



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:56 PM GMT

PDB ID : 2OGX  
Title : The crystal structure of the molybdenum storage protein from *Azotobacter vinelandii* loaded with polyoxotungstates (WSto)  
Authors : Schemberg, J.; Warkentin, E.; Ermler, U.  
Deposited on : 2007-01-09  
Resolution : 1.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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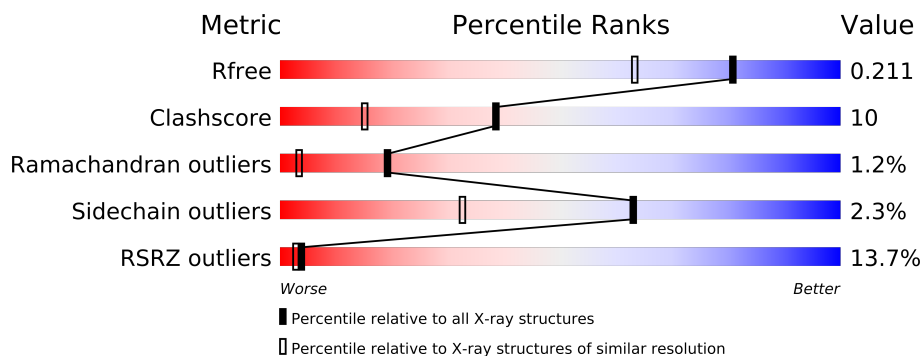
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 1.60 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))
$R_{free}$	66092	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	276	
2	B	270	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	W	A	2025	-	X
7	W	A	2026	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4350 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Molybdenum storage protein subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	Se	0	9	0
			1869	1177	355	334	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	INITIATING METHIONINE	UNP P84308
A	51	MSE	MET	MODIFIED RESIDUE	UNP P84308
A	119	MSE	MET	MODIFIED RESIDUE	UNP P84308
A	236	MSE	MET	MODIFIED RESIDUE	UNP P84308

- Molecule 2 is a protein called Molybdenum storage protein subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	268	Total	C	N	O	S	Se	0	10	0
			2019	1283	354	374	2	6			

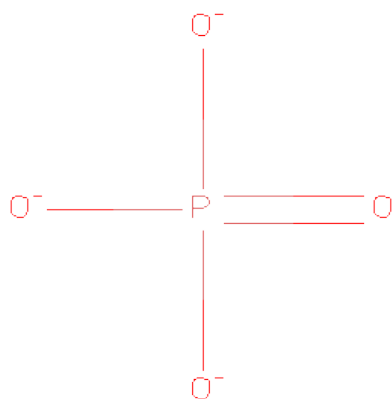
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	MSE	MET	MODIFIED RESIDUE	UNP P84253
B	113	MSE	MET	MODIFIED RESIDUE	UNP P84253
B	149	MSE	MET	MODIFIED RESIDUE	UNP P84253
B	156	MSE	MET	MODIFIED RESIDUE	UNP P84253
B	185	MSE	MET	MODIFIED RESIDUE	UNP P84253
B	216	MSE	MET	MODIFIED RESIDUE	UNP P84253

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

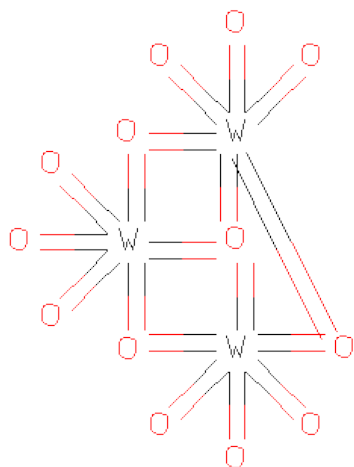
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



