



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:28 PM GMT

PDB ID : 1GQ2
Title : MALIC ENZYME FROM PIGEON LIVER
Authors : Yang, Z.; Zhang, H.; Liang, T.
Deposited on : 2001-11-19
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

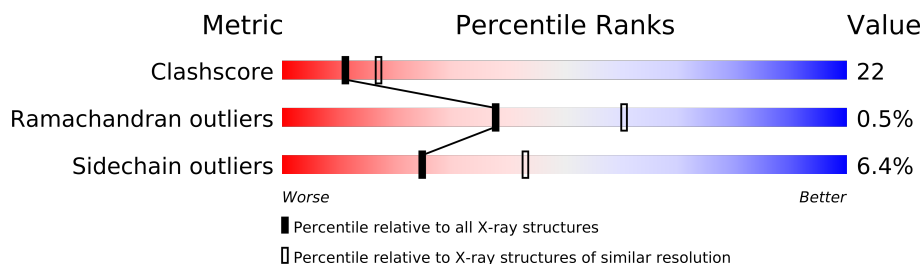
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	555	
1	B	555	
1	C	555	
1	D	555	
1	E	555	
1	F	555	
1	G	555	
1	H	555	
1	I	555	
1	J	555	
1	K	555	
1	L	555	
1	M	555	
1	N	555	
1	O	555	
1	P	555	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 71519 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MALIC ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	B	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	C	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	D	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	E	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	F	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	G	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	H	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	I	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	J	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	K	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	L	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	M	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	N	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	O	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	P	555	Total	C	N	O	S	Se	0	0	0
			4346	2772	742	807	11	14			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	202	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	239	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	248	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	202	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	239	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	248	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
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C	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
D	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	202	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	239	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	248	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
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E	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
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F	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
G	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
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G	248	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
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H	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
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I	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
J	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	202	MSE	MET	MODIFIED RESIDUE	UNP P40927
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J	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
K	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
K	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
K	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
K	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
K	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
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K	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
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L	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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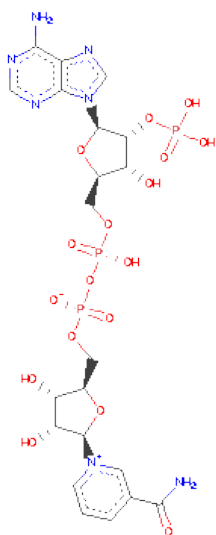
Chain	Residue	Modelled	Actual	Comment	Reference
M	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	202	MSE	MET	MODIFIED RESIDUE	UNP P40927
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M	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
N	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
N	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
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N	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
N	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
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O	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
P	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
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P	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



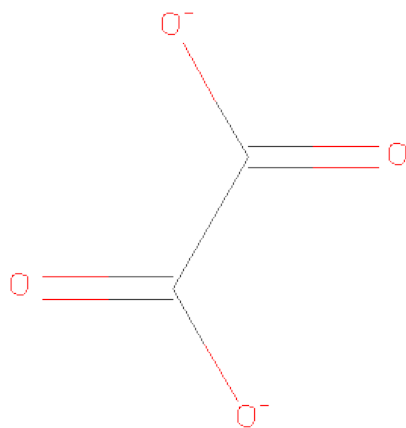
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	M	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	N	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	O	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	P	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C₂O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 2 4	0	0
3	B	1	Total C O 6 2 4	0	0
3	C	1	Total C O 6 2 4	0	0
3	D	1	Total C O 6 2 4	0	0
3	E	1	Total C O 6 2 4	0	0
3	F	1	Total C O 6 2 4	0	0
3	G	1	Total C O 6 2 4	0	0
3	H	1	Total C O 6 2 4	0	0
3	I	1	Total C O 6 2 4	0	0
3	J	1	Total C O 6 2 4	0	0
3	K	1	Total C O 6 2 4	0	0
3	L	1	Total C O 6 2 4	0	0
3	M	1	Total C O 6 2 4	0	0
3	N	1	Total C O 6 2 4	0	0
3	O	1	Total C O 6 2 4	0	0
3	P	1	Total C O 6 2 4	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Mn 1 1	0	0
4	G	1	Total Mn 1 1	0	0
4	J	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	1	Total 1	Mn 1	0	0
4	E	1	Total 1	Mn 1	0	0
4	H	1	Total 1	Mn 1	0	0
4	B	1	Total 1	Mn 1	0	0
4	I	1	Total 1	Mn 1	0	0
4	C	1	Total 1	Mn 1	0	0
4	A	1	Total 1	Mn 1	0	0
4	N	1	Total 1	Mn 1	0	0
4	O	1	Total 1	Mn 1	0	0
4	L	1	Total 1	Mn 1	0	0
4	F	1	Total 1	Mn 1	0	0
4	M	1	Total 1	Mn 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	3	Total 3	Cl 3	0	0
5	G	1	Total 1	Cl 1	0	0
5	J	2	Total 2	Cl 2	0	0
5	K	1	Total 1	Cl 1	0	0
5	E	3	Total 3	Cl 3	0	0
5	H	1	Total 1	Cl 1	0	0
5	B	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	5	Total 5	Cl 5	0	0
5	C	4	Total 4	Cl 4	0	0
5	N	2	Total 2	Cl 2	0	0
5	O	4	Total 4	Cl 4	0	0
5	L	1	Total 1	Cl 1	0	0
5	F	2	Total 2	Cl 2	0	0
5	M	3	Total 3	Cl 3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	5	Total 5	Na 5	0	0
6	G	1	Total 1	Na 1	0	0
6	J	2	Total 2	Na 2	0	0
6	D	2	Total 2	Na 2	0	0
6	K	1	Total 1	Na 1	0	0
6	H	5	Total 5	Na 5	0	0
6	I	2	Total 2	Na 2	0	0
6	C	4	Total 4	Na 4	0	0
6	N	1	Total 1	Na 1	0	0
6	O	4	Total 4	Na 4	0	0
6	L	1	Total 1	Na 1	0	0
6	F	2	Total 2	Na 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	6	Total 6	Na 6	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	35	Total 35	O 35	0	0
7	B	42	Total 42	O 42	0	0
7	C	77	Total 77	O 77	0	0
7	D	49	Total 49	O 49	0	0
7	E	58	Total 58	O 58	0	0
7	F	78	Total 78	O 78	0	0
7	G	65	Total 65	O 65	0	0
7	H	77	Total 77	O 77	0	0
7	I	80	Total 80	O 80	0	0
7	J	63	Total 63	O 63	0	0
7	K	41	Total 41	O 41	0	0
7	L	75	Total 75	O 75	0	0
7	M	81	Total 81	O 81	0	0
7	N	71	Total 71	O 71	0	0
7	O	78	Total 78	O 78	0	0
7	P	79	Total 79	O 79	0	0

