Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 04:35 pm GMT

PDB ID	:	1W9I
Title	:	Myosin II Dictyostelium discoideum motor domain S456Y bound with MgADP-BeFx
Authors	:	Morris, C.A.; Coureux, P.-D.; Wells, A.L.; Houdusse, A.; Sweeney, H.L.
Deposited on	:	2004-10-13
Resolution	:	1.75 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:

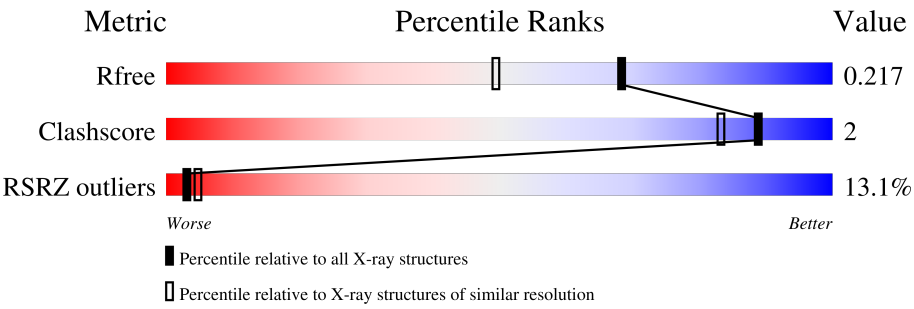
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

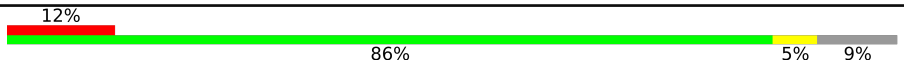
The reported resolution of this entry is 1.75 Å.

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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	A	770	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6489 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 MYOSIN II HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	703	5663	3614	969	1063	17	0	29	1

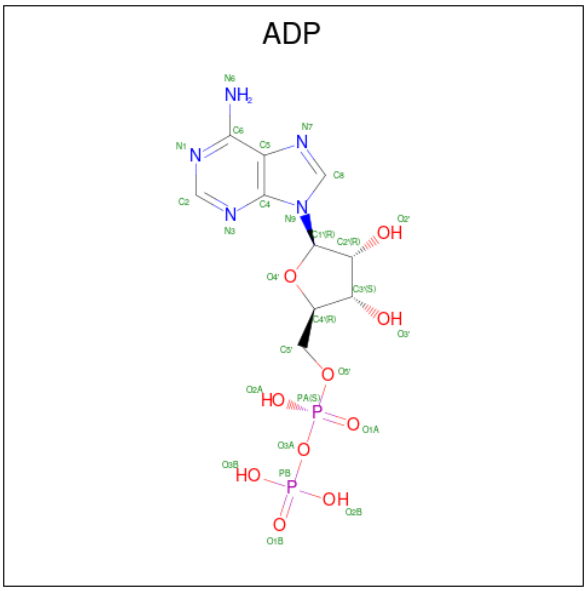
There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	760	LEU	-	expression tag	UNP P08799
A	761	ARG	-	expression tag	UNP P08799
A	762	GLY	-	expression tag	UNP P08799
A	763	ASP	-	expression tag	UNP P08799
A	764	TYR	-	expression tag	UNP P08799
A	765	LYS	-	expression tag	UNP P08799
A	766	ASP	-	expression tag	UNP P08799
A	767	ASP	-	expression tag	UNP P08799
A	768	ASP	-	expression tag	UNP P08799
A	769	ASP	-	expression tag	UNP P08799
A	770	LYS	-	expression tag	UNP P08799
A	456	TYR	SER	engineered mutation	UNP P08799
A	737	PHE	TYR	engineered mutation	UNP P08799

