Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:59 PM GMT

PDB ID	:	4N8X
Title	:	The structure of Nostoc sp. PCC 7120 CcmL
Authors	:	Keeling, T.J.; Kimber, M.S.
Deposited on	:	2013-10-18
Resolution	:	1.93 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

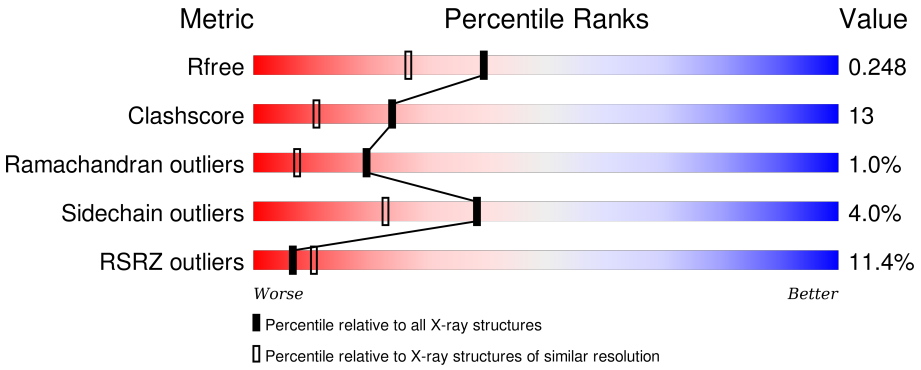
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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))
R_{free}	91344	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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 >=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 <=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.

Mol	Chain	Length	Quality of chain
1	1	109	8% 72% 16% • • 9%
1	2	109	11% 66% 21% • 12%
1	3	109	17% 54% 34% • 9%
1	4	109	16% 60% 28% • 10%
1	A	109	4% 76% 13% • 10%

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Mol	Chain	Length	Quality of chain
1	B	109	4% 74% 15% 9%
1	C	109	10% 75% 13% 10%
1	D	109	15% 67% 19% 10%
1	E	109	11% 61% 26% 11%
1	F	109	17% 60% 28% 10%
1	G	109	11% 72% 17% 11%
1	H	109	6% 70% 17% 10%
1	I	109	6% 67% 23% 10%
1	J	109	10% 69% 17% 12%
1	K	109	21% 63% 25% 10%
1	L	109	12% 65% 23% 10%
1	M	109	6% 69% 19% 10%
1	N	109	6% 70% 17% 10%
1	O	109	12% 63% 24% 12%
1	P	109	17% 64% 26% 9%
1	Q	109	9% 62% 24% 11%
1	R	109	3% 75% 13% 10%
1	S	109	5% 78% 11% 10%
1	T	109	10% 68% 18% 14%
1	U	109	7% 72% 13% 11%
1	V	109	6% 69% 20% 10%
1	W	109	16% 67% 18% 11%
1	X	109	15% 62% 26% 10%
1	Y	109	10% 61% 26% 11%
1	Z	109	9% 67% 20% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24315 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 Carbon dioxide concentrating mechanism protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	99	Total	C	N	O	S	0	0	0
			764	479	136	148	1			
1	2	96	Total	C	N	O	S	0	0	0
			738	464	131	142	1			
1	3	99	Total	C	N	O	S	0	0	0
			764	479	136	148	1			
1	4	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			
1	A	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			
1	B	99	Total	C	N	O	S	0	0	0
			764	479	136	148	1			
1	C	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			
1	D	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			
1	E	97	Total	C	N	O	S	0	0	0
			747	470	133	143	1			
1	F	98	Total	C	N	O	S	0	1	0
			764	482	134	147	1			
1	G	97	Total	C	N	O	S	0	0	0
			747	470	133	143	1			
1	H	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			
1	I	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			
1	J	96	Total	C	N	O	S	0	0	0
			738	464	131	142	1			
1	K	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			
1	L	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			
1	N	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			
1	O	96	Total	C	N	O	S	0	0	0
			738	464	131	142	1			
1	P	99	Total	C	N	O	S	0	0	0
			764	479	136	148	1			
1	Q	97	Total	C	N	O	S	0	0	0
			747	470	133	143	1			
1	R	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			
1	S	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			
1	T	94	Total	C	N	O	S	0	0	0
			719	455	127	136	1			
1	U	97	Total	C	N	O	S	0	0	0
			747	470	133	143	1			
1	V	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			
1	W	97	Total	C	N	O	S	0	0	0
			747	470	133	143	1			
1	X	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			
1	Y	97	Total	C	N	O	S	0	0	0
			747	470	133	143	1			
1	Z	98	Total	C	N	O	S	0	0	0
			755	474	134	146	1			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
1	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
1	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
1	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
1	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
1	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
1	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
1	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
2	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
2	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
2	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2

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Chain	Residue	Modelled	Actual	Comment	Reference
2	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
2	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
2	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
2	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
2	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
3	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
3	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
3	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
3	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
3	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
3	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
3	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
3	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
4	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
4	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
4	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
4	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
4	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
4	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
4	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
4	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
A	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
A	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
A	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
A	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
A	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
A	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
A	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
A	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
B	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
B	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
B	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
B	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
B	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
B	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
B	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
B	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
C	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
C	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
C	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
C	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
C	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
C	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
C	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
D	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
D	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
D	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
D	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
D	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
D	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
D	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
D	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
E	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
E	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
E	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
E	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
E	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
E	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
E	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
E	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
F	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
F	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
F	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
F	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
F	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
F	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
F	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
F	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
G	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
G	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
G	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
G	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
G	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
G	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
G	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
G	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
H	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
H	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
H	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
H	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
H	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
H	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
H	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
I	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
I	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
I	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
I	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
I	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
I	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
I	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
I	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
J	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
J	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
J	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
J	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
J	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
J	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
J	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
J	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
K	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
K	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
K	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
K	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
K	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
K	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
K	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
K	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
L	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
L	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
L	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
L	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
L	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
L	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
L	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
L	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
M	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
M	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
M	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
M	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
M	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
M	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
M	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
M	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
N	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2

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Chain	Residue	Modelled	Actual	Comment	Reference
N	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
N	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
N	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
N	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
N	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
N	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
N	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
O	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
O	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
O	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
O	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
O	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
O	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
O	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
O	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
P	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
P	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
P	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
P	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
P	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
P	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
P	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
P	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Q	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
Q	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
Q	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Q	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Q	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Q	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Q	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Q	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
R	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
R	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
R	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
R	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
R	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
R	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
R	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
R	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
S	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
S	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
S	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2

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Chain	Residue	Modelled	Actual	Comment	Reference
S	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
S	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
S	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
S	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
S	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
T	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
T	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
T	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
T	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
T	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
T	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
T	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
T	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
U	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
U	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
U	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
U	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
U	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
U	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
U	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
U	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
V	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
V	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
V	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
V	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
V	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
V	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
V	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
V	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
W	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
W	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
W	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
W	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
W	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
W	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
W	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
W	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
X	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
X	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
X	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
X	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
X	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2

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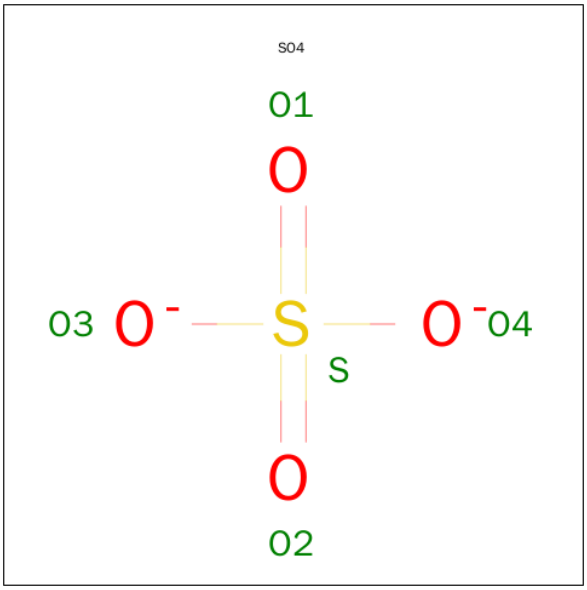
Chain	Residue	Modelled	Actual	Comment	Reference
X	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
X	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
X	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Y	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
Y	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
Y	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Y	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Y	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Y	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Y	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Y	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Z	102	LEU	-	EXPRESSION TAG	UNP Q8YYI2
Z	103	GLU	-	EXPRESSION TAG	UNP Q8YYI2
Z	104	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Z	105	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Z	106	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Z	107	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Z	108	HIS	-	EXPRESSION TAG	UNP Q8YYI2
Z	109	HIS	-	EXPRESSION TAG	UNP Q8YYI2

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1	64	Total O 64 64	0	0
3	2	42	Total O 42 42	0	0
3	3	50	Total O 50 50	0	0
3	4	43	Total O 43 43	0	0
3	A	69	Total O 69 69	0	0
3	B	89	Total O 89 89	0	0
3	C	54	Total O 54 54	0	0
3	D	52	Total O 52 52	0	0
3	E	54	Total O 54 54	0	0
3	F	38	Total O 38 38	0	0
3	G	55	Total O 55 55	0	0
3	H	55	Total O 55 55	0	0
3	I	63	Total O 63 63	0	0
3	J	58	Total O 58 58	0	0
3	K	36	Total O 36 36	0	0
3	L	65	Total O 65 65	0	0
3	M	76	Total O 76 76	0	0
3	N	76	Total O 76 76	0	0
3	O	49	Total O 49 49	0	0
3	P	48	Total O 48 48	0	0
3	Q	64	Total O 64 64	0	0
3	R	81	Total O 81 81	0	0

Continued on next page...

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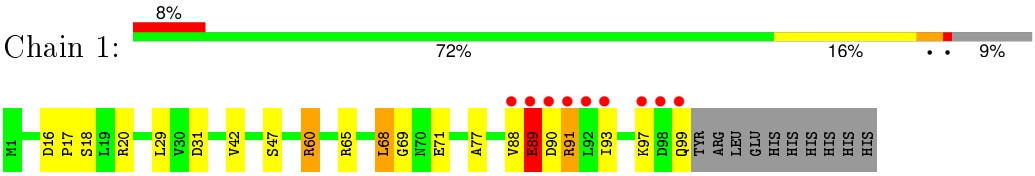
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	S	72	Total O 72 72	0	0
3	T	49	Total O 49 49	0	0
3	U	60	Total O 60 60	0	0
3	V	72	Total O 72 72	0	0
3	W	50	Total O 50 50	0	0
3	X	32	Total O 32 32	0	0
3	Y	62	Total O 62 62	0	0
3	Z	72	Total O 72 72	0	0

3 Residue-property plots (i)

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.

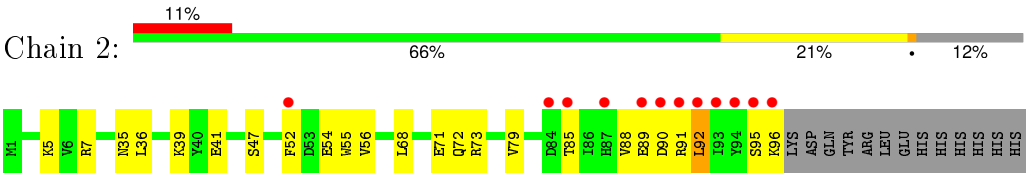
- Molecule 1: Carbon dioxide concentrating mechanism protein

Chain 1:



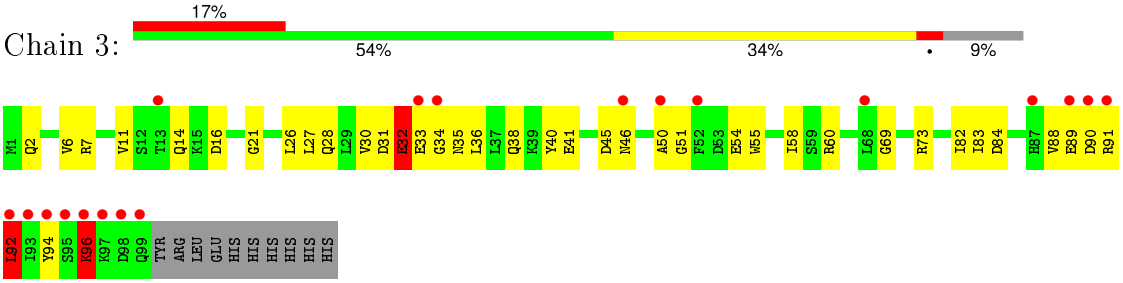
- Molecule 1: Carbon dioxide concentrating mechanism protein

Chain 2:



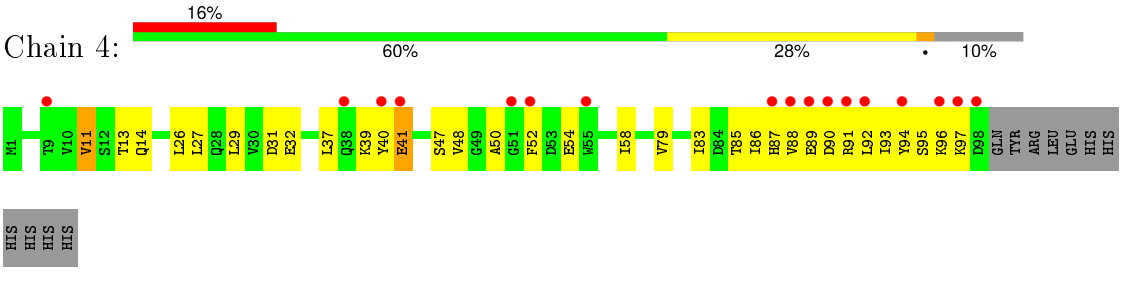
- Molecule 1: Carbon dioxide concentrating mechanism protein

Chain 3:



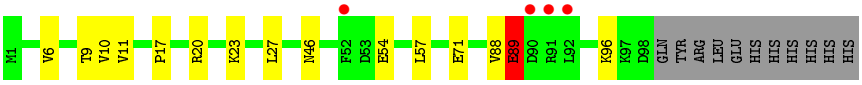
- Molecule 1: Carbon dioxide concentrating mechanism protein

Chain 4:



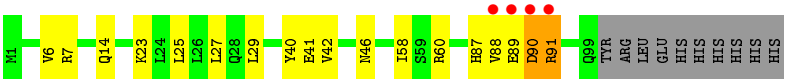
- Molecule 1: Carbon dioxide concentrating mechanism protein

Chain A:



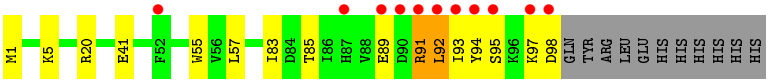
• Molecule 1: Carbon dioxide concentrating mechanism protein

Chain B:



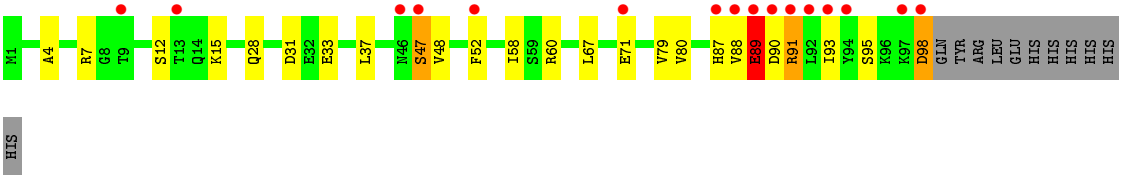
• Molecule 1: Carbon dioxide concentrating mechanism protein

Chain C:



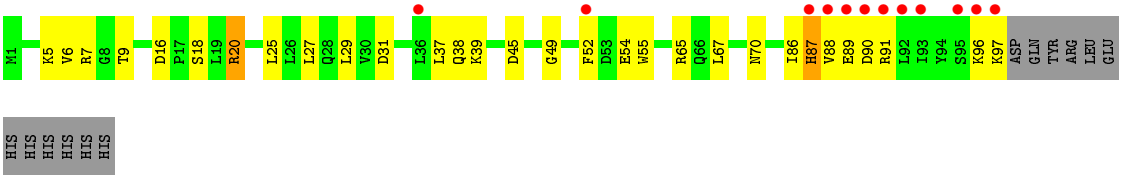
• Molecule 1: Carbon dioxide concentrating mechanism protein

Chain D:



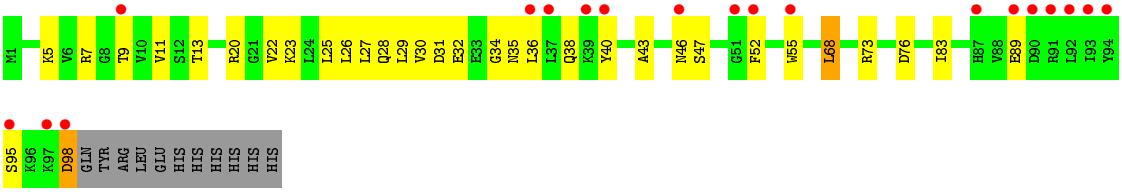
• Molecule 1: Carbon dioxide concentrating mechanism protein

Chain E:



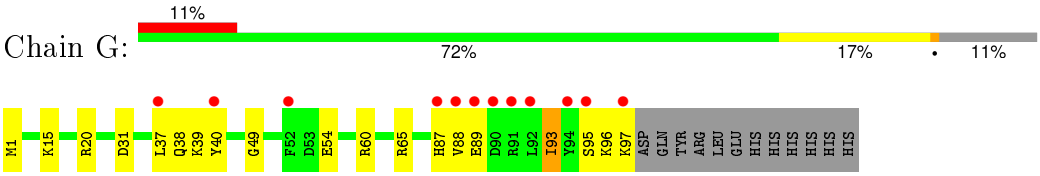
• Molecule 1: Carbon dioxide concentrating mechanism protein

Chain F:



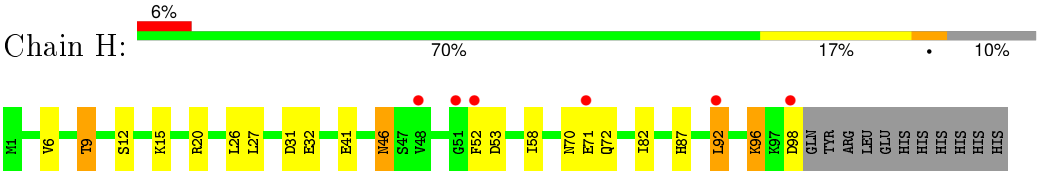
• Molecule 1: Carbon dioxide concentrating mechanism protein

Chain G:



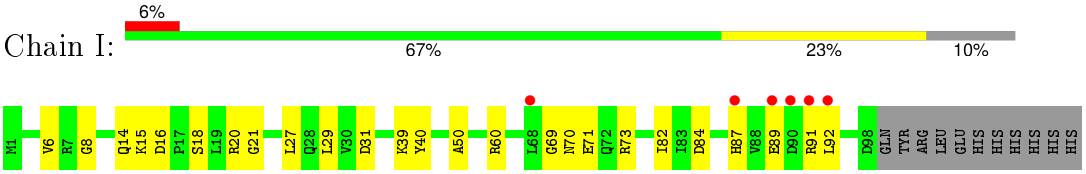
• Molecule 1: Carbon dioxide concentrating mechanism protein

Chain H:



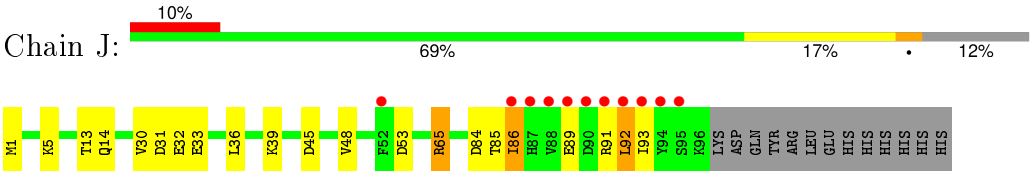
• Molecule 1: Carbon dioxide concentrating mechanism protein

Chain I:



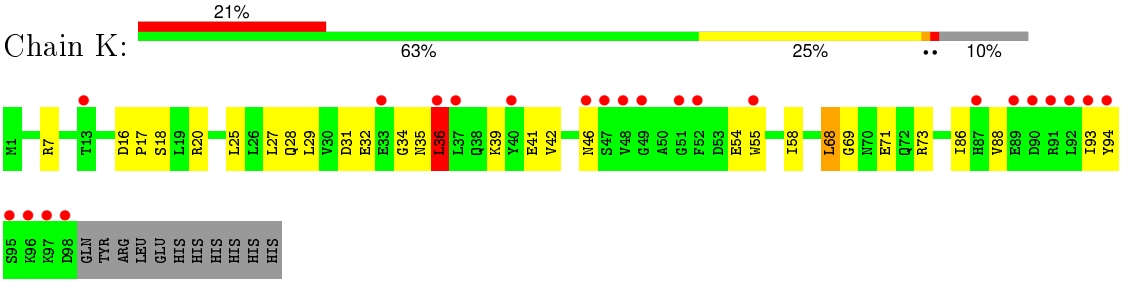
• Molecule 1: Carbon dioxide concentrating mechanism protein

Chain J:



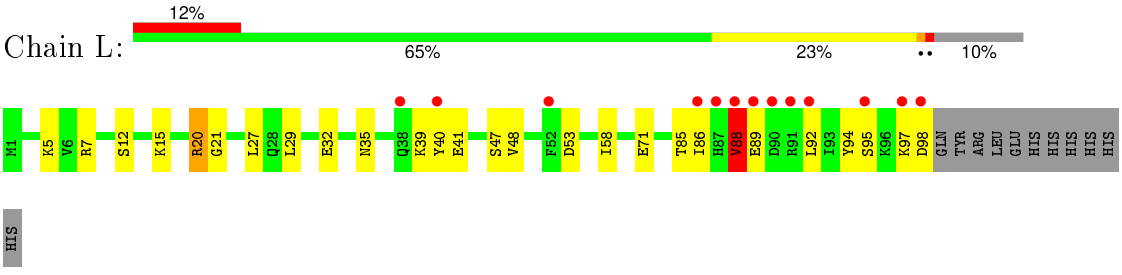
• Molecule 1: Carbon dioxide concentrating mechanism protein

Chain K:



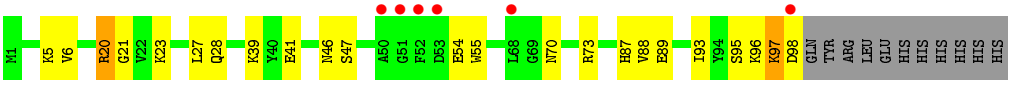
• Molecule 1: Carbon dioxide concentrating mechanism protein

Chain L:

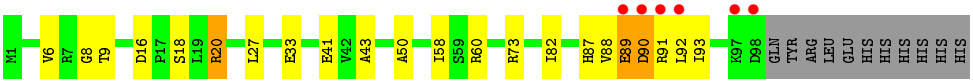


• Molecule 1: Carbon dioxide concentrating mechanism protein

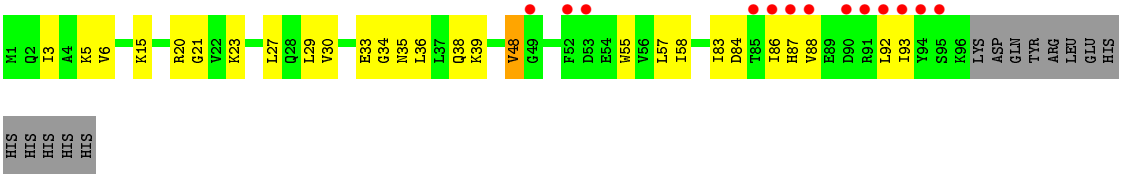
Chain M:



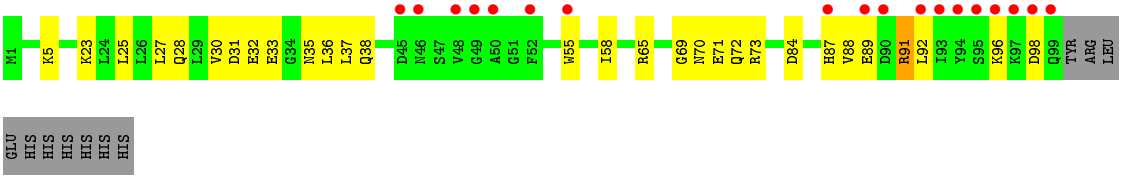
• Molecule 1: Carbon dioxide concentrating mechanism protein



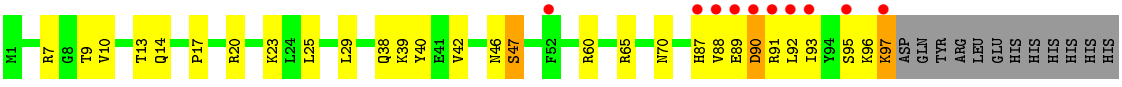
• Molecule 1: Carbon dioxide concentrating mechanism protein



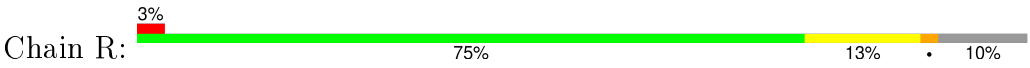
• Molecule 1: Carbon dioxide concentrating mechanism protein

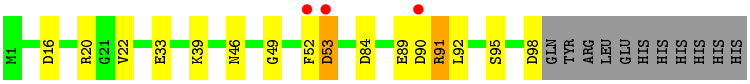


• Molecule 1: Carbon dioxide concentrating mechanism protein

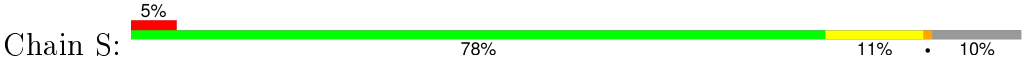


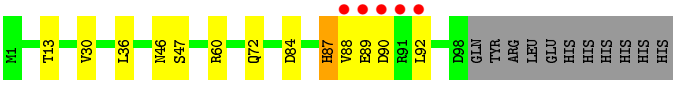
• Molecule 1: Carbon dioxide concentrating mechanism protein



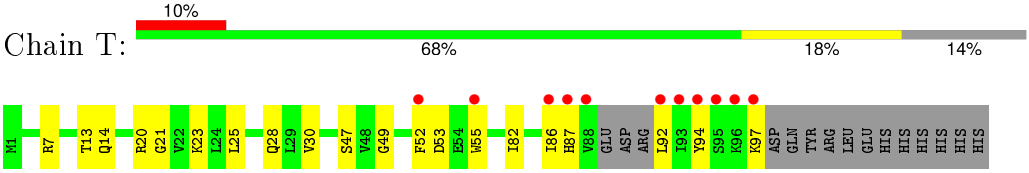


• Molecule 1: Carbon dioxide concentrating mechanism protein

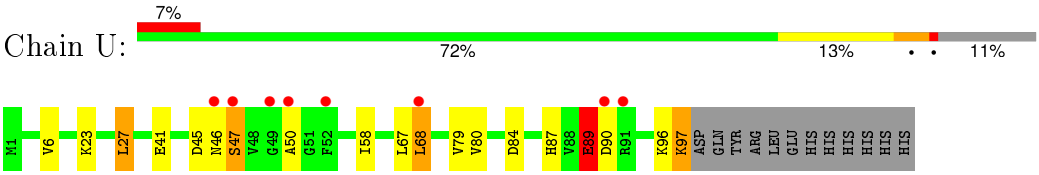




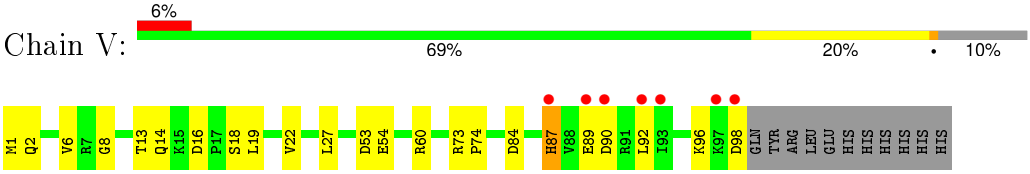
• Molecule 1: Carbon dioxide concentrating mechanism protein



