



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:34 PM GMT

PDB ID : 1PJ4  
Title : Crystal structure of human mitochondrial NAD(P)+-dependent malic enzyme in a pentary complex with natural substrate malate, ATP, Mn++, and allosteric activator fumarate.  
Authors : Tao, X.; Yang, Z.; Tong, L.  
Deposited on : 2003-05-31  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 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

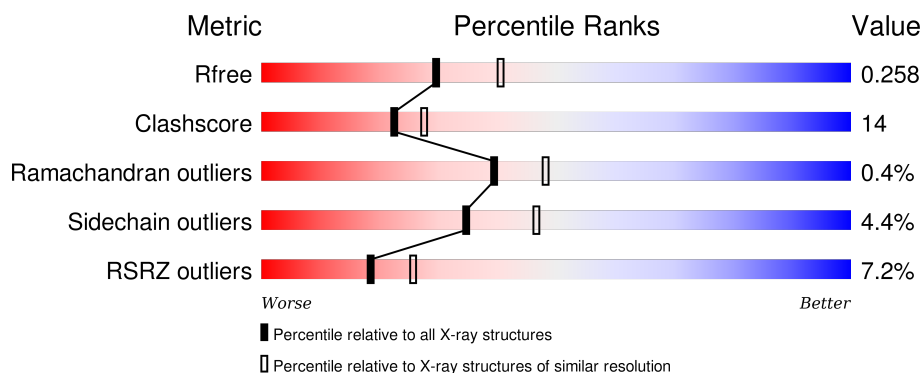
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	564	<div> <div>7%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>
1	B	564	<div> <div>7%</div> <div>69%</div> <div>26%</div> <div>..</div> </div>
1	C	564	<div> <div>7%</div> <div>71%</div> <div>26%</div> <div>..</div> </div>
1	D	564	<div> <div>6%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MLT	A	701	X	-	-	-
2	MLT	B	1701	X	-	-	-
2	MLT	C	2701	X	-	-	-
2	MLT	D	3701	X	-	-	-
5	FUM	A	700	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18442 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 NAD-dependent malic enzyme, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	Se	0	0	0
			4359	2790	743	803	9	14			
1	B	552	Total	C	N	O	S	Se	0	0	0
			4359	2790	743	803	9	14			
1	C	552	Total	C	N	O	S	Se	0	0	0
			4359	2790	743	803	9	14			
1	D	552	Total	C	N	O	S	Se	0	0	0
			4359	2790	743	803	9	14			

There are 56 discrepancies between the modelled and reference sequences:

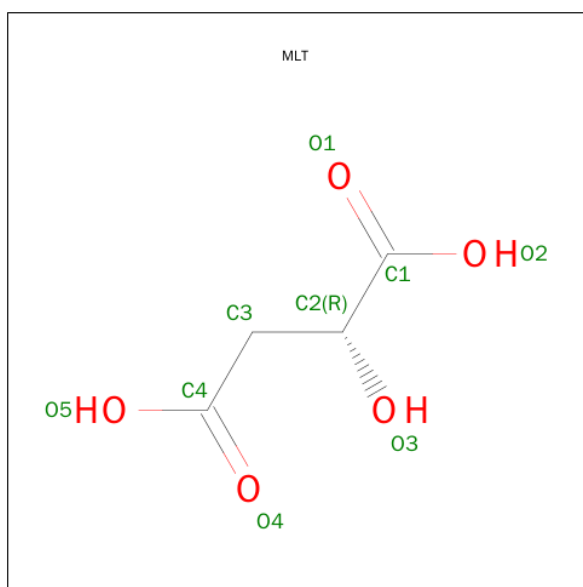
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	177	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	343	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	539	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1029	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1038	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1047	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1075	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1086	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1108	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1177	MSE	MET	MODIFIED RESIDUE	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1219	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1239	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1325	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1327	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1343	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1407	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1539	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2029	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2038	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2047	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2075	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2086	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2108	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2177	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2219	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2239	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2325	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2327	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2343	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2407	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2539	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3029	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3038	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3047	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3075	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3086	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3108	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3177	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3219	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3239	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3325	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3327	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3343	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3407	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3539	MSE	MET	MODIFIED RESIDUE	UNP P23368

- Molecule 2 is MALATE ION (three-letter code: MLT) (formula:  $C_4H_6O_5$ ).