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

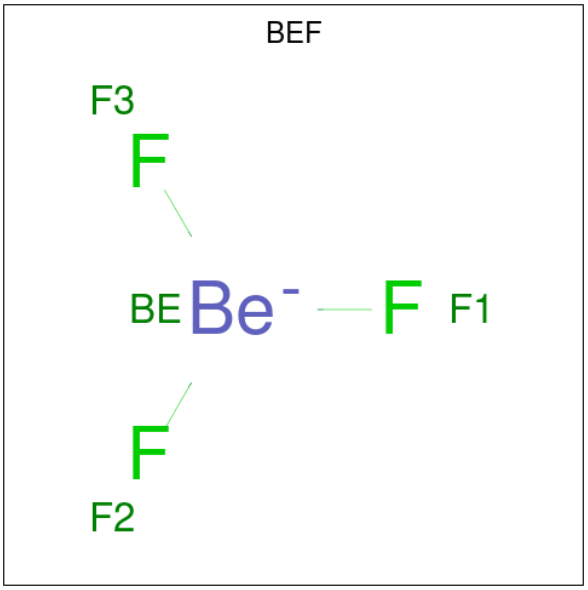
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



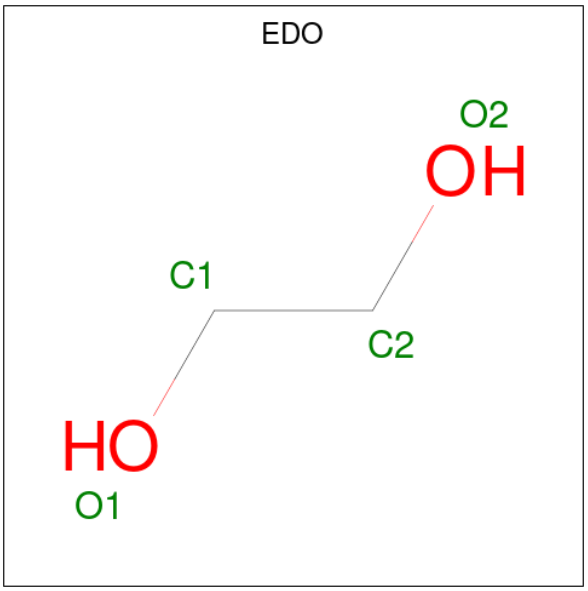
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Be	F		
4	A	1	4	1	3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 6 is water.

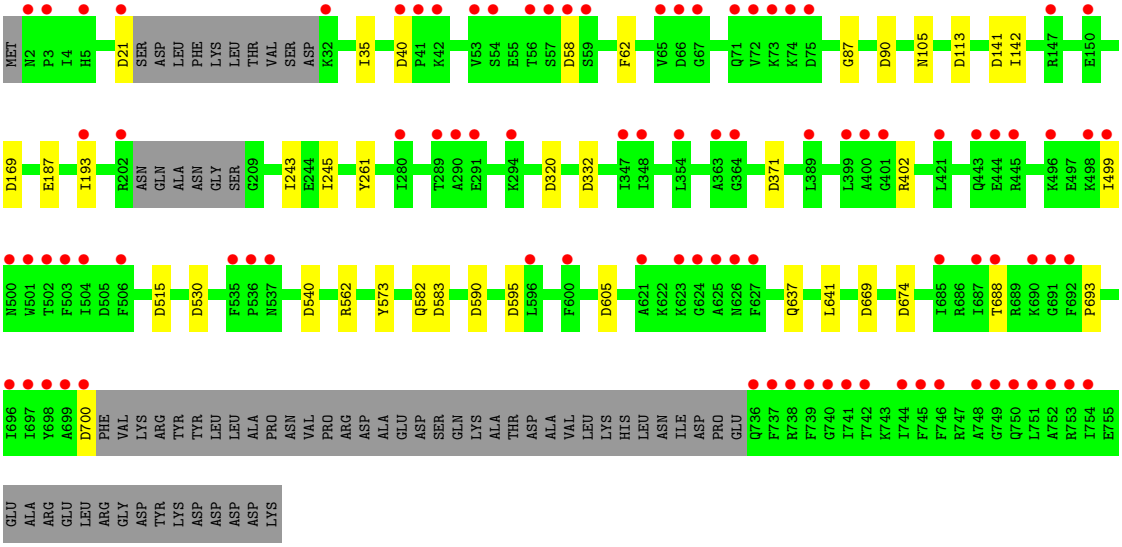
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	734	734	734	0	0

