



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:16 AM UTC

PDB ID : 4ZG4 / pdb_00004zg4
Title : Myosin Vc Pre-powerstroke
Authors : Ropars, V.; Pylypenko, O.; Sweeney, L.; Houdusse, A.
Deposited on : 2015-04-22
Resolution : 2.36 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

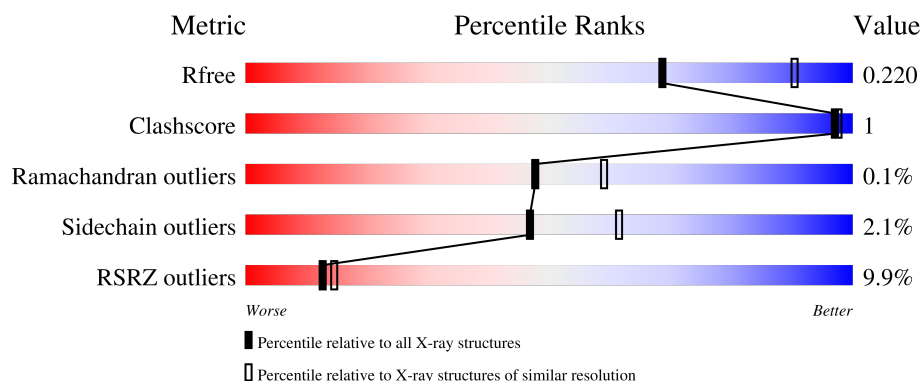
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	B	764	9% 88% 8%
1	E	764	9% 89% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21924 atoms, of which 10274 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-Vc.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	705	Total	C	H	N	O	S	0	5	0
			10590	3480	5116	928	1042	24			
1	E	711	Total	C	H	N	O	S	0	1	0
			10633	3497	5128	938	1047	23			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	756	GLY	-	expression tag	UNP Q9NQX4
B	757	ASP	-	expression tag	UNP Q9NQX4
B	758	TYR	-	expression tag	UNP Q9NQX4
B	759	LYS	-	expression tag	UNP Q9NQX4
B	760	ASP	-	expression tag	UNP Q9NQX4
B	761	ASP	-	expression tag	UNP Q9NQX4
B	762	ASP	-	expression tag	UNP Q9NQX4
B	763	ASP	-	expression tag	UNP Q9NQX4
B	764	LYS	-	expression tag	UNP Q9NQX4
E	756	GLY	-	expression tag	UNP Q9NQX4
E	757	ASP	-	expression tag	UNP Q9NQX4
E	758	TYR	-	expression tag	UNP Q9NQX4
E	759	LYS	-	expression tag	UNP Q9NQX4
E	760	ASP	-	expression tag	UNP Q9NQX4
E	761	ASP	-	expression tag	UNP Q9NQX4
E	762	ASP	-	expression tag	UNP Q9NQX4
E	763	ASP	-	expression tag	UNP Q9NQX4
E	764	LYS	-	expression tag	UNP Q9NQX4

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

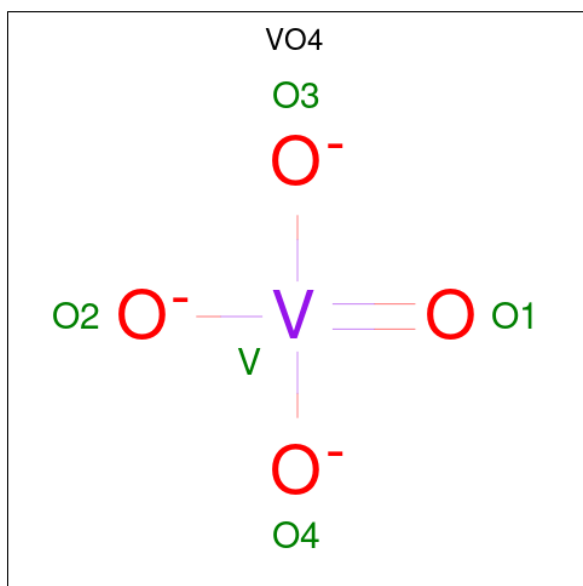
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		

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

- Molecule 3 is VANADATE ION (CCD ID: VO4) (formula: O_4V).



