



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:27 AM EDT

PDB ID : 1W9K / pdb_00001w9k
Title : Dictyostelium discoideum Myosin II motor domain S456E with bound MgADP-BeFx
Authors : Morris, C.A.; Coureux, P.-D.; Wells, A.L.; Houdusse, A.; Sweeney, H.L.
Deposited on : 2004-10-13
Resolution : 2.05 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 ⓘ 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 ⓘ](#)) 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

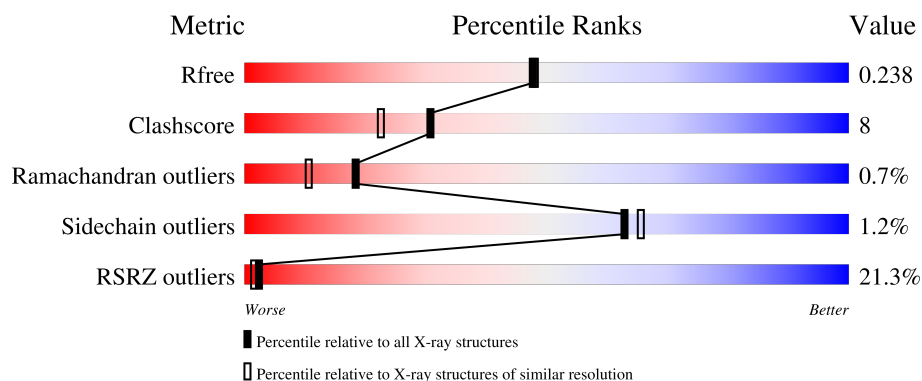
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 $\leq 5\%$. 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	770	20% 78% 14% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6109 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
1	A	719	Total	C	N	O	S	0	7	0
			5612	3577	955	1064	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	443	GLU	GLN	conflict	UNP P08799
A	456	GLU	SER	engineered mutation	UNP P08799
A	737	PHE	TYR	conflict	UNP P08799

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

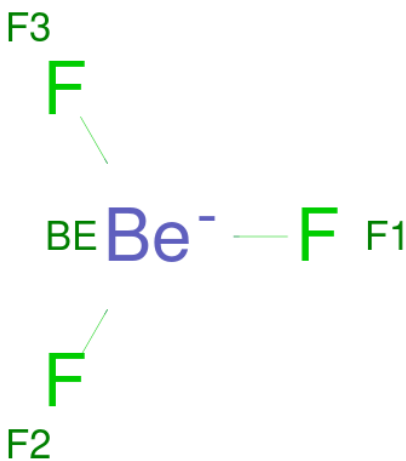
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