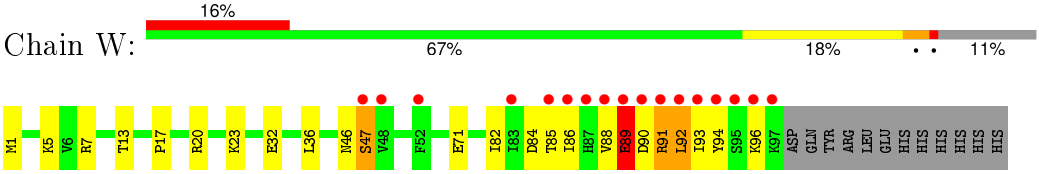
• Molecule 1: Carbon dioxide concentrating mechanism protein



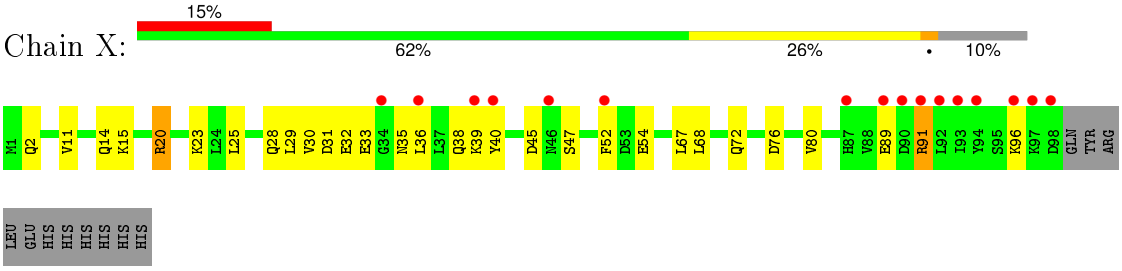
• Molecule 1: Carbon dioxide concentrating mechanism protein



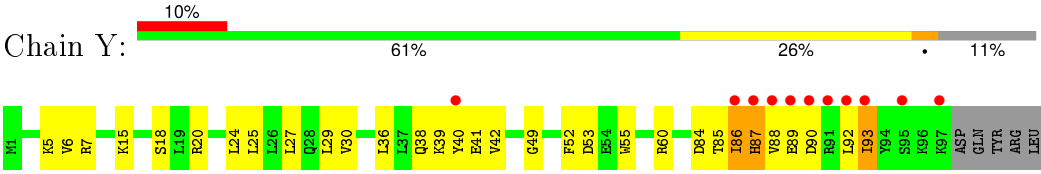
• Molecule 1: Carbon dioxide concentrating mechanism protein



• Molecule 1: Carbon dioxide concentrating mechanism protein



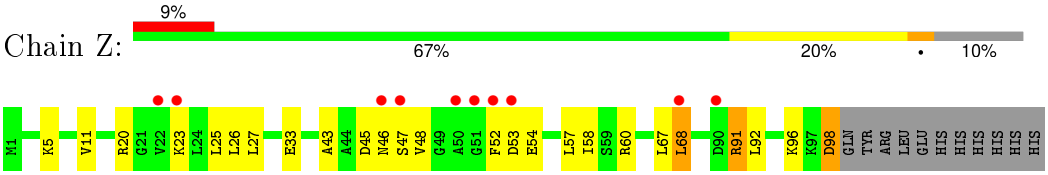
• Molecule 1: Carbon dioxide concentrating mechanism protein



HIS
HIS
HIS

- Molecule 1: Carbon dioxide concentrating mechanism protein

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.88Å 128.12Å 220.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 1.93 48.29 – 1.93	Depositor EDS
% Data completeness (in resolution range)	92.7 (48.29-1.93) 94.0 (48.29-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 1.92Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.206 , 0.247 0.205 , 0.248	Depositor DCC
R_{free} test set	11578 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	112 of 234801 reflections (0.048%)	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	24315	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.03 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.1530e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1	0.64	0/771	0.75	2/1042 (0.2%)
1	2	0.52	0/745	0.71	0/1008
1	3	0.50	0/771	0.74	1/1042 (0.1%)
1	4	0.55	0/762	0.69	0/1030
1	A	0.57	0/762	0.71	0/1030
1	B	0.63	0/771	0.75	0/1042
1	C	0.57	0/762	0.75	0/1030
1	D	0.58	0/762	0.66	0/1030
1	E	0.61	0/754	0.74	0/1019
1	F	0.58	0/775	0.72	0/1048
1	G	0.54	0/754	0.73	0/1019
1	H	0.59	0/762	0.75	0/1030
1	I	0.65	0/762	0.78	0/1030
1	J	0.57	0/745	0.77	1/1008 (0.1%)
1	K	0.51	0/762	0.75	1/1030 (0.1%)
1	L	0.60	0/762	0.71	0/1030
1	M	0.57	0/762	0.70	0/1030
1	N	0.60	0/762	0.73	0/1030
1	O	0.55	0/745	0.74	0/1008
1	P	0.53	0/771	0.73	0/1042
1	Q	0.61	0/754	0.73	0/1019
1	R	0.62	0/762	0.72	0/1030
1	S	0.65	0/762	0.79	0/1030
1	T	0.59	0/725	0.74	0/979
1	U	0.54	0/754	0.78	0/1019
1	V	0.54	0/762	0.71	0/1030
1	W	0.55	0/754	0.70	1/1019 (0.1%)
1	X	0.53	0/762	0.73	0/1030
1	Y	0.56	0/754	0.74	0/1019
1	Z	0.55	0/762	0.71	0/1030
All	All	0.57	0/22773	0.73	6/30783 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Q	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	36	LEU	CA-CB-CG	7.41	132.34	115.30
1	3	92	LEU	CA-CB-CG	6.41	130.03	115.30
1	W	92	LEU	CA-CB-CG	5.82	128.68	115.30
1	J	65	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	1	68	LEU	CA-CB-CG	5.40	127.72	115.30
1	1	60	ARG	NE-CZ-NH1	5.32	122.96	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Q	87	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	764	0	790	19	0
1	2	738	0	765	20	0
1	3	764	0	790	35	2
1	4	755	0	782	25	0
1	A	755	0	782	12	0
1	B	764	0	790	16	0
1	C	755	0	782	12	0
1	D	755	0	782	21	0
1	E	747	0	778	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	764	0	791	29	0
1	G	747	0	778	18	0
1	H	755	0	782	22	0
1	I	755	0	782	23	0
1	J	738	0	765	24	0
1	K	755	0	782	31	0
1	L	755	0	782	27	1
1	M	755	0	782	21	0
1	N	755	0	782	21	0
1	O	738	0	765	25	0
1	P	764	0	790	26	0
1	Q	747	0	778	24	0
1	R	755	0	782	20	0
1	S	755	0	782	10	0
1	T	719	0	754	15	0
1	U	747	0	778	25	0
1	V	755	0	782	23	0
1	W	747	0	778	24	0
1	X	755	0	782	29	1
1	Y	747	0	778	32	0
1	Z	755	0	782	24	0
2	A	5	0	0	0	0
3	1	64	0	0	4	0
3	2	42	0	0	4	0
3	3	50	0	0	12	0
3	4	43	0	0	6	0
3	A	69	0	0	0	0
3	B	89	0	0	2	0
3	C	54	0	0	3	1
3	D	52	0	0	4	0
3	E	54	0	0	5	0
3	F	38	0	0	6	0
3	G	55	0	0	5	0
3	H	55	0	0	2	0
3	I	63	0	0	5	1
3	J	58	0	0	7	1
3	K	36	0	0	8	0
3	L	65	0	0	8	0
3	M	76	0	0	7	1
3	N	76	0	0	3	0
3	O	49	0	0	5	0
3	P	48	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	64	0	0	8	1
3	R	81	0	0	10	0
3	S	72	0	0	4	0
3	T	49	0	0	2	0
3	U	60	0	0	5	0
3	V	72	0	0	9	0
3	W	50	0	0	5	0
3	X	32	0	0	5	1
3	Y	62	0	0	6	0
3	Z	72	0	0	6	0
All	All	24315	0	23398	606	5

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 13.