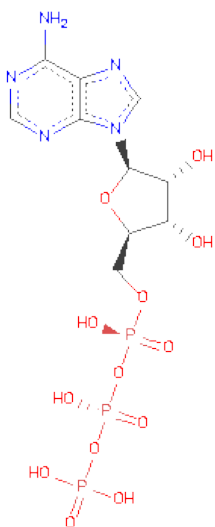
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is TRI-TUNGSTEN(VI) OXIDE COMPLEX (three-letter code: WO3) (formula:  $\text{O}_{13}\text{W}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	W	0	0
			5	4	1		

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 7 is TUNGSTEN ION (three-letter code: W) (formula: W).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	13	Total	W	0	0
			13	13		
7	A	10	Total	W	0	0
			10	10		

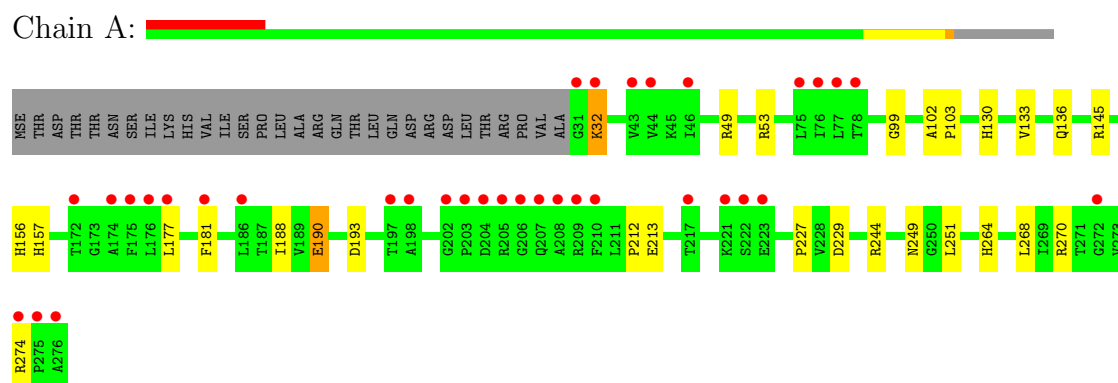
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	198	Total	O	0	0
			198	198		
8	B	193	Total	O	0	1
			194	194		

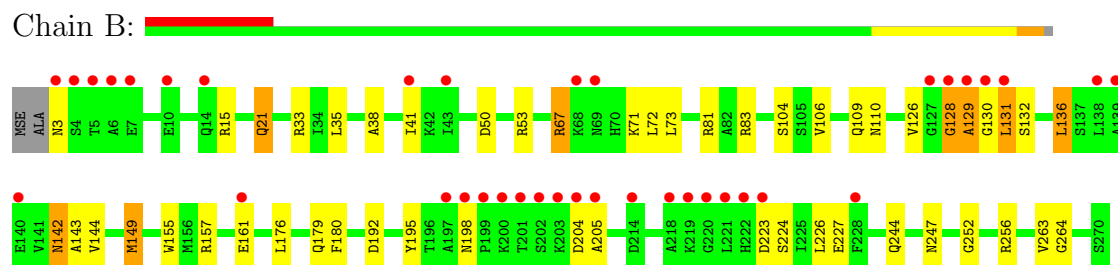
### 3 Residue-property plots

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: Molybdenum storage protein subunit alpha



- Molecule 2: Molybdenum storage protein subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.40Å 114.40Å 233.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 1.60 27.78 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (10.00-1.60) 95.5 (27.78-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	6.50	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.173 , 0.196 0.188 , 0.211	Depositor DCC
$R_{free}$ test set	5695 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 53.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 113025 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4350	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, PO4, W, WO3