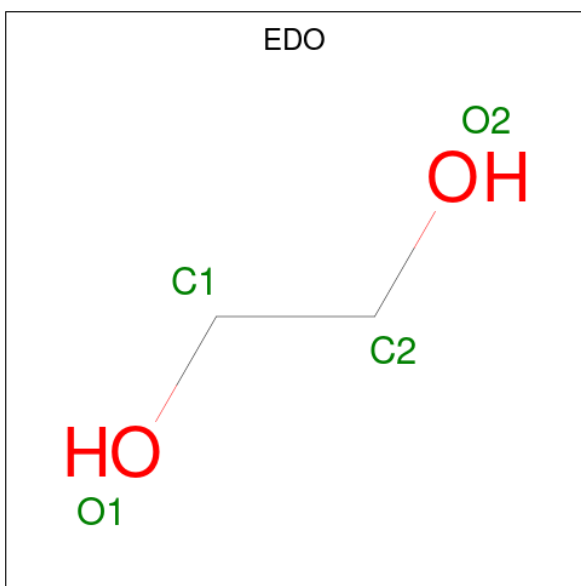
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	V	0	0
			5	4	1		
3	E	1	Total	O	V	0	0
			5	4	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0
4	E	1	Total 39	C 10	H 12	N 5	O 10	P 2	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	B	1	Total	C	H	O	0	0
			10	2	6	2		

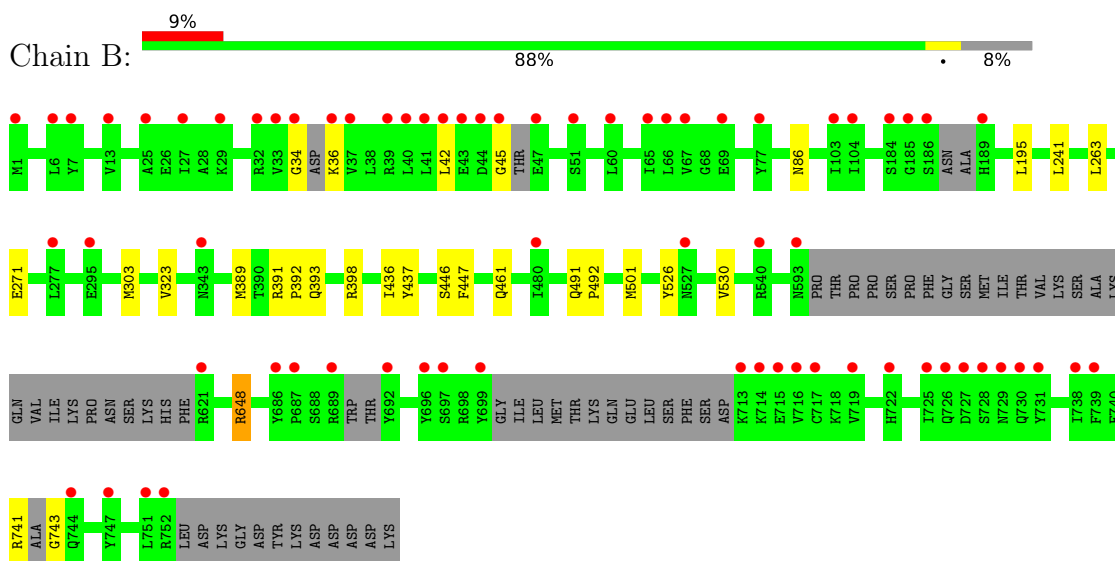
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	363	Total 363	O 363	0	0
6	E	238	Total 238	O 238	0	0