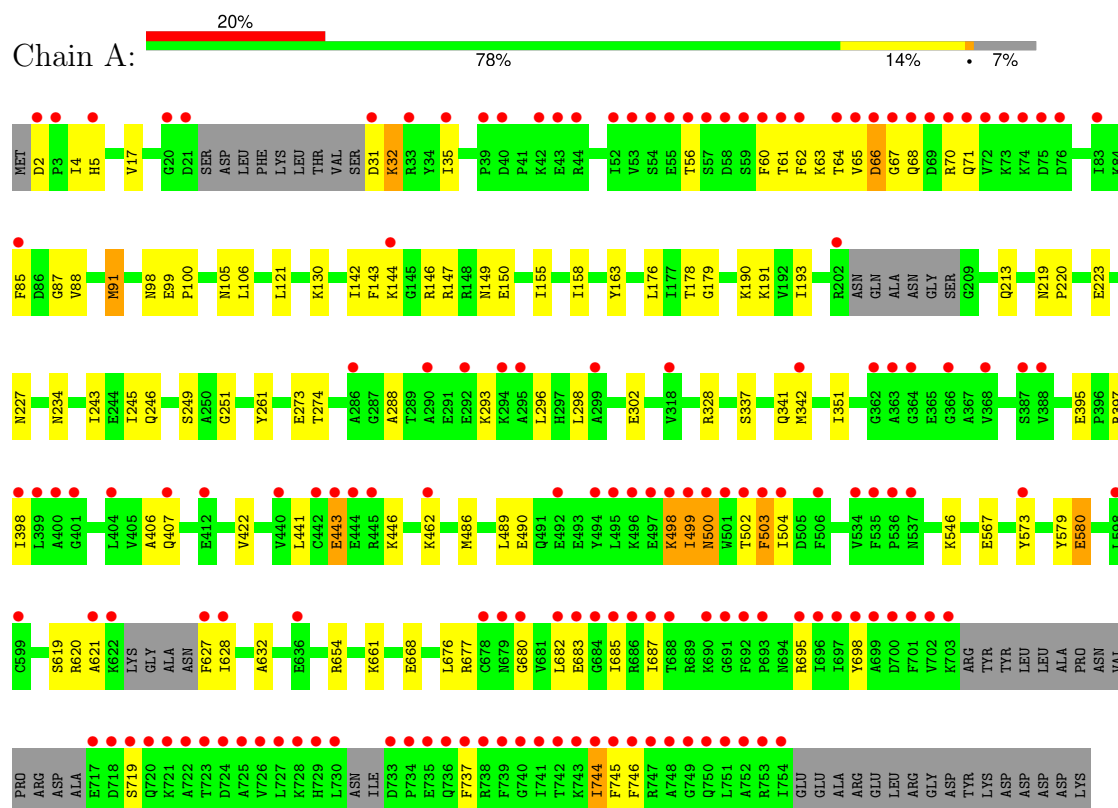
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	437	Total O 437 437	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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.70Å 179.43Å 54.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.05 40.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.1 (40.00-2.05) 98.1 (40.00-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.198 , 0.232 0.206 , 0.238	Depositor DCC
R_{free} test set	3179 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6109	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, EDO, ADP, MG

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	0.66	6/5745 (0.1%)	0.92	12/7774 (0.2%)

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
1	A	1	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	621	ALA	CA-C	10.25	1.66	1.53
1	A	91	MET	SD-CE	-8.23	1.58	1.79
1	A	621	ALA	CA-CB	-5.91	1.44	1.53
1	A	619	SER	CA-C	-5.86	1.45	1.52
1	A	91	MET	CG-SD	-5.16	1.67	1.80
1	A	443	GLU	CA-C	5.07	1.59	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	621	ALA	N-CA-C	10.99	125.52	110.35
1	A	620	ARG	N-CA-C	-9.65	97.52	110.55
1	A	443	GLU	N-CA-C	8.58	129.07	110.80
1	A	621	ALA	CA-C-O	-6.29	114.78	121.88
1	A	500	ASN	N-CA-C	5.90	123.38	110.80
1	A	504	ILE	N-CA-CB	-5.88	102.44	110.56
1	A	620	ARG	CA-C-N	-5.74	110.64	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	620	ARG	C-N-CA	-5.74	110.64	121.66
1	A	680	GLY	N-CA-C	5.51	122.37	115.21
1	A	17	VAL	N-CA-C	-5.44	102.50	109.30
1	A	441	LEU	N-CA-C	5.16	118.03	111.69
1	A	56	THR	N-CA-C	-5.12	99.89	110.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	443	GLU	CA

There are no planarity outliers.

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	5612	0	5409	92	1
2	A	1	0	0	0	0
3	A	27	0	12	0	0
4	A	4	0	0	0	0
5	A	28	0	42	7	0
6	A	437	0	0	11	0
All	All	6109	0	5463	93	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 8.