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: MYOSIN II HEAVY CHAIN

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.02Å 186.51Å 54.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.75 24.19 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.1 (40.00-1.75) 96.1 (24.19-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.182 , 0.207 0.195 , 0.217	Depositor DCC
R_{free} test set	5227 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 75.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6489	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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, EDO, BEF, ADP

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	0.46	0/5887	0.71	21/7948 (0.3%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	ASP	CB-CG-OD2	8.20	125.68	118.30
1	A	540	ASP	CB-CG-OD2	7.62	125.16	118.30
1	A	169	ASP	CB-CG-OD2	7.02	124.62	118.30
1	A	515	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	141	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	40	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	113	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	332	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	58[A]	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	58[B]	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	371	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	21	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	530	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	674	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	583	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	595	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	669	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	590	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	605	ASP	CB-CG-OD2	5.28	123.06	118.30
1	A	700	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	320	ASP	CB-CG-OD2	5.04	122.83	118.30

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	5663	0	5563	22	0
2	A	1	0	0	0	0
3	A	27	0	12	0	0
4	A	4	0	0	0	0
5	A	60	0	90	7	0
6	A	734	0	0	5	1
All	All	6489	0	5665	22	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 2.

All (22) 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:A:573[A]:TYR:OH	6:A:2575:HOH:O	1.90	0.89
1:A:573[B]:TYR:OH	6:A:2576:HOH:O	1.88	0.89
1:A:193[B]:ILE:HD12	1:A:245[B]:ILE:HD11	1.52	0.89
1:A:187:GLU:HB3	5:A:1763:EDO:H12	1.69	0.74
1:A:582:GLN:H	1:A:582:GLN:HE21	1.38	0.71
1:A:402:ARG:O	6:A:2418:HOH:O	2.09	0.70
1:A:637[B]:GLN:NE2	6:A:2643:HOH:O	2.24	0.68
1:A:142:ILE:CD1	5:A:1767:EDO:H21	2.29	0.62
1:A:193[A]:ILE:HD13	5:A:1764:EDO:H22	1.82	0.61
1:A:193[B]:ILE:CD1	1:A:245[B]:ILE:HD11	2.27	0.60
1:A:562[B]:ARG:HD3	6:A:2560:HOH:O	2.02	0.59
1:A:87:GLY:H	1:A:105:ASN:ND2	2.03	0.57
1:A:193[A]:ILE:HD11	1:A:243:ILE:HD13	1.87	0.55
1:A:142:ILE:HD12	5:A:1767:EDO:H21	1.90	0.52
1:A:582:GLN:HE21	1:A:582:GLN:N	2.06	0.52
1:A:142:ILE:HD11	5:A:1767:EDO:H21	1.93	0.49
1:A:641:LEU:HA	5:A:1770:EDO:H12	1.94	0.48
1:A:499:ILE:CG2	1:A:499:ILE:O	2.64	0.45
1:A:187:GLU:HB3	5:A:1763:EDO:C1	2.44	0.44
1:A:261:TYR:HE1	1:A:637[B]:GLN:HG2	1.84	0.43
1:A:688:THR:O	1:A:693:PRO:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HD11	1:A:62:PHE:CD2	2.56	0.41

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)
6:A:2062:HOH:O	6:A:2720:HOH:O[1_556]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