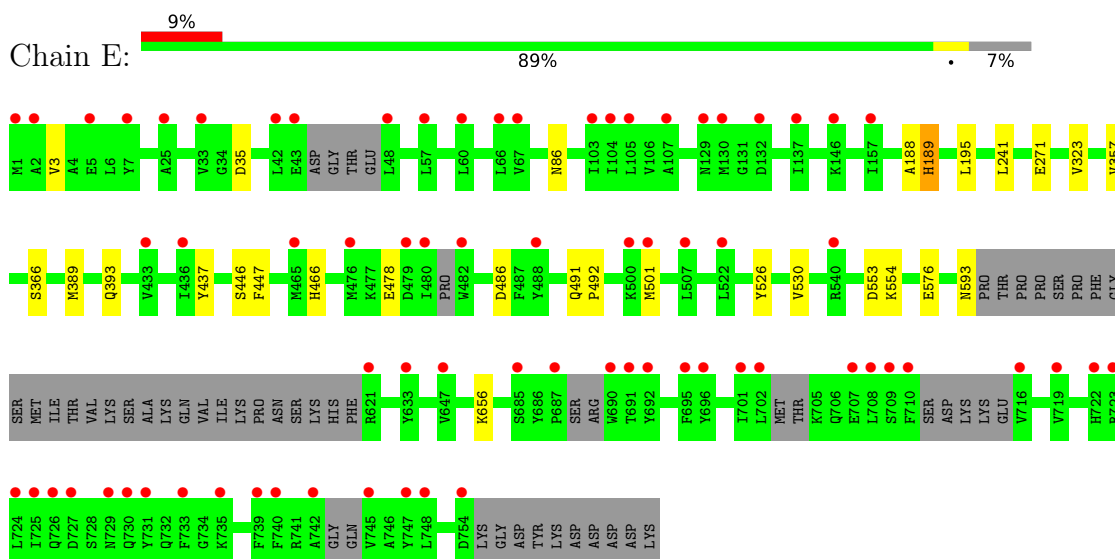
3 Residue-property plots

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-Vc



• Molecule 1: myosin-Vc



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.28Å 67.32Å 133.18Å 90.00° 108.48° 90.00°	Depositor
Resolution (Å)	49.54 – 2.36 49.54 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.54-2.36) 99.5 (49.54-2.36)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.173 , 0.213 0.184 , 0.220	Depositor DCC
R_{free} test set	4094 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21924	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: EDO, MG, VO4, 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	B	0.30	0/5604	0.62	0/7598
1	E	0.29	0/5616	0.63	0/7616
All	All	0.29	0/11220	0.63	0/15214

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	B	5474	5116	5099	12	0
1	E	5505	5128	5128	8	0
2	B	1	0	0	0	0
2	E	1	0	0	0	0
3	B	5	0	0	0	0
3	E	5	0	0	0	0
4	B	27	12	12	0	0
4	E	27	12	12	0	0
5	B	4	6	6	0	0
6	B	363	0	0	2	0
6	E	238	0	0	2	0
All	All	11650	10274	10257	20	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 1.

All (20) 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:B:648:ARG:NH2	6:B:901:HOH:O	2.28	0.66
1:B:34:GLY:O	1:B:36:LYS:N	2.35	0.59
1:B:741:ARG:O	1:B:743:GLY:N	2.36	0.59
1:E:466:HIS:ND1	6:E:901:HOH:O	2.32	0.59
1:E:656:LYS:NZ	6:E:902:HOH:O	2.32	0.58
1:B:461:GLN:NE2	1:B:491:GLN:OE1	2.38	0.56
1:B:42:LEU:N	1:B:45:GLY:O	2.42	0.52
1:E:553:ASP:OD1	1:E:554:LYS:N	2.46	0.49
1:E:188:ALA:HB3	1:E:189:HIS:HA	1.97	0.47
1:B:389:MET:HE2	1:B:393:GLN:HB3	1.99	0.45
1:B:526:TYR:HA	1:B:530:VAL:HG23	1.99	0.45
1:E:491:GLN:N	1:E:492:PRO:CD	2.81	0.44
1:E:446:SER:OG	1:E:447:PHE:N	2.52	0.42
1:B:446:SER:OG	1:B:447:PHE:N	2.50	0.42
1:B:491:GLN:N	1:B:492:PRO:CD	2.83	0.42
1:E:389:MET:HE2	1:E:393:GLN:HB3	2.02	0.42
1:B:263:LEU:HA	1:B:303:MET:HE2	2.03	0.41
1:B:398:ARG:NH2	6:B:911:HOH:O	2.50	0.41
1:E:526:TYR:HA	1:E:530:VAL:HG23	2.03	0.41
1:B:391:ARG:HB3	1:B:392:PRO:HD3	2.03	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	696/764 (91%)	679 (98%)	16 (2%)	1 (0%)	48 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	696/764 (91%)	679 (98%)	16 (2%)	1 (0%)	48 59
All	All	1392/1528 (91%)	1358 (98%)	32 (2%)	2 (0%)	48 59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	241	LEU
1	B	241	LEU

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	B	553/680 (81%)	545 (99%)	8 (1%)	59 73
1	E	553/680 (81%)	538 (97%)	15 (3%)	39 52
All	All	1106/1360 (81%)	1083 (98%)	23 (2%)	47 61

