



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:44 PM GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

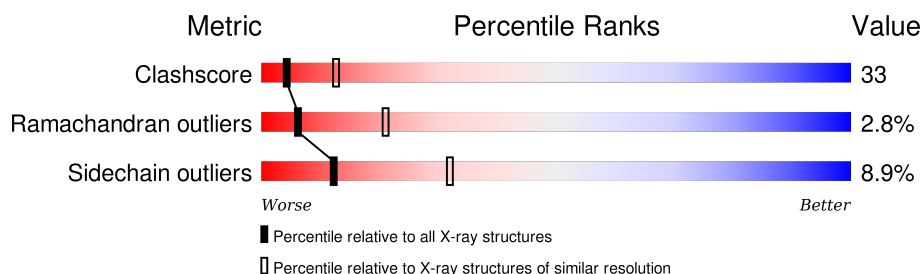
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	166	
1	B	166	
1	C	166	
1	D	166	
1	E	166	
1	F	166	
1	G	166	

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Mol	Chain	Length	Quality of chain
1	H	166	<div><div></div><div>34%46%5%15%</div></div>
1	I	166	<div><div></div><div>31%51%6%12%</div></div>
1	J	166	<div><div></div><div>36%45%5%14%</div></div>

## 2 Entry composition

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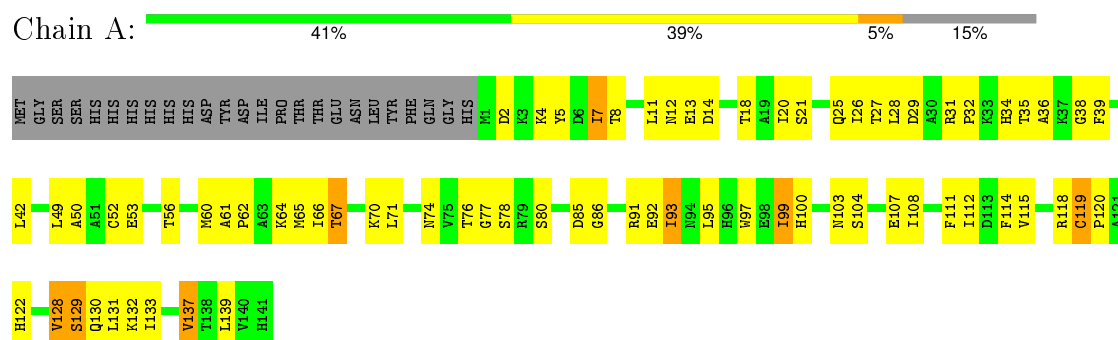
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	21	Total 21	O 21	0	0
2	F	34	Total 34	O 34	0	0
2	G	11	Total 11	O 11	0	0
2	H	16	Total 16	O 16	0	0
2	I	23	Total 23	O 23	0	0
2	J	22	Total 22	O 22	0	0

### 3 Residue-property plots

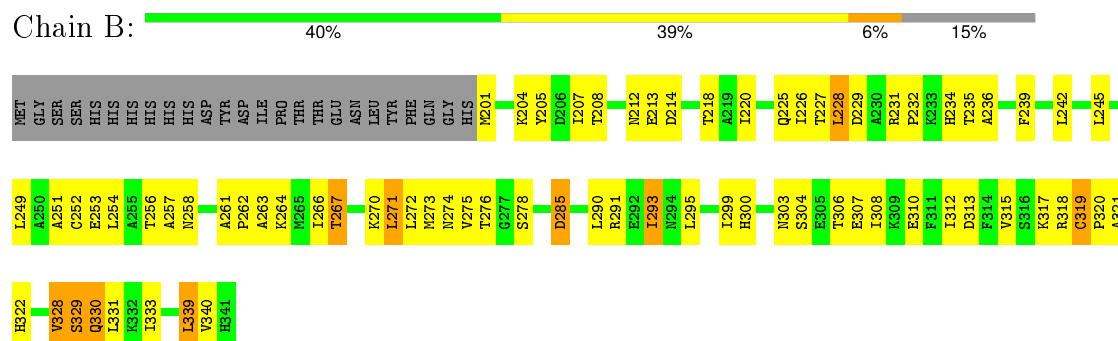
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

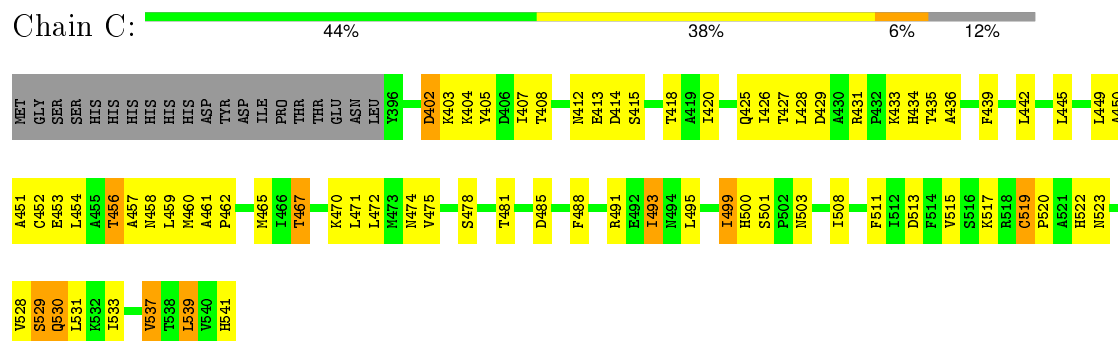
- Molecule 1: osmotical inducible protein C like family



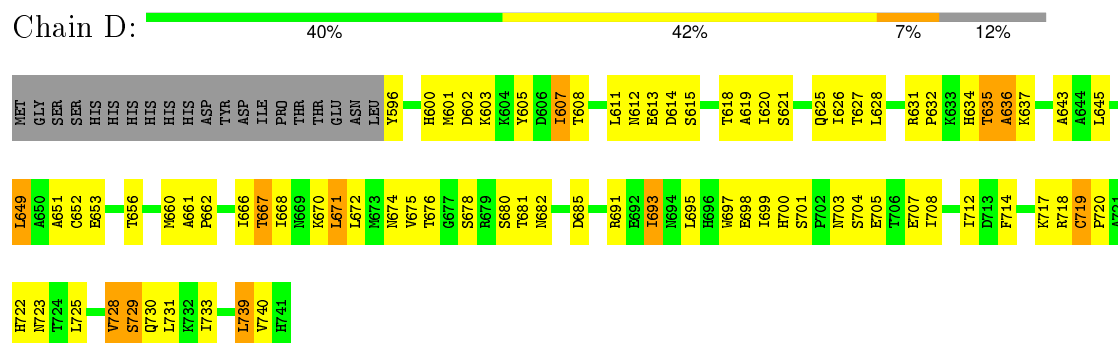
- Molecule 1: osmotical inducible protein C like family



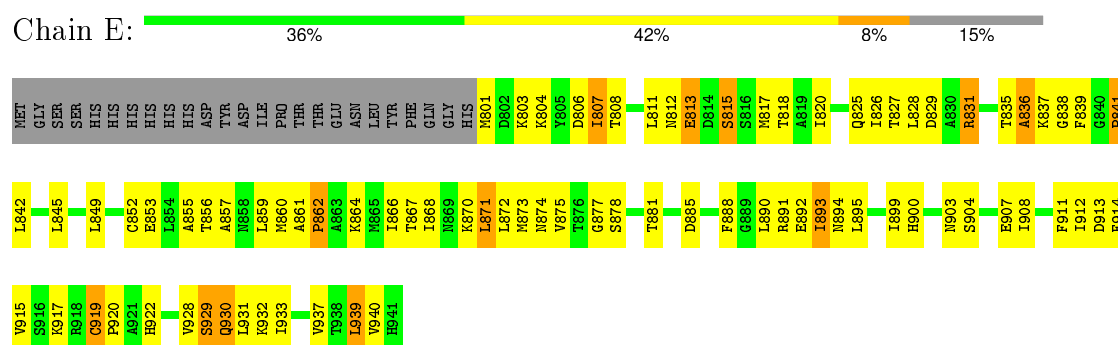
- Molecule 1: osmotical inducible protein C like family



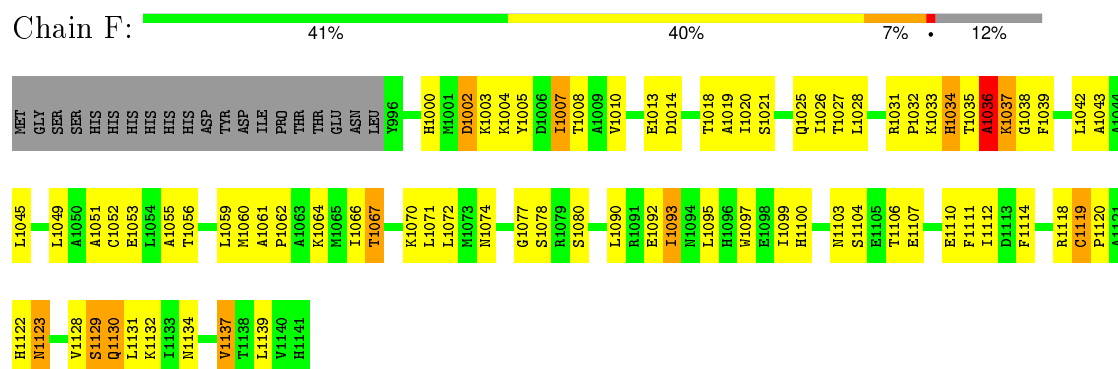
- Molecule 1: osmotical inducible protein C like family



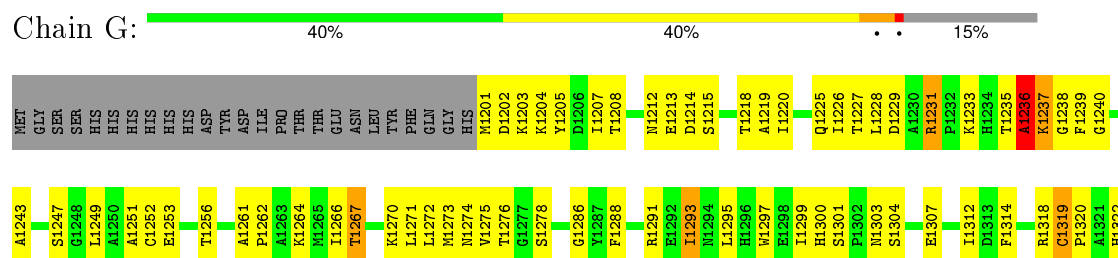
- Molecule 1: osmotical inducible protein C like family