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

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 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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	EDO	A	1762	-	3,3,3	0.28	0	2,2,2	0.35	0
5	EDO	A	1763	-	3,3,3	0.26	0	2,2,2	0.44	0
5	EDO	A	1772	-	3,3,3	0.29	0	2,2,2	0.30	0
5	EDO	A	1771	-	3,3,3	0.30	0	2,2,2	0.28	0
5	EDO	A	1758	-	3,3,3	0.28	0	2,2,2	0.09	0
5	EDO	A	1761	-	3,3,3	0.28	0	2,2,2	0.43	0
5	EDO	A	1764	-	3,3,3	0.31	0	2,2,2	0.31	0
5	EDO	A	1760	-	3,3,3	0.29	0	2,2,2	0.31	0
5	EDO	A	1769	-	3,3,3	0.26	0	2,2,2	0.37	0
5	EDO	A	1767	-	3,3,3	0.28	0	2,2,2	0.42	0
5	EDO	A	1770	-	3,3,3	0.26	0	2,2,2	0.38	0
5	EDO	A	1759	-	3,3,3	0.29	0	2,2,2	0.26	0
5	EDO	A	1768	-	3,3,3	0.29	0	2,2,2	0.18	0
4	BEF	A	1757	3,2	0,3,3	-	-	-		
5	EDO	A	1766	-	3,3,3	0.28	0	2,2,2	0.35	0
3	ADP	A	1756	4,2	24,29,29	1.58	3 (12%)	29,45,45	1.47	4 (13%)
5	EDO	A	1765	-	3,3,3	0.28	0	2,2,2	0.36	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	EDO	A	1762	-	-	0/1/1/1	-
5	EDO	A	1763	-	-	0/1/1/1	-
5	EDO	A	1772	-	-	0/1/1/1	-
5	EDO	A	1771	-	-	1/1/1/1	-
5	EDO	A	1758	-	-	0/1/1/1	-
5	EDO	A	1761	-	-	0/1/1/1	-
5	EDO	A	1764	-	-	0/1/1/1	-
5	EDO	A	1760	-	-	0/1/1/1	-
5	EDO	A	1769	-	-	0/1/1/1	-
5	EDO	A	1767	-	-	0/1/1/1	-
5	EDO	A	1770	-	-	0/1/1/1	-
5	EDO	A	1759	-	-	0/1/1/1	-
5	EDO	A	1768	-	-	0/1/1/1	-
5	EDO	A	1766	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	1756	4,2	-	2/12/32/32	0/3/3/3
5	EDO	A	1765	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1756	ADP	C8-N7	5.57	1.44	1.34
3	A	1756	ADP	PB-O1B	2.24	1.57	1.50
3	A	1756	ADP	C2-N3	2.21	1.35	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1756	ADP	N3-C2-N1	-4.21	122.10	128.68
3	A	1756	ADP	C1'-N9-C4	-2.69	121.92	126.64
3	A	1756	ADP	O3B-PB-O2B	2.48	117.10	107.64
3	A	1756	ADP	O3A-PB-O1B	-2.15	99.24	111.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1756	ADP	PA-O3A-PB-O2B
5	A	1766	EDO	O1-C1-C2-O2
5	A	1771	EDO	O1-C1-C2-O2
3	A	1756	ADP	PA-O3A-PB-O3B

There are no ring outliers.

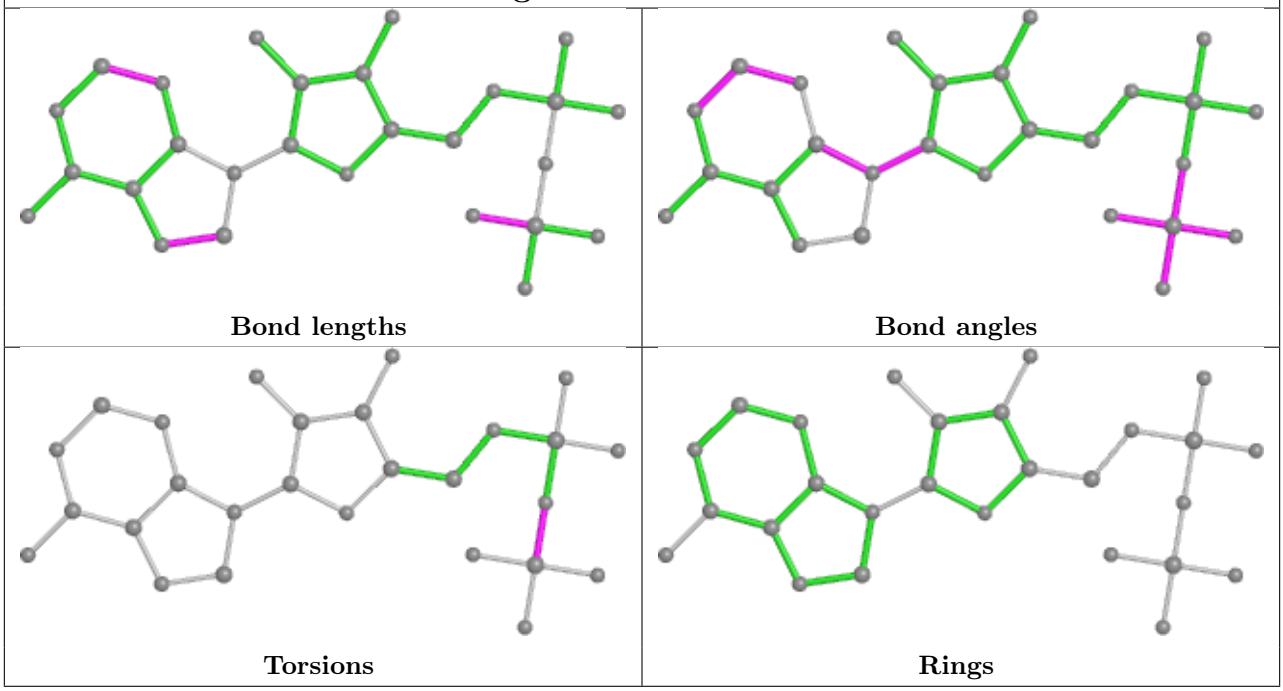
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1763	EDO	2	0
5	A	1764	EDO	1	0
5	A	1767	EDO	3	0
5	A	1770	EDO	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 ADP A 1756



