



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:31 am GMT

PDB ID : 1PJ4  
Title : Crystal structure of human mitochondrial NAD(P)<sup>+</sup>-dependent malic enzyme in a pentary complex with natural substrate malate, ATP, Mn<sup>++</sup>, and allosteric activator fumarate.  
Authors : Tao, X.; Yang, Z.; Tong, L.  
Deposited on : 2003-05-31  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

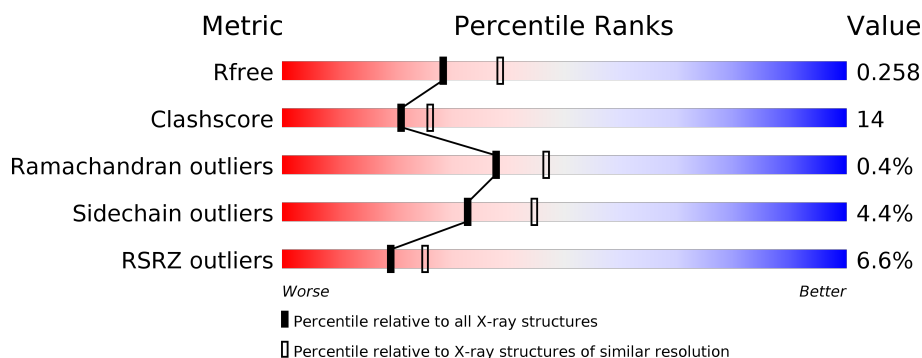
# 1 Overall quality at a glance

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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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>6%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>••</div> </div> </div>
1	B	564	<div> <div>7%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>••</div> </div> </div>
1	C	564	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>••</div> </div> </div>
1	D	564	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>21%</div> <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 crite-

ria:

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:

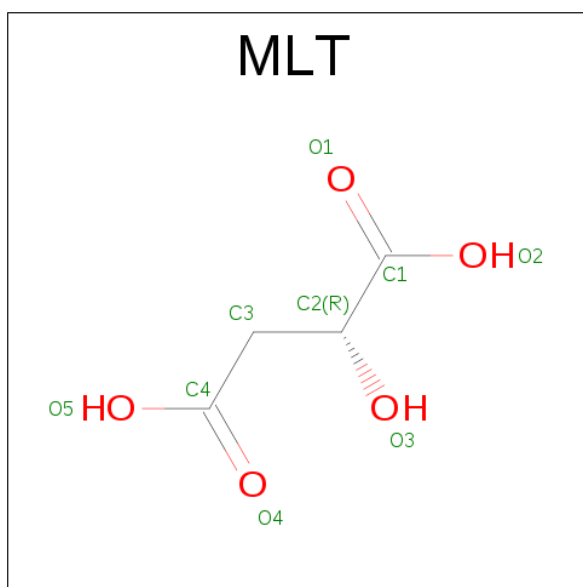
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	177	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:  $C_4H_6O_5$ ).

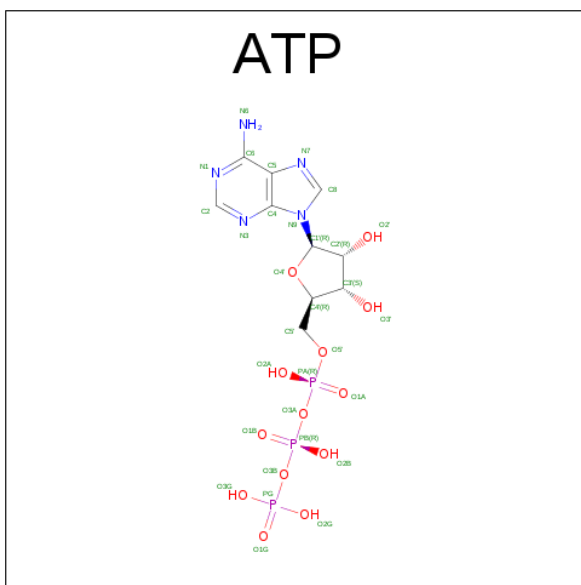


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O	0	0
			9	4	5		
2	C	1	Total	C	O	0	0
			9	4	5		
2	D	1	Total	C	O	0	0
			9	4	5		

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

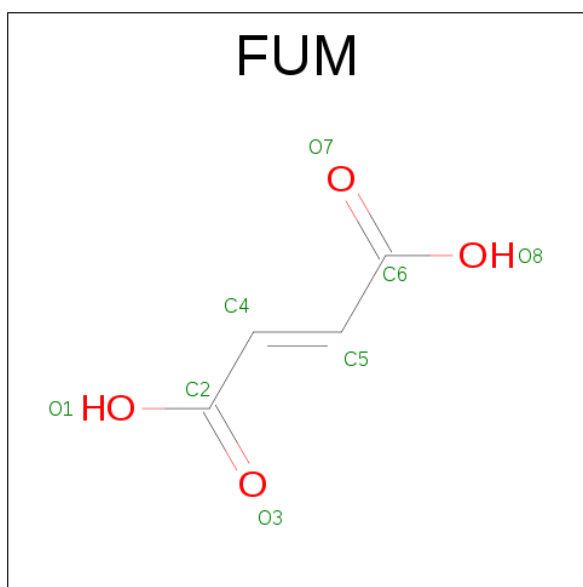
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 5 is FUMARIC ACID (three-letter code: FUM) (formula:  $C_4H_4O_4$ ).



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.

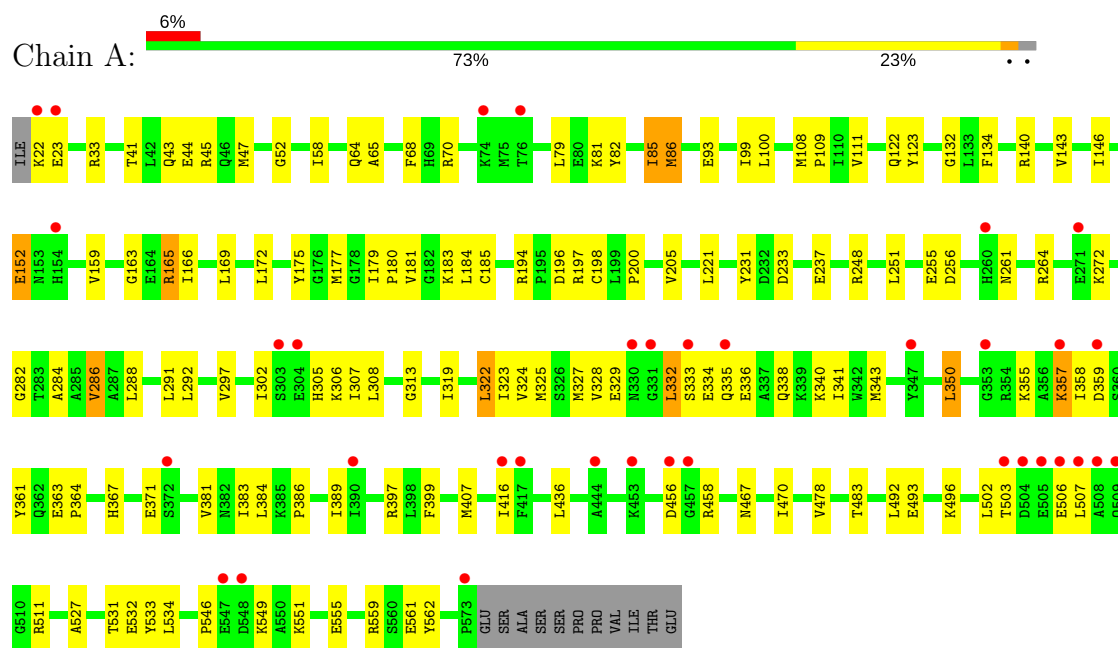
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	165	Total	O	0	0
			165	165		
6	B	176	Total	O	0	0
			176	176		
6	C	169	Total	O	0	0
			169	169		
6	D	176	Total	O	0	0
			176	176		



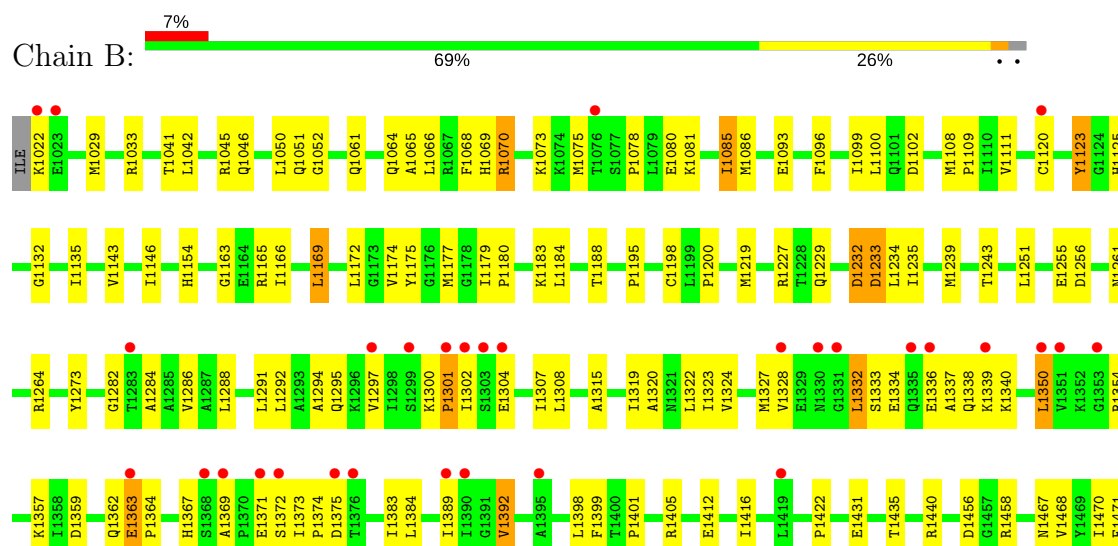
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: NAD-dependent malic enzyme, mitochondrial