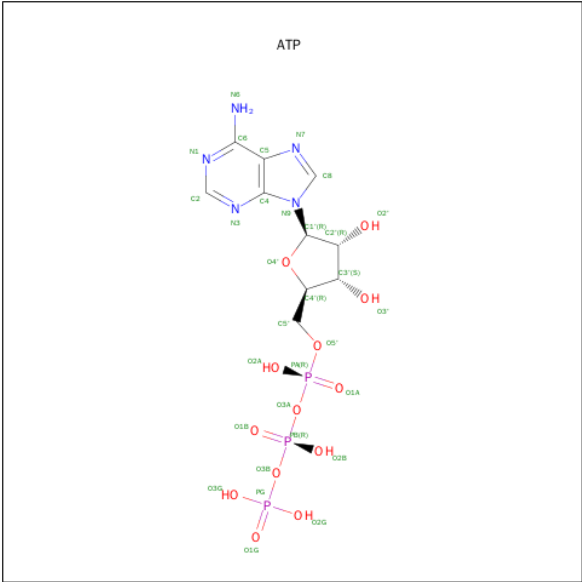


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O	0	0
			9	4	5		
2	C	1	Total	C	O	0	0
			9	4	5		
2	D	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

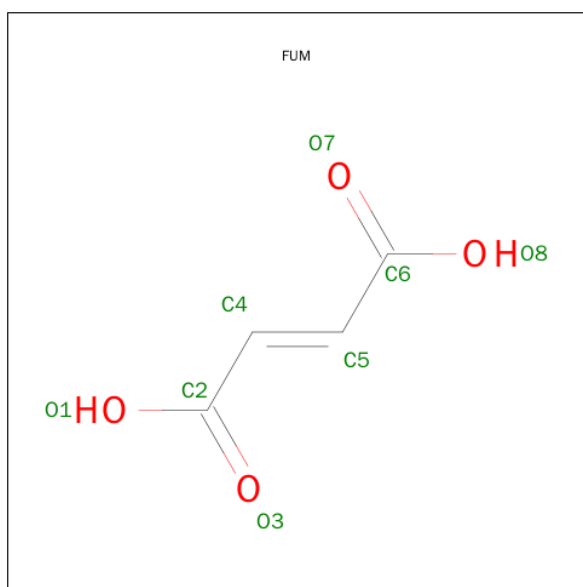
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is FUMARIC ACID (three-letter code: FUM) (formula: C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	B	1	Total	C	O	0	0
			8	4	4		
5	C	1	Total	C	O	0	0
			8	4	4		
5	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is water.