All (606) 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)
1:3:83:ILE:O	1:3:96:LYS:NZ	1.64	1.30
1:R:53:ASP:HB2	3:R:274:HOH:O	1.43	1.12
1:L:12:SER:O	1:L:15:LYS:NZ	1.94	1.00
1:3:2:GLN:NE2	1:4:41:GLU:OE1	1.94	1.00
1:T:20:ARG:NH1	3:T:240:HOH:O	1.95	0.98
1:G:54:GLU:OE2	1:G:96:LYS:NZ	1.97	0.96
1:B:87:HIS:ND1	3:B:269:HOH:O	1.99	0.96
1:Y:5:LYS:NZ	1:Y:53:ASP:OD1	2.01	0.93
1:G:1:MET:N	1:H:41:GLU:OE2	2.03	0.92
1:I:84:ASP:OD2	1:J:13:THR:HG23	1.71	0.90
1:D:12:SER:O	1:D:15:LYS:NZ	2.03	0.90
1:R:84:ASP:OD1	3:R:235:HOH:O	1.87	0.89
1:I:69:GLY:O	1:I:73:ARG:NH2	2.06	0.88
1:K:7:ARG:HG3	1:K:28:GLN:HG2	1.57	0.87
1:Q:10:VAL:O	3:Q:220:HOH:O	1.90	0.87
1:R:16:ASP:OD1	3:R:265:HOH:O	1.92	0.87
1:Y:55:TRP:NE1	3:Y:237:HOH:O	2.03	0.86
1:D:33:GLU:OE2	1:E:38:GLN:NE2	2.08	0.86
1:L:88:VAL:HG22	1:L:89:GLU:H	1.41	0.85
1:Y:89:GLU:HG3	1:Y:90:ASP:H	1.41	0.85
1:1:97:LYS:N	3:1:256:HOH:O	2.10	0.84
1:W:5:LYS:HE3	1:W:7:ARG:HD3	1.60	0.83
1:F:31:ASP:HB3	3:F:232:HOH:O	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:LYS:HD3	1:J:36:LEU:HD21	1.60	0.83
1:D:88:VAL:HG12	1:D:93:ILE:HD11	1.61	0.82
1:K:7:ARG:HD3	1:K:28:GLN:HE21	1.45	0.82
1:3:73:ARG:NH1	3:3:226:HOH:O	2.12	0.82
1:O:84:ASP:OD1	3:O:211:HOH:O	1.98	0.81
1:D:60:ARG:NH1	3:D:230:HOH:O	2.12	0.81
1:G:88:VAL:HG23	1:G:93:ILE:HG21	1.62	0.81
1:3:7:ARG:HG3	1:3:28:GLN:HB2	1.61	0.81
1:O:87:HIS:ND1	3:O:233:HOH:O	2.11	0.81
1:O:23:LYS:NZ	3:O:237:HOH:O	1.97	0.80
1:E:88:VAL:O	1:E:90:ASP:N	2.14	0.80
1:O:33:GLU:HA	1:O:93:ILE:HG12	1.64	0.80
1:K:69:GLY:N	3:K:225:HOH:O	1.85	0.80
1:O:35:ASN:ND2	3:O:221:HOH:O	2.02	0.78
1:E:49:GLY:N	3:E:245:HOH:O	2.13	0.78
1:3:31:ASP:OD1	3:3:244:HOH:O	2.02	0.77
1:1:99:GLN:O	3:1:221:HOH:O	2.02	0.77
1:K:16:ASP:OD1	1:K:18:SER:OG	2.01	0.77
1:P:23:LYS:HE3	1:P:25:LEU:HD21	1.66	0.77
1:C:41:GLU:OE1	3:C:252:HOH:O	2.03	0.77
1:2:41:GLU:OE1	3:2:214:HOH:O	2.02	0.76
1:P:98:ASP:O	3:P:228:HOH:O	2.03	0.76
1:W:85:THR:OG1	1:W:94:TYR:O	2.01	0.76
1:4:54:GLU:OE2	3:4:242:HOH:O	2.02	0.76
1:E:54:GLU:OE2	1:E:96:LYS:NZ	2.14	0.76
1:V:54:GLU:OE2	1:V:96:LYS:NZ	2.17	0.76
1:V:16:ASP:OD1	1:V:18:SER:HB3	1.86	0.75
1:N:33:GLU:OE2	3:N:240:HOH:O	2.04	0.75
1:O:5:LYS:NZ	1:O:30:VAL:HG11	2.02	0.75
1:D:89:GLU:OE1	3:D:221:HOH:O	2.03	0.75
1:X:32:GLU:OE2	1:Y:38:GLN:NE2	2.20	0.74
1:B:60:ARG:NH2	3:C:252:HOH:O	2.14	0.74
1:F:26:LEU:HD22	1:J:86:ILE:HD11	1.70	0.74
1:4:48:VAL:HG11	1:4:79:VAL:HG12	1.69	0.74
1:1:89:GLU:OE2	1:1:91:ARG:HB3	1.88	0.74
1:P:33:GLU:OE1	3:P:223:HOH:O	2.05	0.74
1:P:32:GLU:HB3	3:P:244:HOH:O	1.88	0.73
1:L:20:ARG:HE	1:L:20:ARG:HA	1.52	0.73
1:G:49:GLY:O	3:G:217:HOH:O	2.06	0.73
1:R:20:ARG:NH1	1:Y:18:SER:HB3	2.04	0.73
1:K:29:LEU:HD22	1:K:39:LYS:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:SER:HB3	1:D:98:ASP:HB2	1.71	0.72
1:2:5:LYS:HE2	1:2:55:TRP:HE1	1.55	0.72
3:N:240:HOH:O	1:O:38:GLN:OE1	2.08	0.72
1:J:32:GLU:OE2	3:J:251:HOH:O	2.07	0.71
1:J:32:GLU:OE1	3:J:251:HOH:O	2.08	0.71
1:N:91:ARG:NH1	1:N:93:ILE:HD11	2.05	0.71
1:H:46:ASN:ND2	1:H:70:ASN:OD1	2.23	0.71
1:N:41:GLU:OE2	1:N:58:ILE:HD13	1.89	0.71
1:A:89:GLU:OE1	1:B:7:ARG:NH1	2.17	0.71
1:U:96:LYS:NZ	1:V:14:GLN:HE22	1.89	0.71
1:L:94:TYR:O	3:L:244:HOH:O	2.07	0.71
1:C:20:ARG:NH2	3:C:254:HOH:O	2.22	0.71
1:Z:27:LEU:HD13	1:Z:43:ALA:HB3	1.73	0.70
1:X:47:SER:HB3	1:X:68:LEU:HD11	1.72	0.70
1:L:98:ASP:O	3:L:242:HOH:O	2.09	0.70
1:F:28:GLN:HG2	1:F:36:LEU:HD12	1.74	0.70
1:3:84:ASP:OD2	1:4:13:THR:OG1	2.07	0.70
1:W:96:LYS:O	3:W:249:HOH:O	2.09	0.70
1:E:87:HIS:ND1	3:E:243:HOH:O	2.24	0.69
1:H:82:ILE:HG12	1:I:14:GLN:HB2	1.72	0.69
1:X:28:GLN:HB3	1:X:36:LEU:HD11	1.74	0.69
1:R:84:ASP:CG	3:R:235:HOH:O	2.28	0.69
1:M:88:VAL:HG22	1:M:89:GLU:HG2	1.75	0.69
1:O:27:LEU:HD13	1:O:58:ILE:HD11	1.72	0.69
1:G:65:ARG:NH1	3:G:201:HOH:O	2.26	0.69
1:X:33:GLU:OE2	3:X:206:HOH:O	2.11	0.68
1:V:1:MET:SD	3:W:223:HOH:O	2.51	0.68
1:2:5:LYS:HE2	1:2:55:TRP:NE1	2.08	0.68
1:D:7:ARG:HG3	1:D:28:GLN:HB2	1.76	0.68
1:S:72:GLN:OE1	3:S:262:HOH:O	2.10	0.68
1:2:54:GLU:OE2	1:2:96:LYS:NZ	2.26	0.68
1:P:37:LEU:O	3:P:224:HOH:O	2.11	0.68
1:U:68:LEU:O	3:U:233:HOH:O	2.11	0.68
1:Z:68:LEU:H	1:Z:68:LEU:HD13	1.59	0.67
1:E:87:HIS:CG	3:E:243:HOH:O	2.47	0.67
1:2:54:GLU:HG2	1:2:96:LYS:HZ2	1.60	0.67
1:Y:86:ILE:HD11	1:Y:93:ILE:HD13	1.75	0.67
3:3:247:HOH:O	1:U:89:GLU:HG2	1.94	0.66
1:O:5:LYS:HD2	1:O:36:LEU:HD21	1.75	0.66
1:X:72:GLN:NE2	3:X:221:HOH:O	2.29	0.66
1:Y:84:ASP:OD2	1:Y:85:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:69:GLY:N	1:P:71:GLU:OE2	2.28	0.66
1:1:17:PRO:HA	1:1:20:ARG:NH1	2.11	0.66
1:W:47:SER:O	3:W:239:HOH:O	2.12	0.66
1:E:87:HIS:N	3:E:243:HOH:O	2.25	0.66
1:Q:40:TYR:OH	3:Q:227:HOH:O	2.13	0.66
1:U:96:LYS:NZ	1:V:14:GLN:NE2	2.44	0.65
1:L:92:LEU:HD11	1:L:95:SER:HB2	1.78	0.65
1:X:31:ASP:OD1	1:X:35:ASN:N	2.29	0.65
1:B:14:GLN:NE2	1:R:46:ASN:O	2.30	0.65
1:G:38:GLN:OE1	3:G:246:HOH:O	2.13	0.65
1:E:88:VAL:HG22	1:E:91:ARG:HB2	1.77	0.65
1:N:91:ARG:HH11	1:N:93:ILE:HD11	1.60	0.65
1:1:69:GLY:N	1:1:71:GLU:OE2	2.30	0.65
1:N:16:ASP:OD2	1:N:18:SER:OG	2.11	0.65
1:M:54:GLU:O	3:M:263:HOH:O	2.14	0.65
1:3:94:TYR:HE2	1:3:96:LYS:HZ2	1.43	0.64
1:Z:33:GLU:OE1	3:Z:216:HOH:O	2.15	0.64
1:R:20:ARG:HH12	1:Y:18:SER:HB3	1.61	0.64
1:H:27:LEU:HD13	1:H:58:ILE:HD11	1.78	0.64
1:H:71:GLU:OE1	1:H:71:GLU:N	2.29	0.64
1:O:5:LYS:HZ3	1:O:30:VAL:HG11	1.60	0.64
1:E:5:LYS:HZ2	1:E:55:TRP:HE1	1.46	0.64
1:F:46:ASN:OD1	3:F:211:HOH:O	2.15	0.63
1:J:39:LYS:NZ	3:J:256:HOH:O	2.03	0.63
1:Z:5:LYS:NZ	3:Z:249:HOH:O	2.32	0.63
1:3:34:GLY:N	3:3:244:HOH:O	2.32	0.63
1:J:32:GLU:CD	3:J:251:HOH:O	2.36	0.63
1:3:41:GLU:OE1	3:3:240:HOH:O	2.16	0.63
1:4:47:SER:HB2	3:4:203:HOH:O	1.98	0.63
1:K:32:GLU:N	3:K:230:HOH:O	2.30	0.63
1:P:27:LEU:HG	1:P:58:ILE:HD11	1.80	0.62
1:W:88:VAL:O	1:W:90:ASP:N	2.32	0.62
1:I:69:GLY:N	1:I:71:GLU:OE2	2.32	0.62
1:D:60:ARG:CZ	3:D:230:HOH:O	2.46	0.62
1:K:71:GLU:O	3:K:218:HOH:O	2.15	0.62
1:R:84:ASP:OD2	1:S:13:THR:OG1	2.15	0.62
1:3:94:TYR:HE2	1:3:96:LYS:NZ	1.97	0.62
1:O:20:ARG:NH2	1:O:21:GLY:H	1.97	0.61
1:F:30:VAL:HG12	1:F:31:ASP:O	2.00	0.61
1:U:96:LYS:HZ2	1:V:14:GLN:NE2	1.98	0.61
1:F:98:ASP:N	1:F:98:ASP:OD1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:20:ARG:NH1	1:N:20:ARG:HG3	2.14	0.61
1:K:17:PRO:HA	1:K:20:ARG:HG2	1.81	0.61
1:O:5:LYS:HZ3	1:O:30:VAL:CG1	2.13	0.61
1:U:90:ASP:OD2	3:U:251:HOH:O	2.15	0.61
1:J:86:ILE:O	3:J:250:HOH:O	2.16	0.61
1:H:32:GLU:HG2	1:I:40:TYR:CE1	2.35	0.60
1:3:35:ASN:OD1	3:3:241:HOH:O	2.17	0.60
1:W:91:ARG:NH1	1:W:93:ILE:HG22	2.17	0.60
1:X:15:LYS:HE2	1:X:20:ARG:HD2	1.82	0.60
1:4:26:LEU:HD11	1:4:40:TYR:HB3	1.83	0.60
1:V:16:ASP:OD2	3:V:255:HOH:O	2.17	0.60
1:3:35:ASN:N	3:3:244:HOH:O	2.21	0.60
1:Y:87:HIS:N	1:Y:87:HIS:ND1	2.49	0.60
1:L:20:ARG:HA	1:L:20:ARG:NE	2.17	0.60
1:G:39:LYS:NZ	3:G:248:HOH:O	2.34	0.60
1:2:89:GLU:HG3	1:2:90:ASP:OD1	2.02	0.60
1:L:29:LEU:HD13	1:L:41:GLU:OE1	2.02	0.60
1:G:89:GLU:HG2	1:H:52:PHE:CZ	2.37	0.59
1:R:98:ASP:O	3:R:241:HOH:O	2.16	0.59
1:Q:14:GLN:OE1	3:Q:241:HOH:O	2.17	0.59
1:Q:88:VAL:HG22	1:Q:91:ARG:HB3	1.84	0.59
1:L:39:LYS:HG2	1:L:41:GLU:OE2	2.02	0.59
1:K:46:ASN:ND2	3:K:228:HOH:O	2.35	0.59
1:N:89:GLU:HA	1:N:89:GLU:OE2	2.01	0.59
1:X:28:GLN:NE2	1:X:40:TYR:OH	2.36	0.59
1:Q:88:VAL:O	1:Q:90:ASP:N	2.36	0.59
1:X:96:LYS:HD2	3:X:229:HOH:O	2.02	0.58
1:W:88:VAL:HG23	1:W:93:ILE:HD13	1.85	0.58
1:G:87:HIS:NE2	1:H:9:THR:OG1	2.36	0.58
1:P:28:GLN:OE1	3:P:219:HOH:O	2.17	0.58
1:4:40:TYR:O	3:4:233:HOH:O	2.17	0.58
1:L:40:TYR:OH	3:L:248:HOH:O	2.17	0.58
1:Z:23:LYS:HE3	1:Z:45:ASP:HB3	1.86	0.58
1:U:68:LEU:N	3:U:248:HOH:O	2.37	0.58
1:V:98:ASP:O	3:V:234:HOH:O	2.17	0.58
1:U:96:LYS:HZ1	1:V:14:GLN:HE22	1.52	0.58
1:1:16:ASP:OD2	1:1:18:SER:OG	2.17	0.58
1:Y:5:LYS:HZ3	1:Y:53:ASP:HA	1.69	0.58
1:D:88:VAL:O	1:D:90:ASP:N	2.36	0.58
1:F:35:ASN:N	3:F:231:HOH:O	2.20	0.57
1:4:31:ASP:HB3	1:4:37:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLU:CD	1:B:7:ARG:HH11	2.07	0.57
1:4:50:ALA:O	3:4:217:HOH:O	2.18	0.57
1:I:73:ARG:NH1	3:I:224:HOH:O	2.37	0.57
1:2:88:VAL:O	1:2:89:GLU:HG2	2.05	0.57
1:A:54:GLU:HG2	1:A:96:LYS:HZ3	1.69	0.57
1:M:54:GLU:OE2	1:M:96:LYS:HE2	2.05	0.57
1:X:54:GLU:OE2	3:X:229:HOH:O	2.17	0.57
1:F:32:GLU:HB3	1:G:40:TYR:CD1	2.40	0.57
1:Y:6:VAL:HA	1:Y:27:LEU:HD23	1.87	0.57
1:I:16:ASP:OD2	1:I:18:SER:OG	2.17	0.57
1:1:17:PRO:HA	1:1:20:ARG:HH11	1.70	0.57
1:E:31:ASP:HB3	1:E:37:LEU:HD21	1.86	0.57
1:C:89:GLU:HB2	1:D:52:PHE:CZ	2.39	0.57
1:U:96:LYS:O	1:U:97:LYS:HB2	2.04	0.57
1:Y:86:ILE:HG13	1:Y:93:ILE:HG23	1.86	0.56
1:B:40:TYR:OH	3:B:276:HOH:O	2.11	0.56
1:Y:55:TRP:CD1	3:Y:237:HOH:O	2.54	0.56
1:I:20:ARG:HA	1:I:20:ARG:HH21	1.70	0.56
1:I:20:ARG:NH2	1:I:21:GLY:H	2.02	0.56
1:F:20:ARG:NH1	3:F:213:HOH:O	2.35	0.56
1:V:19:LEU:O	1:V:22:VAL:HG12	2.05	0.56
1:K:7:ARG:CD	1:K:28:GLN:HE21	2.16	0.56
1:P:31:ASP:OD2	1:P:35:ASN:HB2	2.05	0.56
1:U:84:ASP:OD2	1:V:13:THR:HG23	2.05	0.56
1:P:5:LYS:HE3	1:P:30:VAL:HG11	1.87	0.56
1:D:71:GLU:O	3:D:235:HOH:O	2.18	0.56
1:U:67:LEU:HD21	1:U:80:VAL:HG12	1.88	0.56
1:J:14:GLN:HG2	1:T:21:GLY:HA3	1.88	0.56
1:3:89:GLU:HB3	1:4:52:PHE:CZ	2.41	0.56
1:2:47:SER:OG	1:3:16:ASP:OD1	2.21	0.56
1:2:54:GLU:HG2	1:2:96:LYS:NZ	2.20	0.56
1:M:20:ARG:HD3	1:M:21:GLY:N	2.20	0.56
1:U:23:LYS:NZ	3:U:260:HOH:O	2.21	0.55
1:W:5:LYS:NZ	1:W:36:LEU:HD11	2.22	0.55
1:M:20:ARG:NH1	3:M:243:HOH:O	2.26	0.55
1:Y:39:LYS:HA	3:Y:235:HOH:O	2.07	0.55
1:F:40[A]:TYR:CZ	1:J:32:GLU:HB3	2.42	0.54
1:L:86:ILE:N	3:L:244:HOH:O	2.31	0.54
1:E:5:LYS:NZ	1:E:55:TRP:HE1	2.04	0.54
1:W:5:LYS:HZ3	1:W:36:LEU:HD21	1.70	0.54
1:X:23:LYS:HE2	1:X:45:ASP:HB3	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:GLU:OE2	1:E:52:PHE:CD2	2.60	0.54
1:I:71:GLU:CD	1:I:71:GLU:H	2.11	0.54
1:R:33:GLU:OE1	3:R:205:HOH:O	2.18	0.54
1:U:6:VAL:HG22	1:U:27:LEU:HD11	1.90	0.54
1:Q:95:SER:O	1:Q:97:LYS:N	2.41	0.54
1:I:14:GLN:NE2	3:I:223:HOH:O	2.16	0.54
1:W:32:GLU:HB3	1:X:40:TYR:CZ	2.43	0.54
1:F:23:LYS:HE2	1:F:25:LEU:HD21	1.89	0.54
1:M:23:LYS:HG3	3:M:239:HOH:O	2.07	0.54
1:B:88:VAL:HG22	1:B:91:ARG:HG3	1.90	0.54
1:L:92:LEU:HD12	3:L:244:HOH:O	2.06	0.54
1:4:48:VAL:HG11	1:4:79:VAL:CG1	2.38	0.54
1:E:5:LYS:HG2	1:E:55:TRP:CD1	2.43	0.54
1:D:48:VAL:HG11	1:D:79:VAL:HG12	1.90	0.53
1:Y:60:ARG:NH2	3:Y:255:HOH:O	1.99	0.53
1:Y:5:LYS:HZ2	1:Y:7:ARG:HH11	1.57	0.53
1:D:88:VAL:HG23	1:E:7:ARG:O	2.08	0.53
1:2:85:THR:HG22	1:2:95:SER:HA	1.90	0.53
1:V:18:SER:O	1:V:73:ARG:HD3	2.08	0.53
1:H:82:ILE:CG1	1:I:14:GLN:HB2	2.39	0.53
1:K:32:GLU:HB2	1:L:40:TYR:CD2	2.43	0.53
1:N:20:ARG:HG3	1:N:20:ARG:HH11	1.72	0.53
1:I:91:ARG:HG2	1:I:92:LEU:H	1.74	0.53
1:Y:30:VAL:HG22	1:Y:36:LEU:HD23	1.90	0.53
1:A:88:VAL:O	1:A:89:GLU:C	2.47	0.53
1:U:80:VAL:HG11	1:V:74:PRO:HB2	1.90	0.53
1:4:85:THR:OG1	3:4:226:HOH:O	2.19	0.53
1:R:92:LEU:HD21	1:R:95:SER:HB2	1.91	0.53
1:2:72:GLN:OE1	3:2:240:HOH:O	2.18	0.53
1:X:67:LEU:HB3	1:X:68:LEU:HG	1.90	0.53
1:K:32:GLU:HG3	1:L:40:TYR:CE1	2.44	0.53
1:U:45:ASP:OD2	1:U:50:ALA:HB3	2.09	0.52
1:P:5:LYS:HE2	1:P:55:TRP:NE1	2.24	0.52
1:T:23:LYS:HE2	1:T:25:LEU:HD21	1.90	0.52
1:S:46:ASN:ND2	3:S:258:HOH:O	2.43	0.52
1:J:30:VAL:HG12	1:J:36:LEU:HD23	1.92	0.52
1:V:87:HIS:HB2	3:V:220:HOH:O	2.08	0.52
1:S:60:ARG:NH2	3:S:219:HOH:O	2.22	0.52
1:G:89:GLU:HG2	1:H:52:PHE:HZ	1.73	0.52
1:T:52:PHE:O	1:T:53:ASP:HB2	2.10	0.52
1:S:87:HIS:HB3	1:S:92:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:54:GLU:HG2	1:Z:96:LYS:HZ2	1.75	0.52
1:4:27:LEU:CD1	1:4:58:ILE:HD11	2.40	0.52
1:W:1:MET:HE2	1:X:76:ASP:OD1	2.10	0.52
1:P:37:LEU:C	3:P:224:HOH:O	2.46	0.51
1:K:34:GLY:HA3	1:K:55:TRP:CZ2	2.45	0.51
1:I:29:LEU:HD12	1:I:39:LYS:HE2	1.91	0.51
1:P:32:GLU:CB	3:P:244:HOH:O	2.50	0.51
1:V:2:GLN:HG3	3:V:252:HOH:O	2.09	0.51
1:1:71:GLU:H	1:1:71:GLU:CD	2.13	0.51
1:F:22:VAL:HG22	1:F:73:ARG:NH1	2.25	0.51
1:F:32:GLU:OE1	1:F:32:GLU:N	2.43	0.51
1:M:6:VAL:HA	1:M:27:LEU:HD23	1.93	0.51
1:F:76:ASP:H	1:J:1:MET:HE2	1.75	0.51
1:3:32:GLU:O	1:3:34:GLY:N	2.44	0.51
1:Z:23:LYS:HD2	1:Z:25:LEU:HD11	1.92	0.51
1:J:91:ARG:HG2	1:J:92:LEU:H	1.74	0.51
1:M:41:GLU:OE1	3:M:272:HOH:O	2.19	0.51
1:O:5:LYS:HZ2	1:O:30:VAL:HG11	1.74	0.51
1:W:89:GLU:HG2	1:W:90:ASP:OD2	2.11	0.51
1:M:20:ARG:HD3	1:M:21:GLY:H	1.74	0.51
1:U:41:GLU:OE1	3:Y:255:HOH:O	2.19	0.51
1:F:52:PHE:CZ	1:J:89:GLU:HG2	2.46	0.51
1:L:40:TYR:O	3:L:237:HOH:O	2.19	0.51
1:V:60:ARG:HD3	3:V:251:HOH:O	2.11	0.51
1:X:28:GLN:HG3	1:X:40:TYR:CE2	2.47	0.50
1:N:41:GLU:OE2	1:N:58:ILE:CD1	2.58	0.50
1:3:14:GLN:NE2	3:3:237:HOH:O	2.42	0.50
1:2:35:ASN:ND2	3:2:229:HOH:O	2.42	0.50
1:O:3:ILE:HD13	1:O:86:ILE:HD13	1.93	0.50
1:I:50:ALA:HA	1:I:82:ILE:HD11	1.93	0.50
1:C:5:LYS:HE2	1:C:55:TRP:NE1	2.27	0.50
1:U:6:VAL:HA	1:U:27:LEU:HD12	1.93	0.50
1:N:6:VAL:HA	1:N:27:LEU:HD23	1.93	0.50
1:W:71:GLU:HB3	3:W:242:HOH:O	2.11	0.50
1:N:9:THR:OG1	3:N:224:HOH:O	2.20	0.50
1:Z:91:ARG:HG2	1:Z:91:ARG:NH1	2.26	0.50
1:S:88:VAL:HG13	1:T:7:ARG:O	2.12	0.50
1:Y:49:GLY:N	3:Y:236:HOH:O	2.43	0.49