- Molecule 1: osmotical inducible protein C like family



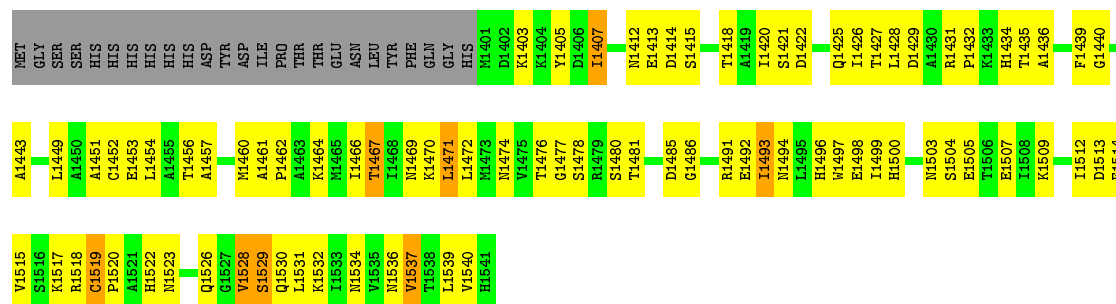
- Molecule 1: osmotical inducible protein C like family





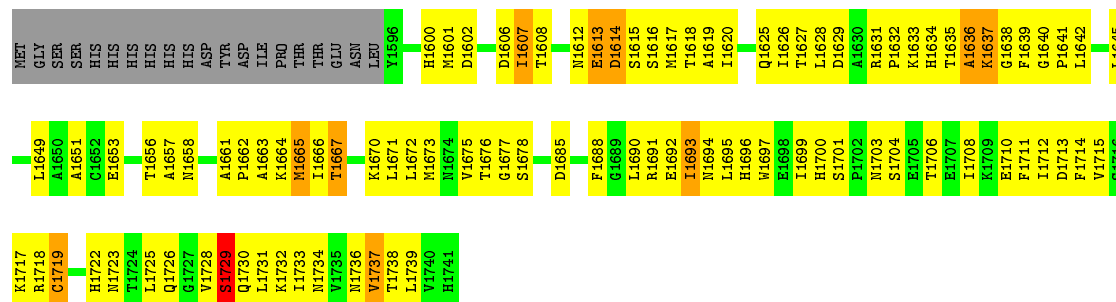
- Molecule 1: osmotical inducible protein C like family

Chain H: 34% 46% 5% 15%



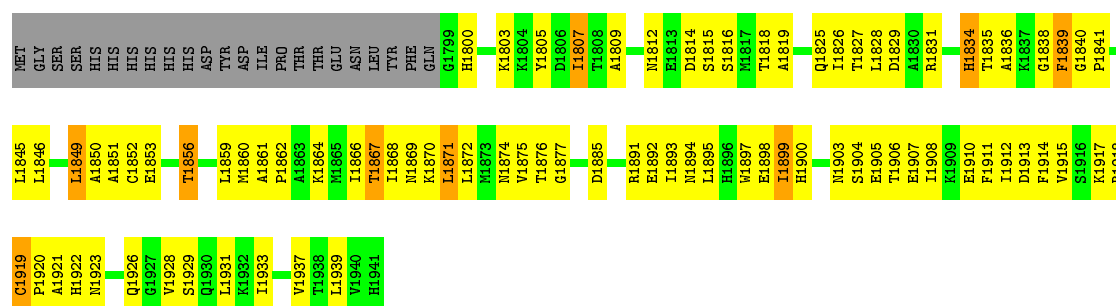
- Molecule 1: osmotical inducible protein C like family

Chain I: 31% 51% 6% 12%



- Molecule 1: osmotical inducible protein C like family

Chain J: 36% 45% 5% 14%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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

All (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
1	H	1486	GLY	N-CA-C	-5.66	98.95	113.10
1	I	1730	GLN	N-CA-C	-5.64	95.77	111.00
1	G	1236	ALA	N-CA-C	5.63	126.19	111.00
1	E	930	GLN	N-CA-C	-5.34	96.58	111.00
1	H	1436	ALA	N-CA-C	5.28	125.26	111.00
1	B	330	GLN	N-CA-CB	-5.20	101.25	110.60
1	G	1286	GLY	N-CA-C	-5.04	100.49	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	GLY	N-CA-C	-5.03	100.52	113.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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.