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	0.85	2/1953 (0.1%)	0.92	2/2652 (0.1%)
2	B	0.80	0/2092	0.95	7/2832 (0.2%)
All	All	0.83	2/4045 (0.0%)	0.93	9/5484 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190[A]	GLU	CB-CG	6.06	1.63	1.52
1	A	190[B]	GLU	CB-CG	6.06	1.63	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	33	ARG	NE-CZ-NH2	-7.30	116.65	120.30
2	B	149	MSE	CG-SE-CE	6.44	113.06	98.90
1	A	49	ARG	NE-CZ-NH1	6.36	123.48	120.30
2	B	157	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	A	229	ASP	CB-CG-OD1	-5.83	113.05	118.30
2	B	136	LEU	CB-CG-CD1	-5.81	101.12	111.00
2	B	33	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	B	50	ASP	CB-CG-OD1	5.16	122.94	118.30
2	B	50	ASP	CB-CG-OD2	-5.09	113.72	118.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1869	0	1910	33	0
2	B	2019	0	2073	49	0
3	A	1	0	0	0	0
4	B	10	0	0	0	0
5	A	5	0	0	0	0
6	A	31	0	12	1	0
7	A	10	0	0	0	0
7	B	13	0	0	0	0
8	A	198	0	0	9	0
8	B	194	0	0	5	0
All	All	4350	0	3995	78	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (78) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:32:LYS:HA	1:A:32:LYS:HE3	1.33	1.11
2:B:129:ALA:HB3	8:B:3452:HOH:O	1.51	1.10
2:B:71:LYS:HG2	2:B:142:ASN:ND2	1.88	0.88
1:A:32:LYS:HA	1:A:32:LYS:CE	2.06	0.85
2:B:71:LYS:HG2	2:B:142:ASN:HD21	1.43	0.81
2:B:224:SER:HB2	2:B:227:GLU:HG2	1.64	0.79
1:A:32:LYS:CA	1:A:32:LYS:HE3	2.12	0.78
2:B:131:LEU:HB2	2:B:180[B]:PHE:CZ	2.21	0.75
2:B:129:ALA:HB1	2:B:131:LEU:HD23	1.68	0.75
2:B:252:GLY:O	2:B:256[B]:ARG:HG3	1.87	0.75
2:B:129:ALA:HB1	2:B:131:LEU:HB3	1.70	0.72
1:A:130:HIS:HE1	8:A:3328:HOH:O	1.70	0.72
2:B:104:SER:HA	2:B:149:MSE:HG3	1.72	0.71
1:A:99:GLY:HA3	2:B:179[B]:GLN:HG2	1.73	0.69
1:A:136[A]:GLN:OE1	8:A:3416:HOH:O	2.09	0.68
2:B:131:LEU:HB2	2:B:180[B]:PHE:HZ	1.60	0.66
2:B:71:LYS:NZ	2:B:142:ASN:HD21	1.93	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:213:GLU:HG2	1:A:270:ARG:NH1	2.12	0.65
2:B:81:ARG:HE	2:B:109:GLN:HE22	1.43	0.64
2:B:73[B]:LEU:HD11	2:B:136:LEU:HD11	1.80	0.63
2:B:53:ARG:NH2	8:B:3033:HOH:O	2.34	0.61
2:B:128:GLY:O	2:B:130:GLY:N	2.34	0.61
2:B:129:ALA:CB	2:B:131:LEU:HD23	2.35	0.56
2:B:71:LYS:HZ2	2:B:142:ASN:HD21	1.52	0.55
2:B:195:TYR:HB3	2:B:205:ALA:HB1	1.88	0.54
1:A:133:VAL:HG11	1:A:177[B]:LEU:HD21	1.90	0.54
1:A:213:GLU:HG2	1:A:270:ARG:HH12	1.72	0.54
2:B:131:LEU:HD13	2:B:180[B]:PHE:CE2	2.43	0.53
2:B:106:VAL:HA	2:B:109:GLN:HE21	1.72	0.53