1:3:84:ASP:HA	1:3:96:LYS:HZ3	1.76	0.49
1:1:20:ARG:NH2	3:1:237:HOH:O	2.45	0.49
1:K:31:ASP:HA	3:K:230:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:ARG:HD3	1:L:48:VAL:O	2.12	0.49
1:C:97:LYS:O	1:C:98:ASP:HB2	2.12	0.49
1:L:88:VAL:HG22	1:L:89:GLU:N	2.18	0.49
1:H:6:VAL:HA	1:H:27:LEU:HD23	1.94	0.49
1:W:5:LYS:HZ1	1:W:36:LEU:HD11	1.77	0.49
1:X:28:GLN:OE1	1:X:36:LEU:HD21	2.12	0.49
1:P:28:GLN:HG2	1:P:36:LEU:HG	1.94	0.49
1:O:3:ILE:HG23	1:O:83:ILE:HD12	1.93	0.49
1:A:6:VAL:HA	1:A:27:LEU:HD23	1.93	0.49
1:D:58:ILE:N	1:D:58:ILE:HD12	2.27	0.49
1:E:96:LYS:O	1:E:97:LYS:HB2	2.12	0.49
1:D:31:ASP:HB3	1:D:37:LEU:HD21	1.94	0.49
1:Q:14:GLN:N	1:Q:14:GLN:OE1	2.46	0.48
1:I:6:VAL:HA	1:I:27:LEU:HD23	1.95	0.48
1:Q:60:ARG:NH1	3:Q:228:HOH:O	2.45	0.48
1:3:45:ASP:HA	3:3:209:HOH:O	2.13	0.48
1:3:60:ARG:NH1	3:3:235:HOH:O	2.45	0.48
1:R:22:VAL:HA	1:R:46:ASN:ND2	2.29	0.48
1:H:71:GLU:HG2	1:H:72:GLN:HG3	1.96	0.48
1:Z:47:SER:OG	1:Z:47:SER:O	2.22	0.48
1:Y:7:ARG:NH1	1:Y:53:ASP:OD1	2.46	0.48
1:2:7:ARG:O	1:2:52:PHE:HE1	1.97	0.48
1:X:30:VAL:HG23	1:X:31:ASP:O	2.13	0.48
1:I:87:HIS:HB3	1:I:89:GLU:O	2.14	0.48
1:I:60:ARG:HD3	3:I:221:HOH:O	2.13	0.48
1:K:31:ASP:CA	3:K:230:HOH:O	2.62	0.48
1:I:18:SER:HB3	3:I:247:HOH:O	2.14	0.48
1:4:29:LEU:HD11	1:4:41:GLU:HG2	1.95	0.47
1:A:88:VAL:HG23	1:B:7:ARG:HB3	1.96	0.47
1:F:13:THR:O	1:F:20:ARG:NH1	2.36	0.47
1:X:29:LEU:HB2	1:X:39:LYS:HB3	1.95	0.47
1:B:41:GLU:OE2	1:B:58:ILE:CD1	2.62	0.47
1:Z:33:GLU:HA	3:Z:221:HOH:O	2.14	0.47
1:Z:46:ASN:OD1	1:Z:47:SER:N	2.47	0.47
1:Z:67:LEU:HD12	1:Z:67:LEU:H	1.78	0.47
1:1:88:VAL:O	1:1:89:GLU:HG3	2.13	0.47
1:F:28:GLN:NE2	1:F:40[A]:TYR:OH	2.48	0.47
1:O:15:LYS:NZ	1:O:20:ARG:NH2	2.62	0.47
1:N:20:ARG:CG	1:N:20:ARG:HH11	2.27	0.47
1:L:97:LYS:HG2	3:L:234:HOH:O	2.14	0.47
1:3:6:VAL:HA	1:3:27:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:18:SER:O	1:K:73:ARG:NH1	2.45	0.47
1:U:23:LYS:CE	3:U:260:HOH:O	2.61	0.47
1:C:57:LEU:HG	1:C:83:ILE:HD11	1.96	0.47
1:3:84:ASP:N	1:4:11:VAL:O	2.45	0.47
1:X:32:GLU:N	1:X:32:GLU:OE1	2.35	0.47
1:R:95:SER:HB3	1:R:98:ASP:HB2	1.97	0.47
1:I:15:LYS:NZ	1:I:20:ARG:NH2	2.62	0.47
1:F:27:LEU:HD13	1:F:43:ALA:HB3	1.97	0.47
1:H:20:ARG:HD2	1:H:20:ARG:HA	1.53	0.47
1:N:87:HIS:O	1:N:87:HIS:ND1	2.47	0.47
1:Y:89:GLU:HG3	1:Y:90:ASP:N	2.20	0.47
1:S:87:HIS:C	1:S:89:GLU:HA	2.35	0.47
1:J:65:ARG:HD3	3:J:201:HOH:O	2.14	0.47
1:M:47:SER:N	3:M:252:HOH:O	2.47	0.47
1:Q:47:SER:HB3	3:R:265:HOH:O	2.13	0.47
1:Y:25:LEU:O	1:Y:42:VAL:HA	2.14	0.47
1:O:29:LEU:HD22	1:O:39:LYS:HE3	1.95	0.47
1:Q:17:PRO:O	1:Q:20:ARG:HG2	2.15	0.47
1:Q:38:GLN:C	3:Q:264:HOH:O	2.52	0.47
1:F:40[B]:TYR:HD2	3:F:235:HOH:O	1.97	0.47
1:W:86:ILE:O	1:W:93:ILE:HG12	2.15	0.47
1:3:27:LEU:HD13	1:3:58:ILE:HD11	1.96	0.46
1:A:10:VAL:HG22	1:E:86:ILE:HG12	1.97	0.46
1:P:38:GLN:OE1	3:P:238:HOH:O	2.20	0.46
1:3:7:ARG:HD2	1:3:28:GLN:OE1	2.16	0.46
1:A:23:LYS:N	1:A:46:ASN:OD1	2.49	0.46
1:Z:98:ASP:OD1	1:Z:98:ASP:N	2.47	0.46
1:W:23:LYS:HG3	1:W:46:ASN:OD1	2.14	0.46
1:Y:5:LYS:NZ	1:Y:7:ARG:NH1	2.62	0.46
1:I:70:ASN:HA	1:I:73:ARG:HD2	1.96	0.46
1:W:5:LYS:CE	1:W:7:ARG:HD3	2.38	0.46
1:V:73:ARG:NH1	3:V:268:HOH:O	2.32	0.46
1:J:93:ILE:N	3:J:250:HOH:O	2.03	0.46
1:K:27:LEU:HG	1:K:58:ILE:HD11	1.98	0.46
1:D:87:HIS:ND1	1:D:91:ARG:O	2.44	0.46
1:J:33:GLU:HA	1:J:93:ILE:HG21	1.98	0.46
1:4:93:ILE:HG13	1:4:94:TYR:N	2.29	0.46
1:E:16:ASP:OD1	1:E:18:SER:OG	2.25	0.46
1:3:30:VAL:HG12	1:3:31:ASP:O	2.16	0.46
1:G:87:HIS:CE1	1:H:9:THR:HG1	2.33	0.46
1:4:88:VAL:HG23	1:4:91:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:88:VAL:O	1:4:90:ASP:N	2.49	0.46
1:T:86:ILE:HD12	1:T:94:TYR:HE2	1.79	0.46
1:X:32:GLU:HB3	1:Y:40:TYR:CD1	2.50	0.46
1:U:87:HIS:O	1:V:8:GLY:HA3	2.15	0.46
1:F:5:LYS:HD3	1:F:7:ARG:HH11	1.81	0.46
1:Q:14:GLN:NE2	3:Q:262:HOH:O	2.41	0.46
1:L:5:LYS:NZ	1:L:53:ASP:OD1	2.46	0.46
1:W:7:ARG:HD2	1:W:7:ARG:HA	1.66	0.46
1:C:89:GLU:OE2	1:C:89:GLU:HA	2.16	0.46
1:E:9:THR:HG22	1:E:25:LEU:HD23	1.97	0.46
1:Q:29:LEU:HD13	1:Q:39:LYS:HG2	1.98	0.46
1:Q:92:LEU:HD21	1:Q:95:SER:HB2	1.98	0.46
1:E:65:ARG:HA	1:E:70:ASN:HB3	1.98	0.46
1:3:34:GLY:HA2	1:3:55:TRP:CH2	2.52	0.45
1:F:32:GLU:HB3	1:G:40:TYR:CG	2.51	0.45
1:Q:95:SER:C	1:Q:97:LYS:H	2.20	0.45
1:N:60:ARG:NH1	1:N:60:ARG:HB3	2.31	0.45
1:K:31:ASP:OD2	1:K:35:ASN:HB2	2.16	0.45
1:Y:29:LEU:HD12	1:Y:39:LYS:HG2	1.98	0.45
1:2:92:LEU:HD13	1:2:92:LEU:HA	1.82	0.45
1:3:69:GLY:O	1:3:73:ARG:HD2	2.16	0.45
1:3:96:LYS:HD2	3:3:207:HOH:O	2.16	0.45
1:G:88:VAL:HG22	1:H:26:LEU:HD23	1.99	0.45
1:F:46:ASN:ND2	1:F:73:ARG:HH12	2.14	0.45
1:H:87:HIS:O	1:I:8:GLY:HA3	2.16	0.45
1:L:85:THR:HB	3:L:244:HOH:O	2.17	0.45
1:S:84:ASP:OD2	1:T:13:THR:HG23	2.17	0.45
1:Z:11:VAL:HA	3:Z:224:HOH:O	2.16	0.45
1:4:32:GLU:HG2	1:Z:26:LEU:HD21	1.98	0.45
1:X:23:LYS:HE3	1:X:25:LEU:HD21	1.98	0.45
1:U:27:LEU:HD21	1:U:79:VAL:CG2	2.46	0.45
1:4:96:LYS:HD2	1:4:96:LYS:HA	1.79	0.45
1:Q:93:ILE:HG21	3:Q:248:HOH:O	2.16	0.45
1:B:25:LEU:O	1:B:42:VAL:HA	2.17	0.45
1:F:68:LEU:H	1:F:68:LEU:HD23	1.81	0.45
1:P:25:LEU:HB2	1:P:27:LEU:CD2	2.47	0.45
1:W:89:GLU:HG2	1:W:90:ASP:N	2.31	0.45
1:O:55:TRP:CZ3	1:O:86:ILE:HD12	2.52	0.45
1:O:55:TRP:HZ3	1:O:86:ILE:HD12	1.82	0.45
1:N:50:ALA:HA	1:N:82:ILE:HD11	1.99	0.45
1:2:56:VAL:HB	1:2:79:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:5:LYS:NZ	1:O:34:GLY:O	2.50	0.44
1:K:86:ILE:HG13	1:K:94:TYR:HB3	1.99	0.44
1:M:87:HIS:O	1:N:8:GLY:HA3	2.17	0.44
1:R:52:PHE:O	1:R:53:ASP:HB3	2.17	0.44
1:2:5:LYS:HD2	1:2:36:LEU:HD21	1.99	0.44
1:M:88:VAL:HG12	1:M:93:ILE:HG23	1.99	0.44
1:P:72:GLN:N	3:P:218:HOH:O	1.86	0.44
1:U:47:SER:HB2	3:V:255:HOH:O	2.17	0.44
1:M:88:VAL:CG2	1:M:89:GLU:HG2	2.45	0.44
1:B:6:VAL:HA	1:B:27:LEU:HD23	1.98	0.44
1:K:29:LEU:CD2	1:K:39:LYS:HB2	2.45	0.44
1:H:31:ASP:HB2	3:H:251:HOH:O	2.16	0.44
1:A:71:GLU:CD	1:A:71:GLU:H	2.21	0.44
1:K:68:LEU:HA	1:K:68:LEU:HD13	1.71	0.44
1:T:87:HIS:CE1	1:T:92:LEU:HB2	2.53	0.44
1:V:84:ASP:OD2	1:W:13:THR:OG1	2.23	0.44
1:P:88:VAL:N	1:P:91:ARG:O	2.50	0.44
1:4:87:HIS:CE1	1:4:92:LEU:HG	2.53	0.44
1:1:31:ASP:HB2	3:2:227:HOH:O	2.17	0.44
1:V:73:ARG:NH2	3:V:268:HOH:O	2.48	0.44
1:Z:20:ARG:O	3:Z:243:HOH:O	2.21	0.44
1:Q:65:ARG:NH2	3:Q:263:HOH:O	2.50	0.44
1:T:28:GLN:OE1	3:T:235:HOH:O	2.21	0.44
1:V:6:VAL:HA	1:V:27:LEU:HD12	1.99	0.44
1:W:89:GLU:HB3	1:X:52:PHE:CZ	2.53	0.44
1:G:31:ASP:HB3	1:G:37:LEU:HD21	2.00	0.44
1:P:25:LEU:HB2	1:P:27:LEU:HD21	2.00	0.43
1:1:65:ARG:NH2	1:1:71:GLU:O	2.51	0.43
1:1:42:VAL:HG21	1:Z:57:LEU:HD21	1.99	0.43
1:U:27:LEU:HD12	1:U:27:LEU:HA	1.81	0.43
1:4:58:ILE:HG23	1:4:58:ILE:HD12	1.70	0.43
1:N:60:ARG:HH11	1:N:60:ARG:HB3	1.84	0.43
1:O:48:VAL:HG22	1:O:48:VAL:O	2.18	0.43
1:T:97:LYS:HA	1:T:97:LYS:HD3	1.84	0.43
1:H:82:ILE:O	1:H:82:ILE:HG13	2.17	0.43
1:L:32:GLU:HG3	1:M:28:GLN:HG3	2.00	0.43
1:M:70:ASN:HA	1:M:73:ARG:HD2	2.00	0.43
1:D:67:LEU:HD11	1:D:80:VAL:HG12	2.01	0.43
1:G:15:LYS:HE2	1:G:20:ARG:NH1	2.34	0.43
1:3:28:GLN:HG3	1:3:40:TYR:CZ	2.54	0.43
1:X:67:LEU:HD11	1:X:80:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:7:ARG:NH1	1:Y:52:PHE:CE1	2.86	0.43
1:Z:27:LEU:HB3	1:Z:58:ILE:HD11	2.00	0.43
1:P:70:ASN:HA	1:P:73:ARG:HD2	2.01	0.43
1:F:34:GLY:HA2	1:F:55:TRP:CH2	2.53	0.43
1:T:87:HIS:NE2	1:T:92:LEU:HD13	2.33	0.43
1:R:91:ARG:NH1	3:R:268:HOH:O	2.51	0.43
1:M:39:LYS:HB3	1:M:39:LYS:HE3	1.76	0.43
1:D:31:ASP:OD1	1:D:31:ASP:C	2.57	0.43
1:X:2:GLN:OE1	1:Y:41:GLU:HG2	2.19	0.43
1:Z:91:ARG:HG2	1:Z:91:ARG:HH11	1.82	0.43
1:K:88:VAL:HG13	1:L:7:ARG:O	2.19	0.43
1:W:17:PRO:HA	1:W:20:ARG:HG3	2.00	0.43
1:W:82:ILE:HB	1:X:14:GLN:HB2	2.00	0.43
1:E:97:LYS:HD2	1:E:97:LYS:HA	1.72	0.42
1:J:86:ILE:HG12	1:J:86:ILE:O	2.18	0.42
1:1:88:VAL:HG23	1:2:7:ARG:O	2.19	0.42
1:X:28:GLN:CB	1:X:36:LEU:HD11	2.46	0.42
1:K:32:GLU:HG3	1:L:40:TYR:CD1	2.54	0.42
1:O:21:GLY:HA3	1:T:14:GLN:HG3	2.00	0.42
1:M:46:ASN:HB2	3:M:252:HOH:O	2.18	0.42
1:S:30:VAL:HG22	1:S:36:LEU:HD23	2.01	0.42
1:J:45:ASP:OD1	1:J:48:VAL:O	2.36	0.42
1:R:20:ARG:NH2	3:R:230:HOH:O	2.51	0.42
1:R:20:ARG:HH12	1:Y:18:SER:CB	2.28	0.42
1:M:54:GLU:N	3:M:263:HOH:O	2.51	0.42
1:Y:15:LYS:HE2	1:Y:20:ARG:NH1	2.34	0.42
1:T:30:VAL:HG11	1:T:55:TRP:HZ3	1.84	0.42
1:X:91:ARG:HD2	1:X:91:ARG:HA	1.89	0.42
1:L:88:VAL:CG2	1:L:89:GLU:H	2.21	0.42
1:2:85:THR:OG1	1:3:11:VAL:HB	2.20	0.42
1:C:91:ARG:HA	1:C:91:ARG:HD2	1.34	0.42
1:L:27:LEU:HD13	1:L:58:ILE:HD11	2.01	0.42
1:Z:68:LEU:CD1	1:Z:68:LEU:H	2.31	0.42
1:F:52:PHE:CE2	1:J:89:GLU:HG2	2.54	0.42
1:E:67:LEU:O	1:E:70:ASN:HB2	2.18	0.42
1:Q:65:ARG:HA	1:Q:70:ASN:HB3	2.00	0.42
1:3:88:VAL:O	1:3:91:ARG:N	2.42	0.42
1:M:23:LYS:HE3	1:M:23:LYS:HB2	1.78	0.42
1:2:68:LEU:HA	1:2:71:GLU:OE2	2.20	0.42
1:3:96:LYS:CD	3:3:207:HOH:O	2.68	0.42
1:K:32:GLU:OE2	1:K:93:ILE:HD13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:ASP:O	1:E:45:ASP:CG	2.58	0.42
1:F:13:THR:HG23	1:J:84:ASP:OD2	2.19	0.42
1:B:88:VAL:O	1:B:88:VAL:HG23	2.18	0.42
1:D:4:ALA:HB3	1:D:58:ILE:HD11	2.00	0.42
1:A:17:PRO:HG2	1:L:71:GLU:CD	2.39	0.42
1:K:25:LEU:O	1:K:42:VAL:HA	2.20	0.42
1:K:28:GLN:CD	1:K:36:LEU:HD11	2.40	0.42
1:Z:91:ARG:HG3	1:Z:92:LEU:N	2.32	0.42
1:B:27:LEU:HD13	1:B:58:ILE:HD11	2.00	0.42
1:C:85:THR:HG22	1:C:95:SER:HA	2.01	0.42
1:G:60:ARG:HG3	3:G:236:HOH:O	2.19	0.42
1:Y:88:VAL:O	1:Y:89:GLU:HB3	2.20	0.42
1:1:88:VAL:C	1:1:89:GLU:HG3	2.40	0.42
1:P:55:TRP:N	3:P:221:HOH:O	2.34	0.42
1:T:30:VAL:HG11	1:T:55:TRP:CZ3	2.54	0.42
1:A:57:LEU:HD12	1:A:57:LEU:HA	1.87	0.42
1:3:26:LEU:HD11	1:3:40:TYR:HB3	2.02	0.42
1:F:38:GLN:HB2	1:F:40[A]:TYR:HE1	1.84	0.42
1:V:87:HIS:CE1	1:V:92:LEU:HG	2.55	0.42
1:4:83:ILE:HD13	1:4:86:ILE:HD11	2.02	0.42
1:3:50:ALA:HA	1:3:82:ILE:HD11	2.01	0.42
1:N:91:ARG:NH1	1:N:93:ILE:CD1	2.80	0.41
1:U:97:LYS:HD2	1:U:97:LYS:HA	1.87	0.41
1:Z:23:LYS:CD	1:Z:25:LEU:HD11	2.50	0.41
1:C:1:MET:HB3	1:C:57:LEU:HD22	2.01	0.41
1:G:95:SER:OG	1:G:97:LYS:HE2	2.19	0.41
1:D:47:SER:OG	1:D:67:LEU:HD23	2.19	0.41
1:Q:25:LEU:O	1:Q:42:VAL:HA	2.20	0.41
1:V:53:ASP:O	3:V:239:HOH:O	2.22	0.41
1:K:28:GLN:OE1	1:K:36:LEU:HD11	2.20	0.41
1:O:6:VAL:HA	1:O:27:LEU:HD23	2.02	0.41
1:M:5:LYS:HE2	1:M:55:TRP:NE1	2.35	0.41
1:3:21:GLY:O	1:3:46:ASN:ND2	2.52	0.41
1:E:29:LEU:HD13	1:E:39:LYS:HG3	2.03	0.41
1:J:5:LYS:HB3	1:J:5:LYS:HE3	1.88	0.41
1:L:20:ARG:NH1	1:L:21:GLY:H	2.18	0.41
1:U:27:LEU:HB3	1:U:58:ILE:HD11	2.02	0.41
1:B:29:LEU:HD21	1:B:41:GLU:OE2	2.20	0.41
1:I:31:ASP:HB2	3:I:216:HOH:O	2.18	0.41
1:N:89:GLU:HB3	1:N:90:ASP:H	1.47	0.41
1:F:29:LEU:HD23	3:F:206:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:84:ASP:OD2	1:Q:13:THR:OG1	2.37	0.41
1:1:60:ARG:NH2	1:Z:60:ARG:HH21	2.19	0.41
1:O:87:HIS:N	3:O:233:HOH:O	2.52	0.41
1:B:41:GLU:OE2	1:B:58:ILE:HD12	2.20	0.41
1:1:60:ARG:CB	3:1:254:HOH:O	2.68	0.41
1:P:27:LEU:CG	1:P:58:ILE:HD11	2.50	0.41
1:X:31:ASP:CG	1:X:35:ASN:HB2	2.41	0.41
1:K:71:GLU:HB2	3:K:215:HOH:O	2.20	0.41
1:H:12:SER:O	1:H:15:LYS:HE3	2.20	0.41
1:B:46:ASN:HA	3:W:247:HOH:O	2.20	0.41
1:Z:23:LYS:HA	3:Z:228:HOH:O	2.20	0.41
1:4:58:ILE:HA	1:4:58:ILE:HD13	1.78	0.41
1:H:15:LYS:HZ2	1:H:20:ARG:HH21	1.67	0.41
1:Q:29:LEU:HD13	1:Q:39:LYS:HD3	2.03	0.41
1:C:85:THR:HA	1:C:94:TYR:O	2.20	0.41
1:P:87:HIS:CE1	1:P:92:LEU:HB3	2.55	0.41
1:Q:7:ARG:HA	1:Q:7:ARG:HD2	1.86	0.41
1:Y:7:ARG:NH1	1:Y:52:PHE:CZ	2.84	0.41
1:E:38:GLN:NE2	3:E:244:HOH:O	2.24	0.41
1:J:91:ARG:CG	1:J:92:LEU:H	2.33	0.41
1:H:87:HIS:CD2	1:H:92:LEU:HG	2.56	0.41
1:P:65:ARG:HA	1:P:70:ASN:HB3	2.03	0.41
1:N:27:LEU:HD11	1:N:43:ALA:HB3	2.03	0.41
1:K:18:SER:HA	1:R:90:ASP:OD2	2.20	0.40
1:J:31:ASP:HB2	1:J:32:GLU:OE1	2.22	0.40
1:K:35:ASN:ND2	3:K:234:HOH:O	2.26	0.40
1:H:71:GLU:CD	3:H:218:HOH:O	2.59	0.40
1:Y:87:HIS:HB3	1:Y:92:LEU:HD12	2.02	0.40
1:P:96:LYS:NZ	1:Q:14:GLN:HE22	2.19	0.40
1:U:27:LEU:HD21	1:U:79:VAL:HG22	2.03	0.40
1:S:47:SER:HB3	3:S:258:HOH:O	2.20	0.40
1:F:55:TRP:HB3	1:F:83:ILE:HD12	2.02	0.40
1:1:60:ARG:HD2	1:1:77:ALA:HB2	2.03	0.40
1:E:6:VAL:HA	1:E:27:LEU:HD23	2.04	0.40
1:A:17:PRO:HA	1:A:20:ARG:HG2	2.03	0.40
1:X:38:GLN:O	3:X:224:HOH:O	2.22	0.40
1:C:92:LEU:C	1:C:93:ILE:HD12	2.42	0.40
1:1:29:LEU:HA	1:1:29:LEU:HD13	1.83	0.40
1:R:20:ARG:NH1	1:Y:18:SER:CB	2.81	0.40
1:2:73:ARG:HH21	1:2:73:ARG:HD2	1.77	0.40
1:Q:23:LYS:N	1:Q:46:ASN:OD1	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:84:ASP:HA	1:W:96:LYS:CD	2.52	0.40
1:N:18:SER:HB2	1:N:73:ARG:HG2	2.03	0.40
1:K:86:ILE:O	1:K:93:ILE:HG12	2.21	0.40
1:R:39:LYS:NZ	3:R:258:HOH:O	2.54	0.40
1:3:51:GLY:N	1:3:54:GLU:OE1	2.25	0.40
1:T:49:GLY:O	1:T:82:ILE:HD11	2.20	0.40
1:O:57:LEU:HA	1:O:57:LEU:HD23	1.92	0.40
1:M:97:LYS:HE2	1:M:97:LYS:HB3	1.68	0.40
1:4:14:GLN:HA	3:4:228:HOH:O	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:244:HOH:O	3:Q:242:HOH:O[4_445]	1.67	0.53
1:L:35:ASN:OD1	3:J:255:HOH:O[3_644]	2.09	0.11
1:3:38:GLN:NE2	1:X:31:ASP:OD2[3_544]	2.10	0.10
3:I:242:HOH:O	3:M:254:HOH:O[3_654]	2.12	0.08
1:3:40:TYR:OH	3:X:206:HOH:O[3_544]	2.15	0.05