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	86	ASN
1	B	195	LEU
1	B	271	GLU
1	B	323	VAL
1	B	436	ILE
1	B	437	TYR
1	B	501	MET
1	B	648	ARG
1	E	3	VAL
1	E	35	ASP
1	E	86	ASN
1	E	189	HIS
1	E	195	LEU
1	E	271	GLU

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Mol	Chain	Res	Type
1	E	323	VAL
1	E	357	VAL
1	E	366	SER
1	E	437	TYR
1	E	478	GLU
1	E	486	ASP
1	E	501	MET
1	E	576	GLU
1	E	593	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	86	ASN
1	B	274	HIS
1	B	320	GLN
1	B	668	GLN
1	E	85	HIS
1	E	230	ASN
1	E	307	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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
3	VO4	E	802	4,2	0,4,4	-	-	-		
3	VO4	B	802	4,2	0,4,4	-	-	-		
5	EDO	B	804	-	3,3,3	0.44	0	2,2,2	0.34	0
4	ADP	E	803	3,2	28,29,29	0.81	1 (3%)	43,45,45	0.95	1 (2%)
4	ADP	B	803	3,2	28,29,29	0.64	1 (3%)	43,45,45	0.97	2 (4%)

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	B	804	-	-	0/1/1/1	-
4	ADP	B	803	3,2	-	1/16/32/32	0/3/3/3
4	ADP	E	803	3,2	-	1/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	803	ADP	PA-O1A	2.43	1.59	1.50
4	B	803	ADP	C4-N9	-2.06	1.33	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	ADP	C2'-C3'-C4'	-3.04	96.73	102.61
4	E	803	ADP	C2'-C3'-C4'	-2.71	97.37	102.61
4	B	803	ADP	O4'-C1'-N9	-2.17	103.92	108.09

There are no chirality outliers.

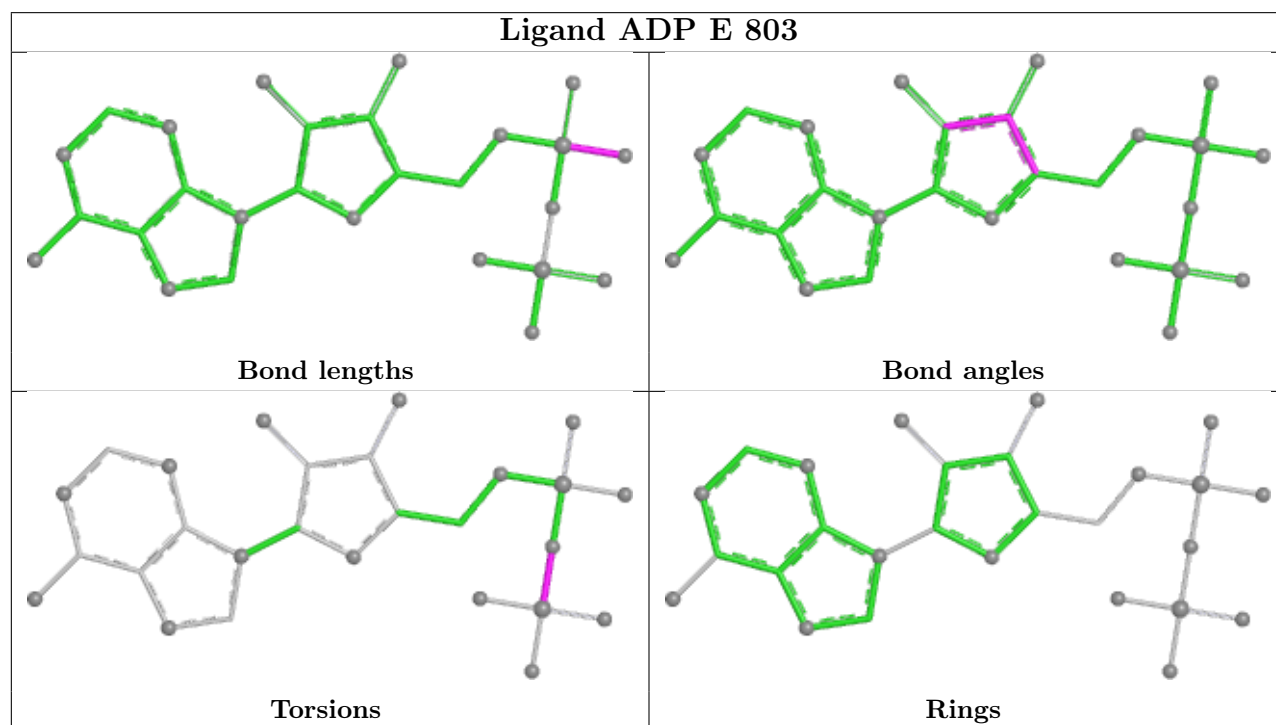
All (2) torsion outliers are listed below:

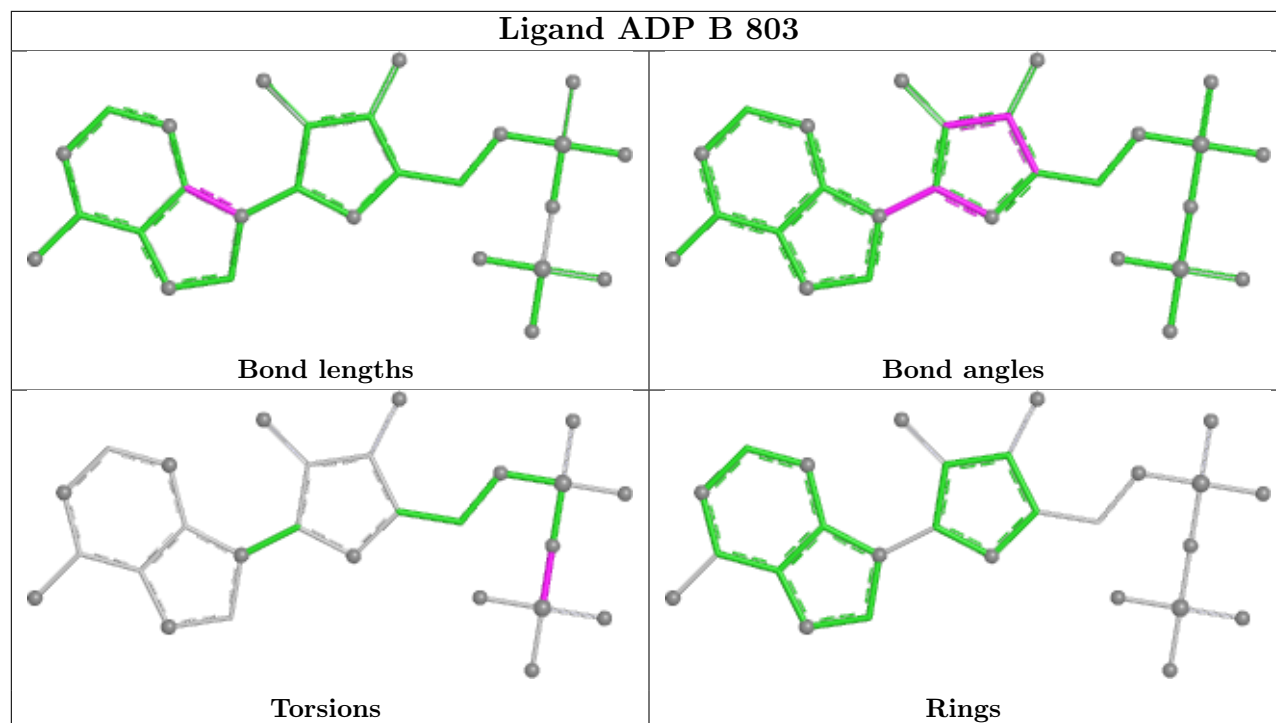
Mol	Chain	Res	Type	Atoms
4	B	803	ADP	PA-O3A-PB-O3B
4	E	803	ADP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