1:A:177[A]:LEU:HG	2:B:155:TRP:NE1	2.24	0.53
2:B:192:ASP:O	2:B:264:GLY:HA2	2.09	0.52
1:A:133:VAL:CG1	1:A:177[B]:LEU:HD21	2.39	0.52
2:B:128:GLY:O	2:B:129:ALA:C	2.46	0.51
1:A:188:ILE:HG22	1:A:190[A]:GLU:HG2	1.92	0.51
2:B:81:ARG:HE	2:B:109:GLN:NE2	2.08	0.50
2:B:71:LYS:NZ	2:B:142:ASN:ND2	2.60	0.50
1:A:130:HIS:HD2	8:A:3318:HOH:O	1.95	0.49
2:B:192:ASP:HA	2:B:247:ASN:HB2	1.95	0.49
1:A:99:GLY:HA3	2:B:179[B]:GLN:CG	2.42	0.49
2:B:35:LEU:HD11	2:B:131:LEU:HD12	1.95	0.48
2:B:129:ALA:HB2	8:B:3211:HOH:O	2.14	0.48
2:B:71:LYS:HZ1	2:B:142:ASN:ND2	2.12	0.47
1:A:156:HIS:HB2	8:B:3367:HOH:O	2.13	0.47
1:A:53[B]:ARG:HD3	1:A:251:LEU:HD21	1.96	0.47
2:B:41[A]:ILE:HD11	2:B:72:LEU:HD22	1.97	0.47
2:B:83:ARG:HD3	8:B:3292:HOH:O	2.13	0.47
2:B:15:ARG:HH22	2:B:21:GLN:HE22	1.62	0.47
1:A:244[B]:ARG:NE	8:A:3219:HOH:O	2.47	0.47
1:A:190[A]:GLU:OE2	6:A:281:ATP:O2B	2.34	0.46
1:A:145[A]:ARG:HD3	8:A:3234:HOH:O	2.15	0.46
1:A:177[B]:LEU:HG	1:A:181:PHE:CE1	2.51	0.46
1:A:188:ILE:HG22	1:A:190[B]:GLU:HG3	1.97	0.46
2:B:129:ALA:HB1	2:B:131:LEU:CD2	2.41	0.45
1:A:103:PRO:HD3	1:A:156:HIS:HA	1.97	0.45
2:B:126:VAL:HG21	2:B:130:GLY:O	2.15	0.45
2:B:104:SER:CA	2:B:149:MSE:HG3	2.44	0.45
2:B:81:ARG:HH22	2:B:110:ASN:ND2	2.15	0.45
2:B:244:GLN:NE2	2:B:263:VAL:O	2.35	0.44
1:A:156:HIS:HE1	8:A:3328:HOH:O	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:73[A]:LEU:HD23	2:B:144:VAL:CG2	2.48	0.44
1:A:130:HIS:CE1	8:A:3328:HOH:O	2.54	0.44
2:B:41[A]:ILE:CD1	2:B:72:LEU:HD22	2.48	0.43
2:B:104:SER:HA	2:B:149:MSE:CG	2.46	0.43
2:B:72:LEU:O	2:B:143:ALA:HA	2.19	0.43
1:A:212:PRO:O	1:A:264:HIS:HE1	2.02	0.43
2:B:38:ALA:HB1	2:B:73[B]:LEU:CD1	2.49	0.43
2:B:176:LEU:HA	2:B:176:LEU:HD12	1.71	0.43
1:A:190[B]:GLU:OE1	1:A:227:PRO:HB2	2.19	0.42
1:A:156:HIS:CE1	8:A:3328:HOH:O	2.72	0.42
1:A:130:HIS:CD2	8:A:3318:HOH:O	2.70	0.42
2:B:15:ARG:HH12	2:B:21:GLN:NE2	2.17	0.42
2:B:67:ARG:C	2:B:67:ARG:HD2	2.40	0.42
1:A:32:LYS:CE	1:A:32:LYS:CA	2.88	0.41
1:A:157:HIS:HB3	2:B:179[A]:GLN:HG2	2.03	0.41
1:A:244[B]:ARG:HD2	1:A:268:LEU:HD22	2.02	0.41
1:A:193:ASP:HA	1:A:249:ASN:HB2	2.02	0.41
1:A:102:ALA:HB3	1:A:103:PRO:HD3	2.02	0.40
2:B:71:LYS:HE3	2:B:136:LEU:O	2.21	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	253/276 (92%)	250 (99%)	3 (1%)	0	100	100
2	B	276/270 (102%)	261 (95%)	9 (3%)	6 (2%)	10	1
All	All	529/546 (97%)	511 (97%)	12 (2%)	6 (1%)	19	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	131	LEU

