wwPDB X-ray Structure Validation Summary Report (i)

Sep 23, 2023 – 04:29 PM EDT

PDB ID	:	5TJR
Title	:	X-ray Crystal structure of a methylmalonate semialdehyde dehydrogenase from Pseudomonas sp. AAC
Authors	:	Peat, T.S.; Newman, J.
Deposited on	:	2016-10-05
Resolution	:	2.95 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

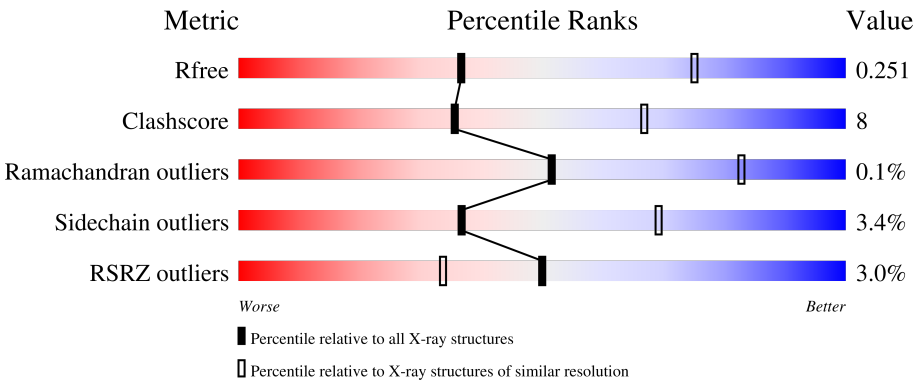
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	A	531	2%, 71%, 14%, •, 13%
1	B	531	2%, 69%, 16%, •, 12%
1	C	531	3%, 70%, 16%, •, 13%
1	D	531	4%, 69%, 18%, •, 12%
1	E	531	3%, 71%, 14%, •, 14%

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Mol	Chain	Length	Quality of chain
1	F	531	2% 69% 15% • 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20975 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 Methylmalonate-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	460	3471	2210	600	646	15	0	0	0
1	B	465	3525	2249	607	654	15	0	1	0
1	C	461	3455	2196	601	643	15	0	0	0
1	D	468	3535	2252	613	655	15	0	0	0
1	E	455	3408	2170	590	633	15	0	0	0
1	F	454	3430	2185	594	636	15	0	0	0