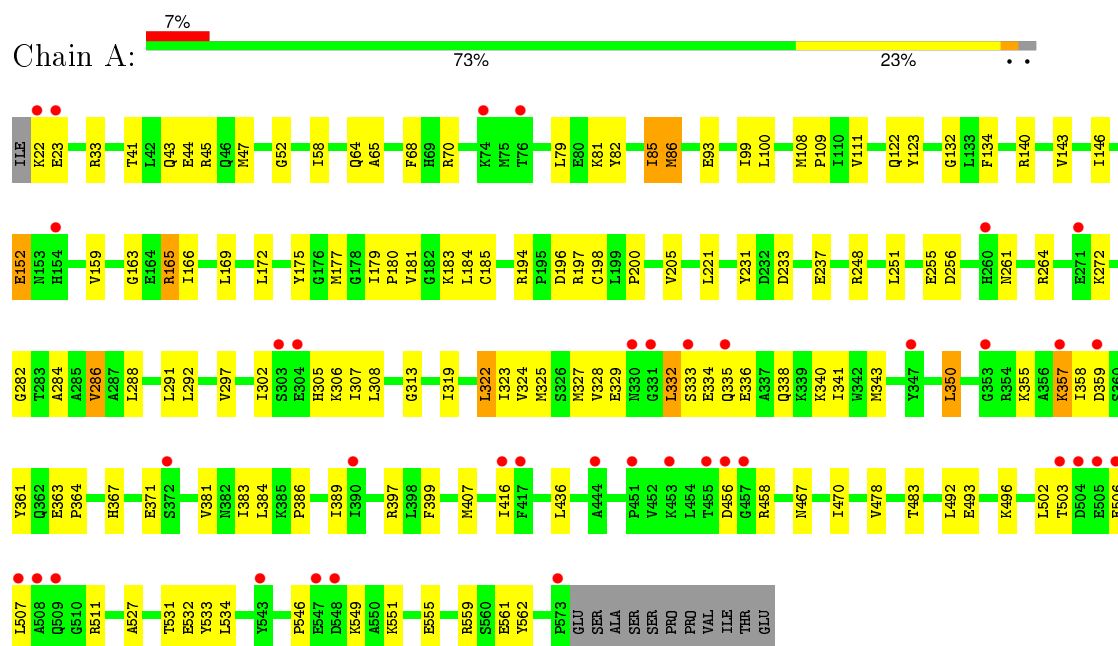
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	165	Total	O	0	0
			165	165		
6	B	176	Total	O	0	0
			176	176		
6	C	169	Total	O	0	0
			169	169		
6	D	176	Total	O	0	0
			176	176		



