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:

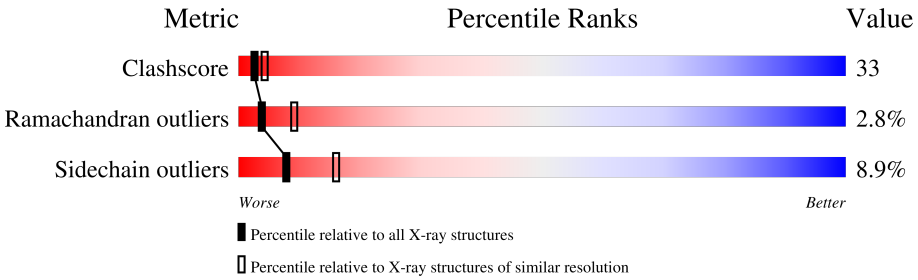
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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.

Mol	Chain	Length	Quality of chain
1	A	166	41% 39% 5% 15%
1	B	166	40% 39% 6% 15%
1	C	166	44% 38% 6% 12%
1	D	166	40% 42% 7% 12%
1	E	166	36% 42% 8% 15%
1	F	166	41% 40% 7% • 12%
1	G	166	40% 40% • • 15%
1	H	166	34% 46% 5% 15%

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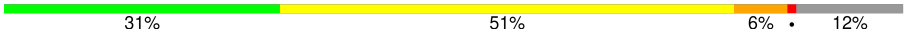
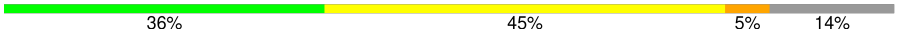
Mol	Chain	Length	Quality of chain
1	I	166	
1	J	166	

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 osmotical inducible protein C like family.

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

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

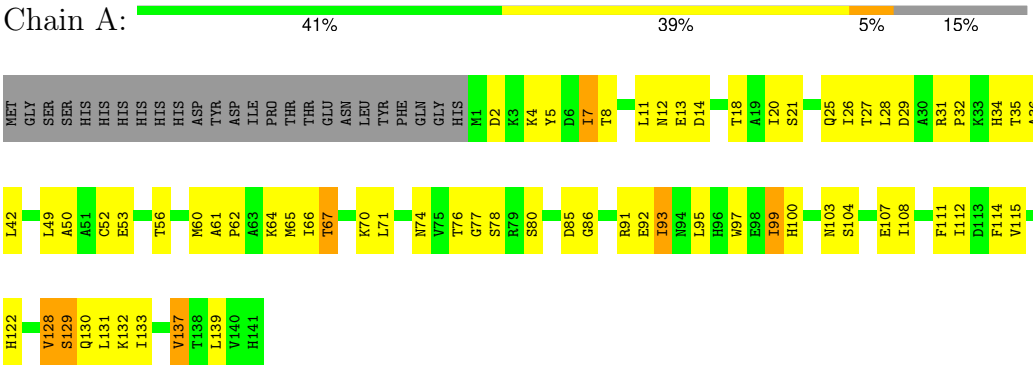
3 Residue-property plots (i)

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. 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.

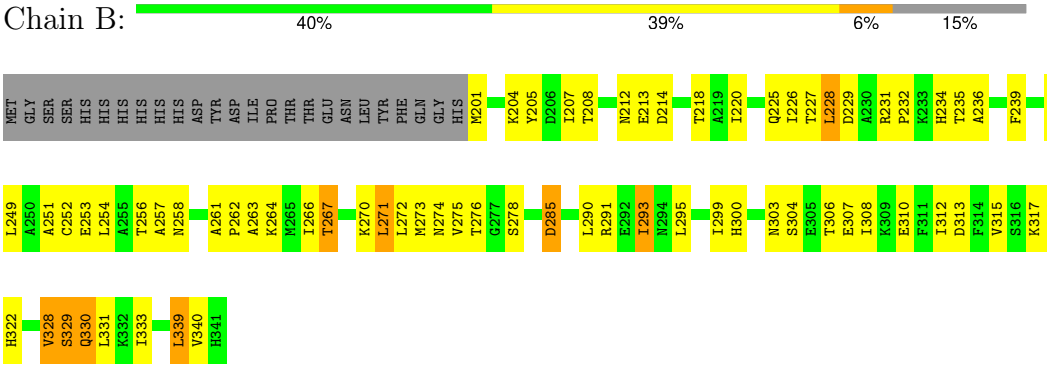
• Molecule 1: osmotical inducible protein C like family