There are 198 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	initiating methionine	UNP A0A081YAY7
A	-31	ARG	-	expression tag	UNP A0A081YAY7
A	-30	GLY	-	expression tag	UNP A0A081YAY7
A	-29	SER	-	expression tag	UNP A0A081YAY7
A	-28	HIS	-	expression tag	UNP A0A081YAY7
A	-27	HIS	-	expression tag	UNP A0A081YAY7
A	-26	HIS	-	expression tag	UNP A0A081YAY7
A	-25	HIS	-	expression tag	UNP A0A081YAY7
A	-24	HIS	-	expression tag	UNP A0A081YAY7
A	-23	HIS	-	expression tag	UNP A0A081YAY7
A	-22	GLY	-	expression tag	UNP A0A081YAY7
A	-21	MET	-	expression tag	UNP A0A081YAY7
A	-20	ALA	-	expression tag	UNP A0A081YAY7
A	-19	SER	-	expression tag	UNP A0A081YAY7
A	-18	MET	-	expression tag	UNP A0A081YAY7
A	-17	THR	-	expression tag	UNP A0A081YAY7
A	-16	GLY	-	expression tag	UNP A0A081YAY7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	expression tag	UNP A0A081YAY7
A	-14	GLN	-	expression tag	UNP A0A081YAY7
A	-13	GLN	-	expression tag	UNP A0A081YAY7
A	-12	MET	-	expression tag	UNP A0A081YAY7
A	-11	GLY	-	expression tag	UNP A0A081YAY7
A	-10	ARG	-	expression tag	UNP A0A081YAY7
A	-9	ASP	-	expression tag	UNP A0A081YAY7
A	-8	LEU	-	expression tag	UNP A0A081YAY7
A	-7	TYR	-	expression tag	UNP A0A081YAY7
A	-6	ASP	-	expression tag	UNP A0A081YAY7
A	-5	ASP	-	expression tag	UNP A0A081YAY7
A	-4	ASP	-	expression tag	UNP A0A081YAY7
A	-3	ASP	-	expression tag	UNP A0A081YAY7
A	-2	LYS	-	expression tag	UNP A0A081YAY7
A	-1	GLY	-	expression tag	UNP A0A081YAY7
A	0	SER	-	expression tag	UNP A0A081YAY7
B	-32	MET	-	initiating methionine	UNP A0A081YAY7
B	-31	ARG	-	expression tag	UNP A0A081YAY7
B	-30	GLY	-	expression tag	UNP A0A081YAY7
B	-29	SER	-	expression tag	UNP A0A081YAY7
B	-28	HIS	-	expression tag	UNP A0A081YAY7
B	-27	HIS	-	expression tag	UNP A0A081YAY7
B	-26	HIS	-	expression tag	UNP A0A081YAY7
B	-25	HIS	-	expression tag	UNP A0A081YAY7
B	-24	HIS	-	expression tag	UNP A0A081YAY7
B	-23	HIS	-	expression tag	UNP A0A081YAY7
B	-22	GLY	-	expression tag	UNP A0A081YAY7
B	-21	MET	-	expression tag	UNP A0A081YAY7
B	-20	ALA	-	expression tag	UNP A0A081YAY7
B	-19	SER	-	expression tag	UNP A0A081YAY7
B	-18	MET	-	expression tag	UNP A0A081YAY7
B	-17	THR	-	expression tag	UNP A0A081YAY7
B	-16	GLY	-	expression tag	UNP A0A081YAY7
B	-15	GLY	-	expression tag	UNP A0A081YAY7
B	-14	GLN	-	expression tag	UNP A0A081YAY7
B	-13	GLN	-	expression tag	UNP A0A081YAY7
B	-12	MET	-	expression tag	UNP A0A081YAY7
B	-11	GLY	-	expression tag	UNP A0A081YAY7
B	-10	ARG	-	expression tag	UNP A0A081YAY7
B	-9	ASP	-	expression tag	UNP A0A081YAY7
B	-8	LEU	-	expression tag	UNP A0A081YAY7
B	-7	TYR	-	expression tag	UNP A0A081YAY7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	ASP	-	expression tag	UNP A0A081YAY7
B	-5	ASP	-	expression tag	UNP A0A081YAY7
B	-4	ASP	-	expression tag	UNP A0A081YAY7
B	-3	ASP	-	expression tag	UNP A0A081YAY7
B	-2	LYS	-	expression tag	UNP A0A081YAY7
B	-1	GLY	-	expression tag	UNP A0A081YAY7
B	0	SER	-	expression tag	UNP A0A081YAY7
C	-32	MET	-	initiating methionine	UNP A0A081YAY7
C	-31	ARG	-	expression tag	UNP A0A081YAY7
C	-30	GLY	-	expression tag	UNP A0A081YAY7
C	-29	SER	-	expression tag	UNP A0A081YAY7
C	-28	HIS	-	expression tag	UNP A0A081YAY7
C	-27	HIS	-	expression tag	UNP A0A081YAY7
C	-26	HIS	-	expression tag	UNP A0A081YAY7
C	-25	HIS	-	expression tag	UNP A0A081YAY7
C	-24	HIS	-	expression tag	UNP A0A081YAY7
C	-23	HIS	-	expression tag	UNP A0A081YAY7
C	-22	GLY	-	expression tag	UNP A0A081YAY7
C	-21	MET	-	expression tag	UNP A0A081YAY7
C	-20	ALA	-	expression tag	UNP A0A081YAY7
C	-19	SER	-	expression tag	UNP A0A081YAY7
C	-18	MET	-	expression tag	UNP A0A081YAY7
C	-17	THR	-	expression tag	UNP A0A081YAY7
C	-16	GLY	-	expression tag	UNP A0A081YAY7
C	-15	GLY	-	expression tag	UNP A0A081YAY7
C	-14	GLN	-	expression tag	UNP A0A081YAY7
C	-13	GLN	-	expression tag	UNP A0A081YAY7
C	-12	MET	-	expression tag	UNP A0A081YAY7
C	-11	GLY	-	expression tag	UNP A0A081YAY7
C	-10	ARG	-	expression tag	UNP A0A081YAY7
C	-9	ASP	-	expression tag	UNP A0A081YAY7
C	-8	LEU	-	expression tag	UNP A0A081YAY7
C	-7	TYR	-	expression tag	UNP A0A081YAY7
C	-6	ASP	-	expression tag	UNP A0A081YAY7
C	-5	ASP	-	expression tag	UNP A0A081YAY7
C	-4	ASP	-	expression tag	UNP A0A081YAY7
C	-3	ASP	-	expression tag	UNP A0A081YAY7
C	-2	LYS	-	expression tag	UNP A0A081YAY7
C	-1	GLY	-	expression tag	UNP A0A081YAY7
C	0	SER	-	expression tag	UNP A0A081YAY7
D	-32	MET	-	initiating methionine	UNP A0A081YAY7
D	-31	ARG	-	expression tag	UNP A0A081YAY7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-30	GLY	-	expression tag	UNP A0A081YAY7
D	-29	SER	-	expression tag	UNP A0A081YAY7
D	-28	HIS	-	expression tag	UNP A0A081YAY7
D	-27	HIS	-	expression tag	UNP A0A081YAY7
D	-26	HIS	-	expression tag	UNP A0A081YAY7
D	-25	HIS	-	expression tag	UNP A0A081YAY7
D	-24	HIS	-	expression tag	UNP A0A081YAY7
D	-23	HIS	-	expression tag	UNP A0A081YAY7
D	-22	GLY	-	expression tag	UNP A0A081YAY7
D	-21	MET	-	expression tag	UNP A0A081YAY7
D	-20	ALA	-	expression tag	UNP A0A081YAY7
D	-19	SER	-	expression tag	UNP A0A081YAY7
D	-18	MET	-	expression tag	UNP A0A081YAY7
D	-17	THR	-	expression tag	UNP A0A081YAY7
D	-16	GLY	-	expression tag	UNP A0A081YAY7
D	-15	GLY	-	expression tag	UNP A0A081YAY7
D	-14	GLN	-	expression tag	UNP A0A081YAY7
D	-13	GLN	-	expression tag	UNP A0A081YAY7
D	-12	MET	-	expression tag	UNP A0A081YAY7
D	-11	GLY	-	expression tag	UNP A0A081YAY7
D	-10	ARG	-	expression tag	UNP A0A081YAY7
D	-9	ASP	-	expression tag	UNP A0A081YAY7
D	-8	LEU	-	expression tag	UNP A0A081YAY7
D	-7	TYR	-	expression tag	UNP A0A081YAY7
D	-6	ASP	-	expression tag	UNP A0A081YAY7
D	-5	ASP	-	expression tag	UNP A0A081YAY7
D	-4	ASP	-	expression tag	UNP A0A081YAY7
D	-3	ASP	-	expression tag	UNP A0A081YAY7
D	-2	LYS	-	expression tag	UNP A0A081YAY7
D	-1	GLY	-	expression tag	UNP A0A081YAY7
D	0	SER	-	expression tag	UNP A0A081YAY7
E	-32	MET	-	initiating methionine	UNP A0A081YAY7
E	-31	ARG	-	expression tag	UNP A0A081YAY7
E	-30	GLY	-	expression tag	UNP A0A081YAY7
E	-29	SER	-	expression tag	UNP A0A081YAY7
E	-28	HIS	-	expression tag	UNP A0A081YAY7
E	-27	HIS	-	expression tag	UNP A0A081YAY7
E	-26	HIS	-	expression tag	UNP A0A081YAY7
E	-25	HIS	-	expression tag	UNP A0A081YAY7
E	-24	HIS	-	expression tag	UNP A0A081YAY7
E	-23	HIS	-	expression tag	UNP A0A081YAY7
E	-22	GLY	-	expression tag	UNP A0A081YAY7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-21	MET	-	expression tag	UNP A0A081YAY7
E	-20	ALA	-	expression tag	UNP A0A081YAY7
E	-19	SER	-	expression tag	UNP A0A081YAY7
E	-18	MET	-	expression tag	UNP A0A081YAY7
E	-17	THR	-	expression tag	UNP A0A081YAY7
E	-16	GLY	-	expression tag	UNP A0A081YAY7
E	-15	GLY	-	expression tag	UNP A0A081YAY7
E	-14	GLN	-	expression tag	UNP A0A081YAY7
E	-13	GLN	-	expression tag	UNP A0A081YAY7
E	-12	MET	-	expression tag	UNP A0A081YAY7
E	-11	GLY	-	expression tag	UNP A0A081YAY7
E	-10	ARG	-	expression tag	UNP A0A081YAY7
E	-9	ASP	-	expression tag	UNP A0A081YAY7
E	-8	LEU	-	expression tag	UNP A0A081YAY7
E	-7	TYR	-	expression tag	UNP A0A081YAY7
E	-6	ASP	-	expression tag	UNP A0A081YAY7
E	-5	ASP	-	expression tag	UNP A0A081YAY7
E	-4	ASP	-	expression tag	UNP A0A081YAY7
E	-3	ASP	-	expression tag	UNP A0A081YAY7
E	-2	LYS	-	expression tag	UNP A0A081YAY7
E	-1	GLY	-	expression tag	UNP A0A081YAY7
E	0	SER	-	expression tag	UNP A0A081YAY7
F	-32	MET	-	initiating methionine	UNP A0A081YAY7
F	-31	ARG	-	expression tag	UNP A0A081YAY7
F	-30	GLY	-	expression tag	UNP A0A081YAY7
F	-29	SER	-	expression tag	UNP A0A081YAY7
F	-28	HIS	-	expression tag	UNP A0A081YAY7
F	-27	HIS	-	expression tag	UNP A0A081YAY7
F	-26	HIS	-	expression tag	UNP A0A081YAY7
F	-25	HIS	-	expression tag	UNP A0A081YAY7
F	-24	HIS	-	expression tag	UNP A0A081YAY7
F	-23	HIS	-	expression tag	UNP A0A081YAY7
F	-22	GLY	-	expression tag	UNP A0A081YAY7
F	-21	MET	-	expression tag	UNP A0A081YAY7
F	-20	ALA	-	expression tag	UNP A0A081YAY7
F	-19	SER	-	expression tag	UNP A0A081YAY7
F	-18	MET	-	expression tag	UNP A0A081YAY7
F	-17	THR	-	expression tag	UNP A0A081YAY7
F	-16	GLY	-	expression tag	UNP A0A081YAY7
F	-15	GLY	-	expression tag	UNP A0A081YAY7
F	-14	GLN	-	expression tag	UNP A0A081YAY7
F	-13	GLN	-	expression tag	UNP A0A081YAY7

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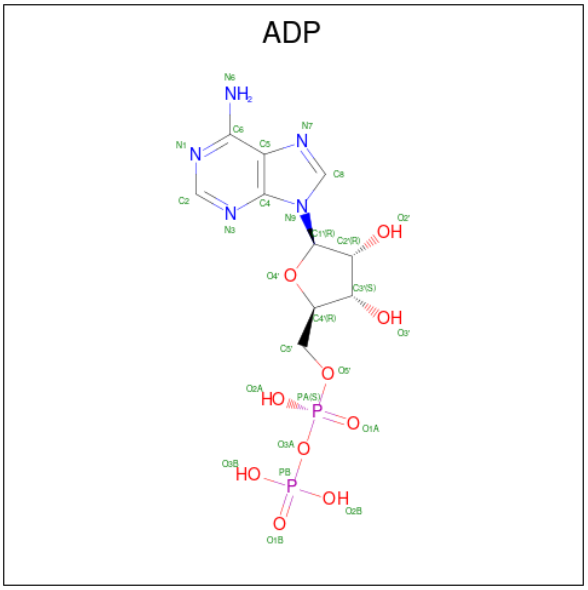
Chain	Residue	Modelled	Actual	Comment	Reference
F	-12	MET	-	expression tag	UNP A0A081YAY7
F	-11	GLY	-	expression tag	UNP A0A081YAY7
F	-10	ARG	-	expression tag	UNP A0A081YAY7
F	-9	ASP	-	expression tag	UNP A0A081YAY7
F	-8	LEU	-	expression tag	UNP A0A081YAY7
F	-7	TYR	-	expression tag	UNP A0A081YAY7
F	-6	ASP	-	expression tag	UNP A0A081YAY7
F	-5	ASP	-	expression tag	UNP A0A081YAY7
F	-4	ASP	-	expression tag	UNP A0A081YAY7
F	-3	ASP	-	expression tag	UNP A0A081YAY7
F	-2	LYS	-	expression tag	UNP A0A081YAY7
F	-1	GLY	-	expression tag	UNP A0A081YAY7
F	0	SER	-	expression tag	UNP A0A081YAY7

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
2	B	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
2	D	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
2	E	1	27	10	5	10	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	F	1	27	10	5	10	2	0	0

- Molecule 3 is water.