All (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
1:F:1036:ALA:O	1:F:1037:LYS:HG3	0.89	1.04
1:I:1612:ASN:HD21	1:I:1618:THR:HG23	1.22	1.04
1:C:412:ASN:HD21	1:C:418:THR:HG23	1.21	1.02
1:H:1493:ILE:HG22	1:H:1531:LEU:HD11	1.43	1.00
1:I:1636:ALA:O	1:I:1637:LYS:HG3	1.60	1.00
1:I:1667:THR:H	1:I:1703:ASN:HD21	1.03	0.97
1:H:1418:THR:HG22	1:H:1427:THR:HG22	1.45	0.96
1:J:1867:THR:H	1:J:1903:ASN:HD21	1.13	0.95
1:F:1036:ALA:C	1:F:1037:LYS:HG3	1.87	0.95
1:C:493:ILE:HG22	1:C:531:LEU:HD11	1.49	0.94
1:C:452:CYS:O	1:C:456:THR:HG23	1.67	0.91
1:A:99:ILE:HD11	1:A:112:ILE:HD11	1.52	0.91
1:B:212:ASN:HD21	1:B:218:THR:HG23	1.35	0.89
1:I:1693:ILE:HG22	1:I:1731:LEU:HD11	1.54	0.89
1:H:1412:ASN:HD21	1:H:1418:THR:HG23	1.36	0.88
1:F:1099:ILE:HD11	1:F:1112:ILE:HD11	1.55	0.88
1:D:620:ILE:HG13	1:D:625:GLN:HG2	1.56	0.87
1:C:503:ASN:HB2	1:C:508:ILE:HD11	1.58	0.85
1:A:67:THR:H	1:A:103:ASN:HD21	1.20	0.85
1:E:831:ARG:NH1	1:E:835:THR:HG21	1.92	0.84
1:G:1252:CYS:O	1:G:1256:THR:HG23	1.79	0.83
1:C:418:THR:HG22	1:C:427:THR:HG22	1.60	0.83
1:A:56:THR:HG21	1:A:119:CYS:HA	1.58	0.83
1:H:1467:THR:H	1:H:1503:ASN:HD21	1.23	0.83
1:G:1231:ARG:NH1	1:G:1235:THR:HG21	1.92	0.83
1:J:1897:TRP:HB3	1:J:1899:ILE:HD11	1.61	0.82
1:B:228:LEU:N	1:B:228:LEU:HD12	1.95	0.81
1:E:888:PHE:H	1:F:1123:ASN:ND2	1.78	0.81
1:E:856:THR:HG21	1:E:919:CYS:HA	1.62	0.81
1:A:12:ASN:ND2	1:A:18:THR:HG23	1.96	0.81
1:I:1667:THR:H	1:I:1703:ASN:ND2	1.78	0.81
1:C:474:ASN:HD22	1:D:608:THR:HG22	1.45	0.80
1:H:1456:THR:HG21	1:H:1519:CYS:HA	1.64	0.80
1:D:661:ALA:HB3	1:D:662:PRO:HD3	1.64	0.80
1:A:32:PRO:HB2	1:A:34:HIS:CE1	2.17	0.80
1:H:1499:ILE:HD11	1:H:1512:ILE:HD11	1.64	0.80
1:I:1618:THR:HG22	1:I:1627:THR:HG22	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1020:ILE:HG13	1:F:1025:GLN:HG2	1.63	0.79
1:I:1626:ILE:HD13	1:J:1839:PHE:CE2	2.18	0.79
1:H:1504:SER:OG	1:H:1507:GLU:HG3	1.83	0.79
1:B:304:SER:OG	1:B:307:GLU:HG3	1.81	0.79
1:I:1628:LEU:HD22	1:J:1851:ALA:HB2	1.66	0.78
1:G:1293:ILE:HG22	1:G:1331:LEU:HD11	1.64	0.78
1:G:1212:ASN:ND2	1:G:1218:THR:HG23	1.95	0.78
1:A:52:CYS:O	1:A:56:THR:HG23	1.84	0.78
1:I:1656:THR:HG21	1:I:1719:CYS:HA	1.65	0.77
1:H:1461:ALA:HB3	1:H:1462:PRO:HD3	1.66	0.77
1:B:252:CYS:O	1:B:256:THR:HG23	1.82	0.77
1:E:818:THR:HG22	1:E:827:THR:HG22	1.66	0.77
1:G:1267:THR:H	1:G:1303:ASN:HD21	1.30	0.77
1:D:652:CYS:O	1:D:656:THR:HG23	1.85	0.77
1:J:1831:ARG:NH1	1:J:1835:THR:HG21	2.00	0.76
1:A:104:SER:OG	1:A:107:GLU:HG3	1.86	0.76
1:C:435:THR:HG22	1:C:435:THR:O	1.84	0.76
1:F:1059:LEU:HG	2:F:2049:HOH:O	1.86	0.76
1:J:1861:ALA:HB3	1:J:1862:PRO:HD3	1.67	0.75
1:E:864:LYS:O	1:E:866:ILE:HD12	1.85	0.75
1:E:870:LYS:HB2	1:E:900:HIS:HB2	1.68	0.75
1:H:1431:ARG:NH1	1:H:1435:THR:HG21	2.01	0.74
1:G:1207:ILE:HD11	1:H:1443:ALA:HB1	1.69	0.74
1:B:231:ARG:HD3	1:B:235:THR:HG22	1.70	0.74
1:C:456:THR:HG21	1:C:519:CYS:HA	1.70	0.73
1:C:412:ASN:ND2	1:C:418:THR:HG23	2.01	0.73
1:C:439:PHE:CE2	1:D:626:ILE:HD13	2.24	0.73
1:G:1226:ILE:HD13	1:H:1439:PHE:CE2	2.24	0.73
1:A:67:THR:H	1:A:103:ASN:ND2	1.85	0.73
1:D:656:THR:HG21	1:D:719:CYS:HA	1.69	0.73
1:E:874:ASN:HD22	1:F:1008:THR:HG22	1.53	0.73
1:F:1097:TRP:HB2	1:F:1137:VAL:HB	1.71	0.73
1:A:61:ALA:HB3	1:A:62:PRO:HD3	1.71	0.73
1:F:1093:ILE:C	1:F:1093:ILE:HD13	2.09	0.72
1:A:70:LYS:HB2	1:A:100:HIS:HB2	1.70	0.72
1:J:1864:LYS:O	1:J:1866:ILE:HD12	1.89	0.72
1:B:229:ASP:OD2	1:B:231:ARG:HD2	1.90	0.72
1:A:93:ILE:HG22	1:A:131:LEU:HD11	1.71	0.72
1:E:893:ILE:HG22	1:E:931:LEU:HD11	1.70	0.72
1:C:499:ILE:N	1:C:499:ILE:HD12	2.05	0.72
1:F:1067:THR:H	1:F:1103:ASN:HD21	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1228:LEU:HD22	1:H:1451:ALA:HB2	1.72	0.70
1:B:328:VAL:O	1:B:329:SER:HB3	1.88	0.70
1:B:226:ILE:HG22	1:B:228:LEU:HD11	1.71	0.70
1:J:1852:CYS:O	1:J:1856:THR:HG23	1.90	0.70
1:I:1699:ILE:HD11	1:I:1712:ILE:HD11	1.71	0.70
1:F:1007:ILE:HD11	1:F:1021:SER:HB2	1.72	0.70
1:G:1208:THR:HG22	1:H:1474:ASN:HD22	1.56	0.70
1:E:839:PHE:CE2	1:F:1026:ILE:HD13	2.26	0.70
1:G:1261:ALA:HB3	1:G:1262:PRO:HD3	1.71	0.70
1:J:1867:THR:N	1:J:1903:ASN:HD21	1.88	0.70
1:D:693:ILE:HG22	1:D:731:LEU:HD11	1.72	0.70
1:J:1911:PHE:O	1:J:1915:VAL:HG23	1.91	0.69
1:E:812:ASN:HD21	1:E:818:THR:HG23	1.55	0.69
1:H:1485:ASP:HB2	1:H:1491:ARG:HH22	1.57	0.69
1:B:212:ASN:ND2	1:B:218:THR:HG23	2.07	0.69
1:E:829:ASP:OD1	1:E:831:ARG:HD2	1.91	0.69
1:B:256:THR:HG21	1:B:319:CYS:HA	1.74	0.69
1:G:1225:GLN:O	1:G:1226:ILE:HD12	1.92	0.69
1:G:1256:THR:HG21	1:G:1319:CYS:HA	1.72	0.69
1:I:1661:ALA:HB3	1:I:1662:PRO:HD3	1.72	0.69
1:C:404:LYS:HD3	1:D:678:SER:HB3	1.75	0.69
1:F:1056:THR:HG21	1:F:1119:CYS:HA	1.75	0.69
1:J:1818:THR:HG22	1:J:1827:THR:HG22	1.74	0.69
1:H:1467:THR:H	1:H:1503:ASN:ND2	1.91	0.68
1:G:1251:ALA:HB2	1:H:1428:LEU:HD22	1.75	0.68
1:I:1675:VAL:HG22	1:I:1695:LEU:HD23	1.74	0.68
1:C:528:VAL:HG12	1:C:530:GLN:H	1.57	0.68
1:D:670:LYS:HB2	1:D:700:HIS:HB2	1.75	0.68
1:I:1632:PRO:HB2	1:I:1634:HIS:CE1	2.27	0.68
1:J:1825:GLN:O	1:J:1826:ILE:HD12	1.92	0.68
1:I:1636:ALA:O	1:I:1637:LYS:CG	2.38	0.68
1:J:1864:LYS:HB3	1:J:1866:ILE:HD13	1.74	0.68
1:B:328:VAL:O	1:B:329:SER:CB	2.41	0.68
1:I:1728:VAL:O	1:I:1729:SER:HB3	1.94	0.68
1:E:867:THR:H	1:E:903:ASN:HD21	1.42	0.68
1:H:1453:GLU:OE1	1:H:1522:HIS:HD2	1.77	0.67
1:H:1493:ILE:CG2	1:H:1531:LEU:HD11	2.23	0.67
1:J:1829:ASP:O	1:J:1840:GLY:HA2	1.94	0.67
1:I:1670:LYS:HB2	1:I:1700:HIS:HB2	1.77	0.67
1:J:1867:THR:H	1:J:1903:ASN:ND2	1.89	0.67
1:C:503:ASN:HB2	1:C:508:ILE:CD1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1228:LEU:N	1:G:1228:LEU:HD12	2.10	0.66
1:E:853:GLU:OE1	1:E:922:HIS:HD2	1.78	0.66
1:C:456:THR:HG21	1:C:519:CYS:HB2	1.76	0.66
1:A:56:THR:O	1:A:60:MET:HG2	1.95	0.66
1:J:1852:CYS:SG	1:J:1920:PRO:HD2	2.35	0.66
1:G:1278:SER:HA	1:H:1403:LYS:O	1.95	0.66
1:F:1070:LYS:HB2	1:F:1100:HIS:HB2	1.77	0.66
1:D:628:LEU:HD12	1:D:628:LEU:N	2.11	0.66
1:A:8:THR:CG2	1:B:274:ASN:HD22	2.08	0.66
1:C:499:ILE:HD13	1:C:537:VAL:HG23	1.77	0.66
1:J:1913:ASP:O	1:J:1917:LYS:HG3	1.96	0.66
1:J:1812:ASN:HD21	1:J:1818:THR:HG23	1.61	0.65
1:D:667:THR:HA	2:D:2059:HOH:O	1.95	0.65
1:E:928:VAL:HG12	1:E:930:GLN:H	1.61	0.65
1:I:1661:ALA:N	2:I:2043:HOH:O	2.28	0.65
1:G:1236:ALA:O	1:G:1237:LYS:HG3	1.95	0.65
1:G:1328:VAL:HG12	1:G:1330:GLN:H	1.61	0.65
1:D:607:ILE:HD11	1:D:621:SER:HB2	1.77	0.65
1:J:1870:LYS:HB2	1:J:1900:HIS:CG	2.31	0.65
1:D:631:ARG:HD3	1:D:635:THR:HG21	1.79	0.65
1:C:453:GLU:OE1	1:C:522:HIS:HD2	1.79	0.65
1:B:299:ILE:HD11	1:B:312:ILE:HD11	1.78	0.65
1:G:1201:MET:N	1:H:1480:SER:HG	1.95	0.65
1:C:402:ASP:OD2	1:D:681:THR:HG23	1.97	0.65
1:D:667:THR:H	1:D:703:ASN:HD21	1.43	0.64
1:A:80:SER:HG	1:B:201:MET:N	1.96	0.64