Chain A:



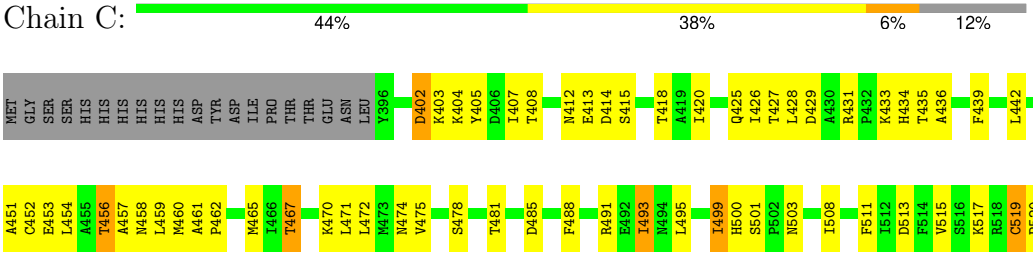
• Molecule 1: osmotical inducible protein C like family

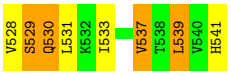
Chain B:



• Molecule 1: osmotical inducible protein C like family

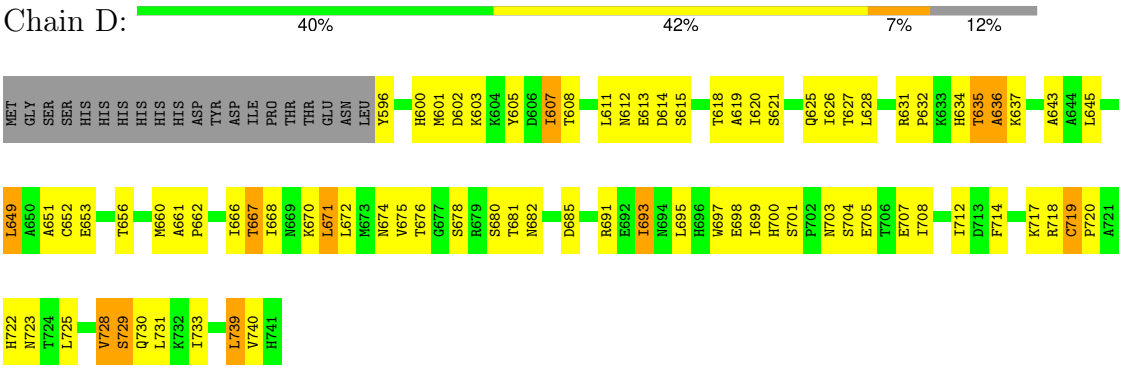
Chain C:





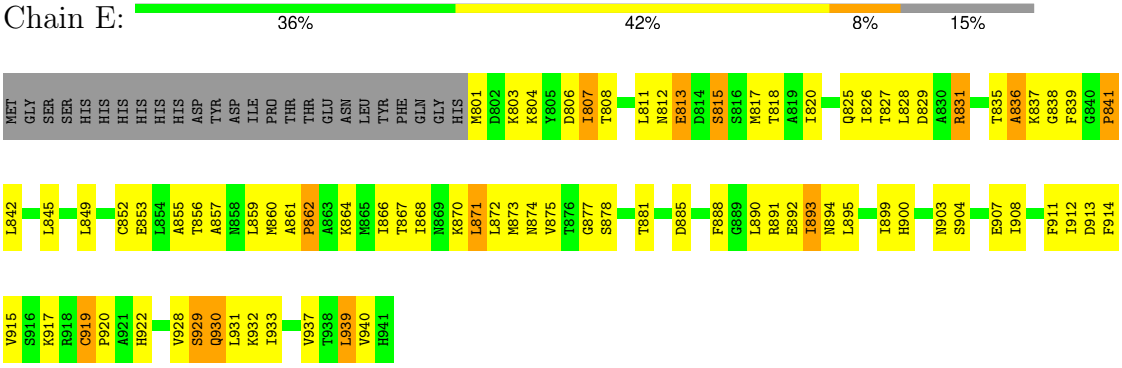
• Molecule 1: osmotical inducible protein C like family