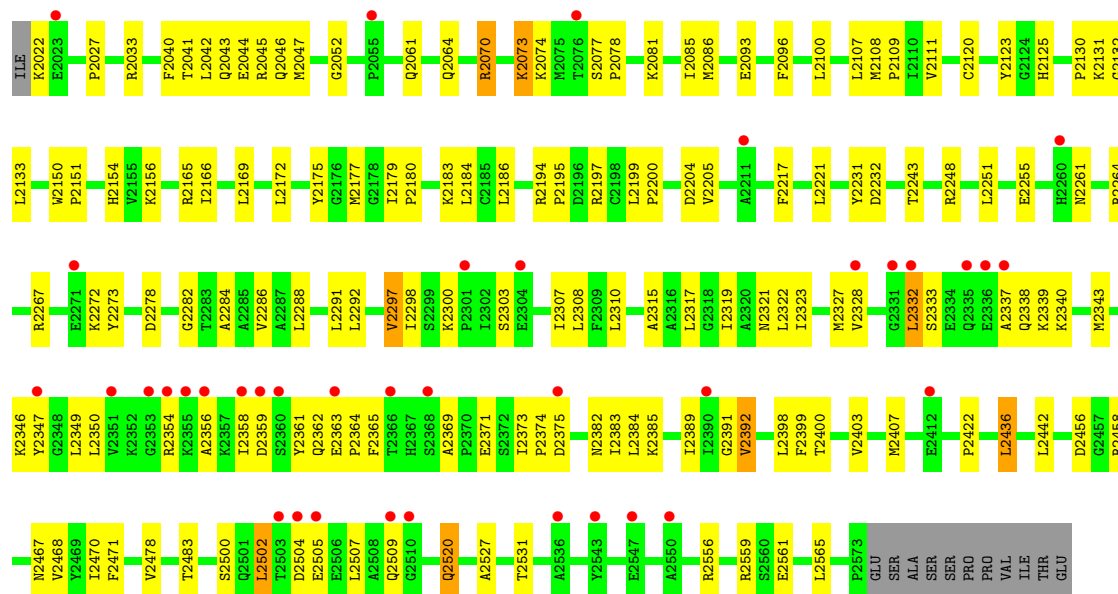


- Molecule 1: NAD-dependent malic enzyme, mitochondrial

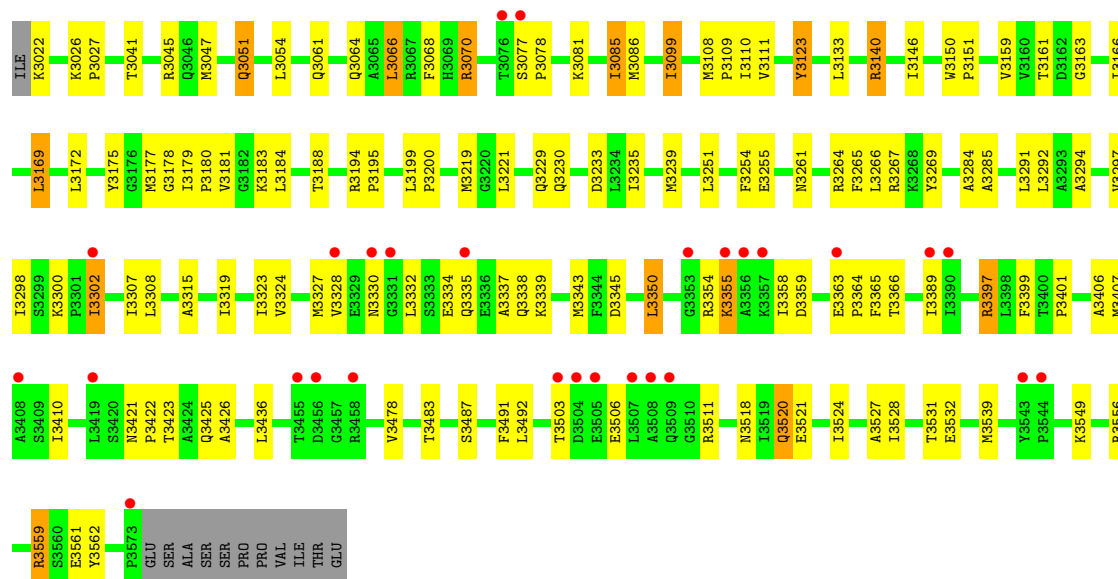
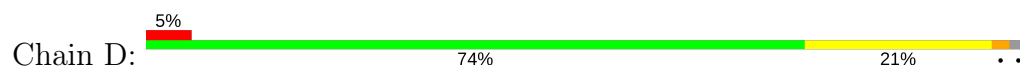




- Molecule 1: NAD-dependent malic enzyme, mitochondrial



- 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
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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: 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.

