Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 10:00 AM EDT

PDB ID	:	4NDR / pdb_00004ndr
Title	:	Crystal structure Molybdenum Storage Protein with fully Mo-loaded cavity
Authors	:	Poppe, J.; Warkentin, E.; Demmer, U.; Ermler, U.
Deposited on	:	2013-10-27
Resolution	:	2.00 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

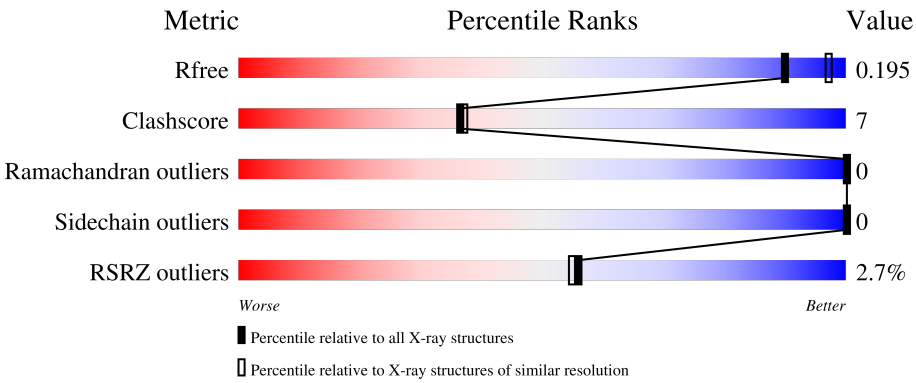
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	B	270	4% 83% 16% •
2	A	276	% 79% 9% 11%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 4401 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.

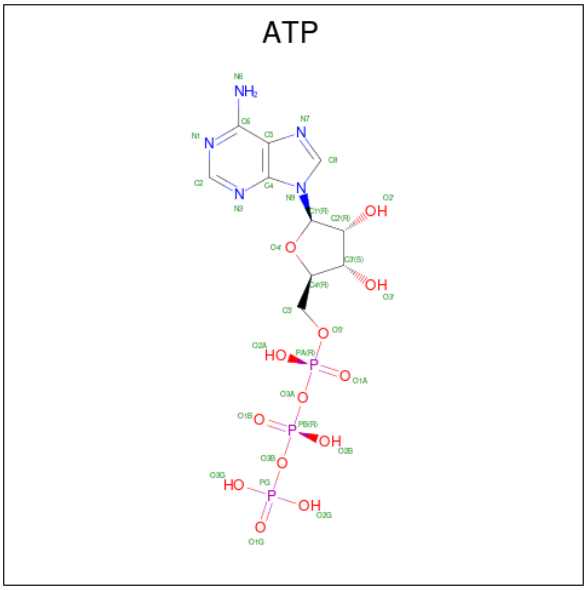
- Molecule 1 is a protein called Molybdenum storage protein subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	268	2021	1286	353	374	8	0	9	0

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

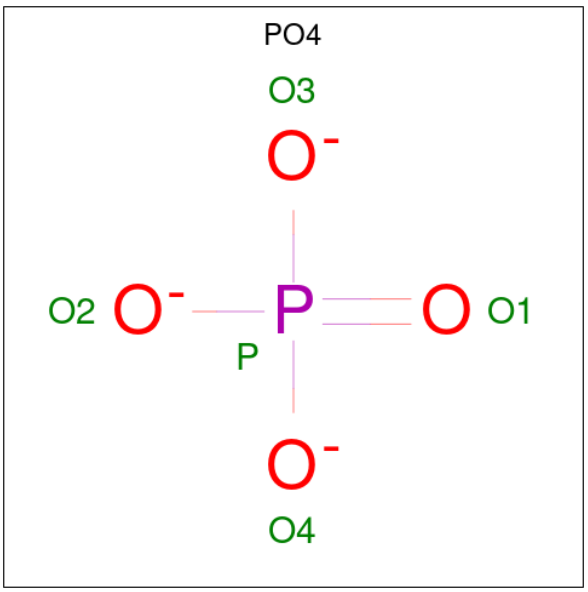
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	245	1858	1177	349	329	3	0	5	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



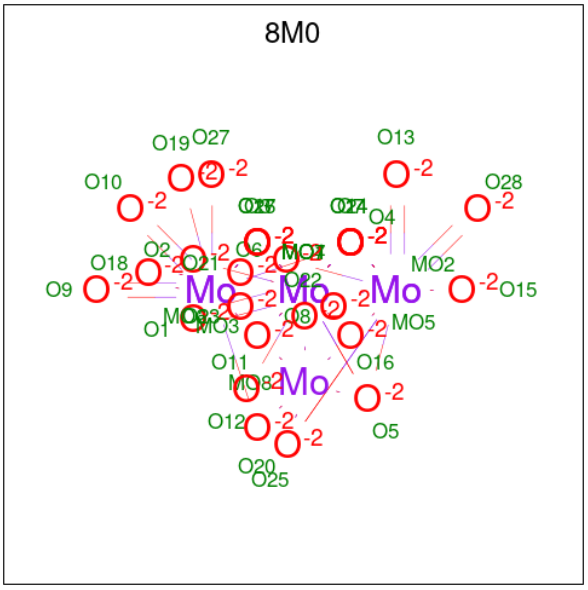
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	31	10	5	13	3	0	0
3	A	1	31	10	5	13	3	0	0

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 5 is bis(mu4-oxo)-tetrakis(mu3-oxo)-hexakis(mu2-oxo)-hexadecaoxo-octamolybdenum (VI) (CCD ID: 8M0) (formula: Mo_8O_{28}).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Mo	O		
5	B	1	36	8	28	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Mo	O		
5	A	1	34	8	26	0	0