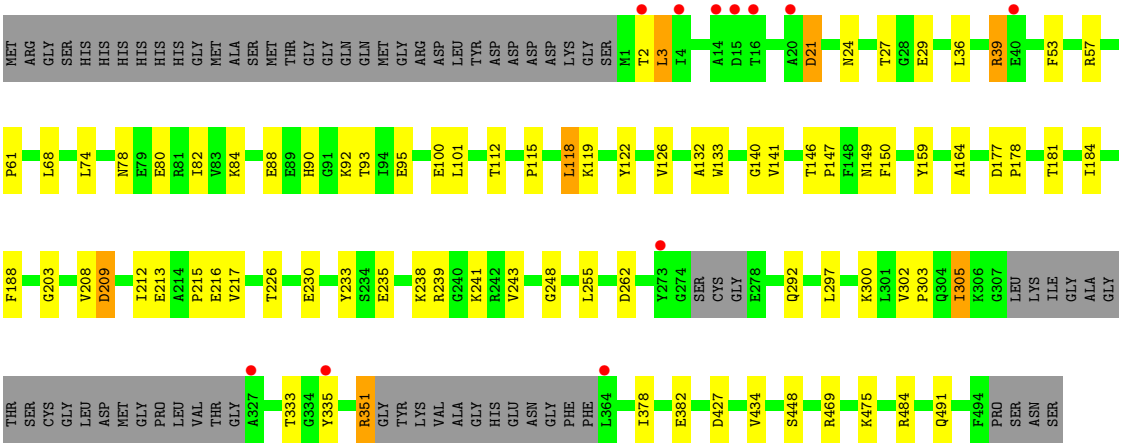
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	3	3	3	0	0
			Total	O		
3	B	5	5	5	0	0
			Total	O		
3	C	2	2	2	0	0
			Total	O		
3	D	3	3	3	0	0
			Total	O		
3	E	1	1	1	0	0
			Total	O		
3	F	2	2	2	0	0

3 Residue-property plots (i)

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

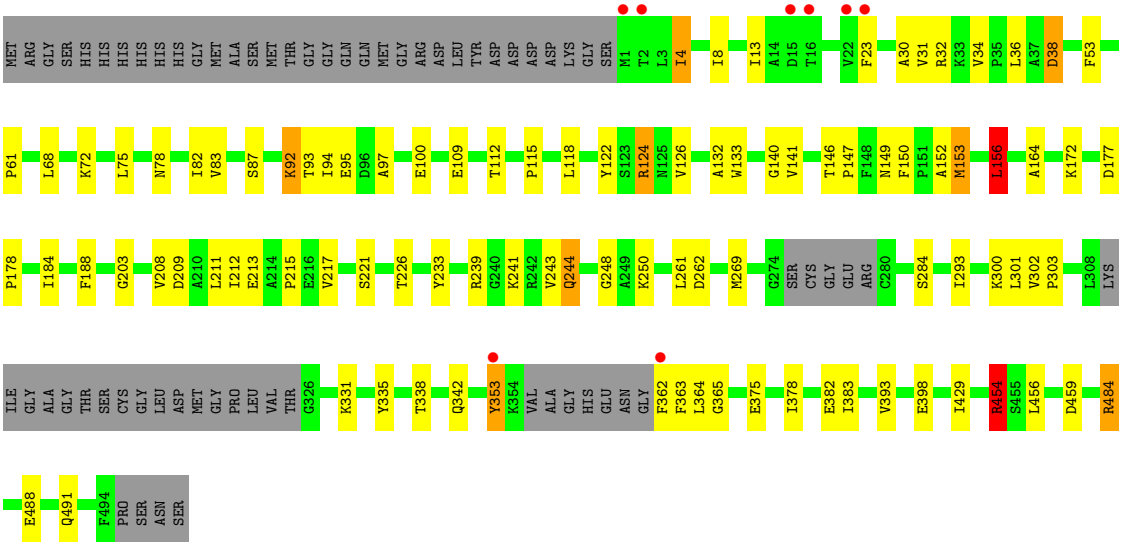
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain A:



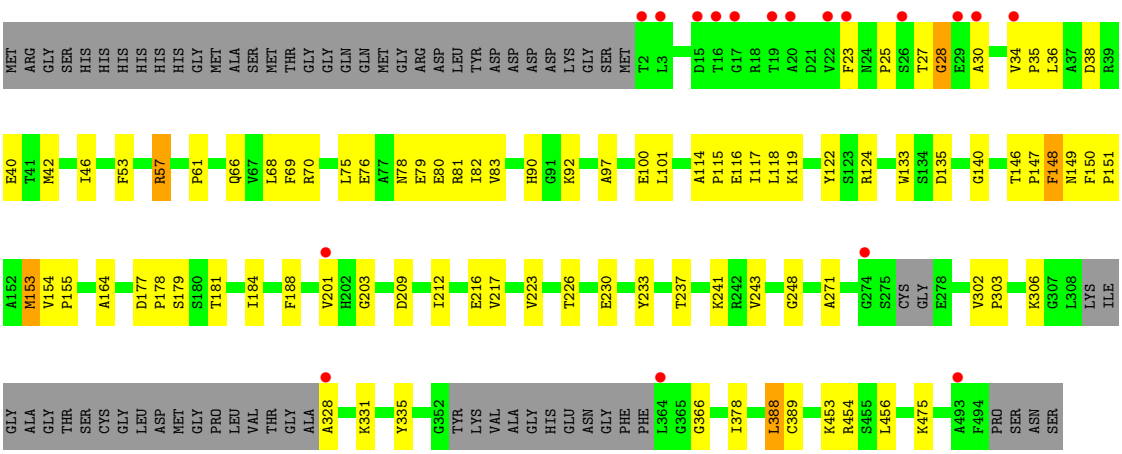
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain B:



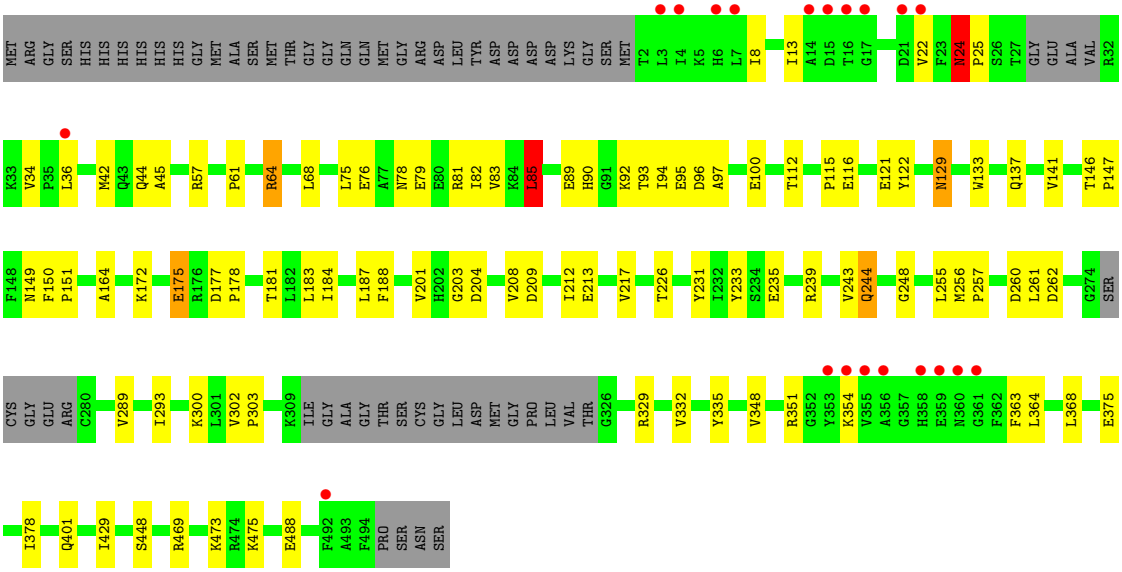
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain C:



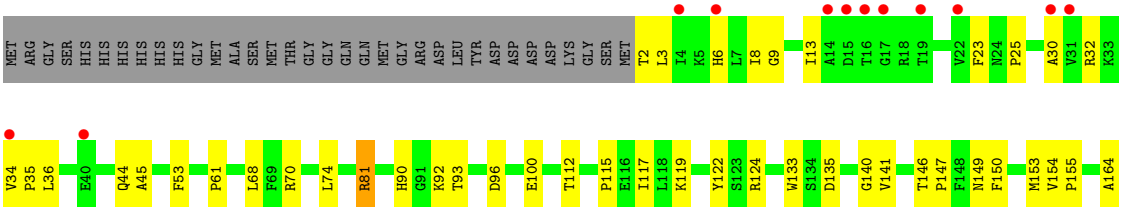
- Molecule 1: Methylmalonate-semialdehyde dehydrogenase

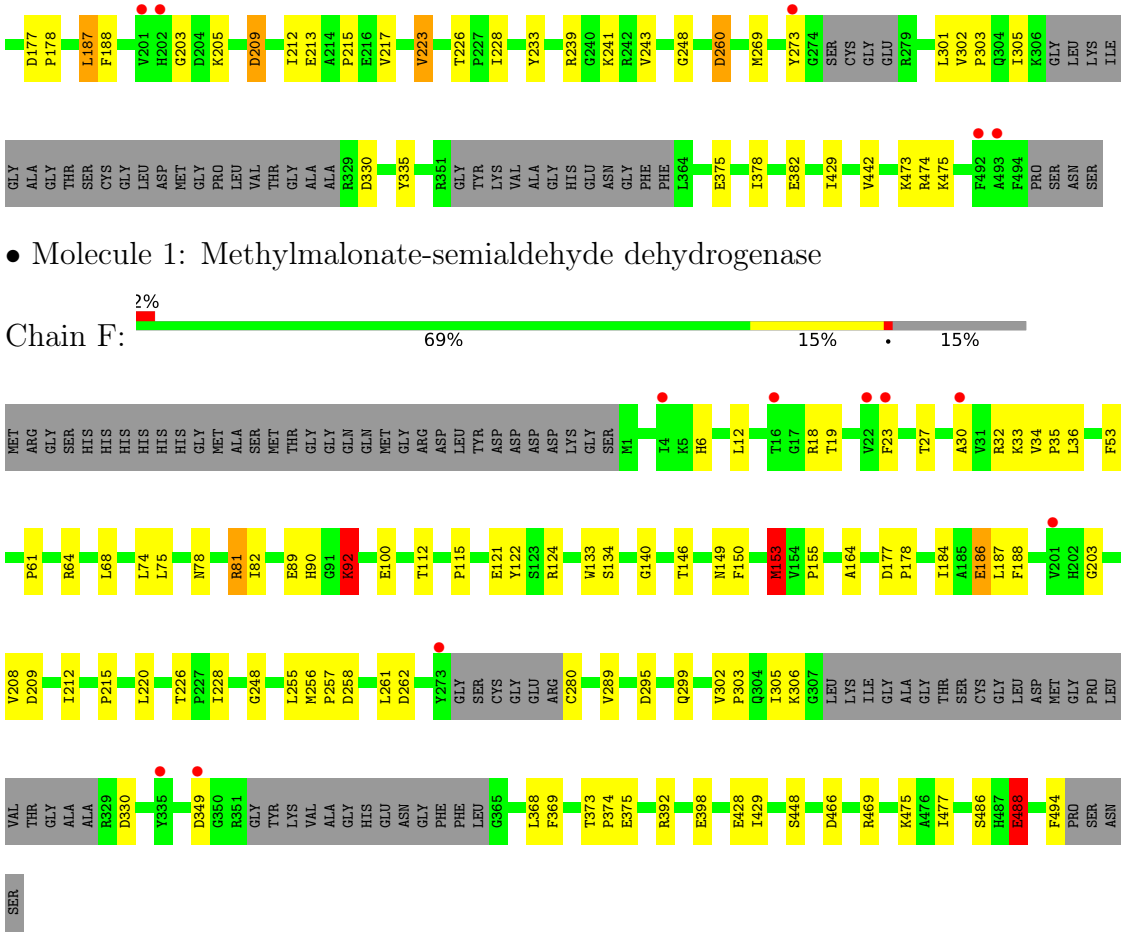
Chain D:



- Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain E:




D177 P178 L187 F188 V201 H202 G203 D204 K205 D209 I212 E213 A214 P215 E216 V217 V223 T226 P227 I228 Y233 R239 G240 K241 R242 V243 G248 D260 M269 Y273 G274 SER CYS GLY GLU R279 L301 V302 P303 Q304 I305 K306 GLY LEU LYS ILE
GLY ALA GLY THR SER CYS GLY LEU ASP MET GLY PRO LEU VAL THR GLY ALA ALA R329 D330 Y335 R351 GLY TYR LYS VAL ALA GLY HIS GLU ASN GLY PHE PHE L364 E375 I378 E382 I429 V442 K473 R474 K475 F492 A493 F494 PRO SER ASN SER
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase
Chain F:
2%
69%
15%
15%
MET ARG GLY SER HIS HIS HIS HIS HIS HIS GLY MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG ASP LEU TYR ASP ASP ASP ASP LYS GLY SER M1 I4 K5 H6 L12 T16 G17 R18 T19 V22 F23 T27 A30 V31 R32 K33 V34 P35 L36 F53
P61 R64 L68 L74 L75 N78 R81 I82 E89 H90 G91 K92 E100 T112 P115 E121 Y122 S123 R124 W133 S134 G140 T146 N149 F150 M153 V154 P155 A164 D177 P178 I184 A185 E186 L187 F188 V201 H202 G203
V208 D209 I212 P215 L220 T226 P227 I228 G248 L255 M256 P257 D258 L261 D262 Y273 GLY SER CYS GLY GLU ARG C280 V289 D295 Q299 V302 P303 Q304 I305 K306 G307 LEU LYS ILE GLY ALA GLY THR SER CYS GLY LEU ASP MET GLY PRO LEU
VAL THR GLY ALA ALA R329 D330 Y335 D349 G350 R351 GLY TYR LYS VAL ALA GLY HIS GLU ASN GLY PHE PHE LEU G365 L368 F369 T373 P374 E375 R392 E398 E428 I429 S448 D466 R469 K475 A476 I477 S486 H487 E488 F494 PRO SER ASN
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.89Å 156.63Å 192.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.95 47.60 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.00-2.95) 99.9 (47.60-2.95)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.212 , 0.249 0.215 , 0.251	Depositor DCC
R_{free} test set	3714 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20975	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.58	0/3542	0.82	7/4810 (0.1%)
1	B	0.61	0/3600	0.84	5/4889 (0.1%)
1	C	0.66	0/3525	0.87	10/4787 (0.2%)
1	D	0.60	0/3610	0.84	8/4900 (0.2%)
1	E	0.58	0/3479	0.85	10/4730 (0.2%)
1	F	0.62	0/3501	0.88	15/4755 (0.3%)
All	All	0.61	0/21257	0.85	55/28871 (0.2%)

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	A	0	2
1	D	0	1
1	E	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	209	ASP	CB-CG-OD1	-11.03	108.37	118.30
1	B	454	ARG	CG-CD-NE	10.00	132.80	111.80
1	E	260	ASP	CB-CG-OD1	9.48	126.83	118.30
1	E	209	ASP	CB-CG-OD2	9.43	126.78	118.30
1	A	209	ASP	CB-CG-OD2	8.92	126.33	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	GLU	Mainchain
1	A	305	ILE	Mainchain
1	D	175	GLU	Mainchain
1	E	260	ASP	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3471	0	3443	54	0
1	B	3525	0	3483	61	0
1	C	3455	0	3410	59	0
1	D	3535	0	3490	67	0
1	E	3408	0	3347	54	0
1	F	3430	0	3405	50	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
2	D	27	0	12	1	0
2	E	27	0	12	1	0
2	F	27	0	12	1	0
3	A	3	0	0	0	0
3	B	5	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
All	All	20975	0	20638	336	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 336 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:A:24:ASN:ND2	1:A:88:GLU:O	1.88	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ILE:CG2	1:C:216:GLU:HG3	1.99	0.92
1:C:23:PHE:O	1:C:25:PRO:HD3	1.74	0.86
1:B:152:ALA:O	1:B:156:LEU:HD12	1.79	0.83
1:F:19:THR:HG22	1:F:33:LYS:HG2	1.60	0.83