All (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
1:A:177:MSE:HE2	1:A:181:VAL:HG23	1.43	1.00
1:A:323:ILE:HG22	1:A:327:MSE:HE2	1.44	1.00
1:D:3343:MSE:HE2	1:D:3365:PHE:HB2	1.43	1.00
1:B:1286:VAL:HG21	1:B:1467:ASN:HA	1.41	0.99
1:D:3140:ARG:HH22	1:D:3233:ASP:HB3	1.29	0.94
1:D:3323:ILE:HG22	1:D:3327:MSE:HE2	1.46	0.94
1:A:177:MSE:HE1	1:A:180:PRO:HB2	1.53	0.91
1:A:286:VAL:HG21	1:A:467:ASN:HA	1.52	0.90
1:D:3177:MSE:HE1	1:D:3200:PRO:CB	2.01	0.90
1:D:3520:GLN:H	1:D:3520:GLN:HE21	1.19	0.90
1:B:1315:ALA:CB	1:B:1392:VAL:HG21	2.02	0.89
1:C:2073:LYS:HA	1:C:2073:LYS:HE3	1.53	0.88
1:A:407:MSE:HE2	1:A:407:MSE:HA	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1069:HIS:O	1:B:1073:LYS:HG2	1.76	0.85
1:C:2343:MSE:HE2	1:C:2365:PHE:HB2	1.60	0.83
1:A:177:MSE:HE3	1:A:177:MSE:O	1.77	0.83
1:A:177:MSE:HE1	1:A:200:PRO:HB2	1.61	0.83
1:B:1066:LEU:HD22	1:B:1070:ARG:NH1	1.93	0.83
1:A:478:VAL:HG13	1:A:483:THR:HB	1.61	0.81
1:C:2520:GLN:HE21	1:C:2520:GLN:H	1.27	0.81
1:B:1334:GLU:O	1:B:1338:GLN:HG3	1.80	0.81
1:B:1369:ALA:HB1	1:B:1373:ILE:HD11	1.60	0.81
1:B:1527:ALA:O	1:B:1531:THR:HG23	1.80	0.81
1:C:2343:MSE:HE3	1:C:2350:LEU:HD12	1.61	0.80
1:A:371:GLU:H	1:A:371:GLU:CD	1.83	0.80
1:A:381:VAL:HG13	1:A:407:MSE:HE3	1.64	0.79
1:B:1315:ALA:HB3	1:B:1392:VAL:CG2	2.09	0.79
1:C:2323:ILE:HG22	1:C:2327:MSE:HE2	1.64	0.79
1:C:2286:VAL:HG22	1:C:2470:ILE:HG12	1.64	0.79
1:D:3123:TYR:HD2	1:D:3219:MSE:HE1	1.45	0.78
1:D:3478:VAL:HG13	1:D:3483:THR:HB	1.65	0.78
1:C:2132:GLY:HA3	1:C:2177:MSE:HE1	1.65	0.77
1:A:381:VAL:CG1	1:A:407:MSE:HE3	2.15	0.77
1:A:177:MSE:CE	1:A:180:PRO:HB2	2.13	0.76
1:C:2184:LEU:HD12	1:C:2200:PRO:HG3	1.66	0.75
1:A:551:LYS:O	1:A:555:GLU:HG3	1.88	0.74
1:D:3239:MSE:HE1	1:D:3254:PHE:HZ	1.51	0.73
1:D:3520:GLN:H	1:D:3520:GLN:NE2	1.86	0.72
1:C:2527:ALA:O	1:C:2531:THR:HG23	1.90	0.72
1:C:2286:VAL:CG2	1:C:2467:ASN:HA	2.19	0.72
1:B:1504:ASP:HA	1:B:1507:LEU:HD12	1.72	0.72
1:D:3177:MSE:CE	1:D:3200:PRO:HB2	2.07	0.71
1:C:2520:GLN:NE2	1:C:2520:GLN:H	1.89	0.71
1:A:456:ASP:OD1	1:A:458:ARG:HD3	1.91	0.70
1:A:81:LYS:O	1:A:85:ILE:HG23	1.92	0.70
1:C:2327:MSE:HE3	1:C:2337:ALA:HB1	1.74	0.70
1:C:2085:ILE:HG13	1:C:2086:MSE:N	2.05	0.69
1:B:1301:PRO:HD2	1:B:1304:GLU:OE2	1.93	0.69
1:C:2354:ARG:NE	1:C:2356:ALA:HB3	2.07	0.69
1:B:1085:ILE:HD11	1:B:1111:VAL:HG22	1.75	0.69
1:C:2392:VAL:HG13	1:C:2392:VAL:O	1.92	0.69
1:D:3140:ARG:NH2	1:D:3233:ASP:HB3	2.06	0.69
1:B:1286:VAL:CG2	1:B:1467:ASN:HA	2.22	0.68
1:B:1108:MSE:HB3	1:B:1109:PRO:HD3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MSE:CE	1:A:200:PRO:HB2	2.24	0.67
1:B:1075:MSE:HE2	1:B:1080:GLU:HG2	1.75	0.67
1:D:3194:ARG:HG2	1:D:3194:ARG:HH11	1.60	0.67
1:C:2338:GLN:NE2	1:C:2364:PRO:HB3	2.09	0.67
1:A:86:MSE:HE1	1:A:185:CYS:SG	2.34	0.67
1:B:1505:GLU:CD	1:B:1505:GLU:H	1.98	0.67
1:C:2179:ILE:HB	1:C:2180:PRO:HD3	1.77	0.67
1:D:3298:ILE:HG22	1:D:3300:LYS:HG2	1.78	0.66
1:B:1374:PRO:HG3	1:B:1383:ILE:HD12	1.77	0.66
1:D:3532:GLU:HG2	1:D:3549:LYS:HG2	1.79	0.65
1:A:108:MSE:HB3	1:A:109:PRO:HD3	1.77	0.65
1:D:3334:GLU:O	1:D:3338:GLN:HG3	1.96	0.65
1:A:288:LEU:HD22	1:A:322:LEU:HD12	1.77	0.65
1:B:1350:LEU:HD22	1:B:1354:ARG:CZ	2.27	0.65
1:B:1492:LEU:HD22	1:B:1496:LYS:HE3	1.77	0.65
1:B:1392:VAL:HG22	1:B:1392:VAL:O	1.97	0.64
1:D:3527:ALA:O	1:D:3531:THR:HG22	1.96	0.63
1:C:2504:ASP:HA	1:C:2507:LEU:HD12	1.80	0.63
1:A:334:GLU:O	1:A:338:GLN:HG3	1.99	0.63
1:B:1085:ILE:C	1:B:1085:ILE:HD12	2.18	0.63
1:C:2315:ALA:CB	1:C:2392:VAL:HG21	2.27	0.63
1:D:3163:GLY:HA2	1:D:3166:ILE:HD11	1.81	0.63
1:A:493:GLU:HG3	1:A:533:TYR:CD1	2.34	0.63
1:D:3179:ILE:HB	1:D:3180:PRO:HD3	1.81	0.63
1:B:1041:THR:O	1:B:1045:ARG:HG3	1.98	0.62
1:A:272:LYS:HB2	1:A:272:LYS:NZ	2.15	0.62
1:C:2073:LYS:CA	1:C:2073:LYS:HE3	2.28	0.62
1:D:3081:LYS:O	1:D:3085:ILE:HG23	1.98	0.62
1:A:363:GLU:HB3	1:A:364:PRO:HD3	1.81	0.62
1:A:407:MSE:CE	1:A:407:MSE:HA	2.29	0.62
1:D:3183:LYS:HE3	1:D:3255:GLU:CD	2.21	0.62
1:A:325:MSE:O	1:A:328:VAL:HG22	1.99	0.61
1:B:1286:VAL:HG22	1:B:1470:ILE:CG1	2.30	0.61
1:B:1232:ASP:OD1	1:B:1264:ARG:NH2	2.34	0.61
1:C:2286:VAL:HG22	1:C:2470:ILE:CG1	2.29	0.61
1:B:1081:LYS:O	1:B:1085:ILE:HG23	2.00	0.61
1:D:3327:MSE:HE3	1:D:3337:ALA:HB1	1.83	0.61
1:B:1401:PRO:O	1:B:1405:ARG:HG3	2.00	0.61
1:C:2371:GLU:CD	1:C:2371:GLU:H	2.03	0.61
1:A:302:ILE:O	1:A:340:LYS:HE2	2.01	0.61
1:A:527:ALA:O	1:A:531:THR:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1075:MSE:HE2	1:B:1080:GLU:CD	2.21	0.61
1:B:1515:PRO:HG2	1:B:1518:ASN:HD22	1.66	0.60
1:A:302:ILE:HA	1:A:305:HIS:HD2	1.67	0.60
1:A:288:LEU:CD2	1:A:322:LEU:HD12	2.31	0.60
1:C:2132:GLY:HA3	1:C:2177:MSE:HE2	1.81	0.60
1:C:2243:THR:HG21	1:C:2273:TYR:CD2	2.37	0.60
1:D:3123:TYR:CD2	1:D:3219:MSE:HE1	2.32	0.59
1:A:41:THR:OG1	1:A:44:GLU:HG3	2.03	0.59
1:B:1478:VAL:HG13	1:B:1483:THR:HB	1.85	0.59
1:C:2315:ALA:HB3	1:C:2392:VAL:HG21	1.84	0.59
1:C:2052:GLY:HA3	1:D:3146:ILE:HG23	1.84	0.59
1:B:1183:LYS:HE3	1:B:1255:GLU:CD	2.22	0.59
1:B:1315:ALA:O	1:B:1319:ILE:HG13	2.03	0.58
1:C:2509:GLN:HG2	6:C:222:HOH:O	2.02	0.58
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.86	0.58
1:A:33:ARG:HD3	1:A:93:GLU:OE2	2.03	0.58
1:B:1286:VAL:HG22	1:B:1470:ILE:HG12	1.86	0.58
1:B:1493:GLU:HG3	1:B:1533:TYR:CD1	2.38	0.58
1:A:532:GLU:HG2	1:A:549:LYS:HG3	1.85	0.58
1:C:2288:LEU:HD22	1:C:2322:LEU:HG	1.86	0.58
1:B:1075:MSE:HE2	1:B:1080:GLU:CG	2.33	0.57
1:A:333:SER:OG	1:A:336:GLU:HG2	2.03	0.57
1:D:3108:MSE:HB3	1:D:3109:PRO:HD3	1.87	0.57
1:D:3406:ALA:O	1:D:3410:ILE:HG13	2.05	0.57
1:A:23:GLU:OE2	1:A:23:GLU:HA	2.04	0.57
1:A:172:LEU:O	1:A:175:TYR:HB2	2.04	0.57