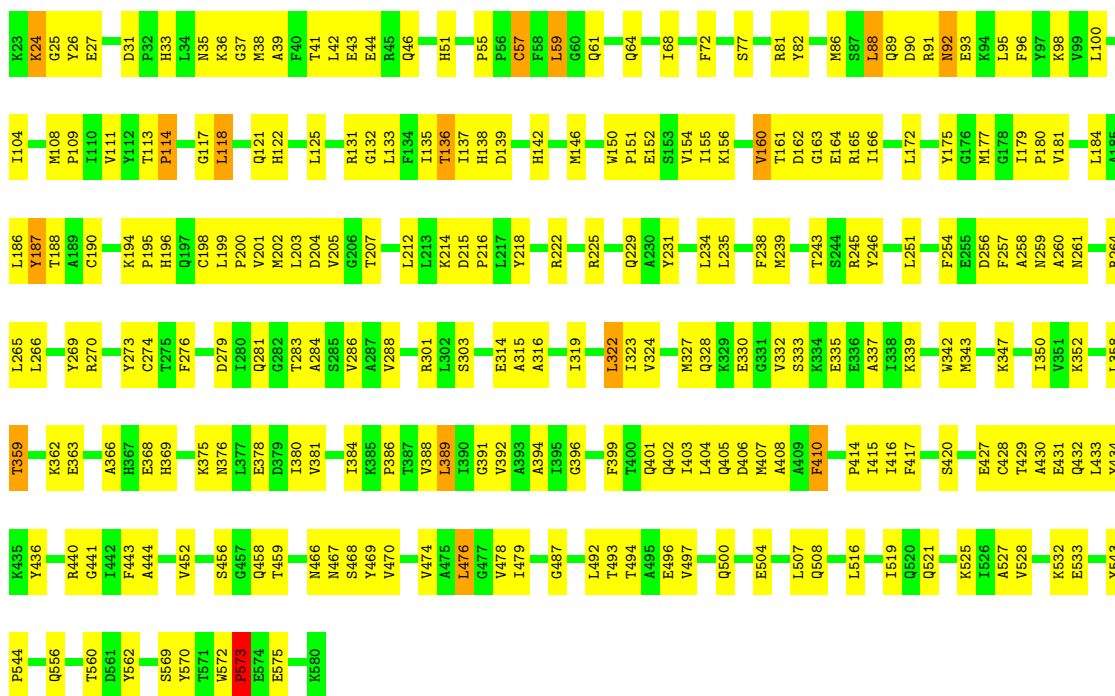
3 Residue-property plots

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.

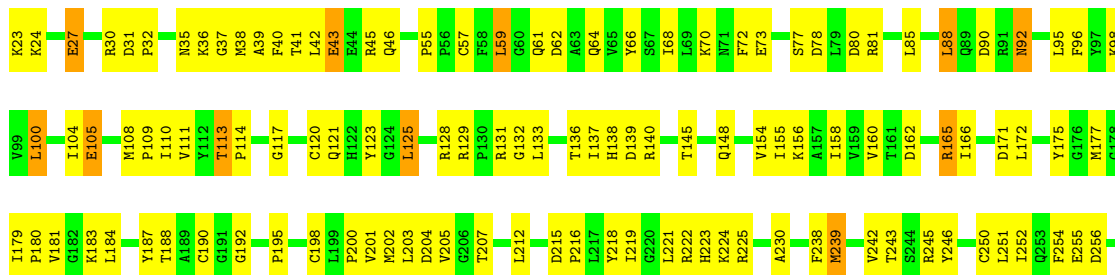
• Molecule 1: MALIC ENZYME

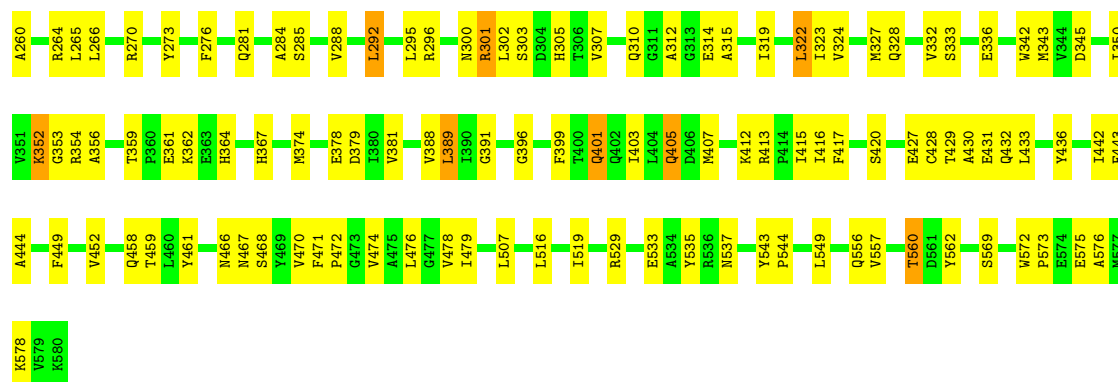
Chain A:



• Molecule 1: MALIC ENZYME

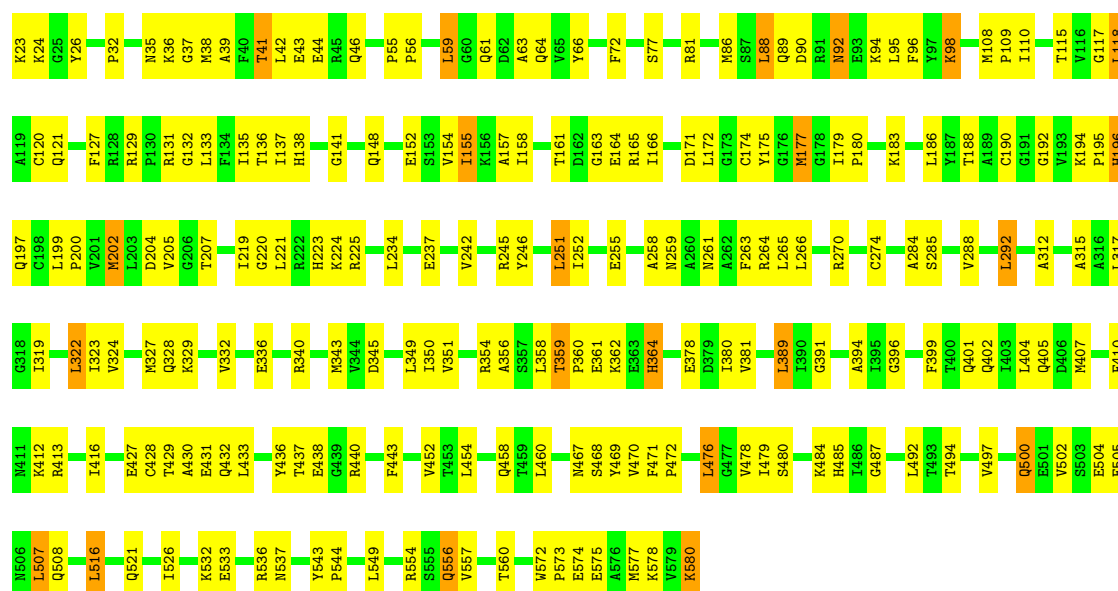
Chain B:





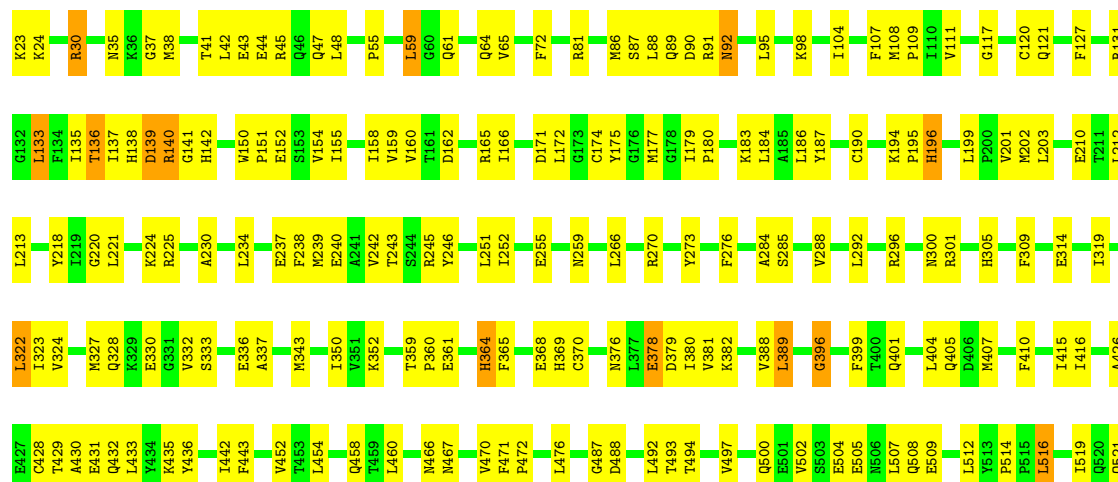
• Molecule 1: MALIC ENZYME

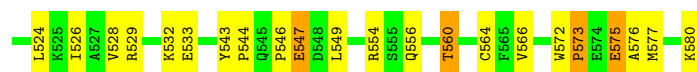
Chain C:



• Molecule 1: MALIC ENZYME

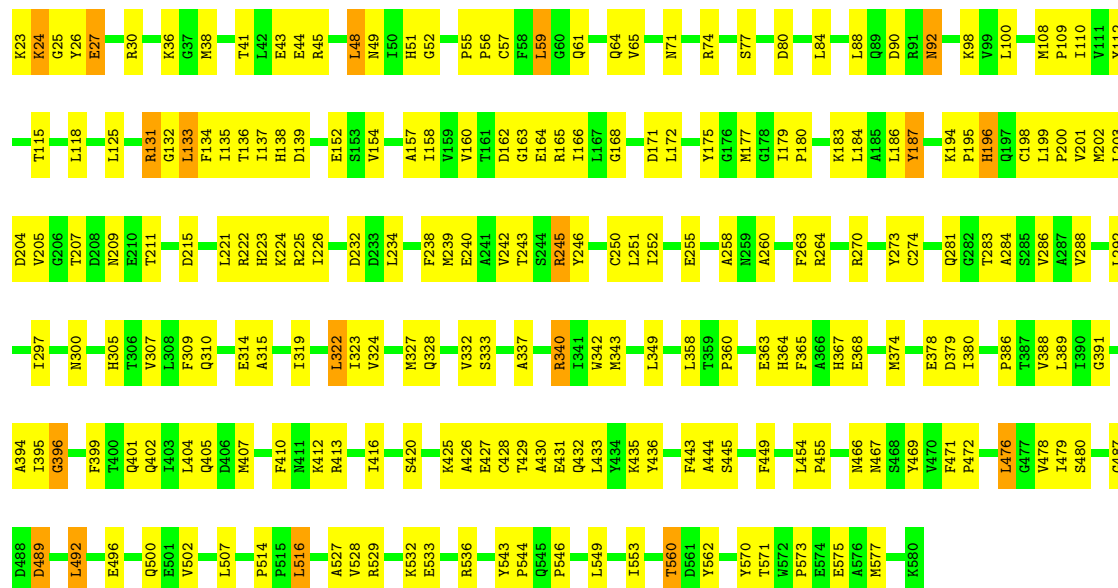
Chain D:





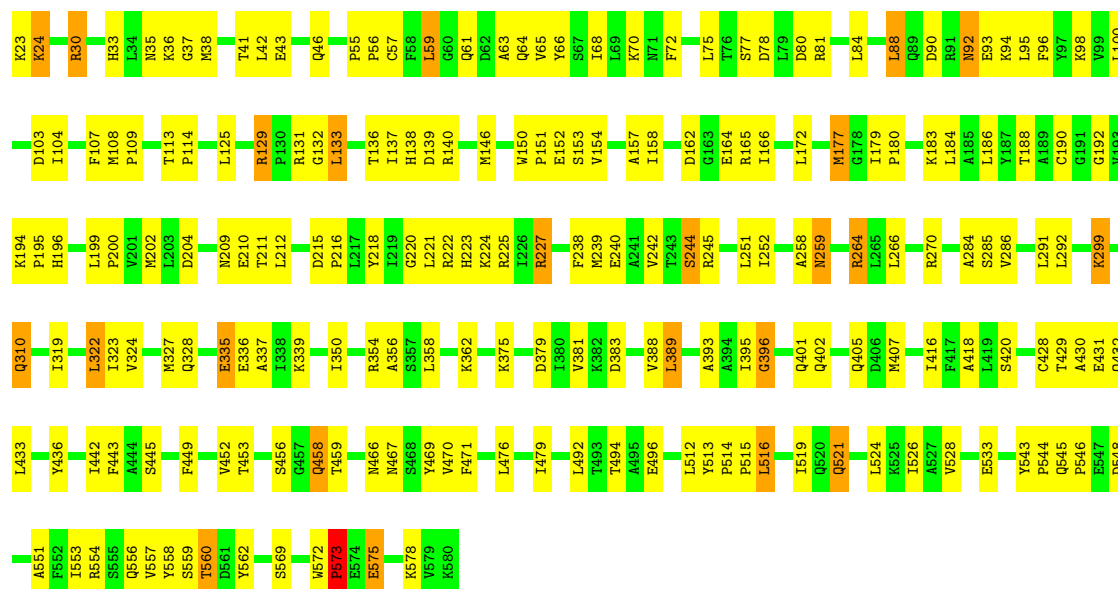
• Molecule 1: MALIC ENZYME

Chain E:



• Molecule 1: MALIC ENZYME

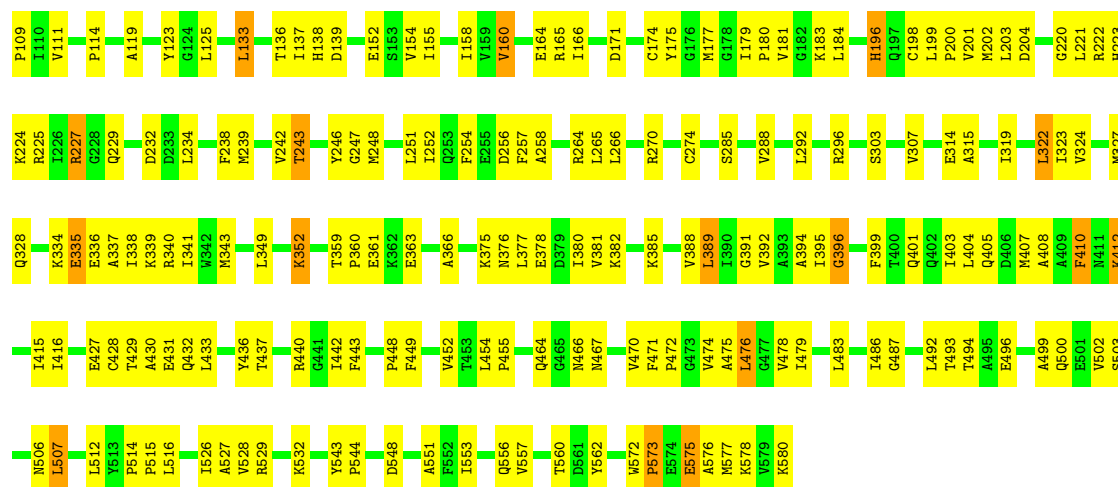
Chain F:



• Molecule 1: MALIC ENZYME

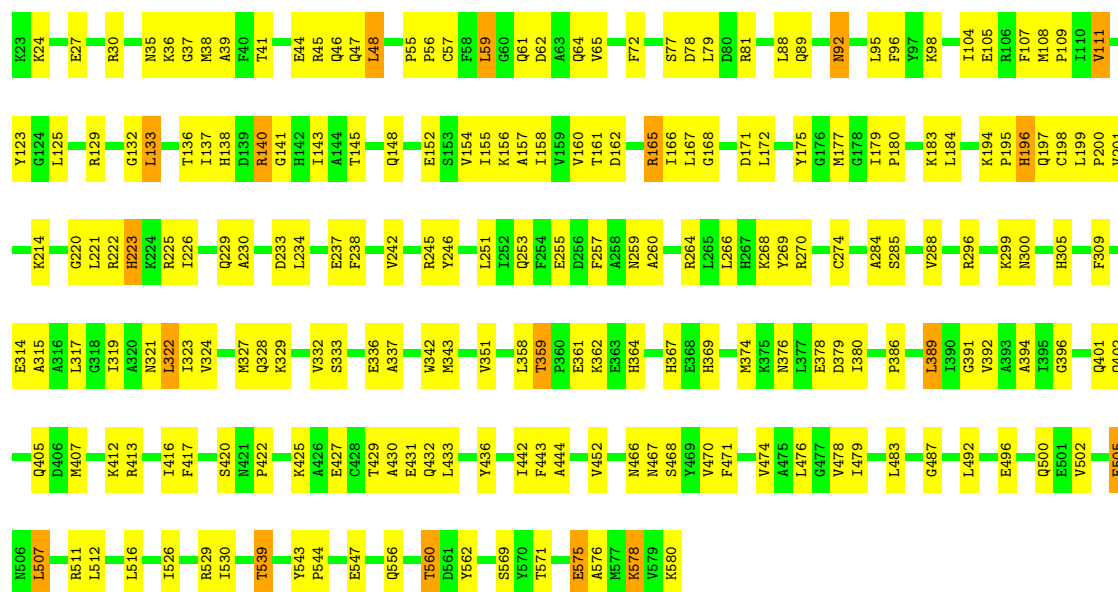
Chain G:





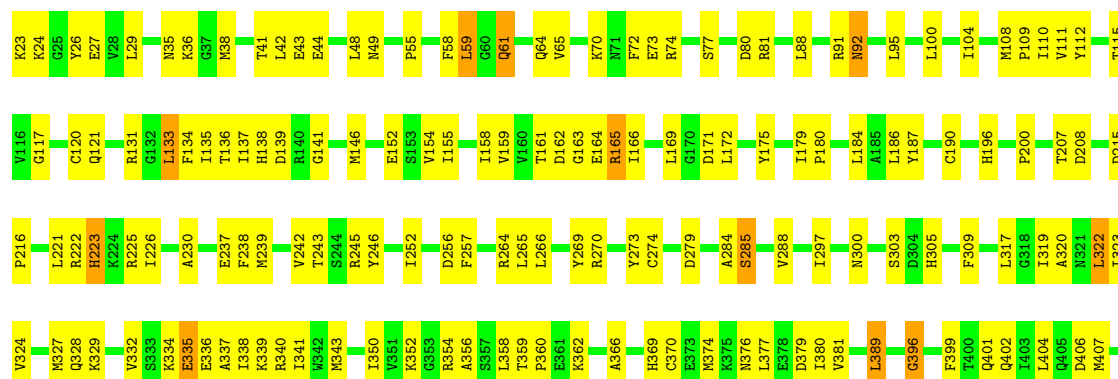
• Molecule 1: MALIC ENZYME

Chain H:



• Molecule 1: MALIC ENZYME

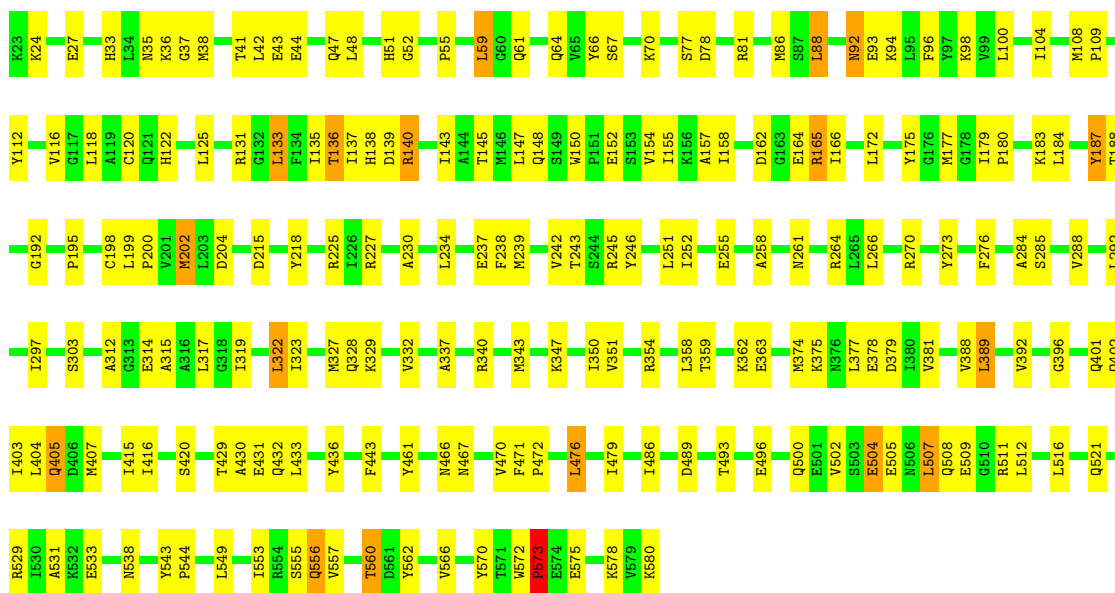
Chain I:





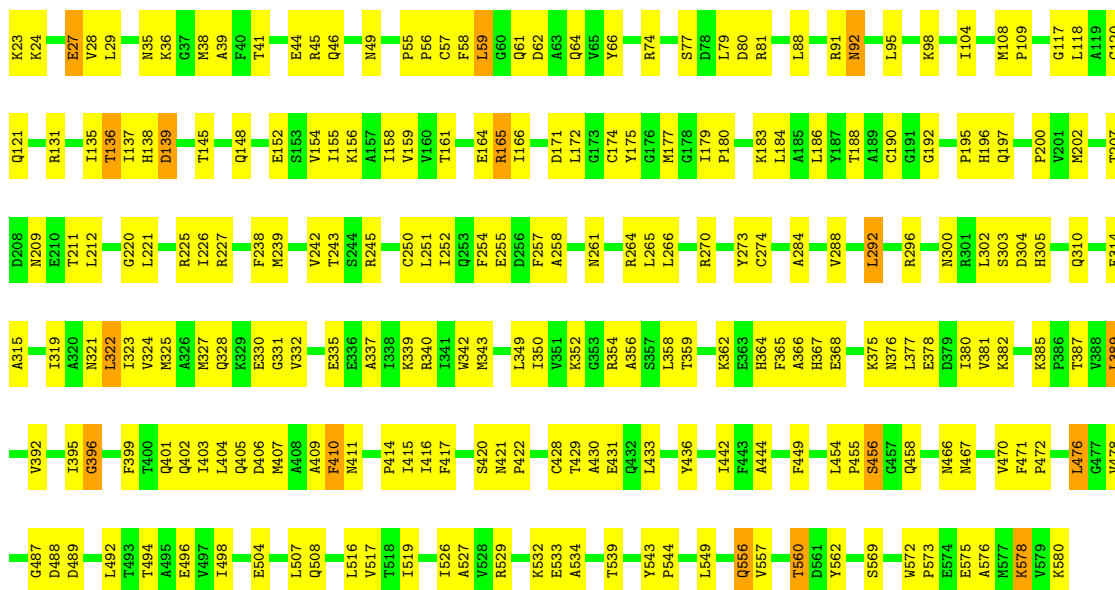
• Molecule 1: MALIC ENZYME

Chain J:



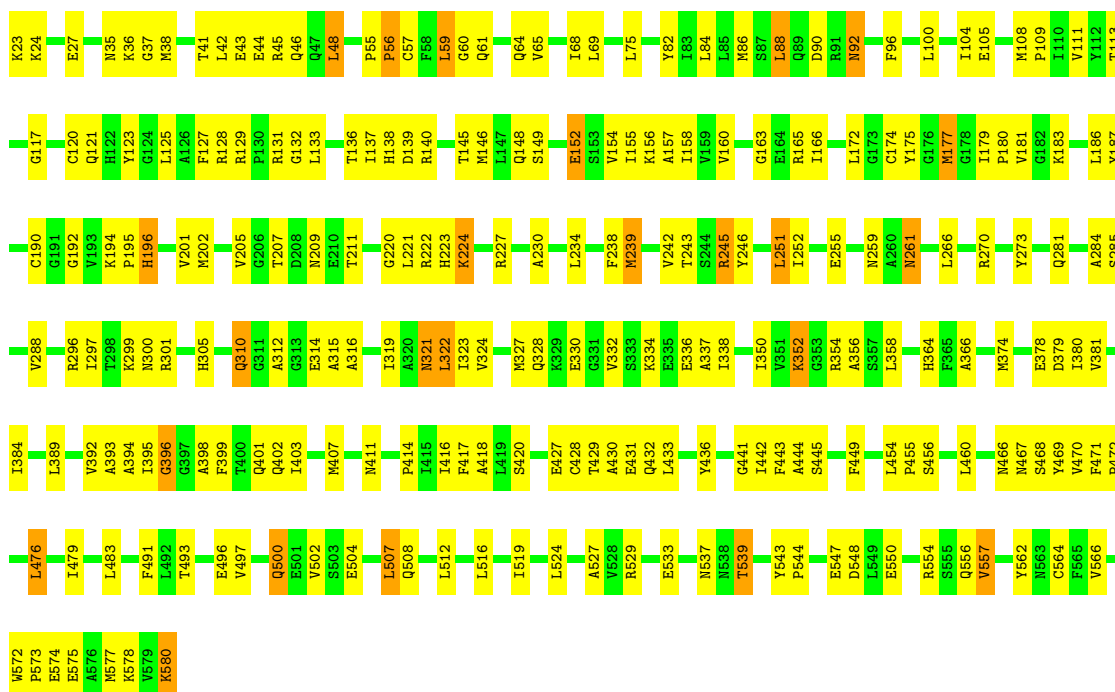
• Molecule 1: MALIC ENZYME

Chain K:



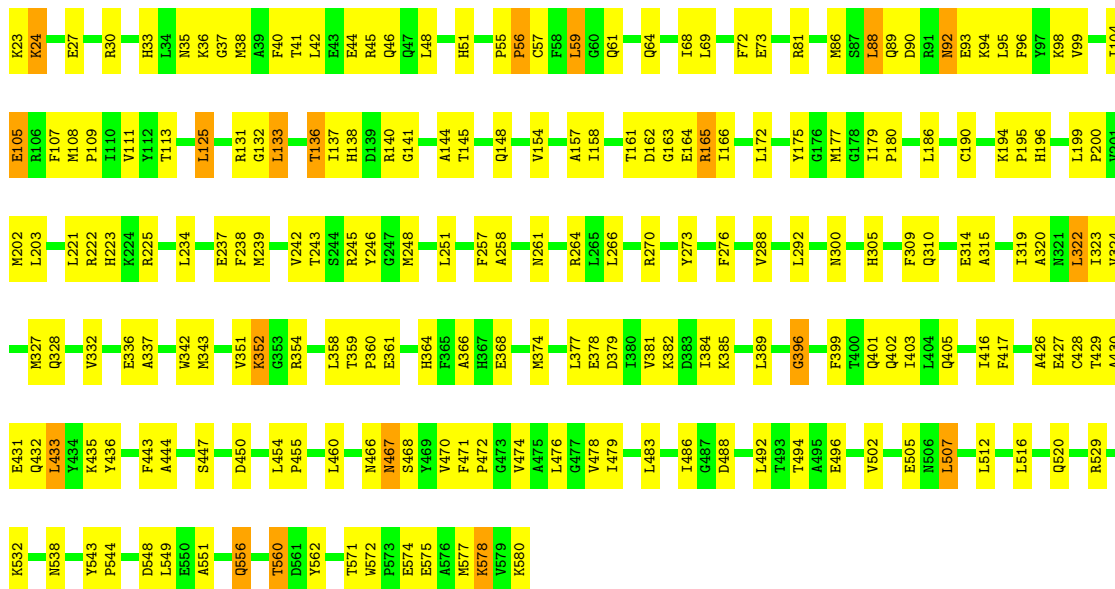
• Molecule 1: MALIC ENZYME

Chain L:



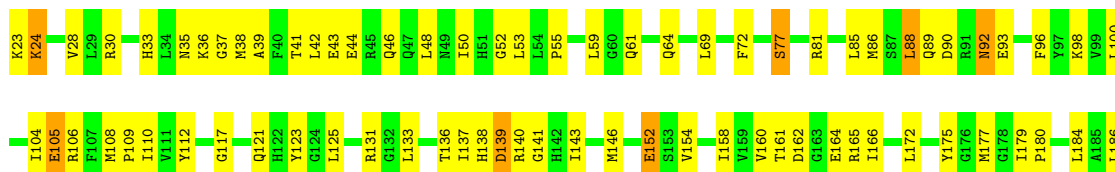
• Molecule 1: MALIC ENZYME

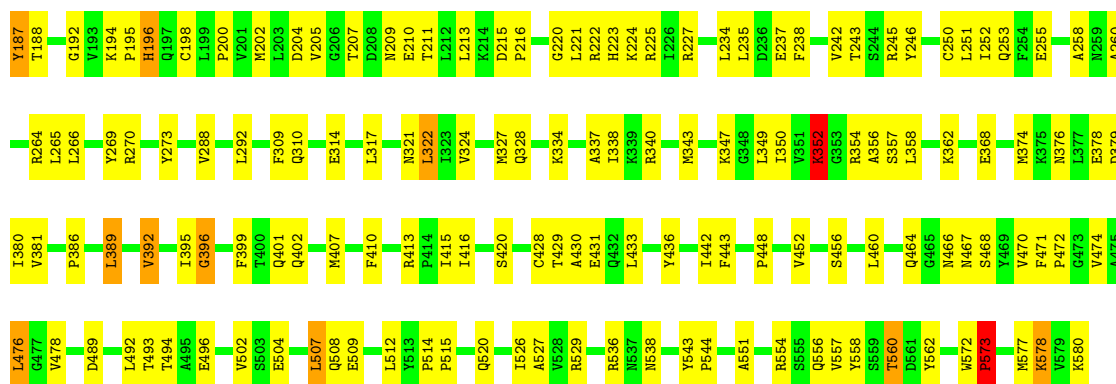
Chain M:



• Molecule 1: MALIC ENZYME

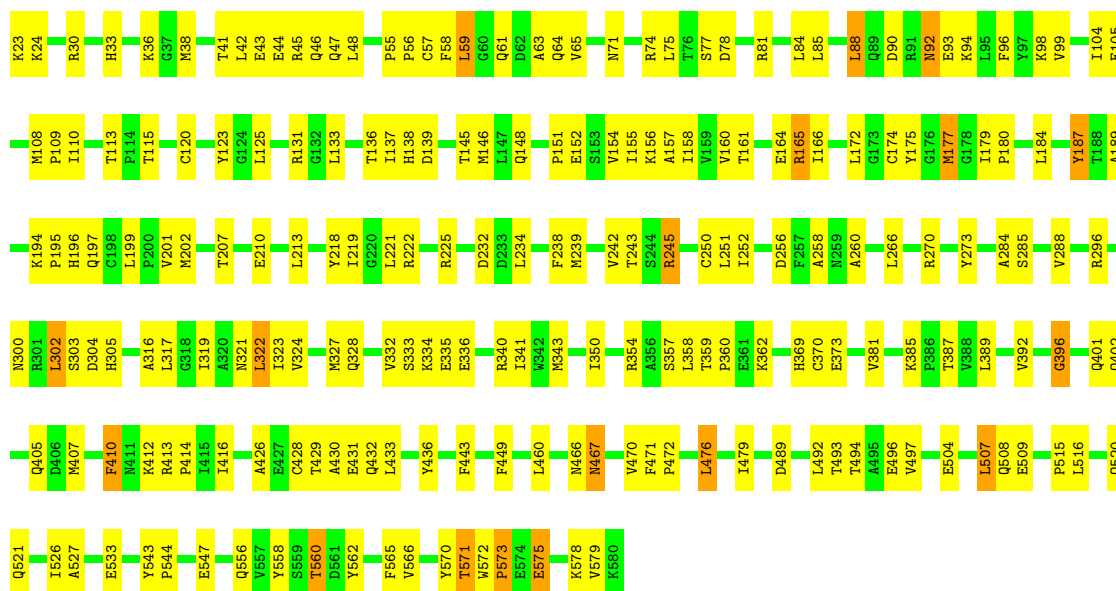
Chain N:





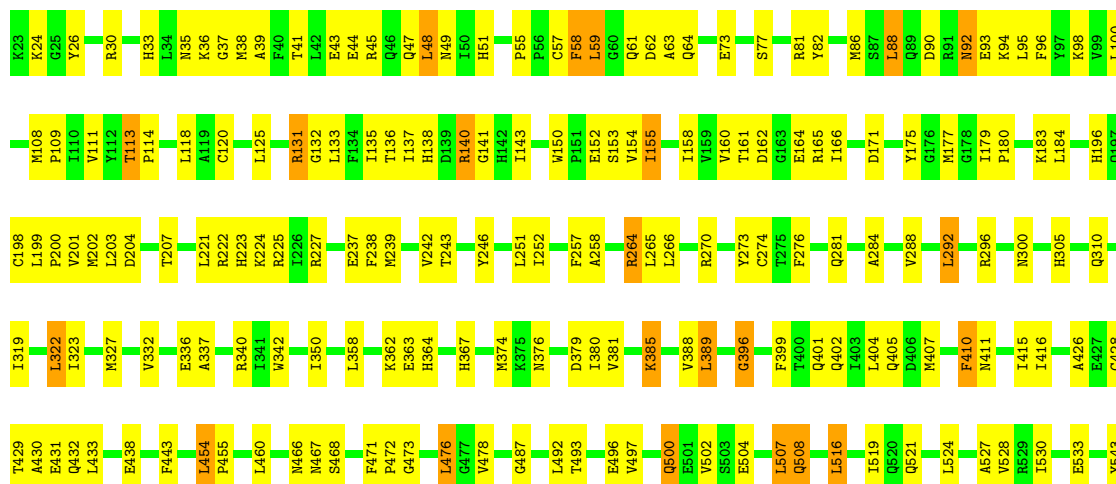
• Molecule 1: MALIC ENZYME

Chain O:



• Molecule 1: MALIC ENZYME

Chain P:





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	124.15Å 140.86Å 167.08Å 90.05° 87.16° 75.63°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	83.0 (10.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	71519	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, NA, NAP, MN, CL

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	0.39	0/4420	0.61	0/5962
1	B	0.38	0/4420	0.61	0/5962
1	C	0.40	0/4420	0.62	1/5962 (0.0%)
1	D	0.40	0/4420	0.62	0/5962
1	E	0.38	0/4420	0.61	0/5962
1	F	0.40	0/4420	0.63	1/5962 (0.0%)
1	G	0.39	0/4420	0.62	0/5962
1	H	0.41	0/4420	0.62	0/5962
1	I	0.40	0/4420	0.63	0/5962
1	J	0.40	0/4420	0.61	0/5962
1	K	0.39	0/4420	0.61	0/5962
1	L	0.39	0/4420	0.62	0/5962
1	M	0.41	0/4420	0.63	0/5962
1	N	0.40	0/4420	0.63	1/5962 (0.0%)
1	O	0.39	0/4420	0.62	0/5962
1	P	0.39	0/4421	0.62	0/5962
All	All	0.39	0/70721	0.62	3/95392 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	LEU	CA-CB-CG	5.19	127.24	115.30
1	F	310	GLN	N-CA-C	-5.11	97.21	111.00
1	N	352	LYS	N-CA-C	5.09	124.75	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4345	0	4366	230	0
1	B	4345	0	4366	216	0
1	C	4345	0	4366	219	0
1	D	4345	0	4366	196	0
1	E	4345	0	4366	189	0
1	F	4345	0	4366	193	0
1	G	4345	0	4366	197	0
1	H	4345	0	4366	178	0
1	I	4345	0	4366	181	0
1	J	4345	0	4366	200	0
1	K	4345	0	4366	208	0
1	L	4345	0	4366	227	0
1	M	4345	0	4366	188	0
1	N	4345	0	4366	207	0
1	O	4345	0	4366	226	0
1	P	4346	0	4366	194	0
2	A	48	0	25	4	0
2	B	48	0	25	4	0
2	C	48	0	25	2	0
2	D	48	0	25	2	0
2	E	48	0	25	3	0
2	F	48	0	25	2	0
2	G	48	0	25	3	0
2	H	48	0	25	3	0
2	I	48	0	25	3	0
2	J	48	0	25	4	0
2	K	48	0	25	5	0
2	L	48	0	25	5	0
2	M	48	0	25	3	0
2	N	48	0	25	3	0
2	O	48	0	25	2	0
2	P	48	0	25	1	0
3	A	6	0	0	1	0
3	B	6	0	0	1	0
3	C	6	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	0	2	0
3	E	6	0	0	1	0
3	F	6	0	0	1	0
3	G	6	0	0	1	0
3	H	6	0	0	1	0
3	I	6	0	0	0	0
3	J	6	0	0	1	0
3	K	6	0	0	1	0
3	L	6	0	0	1	0
3	M	6	0	0	0	0
3	N	6	0	0	1	0
3	O	6	0	0	0	0
3	P	6	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
5	B	1	0	0	0	0
5	C	4	0	0	1	0
5	E	3	0	0	1	0
5	F	2	0	0	1	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	5	0	0	1	0
5	J	2	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	3	0	0	1	0
5	N	2	0	0	1	0
5	O	4	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	3	0	0	3	0
6	C	4	0	0	0	0
6	D	2	0	0	0	0
6	F	2	0	0	0	0
6	G	1	0	0	0	0
6	H	5	0	0	0	0
6	I	2	0	0	0	0
6	J	2	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	6	0	0	0	0
6	N	1	0	0	0	0
6	O	4	0	0	0	0
6	P	5	0	0	0	0
7	A	35	0	0	6	0
7	B	42	0	0	6	0
7	C	77	0	0	7	0
7	D	49	0	0	2	0
7	E	58	0	0	5	0
7	F	78	0	0	6	0
7	G	65	0	0	6	0
7	H	77	0	0	7	0
7	I	80	0	0	7	0
7	J	63	0	0	3	0
7	K	41	0	0	5	0
7	L	75	0	0	7	0
7	M	81	0	0	7	0
7	N	71	0	0	7	0
7	O	78	0	0	8	0
7	P	79	0	0	4	0
All	All	71519	0	70256	3151	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

The worst 5 of 3151 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:136:THR:HG22	1:H:138:HIS:H	1.08	1.17
1:N:136:THR:HG22	1:N:138:HIS:H	1.04	1.17
1:K:98:LYS:HD3	1:K:560:THR:HG21	1.30	1.14
1:F:136:THR:HG22	1:F:138:HIS:H	1.10	1.13
1:B:136:THR:HG22	1:B:138:HIS:H	1.06	1.13