All (93) 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:654:ARG:NH1	6:A:2400:HOH:O	1.93	1.00
1:A:498:LYS:O	1:A:499:ILE:HG13	1.67	0.95
1:A:498:LYS:C	1:A:499:ILE:HG13	1.95	0.91
1:A:342:MET:HE3	1:A:342:MET:HA	1.53	0.90
1:A:744:ILE:HD12	1:A:746:PHE:CE2	2.11	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1763:EDO:H12	6:A:2174:HOH:O	1.76	0.84
1:A:628:ILE:HG12	1:A:632:ALA:HB3	1.59	0.82
1:A:142:ILE:HD11	5:A:1761:EDO:H21	1.59	0.82
1:A:744:ILE:HD12	1:A:746:PHE:CZ	2.13	0.82
1:A:91:MET:HE1	1:A:106:LEU:HG	1.61	0.82
1:A:219:ASN:HB3	1:A:220:PRO:HD3	1.61	0.81
1:A:193[B]:ILE:HD13	5:A:1760:EDO:H22	1.63	0.80
1:A:178[A]:THR:HG22	1:A:179:GLY:N	1.97	0.79
1:A:147:ARG:NH1	1:A:149:ASN:OD1	2.21	0.74
1:A:178[A]:THR:HG22	1:A:179:GLY:H	1.54	0.73
1:A:627:PHE:HB2	6:A:2371:HOH:O	1.91	0.70
1:A:261:TYR:CG	5:A:1764:EDO:H12	2.27	0.69
1:A:219:ASN:HD22	5:A:1760:EDO:HO1	1.41	0.68
1:A:31:ASP:O	1:A:32:LYS:CB	2.42	0.67
1:A:31:ASP:O	1:A:32:LYS:HG3	1.95	0.66
1:A:580:GLU:OE2	6:A:2340:HOH:O	2.13	0.66
1:A:31:ASP:O	1:A:32:LYS:CG	2.43	0.66
1:A:685:ILE:HB	6:A:2421:HOH:O	1.95	0.66
1:A:498:LYS:O	1:A:499:ILE:CG1	2.44	0.64
1:A:35:ILE:HD11	1:A:62:PHE:CD2	2.32	0.64
1:A:628:ILE:HD11	1:A:632:ALA:HB1	1.81	0.63
1:A:87:GLY:H	1:A:105:ASN:ND2	1.97	0.63
1:A:178[A]:THR:CG2	1:A:179:GLY:H	2.12	0.63
1:A:580:GLU:HG3	6:A:2342:HOH:O	2.00	0.61
1:A:121:LEU:HD12	1:A:486:MET:SD	2.42	0.60
1:A:31:ASP:O	1:A:32:LYS:HB2	2.03	0.58
1:A:328:ARG:HD2	6:A:2210:HOH:O	2.03	0.58
1:A:546:LYS:NZ	6:A:2304:HOH:O	2.34	0.58
1:A:744:ILE:C	1:A:744:ILE:HD13	2.29	0.57
1:A:147:ARG:NH2	1:A:150:GLU:OE2	2.37	0.56
1:A:573:TYR:OH	1:A:683:GLU:OE2	2.24	0.56
1:A:628:ILE:CG1	1:A:632:ALA:HB3	2.33	0.54
1:A:66:ASP:OD1	1:A:66:ASP:N	2.36	0.54
1:A:219:ASN:HB3	1:A:220:PRO:CD	2.35	0.53
1:A:85:PHE:O	1:A:88[A]:VAL:HG13	2.09	0.53
1:A:397:ARG:HA	1:A:406:ALA:HA	1.91	0.53
1:A:342:MET:HA	1:A:342:MET:CE	2.33	0.52
1:A:191:LYS:HA	1:A:191:LYS:HE2	1.90	0.52
1:A:744:ILE:HD13	1:A:745:PHE:N	2.25	0.52
1:A:99:GLU:OE1	1:A:677:ARG:NH2	2.43	0.52