1:C:2346:LYS:HE2	1:C:2347:TYR:CE1	2.39	0.57
1:B:1504:ASP:HA	1:B:1507:LEU:CD1	2.33	0.57
1:B:1518:ASN:HB3	1:B:1521:GLU:CD	2.25	0.57
1:B:1556:ARG:HH11	1:B:1556:ARG:HG3	1.70	0.57
1:A:286:VAL:CG2	1:A:467:ASN:HA	2.29	0.56
1:B:1526:ILE:O	1:B:1530:VAL:HG23	2.05	0.56
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.52	0.56
1:B:1179:ILE:HB	1:B:1180:PRO:HD3	1.87	0.56
1:C:2204:ASP:OD2	1:C:2221:LEU:HG	2.04	0.56
1:B:1177:MSE:O	1:B:1180:PRO:HD2	2.05	0.56
1:C:2308:LEU:HB3	1:C:2389:ILE:HD12	1.86	0.56
1:C:2363:GLU:HB3	1:C:2364:PRO:HD3	1.87	0.56
1:C:2154:HIS:O	1:C:2197:ARG:HD2	2.06	0.56
1:C:2383:ILE:HG22	1:C:2384:LEU:HD12	1.87	0.56
1:B:1169:LEU:HD13	1:B:1422:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3177:MSE:O	1:D:3180:PRO:HD2	2.05	0.56
1:D:3350:LEU:HD22	1:D:3354:ARG:CZ	2.36	0.56
1:D:3492:LEU:HD23	1:D:3492:LEU:O	2.06	0.56
1:B:1261:ASN:HD22	1:B:1264:ARG:HD3	1.71	0.56
1:C:2154:HIS:HD2	6:C:231:HOH:O	1.88	0.56
1:A:86:MSE:SE	1:A:111:VAL:HG23	2.56	0.56
1:A:152:GLU:HG2	1:A:196:ASP:O	2.06	0.55
1:C:2061:GLN:HA	1:C:2064:GLN:HE21	1.70	0.55
1:D:3110:ILE:HD12	1:D:3110:ILE:N	2.21	0.55
1:C:2359:ASP:OD2	1:C:2362:GLN:HG3	2.06	0.55
1:A:22:LYS:HG2	1:A:22:LYS:O	2.06	0.55
1:A:307:ILE:HD13	1:A:323:ILE:HD13	1.89	0.55
1:B:1300:LYS:HG3	1:B:1304:GLU:CD	2.27	0.55
1:C:2502:LEU:HD22	1:C:2507:LEU:HG	1.88	0.55
1:D:3068:PHE:CD2	1:D:3099:ILE:HG13	2.41	0.55
1:B:1456:ASP:OD1	1:B:1458:ARG:HD3	2.07	0.55
1:A:132:GLY:CA	1:A:200:PRO:HG2	2.37	0.55
1:A:302:ILE:HA	1:A:305:HIS:CD2	2.42	0.55
1:C:2349:LEU:HD22	1:C:2374:PRO:HG3	1.87	0.55
1:D:3307:ILE:HD13	1:D:3323:ILE:HD13	1.87	0.55
1:D:3528:ILE:O	1:D:3531:THR:CG2	2.55	0.55
1:B:1085:ILE:HD11	1:B:1086:MSE:SE	2.57	0.54
1:C:2315:ALA:O	1:C:2319:ILE:HG13	2.07	0.54
1:C:2040:PHE:HE2	1:C:2565:LEU:HD12	1.72	0.54
1:C:2297:VAL:CG2	1:C:2442:LEU:HD11	2.37	0.54
1:C:2354:ARG:CZ	1:C:2356:ALA:HB3	2.36	0.54
1:C:2500:SER:HB3	6:C:237:HOH:O	2.07	0.54
1:D:3183:LYS:HE3	1:D:3255:GLU:OE2	2.07	0.54
1:B:1559:ARG:HG2	1:B:1559:ARG:HH11	1.72	0.54
1:C:2131:LYS:O	1:C:2177:MSE:HE2	2.07	0.54
1:B:1135:ILE:HD13	1:B:1143:VAL:HG13	1.88	0.54
1:A:506:GLU:O	1:A:511:ARG:HB2	2.08	0.54
1:C:2043:GLN:NE2	1:C:2047:MSE:HE1	2.23	0.54
1:C:2183:LYS:HE2	1:C:2255:GLU:CD	2.28	0.53
1:B:1363:GLU:HB3	1:B:1364:PRO:HD3	1.89	0.53
1:D:3294:ALA:O	1:D:3297:VAL:HG22	2.09	0.53
1:D:3335:GLN:O	1:D:3339:LYS:HG2	2.08	0.53
1:B:1571:GLU:HG3	6:B:670:HOH:O	2.07	0.53
1:C:2165:ARG:O	1:C:2165:ARG:HG2	2.09	0.53
1:B:1066:LEU:HD22	1:B:1070:ARG:HH11	1.70	0.53
1:C:2150:TRP:CE2	1:C:2199:LEU:HD13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1471:PHE:CG	1:B:1472:PRO:HD3	2.44	0.53
1:D:3350:LEU:HD22	1:D:3354:ARG:NH1	2.23	0.53
1:A:350:LEU:HD13	1:A:358:ILE:HD13	1.90	0.53
1:D:3308:LEU:HB3	1:D:3389:ILE:HD12	1.91	0.53
1:A:248:ARG:HH22	1:A:272:LYS:HG3	1.74	0.53
1:B:1261:ASN:HA	1:B:1264:ARG:HD3	1.89	0.53
1:B:1327:MSE:HE3	1:B:1337:ALA:HB1	1.91	0.53
1:C:2108:MSE:HB3	1:C:2109:PRO:HD3	1.89	0.53
1:C:2166:ILE:HG23	1:C:2179:ILE:HG13	1.91	0.53
1:B:1294:ALA:O	1:B:1297:VAL:HG22	2.08	0.52
1:C:2186:LEU:HD13	1:C:2468:VAL:CG2	2.39	0.52
1:B:1389:ILE:HG22	1:B:1416:ILE:HA	1.92	0.52
1:A:350:LEU:HD13	1:A:358:ILE:CD1	2.39	0.52
1:C:2288:LEU:O	1:C:2292:LEU:HD13	2.09	0.52
1:D:3051:GLN:HE21	1:D:3051:GLN:HA	1.75	0.52
1:B:1282:GLY:O	1:B:1286:VAL:HG23	2.09	0.52
1:B:1503:THR:OG1	1:B:1506:GLU:HG3	2.10	0.52
1:D:3169:LEU:HD13	1:D:3422:PRO:HD2	1.92	0.52
1:B:1333:SER:OG	1:B:1336:GLU:HG2	2.10	0.52
1:D:3359:ASP:HB2	6:D:465:HOH:O	2.10	0.52
1:C:2307:ILE:HD12	1:C:2307:ILE:N	2.25	0.51
1:C:2328:VAL:HA	1:C:2332:LEU:O	2.10	0.51
1:D:3315:ALA:HB2	6:D:460:HOH:O	2.10	0.51
1:A:79:LEU:HD22	1:A:122:GLN:HE22	1.75	0.51
1:B:1384:LEU:HD22	1:B:1384:LEU:N	2.25	0.51
1:C:2042:LEU:O	1:C:2046:GLN:HG3	2.11	0.51
1:C:2303:SER:O	1:C:2340:LYS:NZ	2.41	0.51
1:C:2556:ARG:HG3	1:C:2556:ARG:HH11	1.76	0.51
1:B:1302:ILE:HD11	1:B:1327:MSE:HG2	1.93	0.51
1:A:82:TYR:O	1:A:86:MSE:HB2	2.11	0.51
1:A:286:VAL:HG22	1:A:470:ILE:CG1	2.41	0.50
1:A:324:VAL:O	1:A:328:VAL:HG13	2.11	0.50
1:A:297:VAL:CG2	1:A:507:LEU:HG	2.41	0.50
1:B:1132:GLY:CA	1:B:1200:PRO:HG2	2.41	0.50
1:D:3503:THR:OG1	1:D:3506:GLU:HG3	2.11	0.50
1:D:3064:GLN:NE2	1:D:3562:TYR:OH	2.39	0.50
1:B:1075:MSE:CE	1:B:1080:GLU:HG2	2.41	0.50
1:B:1320:ALA:O	1:B:1324:VAL:HG23	2.12	0.50
1:A:546:PRO:O	1:A:549:LYS:HE2	2.11	0.50
1:B:1308:LEU:HB3	1:B:1389:ILE:HD12	1.92	0.50
1:A:492:LEU:O	1:A:492:LEU:HD23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3518:ASN:HB3	1:D:3521:GLU:OE2	2.11	0.50
1:B:1506:GLU:O	1:B:1511:ARG:HB2	2.11	0.50
1:A:503:THR:OG1	1:A:506:GLU:HG3	2.11	0.50
1:D:3041:THR:O	1:D:3045:ARG:HG3	2.11	0.50
1:D:3261:ASN:ND2	1:D:3264:ARG:HH21	2.10	0.50
1:D:3556:ARG:HH11	1:D:3556:ARG:HG3	1.77	0.50
1:B:1099:ILE:HG22	1:B:1100:LEU:HD12	1.93	0.50
1:C:2350:LEU:HD22	1:C:2358:ILE:CD1	2.42	0.50
1:C:2315:ALA:HB3	1:C:2392:VAL:CG2	2.40	0.50
1:D:3332:LEU:H	1:D:3332:LEU:CD1	2.25	0.50
1:D:3528:ILE:O	1:D:3531:THR:HG22	2.12	0.50
1:B:1518:ASN:O	1:B:1521:GLU:HG2	2.12	0.50
1:C:2308:LEU:HD23	1:C:2389:ILE:HD11	1.94	0.50
1:A:79:LEU:HD22	1:A:122:GLN:NE2	2.27	0.49
1:B:1332:LEU:CD1	1:B:1332:LEU:H	2.25	0.49
1:C:2361:TYR:O	1:C:2364:PRO:HD2	2.12	0.49
1:D:3086:MSE:SE	1:D:3111:VAL:HG23	2.62	0.49
1:D:3284:ALA:HA	1:D:3319:ILE:HG12	1.93	0.49
1:A:308:LEU:HB3	1:A:389:ILE:HD12	1.93	0.49
1:B:1033:ARG:HG3	1:B:1033:ARG:HH11	1.77	0.49
1:D:3172:LEU:O	1:D:3175:TYR:HB2	2.11	0.49
1:A:43:GLN:HG2	1:A:47:MSE:HE3	1.94	0.49
1:B:1096:PHE:O	1:B:1100:LEU:HD13	2.12	0.49
1:C:2041:THR:O	1:C:2045:ARG:HG3	2.12	0.49