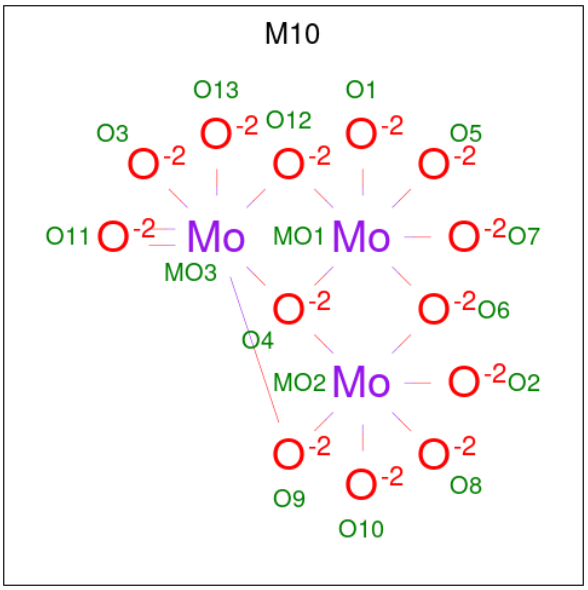
- Molecule 6 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mo		
6	B	16	16	16	0	0
			Total	Mo		
6	A	4	4	4	0	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 8 is (mu3-oxo)-tris(mu2-oxo)-nonakisoxo-trimolybdenum (VI) (CCD ID: M10) (formula: Mo_3O_{13}).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Mo	O		
8	A	1	6	2	4	0	0

- Molecule 9 is water.

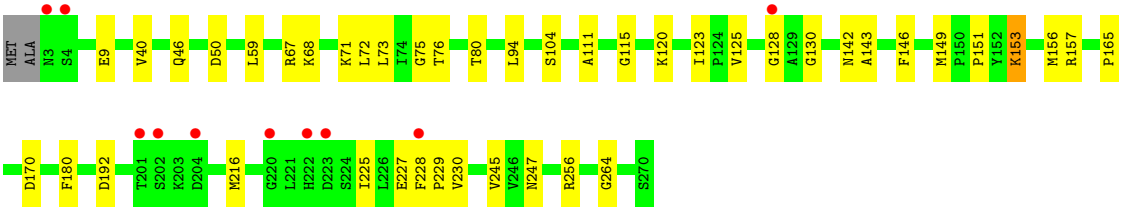
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	B	170	170	170	0	0
			Total	O		
9	A	188	188	188	0	0

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.

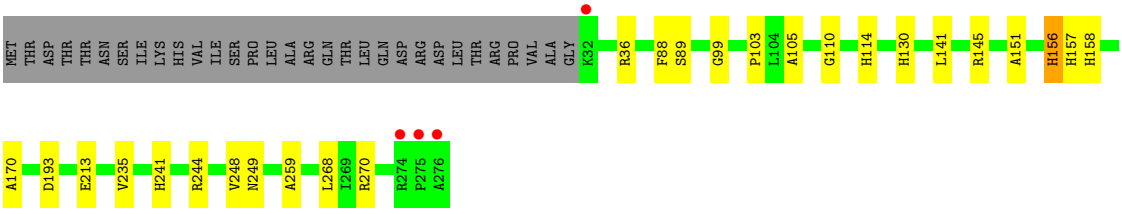
- Molecule 1: Molybdenum storage protein subunit beta

Chain B:



- Molecule 2: Molybdenum storage protein subunit alpha

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	114.27Å 114.27Å 234.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (10.00-2.00) 98.3 (10.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.15 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168), REFMAC	Depositor
R, R_{free}	0.164 , 0.191 0.170 , 0.195	Depositor DCC
R_{free} test set	3078 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4401	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MO, ATP, M10, 8M0, PO4

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	B	0.67	0/2083	0.89	4/2827 (0.1%)
2	A	0.73	0/1913	0.91	1/2606 (0.0%)
All	All	0.70	0/3996	0.90	5/5433 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	156	HIS	CB-CA-C	-7.16	106.32	116.34
1	B	165	PRO	CA-C-N	-6.00	113.58	119.64
1	B	165	PRO	C-N-CA	-6.00	113.58	119.64
1	B	153	LYS	CB-CA-C	-5.83	109.84	116.54
1	B	123	ILE	N-CA-C	5.20	112.69	107.55

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	B	2021	0	2102	33	0
2	A	1858	0	1916	22	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	0	0
5	A	34	0	0	6	0
5	B	36	0	0	4	0
6	A	4	0	0	1	0
6	B	16	0	0	0	0
7	A	1	0	0	0	0
8	A	6	0	0	0	0
9	A	188	0	0	5	0
9	B	170	0	0	5	0
All	All	4401	0	4042	56	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 7.