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	1	97/109 (89%)	92 (95%)	4 (4%)	1 (1%)	19 7
1	2	94/109 (86%)	85 (90%)	9 (10%)	0	100 100
1	3	97/109 (89%)	83 (86%)	10 (10%)	4 (4%)	3 0
1	4	96/109 (88%)	90 (94%)	4 (4%)	2 (2%)	9 2
1	A	96/109 (88%)	91 (95%)	4 (4%)	1 (1%)	19 7
1	B	97/109 (89%)	91 (94%)	4 (4%)	2 (2%)	9 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	96/109 (88%)	88 (92%)	8 (8%)	0	100 100
1	D	96/109 (88%)	92 (96%)	3 (3%)	1 (1%)	19 7
1	E	95/109 (87%)	89 (94%)	5 (5%)	1 (1%)	17 6
1	F	97/109 (89%)	86 (89%)	10 (10%)	1 (1%)	19 7
1	G	95/109 (87%)	93 (98%)	2 (2%)	0	100 100
1	H	96/109 (88%)	90 (94%)	4 (4%)	2 (2%)	9 2
1	I	96/109 (88%)	91 (95%)	5 (5%)	0	100 100
1	J	94/109 (86%)	87 (93%)	7 (7%)	0	100 100
1	K	96/109 (88%)	87 (91%)	9 (9%)	0	100 100
1	L	96/109 (88%)	90 (94%)	5 (5%)	1 (1%)	19 7
1	M	96/109 (88%)	93 (97%)	2 (2%)	1 (1%)	19 7
1	N	96/109 (88%)	91 (95%)	5 (5%)	0	100 100
1	O	94/109 (86%)	88 (94%)	5 (5%)	1 (1%)	17 6
1	P	97/109 (89%)	87 (90%)	9 (9%)	1 (1%)	19 7
1	Q	95/109 (87%)	90 (95%)	2 (2%)	3 (3%)	5 0
1	R	96/109 (88%)	92 (96%)	2 (2%)	2 (2%)	9 2
1	S	96/109 (88%)	91 (95%)	5 (5%)	0	100 100
1	T	90/109 (83%)	87 (97%)	3 (3%)	0	100 100
1	U	95/109 (87%)	87 (92%)	6 (6%)	2 (2%)	9 2
1	V	96/109 (88%)	91 (95%)	4 (4%)	1 (1%)	19 7
1	W	95/109 (87%)	90 (95%)	4 (4%)	1 (1%)	17 6
1	X	96/109 (88%)	91 (95%)	4 (4%)	1 (1%)	19 7
1	Y	95/109 (87%)	94 (99%)	1 (1%)	0	100 100
1	Z	96/109 (88%)	92 (96%)	3 (3%)	1 (1%)	19 7
All	All	2867/3270 (88%)	2689 (94%)	148 (5%)	30 (1%)	19 7