Chain D:



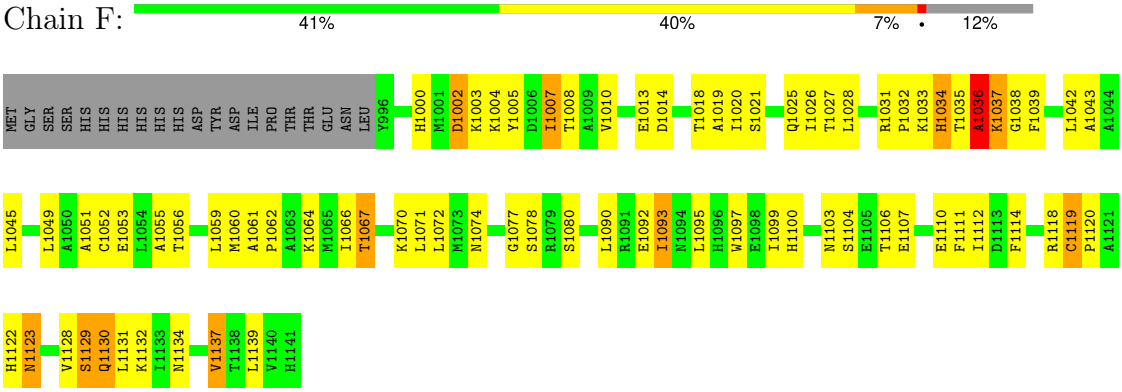
• Molecule 1: osmotical inducible protein C like family

Chain E:



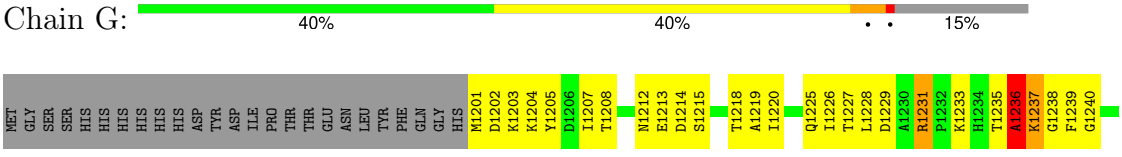
• Molecule 1: osmotical inducible protein C like family

Chain F:



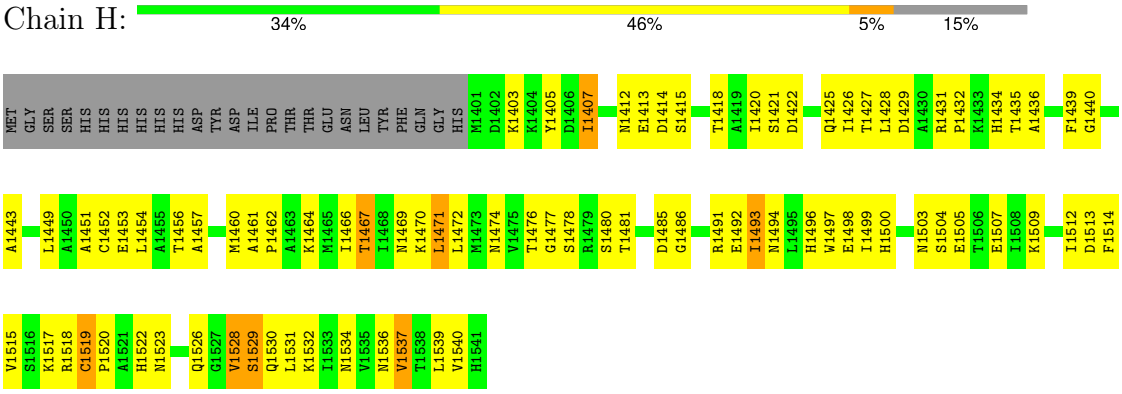
• Molecule 1: osmotical inducible protein C like family