All (56) 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)
6:A:307:MO:MO	9:A:401:HOH:O	1.48	0.84
5:A:303:8M0:O22	9:A:487:HOH:O	2.09	0.70
1:B:256[B]:ARG:NH2	9:B:479:HOH:O	2.25	0.69
1:B:104:SER:HA	1:B:149:MET:HG3	1.78	0.64
2:A:213:GLU:HG2	2:A:270:ARG:NH1	2.13	0.64
1:B:71[A]:LYS:NZ	9:B:562:HOH:O	2.34	0.60
1:B:192:ASP:O	1:B:264:GLY:HA2	2.01	0.60
1:B:67:ARG:HE	1:B:68[B]:LYS:NZ	2.01	0.58
5:B:303:8M0:O14	2:A:158:HIS:HE1	1.85	0.58
1:B:151:PRO:HB3	5:B:303:8M0:O4	2.04	0.57
1:B:170:ASP:HB3	1:B:230:VAL:HG21	1.87	0.57
2:A:244[B]:ARG:HD2	2:A:268:LEU:HD22	1.87	0.56
1:B:50:ASP:OD2	1:B:80[B]:THR:HG23	2.07	0.55
1:B:192:ASP:HA	1:B:247:ASN:HB2	1.89	0.55
2:A:130:HIS:HB2	5:A:303:8M0:O21	2.08	0.53
1:B:225:ILE:HD13	1:B:245:VAL:HG11	1.91	0.53
1:B:71[A]:LYS:HG2	1:B:142:ASN:OD1	2.09	0.53
1:B:170:ASP:HB2	1:B:227:GLU:CD	2.34	0.52
2:A:36:ARG:NH2	9:A:488:HOH:O	2.42	0.52
3:B:301:ATP:O3G	9:B:402:HOH:O	2.19	0.50
2:A:145[A]:ARG:HD3	9:A:564:HOH:O	2.12	0.49
1:B:115:GLY:HA3	1:B:125:VAL:CG2	2.43	0.49
2:A:103:PRO:HD3	2:A:156:HIS:HA	1.95	0.49
1:B:76:THR:HG21	1:B:111:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:303:8M0:O24	2:A:156:HIS:ND1	2.30	0.49
1:B:130:GLY:HA3	1:B:180:PHE:CE1	2.48	0.49
2:A:110:GLY:HA3	5:A:303:8M0:O24	2.12	0.48
1:B:228:PHE:CG	1:B:229:PRO:HD3	2.48	0.48
1:B:72:LEU:O	1:B:143:ALA:HA	2.15	0.47
2:A:151:ALA:HB3	2:A:170:ALA:HB1	1.97	0.46
1:B:75:GLY:HA2	1:B:146:PHE:O	2.16	0.46
2:A:156:HIS:HE1	5:A:303:8M0:O23	1.99	0.46
2:A:241:HIS:HD2	9:A:516:HOH:O	1.99	0.46
1:B:229:PRO:HB2	9:B:507:HOH:O	2.15	0.45
1:B:227:GLU:HB2	1:B:230:VAL:HG23	1.99	0.45
2:A:114:HIS:HE1	5:A:303:8M0:O10	1.99	0.45
1:B:151:PRO:O	1:B:153:LYS:HG3	2.16	0.45
1:B:216:MET:HE2	1:B:216:MET:HB3	1.90	0.45
2:A:114:HIS:CE1	5:A:303:8M0:O10	2.70	0.44
1:B:120:LYS:NZ	9:B:563:HOH:O	2.50	0.44
1:B:67:ARG:HE	1:B:68[B]:LYS:HZ2	1.66	0.43
1:B:157:ARG:HG2	2:A:235:VAL:HG12	2.00	0.43
1:B:228:PHE:CD2	1:B:229:PRO:HD3	2.53	0.43
1:B:40:VAL:HG22	1:B:73[A]:LEU:HD12	2.00	0.43
1:B:128:GLY:HA2	5:B:303:8M0:O16	2.18	0.43
2:A:213:GLU:HG2	2:A:270:ARG:HH11	1.82	0.43
2:A:99:GLY:O	2:A:157:HIS:HD2	2.02	0.42
1:B:46:GLN:OE1	1:B:80[B]:THR:HG22	2.20	0.42
2:A:88:PHE:CE1	2:A:105:ALA:HB2	2.54	0.42
1:B:9:GLU:HG3	2:A:89[B]:SER:HB2	2.02	0.42
1:B:156:MET:HE2	1:B:156:MET:HB2	2.00	0.42
2:A:193:ASP:HA	2:A:249:ASN:HB2	2.01	0.41
1:B:94:LEU:HD23	1:B:94:LEU:HA	1.94	0.41
2:A:141:LEU:HA	2:A:141:LEU:HD23	1.82	0.40
1:B:59:LEU:HD23	1:B:59:LEU:HA	1.85	0.40
2:A:248:VAL:HG11	2:A:259:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	275/270 (102%)	266 (97%)	9 (3%)	0	100	100
2	A	248/276 (90%)	243 (98%)	5 (2%)	0	100	100
All	All	523/546 (96%)	509 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	B	214/206 (104%)	214 (100%)	0	100	100
2	A	192/216 (89%)	192 (100%)	0	100	100
All	All	406/422 (96%)	406 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3	ASN
1	B	14	GLN
1	B	101	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 21 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	$\#\|Z\| > 2$
5	8M0	B	303	6	34,48,48	3.43	11 (32%)	-		
5	8M0	A	303	2	21,46,48	3.76	10 (47%)	-		
3	ATP	B	301	-	32,33,33	1.43	4 (12%)	48,52,52	1.92	11 (22%)
4	PO4	B	302	-	4,4,4	0.85	0	6,6,6	0.51	0
3	ATP	A	301	7	32,33,33	1.23	2 (6%)	48,52,52	1.95	12 (25%)
8	M10	A	304	2	0,5,18	-	-	-		

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
3	ATP	B	301	-	-	6/22/38/38	0/3/3/3
3	ATP	A	301	7	-	3/22/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	303	8M0	O23-MO7	9.66	1.92	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	303	8M0	O23-MO7	9.16	1.91	1.71
5	B	303	8M0	O1-MO1	9.11	1.91	1.71
5	B	303	8M0	O18-MO6	8.27	1.89	1.71
5	A	303	8M0	O1-MO1	8.12	1.88	1.71
5	B	303	8M0	O8-MO2	7.51	1.87	1.71
5	A	303	8M0	O8-MO2	7.17	1.86	1.71
5	B	303	8M0	O28-MO5	6.32	2.30	1.72
5	A	303	8M0	O18-MO6	5.95	1.84	1.71
3	B	301	ATP	C5-C4	5.03	1.48	1.39
3	A	301	ATP	C5-C4	4.18	1.46	1.39
5	A	303	8M0	O20-MO6	3.51	2.22	1.89
5	A	303	8M0	O3-MO3	3.45	1.99	1.86
5	B	303	8M0	O15-MO5	-3.04	1.90	2.34
5	B	303	8M0	O20-MO6	3.02	2.18	1.89
5	B	303	8M0	O14-MO5	2.90	2.03	1.93
3	B	301	ATP	C5-C6	2.61	1.48	1.41
5	A	303	8M0	O10-MO3	2.40	1.88	1.71
5	B	303	8M0	O20-MO8	2.36	2.04	1.80
5	B	303	8M0	O7-MO4	2.33	2.04	1.80
3	B	301	ATP	C5-N7	-2.28	1.34	1.39
5	A	303	8M0	O9-MO3	2.26	1.87	1.71
5	B	303	8M0	O3-MO3	2.22	2.01	1.93
3	A	301	ATP	C8-N7	2.20	1.35	1.31
3	B	301	ATP	C8-N7	2.19	1.35	1.31
5	A	303	8M0	O20-MO8	2.10	2.02	1.80
5	A	303	8M0	O7-MO4	2.09	2.02	1.80

