



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 17, 2023 – 03:26 AM EST

PDB ID : 2ONK  
Title : ABC transporter ModBC in complex with its binding protein ModA  
Authors : Hollenstein, K.; Frei, D.C.; Locher, K.P.  
Deposited on : 2007-01-24  
Resolution : 3.10 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)

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

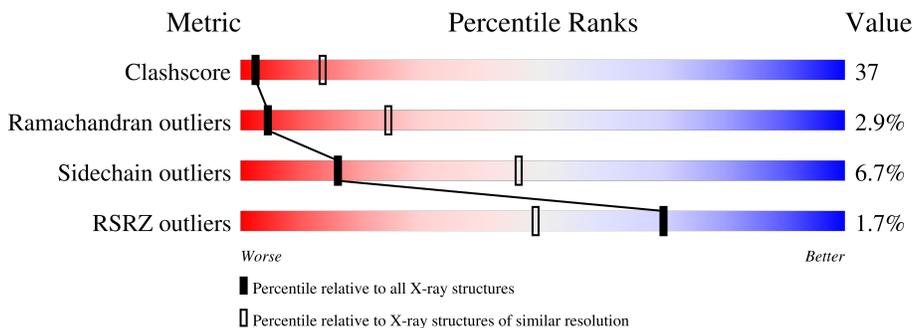
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	240	 2% 42% 52% 6%
1	B	240	 2% 41% 52% 6%
1	F	240	 2% 39% 54% 7%
1	G	240	 7% 39% 55% 6%
2	C	284	 45% 38% 5% 11%
2	D	284	 45% 38% 5% 11%

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Mol	Chain	Length	Quality of chain
2	H	284	
2	I	284	
3	E	314	
3	J	314	

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
4	PO4	B	802	-	X	-	-
4	PO4	F	803	-	X	-	-
4	PO4	G	804	-	X	-	-
6	WO4	E	701	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 20218 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 Molybdate/tungstate ABC transporter, ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	240	1902	1212	349	334	7	0	0	0
1	B	240	1902	1212	349	334	7	0	0	0
1	F	240	1902	1212	349	334	7	0	0	0
1	G	240	1902	1212	349	334	7	0	0	0

- Molecule 2 is a protein called Molybdate/tungstate ABC transporter, permease protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	252	1901	1279	297	320	5	0	0	0
2	D	252	1901	1279	297	320	5	0	0	0
2	H	252	1901	1279	297	320	5	0	0	0
2	I	252	1901	1279	297	320	5	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	cloning artifact	UNP O30143
C	-21	GLY	-	cloning artifact	UNP O30143
C	-20	HIS	-	expression tag	UNP O30143
C	-19	HIS	-	expression tag	UNP O30143
C	-18	HIS	-	expression tag	UNP O30143
C	-17	HIS	-	expression tag	UNP O30143
C	-16	HIS	-	expression tag	UNP O30143
C	-15	HIS	-	expression tag	UNP O30143