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	B	705/764 (92%)	0.41	68 (9%) 13 16	28, 68, 148, 198	3 (0%)
1	E	711/764 (93%)	0.57	72 (10%) 12 14	31, 82, 148, 189	1 (0%)
All	All	1416/1528 (92%)	0.49	140 (9%) 13 14	28, 76, 148, 198	4 (0%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	SER	6.9
1	E	103	ILE	5.2
1	E	43	GLU	5.1
1	E	692	TYR	5.0
1	E	48	LEU	5.0
1	E	710	PHE	4.7
1	B	687	PRO	4.6
1	B	103	ILE	4.5
1	B	717	CYS	4.5
1	E	42	LEU	4.4
1	E	725	ILE	4.4
1	E	727	ASP	4.2
1	E	480	ILE	4.1
1	B	730	GLN	4.1
1	B	13	VAL	4.0
1	E	479	ASP	3.9
1	E	748	LEU	3.8
1	B	696	TYR	3.7
1	E	621	ARG	3.7
1	E	522	LEU	3.7
1	B	65	ILE	3.6
1	B	34	GLY	3.6
1	E	716	VAL	3.6
1	B	752	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	729	ASN	3.6
1	B	44	ASP	3.6
1	B	738	ILE	3.5
1	E	132	ASP	3.5
1	B	25	ALA	3.5
1	B	185	GLY	3.5
1	E	739	PHE	3.5
1	E	708	LEU	3.4
1	B	37	VAL	3.4
1	B	45	GLY	3.4
1	E	476	MET	3.3
1	E	687	PRO	3.3
1	E	691	THR	3.3
1	B	60	LEU	3.3
1	B	32	ARG	3.3
1	E	60	LEU	3.2
1	B	343	ASN	3.2
1	B	7	TYR	3.2
1	B	41	LEU	3.2
1	E	137	ILE	3.2
1	E	733	PHE	3.1
1	B	40	LEU	3.1
1	B	36	LYS	3.1
1	B	714	LYS	3.1
1	E	740	PHE	3.1
1	E	488	TYR	3.1
1	E	507	LEU	3.1
1	E	724	LEU	3.1
1	E	696	TYR	3.0
1	E	5	GLU	3.0
1	B	697	SER	3.0
1	B	729	ASN	3.0
1	E	702	LEU	3.0
1	B	29	LYS	3.0
1	B	184	SER	3.0
1	B	731	TYR	2.9
1	B	51	SER	2.9
1	B	6	LEU	2.9
1	E	67	VAL	2.9
1	E	129	ASN	2.9
1	B	42	LEU	2.9
1	E	709	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	747	TYR	2.8
1	B	69[A]	GLU	2.8
1	E	726	GLN	2.8
1	B	1	MET	2.8
1	B	27	ILE	2.8
1	E	730	GLN	2.8
1	E	1	MET	2.8
1	E	501	MET	2.8
1	E	130	MET	2.8
1	E	465	MET	2.8
1	B	33	VAL	2.8
1	E	747	TYR	2.7
1	E	745	VAL	2.7
1	E	2	ALA	2.7
1	B	593	ASN	2.7
1	E	25	ALA	2.6
1	E	7	TYR	2.6
1	E	690	TRP	2.6
1	E	105	LEU	2.6
1	E	754	ASP	2.5
1	B	713	LYS	2.5
1	B	716	VAL	2.5
1	E	731	TYR	2.5
1	B	621	ARG	2.5
1	E	104	ILE	2.5
1	E	723	ARG	2.5
1	B	686	TYR	2.5
1	E	719	VAL	2.4
1	B	751	LEU	2.4
1	B	689	ARG	2.4
1	B	728	SER	2.4
1	B	295	GLU	2.4
1	E	735	LYS	2.4
1	B	719	VAL	2.4
1	E	742	ALA	2.4
1	B	727	ASP	2.3
1	E	685	SER	2.3
1	E	436	ILE	2.3
1	B	692	TYR	2.3
1	B	722	HIS	2.3
1	E	157	ILE	2.3
1	E	33	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	57	LEU	2.2
1	E	695	PHE	2.2
1	B	189	HIS	2.2
1	E	722	HIS	2.2
1	E	146	LYS	2.2
1	B	540	ARG	2.2
1	B	480	ILE	2.2
1	E	500	LYS	2.2
1	B	699	TYR	2.2
1	B	739	PHE	2.2
1	E	707	GLU	2.2
1	B	77	TYR	2.1
1	E	66	LEU	2.1
1	E	433	VAL	2.1
1	B	47	GLU	2.1
1	E	482	TRP	2.1
1	E	647	VAL	2.1
1	B	726	GLN	2.1
1	E	540	ARG	2.1
1	E	633	TYR	2.1
1	B	744	GLN	2.1
1	B	104	ILE	2.1
1	B	67	VAL	2.1
1	B	39	ARG	2.1
1	B	43	GLU	2.0
1	B	715	GLU	2.0
1	E	107	ALA	2.0
1	B	527	ASN	2.0
1	E	701	ILE	2.0
1	B	66	LEU	2.0
1	B	277	LEU	2.0
1	B	725	ILE	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 ⓘ