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	301	ATP	C5-C4-N3	-6.45	117.83	126.72
3	B	301	ATP	N3-C4-N9	5.75	136.95	127.17
3	A	301	ATP	C5-C4-N3	-5.22	119.53	126.72
3	A	301	ATP	N3-C4-N9	5.17	135.96	127.17
3	A	301	ATP	C4-N9-C8	4.20	110.15	105.74
3	B	301	ATP	C2-N3-C4	3.85	121.22	111.83
3	B	301	ATP	N3-C2-N1	-3.55	123.21	128.58
3	A	301	ATP	N3-C2-N1	-3.37	123.48	128.58
3	A	301	ATP	C2-N3-C4	3.35	120.02	111.83
3	A	301	ATP	O5'-C5'-C4'	-3.22	98.03	108.99
3	B	301	ATP	C4-N9-C8	2.86	108.74	105.74
3	B	301	ATP	C4-C5-N7	-2.76	107.42	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	ATP	O3A-PB-O1B	-2.52	103.11	110.70
3	A	301	ATP	N9-C8-N7	-2.48	110.42	113.94
3	A	301	ATP	C4'-O4'-C1'	-2.47	104.02	109.47
3	B	301	ATP	C5-N7-C8	2.41	107.24	103.45
3	A	301	ATP	N6-C6-N1	2.39	123.69	118.38
3	A	301	ATP	O2A-PA-O3A	2.36	113.66	107.27
3	B	301	ATP	C1'-N9-C8	-2.28	122.04	127.09
3	A	301	ATP	C5-C6-N6	-2.20	117.83	123.29
3	B	301	ATP	C3'-C2'-C1'	2.20	105.62	101.46
3	B	301	ATP	O3B-PG-O1G	-2.09	100.06	111.04
3	B	301	ATP	N6-C6-N1	2.05	122.93	118.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	ATP	C3'-C4'-C5'-O5'
3	B	301	ATP	C2'-C1'-N9-C4
3	B	301	ATP	C2'-C1'-N9-C8
3	A	301	ATP	C2'-C1'-N9-C4
3	B	301	ATP	C4'-C5'-O5'-PA
3	A	301	ATP	C2'-C1'-N9-C8
3	B	301	ATP	O4'-C1'-N9-C8
3	A	301	ATP	O4'-C1'-N9-C8
3	B	301	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

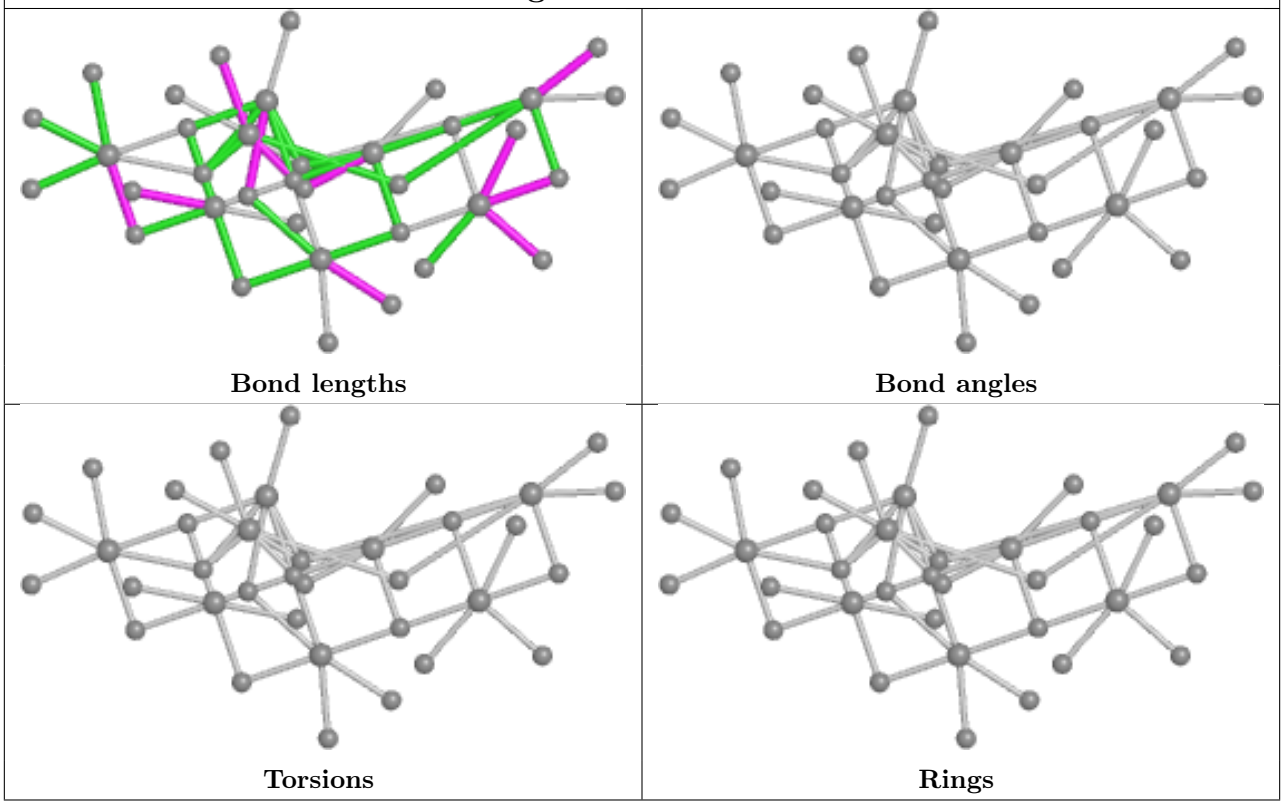
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	303	8M0	4	0
5	A	303	8M0	6	0
3	B	301	ATP	1	0