1:D:3397:ARG:HD3	1:D:3426:ALA:O	2.12	0.49
1:A:332:LEU:HA	1:A:336:GLU:OE2	2.13	0.49
1:C:2392:VAL:HG13	6:C:120:HOH:O	2.12	0.49
1:C:2165:ARG:O	1:C:2165:ARG:NH1	2.46	0.49
1:C:2177:MSE:CE	1:C:2200:PRO:HB2	2.43	0.49
1:C:2298:ILE:HG22	1:C:2300:LYS:HB2	1.95	0.49
1:D:3520:GLN:N	1:D:3520:GLN:HE21	1.99	0.49
1:A:389:ILE:HG23	1:A:399:PHE:CZ	2.48	0.48
1:A:43:GLN:CG	1:A:47:MSE:HE3	2.42	0.48
1:B:1068:PHE:CD2	1:B:1099:ILE:HG13	2.49	0.48
1:B:1288:LEU:O	1:B:1292:LEU:HD13	2.12	0.48
1:D:3506:GLU:O	1:D:3511:ARG:HB2	2.12	0.48
1:B:1392:VAL:HG23	4:B:1601:ATP:O3G	2.14	0.48
1:C:2248:ARG:HH21	1:C:2272:LYS:HG2	1.78	0.48
1:C:2389:ILE:HG23	1:C:2399:PHE:CZ	2.49	0.48
1:A:177:MSE:O	1:A:180:PRO:HD2	2.14	0.48
1:B:1184:LEU:HD12	1:B:1200:PRO:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3188:THR:HG21	1:D:3195:PRO:HG3	1.95	0.48
1:D:3358:ILE:HD13	1:D:3366:THR:OG1	2.13	0.48
1:A:308:LEU:HD23	1:A:389:ILE:HD11	1.94	0.48
1:B:1235:ILE:O	1:B:1239:MSE:HG2	2.13	0.48
1:C:2338:GLN:HE22	1:C:2364:PRO:HB3	1.79	0.48
1:D:3324:VAL:HA	1:D:3327:MSE:HE3	1.96	0.48
1:B:1123:TYR:CD2	1:B:1219:MSE:HE1	2.49	0.48
1:B:1389:ILE:HG23	1:B:1399:PHE:CE1	2.49	0.48
1:C:2371:GLU:N	1:C:2371:GLU:OE2	2.39	0.48
1:C:2310:LEU:HD21	1:C:2398:LEU:HB2	1.96	0.48
1:D:3487:SER:OG	1:D:3539:MSE:HE1	2.13	0.48
1:B:1302:ILE:O	1:B:1340:LYS:HE3	2.13	0.48
1:A:177:MSE:CE	1:A:181:VAL:HG23	2.28	0.48
1:A:282:GLY:O	1:A:286:VAL:HG23	2.13	0.48
1:A:146:ILE:HG23	1:B:1052:GLY:HA3	1.96	0.48
1:B:1511:ARG:NH1	6:B:34:HOH:O	2.46	0.47
1:A:332:LEU:CD1	1:A:332:LEU:H	2.27	0.47
1:A:64:GLN:NE2	1:A:562:TYR:OH	2.39	0.47
1:B:1120:CYS:O	1:B:1175:TYR:HB3	2.14	0.47
1:B:1188:THR:HG21	1:B:1195:PRO:HG3	1.95	0.47
1:A:371:GLU:N	1:A:371:GLU:OE2	2.43	0.47
1:C:2081:LYS:O	1:C:2085:ILE:HG23	2.15	0.47
1:B:1468:VAL:HA	1:B:1471:PHE:CE2	2.50	0.47
1:C:2033:ARG:HD3	1:C:2093:GLU:OE2	2.14	0.47
1:A:324:VAL:HA	1:A:327:MSE:HE3	1.97	0.47
1:B:1286:VAL:HG22	1:B:1470:ILE:HG13	1.97	0.47
1:B:1350:LEU:HD22	1:B:1354:ARG:NH2	2.27	0.47
1:A:140:ARG:NH2	1:A:233:ASP:OD2	2.48	0.47
1:A:165:ARG:O	1:A:256:ASP:HB3	2.14	0.47
1:C:2177:MSE:HE1	1:C:2200:PRO:HB2	1.97	0.47
1:A:163:GLY:HA2	1:A:166:ILE:HD11	1.97	0.47
1:B:1233:ASP:CG	1:B:1234:LEU:N	2.67	0.47
1:A:65:ALA:HA	1:A:99:ILE:HD11	1.97	0.47
1:C:2507:LEU:HB2	6:C:121:HOH:O	2.14	0.47
1:C:2556:ARG:NH1	1:C:2556:ARG:HG3	2.30	0.47
1:A:45:ARG:NH2	1:A:58:ILE:HD13	2.30	0.47
1:A:492:LEU:CD2	1:A:496:LYS:HE2	2.45	0.47
1:A:483:THR:OG1	1:A:534:LEU:HD13	2.15	0.47
1:B:1078:PRO:HD2	6:B:115:HOH:O	2.14	0.47
1:C:2346:LYS:HE2	1:C:2347:TYR:CZ	2.50	0.46
1:D:3235:ILE:HG13	1:D:3265:PHE:CZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2315:ALA:HB2	6:C:424:HOH:O	2.14	0.46
1:C:2505:GLU:CD	1:C:2505:GLU:H	2.19	0.46
1:B:1229:GLN:HA	1:B:1229:GLN:NE2	2.31	0.46
1:C:2172:LEU:O	1:C:2175:TYR:HB2	2.14	0.46
1:A:286:VAL:HG22	1:A:470:ILE:HG13	1.96	0.46
1:C:2458:ARG:HD2	6:C:663:HOH:O	2.14	0.46
1:B:1029:MSE:SE	1:B:1050:LEU:HD22	2.65	0.46
1:B:1046:GLN:HG2	1:B:1051:GLN:HG3	1.97	0.46
1:B:1308:LEU:HD23	1:B:1389:ILE:HD11	1.97	0.46
1:D:3140:ARG:HH22	1:D:3233:ASP:CB	2.13	0.46
1:D:3161:THR:HG22	1:D:3180:PRO:HG2	1.97	0.46
1:D:3332:LEU:HD12	1:D:3332:LEU:N	2.31	0.46
1:B:1243:THR:HG21	1:B:1273:TYR:CD2	2.51	0.46
1:B:1359:ASP:OD2	1:B:1362:GLN:HG3	2.15	0.46
1:B:1556:ARG:HG3	1:B:1556:ARG:NH1	2.30	0.46
1:C:2073:LYS:HA	1:C:2073:LYS:CE	2.36	0.46
1:B:1085:ILE:HD12	1:B:1086:MSE:N	2.31	0.46
1:B:1307:ILE:N	1:B:1307:ILE:HD12	2.31	0.46
1:C:2156:LYS:HA	1:C:2156:LYS:HE2	1.97	0.46
1:C:2369:ALA:HB1	1:C:2373:ILE:HD11	1.98	0.46
1:A:328:VAL:HA	1:A:332:LEU:O	2.16	0.45
1:A:41:THR:O	1:A:45:ARG:HG3	2.16	0.45
1:B:1284:ALA:HA	1:B:1319:ILE:HG12	1.98	0.45
1:A:177:MSE:O	1:A:177:MSE:CE	2.56	0.45
1:B:1261:ASN:ND2	1:B:1264:ARG:HH11	2.14	0.45
1:C:2183:LYS:HE2	1:C:2255:GLU:OE2	2.16	0.45
1:C:2350:LEU:HD23	1:C:2354:ARG:NH1	2.32	0.45
1:D:3169:LEU:HD13	1:D:3422:PRO:CD	2.47	0.45
1:D:3239:MSE:HE3	1:D:3269:TYR:CE1	2.52	0.45
1:A:323:ILE:CG2	1:A:327:MSE:HE2	2.31	0.45
1:A:306:LYS:HB3	1:A:386:PRO:HA	1.99	0.45
1:C:2315:ALA:HB1	1:C:2392:VAL:HG21	1.97	0.45
1:D:3524:ILE:O	1:D:3528:ILE:HG13	2.16	0.45
1:A:183:LYS:HE3	1:A:255:GLU:CD	2.36	0.45
1:B:1075:MSE:HE2	1:B:1080:GLU:OE1	2.17	0.45
1:B:1172:LEU:O	1:B:1175:TYR:HB2	2.17	0.45
1:C:2310:LEU:HB3	1:C:2391:GLY:HA2	1.97	0.45
1:D:3140:ARG:HD2	6:D:637:HOH:O	2.15	0.45
1:D:3239:MSE:HE1	1:D:3254:PHE:CZ	2.40	0.45
1:A:143:VAL:HB	1:A:237:GLU:HG2	1.98	0.45
1:A:284:ALA:HA	1:A:319:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1328:VAL:HA	1:B:1332:LEU:O	2.16	0.45
1:C:2186:LEU:HD13	1:C:2468:VAL:HG23	1.99	0.45
1:B:1033:ARG:NH1	1:B:1093:GLU:OE2	2.49	0.45
1:C:2520:GLN:HB2	6:C:265:HOH:O	2.17	0.45
1:C:2468:VAL:HA	1:C:2471:PHE:CE2	2.52	0.45
1:C:2297:VAL:HG21	1:C:2442:LEU:HD11	1.99	0.45
1:C:2120:CYS:O	1:C:2175:TYR:HB3	2.17	0.44
1:D:3267:ARG:HD2	6:D:109:HOH:O	2.17	0.44
1:A:132:GLY:HA2	1:A:200:PRO:HG2	1.99	0.44
1:A:184:LEU:HD22	1:A:198:CYS:HB3	1.98	0.44
1:B:1061:GLN:HA	1:B:1064:GLN:HE21	1.82	0.44
1:B:1166:ILE:HG23	1:B:1179:ILE:HG13	1.98	0.44
1:A:335:GLN:HB2	6:A:4635:HOH:O	2.18	0.44
1:C:2041:THR:OG1	1:C:2044:GLU:HG3	2.16	0.44
1:C:2520:GLN:HE21	1:C:2520:GLN:N	2.05	0.44
1:D:3150:TRP:HA	1:D:3151:PRO:HD3	1.75	0.44
1:A:313:GLY:HA2	6:A:4711:HOH:O	2.17	0.44
1:B:1551:LYS:NZ	6:B:569:HOH:O	2.50	0.44
1:D:3159:VAL:HG23	1:D:3184:LEU:HD21	1.99	0.44
1:C:2478:VAL:HG13	1:C:2483:THR:HB	2.00	0.44
1:D:3194:ARG:HG2	1:D:3194:ARG:NH1	2.28	0.44
1:A:341:ILE:O	1:A:367:HIS:HE1	2.01	0.44
1:A:389:ILE:HG22	1:A:416:ILE:HA	2.00	0.44
1:B:1154:HIS:HD2	6:B:259:HOH:O	2.01	0.44