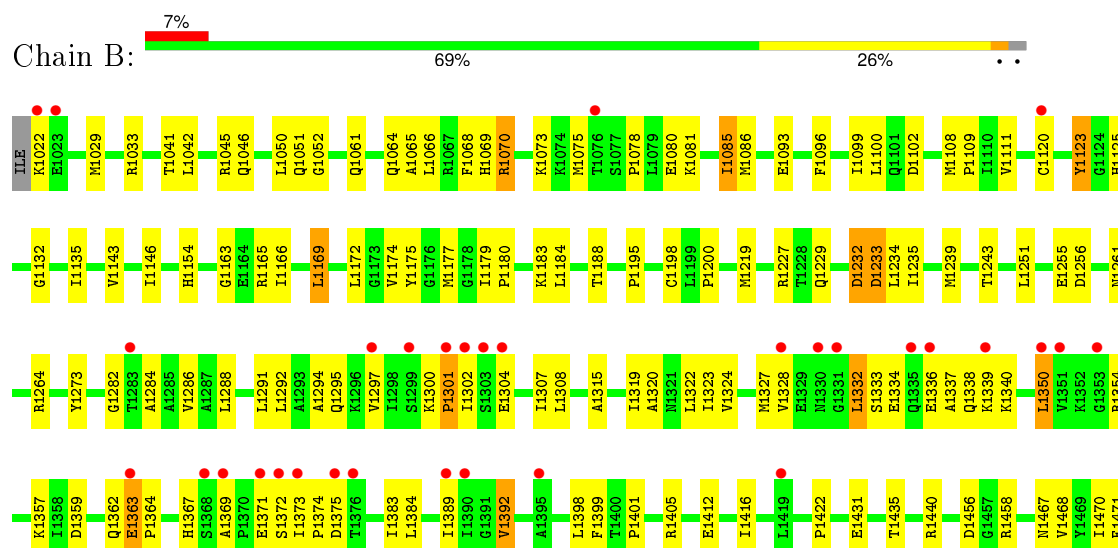
### 3 Residue-property plots

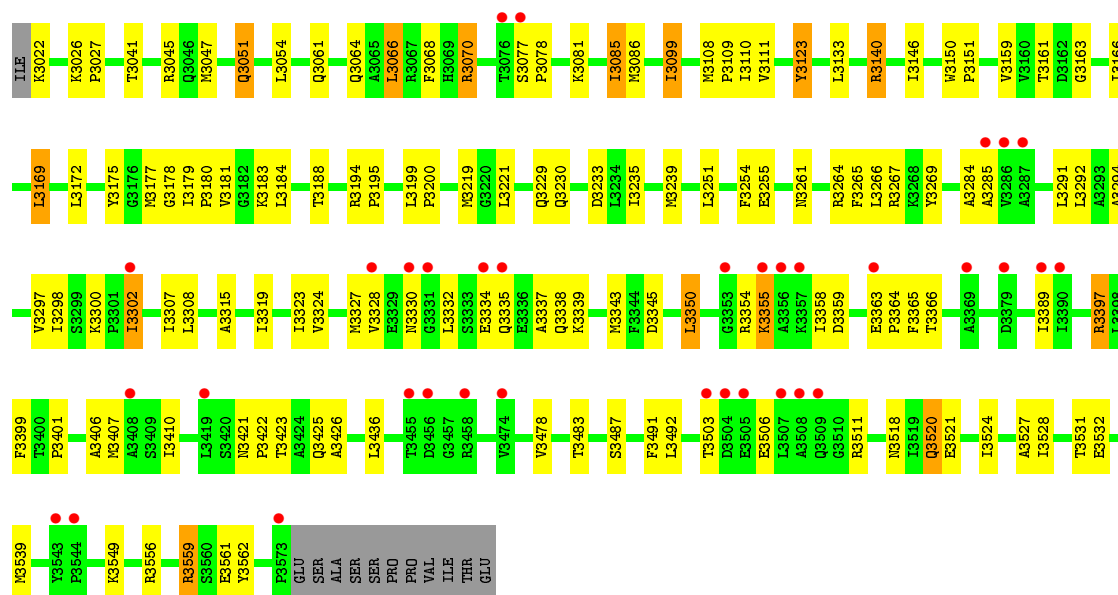
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

- Molecule 1: NAD-dependent malic enzyme, mitochondrial



- Molecule 1: NAD-dependent malic enzyme, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	226.05Å 117.34Å 111.31Å 90.00° 109.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.30 29.55 – 2.29	Depositor EDS
% Data completeness (in resolution range)	92.7 (19.94-2.30) 96.7 (29.55-2.29)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.211 , 0.252 0.217 , 0.258	Depositor DCC
$R_{free}$ test set	8936 reflections (7.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 119545 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18442	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FUM, MLT, ATP, MN

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	0.36	0/4439	0.60	0/5987
1	B	0.36	0/4439	0.60	0/5987
1	C	0.36	0/4439	0.60	0/5987
1	D	0.36	0/4439	0.60	0/5987
All	All	0.36	0/17756	0.60	0/23948

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4359	0	4396	112	0
1	B	4359	0	4396	138	0
1	C	4359	0	4396	131	0
1	D	4359	0	4396	111	0
2	A	9	0	3	0	0
2	B	9	0	3	0	0
2	C	9	0	3	0	0
2	D	9	0	3	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	1	0
4	B	62	0	24	1	0
4	C	62	0	24	1	0
4	D	62	0	24	1	0
5	A	8	0	2	0	0
5	B	8	0	2	0	0
5	C	8	0	2	0	0
5	D	8	0	2	0	0
6	A	165	0	0	2	0
6	B	176	0	0	7	0
6	C	169	0	0	8	0
6	D	176	0	0	4	0
All	All	18442	0	17700	485	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 14.