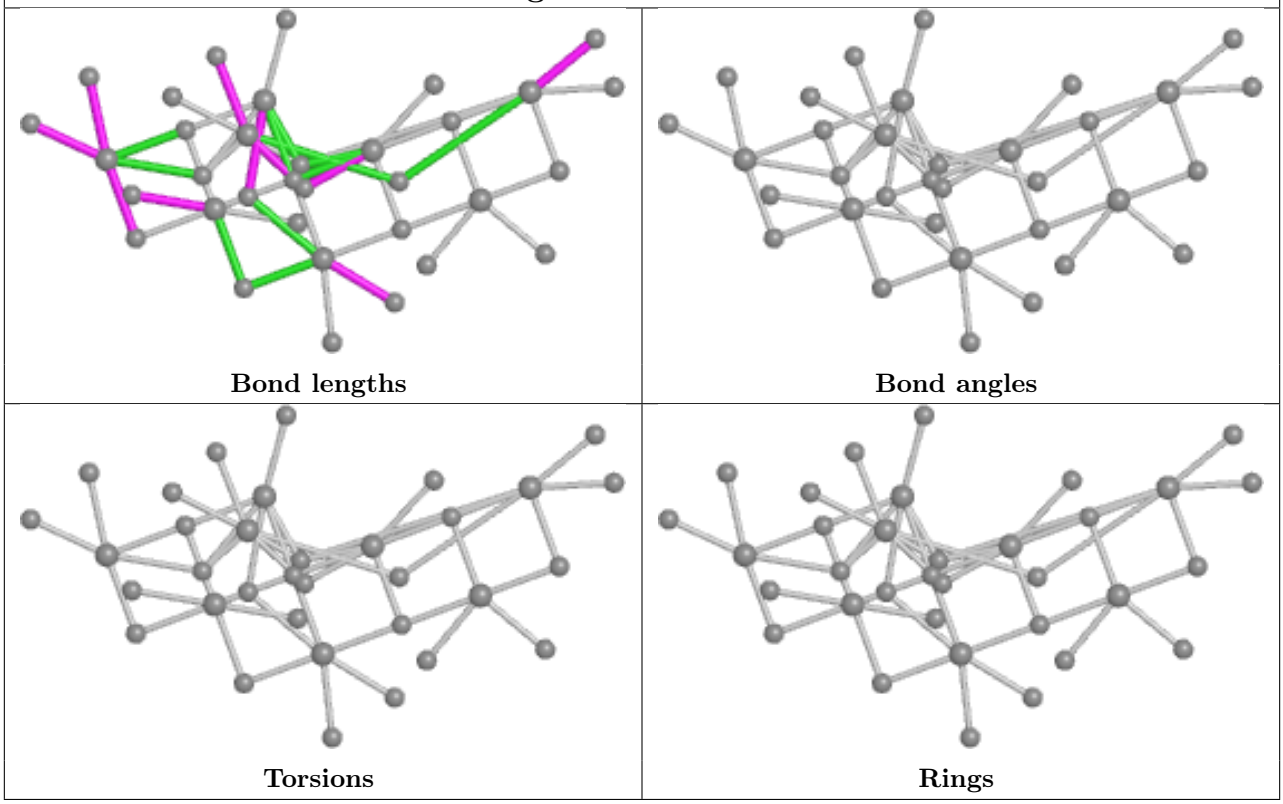
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