1:D:626:ILE:HG22	1:D:628:LEU:CD1	2.27	0.64
1:G:1293:ILE:HD13	1:G:1293:ILE:C	2.17	0.64
1:F:1052:CYS:O	1:F:1056:THR:HG23	1.96	0.64
1:D:631:ARG:HD3	1:D:635:THR:CG2	2.28	0.64
1:E:828:LEU:HD22	1:F:1051:ALA:HB2	1.79	0.64
1:C:407:ILE:HD11	1:D:643:ALA:HB1	1.78	0.64
1:E:899:ILE:HD11	1:E:912:ILE:HD11	1.80	0.64
1:I:1627:THR:O	1:I:1638:GLY:HA3	1.97	0.63
1:I:1631:ARG:HH11	1:I:1635:THR:HG21	1.63	0.63
1:I:1631:ARG:NH1	1:I:1635:THR:HG21	2.12	0.63
1:G:1227:THR:O	1:G:1238:GLY:HA3	1.99	0.63
1:B:285:ASP:HB2	1:B:291:ARG:HH22	1.62	0.63
1:D:672:LEU:HG	1:D:698:GLU:HB3	1.81	0.63
1:B:218:THR:HG22	1:B:227:THR:HG22	1.80	0.63
1:C:474:ASN:HD22	1:D:608:THR:CG2	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1431:ARG:HH11	1:H:1435:THR:HG21	1.62	0.63
1:B:227:THR:C	1:B:228:LEU:HD12	2.18	0.63
1:J:1870:LYS:HB2	1:J:1900:HIS:HB2	1.79	0.63
1:A:56:THR:OG1	1:A:115:VAL:HG13	1.98	0.63
1:F:1026:ILE:HG22	1:F:1028:LEU:CD1	2.27	0.63
1:G:1202:ASP:HB2	1:H:1481:THR:HG23	1.81	0.63
1:B:252:CYS:SG	1:B:320:PRO:HD2	2.39	0.63
1:C:470:LYS:HB2	1:C:500:HIS:HB2	1.79	0.63
1:J:1856:THR:HG21	1:J:1919:CYS:HA	1.80	0.62
1:E:867:THR:H	1:E:903:ASN:ND2	1.97	0.62
1:C:513:ASP:O	1:C:517:LYS:HG3	1.98	0.62
1:I:1626:ILE:HG22	1:I:1628:LEU:CD1	2.29	0.62
1:E:874:ASN:HD22	1:F:1008:THR:CG2	2.12	0.62
1:G:1270:LYS:HB2	1:G:1300:HIS:HB2	1.80	0.62
1:E:801:MET:N	1:F:1080:SER:HG	1.98	0.62
1:E:839:PHE:CD2	1:F:1026:ILE:HD13	2.33	0.62
1:E:826:ILE:HG22	1:E:828:LEU:CD1	2.28	0.62
1:D:699:ILE:HD11	1:D:712:ILE:CD1	2.16	0.62
1:G:1276:THR:HA	1:H:1405:TYR:O	2.00	0.62
1:J:1834:HIS:CD2	1:J:1834:HIS:H	2.16	0.62
1:F:1132:LYS:HE3	1:F:1134:ASN:OD1	1.99	0.61
1:B:231:ARG:NH1	1:B:235:THR:HG21	2.15	0.61
1:J:1853:GLU:OE1	1:J:1922:HIS:HD2	1.83	0.61
1:D:667:THR:H	1:D:703:ASN:ND2	1.99	0.61
1:C:453:GLU:OE1	1:C:522:HIS:CD2	2.54	0.61
1:E:835:THR:O	1:E:836:ALA:O	2.18	0.61
1:G:1205:TYR:O	1:H:1476:THR:HA	2.00	0.61
1:B:339:LEU:HD23	1:B:340:VAL:N	2.16	0.61
1:D:670:LYS:HB2	1:D:700:HIS:CG	2.36	0.61
1:I:1693:ILE:HD13	1:I:1693:ILE:C	2.21	0.61
1:B:270:LYS:HB2	1:B:300:HIS:HB2	1.82	0.61
1:C:499:ILE:HD12	1:C:499:ILE:H	1.64	0.61
1:F:1018:THR:HG22	1:F:1027:THR:HG22	1.83	0.61
1:C:460:MET:CE	1:I:1663:ALA:HA	2.31	0.61
1:H:1493:ILE:C	1:H:1493:ILE:HD13	2.21	0.60
1:G:1208:THR:HG22	1:H:1474:ASN:ND2	2.14	0.60
1:G:1226:ILE:HD13	1:H:1439:PHE:CD2	2.36	0.60
1:J:1905:GLU:HG3	2:J:2096:HOH:O	2.00	0.60
1:I:1612:ASN:ND2	1:I:1618:THR:HG23	2.05	0.60
1:G:1291:ARG:HH11	1:G:1291:ARG:HG2	1.67	0.60
1:J:1856:THR:HG21	1:J:1919:CYS:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:672:LEU:C	1:D:672:LEU:HD12	2.22	0.60
1:D:632:PRO:HB2	1:D:634:HIS:CE1	2.36	0.60
1:C:493:ILE:HD13	1:C:493:ILE:C	2.21	0.60
1:C:467:THR:H	1:C:503:ASN:HD21	1.49	0.60
1:H:1470:LYS:HB2	1:H:1500:HIS:HB2	1.82	0.60
1:B:253:GLU:OE1	1:B:322:HIS:HD2	1.83	0.60
1:H:1432:PRO:HB2	1:H:1434:HIS:CE1	2.36	0.60
1:I:1711:PHE:O	1:I:1714:PHE:HB3	2.02	0.60
1:I:1628:LEU:N	1:I:1628:LEU:HD12	2.17	0.59
1:F:1128:VAL:HB	1:F:1131:LEU:HB3	1.84	0.59
1:I:1633:LYS:O	1:I:1636:ALA:HB2	2.02	0.59
1:B:226:ILE:HG22	1:B:228:LEU:CD1	2.33	0.59
1:G:1231:ARG:HH11	1:G:1235:THR:HG21	1.66	0.59
1:F:1000:HIS:HB2	2:F:2004:HOH:O	2.02	0.59
1:E:904:SER:OG	1:E:907:GLU:HG3	2.03	0.59
1:H:1425:GLN:O	1:H:1426:ILE:HD12	2.02	0.59
1:F:1104:SER:OG	1:F:1107:GLU:HG3	2.02	0.59
1:A:8:THR:HG22	1:B:274:ASN:HD22	1.68	0.59
1:H:1454:LEU:HD22	1:H:1471:LEU:HD13	1.83	0.59
1:G:1229:ASP:OD2	1:G:1231:ARG:HD2	2.03	0.59
1:F:1067:THR:H	1:F:1103:ASN:ND2	2.00	0.59
1:A:29:ASP:OD2	1:A:31:ARG:HD2	2.03	0.59
1:B:293:ILE:CG2	1:B:333:ILE:HG12	2.33	0.59
1:D:636:ALA:O	1:D:637:LYS:HG3	2.03	0.58
1:C:408:THR:HG22	1:D:674:ASN:HD22	1.68	0.58
1:C:408:THR:CG2	1:D:674:ASN:HD22	2.16	0.58
1:C:470:LYS:HB2	1:C:500:HIS:CG	2.38	0.58
1:C:533:ILE:HD12	1:C:533:ILE:N	2.18	0.58
1:B:306:THR:O	1:B:310:GLU:HG3	2.03	0.58
1:F:1026:ILE:HG22	1:F:1028:LEU:HD11	1.85	0.58
1:A:97:TRP:HB2	1:A:137:VAL:HB	1.85	0.58
1:A:128:VAL:O	1:A:129:SER:CB	2.51	0.58
1:H:1464:LYS:HB3	1:H:1466:ILE:HD13	1.86	0.58
1:E:888:PHE:H	1:F:1123:ASN:HD22	1.51	0.58
1:H:1429:ASP:O	1:H:1440:GLY:HA2	2.03	0.58
1:I:1625:GLN:O	1:I:1626:ILE:HD12	2.03	0.58
1:B:231:ARG:HH11	1:B:235:THR:HG21	1.67	0.58
1:A:26:ILE:HG22	1:A:28:LEU:CD1	2.34	0.58
1:E:826:ILE:HD13	1:F:1039:PHE:CE2	2.39	0.58
1:I:1626:ILE:HD13	1:J:1839:PHE:CD2	2.39	0.58
1:H:1428:LEU:N	1:H:1428:LEU:HD12	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:LYS:HB3	1:B:266:ILE:HD13	1.86	0.58
1:H:1407:ILE:HD11	1:H:1421:SER:HB2	1.86	0.57
1:C:439:PHE:CD2	1:D:626:ILE:HD13	2.39	0.57
1:D:613:GLU:O	1:D:615:SER:N	2.38	0.57
1:H:1452:CYS:SG	1:H:1520:PRO:HD2	2.45	0.57
1:C:428:LEU:N	1:C:428:LEU:HD12	2.19	0.57
1:F:1031:ARG:HB2	1:F:1036:ALA:H	1.70	0.57
1:C:499:ILE:CD1	1:C:537:VAL:HG23	2.34	0.57
1:E:853:GLU:OE1	1:E:922:HIS:CD2	2.58	0.57
1:E:911:PHE:O	1:E:914:PHE:HB3	2.04	0.57
1:E:893:ILE:C	1:E:893:ILE:HD13	2.25	0.57
1:H:1509:LYS:O	1:H:1509:LYS:HD3	2.05	0.57
1:E:820:ILE:HD12	1:E:820:ILE:N	2.20	0.57
1:B:257:ALA:HA	1:B:315:VAL:CG2	2.35	0.57
1:D:613:GLU:C	1:D:615:SER:H	2.08	0.57
1:F:1128:VAL:HG12	1:F:1130:GLN:H	1.70	0.56
1:F:1027:THR:O	1:F:1038:GLY:HA3	2.05	0.56
1:H:1425:GLN:C	1:H:1426:ILE:HD12	2.24	0.56
1:E:878:SER:HB3	1:F:1004:LYS:HD3	1.87	0.56
1:C:481:THR:HG23	1:D:602:ASP:HB2	1.86	0.56
1:C:456:THR:CG2	1:C:519:CYS:HB2	2.35	0.56
1:I:1626:ILE:HG22	1:I:1628:LEU:HD11	1.87	0.56
1:B:229:ASP:CG	1:B:231:ARG:HD2	2.25	0.56
1:J:1919:CYS:SG	1:J:1921:ALA:HB3	2.45	0.56
1:E:939:LEU:HD23	1:E:940:VAL:N	2.20	0.56
1:F:1061:ALA:HB3	1:F:1062:PRO:HD3	1.87	0.56
1:C:485:ASP:OD2	1:C:491:ARG:NH2	2.38	0.56
1:B:213:GLU:O	1:B:214:ASP:CG	2.43	0.56
1:D:699:ILE:HD12	1:D:708:ILE:CG2	2.36	0.56
1:F:1034:HIS:O	1:F:1035:THR:C	2.43	0.56
1:E:872:LEU:HD12	1:E:872:LEU:O	2.05	0.56
1:C:442:LEU:HD12	1:D:605:TYR:CZ	2.40	0.56
1:G:1247:SER:OG	1:H:1407:ILE:HG12	2.06	0.56
1:A:20:ILE:HG13	1:A:25:GLN:HG2	1.88	0.56
1:A:12:ASN:HB3	2:A:2100:HOH:O	2.06	0.56
1:H:1412:ASN:ND2	1:H:1418:THR:HG23	2.15	0.56
1:I:1713:ASP:HB3	1:I:1717:LYS:NZ	2.21	0.56
1:J:1897:TRP:HB2	1:J:1937:VAL:HB	1.88	0.56
1:D:728:VAL:O	1:D:729:SER:CB	2.54	0.56
1:G:1304:SER:OG	1:G:1307:GLU:HG3	2.05	0.56
1:F:1032:PRO:O	1:F:1034:HIS:N	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1213:GLU:O	1:G:1214:ASP:CG	2.45	0.55
1:A:74:ASN:HD22	1:B:208:THR:CG2	2.19	0.55
1:E:864:LYS:HB3	1:E:866:ILE:CD1	2.36	0.55
1:C:460:MET:HE1	1:I:1663:ALA:HA	1.88	0.55
1:H:1505:GLU:CG	2:H:2000:HOH:O	2.53	0.55
1:A:4:LYS:HD3	1:B:278:SER:HB3	1.87	0.55
1:J:1828:LEU:N	1:J:1828:LEU:HD12	2.21	0.55
1:D:699:ILE:HD12	1:D:708:ILE:HG23	1.88	0.55
1:E:829:ASP:CG	1:E:831:ARG:HD2	2.27	0.55
1:A:93:ILE:CG2	1:A:133:ILE:HG12	2.36	0.55