1:D:3285:ALA:HB2	1:D:3491:PHE:HB3	1.98	0.44
1:C:2022:LYS:NZ	1:C:2022:LYS:HB3	2.32	0.44
1:C:2382:ASN:O	1:C:2385:LYS:HD2	2.18	0.44
1:D:3421:ASN:ND2	2:D:3701:MLT:H32	2.33	0.44
1:A:159:VAL:HG23	1:A:184:LEU:HD21	1.99	0.44
1:A:205:VAL:HG11	1:A:231:TYR:HD1	1.81	0.44
1:C:2317:LEU:O	1:C:2321:ASN:ND2	2.51	0.44
1:D:3123:TYR:HD2	1:D:3219:MSE:CE	2.24	0.44
1:B:1132:GLY:HA3	1:B:1200:PRO:HG2	2.00	0.43
1:C:2085:ILE:CG1	1:C:2086:MSE:N	2.77	0.43
1:D:3324:VAL:O	1:D:3328:VAL:HG23	2.18	0.43
1:A:272:LYS:HZ3	1:A:272:LYS:HB2	1.83	0.43
1:A:302:ILE:HD12	1:A:305:HIS:HD2	1.83	0.43
1:B:1354:ARG:HB2	6:B:653:HOH:O	2.17	0.43
1:C:2217:PHE:CZ	1:D:3066:LEU:HD23	2.53	0.43
1:B:1069:HIS:HE1	1:B:1102:ASP:OD2	2.01	0.43
1:B:1108:MSE:HE3	1:B:1516:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3492:LEU:HD23	1:D:3492:LEU:C	2.38	0.43
1:B:1169:LEU:HD13	1:B:1422:PRO:CD	2.48	0.43
1:B:1350:LEU:HD22	1:B:1354:ARG:NH1	2.33	0.43
1:C:2070:ARG:O	1:C:2074:LYS:HD3	2.19	0.43
1:D:3345:ASP:HB2	4:D:3601:ATP:O2'	2.19	0.43
1:B:1065:ALA:HA	1:B:1099:ILE:HD11	2.01	0.43
1:C:2436:LEU:HD12	1:C:2436:LEU:HA	1.79	0.43
1:B:1166:ILE:HA	1:B:1256:ASP:OD2	2.19	0.43
1:B:1372:SER:O	1:B:1374:PRO:HD3	2.18	0.43
1:B:1412:GLU:O	1:B:1440:ARG:NH1	2.48	0.43
1:D:3528:ILE:O	1:D:3531:THR:HG23	2.18	0.43
1:A:22:LYS:HZ1	1:C:2027:PRO:HG2	1.83	0.43
1:A:341:ILE:O	1:A:367:HIS:CE1	2.72	0.43
1:A:383:ILE:HG22	1:A:384:LEU:HD12	1.99	0.43
1:B:1227:ARG:HG2	1:B:1227:ARG:HH11	1.84	0.43
1:B:1300:LYS:CG	1:B:1304:GLU:HG3	2.48	0.43
1:D:3559:ARG:HB2	1:D:3559:ARG:HE	1.73	0.43
1:B:1315:ALA:HB2	6:B:272:HOH:O	2.18	0.43
1:B:1431:GLU:O	1:B:1435:THR:HG23	2.18	0.43
1:D:3363:GLU:HB2	1:D:3364:PRO:HD3	2.00	0.43
1:C:2096:PHE:O	1:C:2100:LEU:HD13	2.19	0.42
1:C:2319:ILE:O	1:C:2323:ILE:HG13	2.19	0.42
1:D:3061:GLN:HA	1:D:3064:GLN:HE21	1.84	0.42
1:B:1085:ILE:HD12	1:B:1096:PHE:HE1	1.83	0.42
1:B:1288:LEU:HD22	1:B:1322:LEU:HG	2.00	0.42
1:C:2261:ASN:ND2	1:C:2264:ARG:NH2	2.68	0.42
1:D:3051:GLN:NE2	1:D:3051:GLN:HA	2.34	0.42
1:D:3140:ARG:NH2	1:D:3230:GLN:O	2.50	0.42
1:D:3315:ALA:O	1:D:3319:ILE:HG13	2.19	0.42
1:D:3397:ARG:HA	1:D:3397:ARG:HD3	1.92	0.42
1:B:1184:LEU:HD22	1:B:1198:CYS:HB3	2.00	0.42
1:B:1322:LEU:HD12	1:B:1322:LEU:HA	1.83	0.42
1:C:2077:SER:HA	1:C:2078:PRO:HD3	1.92	0.42
1:C:2284:ALA:HA	1:C:2319:ILE:HG12	2.00	0.42
1:C:2150:TRP:HA	1:C:2151:PRO:HD3	1.83	0.42
1:C:2297:VAL:HG22	1:C:2442:LEU:HD11	2.02	0.42
1:C:2130:PRO:HG3	1:D:3054:LEU:HD23	2.02	0.42
1:D:3066:LEU:HD21	1:D:3070:ARG:HH21	1.84	0.42
1:A:194:ARG:NH1	1:A:197:ARG:NH2	2.67	0.42
1:A:328:VAL:HG23	1:A:329:GLU:N	2.34	0.42
1:D:3363:GLU:CB	1:D:3364:PRO:HD3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MSE:HE2	1:A:181:VAL:CG2	2.30	0.42
1:B:1046:GLN:HG2	1:B:1051:GLN:CG	2.50	0.42
1:B:1042:LEU:O	1:B:1046:GLN:HG3	2.20	0.42
1:B:1295:GLN:HA	1:B:1295:GLN:OE1	2.20	0.42
1:D:3302:ILE:HD11	1:D:3327:MSE:HG2	2.02	0.42
1:D:3389:ILE:HG23	1:D:3399:PHE:CE1	2.54	0.42
1:B:1559:ARG:CG	1:B:1559:ARG:HH11	2.32	0.41
1:D:3199:LEU:HA	1:D:3200:PRO:HD3	1.90	0.41
1:D:3308:LEU:HD23	1:D:3389:ILE:HD11	2.02	0.41
1:D:3528:ILE:HA	1:D:3531:THR:CG2	2.50	0.41
1:C:2243:THR:HG21	1:C:2273:TYR:HD2	1.82	0.41
1:C:2400:THR:OG1	1:C:2403:VAL:HG23	2.20	0.41
1:D:3051:GLN:HE21	1:D:3051:GLN:CA	2.33	0.41
1:D:3401:PRO:HA	1:D:3436:LEU:CD1	2.50	0.41
1:A:359:ASP:OD2	1:A:361:TYR:HD1	2.03	0.41
1:A:381:VAL:HG13	1:A:407:MSE:CE	2.44	0.41
1:B:1022:LYS:C	1:B:1022:LYS:HD3	2.40	0.41
1:C:2166:ILE:HD12	1:C:2179:ILE:HG13	2.02	0.41
1:C:2205:VAL:HG11	1:C:2231:TYR:HD1	1.86	0.41
1:C:2456:ASP:OD1	1:C:2458:ARG:HD3	2.21	0.41
1:D:3178:GLY:O	1:D:3181:VAL:HG13	2.20	0.41
1:D:3298:ILE:CG2	1:D:3300:LYS:HG2	2.48	0.41
1:D:3332:LEU:N	1:D:3332:LEU:CD1	2.84	0.41
1:B:1174:VAL:O	1:B:1174:VAL:HG12	2.20	0.41
1:C:2107:LEU:O	1:C:2111:VAL:HG12	2.20	0.41
1:D:3026:LYS:HB3	1:D:3027:PRO:HD3	2.02	0.41
1:C:2261:ASN:ND2	1:C:2264:ARG:HH21	2.18	0.41
1:D:3239:MSE:CE	1:D:3254:PHE:HZ	2.28	0.41
1:D:3528:ILE:HA	1:D:3531:THR:HG22	2.02	0.41
1:A:343:MSE:HE3	1:A:350:LEU:HG	2.02	0.41
1:B:1163:GLY:HA2	1:B:1166:ILE:HD11	2.01	0.41
1:C:2186:LEU:HD13	1:C:2468:VAL:HG21	2.02	0.41
1:C:2183:LYS:HE3	1:C:2278:ASP:OD2	2.20	0.41
1:D:3407:MSE:HB2	1:D:3407:MSE:HE2	1.90	0.41
1:B:1332:LEU:CD1	1:B:1332:LEU:N	2.83	0.41
1:C:2389:ILE:HB	1:C:2407:MSE:HE2	2.03	0.41
1:D:3177:MSE:O	1:D:3181:VAL:HG12	2.21	0.41
1:D:3300:LYS:HB3	1:D:3300:LYS:HE3	1.89	0.41
1:A:389:ILE:HG23	1:A:399:PHE:CE1	2.55	0.41
1:C:2169:LEU:CD2	1:C:2422:PRO:HD3	2.51	0.41
1:A:134:PHE:O	1:B:1052:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1357:LYS:HD3	1:B:1357:LYS:N	2.35	0.41
1:B:1502:LEU:HD13	1:B:1507:LEU:HD23	2.02	0.41
1:C:2322:LEU:HA	1:C:2322:LEU:HD12	1.87	0.41
1:B:1339:LYS:HA	1:B:1367:HIS:CE1	2.56	0.40
1:C:2154:HIS:O	1:C:2197:ARG:CD	2.69	0.40
1:A:165:ARG:NH1	4:A:4601:ATP:O1G	2.54	0.40
1:C:2194:ARG:HA	1:C:2195:PRO:HD2	1.91	0.40
1:D:3556:ARG:NH1	1:D:3556:ARG:HG3	2.36	0.40
1:D:3077:SER:HA	1:D:3078:PRO:HD3	1.91	0.40
1:D:3177:MSE:C	1:D:3180:PRO:HD2	2.42	0.40
1:D:3355:LYS:HB2	1:D:3355:LYS:NZ	2.37	0.40
1:A:196:ASP:OD1	1:A:197:ARG:HG3	2.21	0.40
1:A:68:PHE:CD2	1:A:99:ILE:HG13	2.57	0.40
1:A:52:GLY:HA3	1:B:1146:ILE:HG23	2.04	0.40
1:C:2282:GLY:O	1:C:2286:VAL:HG23	2.21	0.40
1:C:2194:ARG:HG3	4:C:2602:ATP:C6	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/564 (98%)	531 (96%)	16 (3%)	3 (0%)	32	39
1	B	550/564 (98%)	534 (97%)	14 (2%)	2 (0%)	38	47
1	C	550/564 (98%)	532 (97%)	16 (3%)	2 (0%)	38	47
1	D	550/564 (98%)	531 (96%)	17 (3%)	2 (0%)	38	47
All	All	2200/2256 (98%)	2128 (97%)	63 (3%)	9 (0%)	38	47