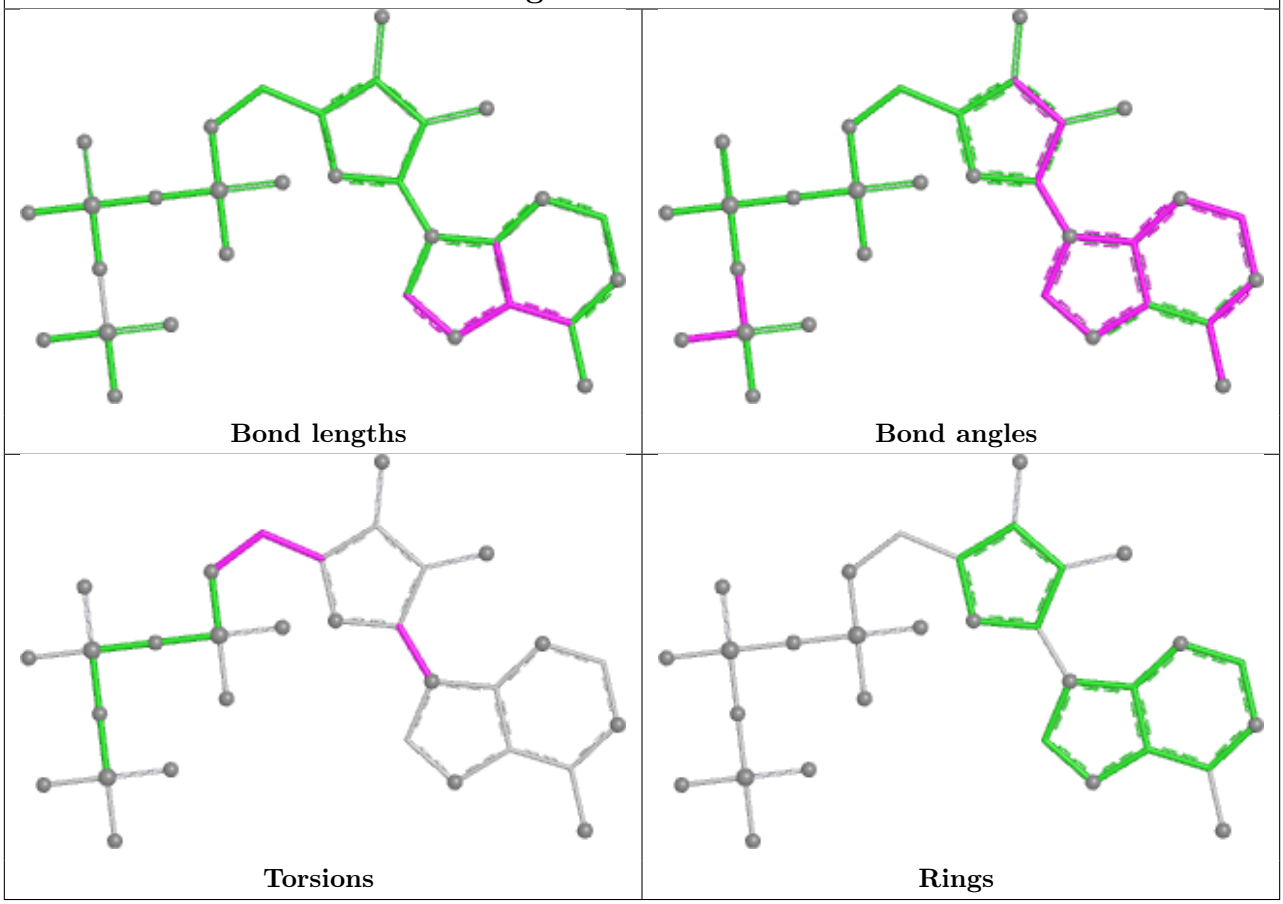
Ligand 8M0 B 303



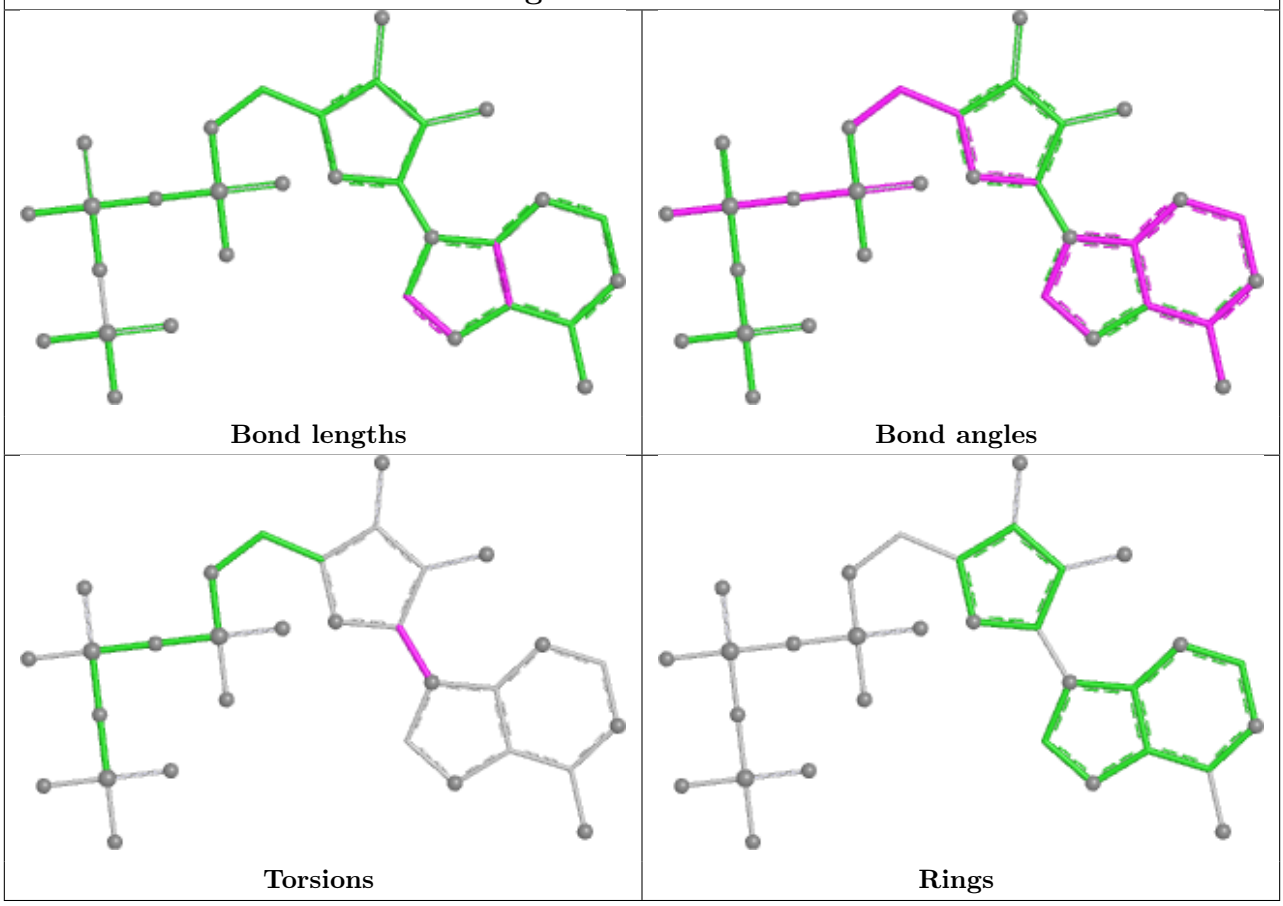
Ligand 8M0 A 303



Ligand ATP B 301



Ligand ATP A 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	B	268/270 (99%)	-0.45	10 (3%)	45	44	13, 29, 66, 102	9 (3%)
2	A	245/276 (88%)	-0.75	4 (1%)	70	70	14, 25, 49, 94	5 (2%)
All	All	513/546 (93%)	-0.59	14 (2%)	56	55	13, 27, 61, 102	14 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	HIS	5.8
1	B	3	ASN	3.3
1	B	223	ASP	2.9
1	B	228	PHE	2.8
2	A	276	ALA	2.7
1	B	128	GLY	2.6
1	B	4	SER	2.6
2	A	275	PRO	2.3
1	B	201	THR	2.3
2	A	32	LYS	2.2
1	B	202	SER	2.2
2	A	274	ARG	2.1
1	B	204	ASP	2.1
1	B	220	GLY	2.1

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 oligosaccharides in this entry.