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	452/531 (85%)	432 (96%)	20 (4%)	0	100	100
1	B	458/531 (86%)	438 (96%)	20 (4%)	0	100	100
1	C	453/531 (85%)	430 (95%)	21 (5%)	2 (0%)	34	69
1	D	460/531 (87%)	444 (96%)	16 (4%)	0	100	100
1	E	447/531 (84%)	428 (96%)	19 (4%)	0	100	100
1	F	446/531 (84%)	423 (95%)	23 (5%)	0	100	100
All	All	2716/3186 (85%)	2595 (96%)	119 (4%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	28	GLY
1	C	271	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/416 (85%)	343 (97%)	10 (3%)	43	74
1	B	358/416 (86%)	342 (96%)	16 (4%)	27	61
1	C	349/416 (84%)	338 (97%)	11 (3%)	39	71
1	D	358/416 (86%)	343 (96%)	15 (4%)	30	63
1	E	343/416 (82%)	334 (97%)	9 (3%)	46	75
1	F	350/416 (84%)	338 (97%)	12 (3%)	37	69
All	All	2111/2496 (85%)	2038 (96%)	73 (4%)	37	68

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	223	VAL
1	F	488	GLU
1	E	473	LYS
1	F	188	PHE
1	B	454	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	24	ASN
1	D	202	HIS
1	B	129	ASN
1	B	244	GLN
1	B	342	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are 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	ADP	A	501	-	24,29,29	1.03	2 (8%)	29,45,45	1.63	7 (24%)
2	ADP	F	501	-	24,29,29	1.00	2 (8%)	29,45,45	1.53	6 (20%)
2	ADP	E	501	-	24,29,29	1.10	2 (8%)	29,45,45	1.41	5 (17%)
2	ADP	B	501	-	24,29,29	1.08	2 (8%)	29,45,45	1.57	7 (24%)
2	ADP	D	501	-	24,29,29	1.06	1 (4%)	29,45,45	1.64	4 (13%)

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	ADP	A	501	-	-	6/12/32/32	0/3/3/3
2	ADP	F	501	-	-	8/12/32/32	0/3/3/3
2	ADP	E	501	-	-	0/12/32/32	0/3/3/3
2	ADP	B	501	-	-	4/12/32/32	0/3/3/3
2	ADP	D	501	-	-	5/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	ADP	C2-N3	2.92	1.36	1.32
2	A	501	ADP	C2-N3	2.63	1.36	1.32
2	F	501	ADP	C2-N3	2.62	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	ADP	C5-C4	2.45	1.47	1.40
2	D	501	ADP	C5-C4	2.35	1.47	1.40

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	ADP	N3-C2-N1	-4.31	121.94	128.68
2	A	501	ADP	C4-C5-N7	-3.84	105.40	109.40
2	E	501	ADP	C3'-C2'-C1'	3.67	106.50	100.98
2	F	501	ADP	N3-C2-N1	-3.65	122.97	128.68
2	D	501	ADP	PA-O3A-PB	-3.65	120.30	132.83

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ADP	PA-O3A-PB-O2B
2	A	501	ADP	C5'-O5'-PA-O3A
2	A	501	ADP	O4'-C4'-C5'-O5'
2	B	501	ADP	PA-O3A-PB-O3B
2	D	501	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

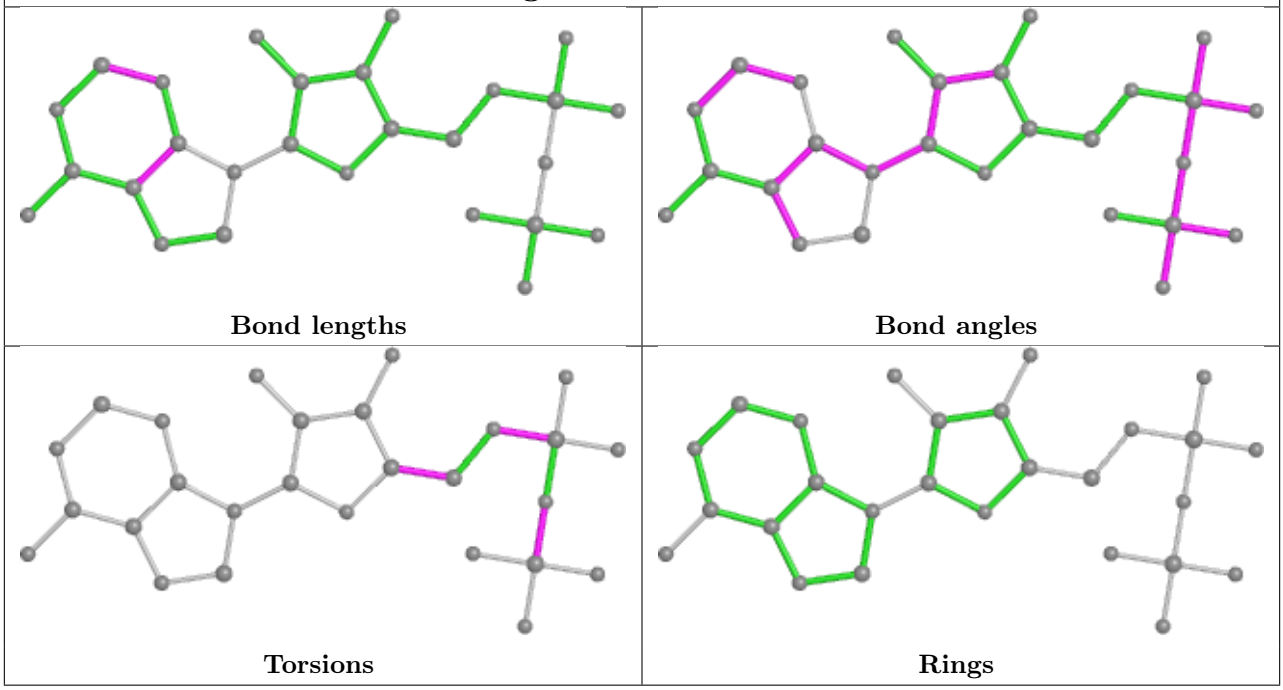
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	ADP	1	0
2	E	501	ADP	1	0
2	B	501	ADP	1	0
2	D	501	ADP	1	0

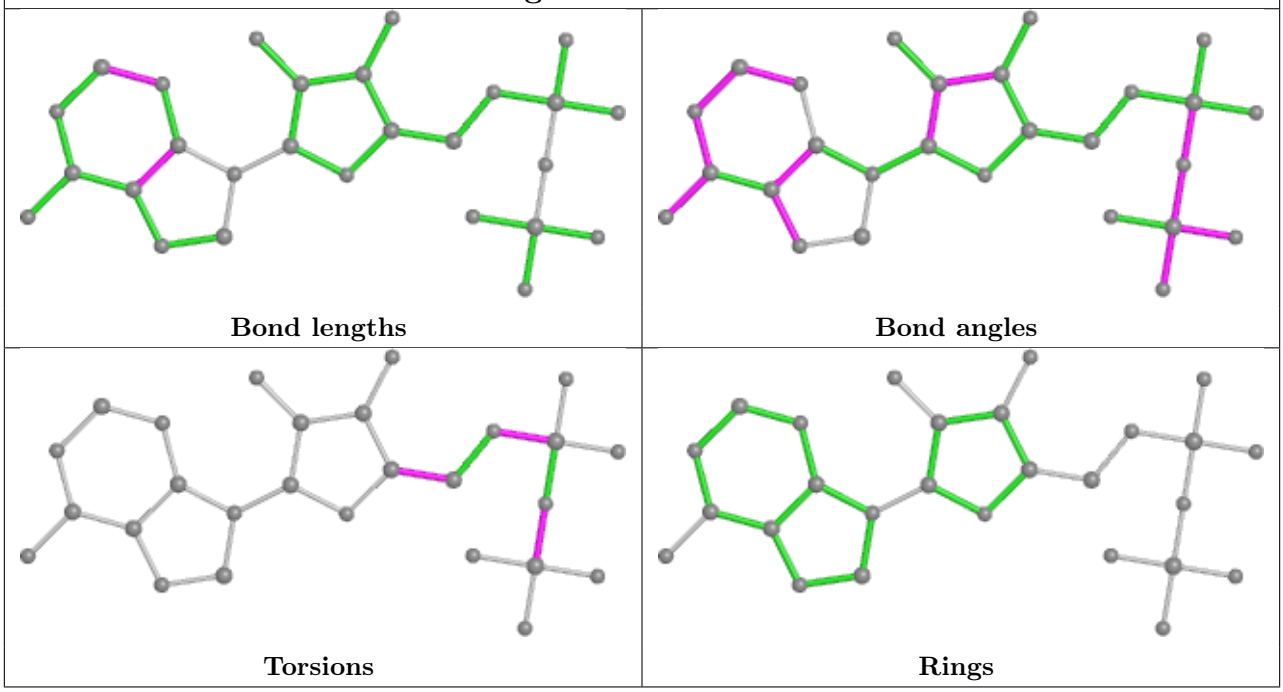
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