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	expression tag	UNP O30143
C	-13	HIS	-	expression tag	UNP O30143
C	-12	HIS	-	expression tag	UNP O30143
C	-11	HIS	-	expression tag	UNP O30143
C	-10	SER	-	cloning artifact	UNP O30143
C	-9	SER	-	cloning artifact	UNP O30143
C	-8	GLY	-	cloning artifact	UNP O30143
C	-7	GLU	-	cloning artifact	UNP O30143
C	-6	ASN	-	cloning artifact	UNP O30143
C	-5	LEU	-	cloning artifact	UNP O30143
C	-4	TYR	-	cloning artifact	UNP O30143
C	-3	PHE	-	cloning artifact	UNP O30143
C	-2	GLN	-	cloning artifact	UNP O30143
C	-1	GLY	-	cloning artifact	UNP O30143
C	0	HIS	-	cloning artifact	UNP O30143
D	-22	MET	-	cloning artifact	UNP O30143
D	-21	GLY	-	cloning artifact	UNP O30143
D	-20	HIS	-	expression tag	UNP O30143
D	-19	HIS	-	expression tag	UNP O30143
D	-18	HIS	-	expression tag	UNP O30143
D	-17	HIS	-	expression tag	UNP O30143
D	-16	HIS	-	expression tag	UNP O30143
D	-15	HIS	-	expression tag	UNP O30143
D	-14	HIS	-	expression tag	UNP O30143
D	-13	HIS	-	expression tag	UNP O30143
D	-12	HIS	-	expression tag	UNP O30143
D	-11	HIS	-	expression tag	UNP O30143
D	-10	SER	-	cloning artifact	UNP O30143
D	-9	SER	-	cloning artifact	UNP O30143
D	-8	GLY	-	cloning artifact	UNP O30143
D	-7	GLU	-	cloning artifact	UNP O30143
D	-6	ASN	-	cloning artifact	UNP O30143
D	-5	LEU	-	cloning artifact	UNP O30143
D	-4	TYR	-	cloning artifact	UNP O30143
D	-3	PHE	-	cloning artifact	UNP O30143
D	-2	GLN	-	cloning artifact	UNP O30143
D	-1	GLY	-	cloning artifact	UNP O30143
D	0	HIS	-	cloning artifact	UNP O30143
H	-22	MET	-	cloning artifact	UNP O30143
H	-21	GLY	-	cloning artifact	UNP O30143
H	-20	HIS	-	expression tag	UNP O30143
H	-19	HIS	-	expression tag	UNP O30143

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-18	HIS	-	expression tag	UNP O30143
H	-17	HIS	-	expression tag	UNP O30143
H	-16	HIS	-	expression tag	UNP O30143
H	-15	HIS	-	expression tag	UNP O30143
H	-14	HIS	-	expression tag	UNP O30143
H	-13	HIS	-	expression tag	UNP O30143
H	-12	HIS	-	expression tag	UNP O30143
H	-11	HIS	-	expression tag	UNP O30143
H	-10	SER	-	cloning artifact	UNP O30143
H	-9	SER	-	cloning artifact	UNP O30143
H	-8	GLY	-	cloning artifact	UNP O30143
H	-7	GLU	-	cloning artifact	UNP O30143
H	-6	ASN	-	cloning artifact	UNP O30143
H	-5	LEU	-	cloning artifact	UNP O30143
H	-4	TYR	-	cloning artifact	UNP O30143
H	-3	PHE	-	cloning artifact	UNP O30143
H	-2	GLN	-	cloning artifact	UNP O30143
H	-1	GLY	-	cloning artifact	UNP O30143
H	0	HIS	-	cloning artifact	UNP O30143
I	-22	MET	-	cloning artifact	UNP O30143
I	-21	GLY	-	cloning artifact	UNP O30143
I	-20	HIS	-	expression tag	UNP O30143
I	-19	HIS	-	expression tag	UNP O30143
I	-18	HIS	-	expression tag	UNP O30143
I	-17	HIS	-	expression tag	UNP O30143
I	-16	HIS	-	expression tag	UNP O30143
I	-15	HIS	-	expression tag	UNP O30143
I	-14	HIS	-	expression tag	UNP O30143
I	-13	HIS	-	expression tag	UNP O30143
I	-12	HIS	-	expression tag	UNP O30143
I	-11	HIS	-	expression tag	UNP O30143
I	-10	SER	-	cloning artifact	UNP O30143
I	-9	SER	-	cloning artifact	UNP O30143
I	-8	GLY	-	cloning artifact	UNP O30143
I	-7	GLU	-	cloning artifact	UNP O30143
I	-6	ASN	-	cloning artifact	UNP O30143
I	-5	LEU	-	cloning artifact	UNP O30143
I	-4	TYR	-	cloning artifact	UNP O30143
I	-3	PHE	-	cloning artifact	UNP O30143
I	-2	GLN	-	cloning artifact	UNP O30143
I	-1	GLY	-	cloning artifact	UNP O30143
I	0	HIS	-	cloning artifact	UNP O30143