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3	32	GLU
1	D	89	GLU
1	E	89	GLU
1	O	88	VAL
1	Q	89	GLU

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Mol	Chain	Res	Type
1	Q	96	LYS
1	U	47	SER
1	W	89	GLU
1	3	33	GLU
1	4	89	GLU
1	B	89	GLU
1	F	89	GLU
1	H	96	LYS
1	L	88	VAL
1	M	97	LYS
1	R	89	GLU
1	Z	53	ASP
1	3	96	LYS
1	A	89	GLU
1	B	90	ASP
1	P	89	GLU
1	V	89	GLU
1	X	89	GLU
1	3	92	LEU
1	H	46	ASN
1	Q	90	ASP
1	1	89	GLU
1	4	39	LYS
1	U	89	GLU
1	R	49	GLY

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	1	83/93 (89%)	77 (93%)	6 (7%)	18 5
1	2	80/93 (86%)	77 (96%)	3 (4%)	40 24
1	3	83/93 (89%)	78 (94%)	5 (6%)	24 9
1	4	82/93 (88%)	78 (95%)	4 (5%)	31 14
1	A	82/93 (88%)	79 (96%)	3 (4%)	41 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	83/93 (89%)	80 (96%)	3 (4%)	42 27
1	C	82/93 (88%)	80 (98%)	2 (2%)	57 46
1	D	82/93 (88%)	78 (95%)	4 (5%)	31 14
1	E	81/93 (87%)	79 (98%)	2 (2%)	55 44
1	F	83/93 (89%)	77 (93%)	6 (7%)	18 5
1	G	81/93 (87%)	80 (99%)	1 (1%)	78 74
1	H	82/93 (88%)	77 (94%)	5 (6%)	23 9
1	I	82/93 (88%)	82 (100%)	0	100 100
1	J	80/93 (86%)	76 (95%)	4 (5%)	30 14
1	K	82/93 (88%)	78 (95%)	4 (5%)	31 14
1	L	82/93 (88%)	79 (96%)	3 (4%)	41 26
1	M	82/93 (88%)	79 (96%)	3 (4%)	41 26
1	N	82/93 (88%)	77 (94%)	5 (6%)	23 9
1	O	80/93 (86%)	78 (98%)	2 (2%)	55 44
1	P	83/93 (89%)	82 (99%)	1 (1%)	78 74
1	Q	81/93 (87%)	78 (96%)	3 (4%)	41 26
1	R	82/93 (88%)	80 (98%)	2 (2%)	57 46
1	S	82/93 (88%)	80 (98%)	2 (2%)	57 46
1	T	78/93 (84%)	77 (99%)	1 (1%)	76 71
1	U	81/93 (87%)	76 (94%)	5 (6%)	23 8
1	V	82/93 (88%)	80 (98%)	2 (2%)	57 46
1	W	81/93 (87%)	77 (95%)	4 (5%)	31 14
1	X	82/93 (88%)	79 (96%)	3 (4%)	41 26
1	Y	81/93 (87%)	77 (95%)	4 (5%)	31 14
1	Z	82/93 (88%)	77 (94%)	5 (6%)	23 9
All	All	2449/2790 (88%)	2352 (96%)	97 (4%)	38 22

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

Mol	Chain	Res	Type
1	1	47	SER
1	1	68	LEU
1	1	89	GLU

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Mol	Chain	Res	Type
1	1	90	ASP
1	1	91	ARG
1	1	93	ILE
1	2	39	LYS
1	2	91	ARG
1	2	92	LEU
1	3	32	GLU
1	3	36	LEU
1	3	90	ASP
1	3	92	LEU
1	3	96	LYS
1	4	11	VAL
1	4	41	GLU
1	4	95	SER
1	4	97	LYS
1	A	9	THR
1	A	11	VAL
1	A	89	GLU
1	B	23	LYS
1	B	90	ASP
1	B	91	ARG
1	C	91	ARG
1	C	92	LEU
1	D	47	SER
1	D	89	GLU
1	D	91	ARG
1	D	98	ASP
1	E	20	ARG
1	E	87	HIS
1	F	9	THR
1	F	11	VAL
1	F	47	SER
1	F	68	LEU
1	F	95	SER
1	F	98	ASP
1	G	93	ILE
1	H	9	THR
1	H	53	ASP
1	H	92	LEU
1	H	96	LYS
1	H	98	ASP
1	J	53	ASP

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Mol	Chain	Res	Type
1	J	85	THR
1	J	86	ILE
1	J	92	LEU
1	K	36	LEU
1	K	41	GLU
1	K	54	GLU
1	K	68	LEU
1	L	20	ARG
1	L	47	SER
1	L	88	VAL
1	M	20	ARG
1	M	95	SER
1	M	98	ASP
1	N	20	ARG
1	N	88	VAL
1	N	89	GLU
1	N	90	ASP
1	N	92	LEU
1	O	48	VAL
1	O	92	LEU
1	P	91	ARG
1	Q	9	THR
1	Q	47	SER
1	Q	97	LYS
1	R	53	ASP
1	R	91	ARG
1	S	87	HIS
1	S	90	ASP
1	T	47	SER
1	U	27	LEU
1	U	46	ASN
1	U	68	LEU
1	U	89	GLU
1	U	97	LYS
1	V	87	HIS
1	V	90	ASP
1	W	47	SER
1	W	89	GLU
1	W	91	ARG
1	W	92	LEU
1	X	11	VAL
1	X	20	ARG

