081	T718	M712	A713	C714	E715	P714	2088
2081	T718	M712	A713	C714	E715	P714	2088	T719	M713	A714	C715	E716</b		

H722
N723
T724
L725
V728
S729
Q730
L731
K732
I733
L739
V740
H741

- Molecule 1: osmotically inducible protein C like family

Chain E:



V915
S916
K917
R918
C919
P920
A921
H922

V928
S929
Q930

L931
K932
I933

V937
T938
L939
V940
H941

- Molecule 1: osmotically inducible protein C like family

Chain F:



04065 04066 04067 04068 04069 04070 04071 04072 04073 04074 04075 04076 04077 04078 04079 04080 04081 04082 04083 04084 04085 04086 04087 04088 04089 04090 04091 04092 04093 04094 04095 04096 04097 04098 04099 04100 04101 04102 04103 04104 04105 04106 04107 04108 04109 04110 04111 04112 04113 04114 04115 04116 04117 04118 04119 04120

Diagram illustrating the distribution of various labels across 12 segments. The segments are color-coded: yellow (1-3), orange (4-5), green (6-7), red (8-9), blue (10-11), and purple (12). A green bar highlights segments 4 through 7.

Segment	Label
1	H1122
2	N1123
3	V1128
4	S1129
5	Q1130
6	L1131
7	K1132
8	I1133
9	N1134
10	V1137
11	T1138
12	L1139
13	V1140
14	H1141

- Molecule 1: osmotically inducible protein C like family

Chain G.



MET
GLY
SER
HIS
HIS
HIS
HIS
HIS
ASP
TYR
ASP
ILE
PRO
THR
THR
GLU
ASN
LEU
TYR
PHE
GLN
GLY
HIS
M1201
D1202
K1203
K1204
I1205
D1206
I1207
T1208



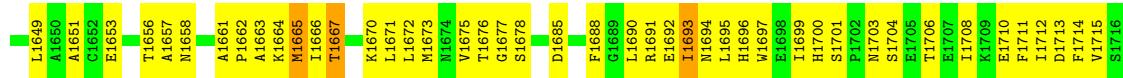
- Molecule 1: osmotically inducible protein C like family

Chain H: 34% 46% 5% 15%



- Molecule 1: osmotically inducible protein C like family

Chain I: 31% 51% 6% 12%



- Molecule 1: osmotically inducible protein C like family

Chain J: 36% 45% 5% 14%



4 Data and refinement statistics [\(i\)](#)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.36 Å 95.60 Å 308.48 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.85	Depositor
% Data completeness (in resolution range)	94.1 (19.91-2.85)	Depositor
R _{merge}	(Not available)	Depositor
R _{sym}	0.09	Depositor
Refinement program	CNS	Depositor
R, R _{free}	0.217 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11257	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

5 Model quality [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/1103	0.75	1/1494 (0.1%)
1	B	0.45	0/1103	0.77	1/1494 (0.1%)
1	C	0.45	1/1152 (0.1%)	0.75	1/1560 (0.1%)
1	D	0.43	0/1152	0.71	0/1560
1	E	0.44	0/1103	0.74	1/1494 (0.1%)
1	F	0.46	0/1152	0.77	2/1560 (0.1%)
1	G	0.45	0/1103	0.77	3/1494 (0.2%)
1	H	0.42	0/1103	0.77	2/1494 (0.1%)
1	I	0.48	1/1152 (0.1%)	0.74	2/1560 (0.1%)
1	J	0.43	0/1118	0.75	0/1514
All	All	0.44	2/11241 (0.0%)	0.75	13/15224 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1636	ALA	N-CA	5.39	1.57	1.46
1	C	436	ALA	N-CA	5.07	1.56	1.46

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1330	GLN	N-CA-C	-6.99	92.12	111.00
1	F	1130	GLN	N-CA-C	-6.08	94.59	111.00
1	C	530	GLN	N-CA-C	-6.07	94.62	111.00
1	F	1036	ALA	N-CA-C	5.84	126.78	111.00
1	I	1636	ALA	N-CA-C	5.81	126.69	111.00

There are no chirality outliers.