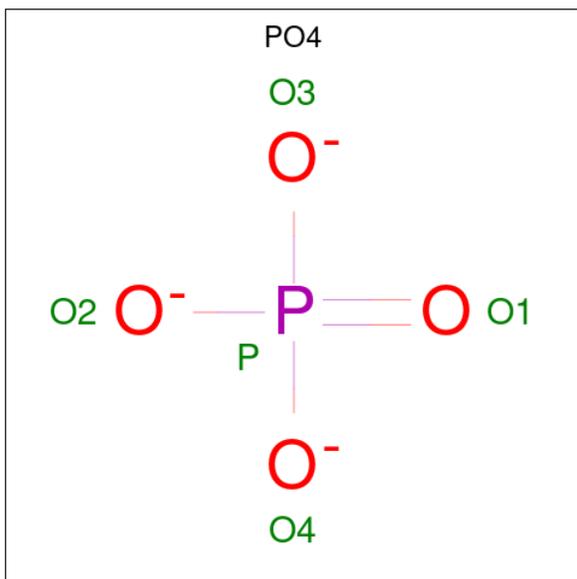
- Molecule 3 is a protein called Molybdate/tungstate binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	311	Total 2489	C 1590	N 414	O 474	S 11	0	0	0
3	J	310	Total 2481	C 1585	N 415	O 469	S 12	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	29	GLY	-	cloning artifact	UNP O30142
E	30	HIS	-	cloning artifact	UNP O30142
E	31	MET	-	cloning artifact	UNP O30142
J	29	GLY	-	cloning artifact	UNP O30142
J	30	HIS	-	cloning artifact	UNP O30142
J	31	MET	-	cloning artifact	UNP O30142

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

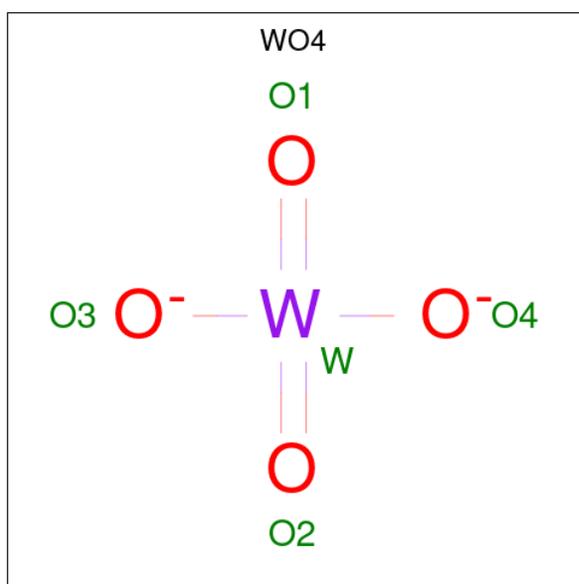


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
4	A	1	Total 5	O 4	P 1	0	0
4	B	1	Total 5	O 4	P 1	0	0
4	F	1	Total 5	O 4	P 1	0	0
4	G	1	Total 5	O 4	P 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0
5	G	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0
5	J	1	Total Mg 1 1	0	0

- Molecule 6 is TUNGSTATE(VI)ION (three-letter code: WO4) (formula: O<sub>4</sub>W).