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	A	703/770 (91%)	0.75	92 (13%) 3 5	11, 22, 61, 87	1 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	752	ALA	12.2
1	A	744	ILE	10.1
1	A	698	TYR	9.3
1	A	699	ALA	9.0
1	A	751	LEU	8.9
1	A	697	ILE	8.3
1	A	400	ALA	7.0
1	A	749	GLY	6.8
1	A	741	ILE	6.4
1	A	739	PHE	6.0
1	A	700	ASP	5.9
1	A	536	PRO	5.7
1	A	502	THR	5.7
1	A	399	LEU	5.4
1	A	621	ALA	5.4
1	A	501	TRP	5.1
1	A	504	ILE	5.0
1	A	692	PHE	5.0
1	A	691	GLY	4.9
1	A	42	LYS	4.9
1	A	500	ASN	4.9
1	A	745	PHE	4.9
1	A	444	GLU	4.8
1	A	742	THR	4.8
1	A	753	ARG	4.6
1	A	754	ILE	4.5
1	A	737	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	2	ASN	4.5
1	A	738	ARG	4.2
1	A	58[A]	ASP	4.2
1	A	537	ASN	4.2
1	A	5	HIS	3.9
1	A	363	ALA	3.8
1	A	625	ALA	3.8
1	A	445	ARG	3.8
1	A	740	GLY	3.8
1	A	535	PHE	3.8
1	A	624	GLY	3.7
1	A	290	ALA	3.7
1	A	506	PHE	3.7
1	A	443	GLN	3.6
1	A	688	THR	3.6
1	A	67	GLY	3.5
1	A	750	GLN	3.4
1	A	289	THR	3.3
1	A	202	ARG	3.3
1	A	40	ASP	3.3
1	A	626	ASN	3.3
1	A	746	PHE	3.2
1	A	57	SER	3.2
1	A	21	ASP	3.1
1	A	32	LYS	3.1
1	A	75	ASP	3.1
1	A	685	ILE	3.0
1	A	690	LYS	3.0
1	A	748	ALA	3.0
1	A	499	ILE	2.9
1	A	364	GLY	2.9
1	A	401	GLY	2.9
1	A	65[A]	VAL	2.8
1	A	736	GLN	2.8
1	A	503	PHE	2.7
1	A	71	GLN	2.7
1	A	66[A]	ASP	2.6
1	A	348	ILE	2.6
1	A	696	ILE	2.6
1	A	59	SER	2.6
1	A	53	VAL	2.5
1	A	193[A]	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	291	GLU	2.5
1	A	354	LEU	2.4
1	A	596	LEU	2.4
1	A	496	LYS	2.4
1	A	389	LEU	2.4
1	A	147	ARG	2.3
1	A	498	LYS	2.2
1	A	623	LYS	2.2
1	A	280	ILE	2.2
1	A	687	ILE	2.2
1	A	41	PRO	2.2
1	A	421	LEU	2.2
1	A	56	THR	2.2
1	A	3	PRO	2.1
1	A	600	PHE	2.1
1	A	72	VAL	2.1
1	A	627	PHE	2.1
1	A	74	LYS	2.1
1	A	150[A]	GLU	2.1
1	A	73	LYS	2.0
1	A	54	SER	2.0
1	A	294	LYS	2.0
1	A	347	ILE	2.0

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, 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.