All (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
1	D	3397	ARG
1	B	1392	VAL
1	D	3302	ILE
1	C	2392	VAL

### 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	468/465 (101%)	447 (96%)	21 (4%)	32	44
1	B	468/465 (101%)	449 (96%)	19 (4%)	35	48
1	C	468/465 (101%)	450 (96%)	18 (4%)	38	52
1	D	468/465 (101%)	443 (95%)	25 (5%)	26	35
All	All	1872/1860 (101%)	1789 (96%)	83 (4%)	33	45

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	85	ILE
1	A	86	MSE
1	A	100	LEU
1	A	123	TYR
1	A	152	GLU
1	A	165	ARG
1	A	169	LEU
1	A	221	LEU
1	A	251	LEU
1	A	286	VAL
1	A	291	LEU
1	A	292	LEU

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Mol	Chain	Res	Type
1	A	322	LEU
1	A	350	LEU
1	A	355	LYS
1	A	357	LYS
1	A	436	LEU
1	A	502	LEU
1	A	559	ARG
1	A	561	GLU
1	B	1070	ARG
1	B	1085	ILE
1	B	1123	TYR
1	B	1125	HIS
1	B	1165	ARG
1	B	1169	LEU
1	B	1232	ASP
1	B	1233	ASP
1	B	1251	LEU
1	B	1291	LEU
1	B	1301	PRO
1	B	1350	LEU
1	B	1363	GLU
1	B	1371	GLU
1	B	1375	ASP
1	B	1398	LEU
1	B	1492	LEU
1	B	1502	LEU
1	B	1504	ASP
1	C	2070	ARG
1	C	2073	LYS
1	C	2123	TYR
1	C	2125	HIS
1	C	2133	LEU
1	C	2232	ASP
1	C	2251	LEU
1	C	2267	ARG
1	C	2291	LEU
1	C	2297	VAL
1	C	2333	SER
1	C	2339	LYS
1	C	2375	ASP
1	C	2436	LEU
1	C	2502	LEU

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Mol	Chain	Res	Type
1	C	2520	GLN
1	C	2559	ARG
1	C	2561	GLU
1	D	3022	LYS
1	D	3047	MSE
1	D	3051	GLN
1	D	3066	LEU
1	D	3070	ARG
1	D	3085	ILE
1	D	3099	ILE
1	D	3123	TYR
1	D	3133	LEU
1	D	3140	ARG
1	D	3169	LEU
1	D	3221	LEU
1	D	3229	GLN
1	D	3251	LEU
1	D	3266	LEU
1	D	3291	LEU
1	D	3292	LEU
1	D	3330	ASN
1	D	3350	LEU
1	D	3355	LYS
1	D	3423	THR
1	D	3425	GLN
1	D	3520	GLN
1	D	3559	ARG
1	D	3561	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	64	GLN
1	A	122	GLN
1	A	125	HIS
1	A	154	HIS
1	A	230	GLN
1	A	261	ASN
1	A	330	ASN
1	A	335	GLN
1	A	482	ASN

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Mol	Chain	Res	Type
1	B	1051	GLN
1	B	1064	GLN
1	B	1069	HIS
1	B	1154	HIS
1	B	1229	GLN
1	B	1230	GLN
1	B	1261	ASN
1	B	1482	ASN
1	B	1518	ASN
1	C	2043	GLN
1	C	2064	GLN
1	C	2069	HIS
1	C	2122	GLN
1	C	2154	HIS
1	C	2229	GLN
1	C	2230	GLN
1	C	2261	ASN
1	C	2338	GLN
1	C	2520	GLN
1	D	3051	GLN
1	D	3064	GLN
1	D	3069	HIS
1	D	3089	GLN
1	D	3122	GLN
1	D	3230	GLN
1	D	3261	ASN
1	D	3330	ASN
1	D	3338	GLN
1	D	3425	GLN
1	D	3482	ASN
1	D	3520	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	-	27,33,33	1.75	7 (25%)	25,52,52	2.25	2 (8%)
4	ATP	A	4602	-	27,33,33	1.59	6 (22%)	25,52,52	2.26	2 (8%)
5	FUM	A	700	-	1,7,7	1.64	0	0,8,8	0.00	-
2	MLT	A	701	3	2,8,8	0.96	0	4,10,10	1.33	1 (25%)
4	ATP	B	1601	-	27,33,33	1.87	7 (25%)	25,52,52	2.28	3 (12%)
4	ATP	B	1602	-	27,33,33	1.57	6 (22%)	25,52,52	2.31	2 (8%)
5	FUM	B	1700	-	1,7,7	1.57	0	0,8,8	0.00	-
2	MLT	B	1701	3	2,8,8	0.83	0	4,10,10	1.72	1 (25%)
4	ATP	C	2601	-	27,33,33	1.64	7 (25%)	25,52,52	2.33	3 (12%)
4	ATP	C	2602	-	27,33,33	1.50	4 (14%)	25,52,52	2.25	2 (8%)
5	FUM	C	2700	-	1,7,7	1.83	0	0,8,8	0.00	-
2	MLT	C	2701	3	2,8,8	1.03	0	4,10,10	1.12	1 (25%)
4	ATP	D	3601	-	27,33,33	1.68	7 (25%)	25,52,52	2.26	3 (12%)
4	ATP	D	3602	-	27,33,33	1.60	5 (18%)	25,52,52	2.28	2 (8%)
5	FUM	D	3700	-	1,7,7	1.69	0	0,8,8	0.00	-
2	MLT	D	3701	3	2,8,8	0.59	0	4,10,10	1.70	1 (25%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (49) 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	D	3601	ATP	C2'-C1'	-3.10	1.48	1.53
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
4	D	3601	ATP	C5-C4	-2.83	1.34	1.40
4	A	4602	ATP	C5-C4	-2.82	1.34	1.40
4	B	1601	ATP	C2'-C1'	-2.81	1.49	1.53
4	A	4601	ATP	C5-C4	-2.79	1.34	1.40
4	B	1602	ATP	C5-N7	-2.63	1.30	1.39
4	A	4602	ATP	C5-N7	-2.54	1.30	1.39
4	C	2602	ATP	C5-N7	-2.45	1.31	1.39
4	D	3602	ATP	C5-N7	-2.44	1.31	1.39
4	A	4601	ATP	C2'-C1'	-2.42	1.49	1.53
4	D	3601	ATP	C5-N7	-2.41	1.31	1.39
4	A	4601	ATP	C5-N7	-2.41	1.31	1.39
4	C	2601	ATP	C2'-C1'	-2.39	1.49	1.53
4	B	1601	ATP	C5-N7	-2.39	1.31	1.39
4	C	2601	ATP	C5-N7	-2.22	1.31	1.39
4	C	2601	ATP	C2-N1	2.02	1.37	1.33
4	B	1602	ATP	C2-N1	2.04	1.37	1.33
4	B	1601	ATP	C2-N1	2.05	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4602	ATP	C2-N1	2.12	1.37	1.33
4	D	3601	ATP	C2-N1	2.13	1.37	1.33
4	B	1602	ATP	PG-O3B	2.21	1.63	1.60
4	A	4601	ATP	C2-N1	2.24	1.38	1.33
4	A	4602	ATP	PG-O3B	2.30	1.63	1.60
4	D	3602	ATP	C2-N1	2.32	1.38	1.33
4	D	3601	ATP	O4'-C1'	2.84	1.45	1.41
4	C	2601	ATP	C2-N3	3.00	1.37	1.32
4	C	2602	ATP	O4'-C1'	3.05	1.45	1.41
4	D	3602	ATP	C2-N3	3.08	1.37	1.32
4	C	2602	ATP	C2-N3	3.14	1.37	1.32
4	A	4602	ATP	C2-N3	3.14	1.37	1.32
4	C	2601	ATP	O4'-C1'	3.24	1.45	1.41
4	A	4601	ATP	C2-N3	3.31	1.37	1.32
4	B	1602	ATP	C2-N3	3.35	1.37	1.32
4	B	1601	ATP	C2-N3	3.38	1.37	1.32
4	B	1602	ATP	O4'-C1'	3.43	1.46	1.41
4	A	4602	ATP	O4'-C1'	3.50	1.46	1.41
4	D	3601	ATP	C2-N3	3.53	1.38	1.32
4	A	4601	ATP	O4'-C1'	3.59	1.46	1.41
4	B	1601	ATP	O4'-C1'	3.77	1.46	1.41
4	D	3601	ATP	PG-O3B	3.78	1.66	1.60
4	C	2601	ATP	PG-O3B	3.87	1.66	1.60
4	D	3602	ATP	O4'-C1'	4.36	1.47	1.41
4	A	4601	ATP	PG-O3B	4.36	1.67	1.60
4	B	1601	ATP	PG-O3B	5.05	1.68	1.60