6.4 Ligands (i)

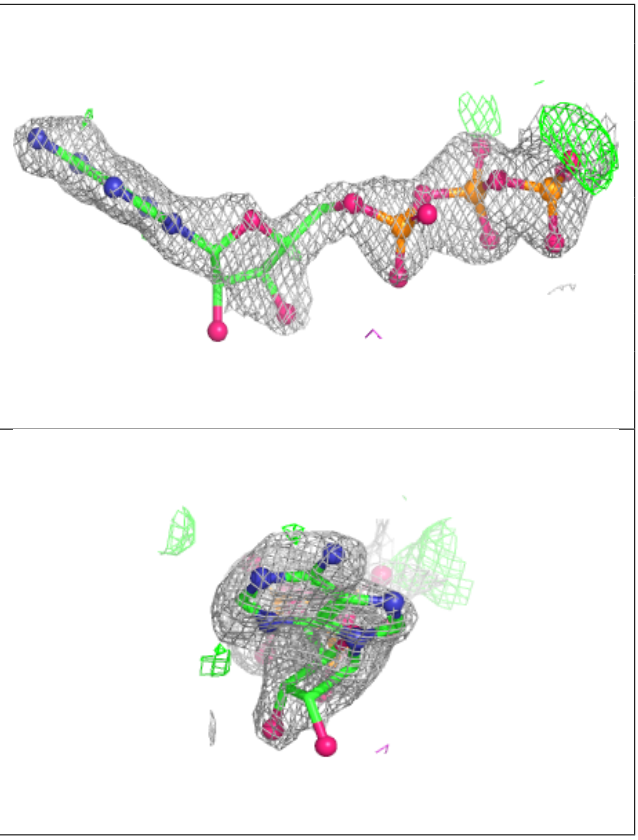
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MO	B	305	1/1	0.42	0.15	105,105,105,105	0
6	MO	B	319	1/1	0.48	0.15	94,94,94,94	1
6	MO	B	315	1/1	0.73	0.15	128,128,128,128	1
4	PO4	B	302	5/5	0.76	0.13	80,82,82,83	0
6	MO	B	317	1/1	0.82	0.07	62,62,62,62	1
6	MO	B	306	1/1	0.84	0.13	106,106,106,106	1
6	MO	B	318	1/1	0.86	0.07	50,50,50,50	1
6	MO	B	308	1/1	0.87	0.07	62,62,62,62	1
6	MO	B	313	1/1	0.87	0.08	46,46,46,46	1
6	MO	B	307	1/1	0.88	0.08	67,67,67,67	1
6	MO	B	304	1/1	0.90	0.05	53,53,53,53	1
6	MO	B	309	1/1	0.90	0.06	65,65,65,65	1
6	MO	B	316	1/1	0.90	0.05	52,52,52,52	1
6	MO	B	312	1/1	0.93	0.09	49,49,49,49	1
6	MO	B	311	1/1	0.95	0.05	54,54,54,54	1
6	MO	B	310	1/1	0.95	0.07	46,46,46,46	1
3	ATP	B	301	31/31	0.96	0.09	32,41,46,58	28
5	8M0	B	303	36/36	0.99	0.07	17,27,44,50	36
3	ATP	A	301	31/31	0.99	0.04	20,25,29,32	0
6	MO	A	306	1/1	0.99	0.04	56,56,56,56	1
7	MG	A	302	1/1	0.99	0.03	25,25,25,25	0
6	MO	A	305	1/1	1.00	0.01	40,40,40,40	1
6	MO	B	314	1/1	1.00	0.02	30,30,30,30	1
6	MO	A	307	1/1	1.00	0.03	37,37,37,37	1
6	MO	A	308	1/1	1.00	0.05	37,37,37,37	1
5	8M0	A	303	34/36	1.00	0.04	20,24,32,34	0
8	M10	A	304	6/16	1.00	0.05	21,22,24,101	2

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

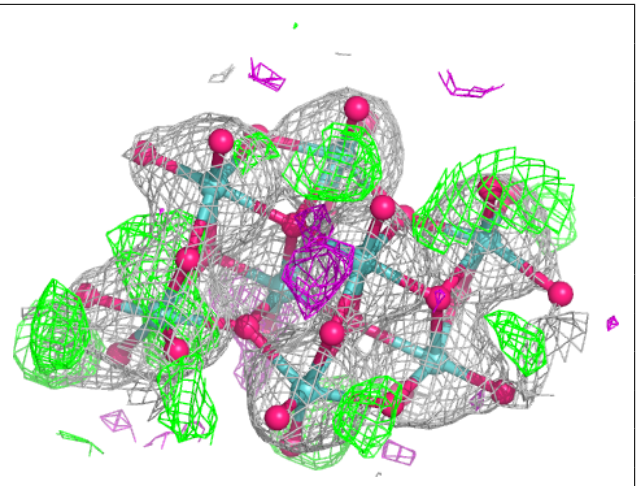
Electron density around ATP B 301:

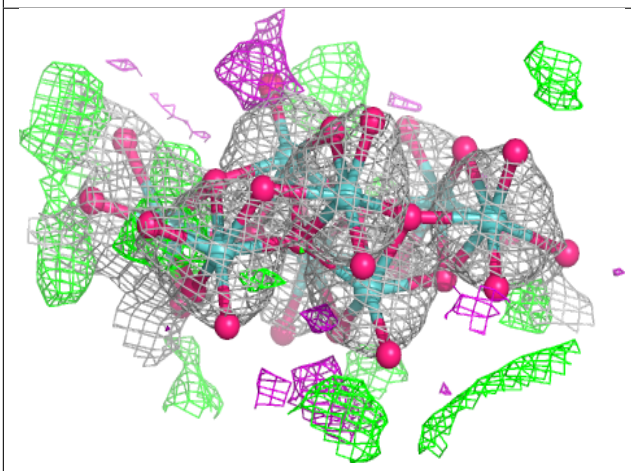
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