1:A:142:ILE:CD1	5:A:1761:EDO:H21	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LEU:HD12	1:A:176:LEU:N	2.26	0.51
1:A:490:GLU:HB3	1:A:503:PHE:CE1	2.46	0.51
1:A:246:GLN:HG2	1:A:446:LYS:HD2	1.93	0.51
1:A:462:LYS:HD3	1:A:462:LYS:H	1.76	0.50
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.94	0.50
1:A:147:ARG:CZ	1:A:150:GLU:OE2	2.61	0.49
1:A:87:GLY:H	1:A:105:ASN:HD21	1.60	0.49
1:A:64:THR:OG1	1:A:66:ASP:OD1	2.30	0.49
1:A:193[B]:ILE:HD11	1:A:243:ILE:HD13	1.95	0.48
1:A:63:LYS:HA	1:A:68:GLN:O	2.12	0.48
1:A:490:GLU:HB3	1:A:503:PHE:HE1	1.78	0.48
1:A:261:TYR:CB	5:A:1764:EDO:H12	2.44	0.47
1:A:60:PHE:O	1:A:71:GLN:HA	2.13	0.47
1:A:190:LYS:HE3	1:A:223:GLU:OE2	2.13	0.47
1:A:121:LEU:CD1	1:A:486:MET:SD	3.03	0.47
1:A:4:ILE:HD12	1:A:146:ARG:NE	2.29	0.47
1:A:65:VAL:C	1:A:67:GLY:H	2.24	0.46
1:A:737:PHE:HA	1:A:745:PHE:O	2.15	0.46
1:A:2:ASP:OD2	1:A:5:HIS:HD2	1.99	0.46
1:A:98:ASN:OD1	1:A:100:PRO:HG2	2.15	0.46
1:A:193[A]:ILE:HD12	1:A:245:ILE:HD11	1.99	0.44
1:A:4:ILE:HD12	1:A:146:ARG:CZ	2.47	0.44
1:A:676:LEU:HB3	1:A:682:LEU:HG	2.00	0.44
1:A:155:ILE:O	1:A:158:ILE:HG22	2.18	0.43
1:A:302:GLU:H	1:A:302:GLU:CD	2.25	0.43
1:A:91:MET:HE1	1:A:106:LEU:CG	2.42	0.43
1:A:567:GLU:HA	1:A:579:TYR:O	2.19	0.43
1:A:398:ILE:HG12	1:A:407:GLN:HG2	2.00	0.43
1:A:661:LYS:NZ	1:A:668:GLU:OE2	2.47	0.43
1:A:130:LYS:HE2	6:A:2081:HOH:O	2.18	0.42
1:A:234:ASN:ND2	6:A:2154:HOH:O	2.52	0.42
1:A:99:GLU:N	1:A:100:PRO:HD2	2.35	0.42
1:A:273:GLU:C	1:A:274:THR:HG23	2.43	0.42
1:A:288:ALA:O	1:A:293:LYS:HE3	2.19	0.42
1:A:695:ARG:HG2	1:A:745:PHE:CD2	2.55	0.42
1:A:698:TYR:HB3	1:A:719:SER:CB	2.49	0.42
1:A:489:LEU:HD11	6:A:2270:HOH:O	2.18	0.42
1:A:61:THR:HA	1:A:70:ARG:O	2.20	0.42
1:A:296:LEU:HB2	1:A:298:LEU:HG	2.03	0.41
1:A:337:SER:O	1:A:341:GLN:HG3	2.20	0.41
1:A:395:GLU:HA	1:A:407:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:CD1	1:A:146:ARG:NE	2.84	0.41
1:A:143:PHE:O	1:A:144:LYS:C	2.63	0.41
1:A:223:GLU:O	1:A:227:ASN:HB2	2.21	0.41
1:A:163:TYR:OH	1:A:251:GLY:O	2.37	0.40
1:A:503:PHE:N	1:A:503:PHE:CD2	2.90	0.40
1:A:31:ASP:OD1	1:A:32:LYS:N	2.52	0.40