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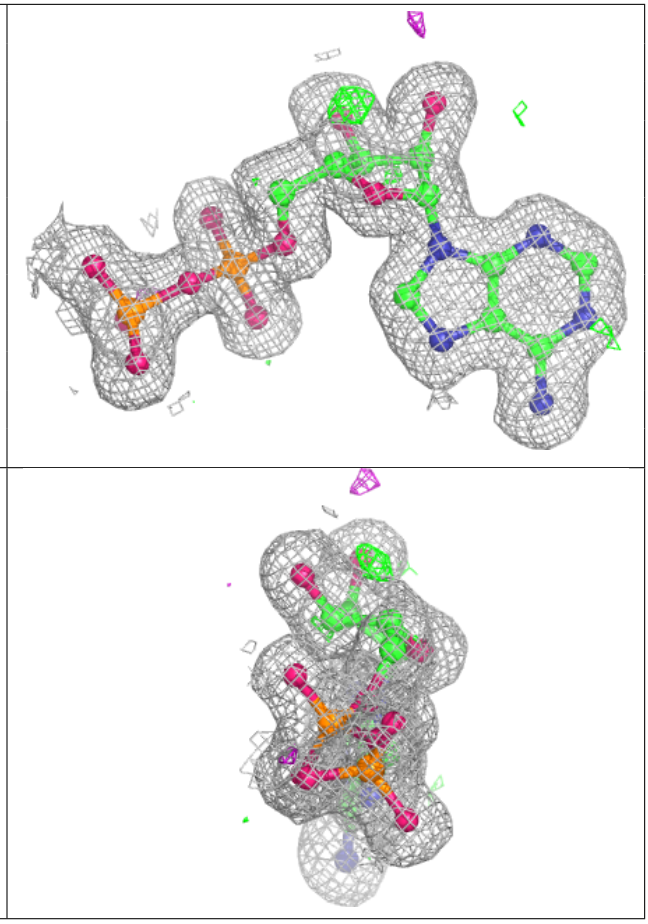
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	1763	4/4	0.74	0.17	47,47,48,49	0
5	EDO	A	1772	4/4	0.74	0.26	54,54,55,55	0
5	EDO	A	1771	4/4	0.77	0.30	56,56,57,57	0
5	EDO	A	1769	4/4	0.79	0.17	31,31,32,34	0
5	EDO	A	1768	4/4	0.83	0.17	27,31,34,36	0
5	EDO	A	1765	4/4	0.85	0.15	22,26,28,31	0
5	EDO	A	1770	4/4	0.85	0.20	40,40,40,41	0
5	EDO	A	1759	4/4	0.86	0.14	31,31,32,33	0
5	EDO	A	1762	4/4	0.87	0.17	35,36,36,38	0
5	EDO	A	1766	4/4	0.88	0.19	45,45,45,45	0
5	EDO	A	1767	4/4	0.93	0.12	32,35,35,37	0
5	EDO	A	1758	4/4	0.94	0.09	25,27,27,29	0
5	EDO	A	1760	4/4	0.94	0.09	28,28,30,30	0
5	EDO	A	1764	4/4	0.96	0.13	25,26,26,28	0
5	EDO	A	1761	4/4	0.97	0.08	34,35,35,37	0
3	ADP	A	1756	27/27	0.98	0.07	9,12,15,15	0
4	BEF	A	1757	4/4	0.99	0.09	10,11,11,12	0
2	MG	A	1755	1/1	1.00	0.06	10,10,10,10	0

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 ADP A 1756:

$2mF_o$-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.