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Mol	Chain	Res	Type
2	B	132	SER
2	B	129	ALA
2	B	204	ASP
2	B	223	ASP
2	B	128	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/212 (93%)	195 (99%)	2 (1%)	85	70
2	B	215/199 (108%)	208 (97%)	7 (3%)	50	20
All	All	412/411 (100%)	403 (98%)	9 (2%)	63	34

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	274	ARG
2	B	3	ASN
2	B	21	GLN
2	B	67	ARG
2	B	142	ASN
2	B	161	GLU
2	B	198	ASN
2	B	226	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	HIS
1	A	264	HIS
2	B	3	ASN
2	B	21	GLN
2	B	101	GLN
2	B	109	GLN

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Mol	Chain	Res	Type
2	B	110	ASN
2	B	142	ASN
2	B	198	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 24 are monoatomic - leaving 4 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	$\# Z  > 2$
5	WO3	A	2008	1	4,4,18	3.63	2 (50%)	0,6,51	0.00	-
6	ATP	A	281	3	33,33,33	1.10	1 (3%)	52,52,52	2.26	11 (21%)
4	PO4	B	292	-	4,4,4	0.80	0	6,6,6	0.34	0
4	PO4	B	293	-	4,4,4	1.07	0	6,6,6	0.39	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
5	WO3	A	2008	1	-	0/0/0/60	0/0/0/3
6	ATP	A	281	3	-	0/22/38/38	0/1/3/3
4	PO4	B	292	-	-	0/0/0/0	0/0/0/0
4	PO4	B	293	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2008	WO3	WA-O4A	6.11	2.23	1.72
5	A	2008	WO3	WA-O3A	3.76	2.03	1.72
6	A	281	ATP	C5-C4	2.77	1.46	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	281	ATP	C4'-O4'-C1'	-8.47	100.55	109.75
6	A	281	ATP	N3-C2-N1	-7.52	122.42	128.71
6	A	281	ATP	N3-C4-N9	5.33	135.05	125.43
6	A	281	ATP	C8-N9-C4	4.35	110.22	106.90
6	A	281	ATP	O5'-C5'-C4'	-3.18	97.25	108.94
6	A	281	ATP	N6-C6-N1	2.44	124.15	119.36
6	A	281	ATP	C5-C4-N3	-2.28	120.74	125.70
6	A	281	ATP	C5-C4-N9	-2.11	104.11	107.16
6	A	281	ATP	C2-N1-C6	2.07	122.50	118.77
6	A	281	ATP	C4-C5-N7	-2.05	107.77	109.52
6	A	281	ATP	C2-N3-C4	2.01	119.74	114.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	246/276 (89%)	0.44	35 (14%) 3 2	15, 20, 39, 49	0
2	B	268/270 (99%)	0.59	37 (13%) 4 3	17, 23, 56, 75	0
All	All	514/546 (94%)	0.52	72 (14%) 4 3	15, 21, 47, 75	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	203	LYS	12.4
2	B	127	GLY	11.2
2	B	201	THR	10.9
2	B	222	HIS	10.1
2	B	3	ASN	8.6
2	B	202	SER	7.6
2	B	204	ASP	7.0
2	B	129	ALA	6.9
2	B	128	GLY	6.7
1	A	221	LYS	6.3
1	A	276	ALA	5.6
1	A	207	GLN	5.6
2	B	228	PHE	5.5