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:249:SER:OG	1:A:580:GLU:OE1[1_554]	2.19	0.01

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	714/770 (93%)	695 (97%)	14 (2%)	5 (1%)	18 10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	499	ILE
1	A	500	ASN
1	A	443	GLU
1	A	498	LYS

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	587/673 (87%)	580 (99%)	7 (1%)	63 65

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASP
1	A	213	GLN
1	A	502	THR
1	A	503	PHE
1	A	580	GLU
1	A	687	ILE
1	A	744	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	79	GLN
1	A	105	ASN
1	A	112	GLN
1	A	188	ASN
1	A	219	ASN
1	A	234	ASN
1	A	329	GLN
1	A	376	ASN
1	A	439	ASN
1	A	532	GLN
1	A	594	GLN
1	A	613	ASN
1	A	694	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	BEF	A	1757	2,3	0,3,3	-	-	-		
5	EDO	A	1758	-	3,3,3	0.33	0	2,2,2	0.51	0
5	EDO	A	1760	-	3,3,3	0.34	0	2,2,2	0.13	0
3	ADP	A	1756	2,4	28,29,29	2.33	5 (17%)	43,45,45	1.97	10 (23%)
5	EDO	A	1759	-	3,3,3	0.26	0	2,2,2	0.45	0
5	EDO	A	1761	-	3,3,3	0.30	0	2,2,2	0.40	0
5	EDO	A	1764	-	3,3,3	0.23	0	2,2,2	0.05	0
5	EDO	A	1763	-	3,3,3	0.26	0	2,2,2	0.39	0
5	EDO	A	1762	-	3,3,3	0.32	0	2,2,2	0.16	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	1758	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1760	-	-	0/1/1/1	-
3	ADP	A	1756	2,4	-	3/16/32/32	0/3/3/3
5	EDO	A	1759	-	-	1/1/1/1	-
5	EDO	A	1761	-	-	0/1/1/1	-
5	EDO	A	1764	-	-	1/1/1/1	-
5	EDO	A	1763	-	-	0/1/1/1	-
5	EDO	A	1762	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1756	ADP	C8-N7	6.94	1.45	1.31
3	A	1756	ADP	C8-N9	6.13	1.48	1.37
3	A	1756	ADP	PA-O3A	5.81	1.65	1.59
3	A	1756	ADP	PB-O1B	3.57	1.61	1.50
3	A	1756	ADP	PA-O1A	2.20	1.58	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1756	ADP	N9-C8-N7	-7.18	103.75	113.94
3	A	1756	ADP	N3-C2-N1	-4.60	121.62	128.58
3	A	1756	ADP	C5-C4-N3	-3.70	121.62	126.72
3	A	1756	ADP	C5-C4-N9	3.36	109.47	105.81
3	A	1756	ADP	C4-N9-C1'	-2.80	120.09	126.63
3	A	1756	ADP	C5-N7-C8	2.50	107.38	103.45
3	A	1756	ADP	C2'-C1'-N9	-2.43	107.26	113.30
3	A	1756	ADP	C2-N3-C4	2.43	117.77	111.83
3	A	1756	ADP	O3B-PB-O2B	2.09	115.64	107.80
3	A	1756	ADP	C6-C5-C4	2.03	119.95	117.18

There are no chirality outliers.

All (6) torsion outliers are listed below:

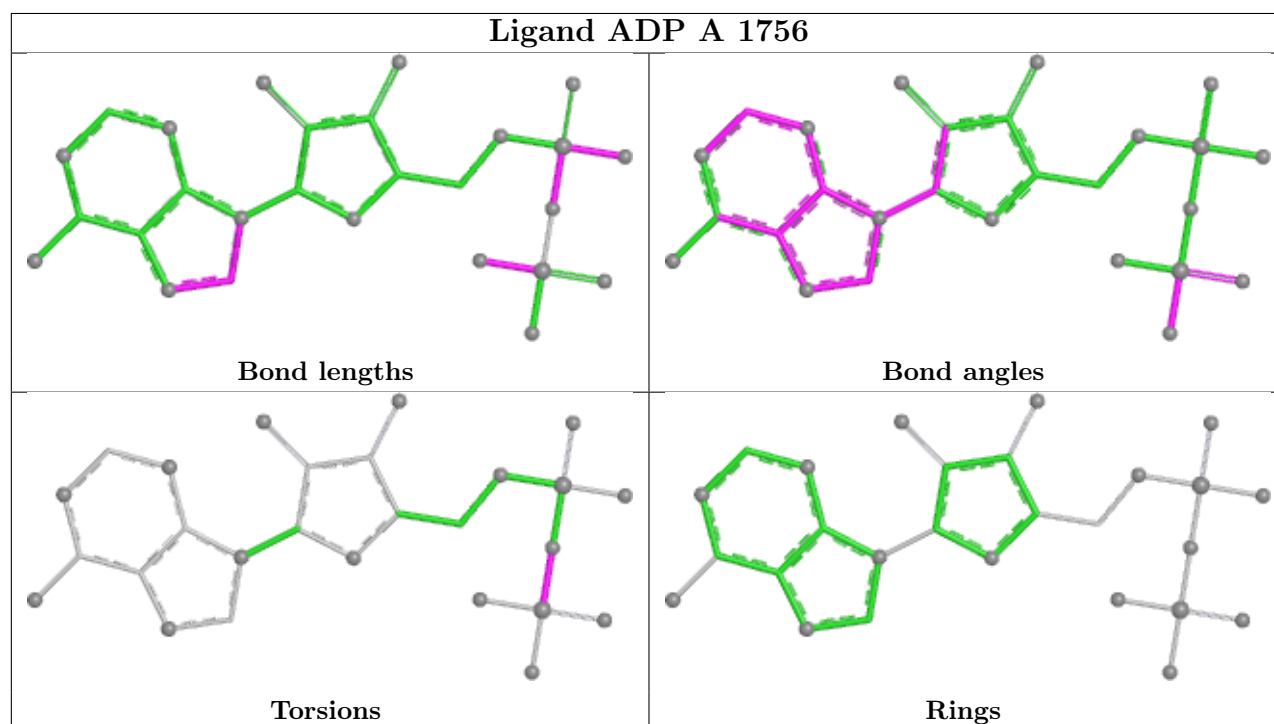
Mol	Chain	Res	Type	Atoms
3	A	1756	ADP	PA-O3A-PB-O2B
5	A	1758	EDO	O1-C1-C2-O2
5	A	1764	EDO	O1-C1-C2-O2
3	A	1756	ADP	PA-O3A-PB-O3B
3	A	1756	ADP	PA-O3A-PB-O1B
5	A	1759	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1760	EDO	2	0
5	A	1761	EDO	2	0
5	A	1764	EDO	2	0
5	A	1763	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 than 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.