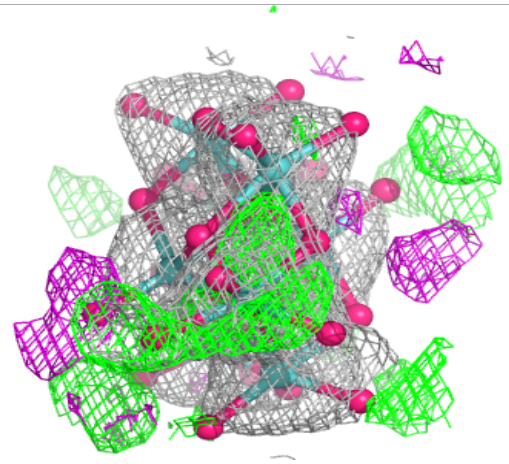


Electron density around 8M0 B 303:

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

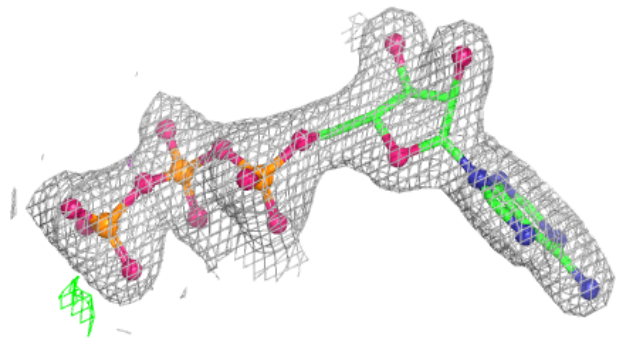


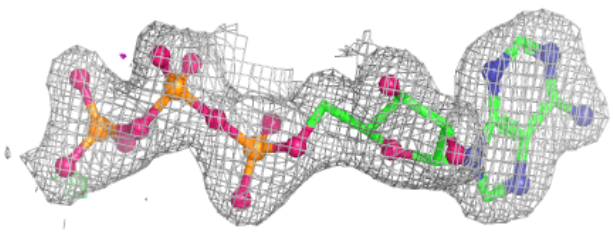


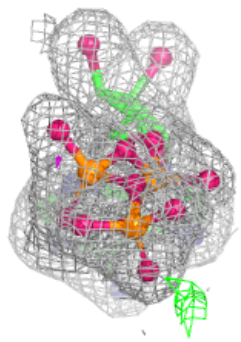


Electron density around ATP A 301:

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

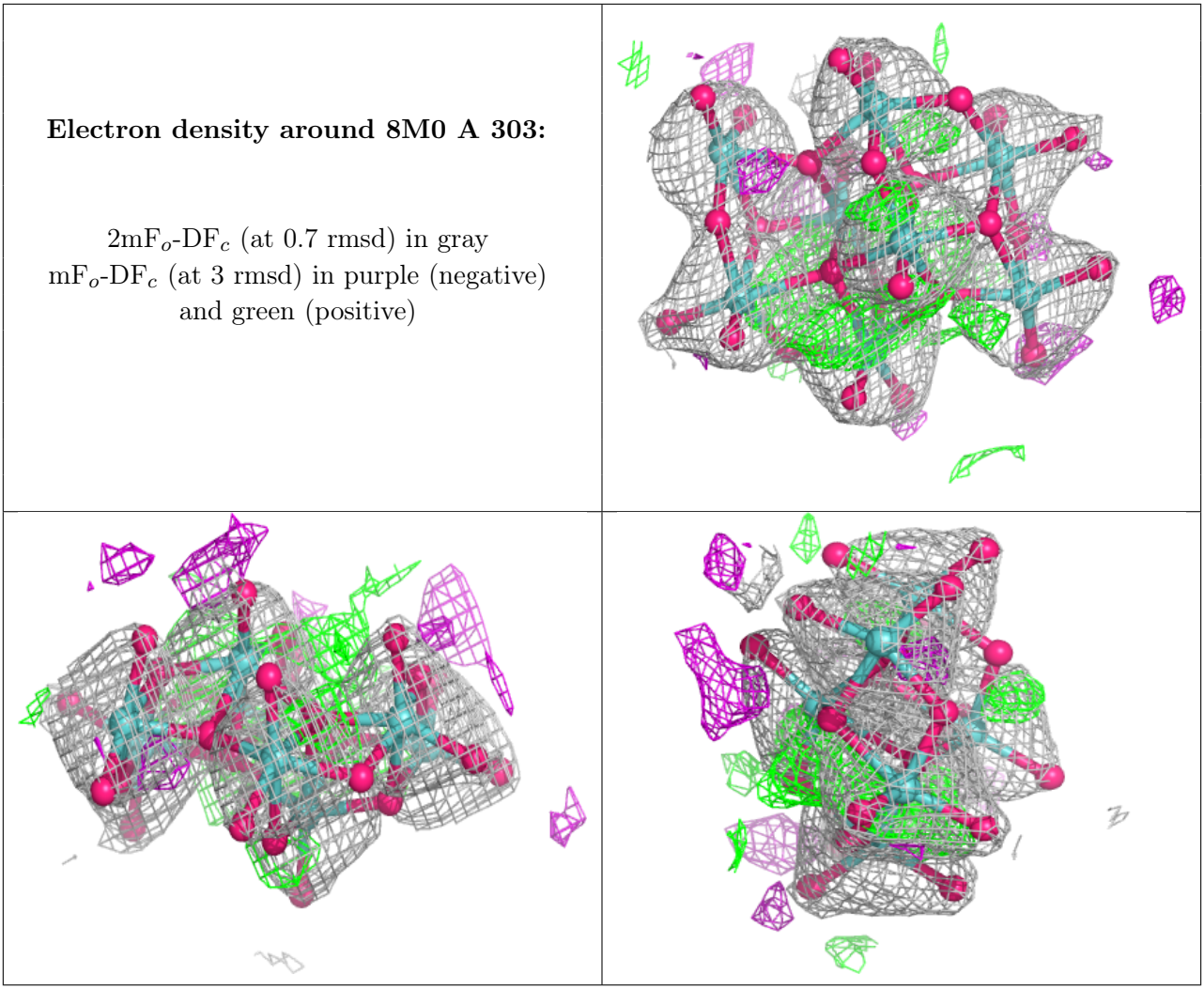






Electron density around 8M0 A 303:

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



6.5 Other polymers (i)

There are no such residues in this entry.