The worst 5 of 485 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:B:1315:ALA:HB3	1:B:1392:VAL:HG21	1.25	1.14
1:D:3177:MSE:HE1	1:D:3200:PRO:HB2	1.14	1.07
1:C:2286:VAL:HG21	1:C:2467:ASN:HA	1.38	1.05
1:B:1323:ILE:HG22	1:B:1327:MSE:HE2	1.40	1.03
1:C:2132:GLY:HA3	1:C:2177:MSE:CE	1.89	1.01

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	550/564 (98%)	531 (96%)	16 (3%)	3 (0%)	34	41
1	B	550/564 (98%)	534 (97%)	14 (2%)	2 (0%)	39	48
1	C	550/564 (98%)	532 (97%)	16 (3%)	2 (0%)	39	48
1	D	550/564 (98%)	531 (96%)	17 (3%)	2 (0%)	39	48
All	All	2200/2256 (98%)	2128 (97%)	63 (3%)	9 (0%)	39	48

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	LYS
1	C	2332	LEU
1	A	397	ARG
1	B	1332	LEU
1	A	332	LEU

### 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	468/465 (101%)	447 (96%)	21 (4%)	34	46
1	B	468/465 (101%)	449 (96%)	19 (4%)	37	50
1	C	468/465 (101%)	450 (96%)	18 (4%)	40	54
1	D	468/465 (101%)	443 (95%)	25 (5%)	28	37
All	All	1872/1860 (101%)	1789 (96%)	83 (4%)	35	46

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1492	LEU
1	C	2251	LEU
1	D	3350	LEU
1	B	1502	LEU
1	C	2123	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1518	ASN
1	C	2122	GLN
1	D	3338	GLN
1	C	2043	GLN
1	C	2064	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](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\# Z  > 2$
4	ATP	A	4601	-	24,33,33	1.60	5 (20%)	31,52,52	2.28	3 (9%)
4	ATP	A	4602	-	24,33,33	1.61	5 (20%)	31,52,52	2.26	2 (6%)
5	FUM	A	700	-	1,7,7	1.67	0	0,8,8	0.00	-
2	MLT	A	701	3	1,8,8	0.22	0	2,10,10	0.30	0
4	ATP	B	1601	-	24,33,33	1.64	5 (20%)	31,52,52	2.30	3 (9%)
4	ATP	B	1602	-	24,33,33	1.62	5 (20%)	31,52,52	2.33	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	FUM	B	1700	-	1,7,7	1.59	0	0,8,8	0.00	-
2	MLT	B	1701	3	1,8,8	0.35	0	2,10,10	0.36	0
4	ATP	C	2601	-	24,33,33	1.50	4 (16%)	31,52,52	2.35	3 (9%)
4	ATP	C	2602	-	24,33,33	1.57	4 (16%)	31,52,52	2.27	2 (6%)
5	FUM	C	2700	-	1,7,7	1.86	0	0,8,8	0.00	-
2	MLT	C	2701	3	1,8,8	0.19	0	2,10,10	0.37	0
4	ATP	D	3601	-	24,33,33	1.51	5 (20%)	31,52,52	2.28	4 (12%)
4	ATP	D	3602	-	24,33,33	1.69	5 (20%)	31,52,52	2.29	2 (6%)
5	FUM	D	3700	-	1,7,7	1.72	0	0,8,8	0.00	-
2	MLT	D	3701	3	1,8,8	0.25	0	2,10,10	0.43	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
4	ATP	A	4601	-	-	0/18/38/38	0/3/3/3
4	ATP	A	4602	-	-	0/18/38/38	0/3/3/3
5	FUM	A	700	-	-	0/0/5/5	0/0/0/0
2	MLT	A	701	3	1/1/3/3	0/2/8/8	0/0/0/0
4	ATP	B	1601	-	-	0/18/38/38	0/3/3/3
4	ATP	B	1602	-	-	0/18/38/38	0/3/3/3
5	FUM	B	1700	-	-	0/0/5/5	0/0/0/0
2	MLT	B	1701	3	1/1/3/3	0/2/8/8	0/0/0/0
4	ATP	C	2601	-	-	0/18/38/38	0/3/3/3
4	ATP	C	2602	-	-	0/18/38/38	0/3/3/3
5	FUM	C	2700	-	-	0/0/5/5	0/0/0/0
2	MLT	C	2701	3	1/1/3/3	0/2/8/8	0/0/0/0
4	ATP	D	3601	-	-	0/18/38/38	0/3/3/3
4	ATP	D	3602	-	-	0/18/38/38	0/3/3/3
5	FUM	D	3700	-	-	0/0/5/5	0/0/0/0
2	MLT	D	3701	3	1/1/3/3	0/2/8/8	0/0/0/0