5.7 Other polymers [i](#)

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, 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	719/770 (93%)	0.96	153 (21%) 2 1	14, 33, 80, 89	7 (0%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	685	ILE	8.1
1	A	701	PHE	7.4
1	A	497	GLU	7.2
1	A	718	ASP	7.0
1	A	739	PHE	6.6
1	A	730	LEU	6.5
1	A	744	ILE	6.1
1	A	733	ASP	6.0
1	A	503	PHE	6.0
1	A	726	VAL	5.9
1	A	534	VAL	5.9
1	A	702	VAL	5.8
1	A	752	ALA	5.8
1	A	738	ARG	5.7
1	A	72	VAL	5.7
1	A	725	ALA	5.6
1	A	746	PHE	5.4
1	A	741	ILE	5.4
1	A	622	LYS	5.3
1	A	745	PHE	5.1
1	A	722	ALA	5.1
1	A	499	ILE	5.1
1	A	65	VAL	5.0
1	A	717	GLU	5.0
1	A	599	CYS	5.0
1	A	621	ALA	4.9
1	A	498	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	723	THR	4.8
1	A	202	ARG	4.8
1	A	21	ASP	4.7
1	A	697	ILE	4.7
1	A	501	TRP	4.7
1	A	43	GLU	4.7
1	A	444	GLU	4.7
1	A	729	HIS	4.6
1	A	443	GLU	4.5
1	A	502	THR	4.5
1	A	52	ILE	4.5
1	A	719	SER	4.5
1	A	61	THR	4.5
1	A	692	PHE	4.5
1	A	362	GLY	4.4
1	A	754	ILE	4.4
1	A	742	THR	4.3
1	A	69	ASP	4.3
1	A	495	LEU	4.3
1	A	698	TYR	4.3
1	A	721	LYS	4.2
1	A	720	GLN	4.2
1	A	74	LYS	4.2
1	A	700	ASP	4.1
1	A	363	ALA	4.1
1	A	751	LEU	4.1
1	A	71	GLN	4.1
1	A	73	LYS	4.0
1	A	494	TYR	4.0
1	A	688	THR	4.0
1	A	535	PHE	3.9
1	A	537	ASN	3.9
1	A	691	GLY	3.9
1	A	687	ILE	3.9
1	A	66	ASP	3.8
1	A	67	GLY	3.8
1	A	678	CYS	3.8
1	A	683	GLU	3.8
1	A	627	PHE	3.8
1	A	728	LYS	3.7
1	A	536	PRO	3.7
1	A	727	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	31	ASP	3.6
1	A	684	GLY	3.6
1	A	399	LEU	3.6
1	A	500	ASN	3.5
1	A	387	SER	3.4
1	A	686	ARG	3.4
1	A	753	ARG	3.4
1	A	60	PHE	3.4
1	A	299	ALA	3.4
1	A	680	GLY	3.3
1	A	696	ILE	3.3
1	A	290	ALA	3.3
1	A	295	ALA	3.3
1	A	573	TYR	3.3
1	A	699	ALA	3.3
1	A	53	VAL	3.2
1	A	57	SER	3.2
1	A	368	VAL	3.2
1	A	42	LYS	3.1
1	A	33	ARG	3.1
1	A	62	PHE	3.1
1	A	58	ASP	3.0
1	A	690	LYS	3.0
1	A	735	GLU	3.0
1	A	737	PHE	3.0
1	A	412	GLU	3.0
1	A	703	LYS	3.0
1	A	445	ARG	2.9
1	A	695	ARG	2.9
1	A	364	GLY	2.9
1	A	736	GLN	2.9
1	A	398	ILE	2.9
1	A	39	PRO	2.9
1	A	506	PHE	2.9
1	A	724	ASP	2.8
1	A	35	ILE	2.8
1	A	59	SER	2.8
1	A	628	ILE	2.8
1	A	44	ARG	2.7
1	A	747	ARG	2.7
1	A	3	PRO	2.7
1	A	294	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	401	GLY	2.6
1	A	504	ILE	2.6
1	A	68	GLN	2.6
1	A	342	MET	2.6
1	A	64	THR	2.6
1	A	407	GLN	2.6
1	A	496	LYS	2.5
1	A	54	SER	2.5
1	A	462	LYS	2.5
1	A	85	PHE	2.5
1	A	750	GLN	2.5
1	A	5	HIS	2.5
1	A	56	THR	2.4
1	A	743	LYS	2.4
1	A	748	ALA	2.4
1	A	679	ASN	2.4
1	A	2	ASP	2.4
1	A	70	ARG	2.4
1	A	366	GLY	2.4
1	A	75	ASP	2.4
1	A	442	CYS	2.4
1	A	400	ALA	2.3
1	A	318	VAL	2.3
1	A	492	GLU	2.3
1	A	636	GLU	2.3
1	A	286	ALA	2.3
1	A	83	ILE	2.3
1	A	388	VAL	2.2
1	A	76	ASP	2.2
1	A	734	PRO	2.2
1	A	740	GLY	2.2
1	A	682	LEU	2.2
1	A	440	VAL	2.1
1	A	20	GLY	2.1
1	A	404	LEU	2.1
1	A	55	GLU	2.1
1	A	292	GLU	2.1
1	A	693	PRO	2.1
1	A	40	ASP	2.1
1	A	749	GLY	2.0
1	A	598	LEU	2.0
1	A	144	LYS	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](#)