Chain G:



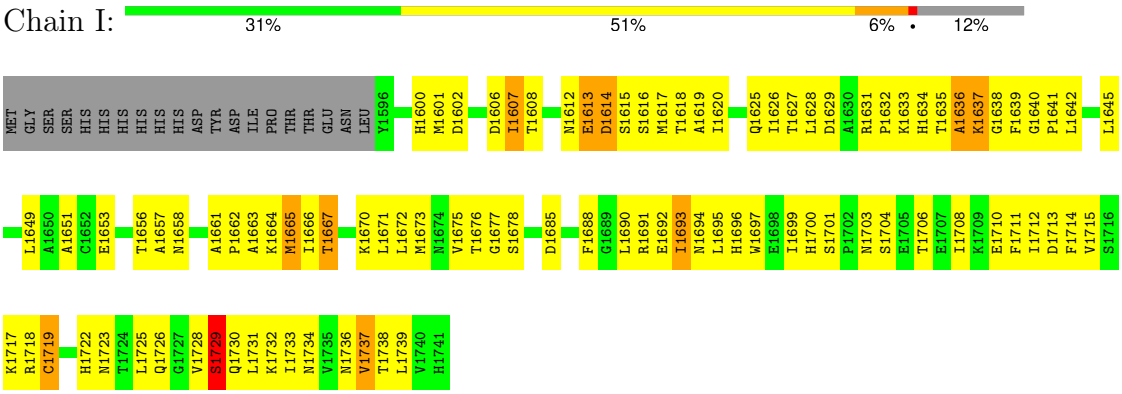
• Molecule 1: osmotical inducible protein C like family

Chain H:



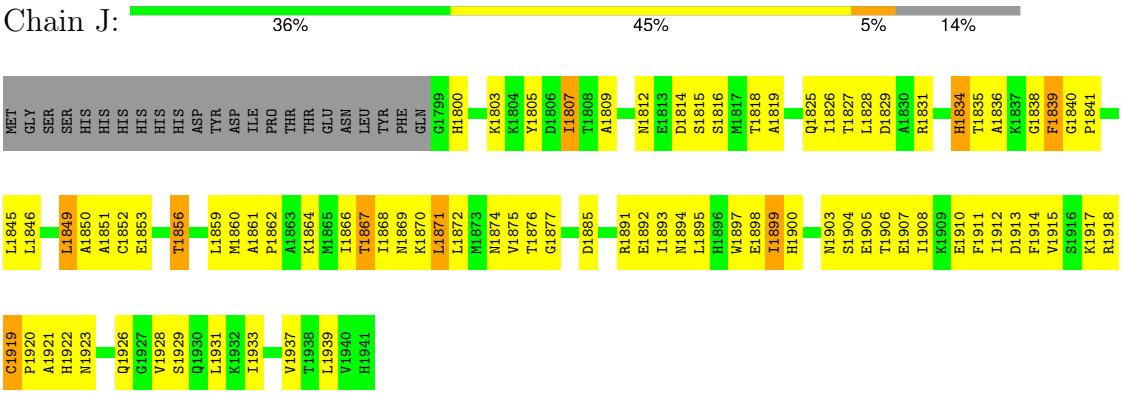
• Molecule 1: osmotical inducible protein C like family

Chain I:



• Molecule 1: osmotical inducible protein C like family

Chain J:



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	66.36Å 95.60Å 308.48Å 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.43	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(^{o})	Ideal(^{o})
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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.