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2601	ATP	C5-C4	-3.13	1.33	1.40
4	B	1601	ATP	C5-C4	-3.10	1.33	1.40
4	C	2602	ATP	C5-C4	-3.09	1.33	1.40
4	B	1602	ATP	C5-C4	-3.00	1.33	1.40
4	D	3602	ATP	C5-C4	-2.84	1.34	1.40



The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1602	ATP	N3-C2-N1	-11.04	120.44	128.89
4	C	2601	ATP	N3-C2-N1	-10.92	120.53	128.89
4	D	3602	ATP	N3-C2-N1	-10.86	120.58	128.89
4	C	2602	ATP	N3-C2-N1	-10.75	120.66	128.89
4	A	4602	ATP	N3-C2-N1	-10.69	120.71	128.89

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	3701	MLT	C2
2	A	701	MLT	C2
2	B	1701	MLT	C2
2	C	2701	MLT	C2

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4601	ATP	1	0
4	B	1601	ATP	1	0
4	C	2602	ATP	1	0
4	D	3601	ATP	1	0
2	D	3701	MLT	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	538/564 (95%)	0.40	38 (7%) 19 26	16, 27, 52, 66	0
1	B	538/564 (95%)	0.52	42 (7%) 16 22	16, 27, 53, 68	0
1	C	538/564 (95%)	0.43	40 (7%) 17 25	16, 28, 52, 60	0
1	D	538/564 (95%)	0.40	35 (6%) 22 30	15, 28, 52, 67	0
All	All	2152/2256 (95%)	0.44	155 (7%) 18 26	15, 27, 52, 68	0

The worst 5 of 155 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3353	GLY	6.2
1	B	1510	GLY	6.1
1	C	2358	ILE	5.5
1	A	507	LEU	4.8
1	B	1301	PRO	4.5

### 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	FUM	A	700	8/8	0.95	0.23	2.01	35,37,38,38	0
5	FUM	D	3700	8/8	0.96	0.21	1.57	35,38,38,39	0
5	FUM	C	2700	8/8	0.94	0.17	1.44	35,37,39,39	0
4	ATP	C	2602	31/31	0.88	0.17	1.38	24,35,73,75	0
2	MLT	C	2701	9/9	0.89	0.17	0.98	26,30,32,32	0
4	ATP	D	3602	31/31	0.87	0.17	0.98	23,37,73,75	0
4	ATP	A	4601	31/31	0.88	0.18	0.92	25,28,60,62	0
4	ATP	C	2601	31/31	0.86	0.19	0.77	30,32,60,61	0
4	ATP	A	4602	31/31	0.87	0.17	0.67	21,35,73,74	0
4	ATP	D	3601	31/31	0.90	0.16	0.33	27,30,59,60	0
4	ATP	B	1602	31/31	0.88	0.15	0.31	24,34,71,73	0
2	MLT	D	3701	9/9	0.93	0.17	0.26	27,29,31,33	0
4	ATP	B	1601	31/31	0.90	0.18	0.22	28,30,59,60	0
5	FUM	B	1700	8/8	0.94	0.14	0.22	35,39,39,40	0
2	MLT	A	701	9/9	0.95	0.14	-0.17	25,28,31,33	0
2	MLT	B	1701	9/9	0.96	0.15	-0.61	27,30,34,34	0
3	MN	C	2604	1/1	0.99	0.12	-1.24	29,29,29,29	0
3	MN	B	1604	1/1	0.99	0.13	-1.72	28,28,28,28	0
3	MN	A	4604	1/1	1.00	0.09	-1.91	23,23,23,23	0
3	MN	D	3604	1/1	0.99	0.08	-2.67	28,28,28,28	0

## 6.5 Other polymers

There are no such residues in this entry.