There are no planarity outliers.

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	A	1084	0	1094	72	0
1	B	1084	0	1091	81	0
1	C	1130	0	1127	87	0
1	D	1130	0	1127	86	0
1	E	1084	0	1091	88	0
1	F	1130	0	1127	78	0
1	G	1084	0	1091	79	0
1	H	1084	0	1091	90	0
1	I	1130	0	1127	101	0
1	J	1098	0	1101	87	0
2	A	25	0	0	2	0
2	B	34	0	0	2	0
2	C	17	0	0	1	0
2	D	16	0	0	3	0
2	E	21	0	0	1	0
2	F	34	0	0	2	0
2	G	11	0	0	0	0
2	H	16	0	0	5	0
2	I	23	0	0	5	0
2	J	22	0	0	2	0
All	All	11257	0	11067	731	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 33.

The worst 5 of 731 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1036:ALA:O	1:F:1037:LYS:CG	1.81	1.28
1:G:1212:ASN:HD21	1:G:1218:THR:HG23	1.10	1.11
1:D:699:ILE:HD11	1:D:712:ILE:HD11	1.27	1.09
1:A:12:ASN:HD21	1:A:18:THR:HG23	1.18	1.08
1:F:1093:ILE:HG22	1:F:1131:LEU:HD11	1.33	1.07

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	139/166 (84%)	124 (89%)	12 (9%)	3 (2%)	5 12
1	B	139/166 (84%)	129 (93%)	7 (5%)	3 (2%)	5 12
1	C	144/166 (87%)	133 (92%)	10 (7%)	1 (1%)	19 36
1	D	144/166 (87%)	132 (92%)	7 (5%)	5 (4%)	3 6
1	E	139/166 (84%)	124 (89%)	9 (6%)	6 (4%)	2 4
1	F	144/166 (87%)	130 (90%)	10 (7%)	4 (3%)	4 9
1	G	139/166 (84%)	129 (93%)	6 (4%)	4 (3%)	3 8
1	H	139/166 (84%)	127 (91%)	9 (6%)	3 (2%)	5 12
1	I	144/166 (87%)	131 (91%)	7 (5%)	6 (4%)	2 4
1	J	141/166 (85%)	127 (90%)	10 (7%)	4 (3%)	4 9
All	All	1412/1660 (85%)	1286 (91%)	87 (6%)	39 (3%)	4 9

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	328	VAL
1	E	836	ALA
1	F	1036	ALA
1	F	1037	LYS
1	G	1236	ALA

5.3.2 Protein sidechains [\(i\)](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	121/144 (84%)	110 (91%)	11 (9%)	7	15
1	B	121/144 (84%)	111 (92%)	10 (8%)	9	19
1	C	125/144 (87%)	113 (90%)	12 (10%)	7	13
1	D	125/144 (87%)	115 (92%)	10 (8%)	10	20
1	E	121/144 (84%)	112 (93%)	9 (7%)	11	24
1	F	125/144 (87%)	113 (90%)	12 (10%)	7	13
1	G	121/144 (84%)	112 (93%)	9 (7%)	11	24
1	H	121/144 (84%)	111 (92%)	10 (8%)	9	19
1	I	125/144 (87%)	112 (90%)	13 (10%)	5	11
1	J	122/144 (85%)	109 (89%)	13 (11%)	5	10
All	All	1227/1440 (85%)	1118 (91%)	109 (9%)	8	16

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1071	LEU
1	G	1326	GLN
1	J	1849	LEU
1	F	1118	ARG
1	G	1249	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	1523	ASN
1	J	1874	ASN
1	I	1598	GLN
1	I	1722	HIS
1	C	522	HIS

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [\(i\)](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [\(i\)](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [\(i\)](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [\(i\)](#)

EDS was not executed - this section is therefore empty.