1:B:261:ALA:HB3	1:B:262:PRO:HD3	1.88	0.55
1:G:1272:LEU:C	1:G:1272:LEU:HD12	2.26	0.55
1:B:313:ASP:O	1:B:317:LYS:HG3	2.06	0.55
1:B:328:VAL:HG12	1:B:329:SER:N	2.21	0.55
1:E:885:ASP:OD2	1:E:891:ARG:NH2	2.40	0.55
1:B:267:THR:H	1:B:303:ASN:HD21	1.54	0.55
1:C:474:ASN:ND2	1:D:608:THR:HG22	2.18	0.54
1:H:1493:ILE:HD13	1:H:1494:ASN:N	2.23	0.54
1:A:128:VAL:O	1:A:129:SER:HB3	2.07	0.54
1:D:670:LYS:HB2	1:D:700:HIS:CB	2.37	0.54
1:A:7:ILE:HD11	1:A:21:SER:HB2	1.88	0.54
1:E:803:LYS:O	1:F:1078:SER:HA	2.07	0.54
1:H:1528:VAL:O	1:H:1529:SER:CB	2.55	0.54
1:C:456:THR:HG21	1:C:519:CYS:CA	2.37	0.54
1:H:1431:ARG:HD3	1:H:1435:THR:HG22	1.88	0.54
1:J:1919:CYS:SG	1:J:1921:ALA:N	2.80	0.54
1:D:728:VAL:HG12	1:D:730:GLN:H	1.71	0.54
1:G:1204:LYS:HD3	1:H:1478:SER:HB3	1.89	0.54
1:H:1453:GLU:OE1	1:H:1522:HIS:CD2	2.59	0.54
1:C:420:ILE:HG13	1:C:425:GLN:HG2	1.88	0.54
1:A:111:PHE:O	1:A:114:PHE:HB3	2.07	0.54
1:D:626:ILE:HG22	1:D:628:LEU:HD12	1.89	0.54
1:G:1220:ILE:HD12	1:G:1220:ILE:N	2.23	0.54
1:H:1505:GLU:HG2	2:H:2000:HOH:O	2.08	0.54
1:I:1678:SER:HA	1:J:1803:LYS:O	2.08	0.54
1:B:228:LEU:N	1:B:228:LEU:CD1	2.68	0.54
1:E:852:CYS:O	1:E:856:THR:HG23	2.08	0.54
1:A:31:ARG:HH22	1:C:431:ARG:HH22	1.56	0.54
1:E:826:ILE:HG22	1:E:828:LEU:HD11	1.90	0.54
1:A:26:ILE:HD13	1:B:239:PHE:CE2	2.43	0.54
1:J:1866:ILE:CG2	1:J:1868:ILE:HD11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:875:VAL:HG13	1:E:893:ILE:HD11	1.90	0.53
1:A:26:ILE:HD13	1:B:239:PHE:CD2	2.43	0.53
1:A:13:GLU:O	1:A:14:ASP:CG	2.46	0.53
1:C:456:THR:HG21	1:C:519:CYS:CB	2.38	0.53
1:B:254:LEU:HD22	1:B:271:LEU:HD13	1.91	0.53
1:E:881:THR:HG23	1:F:1002:ASP:HB2	1.91	0.53
1:E:873:MET:SD	1:E:895:LEU:HD22	2.49	0.53
1:E:855:ALA:O	1:E:859:LEU:HG	2.08	0.53
1:F:1028:LEU:N	1:F:1028:LEU:HD12	2.24	0.53
1:H:1523:ASN:HA	2:H:2170:HOH:O	2.08	0.53
1:A:53:GLU:OE1	1:A:122:HIS:HD2	1.92	0.53
1:I:1696:HIS:CD2	1:I:1736:ASN:ND2	2.77	0.53
1:A:39:PHE:CD2	1:B:226:ILE:HD13	2.44	0.53
1:H:1452:CYS:O	1:H:1456:THR:HG23	2.07	0.53
1:H:1431:ARG:NE	2:H:2002:HOH:O	2.41	0.53
1:B:242:LEU:HD13	1:B:290:LEU:HD21	1.91	0.53
1:J:1872:LEU:HD12	1:J:1872:LEU:C	2.29	0.53
1:I:1664:LYS:HB3	1:I:1666:ILE:HD13	1.90	0.53
1:D:653:GLU:OE1	1:D:722:HIS:HD2	1.92	0.53
1:G:1212:ASN:HD21	1:G:1218:THR:CG2	2.02	0.53
1:A:52:CYS:SG	1:A:120:PRO:HD2	2.48	0.53
1:J:1831:ARG:HH11	1:J:1835:THR:HG21	1.74	0.53
1:H:1429:ASP:OD1	1:H:1431:ARG:HD2	2.09	0.53
1:F:1032:PRO:C	1:F:1034:HIS:H	2.12	0.53
1:J:1852:CYS:O	1:J:1856:THR:CG2	2.56	0.53
1:E:893:ILE:HD13	1:E:894:ASN:N	2.23	0.53
1:G:1239:PHE:CE2	1:H:1426:ILE:HD13	2.44	0.53
1:B:256:THR:OG1	1:B:315:VAL:HG13	2.08	0.52
1:A:8:THR:HG22	1:B:274:ASN:HA	1.90	0.52
1:D:613:GLU:C	1:D:615:SER:N	2.62	0.52
1:J:1872:LEU:O	1:J:1872:LEU:HD12	2.10	0.52
1:C:458:ASN:HD22	1:D:611:LEU:HD21	1.74	0.52
1:B:313:ASP:HB3	1:B:317:LYS:NZ	2.24	0.52
1:B:272:LEU:HD12	1:B:272:LEU:C	2.30	0.52
1:D:675:VAL:HG22	1:D:695:LEU:HD23	1.91	0.52
1:H:1456:THR:OG1	1:H:1515:VAL:HG13	2.09	0.52
1:C:434:HIS:HD2	1:C:435:THR:OG1	1.92	0.52
1:I:1713:ASP:O	1:I:1717:LYS:HG3	2.10	0.52
1:A:42:LEU:HD12	1:B:205:TYR:OH	2.08	0.52
1:B:257:ALA:HA	1:B:315:VAL:HG21	1.90	0.52
1:I:1728:VAL:O	1:I:1729:SER:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1849:LEU:HD12	1:J:1893:ILE:HD11	1.91	0.52
1:H:1477:GLY:HA2	1:H:1492:GLU:O	2.09	0.52
1:F:1093:ILE:CG2	1:F:1131:LEU:HD11	2.24	0.52
1:H:1505:GLU:OE2	1:I:1704:SER:HB2	2.10	0.52
1:I:1672:LEU:C	1:I:1672:LEU:HD12	2.30	0.52
1:A:128:VAL:HG12	1:A:130:GLN:H	1.75	0.52
1:D:693:ILE:HD13	1:D:693:ILE:C	2.30	0.52
1:H:1456:THR:O	1:H:1460:MET:HG2	2.10	0.52
1:B:328:VAL:HG12	1:B:330:GLN:H	1.75	0.52
1:A:7:ILE:HD11	1:A:21:SER:CB	2.40	0.52
1:G:1231:ARG:HG2	1:G:1231:ARG:HH11	1.74	0.52
1:I:1673:MET:HE2	1:I:1695:LEU:HB3	1.92	0.51
1:G:1225:GLN:C	1:G:1226:ILE:HD12	2.31	0.51
1:A:70:LYS:HB2	1:A:100:HIS:CB	2.40	0.51
1:C:472:LEU:HD12	1:C:472:LEU:C	2.30	0.51
1:J:1908:ILE:O	1:J:1912:ILE:HD13	2.09	0.51
1:G:1253:GLU:OE1	1:G:1322:HIS:HB2	2.10	0.51
1:I:1693:ILE:HD13	1:I:1694:ASN:N	2.25	0.51
1:F:1020:ILE:HG13	1:F:1025:GLN:CG	2.37	0.51
1:A:131:LEU:HD12	1:A:132:LYS:H	1.75	0.51
1:A:8:THR:HG22	1:B:274:ASN:ND2	2.25	0.51
1:J:1853:GLU:OE1	1:J:1922:HIS:CD2	2.63	0.51
1:D:725:LEU:O	1:D:728:VAL:HG23	2.10	0.51
1:E:861:ALA:HB3	1:E:862:PRO:HD3	1.92	0.51
1:G:1299:ILE:HD11	1:G:1312:ILE:HD11	1.93	0.51
1:I:1706:THR:O	1:I:1710:GLU:HG3	2.11	0.51
1:A:39:PHE:CE2	1:B:226:ILE:HD13	2.46	0.51
1:I:1696:HIS:HD2	1:I:1736:ASN:ND2	2.09	0.51
1:F:1031:ARG:CB	1:F:1036:ALA:H	2.24	0.51
1:J:1906:THR:O	1:J:1910:GLU:HG3	2.10	0.51
1:J:1933:ILE:N	1:J:1933:ILE:HD12	2.26	0.51
1:H:1467:THR:N	1:H:1503:ASN:HD21	2.01	0.51
1:G:1231:ARG:NH1	1:G:1231:ARG:HG2	2.26	0.51
1:G:1226:ILE:HG22	1:G:1228:LEU:CD1	2.41	0.51
1:D:668:ILE:HG21	1:D:671:LEU:HB2	1.92	0.51
1:F:1128:VAL:O	1:F:1129:SER:CB	2.60	0.50
1:E:826:ILE:HG22	1:E:828:LEU:HD12	1.92	0.50
1:A:12:ASN:HD21	1:A:18:THR:CG2	2.06	0.50
1:F:1026:ILE:HG22	1:F:1028:LEU:HD12	1.92	0.50
1:E:870:LYS:HB2	1:E:900:HIS:CB	2.39	0.50
1:B:229:ASP:OD1	1:B:231:ARG:HD2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1457:ALA:HA	1:H:1515:VAL:CG2	2.41	0.50
1:D:700:HIS:HA	1:D:740:VAL:O	2.12	0.50
1:D:653:GLU:OE1	1:D:722:HIS:CD2	2.64	0.50
1:C:445:LEU:HG	1:D:645:LEU:HG	1.93	0.50
1:G:1228:LEU:HD22	1:H:1451:ALA:CB	2.41	0.50
1:G:1208:THR:CG2	1:H:1474:ASN:HD22	2.23	0.50
1:C:459:LEU:O	1:I:1663:ALA:HB2	2.12	0.50
1:A:85:ASP:OD2	1:A:91:ARG:NH2	2.45	0.50
1:D:619:ALA:C	1:D:620:ILE:HD12	2.32	0.50
1:I:1639:PHE:CE2	1:J:1826:ILE:HD13	2.47	0.50
1:J:1870:LYS:HB2	1:J:1900:HIS:CB	2.41	0.50
1:E:807:ILE:HD11	1:F:1043:ALA:HB1	1.94	0.50
1:I:1688:PHE:H	1:J:1923:ASN:ND2	2.10	0.50
1:H:1528:VAL:HG11	1:H:1531:LEU:HB3	1.93	0.50
1:C:475:VAL:HG13	1:C:493:ILE:HD11	1.92	0.50
1:E:872:LEU:C	1:E:872:LEU:HD12	2.32	0.50
1:E:932:LYS:HD3	2:E:2081:HOH:O	2.10	0.50
1:J:1904:SER:OG	1:J:1907:GLU:HG3	2.12	0.50
1:F:1106:THR:O	1:F:1110:GLU:HG3	2.12	0.50
1:E:913:ASP:O	1:E:917:LYS:HG3	2.11	0.50
1:I:1693:ILE:CG2	1:I:1733:ILE:HG12	2.42	0.50
1:C:451:ALA:HB2	1:D:628:LEU:HD22	1.93	0.50
1:C:465:MET:HE2	1:I:1718:ARG:HH22	1.75	0.50
1:E:857:ALA:HA	1:E:915:VAL:HG22	1.93	0.50
1:D:635:THR:HG22	1:D:636:ALA:N	2.26	0.49
1:B:306:THR:HG23	2:B:2019:HOH:O	2.12	0.49
1:E:806:ASP:O	1:E:807:ILE:HD12	2.12	0.49
1:I:1737:VAL:CG2	1:I:1738:THR:N	2.74	0.49
1:B:232:PRO:HB2	1:B:234:HIS:CE1	2.47	0.49
1:C:528:VAL:O	1:C:529:SER:CB	2.60	0.49
1:E:820:ILE:HG13	1:E:825:GLN:HG2	1.94	0.49
1:I:1612:ASN:C	1:I:1613:GLU:O	2.48	0.49
1:E:829:ASP:OD2	1:E:831:ARG:HD2	2.13	0.49
1:G:1303:ASN:O	1:G:1341:HIS:HE1	1.95	0.49
1:G:1300:HIS:HA	1:G:1340:VAL:O	2.11	0.49
1:E:808:THR:HG22	1:F:1074:ASN:HD22	1.77	0.49