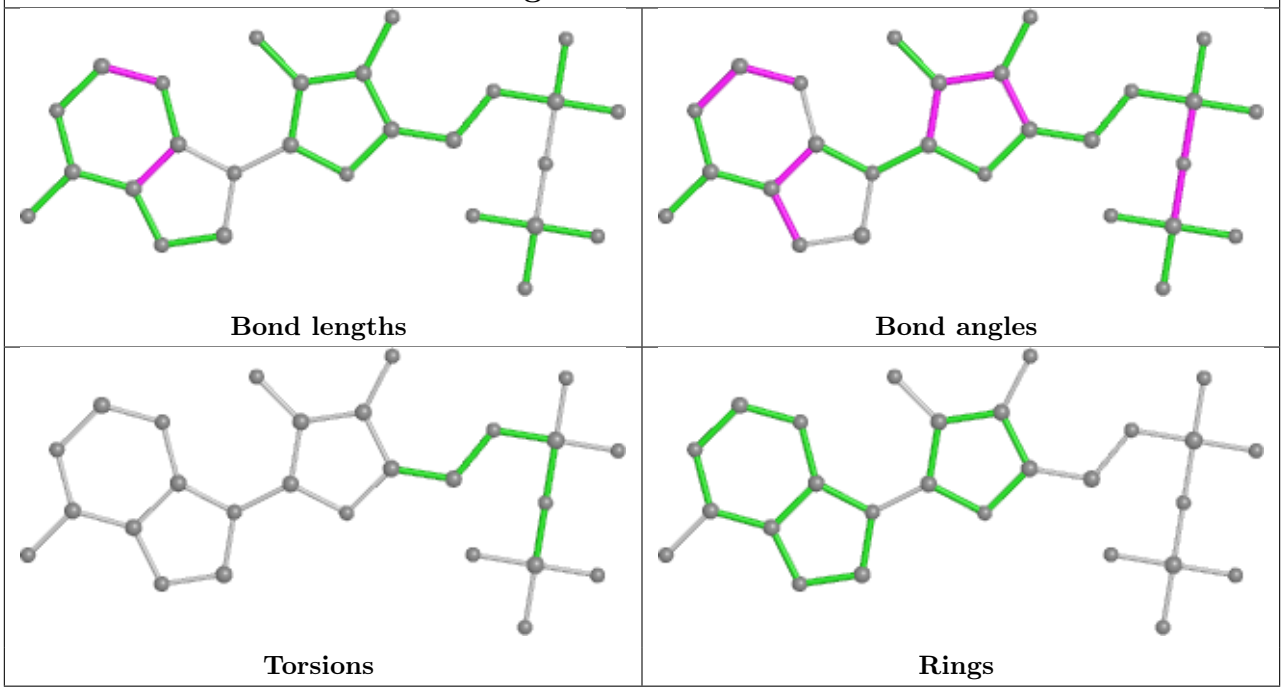
Ligand ADP A 501



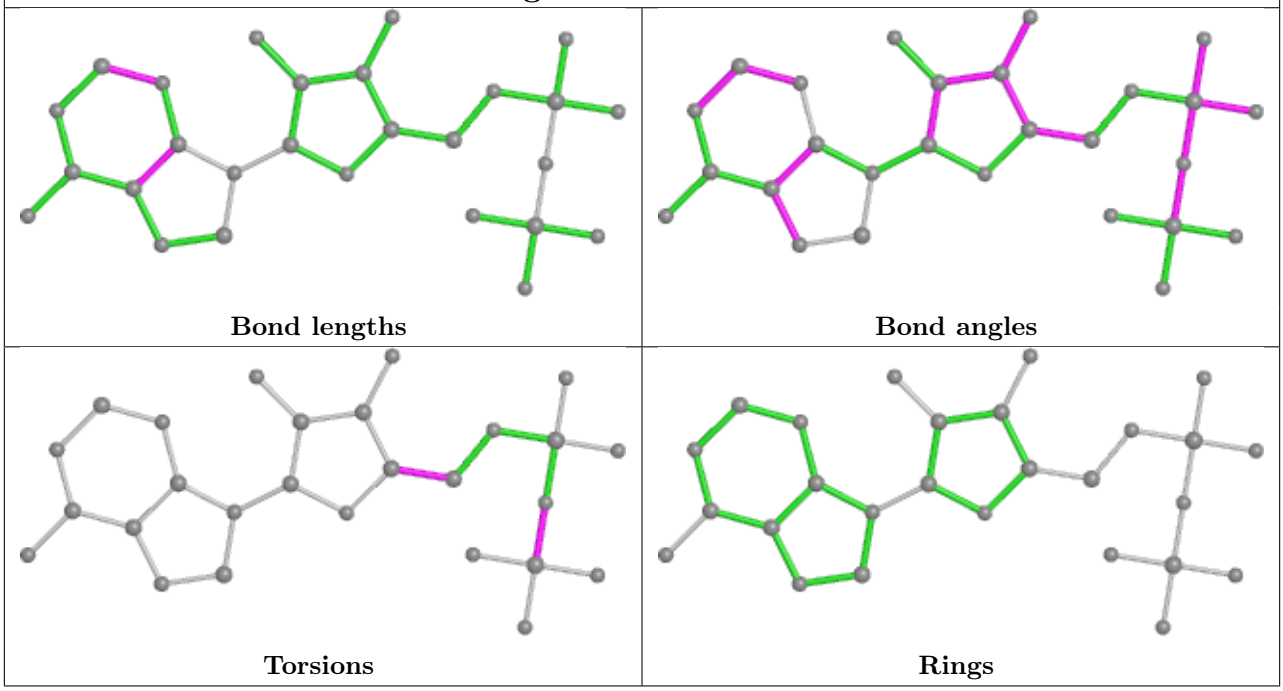
Ligand ADP F 501

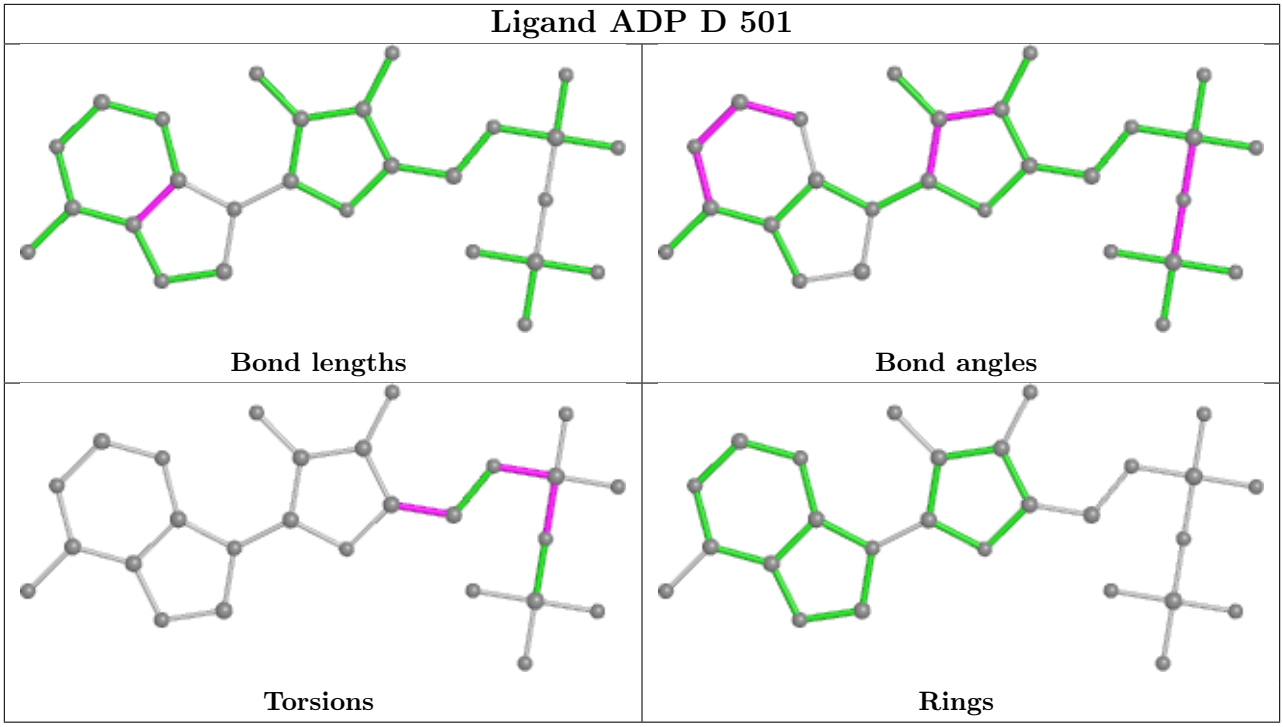


Ligand ADP E 501



Ligand ADP B 501





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	A	460/531 (86%)	0.11	11 (2%)	59	42	38, 65, 115, 157	0
1	B	465/531 (87%)	-0.02	8 (1%)	70	53	36, 65, 118, 149	0
1	C	461/531 (86%)	0.03	18 (3%)	39	25	34, 67, 114, 148	0
1	D	468/531 (88%)	0.00	20 (4%)	35	22	36, 67, 114, 141	0
1	E	455/531 (85%)	0.08	17 (3%)	41	27	39, 73, 126, 157	0
1	F	454/531 (85%)	0.05	9 (1%)	65	48	39, 69, 111, 139	0
All	All	2763/3186 (86%)	0.04	83 (3%)	50	34	34, 68, 118, 157	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	273	TYR	5.9