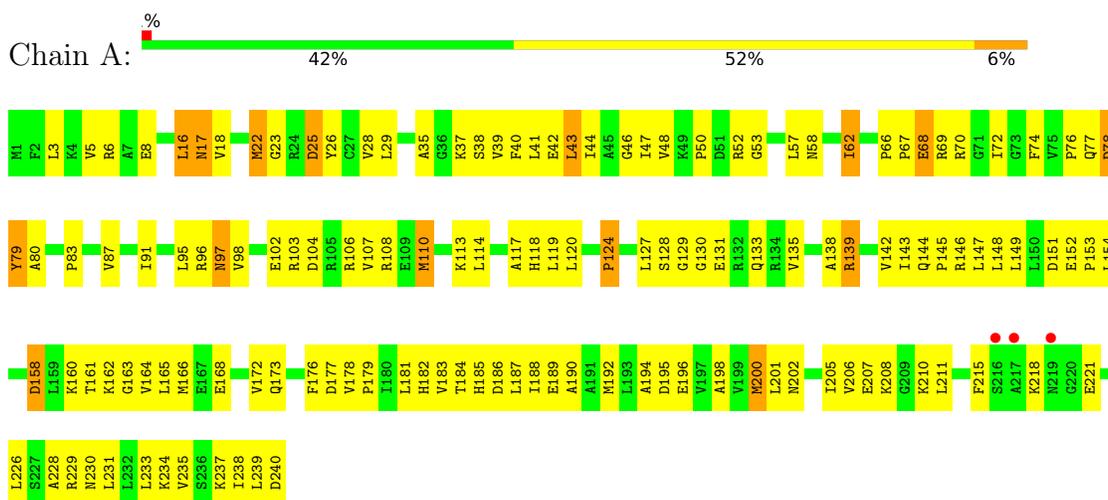


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total O W 5 4 1	0	0
6	J	1	Total O W 5 4 1	0	0

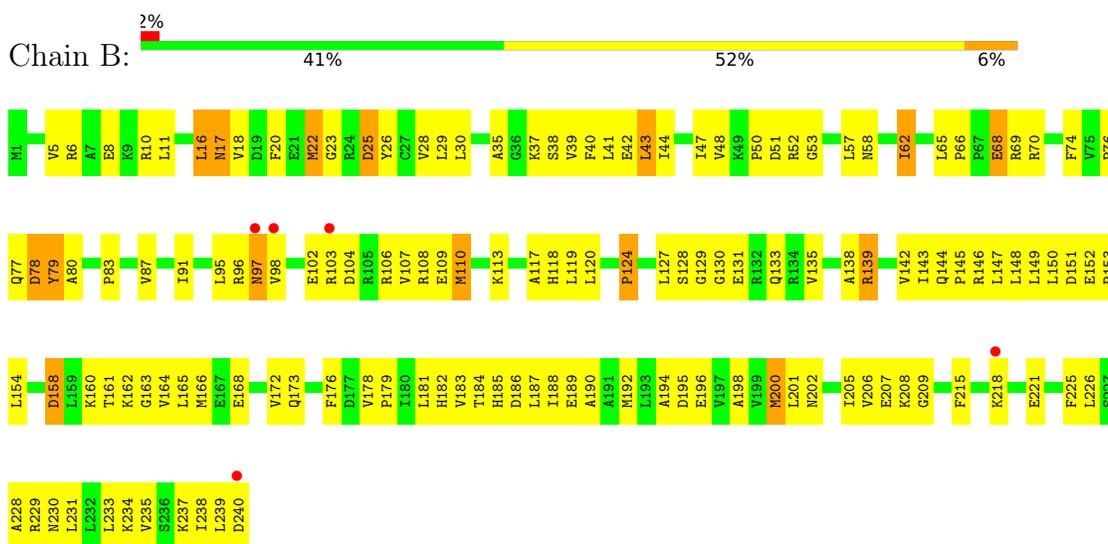
### 3 Residue-property plots [i](#)

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: Molybdate/tungstate ABC transporter, ATP-binding protein