1:G:1243:ALA:HB1	1:H:1407:ILE:CD1	2.42	0.49
1:F:1052:CYS:SG	1:F:1120:PRO:HD2	2.53	0.49
1:J:1814:ASP:OD1	1:J:1816:SER:HB3	2.12	0.49
1:E:852:CYS:SG	1:E:920:PRO:HD2	2.52	0.49
1:F:1019:ALA:C	1:F:1020:ILE:HD12	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1831:ARG:HD3	1:J:1835:THR:HG22	1.93	0.49
1:E:870:LYS:HB2	1:E:900:HIS:CG	2.47	0.49
1:E:881:THR:CG2	1:F:1003:LYS:HG2	2.43	0.49
1:H:1540:VAL:HG12	2:H:2127:HOH:O	2.11	0.49
1:I:1662:PRO:CD	2:I:2043:HOH:O	2.60	0.49
1:C:457:ALA:O	1:C:511:PHE:HZ	1.96	0.49
1:A:70:LYS:HB2	1:A:100:HIS:CG	2.47	0.48
1:I:1725:LEU:O	1:I:1728:VAL:HG23	2.12	0.48
1:D:704:SER:OG	1:D:707:GLU:HG3	2.12	0.48
1:G:1328:VAL:O	1:G:1329:SER:CB	2.60	0.48
1:I:1651:ALA:HB2	1:J:1828:LEU:HD22	1.95	0.48
1:C:470:LYS:HB2	1:C:500:HIS:CB	2.43	0.48
1:F:1053:GLU:OE1	1:F:1122:HIS:HD2	1.95	0.48
1:H:1413:GLU:O	1:H:1414:ASP:CG	2.51	0.48
1:J:1831:ARG:HB3	1:J:1835:THR:HB	1.94	0.48
1:F:1111:PHE:O	1:F:1114:PHE:HB3	2.13	0.48
1:C:454:LEU:O	1:C:457:ALA:HB3	2.12	0.48
1:G:1226:ILE:HG22	1:G:1228:LEU:HD12	1.95	0.48
1:E:913:ASP:HB3	1:E:917:LYS:NZ	2.28	0.48
1:J:1831:ARG:HG2	1:J:1831:ARG:HH11	1.78	0.48
1:J:1859:LEU:O	1:J:1862:PRO:HD2	2.13	0.48
1:A:8:THR:CG2	1:B:274:ASN:ND2	2.77	0.48
1:I:1645:LEU:HG	1:J:1845:LEU:HG	1.95	0.48
1:J:1826:ILE:HG22	1:J:1828:LEU:CD1	2.44	0.48
1:C:478:SER:HA	1:D:603:LYS:O	2.14	0.48
1:F:1020:ILE:HD12	1:F:1020:ILE:N	2.29	0.48
1:G:1251:ALA:CB	1:H:1428:LEU:HD22	2.42	0.48
1:I:1693:ILE:CD1	1:I:1695:LEU:HG	2.44	0.48
1:D:666:ILE:HA	1:D:703:ASN:ND2	2.28	0.48
1:D:701:SER:OG	1:D:703:ASN:HB2	2.14	0.48
1:D:685:ASP:OD2	1:D:691:ARG:NH2	2.47	0.48
1:I:1619:ALA:C	1:I:1620:ILE:HD12	2.34	0.48
1:C:429:ASP:OD1	1:C:431:ARG:HD2	2.14	0.48
1:C:472:LEU:HD12	1:C:472:LEU:O	2.14	0.48
1:C:465:MET:HG3	1:I:1718:ARG:NH2	2.29	0.48
1:E:845:LEU:HG	1:F:1045:LEU:HG	1.96	0.48
1:H:1485:ASP:CB	1:H:1491:ARG:HH22	2.27	0.47
1:C:451:ALA:CB	1:D:628:LEU:HD22	2.44	0.47
1:I:1699:ILE:HD12	1:I:1708:ILE:CG2	2.44	0.47
1:F:1013:GLU:O	1:F:1014:ASP:CG	2.52	0.47
1:J:1831:ARG:HG2	1:J:1831:ARG:NH1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1236:ALA:O	1:G:1237:LYS:CG	2.62	0.47
1:C:491:ARG:HH11	1:C:491:ARG:HG2	1.78	0.47
1:D:671:LEU:HD21	1:D:697:TRP:HE3	1.79	0.47
1:E:842:LEU:HD12	1:F:1005:TYR:CZ	2.49	0.47
1:C:456:THR:OG1	1:C:515:VAL:HG13	2.13	0.47
1:H:1426:ILE:HG22	1:H:1428:LEU:CD1	2.44	0.47
1:J:1856:THR:O	1:J:1860:MET:HG2	2.14	0.47
1:D:649:LEU:HD13	1:D:695:LEU:HD21	1.97	0.47
1:A:28:LEU:HD22	1:B:251:ALA:CB	2.44	0.47
1:C:465:MET:CE	1:I:1718:ARG:HH22	2.27	0.47
1:C:405:TYR:O	1:D:676:THR:HA	2.13	0.47
1:J:1885:ASP:HB2	1:J:1891:ARG:HH22	1.78	0.47
1:E:828:LEU:N	1:E:828:LEU:HD12	2.29	0.47
1:H:1470:LYS:HB2	1:H:1500:HIS:CG	2.50	0.47
1:D:652:CYS:SG	1:D:720:PRO:HD2	2.55	0.47
1:D:626:ILE:HG22	1:D:628:LEU:HD11	1.95	0.47
1:E:875:VAL:HB	1:F:1007:ILE:HG22	1.96	0.47
1:I:1662:PRO:HD3	2:I:2043:HOH:O	2.15	0.47
1:E:828:LEU:HD22	1:F:1051:ALA:CB	2.43	0.47
1:I:1631:ARG:HD3	1:I:1635:THR:HG22	1.97	0.47
1:J:1891:ARG:HH11	1:J:1891:ARG:HG2	1.80	0.47
1:B:220:ILE:HG13	1:B:225:GLN:HG2	1.97	0.47
1:H:1497:TRP:HB2	1:H:1537:VAL:HB	1.97	0.47
1:D:618:THR:HG22	1:D:627:THR:HG22	1.96	0.47
1:I:1628:LEU:HD22	1:J:1851:ALA:CB	2.41	0.47
1:G:1229:ASP:O	1:G:1240:GLY:HA2	2.15	0.47
1:E:928:VAL:O	1:E:929:SER:CB	2.62	0.47
1:D:671:LEU:HD21	1:D:697:TRP:CE3	2.50	0.47
1:J:1814:ASP:O	1:J:1816:SER:N	2.48	0.47
1:E:842:LEU:HD13	1:E:890:LEU:HD21	1.96	0.47
1:G:1314:PHE:O	1:G:1318:ARG:HB2	2.15	0.47
1:J:1897:TRP:HB2	1:J:1937:VAL:CB	2.44	0.46
1:A:128:VAL:HB	1:A:131:LEU:HB3	1.96	0.46
1:D:693:ILE:CG2	1:D:731:LEU:HD11	2.45	0.46
1:J:1866:ILE:HA	1:J:1903:ASN:ND2	2.31	0.46
1:G:1219:ALA:C	1:G:1220:ILE:HD12	2.35	0.46
1:E:875:VAL:CG1	1:E:893:ILE:HD11	2.45	0.46
1:A:28:LEU:N	1:A:28:LEU:HD12	2.30	0.46
1:C:491:ARG:NH1	1:C:491:ARG:HG2	2.31	0.46
1:H:1528:VAL:CG1	1:H:1531:LEU:HB3	2.46	0.46
1:I:1658:ASN:C	2:I:2043:HOH:O	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:841:PRO:HG3	1:F:1051:ALA:HB1	1.98	0.46
1:B:275:VAL:HG13	1:B:295:LEU:HD23	1.97	0.46
1:I:1697:TRP:HB2	1:I:1737:VAL:HB	1.98	0.46
1:C:503:ASN:O	1:C:541:HIS:HE1	1.98	0.46
1:B:231:ARG:HD3	1:B:235:THR:CG2	2.44	0.46
1:B:273:MET:SD	1:B:295:LEU:HD22	2.56	0.46
1:J:1876:THR:O	1:J:1893:ILE:HA	2.16	0.46
1:G:1275:VAL:HG13	1:G:1295:LEU:HD23	1.97	0.46
1:C:435:THR:CG2	1:C:435:THR:O	2.55	0.46
1:J:1825:GLN:C	1:J:1826:ILE:HD12	2.37	0.46
1:A:26:ILE:HG22	1:A:28:LEU:HD11	1.96	0.46
1:B:270:LYS:HB2	1:B:300:HIS:CG	2.51	0.45
1:B:303:ASN:H	1:B:303:ASN:HD22	1.64	0.45
1:I:1642:LEU:HD13	1:I:1690:LEU:HD21	1.98	0.45
1:J:1850:ALA:O	1:J:1853:GLU:HB2	2.15	0.45
1:C:508:ILE:HD13	1:C:539:LEU:HD11	1.97	0.45
1:J:1869:ASN:O	1:J:1870:LYS:HD3	2.16	0.45
1:D:705:GLU:HA	1:D:739:LEU:HD12	1.98	0.45
1:E:817:MET:CE	1:F:1055:ALA:HB2	2.47	0.45
1:I:1617:MET:O	1:I:1628:LEU:N	2.50	0.45
1:H:1431:ARG:HD3	1:H:1435:THR:CG2	2.46	0.45
1:B:293:ILE:C	1:B:293:ILE:HD13	2.37	0.45
1:F:1072:LEU:C	1:F:1072:LEU:HD12	2.36	0.45
1:D:728:VAL:O	1:D:729:SER:HB3	2.17	0.45
1:A:64:LYS:O	1:A:65:MET:HB2	2.16	0.45
1:E:928:VAL:HB	1:E:931:LEU:HB3	1.99	0.45
1:F:1070:LYS:HB2	1:F:1100:HIS:CG	2.50	0.45
1:I:1606:ASP:O	1:I:1607:ILE:HD12	2.16	0.45
1:F:1031:ARG:HB3	1:F:1035:THR:HB	1.97	0.45
1:F:1025:GLN:O	1:F:1026:ILE:HD12	2.17	0.45
1:I:1713:ASP:HA	2:I:2186:HOH:O	2.16	0.45
1:A:99:ILE:HD12	1:A:108:ILE:HG23	1.98	0.45
1:G:1328:VAL:HB	1:G:1331:LEU:HB3	1.99	0.45
1:A:93:ILE:HD11	1:A:95:LEU:HD21	1.99	0.45
1:A:5:TYR:CZ	1:B:242:LEU:HD12	2.51	0.45
1:I:1600:HIS:CD2	1:I:1601:MET:H	2.35	0.45
1:E:811:LEU:HD11	1:E:815:SER:HA	1.98	0.45
1:G:1231:ARG:HD3	1:G:1235:THR:HG22	1.98	0.45
1:J:1897:TRP:HB3	1:J:1899:ILE:CD1	2.41	0.45
1:A:132:LYS:HD3	2:A:2068:HOH:O	2.17	0.45
1:J:1856:THR:HG21	1:J:1919:CYS:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:620:ILE:HD12	1:D:620:ILE:N	2.32	0.45
1:B:245:LEU:HD23	1:B:245:LEU:C	2.37	0.45
1:H:1528:VAL:HG12	1:H:1530:GLN:H	1.81	0.44
1:E:831:ARG:NH1	1:E:835:THR:CG2	2.74	0.44
1:I:1608:THR:HG22	1:J:1874:ASN:HD22	1.81	0.44
1:J:1877:GLY:HA2	1:J:1892:GLU:O	2.16	0.44
1:A:66:ILE:HD12	1:A:66:ILE:N	2.32	0.44
1:I:1625:GLN:C	1:I:1626:ILE:HD12	2.37	0.44
1:I:1619:ALA:O	1:I:1625:GLN:HA	2.18	0.44
1:C:402:ASP:OD2	1:D:681:THR:CG2	2.65	0.44
1:J:1809:ALA:HA	1:J:1819:ALA:HA	2.00	0.44
1:G:1337:VAL:HG22	1:G:1338:THR:N	2.32	0.44
1:I:1701:SER:HG	1:I:1703:ASN:HD22	1.64	0.44
1:I:1673:MET:CE	1:I:1695:LEU:HB3	2.47	0.44
1:F:1070:LYS:HB2	1:F:1100:HIS:CB	2.47	0.44
1:I:1629:ASP:O	1:I:1640:GLY:HA2	2.17	0.44
1:J:1872:LEU:HG	1:J:1898:GLU:HB3	1.99	0.44
1:F:1064:LYS:O	1:F:1066:ILE:HD12	2.17	0.44
1:I:1620:ILE:HG13	1:I:1625:GLN:HG2	2.00	0.44