1	F	30	ALA	4.6
1	E	493	ALA	4.6
1	C	34	VAL	4.4
1	A	364	LEU	4.4

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 monosaccharides in this entry.

6.4 Ligands (i)

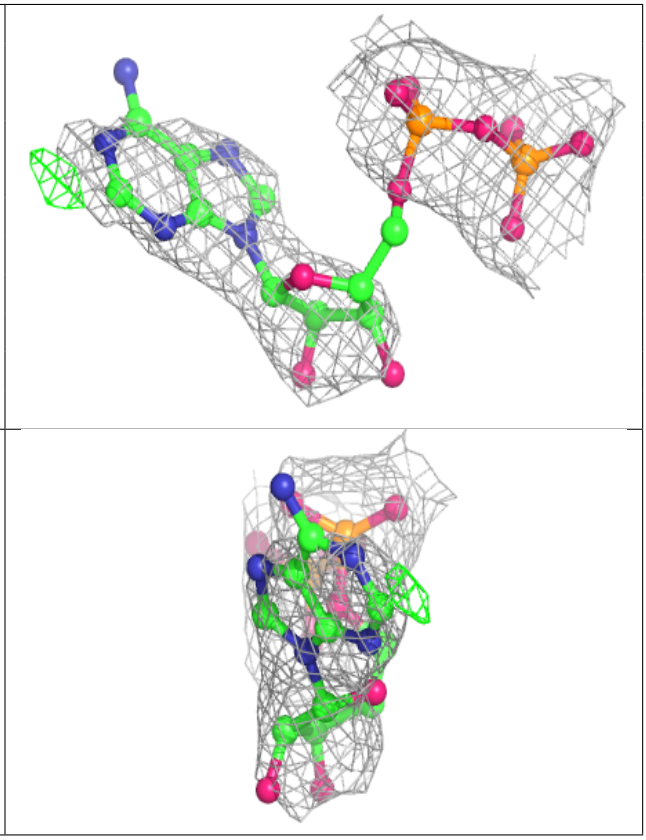
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	E	501	27/27	0.80	0.28	83,95,105,108	27
2	ADP	A	501	27/27	0.85	0.27	76,91,100,105	27
2	ADP	F	501	27/27	0.89	0.21	65,80,89,95	27
2	ADP	D	501	27/27	0.90	0.20	59,67,74,77	27
2	ADP	B	501	27/27	0.91	0.22	61,67,72,76	27

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

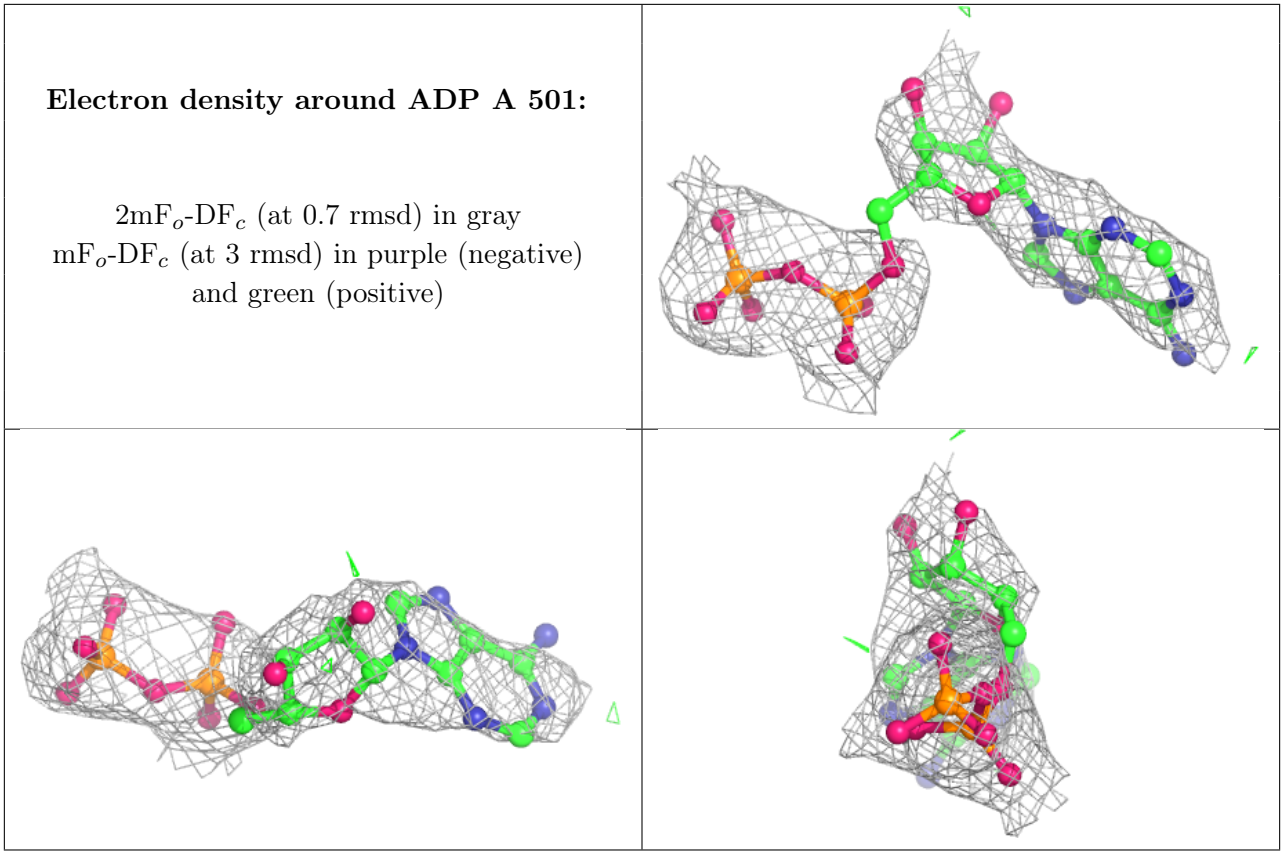
Electron density around ADP E 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