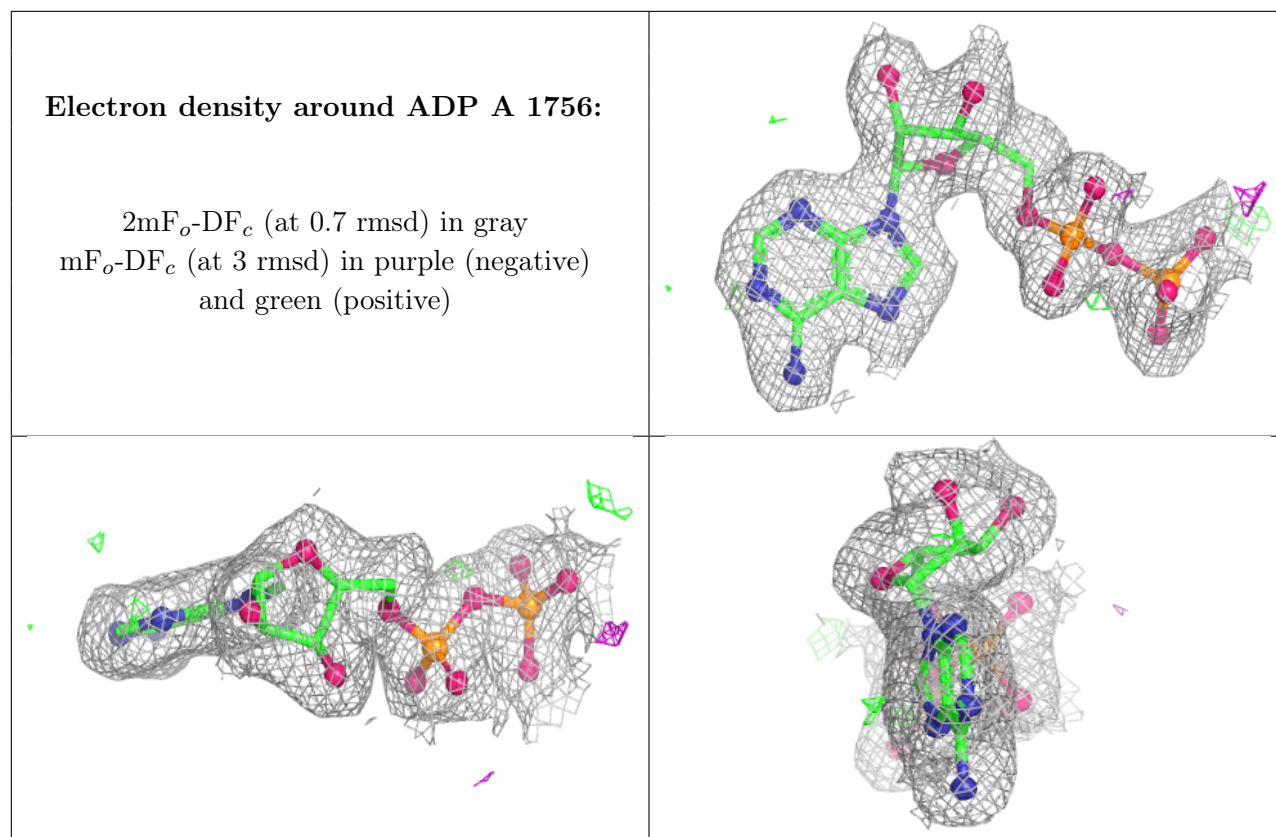
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
5	EDO	A	1761	4/4	0.89	0.18	45,51,52,56	0
5	EDO	A	1763	4/4	0.90	0.13	54,55,57,57	0
5	EDO	A	1759	4/4	0.91	0.14	40,42,43,44	0
5	EDO	A	1760	4/4	0.91	0.10	36,38,38,38	0
5	EDO	A	1762	4/4	0.92	0.13	25,38,42,46	0
5	EDO	A	1758	4/4	0.93	0.17	29,36,37,41	0
2	MG	A	1755	1/1	0.96	0.04	20,20,20,20	0
4	BEF	A	1757	4/4	0.97	0.06	17,19,21,21	0
3	ADP	A	1756	27/27	0.98	0.05	15,20,23,24	0
5	EDO	A	1764	4/4	0.98	0.04	21,21,23,24	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.