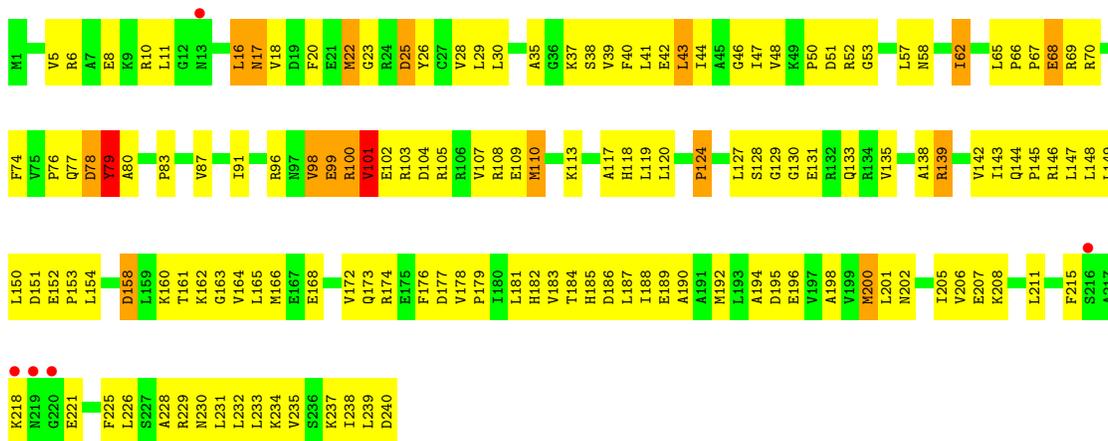


- Molecule 1: Molybdate/tungstate ABC transporter, ATP-binding protein

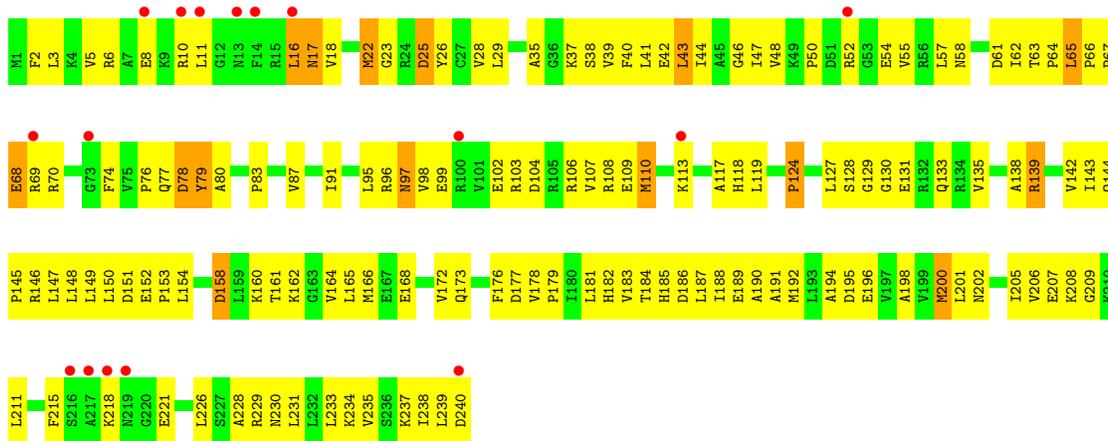


- Molecule 1: Molybdate/tungstate ABC transporter, ATP-binding protein

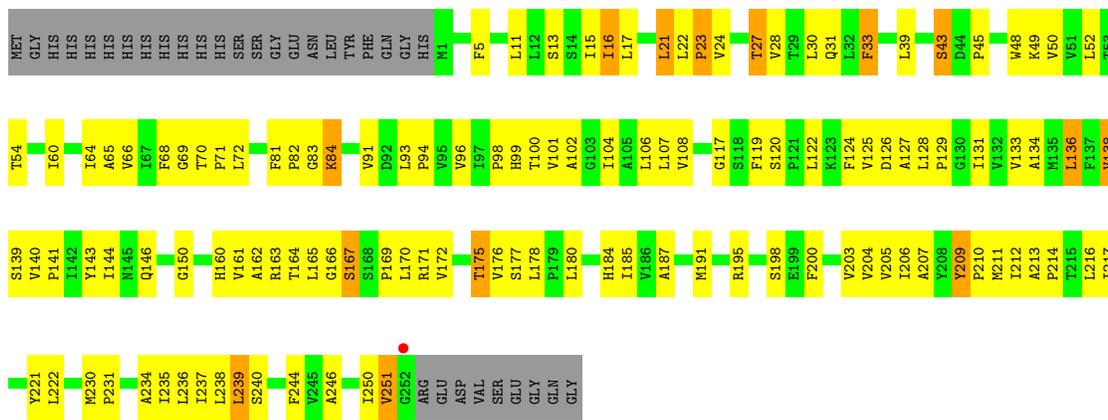




• Molecule 1: Molybdate/tungstate ABC transporter, ATP-binding protein



• Molecule 2: Molybdate/tungstate ABC transporter, permease protein



• Molecule 2: Molybdate/tungstate ABC transporter, permease protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.03Å 171.20Å 158.47Å 90.00° 98.79° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 29.69 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.10) 100.0 (29.69-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 3.11Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.256 , 0.283 0.243 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	92.1	Xtrriage
Anisotropy	0.095	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 92.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	20218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: PO4, MG, WO4