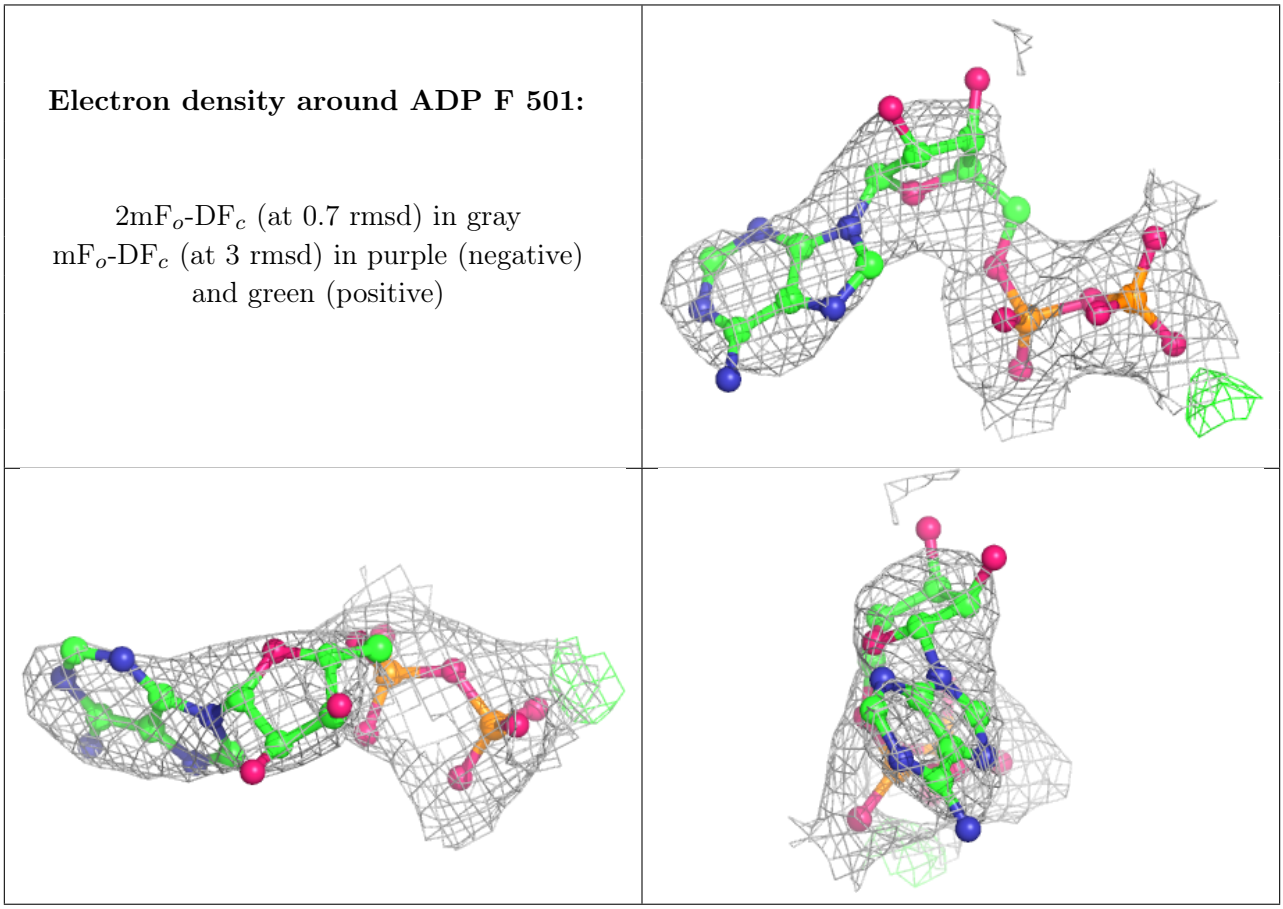
Electron density around ADP A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



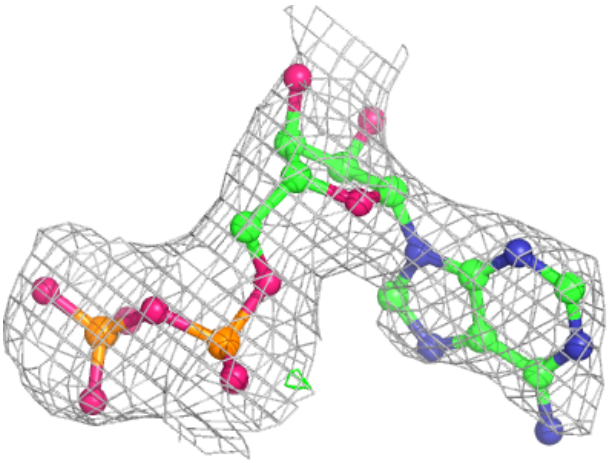
Electron density around ADP F 501:

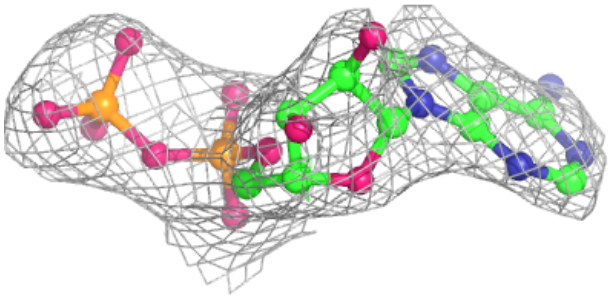
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

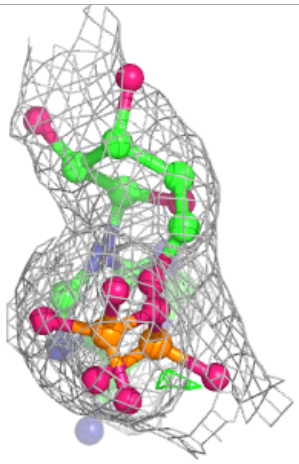


Electron density around ADP D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

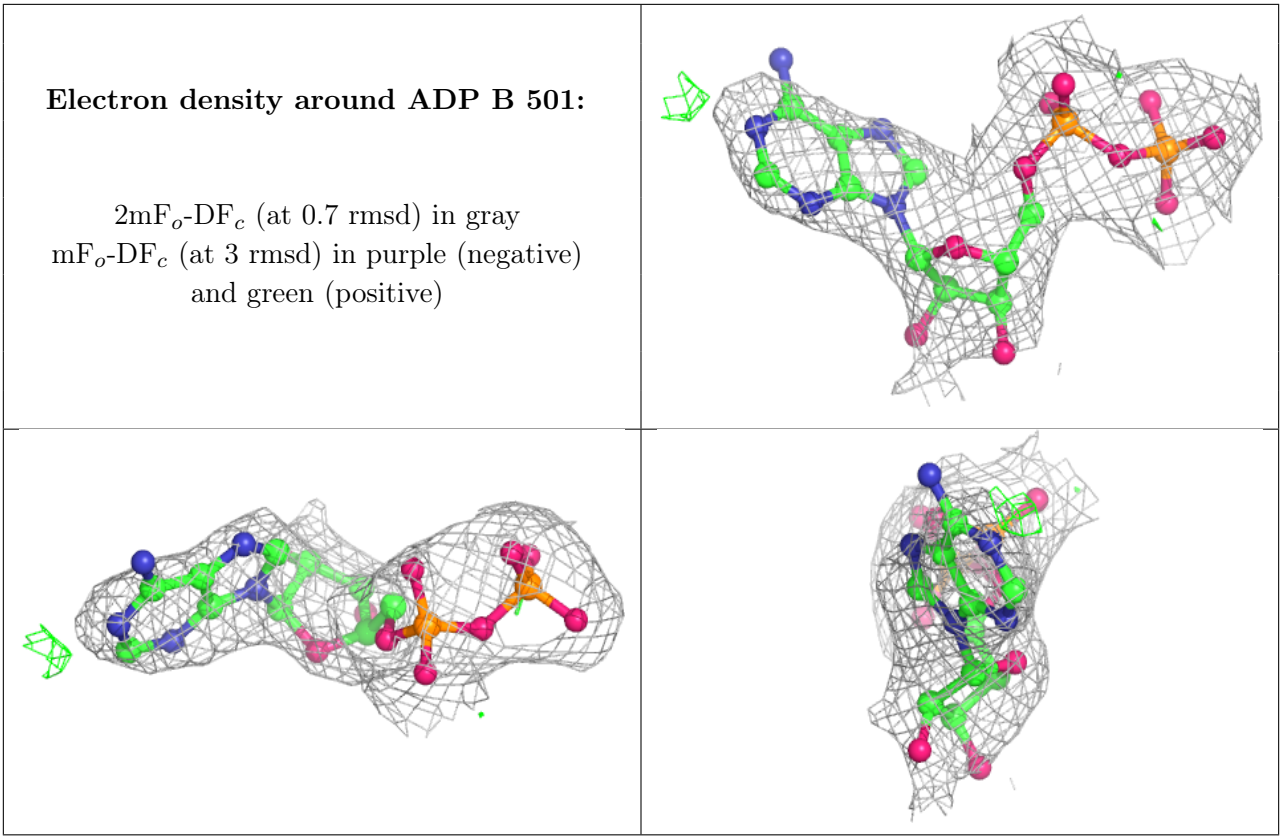






Electron density around ADP B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.