1:C:491:ARG:HD2	1:D:601:MET:HG2	2.00	0.44
1:H:1528:VAL:O	1:H:1529:SER:HB3	2.17	0.44
1:B:263:ALA:O	1:D:718:ARG:NH2	2.51	0.44
1:I:1696:HIS:CD2	1:I:1736:ASN:HD21	2.36	0.44
1:A:93:ILE:C	1:A:93:ILE:HD13	2.38	0.44
1:C:428:LEU:HD22	1:D:651:ALA:HB2	2.00	0.44
1:C:465:MET:HG3	1:I:1718:ARG:HH21	1.82	0.44
1:I:1675:VAL:HB	1:J:1807:ILE:HG22	2.00	0.44
1:J:1911:PHE:O	1:J:1914:PHE:HB3	2.18	0.44
1:C:452:CYS:SG	1:C:520:PRO:HD2	2.57	0.43
1:G:1228:LEU:CD1	1:G:1228:LEU:N	2.80	0.43
1:E:939:LEU:HD23	1:E:940:VAL:H	1.81	0.43
1:J:1827:THR:O	1:J:1838:GLY:HA3	2.18	0.43
1:B:319:CYS:SG	1:B:321:ALA:HB3	2.58	0.43
1:D:660:MET:SD	1:D:714:PHE:HE1	2.41	0.43
1:G:1203:LYS:O	1:H:1478:SER:HA	2.19	0.43
1:G:1253:GLU:OE1	1:G:1322:HIS:CD2	2.71	0.43
1:E:857:ALA:HA	1:E:915:VAL:CG2	2.48	0.43
1:C:493:ILE:HD11	1:C:495:LEU:CD2	2.48	0.43
1:H:1457:ALA:HA	1:H:1515:VAL:HG21	2.01	0.43
1:G:1239:PHE:CD2	1:H:1426:ILE:HD13	2.53	0.43
1:C:460:MET:HE2	1:I:1663:ALA:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:ILE:HG22	1:C:428:LEU:CD1	2.49	0.43
1:D:612:ASN:HD21	1:D:618:THR:HG23	1.83	0.43
1:I:1608:THR:CG2	1:J:1874:ASN:HD22	2.31	0.43
1:G:1337:VAL:CG2	1:G:1338:THR:N	2.81	0.43
1:D:600:HIS:HA	2:D:2092:HOH:O	2.18	0.43
1:E:893:ILE:HG23	1:E:933:ILE:HG23	2.00	0.43
1:I:1657:ALA:HB2	1:I:1715:VAL:HG11	2.01	0.43
1:F:1042:LEU:HD13	1:F:1090:LEU:HD21	2.00	0.43
1:H:1420:ILE:HD12	1:H:1420:ILE:N	2.33	0.43
1:I:1626:ILE:HG22	1:I:1628:LEU:HD12	1.99	0.43
1:H:1485:ASP:OD2	1:H:1491:ARG:NH2	2.52	0.43
1:A:5:TYR:O	1:B:276:THR:HA	2.19	0.43
1:I:1614:ASP:OD1	1:I:1616:SER:HB3	2.19	0.43
1:J:1875:VAL:HG22	1:J:1895:LEU:HD23	2.00	0.43
1:A:78:SER:HB3	1:B:204:LYS:HD3	2.00	0.43
1:H:1472:LEU:CD1	1:H:1498:GLU:HB3	2.49	0.43
1:G:1233:LYS:O	1:G:1236:ALA:HB2	2.18	0.43
1:I:1737:VAL:HG22	1:I:1738:THR:N	2.34	0.43
1:G:1301:SER:HG	1:G:1303:ASN:HD22	1.67	0.43
1:H:1472:LEU:C	1:H:1472:LEU:HD12	2.40	0.43
1:A:27:THR:O	1:A:38:GLY:HA3	2.18	0.43
1:I:1732:LYS:HE3	1:I:1734:ASN:OD1	2.19	0.43
1:E:812:ASN:C	1:E:813:GLU:O	2.57	0.43
1:J:1856:THR:CG2	1:J:1919:CYS:HB2	2.46	0.43
1:A:93:ILE:CG2	1:A:131:LEU:HD11	2.44	0.42
1:A:7:ILE:HG22	1:B:275:VAL:HB	2.00	0.42
1:G:1272:LEU:HD12	1:G:1272:LEU:O	2.19	0.42
1:D:717:LYS:HD2	2:D:2204:HOH:O	2.19	0.42
1:E:874:ASN:ND2	1:F:1008:THR:HG22	2.28	0.42
1:J:1928:VAL:HB	1:J:1931:LEU:HB3	2.00	0.42
1:J:1893:ILE:HG22	1:J:1931:LEU:HD11	2.02	0.42
1:F:1077:GLY:HA2	1:F:1092:GLU:O	2.19	0.42
1:C:413:GLU:C	1:C:415:SER:N	2.71	0.42
1:I:1699:ILE:HD12	1:I:1708:ILE:HG23	2.00	0.42
1:B:271:LEU:HA	1:B:271:LEU:HD23	1.85	0.42
1:G:1273:MET:HE3	1:G:1297:TRP:CE2	2.54	0.42
1:D:693:ILE:CG2	1:D:733:ILE:HG12	2.49	0.42
1:F:1031:ARG:HA	1:F:1032:PRO:HD3	1.85	0.42
1:I:1636:ALA:O	1:I:1637:LYS:CB	2.67	0.42
1:E:831:ARG:HH11	1:E:831:ARG:HG2	1.85	0.42
1:B:267:THR:HA	2:B:2031:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:804:LYS:HD3	1:F:1078:SER:HB3	2.02	0.42
1:I:1642:LEU:HD12	1:J:1805:TYR:CZ	2.54	0.42
1:I:1685:ASP:OD2	1:I:1691:ARG:NH2	2.52	0.42
1:F:1093:ILE:CD1	1:F:1093:ILE:C	2.81	0.42
1:I:1676:THR:HA	1:J:1805:TYR:O	2.20	0.42
1:C:413:GLU:O	1:C:414:ASP:CG	2.57	0.42
1:H:1513:ASP:O	1:H:1517:LYS:HG3	2.19	0.42
1:E:868:ILE:HG21	1:E:871:LEU:HB2	2.02	0.42
1:G:1291:ARG:NH1	1:G:1291:ARG:HG2	2.32	0.42
1:F:1056:THR:O	1:F:1060:MET:HG2	2.20	0.42
1:H:1505:GLU:CD	1:I:1704:SER:HB2	2.40	0.42
1:A:76:THR:HA	1:B:205:TYR:O	2.20	0.42
1:H:1496:HIS:HA	1:H:1536:ASN:O	2.19	0.42
1:E:877:GLY:HA2	1:E:892:GLU:O	2.18	0.42
1:A:77:GLY:HA2	1:A:92:GLU:O	2.19	0.42
1:H:1491:ARG:O	1:H:1531:LEU:HA	2.19	0.42
1:I:1629:ASP:OD2	1:I:1631:ARG:HD2	2.20	0.42
1:E:908:ILE:HG13	1:E:939:LEU:HG	2.00	0.42
1:I:1677:GLY:HA2	1:I:1692:GLU:O	2.20	0.42
1:H:1460:MET:SD	1:H:1514:PHE:HE1	2.43	0.42
1:B:272:LEU:O	1:B:272:LEU:HD12	2.20	0.42
1:C:433:LYS:HB2	2:C:2126:HOH:O	2.18	0.42
1:D:661:ALA:HB3	1:D:662:PRO:CD	2.43	0.41
1:G:1253:GLU:OE1	1:G:1322:HIS:HD2	2.03	0.41
1:A:11:LEU:HD21	1:B:258:ASN:HD22	1.85	0.41
1:C:461:ALA:HB3	1:C:462:PRO:HD3	2.01	0.41
1:H:1532:LYS:HE3	1:H:1534:ASN:OD1	2.19	0.41
1:E:825:GLN:O	1:E:826:ILE:HD12	2.21	0.41
1:E:831:ARG:NH1	1:E:831:ARG:HG2	2.35	0.41
1:B:263:ALA:HA	1:D:660:MET:SD	2.61	0.41
1:J:1831:ARG:HD3	1:J:1835:THR:CG2	2.50	0.41
1:J:1871:LEU:HD23	1:J:1871:LEU:HA	1.88	0.41
1:A:99:ILE:HD11	1:A:112:ILE:CD1	2.38	0.41
1:D:656:THR:O	1:D:660:MET:HG2	2.20	0.41
1:J:1875:VAL:HA	1:J:1894:ASN:O	2.20	0.41
1:J:1864:LYS:HA	1:J:1864:LYS:HD3	1.89	0.41
1:G:1256:THR:HG21	1:G:1319:CYS:HB2	2.02	0.41
1:G:1243:ALA:HB1	1:H:1407:ILE:HD11	2.00	0.41
1:E:872:LEU:CB	1:F:1010:VAL:HG22	2.50	0.41
1:F:1093:ILE:HD11	1:F:1095:LEU:CD2	2.50	0.41
1:D:675:VAL:HG13	1:D:693:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1264:LYS:HB3	1:G:1266:ILE:HD13	2.02	0.41
1:I:1653:GLU:OE1	1:I:1722:HIS:HB2	2.20	0.41
1:G:1291:ARG:O	1:G:1331:LEU:HA	2.21	0.41
1:I:1631:ARG:HG2	1:I:1631:ARG:NH1	2.36	0.41
1:B:291:ARG:O	1:B:331:LEU:HA	2.20	0.41
1:A:50:ALA:O	1:A:53:GLU:HB2	2.20	0.41
1:I:1620:ILE:N	1:I:1620:ILE:HD12	2.36	0.41
1:E:875:VAL:HG13	1:E:895:LEU:HD23	2.03	0.41
1:A:26:ILE:HG22	1:A:28:LEU:HD12	2.03	0.41
1:J:1906:THR:HG21	2:J:2132:HOH:O	2.19	0.41
1:C:503:ASN:CB	1:C:508:ILE:CD1	2.97	0.41
1:B:299:ILE:HD12	1:B:308:ILE:HG23	2.03	0.41
1:C:481:THR:CG2	1:D:603:LYS:HG2	2.51	0.41
1:I:1665:MET:HE3	1:I:1665:MET:HB2	1.71	0.41
1:C:403:LYS:HD3	1:C:403:LYS:HA	1.90	0.41
1:A:35:THR:HG22	1:A:35:THR:O	2.21	0.41
1:C:450:ALA:HB2	1:C:475:VAL:HG21	2.03	0.40
1:G:1252:CYS:SG	1:G:1320:PRO:HD2	2.61	0.40
1:G:1288:PHE:H	1:H:1523:ASN:ND2	2.19	0.40
1:I:1653:GLU:OE1	1:I:1722:HIS:HD2	2.04	0.40
1:I:1701:SER:OG	1:I:1703:ASN:HB2	2.21	0.40
1:H:1421:SER:O	1:H:1422:ASP:C	2.60	0.40
1:A:42:LEU:HD12	1:B:205:TYR:CZ	2.56	0.40
1:C:488:PHE:H	1:D:723:ASN:ND2	2.19	0.40
1:E:856:THR:O	1:E:860:MET:HG2	2.22	0.40
1:I:1631:ARG:HD3	1:I:1635:THR:CG2	2.51	0.40
1:G:1231:ARG:CG	1:G:1231:ARG:HH11	2.33	0.40
1:H:1469:ASN:O	1:H:1470:LYS:HD3	2.21	0.40
1:B:257:ALA:HA	1:B:315:VAL:HG22	2.03	0.40
1:E:827:THR:O	1:E:838:GLY:HA3	2.21	0.40
1:G:1270:LYS:HB2	1:G:1300:HIS:CG	2.57	0.40
1:J:1846:LEU:HD22	1:J:1893:ILE:HD11	2.03	0.40
1:C:413:GLU:C	1:C:415:SER:H	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	8	27
1	B	139/166 (84%)	129 (93%)	7 (5%)	3 (2%)	8	27
1	C	144/166 (87%)	133 (92%)	10 (7%)	1 (1%)	26	59
1	D	144/166 (87%)	132 (92%)	7 (5%)	5 (4%)	4	16
1	E	139/166 (84%)	124 (89%)	9 (6%)	6 (4%)	3	11
1	F	144/166 (87%)	130 (90%)	10 (7%)	4 (3%)	6	21
1	G	139/166 (84%)	129 (93%)	6 (4%)	4 (3%)	6	20
1	H	139/166 (84%)	127 (91%)	9 (6%)	3 (2%)	8	27
1	I	144/166 (87%)	131 (91%)	7 (5%)	6 (4%)	3	11
1	J	141/166 (85%)	127 (90%)	10 (7%)	4 (3%)	6	21
All	All	1412/1660 (85%)	1286 (91%)	87 (6%)	39 (3%)	6	21