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1602	ATP	N3-C2-N1	-9.67	120.44	128.86
4	C	2601	ATP	N3-C2-N1	-9.56	120.53	128.86
4	D	3602	ATP	N3-C2-N1	-9.51	120.58	128.86
4	C	2602	ATP	N3-C2-N1	-9.41	120.66	128.86
4	A	4602	ATP	N3-C2-N1	-9.35	120.71	128.86
4	B	1601	ATP	N3-C2-N1	-9.33	120.74	128.86
4	A	4601	ATP	N3-C2-N1	-9.29	120.77	128.86
4	D	3601	ATP	N3-C2-N1	-9.27	120.79	128.86
2	B	1701	MLT	C4-C3-C2	-3.40	109.61	113.96
2	D	3701	MLT	C4-C3-C2	-3.34	109.69	113.96
2	A	701	MLT	C4-C3-C2	-2.57	110.67	113.96
4	C	2601	ATP	C4'-O4'-C1'	-2.38	107.24	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3601	ATP	C4'-O4'-C1'	-2.17	107.46	109.77
2	C	2701	MLT	C4-C3-C2	-2.09	111.29	113.96
4	B	1601	ATP	C4'-O4'-C1'	-2.00	107.64	109.77
4	D	3602	ATP	C4-C5-N7	4.39	113.65	109.41
4	D	3601	ATP	C4-C5-N7	4.45	113.71	109.41
4	C	2602	ATP	C4-C5-N7	4.47	113.73	109.41
4	A	4601	ATP	C4-C5-N7	4.50	113.75	109.41
4	B	1601	ATP	C4-C5-N7	4.51	113.77	109.41
4	A	4602	ATP	C4-C5-N7	4.53	113.78	109.41
4	C	2601	ATP	C4-C5-N7	4.54	113.80	109.41
4	B	1602	ATP	C4-C5-N7	4.57	113.83	109.41

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	0.34	35 (6%)	20 26	16, 27, 52, 66	0
1	B	538/564 (95%)	0.46	41 (7%)	15 20	16, 27, 53, 68	0
1	C	538/564 (95%)	0.37	38 (7%)	17 22	16, 28, 52, 60	0
1	D	538/564 (95%)	0.34	28 (5%)	28 35	15, 28, 52, 67	0
All	All	2152/2256 (95%)	0.38	142 (6%)	19 25	15, 27, 52, 68	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3353	GLY	6.0
1	B	1510	GLY	5.8
1	C	2358	ILE	5.3
1	A	507	LEU	4.6
1	B	1301	PRO	4.4
1	B	1076	THR	4.0
1	C	2355	LYS	4.0
1	A	353	GLY	4.0
1	C	2510	GLY	4.0
1	A	331	GLY	4.0
1	C	2356	ALA	3.9
1	A	372	SER	3.8
1	B	1543	TYR	3.7
1	D	3455	THR	3.7
1	B	1503	THR	3.7
1	B	1304	GLU	3.6
1	B	1328	VAL	3.6
1	D	3331	GLY	3.6
1	D	3508	ALA	3.6
1	B	1550	ALA	3.5
1	B	1505	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	1375	ASP	3.5
1	A	509	GLN	3.4
1	C	2304	GLU	3.4
1	C	2301	PRO	3.3
1	D	3507	LEU	3.3
1	B	1372	SER	3.3
1	C	2375	ASP	3.3
1	C	2076	THR	3.3
1	A	503	THR	3.2
1	C	2331	GLY	3.2
1	D	3302	ILE	3.2
1	B	1390	ILE	3.1
1	D	3504	ASP	3.1
1	C	2335	GLN	3.1
1	D	3363	GLU	3.1
1	B	1339	LYS	3.1
1	B	1331	GLY	3.0
1	B	1508	ALA	3.0
1	C	2360	SER	3.0
1	D	3328	VAL	3.0
1	D	3543	TYR	3.0
1	B	1371	GLU	3.0
1	C	2336	GLU	2.9
1	C	2504	ASP	2.9
1	A	335	GLN	2.9
1	C	2359	ASP	2.9
1	A	390	ILE	2.9
1	C	2337	ALA	2.8
1	C	2368	SER	2.8
1	D	3390	ILE	2.8
1	D	3335	GLN	2.8
1	A	416	ILE	2.8
1	B	1120	CYS	2.8
1	A	22	LYS	2.8
1	B	1330	ASN	2.7
1	D	3356	ALA	2.7
1	A	504	ASP	2.7
1	A	573	PRO	2.7
1	B	1023	GLU	2.6
1	B	1376	THR	2.6
1	B	1335	GLN	2.6
1	D	3076	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	3330	ASN	2.6
1	C	2547	GLU	2.5
1	C	2536	ALA	2.5
1	C	2503	THR	2.5
1	A	304	GLU	2.5
1	C	2366	THR	2.5
1	C	2363	GLU	2.4
1	D	3544	PRO	2.4
1	A	333	SER	2.4
1	B	1389	ILE	2.4
1	A	76	THR	2.4
1	D	3389	ILE	2.4
1	B	1299	SER	2.4
1	B	1368	SER	2.4
1	A	23	GLU	2.4
1	B	1303	SER	2.4
1	B	1363	GLU	2.4
1	C	2260	HIS	2.4
1	B	1302	ILE	2.3
1	B	1351	VAL	2.3
1	A	154	HIS	2.3
1	B	1571	GLU	2.3
1	C	2390	ILE	2.3
1	D	3505	GLU	2.3
1	C	2347	TYR	2.3
1	D	3503	THR	2.3
1	A	505	GLU	2.3
1	C	2505	GLU	2.3
1	D	3077	SER	2.3
1	C	2023	GLU	2.3
1	A	457	GLY	2.3
1	A	260	HIS	2.3
1	B	1336	GLU	2.2
1	C	2353	GLY	2.2
1	D	3458	ARG	2.2
1	B	1509	GLN	2.2
1	A	303	SER	2.2
1	C	2211	ALA	2.2
1	C	2351	VAL	2.2
1	A	357	LYS	2.2
1	C	2543	TYR	2.2
1	A	271	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1504	ASP	2.2
1	B	1283	THR	2.2
1	A	74	LYS	2.2
1	A	506	GLU	2.2
1	D	3357	LYS	2.2
1	D	3509	GLN	2.2
1	A	347	TYR	2.1
1	A	508	ALA	2.1
1	B	1419	LEU	2.1
1	C	2332	LEU	2.1
1	A	444	ALA	2.1
1	B	1297	VAL	2.1
1	C	2328	VAL	2.1
1	A	453	LYS	2.1
1	B	1022	LYS	2.1
1	A	359	ASP	2.1
1	A	417	PHE	2.1
1	A	547	GLU	2.1
1	C	2055	PRO	2.1
1	B	1369	ALA	2.1
1	B	1353	GLY	2.1
1	D	3355	LYS	2.1
1	B	1350	LEU	2.1
1	D	3419	LEU	2.1
1	A	548	ASP	2.1
1	C	2354	ARG	2.1
1	A	330	ASN	2.0
1	C	2550	ALA	2.0
1	C	2509	GLN	2.0
1	D	3573	PRO	2.0
1	B	1511	ARG	2.0
1	C	2271	GLU	2.0
1	B	1395	ALA	2.0
1	D	3408	ALA	2.0
1	C	2412	GLU	2.0
1	A	456	ASP	2.0
1	D	3456	ASP	2.0

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

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(Å <sup>2</sup> )	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	1.58	35,38,38,39	0
5	FUM	C	2700	8/8	0.94	0.17	1.46	35,37,39,39	0
4	ATP	C	2602	31/31	0.88	0.17	1.37	24,35,73,75	0
2	MLT	C	2701	9/9	0.89	0.17	1.02	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	0.91	25,28,60,62	0
4	ATP	C	2601	31/31	0.86	0.19	0.76	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	0.30	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	0.21	28,30,59,60	0
5	FUM	B	1700	8/8	0.94	0.14	0.20	35,39,39,40	0
2	MLT	A	701	9/9	0.95	0.14	-0.18	25,28,31,33	0
2	MLT	B	1701	9/9	0.96	0.15	-0.58	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	-1.73	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	-2.69	28,28,28,28	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.