1	A	203	PRO	5.5
1	A	205	ARG	5.3
1	A	206	GLY	5.0
1	A	32	LYS	5.0
2	B	198	ASN	4.9
2	B	5	THR	4.9
2	B	6	ALA	4.7
1	A	274	ARG	4.6
2	B	139	ALA	4.5
2	B	197	ALA	4.5
1	A	204	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	202	GLY	4.3
2	B	219	LYS	4.0
2	B	138	LEU	3.9
2	B	130	GLY	3.9
2	B	200	LYS	3.9
1	A	275	PRO	3.8
2	B	218	ALA	3.7
2	B	199	PRO	3.6
1	A	31	GLY	3.5
1	A	223	GLU	3.4
1	A	77	LEU	3.3
2	B	140	GLU	3.2
2	B	223	ASP	3.2
2	B	205	ALA	3.1
1	A	177[A]	LEU	3.1
2	B	131	LEU	2.9
1	A	174	ALA	2.9
1	A	222	SER	2.9
2	B	221	LEU	2.8
2	B	220	GLY	2.8
2	B	41[A]	ILE	2.7
1	A	209	ARG	2.7
1	A	186	LEU	2.6
1	A	210	PHE	2.6
2	B	43	ILE	2.6
1	A	217	THR	2.6
2	B	68	LYS	2.6
1	A	272	GLY	2.5
1	A	181	PHE	2.5
2	B	7	GLU	2.5
1	A	43	VAL	2.4
2	B	4	SER	2.4
1	A	75	LEU	2.4
2	B	14	GLN	2.3
2	B	69	ASN	2.3
1	A	175	PHE	2.3
2	B	214	ASP	2.2
1	A	197	THR	2.2
1	A	76	ILE	2.1
1	A	198	ALA	2.1
2	B	161	GLU	2.1
1	A	44	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	10	GLU	2.1
1	A	208	ALA	2.0
1	A	46	ILE	2.0
1	A	78	THR	2.0
1	A	172	THR	2.0
1	A	176	LEU	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	W	A	2025	1/1	0.26	18.89	30,30,30,30	1
7	W	A	2026	1/1	0.25	5.52	31,31,31,31	1
7	W	A	2015	1/1	0.15	1.32	27,27,27,27	1
7	W	A	2012	1/1	0.11	0.32	49,49,49,49	1
4	PO4	B	293	5/5	0.10	0.23	27,30,36,38	0
5	WO3	A	2008	5/16	0.09	-0.51	19,23,24,27	5
7	W	A	2017	1/1	0.06	-0.66	33,33,33,33	1
6	ATP	A	281	31/31	0.07	-0.84	18,24,28,32	0
4	PO4	B	292	5/5	0.06	-0.89	28,32,33,34	0
7	W	A	2004	1/1	0.06	-0.96	27,27,27,27	1
7	W	B	2001	1/1	0.02	-1.10	38,38,38,38	1
3	MG	A	291	1/1	0.10	-1.11	29,29,29,29	0
7	W	A	2014	1/1	0.14	-1.39	31,31,31,31	1
7	W	B	2006	1/1	0.03	-1.50	30,30,30,30	1
7	W	B	2007	1/1	0.04	-1.71	33,33,33,33	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	W	B	2002	1/1	0.09	-1.73	35,35,35,35	1
7	W	B	2028	1/1	0.06	-1.74	26,26,26,26	1
7	W	B	2027	1/1	0.04	-1.84	22,22,22,22	1
7	W	A	2005	1/1	0.04	-2.19	29,29,29,29	1
7	W	B	2003	1/1	0.02	-2.29	40,40,40,40	1
7	W	A	2013	1/1	0.02	-2.38	33,33,33,33	1
7	W	B	2009	1/1	0.04	-6.98	43,43,43,43	1
7	W	A	2016	1/1	0.07	-8.52	34,34,34,34	1
7	W	B	2010	1/1	0.06	-20.86	41,41,41,41	1
7	W	B	2031	1/1	0.20	-	40,40,40,40	1
7	W	B	2030	1/1	0.15	-	48,48,48,48	1
7	W	B	2029	1/1	0.05	-	36,36,36,36	1
7	W	B	2011	1/1	0.08	-	25,25,25,25	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.