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	0.43	0/1930	0.75	1/2596 (0.0%)
1	B	0.41	0/1930	0.74	2/2596 (0.1%)
1	F	0.44	0/1930	0.76	2/2596 (0.1%)
1	G	0.42	0/1930	0.74	2/2596 (0.1%)
2	C	0.45	0/1945	0.66	1/2662 (0.0%)
2	D	0.48	0/1945	0.71	1/2662 (0.0%)
2	H	0.42	0/1945	0.65	1/2662 (0.0%)
2	I	0.46	0/1945	0.70	1/2662 (0.0%)
3	E	0.44	0/2540	0.68	0/3435
3	J	0.43	0/2533	0.68	0/3425
All	All	0.44	0/20573	0.71	11/27892 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	I	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ASP	CB-CG-OD1	5.80	123.52	118.30
1	F	78	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	78	ASP	CB-CG-OD1	5.76	123.48	118.30
2	D	210	PRO	N-CA-C	-5.66	97.39	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	210	PRO	N-CA-C	-5.63	97.46	112.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	209	TYR	Sidechain
2	I	209	TYR	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	1902	0	2002	175	1
1	B	1902	0	2002	158	0
1	F	1902	0	2002	184	1
1	G	1902	0	2002	182	0
2	C	1901	0	2044	161	0
2	D	1901	0	2044	152	0
2	H	1901	0	2044	165	0
2	I	1901	0	2044	161	0
3	E	2489	0	2487	196	0
3	J	2481	0	2477	197	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
4	F	5	0	0	1	0
4	G	5	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
6	E	5	0	0	2	0
6	J	5	0	0	1	0
All	All	20218	0	21148	1547	1

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 37.

The worst 5 of 1547 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:G:166:MET:HE1	1:G:189:GLU:HA	1.20	1.17
1:B:187:LEU:HB3	1:B:229:ARG:NH1	1.62	1.15
1:A:187:LEU:HB3	1:A:229:ARG:NH1	1.62	1.15
1:B:166:MET:HE1	1:B:189:GLU:HA	1.21	1.14
1:G:187:LEU:HB3	1:G:229:ARG:NH1	1.62	1.14

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:NZ	1:F:174:ARG:O[1_546]	2.14	0.06

## 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	238/240 (99%)	203 (85%)	31 (13%)	4 (2%)	9	36
1	B	238/240 (99%)	202 (85%)	32 (13%)	4 (2%)	9	36
1	F	238/240 (99%)	202 (85%)	29 (12%)	7 (3%)	4	24
1	G	238/240 (99%)	194 (82%)	40 (17%)	4 (2%)	9	36
2	C	250/284 (88%)	193 (77%)	50 (20%)	7 (3%)	5	25
2	D	250/284 (88%)	192 (77%)	48 (19%)	10 (4%)	3	17
2	H	250/284 (88%)	194 (78%)	49 (20%)	7 (3%)	5	25
2	I	250/284 (88%)	192 (77%)	49 (20%)	9 (4%)	3	20
3	E	309/314 (98%)	254 (82%)	44 (14%)	11 (4%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	308/314 (98%)	254 (82%)	43 (14%)	11 (4%)	3	20
All	All	2569/2724 (94%)	2080 (81%)	415 (16%)	74 (3%)	4	24

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	100	ARG
2	C	84	LYS
2	D	84	LYS
2	D	115	LEU
2	H	84	LYS