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	553/555 (100%)	524 (95%)	23 (4%)	6 (1%)	21	34
1	B	553/555 (100%)	530 (96%)	21 (4%)	2 (0%)	43	66
1	C	553/555 (100%)	530 (96%)	21 (4%)	2 (0%)	43	66
1	D	553/555 (100%)	530 (96%)	21 (4%)	2 (0%)	43	66
1	E	553/555 (100%)	530 (96%)	22 (4%)	1 (0%)	56	79
1	F	553/555 (100%)	529 (96%)	22 (4%)	2 (0%)	43	66
1	G	553/555 (100%)	531 (96%)	19 (3%)	3 (0%)	38	60
1	H	553/555 (100%)	534 (97%)	16 (3%)	3 (0%)	38	60
1	I	553/555 (100%)	535 (97%)	17 (3%)	1 (0%)	56	79
1	J	553/555 (100%)	531 (96%)	19 (3%)	3 (0%)	38	60
1	K	553/555 (100%)	524 (95%)	27 (5%)	2 (0%)	43	66
1	L	553/555 (100%)	534 (97%)	14 (2%)	5 (1%)	25	42
1	M	553/555 (100%)	528 (96%)	23 (4%)	2 (0%)	43	66
1	N	553/555 (100%)	528 (96%)	21 (4%)	4 (1%)	30	50
1	O	553/555 (100%)	531 (96%)	18 (3%)	4 (1%)	30	50
1	P	553/555 (100%)	532 (96%)	18 (3%)	3 (0%)	38	60
All	All	8848/8880 (100%)	8481 (96%)	322 (4%)	45 (0%)	38	60

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	GLY
1	A	573	PRO
1	B	396	GLY
1	C	396	GLY
1	D	396	GLY

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	467/453 (103%)	438 (94%)	29 (6%)	26	45
1	B	467/453 (103%)	438 (94%)	29 (6%)	26	45
1	C	467/453 (103%)	437 (94%)	30 (6%)	25	43
1	D	467/453 (103%)	439 (94%)	28 (6%)	27	47
1	E	467/453 (103%)	431 (92%)	36 (8%)	18	33
1	F	467/453 (103%)	434 (93%)	33 (7%)	21	37
1	G	467/453 (103%)	441 (94%)	26 (6%)	30	51
1	H	467/453 (103%)	437 (94%)	30 (6%)	25	43
1	I	467/453 (103%)	439 (94%)	28 (6%)	27	47
1	J	467/453 (103%)	437 (94%)	30 (6%)	25	43
1	K	467/453 (103%)	443 (95%)	24 (5%)	33	57
1	L	467/453 (103%)	437 (94%)	30 (6%)	25	43
1	M	467/453 (103%)	432 (92%)	35 (8%)	19	34
1	N	467/453 (103%)	443 (95%)	24 (5%)	33	57
1	O	467/453 (103%)	437 (94%)	30 (6%)	25	43
1	P	467/453 (103%)	430 (92%)	37 (8%)	18	31
All	All	7472/7248 (103%)	6993 (94%)	479 (6%)	25	43

5 of 479 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	62	ASP
1	I	578	LYS
1	P	48	LEU
1	H	196	HIS
1	I	59	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 286 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	92	ASN
1	I	467	ASN
1	O	405	GLN
1	H	271	ASN
1	H	545	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 117 ligands modelled in this entry, 85 are monoatomic - leaving 32 for Mogul analysis.

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	NAP	A	1581	-	52,52,52	1.66	11 (21%)	80,80,80	2.00	14 (17%)
3	OXL	A	1583	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	B	1581	-	52,52,52	1.65	10 (19%)	80,80,80	2.00	14 (17%)
3	OXL	B	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	C	1581	-	52,52,52	1.76	11 (21%)	80,80,80	2.00	15 (18%)
3	OXL	C	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	D	1581	-	52,52,52	1.75	11 (21%)	80,80,80	2.03	15 (18%)
3	OXL	D	1582	4,6	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	E	1581	-	52,52,52	1.77	10 (19%)	80,80,80	2.01	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXL	E	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	F	1581	-	52,52,52	1.71	11 (21%)	80,80,80	2.07	16 (20%)
3	OXL	F	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	G	1581	-	52,52,52	1.67	10 (19%)	80,80,80	2.01	15 (18%)
3	OXL	G	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	H	1581	-	52,52,52	1.71	12 (23%)	80,80,80	2.04	15 (18%)
3	OXL	H	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	I	1581	-	52,52,52	1.79	12 (23%)	80,80,80	2.05	14 (17%)
3	OXL	I	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	J	1581	-	52,52,52	1.75	10 (19%)	80,80,80	2.06	16 (20%)
3	OXL	J	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	K	1581	-	52,52,52	1.75	11 (21%)	80,80,80	2.06	15 (18%)
3	OXL	K	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	L	1581	-	52,52,52	1.80	12 (23%)	80,80,80	2.03	14 (17%)
3	OXL	L	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	M	1581	-	52,52,52	1.65	10 (19%)	80,80,80	1.98	15 (18%)
3	OXL	M	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	N	1581	-	52,52,52	1.73	10 (19%)	80,80,80	2.10	14 (17%)
3	OXL	N	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	O	1581	-	52,52,52	1.71	11 (21%)	80,80,80	2.06	14 (17%)
3	OXL	O	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	P	1581	-	52,52,52	1.72	11 (21%)	80,80,80	1.99	14 (17%)
3	OXL	P	1582	4	0,5,5	0.00	-	0,6,6	0.00	-

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	NAP	A	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	A	1583	4	-	0/0/4/4	0/0/0/0
2	NAP	B	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	B	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	C	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	C	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	D	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	D	1582	4,6	-	0/0/4/4	0/0/0/0
2	NAP	E	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	E	1582	4	-	0/0/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	F	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	F	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	G	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	G	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	H	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	H	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	I	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	I	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	J	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	J	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	K	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	K	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	L	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	L	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	M	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	M	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	N	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	N	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	O	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	O	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	P	1581	-	-	0/35/67/67	0/3/5/5
3	OXL	P	1582	4	-	0/0/4/4	0/0/0/0

The worst 5 of 173 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1581	NAP	C2N-N1N	6.60	1.43	1.35
2	J	1581	NAP	C2N-N1N	6.52	1.43	1.35
2	P	1581	NAP	C2N-N1N	6.35	1.43	1.35
2	E	1581	NAP	C2N-N1N	6.35	1.43	1.35
2	D	1581	NAP	C2N-N1N	6.19	1.43	1.35

The worst 5 of 234 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1581	NAP	N3A-C2A-N1A	-10.27	120.13	128.71
2	J	1581	NAP	N3A-C2A-N1A	-9.95	120.39	128.71
2	G	1581	NAP	N3A-C2A-N1A	-9.91	120.43	128.71
2	L	1581	NAP	N3A-C2A-N1A	-9.85	120.47	128.71
2	H	1581	NAP	N3A-C2A-N1A	-9.81	120.50	128.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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.