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Mol	Chain	Res	Type
1	X	91	ARG
1	Y	24	LEU
1	Y	86	ILE
1	Y	87	HIS
1	Y	93	ILE
1	Z	48	VAL
1	Z	52	PHE
1	Z	68	LEU
1	Z	91	ARG
1	Z	98	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	35	ASN
1	K	28	GLN
1	O	87	HIS
1	R	2	GLN
1	U	2	GLN
1	V	14	GLN
1	X	28	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	201	-	4,4,4	0.29	0	6,6,6	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	201	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	99/109 (90%)	0.43	9 (9%) 11 17	13, 24, 65, 79	0
1	2	96/109 (88%)	0.67	12 (12%) 5 8	19, 31, 78, 106	0
1	3	99/109 (90%)	1.03	19 (19%) 2 2	23, 43, 82, 93	0
1	4	98/109 (89%)	0.80	17 (17%) 2 3	20, 40, 66, 90	0
1	A	98/109 (89%)	0.25	4 (4%) 41 50	15, 30, 51, 68	0
1	B	99/109 (90%)	0.22	4 (4%) 42 51	14, 23, 56, 81	0
1	C	98/109 (89%)	0.64	11 (11%) 7 11	16, 27, 77, 93	0
1	D	98/109 (89%)	0.87	16 (16%) 2 3	18, 38, 70, 88	0
1	E	97/109 (88%)	0.84	12 (12%) 5 8	16, 32, 74, 96	0
1	F	98/109 (89%)	0.99	19 (19%) 1 2	20, 40, 76, 97	0
1	G	97/109 (88%)	0.70	12 (12%) 5 8	18, 33, 78, 87	0
1	H	98/109 (89%)	0.34	6 (6%) 25 32	18, 33, 53, 75	0
1	I	98/109 (89%)	0.29	6 (6%) 25 32	13, 25, 63, 83	0
1	J	96/109 (88%)	0.66	11 (11%) 6 10	16, 30, 77, 96	0
1	K	98/109 (89%)	1.26	23 (23%) 1 1	21, 46, 80, 91	0
1	L	98/109 (89%)	0.71	13 (13%) 4 7	18, 36, 68, 88	0
1	M	98/109 (89%)	0.43	6 (6%) 25 32	17, 32, 63, 75	0
1	N	98/109 (89%)	0.22	6 (6%) 25 32	14, 24, 69, 82	0
1	O	96/109 (88%)	0.64	13 (13%) 4 6	16, 29, 75, 91	0
1	P	99/109 (90%)	1.15	18 (18%) 2 2	19, 42, 76, 84	0
1	Q	97/109 (88%)	0.57	10 (10%) 9 13	16, 33, 61, 83	0
1	R	98/109 (89%)	0.22	3 (3%) 52 61	16, 28, 49, 64	0
1	S	98/109 (89%)	0.21	5 (5%) 32 41	14, 23, 58, 74	0
1	T	94/109 (86%)	0.58	11 (11%) 6 9	16, 27, 70, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	U	97/109 (88%)	0.43	8 (8%) 14 21	19, 34, 67, 75	0
1	V	98/109 (89%)	0.41	7 (7%) 19 27	20, 34, 65, 82	0
1	W	97/109 (88%)	0.87	17 (17%) 2 3	18, 36, 76, 96	0
1	X	98/109 (89%)	0.91	16 (16%) 2 3	19, 42, 71, 83	0
1	Y	97/109 (88%)	0.65	11 (11%) 7 10	17, 30, 73, 94	0
1	Z	98/109 (89%)	0.63	10 (10%) 9 13	18, 34, 70, 78	0
All	All	2928/3270 (89%)	0.62	335 (11%) 7 10	13, 33, 70, 106	0

All (335) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	92	LEU	10.1
1	T	92	LEU	9.6
1	T	94	TYR	8.9
1	Z	52	PHE	8.9
1	G	92	LEU	8.4
1	I	90	ASP	8.3
1	C	90	ASP	7.4
1	P	92	LEU	7.4
1	E	92	LEU	7.2
1	W	92	LEU	7.0
1	Y	90	ASP	6.9
1	F	90	ASP	6.8
1	L	92	LEU	6.8
1	J	90	ASP	6.6
1	2	92	LEU	6.6
1	W	90	ASP	6.6
1	E	88	VAL	6.5
1	J	92	LEU	6.5
1	E	90	ASP	6.4
1	3	92	LEU	6.4
1	K	90	ASP	6.4
1	Y	88	VAL	6.4
1	3	90	ASP	6.3
1	C	92	LEU	6.2
1	E	87	HIS	6.2
1	F	40[A]	TYR	6.0
1	P	99	GLN	6.0
1	K	97	LYS	5.9
1	G	88	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
1	J	93	ILE	5.8
1	C	94	TYR	5.8
1	Q	91	ARG	5.8
1	K	92	LEU	5.8
1	Y	95	SER	5.7
1	P	90	ASP	5.6
1	3	99	GLN	5.4
1	Q	90	ASP	5.3
1	2	90	ASP	5.3
1	D	92	LEU	5.3
1	D	90	ASP	5.3
1	3	93	ILE	5.2
1	K	93	ILE	5.2
1	D	97	LYS	5.2
1	N	90	ASP	5.2
1	L	90	ASP	5.2
1	V	92	LEU	5.1
1	B	89	GLU	5.1
1	P	97	LYS	5.1
1	O	90	ASP	5.1
1	1	99	GLN	5.1
1	P	93	ILE	5.1
1	C	95	SER	5.0
1	Q	92	LEU	5.0
1	H	98	ASP	4.9
1	S	90	ASP	4.9
1	E	91	ARG	4.8
1	1	92	LEU	4.8
1	M	52	PHE	4.8
1	X	90	ASP	4.8
1	4	92	LEU	4.8
1	O	93	ILE	4.7
1	U	68	LEU	4.7
1	O	87	HIS	4.7
1	1	90	ASP	4.7
1	W	85	THR	4.7
1	P	98	ASP	4.6
1	E	95	SER	4.6
1	P	94	TYR	4.6
1	E	93	ILE	4.6
1	C	98	ASP	4.6
1	J	87	HIS	4.6

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Mol	Chain	Res	Type	RSRZ
1	3	96	LYS	4.6
1	K	49	GLY	4.5
1	C	91	ARG	4.5
1	Z	47	SER	4.5
1	P	95	SER	4.5
1	G	87	HIS	4.5
1	G	91	ARG	4.5
1	2	91	ARG	4.4
1	P	89	GLU	4.4
1	G	89	GLU	4.4
1	G	95	SER	4.4
1	I	89	GLU	4.4
1	J	94	TYR	4.4
1	Y	91	ARG	4.4
1	K	98	ASP	4.3
1	K	46	ASN	4.3
1	2	94	TYR	4.3
1	D	89	GLU	4.2
1	L	52	PHE	4.2
1	2	93	ILE	4.2
1	W	89	GLU	4.2
1	W	87	HIS	4.2
1	B	90	ASP	4.2
1	T	87	HIS	4.2
1	K	91	ARG	4.1
1	3	98	ASP	4.1
1	4	90	ASP	4.1
1	V	89	GLU	4.1
1	R	90	ASP	4.0
1	J	95	SER	4.0
1	O	94	TYR	4.0
1	Y	86	ILE	4.0
1	4	89	GLU	4.0
1	S	89	GLU	4.0
1	2	89	GLU	4.0
1	K	94	TYR	4.0
1	1	98	ASP	3.9
1	Z	46	ASN	3.9
1	F	91	ARG	3.9
1	W	93	ILE	3.9
1	D	87	HIS	3.8
1	M	50	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	52	PHE	3.8
1	F	97	LYS	3.8
1	2	87	HIS	3.7
1	W	94	TYR	3.7
1	K	51	GLY	3.7
1	F	95	SER	3.7
1	W	48	VAL	3.7
1	T	97	LYS	3.7
1	M	51	GLY	3.7
1	O	53	ASP	3.7
1	X	34	GLY	3.7
1	3	95	SER	3.7
1	T	93	ILE	3.6
1	X	92	LEU	3.6
1	4	52	PHE	3.6
1	L	97	LYS	3.6
1	H	52	PHE	3.6
1	W	91	ARG	3.6
1	K	40	TYR	3.6
1	L	87	HIS	3.6
1	F	93	ILE	3.5
1	Q	93	ILE	3.5
1	2	52	PHE	3.5
1	X	98	ASP	3.5
1	C	93	ILE	3.5
1	W	95	SER	3.4
1	Y	97	LYS	3.4
1	2	95	SER	3.4
1	3	97	LYS	3.4
1	F	98	ASP	3.4
1	K	96	LYS	3.4
1	F	94	TYR	3.4
1	A	91	ARG	3.3
1	G	52	PHE	3.3
1	L	98	ASP	3.3
1	L	89	GLU	3.3
1	4	91	ARG	3.3
1	K	48	VAL	3.3
1	F	55	TRP	3.3
1	4	97	LYS	3.3
1	X	91	ARG	3.3
1	P	49	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	O	91	ARG	3.2
1	C	87	HIS	3.2
1	2	96	LYS	3.2
1	X	89	GLU	3.2
1	K	87	HIS	3.2
1	X	93	ILE	3.2
1	F	92	LEU	3.2
1	3	89	GLU	3.2
1	W	88	VAL	3.2
1	Z	50	ALA	3.2
1	X	46	ASN	3.1
1	3	34	GLY	3.1
1	N	92	LEU	3.1
1	Z	68	LEU	3.1
1	O	52	PHE	3.1
1	E	89	GLU	3.1
1	K	52	PHE	3.1
1	3	46	ASN	3.1
1	L	88	VAL	3.1
1	3	33	GLU	3.1
1	Q	89	GLU	3.1
1	3	68	LEU	3.1
1	Y	87	HIS	3.1
1	1	89	GLU	3.1
1	4	40	TYR	3.1
1	T	52	PHE	3.0
1	1	91	ARG	3.0
1	3	94	TYR	3.0
1	G	97	LYS	3.0
1	M	68	LEU	3.0
1	N	98	ASP	3.0
1	V	98	ASP	3.0
1	E	52	PHE	2.9
1	3	87	HIS	2.9
1	A	52	PHE	2.9
1	E	97	LYS	2.9
1	J	86	ILE	2.9
1	3	91	ARG	2.9
1	L	95	SER	2.9
1	X	94	TYR	2.9
1	G	90	ASP	2.9
1	Q	87	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	X	40	TYR	2.9
1	C	97	LYS	2.8
1	X	52	PHE	2.8
1	Y	40	TYR	2.8
1	O	86	ILE	2.8
1	K	33	GLU	2.8
1	1	88	VAL	2.8
1	Z	51	GLY	2.8
1	X	97	LYS	2.8
1	4	98	ASP	2.8
1	D	98	ASP	2.7
1	D	88	VAL	2.7
1	2	84	ASP	2.7
1	M	98	ASP	2.7
1	1	97	LYS	2.7
1	F	52	PHE	2.7
1	K	37	LEU	2.7
1	T	86	ILE	2.7
1	X	96	LYS	2.7
1	T	95	SER	2.7
1	T	96	LYS	2.7
1	F	87	HIS	2.7
1	4	88	VAL	2.7
1	D	91	ARG	2.7
1	H	48	VAL	2.6
1	J	88	VAL	2.6
1	N	97	LYS	2.6
1	T	88	VAL	2.6
1	L	91	ARG	2.6
1	I	92	LEU	2.6
1	Y	92	LEU	2.6
1	F	89	GLU	2.6
1	P	87	HIS	2.6
1	4	94	TYR	2.6
1	F	51	GLY	2.6
1	U	49	GLY	2.6
1	I	91	ARG	2.6
1	R	52	PHE	2.6
1	A	90	ASP	2.6
1	H	71	GLU	2.6
1	J	89	GLU	2.6
1	N	91	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	X	36	LEU	2.6
1	W	97	LYS	2.5
1	K	36	LEU	2.5
1	1	93	ILE	2.5
1	F	39	LYS	2.5
1	4	51	GLY	2.5
1	U	46	ASN	2.5
1	O	95	SER	2.5
1	D	46	ASN	2.5
1	J	91	ARG	2.5
1	Q	88	VAL	2.5
1	Y	93	ILE	2.5
1	4	38	GLN	2.5
1	T	55	TRP	2.4
1	X	87	HIS	2.4
1	P	96	LYS	2.4
1	V	97	LYS	2.4
1	X	39	LYS	2.4
1	O	88	VAL	2.4
1	B	91	ARG	2.4
1	U	50	ALA	2.4
1	U	91	ARG	2.4
1	D	94	TYR	2.4
1	V	90	ASP	2.4
1	P	52	PHE	2.4
1	P	50	ALA	2.4
1	K	13	THR	2.4
1	L	40	TYR	2.4
1	M	53	ASP	2.4
1	H	92	LEU	2.4
1	L	86	ILE	2.4
1	4	87	HIS	2.4
1	Q	97	LYS	2.3
1	W	52	PHE	2.3
1	P	55	TRP	2.3
1	4	41	GLU	2.3
1	S	92	LEU	2.3
1	D	13	THR	2.3
1	Z	53	ASP	2.3
1	O	49	GLY	2.3
1	W	96	LYS	2.3
1	Z	22	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	89	GLU	2.3
1	D	52	PHE	2.3
1	2	85	THR	2.3
1	V	93	ILE	2.3
1	4	55	TRP	2.2
1	K	95	SER	2.2
1	I	87	HIS	2.2
1	Y	89	GLU	2.2
1	D	47	SER	2.2
1	K	47	SER	2.2
1	C	89	GLU	2.2
1	F	46	ASN	2.2
1	Z	23	LYS	2.2
1	K	89	GLU	2.2
1	L	38	GLN	2.2
1	3	52	PHE	2.2
1	C	52	PHE	2.2
1	P	48	VAL	2.2
1	W	86	ILE	2.2
1	E	36	LEU	2.2
1	F	36	LEU	2.2
1	O	85	THR	2.2
1	U	90	ASP	2.1
1	U	52	PHE	2.1
1	W	83	ILE	2.1
1	3	13	THR	2.1
1	G	94	TYR	2.1
1	I	68	LEU	2.1
1	U	47	SER	2.1
1	P	46	ASN	2.1
1	D	71	GLU	2.1
1	D	9	THR	2.1
1	F	9	THR	2.1
1	S	88	VAL	2.1
1	D	93	ILE	2.1
1	S	91	ARG	2.1
1	3	50	ALA	2.1
1	P	45	ASP	2.1
1	4	9	THR	2.1
1	Q	52	PHE	2.1
1	F	37	LEU	2.1
1	R	53	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	4	96	LYS	2.1
1	V	87	HIS	2.1
1	E	96	LYS	2.0
1	Z	90	ASP	2.1
1	K	55	TRP	2.0
1	B	88	VAL	2.0
1	H	51	GLY	2.0
1	W	47	SER	2.0
1	A	92	LEU	2.0
1	G	37	LEU	2.0
1	G	40	TYR	2.0
1	Q	95	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	201	5/5	0.97	0.07	-1.81	51,51,53,58	0

6.5 Other polymers (i)

There are no such residues in this entry.