### 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	202/202 (100%)	187 (93%)	15 (7%)	13	42
1	B	202/202 (100%)	187 (93%)	15 (7%)	13	42
1	F	202/202 (100%)	186 (92%)	16 (8%)	12	40
1	G	202/202 (100%)	189 (94%)	13 (6%)	17	48
2	C	206/233 (88%)	193 (94%)	13 (6%)	18	48
2	D	206/233 (88%)	193 (94%)	13 (6%)	18	48
2	H	206/233 (88%)	193 (94%)	13 (6%)	18	48
2	I	206/233 (88%)	193 (94%)	13 (6%)	18	48
3	E	273/275 (99%)	256 (94%)	17 (6%)	18	49
3	J	271/275 (98%)	254 (94%)	17 (6%)	18	48
All	All	2176/2290 (95%)	2031 (93%)	145 (7%)	16	46

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	113	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	J	329	ASP
3	E	185	ASN
3	J	109	MET
1	G	22	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	185	ASN
3	J	130	ASN
3	E	192	ASN
3	E	274	ASN
3	J	183	ASN

### 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](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	PO4	F	803	5	4,4,4	2.89	4 (100%)	6,6,6	0.47	0
6	WO4	J	702	3	2,4,4	11.58	2 (100%)	-		
6	WO4	E	701	3	2,4,4	11.54	2 (100%)	-		
4	PO4	A	801	5	4,4,4	3.01	3 (75%)	6,6,6	0.49	0
4	PO4	G	804	5	4,4,4	2.95	4 (100%)	6,6,6	0.48	0
4	PO4	B	802	5	4,4,4	2.80	4 (100%)	6,6,6	0.39	0

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	701	WO4	W-O2	12.11	2.03	1.74
6	J	702	WO4	W-O2	12.11	2.03	1.74
6	J	702	WO4	W-O1	11.03	2.00	1.74
6	E	701	WO4	W-O1	10.94	2.00	1.74
4	A	801	PO4	P-O1	4.49	1.61	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	803	PO4	1	0
6	J	702	WO4	1	0
6	E	701	WO4	2	0
4	A	801	PO4	1	0
4	G	804	PO4	1	0
4	B	802	PO4	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	240/240 (100%)	-0.44	3 (1%) 77 59	32, 73, 148, 178	0
1	B	240/240 (100%)	-0.11	5 (2%) 63 43	60, 115, 183, 200	0
1	F	240/240 (100%)	-0.25	5 (2%) 63 43	38, 96, 168, 197	0
1	G	240/240 (100%)	0.14	16 (6%) 17 7	62, 134, 188, 200	0
2	C	252/284 (88%)	-0.56	1 (0%) 92 84	33, 66, 134, 200	0
2	D	252/284 (88%)	-0.52	3 (1%) 79 61	39, 76, 146, 200	0
2	H	252/284 (88%)	-0.24	5 (1%) 65 44	40, 93, 175, 199	0
2	I	252/284 (88%)	-0.29	2 (0%) 86 72	52, 102, 169, 200	0
3	E	311/314 (99%)	-0.48	1 (0%) 94 88	36, 81, 148, 188	0
3	J	310/314 (98%)	-0.24	3 (0%) 82 67	32, 87, 156, 198	0
All	All	2589/2724 (95%)	-0.31	44 (1%) 70 49	32, 91, 169, 200	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	240	ASP	4.5
1	G	13	ASN	4.1
1	F	216	SER	3.9
2	H	2	ARG	3.6
1	G	218	LYS	3.6

### 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	E	705	1/1	0.85	0.13	86,86,86,86	0
5	MG	F	703	1/1	0.86	0.24	89,89,89,89	0
5	MG	G	704	1/1	0.90	0.12	83,83,83,83	0
5	MG	B	702	1/1	0.90	0.21	87,87,87,87	0
4	PO4	G	804	5/5	0.92	0.11	99,99,99,99	0
4	PO4	B	802	5/5	0.96	0.14	84,84,84,84	0
5	MG	A	701	1/1	0.96	0.13	75,75,75,75	0
4	PO4	F	803	5/5	0.97	0.13	60,60,60,60	0
5	MG	J	706	1/1	0.97	0.25	42,42,42,42	0
4	PO4	A	801	5/5	0.98	0.10	60,60,60,60	0
6	WO4	E	701	5/5	0.99	0.19	49,49,49,49	0
6	WO4	J	702	5/5	0.99	0.20	48,48,48,48	0

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

There are no such residues in this entry.