All (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
1	G	1237	LYS
1	I	1637	LYS
1	J	1815	SER
1	J	1836	ALA
1	A	129	SER
1	B	329	SER
1	D	614	ASP
1	D	635	THR
1	D	636	ALA

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Mol	Chain	Res	Type
1	F	1033	LYS
1	I	1615	SER
1	A	128	VAL
1	C	529	SER
1	D	729	SER
1	E	815	SER
1	E	837	LYS
1	E	929	SER
1	F	1129	SER
1	G	1329	SER
1	H	1529	SER
1	I	1613	GLU
1	I	1729	SER
1	A	36	ALA
1	B	236	ALA
1	E	813	GLU
1	E	862	PRO
1	G	1215	SER
1	H	1415	SER
1	J	1839	PHE
1	I	1614	ASP
1	J	1841	PRO
1	D	728	VAL
1	H	1528	VAL
1	I	1641	PRO

### 5.3.2 Protein sidechains ⓘ

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%)	12	31
1	B	121/144 (84%)	111 (92%)	10 (8%)	14	36
1	C	125/144 (87%)	113 (90%)	12 (10%)	10	28
1	D	125/144 (87%)	115 (92%)	10 (8%)	15	38
1	E	121/144 (84%)	112 (93%)	9 (7%)	17	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	125/144 (87%)	113 (90%)	12 (10%)	10	28
1	G	121/144 (84%)	112 (93%)	9 (7%)	17	42
1	H	121/144 (84%)	111 (92%)	10 (8%)	14	36
1	I	125/144 (87%)	112 (90%)	13 (10%)	9	23
1	J	122/144 (85%)	109 (89%)	13 (11%)	8	22
All	All	1227/1440 (85%)	1118 (91%)	109 (9%)	12	32

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	7	ILE
1	A	49	LEU
1	A	67	THR
1	A	71	LEU
1	A	93	ILE
1	A	99	ILE
1	A	118	ARG
1	A	119	CYS
1	A	137	VAL
1	A	139	LEU
1	B	207	ILE
1	B	228	LEU
1	B	249	LEU
1	B	267	THR
1	B	271	LEU
1	B	285	ASP
1	B	293	ILE
1	B	318	ARG
1	B	319	CYS
1	B	339	LEU
1	C	402	ASP
1	C	449	LEU
1	C	456	THR
1	C	467	THR
1	C	471	LEU
1	C	493	ILE
1	C	499	ILE
1	C	501	SER
1	C	519	CYS

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Mol	Chain	Res	Type
1	C	523	ASN
1	C	537	VAL
1	C	539	LEU
1	D	596	TYR
1	D	607	ILE
1	D	649	LEU
1	D	667	THR
1	D	671	LEU
1	D	680	SER
1	D	682	ASN
1	D	693	ILE
1	D	719	CYS
1	D	739	LEU
1	E	807	ILE
1	E	831	ARG
1	E	841	PRO
1	E	849	LEU
1	E	871	LEU
1	E	893	ILE
1	E	919	CYS
1	E	937	VAL
1	E	939	LEU
1	F	1002	ASP
1	F	1007	ILE
1	F	1034	HIS
1	F	1049	LEU
1	F	1067	THR
1	F	1071	LEU
1	F	1093	ILE
1	F	1118	ARG
1	F	1119	CYS
1	F	1123	ASN
1	F	1137	VAL
1	F	1139	LEU
1	G	1231	ARG
1	G	1249	LEU
1	G	1267	THR
1	G	1271	LEU
1	G	1274	ASN
1	G	1293	ILE
1	G	1319	CYS
1	G	1326	GLN

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Mol	Chain	Res	Type
1	G	1339	LEU
1	H	1407	ILE
1	H	1449	LEU
1	H	1467	THR
1	H	1471	LEU
1	H	1493	ILE
1	H	1518	ARG
1	H	1519	CYS
1	H	1526	GLN
1	H	1537	VAL
1	H	1539	LEU
1	I	1602	ASP
1	I	1607	ILE
1	I	1649	LEU
1	I	1665	MET
1	I	1667	THR
1	I	1671	LEU
1	I	1693	ILE
1	I	1719	CYS
1	I	1723	ASN
1	I	1726	GLN
1	I	1729	SER
1	I	1737	VAL
1	I	1739	LEU
1	J	1800	HIS
1	J	1807	ILE
1	J	1834	HIS
1	J	1849	LEU
1	J	1856	THR
1	J	1867	THR
1	J	1871	LEU
1	J	1899	ILE
1	J	1918	ARG
1	J	1919	CYS
1	J	1926	GLN
1	J	1929	SER
1	J	1939	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN

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Mol	Chain	Res	Type
1	A	34	HIS
1	A	69	ASN
1	A	74	ASN
1	A	103	ASN
1	A	122	HIS
1	A	123	ASN
1	A	126	GLN
1	A	141	HIS
1	B	212	ASN
1	B	234	HIS
1	B	258	ASN
1	B	269	ASN
1	B	274	ASN
1	B	303	ASN
1	B	322	HIS
1	B	323	ASN
1	B	341	HIS
1	C	400	HIS
1	C	412	ASN
1	C	434	HIS
1	C	458	ASN
1	C	474	ASN
1	C	503	ASN
1	C	522	HIS
1	C	541	HIS
1	D	612	ASN
1	D	674	ASN
1	D	703	ASN
1	D	722	HIS
1	D	723	ASN
1	D	741	HIS
1	E	812	ASN
1	E	834	HIS
1	E	874	ASN
1	E	903	ASN
1	E	922	HIS
1	E	923	ASN
1	E	941	HIS
1	F	1012	ASN
1	F	1069	ASN
1	F	1074	ASN
1	F	1100	HIS

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Mol	Chain	Res	Type
1	F	1103	ASN
1	F	1122	HIS
1	F	1123	ASN
1	G	1212	ASN
1	G	1274	ASN
1	G	1303	ASN
1	G	1322	HIS
1	G	1323	ASN
1	G	1341	HIS
1	H	1412	ASN
1	H	1434	HIS
1	H	1474	ASN
1	H	1503	ASN
1	H	1522	HIS
1	H	1523	ASN
1	H	1541	HIS
1	I	1598	GLN
1	I	1600	HIS
1	I	1612	ASN
1	I	1634	HIS
1	I	1696	HIS
1	I	1703	ASN
1	I	1722	HIS
1	I	1736	ASN
1	I	1741	HIS
1	J	1812	ASN
1	J	1834	HIS
1	J	1858	ASN
1	J	1874	ASN
1	J	1903	ASN
1	J	1922	HIS
1	J	1923	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.