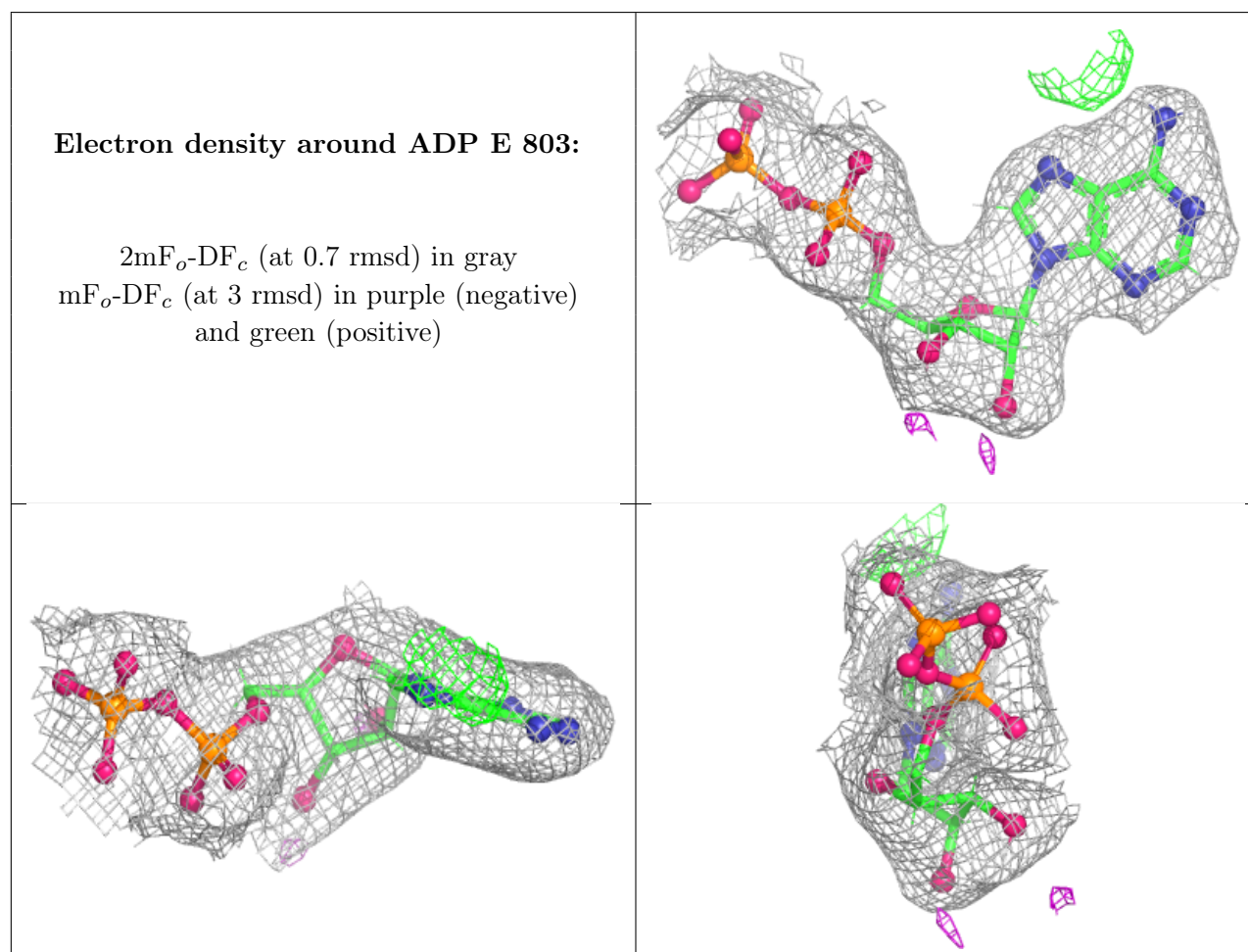
There are no oligosaccharides in this entry.

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. 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.

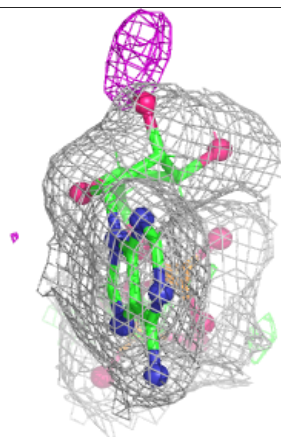
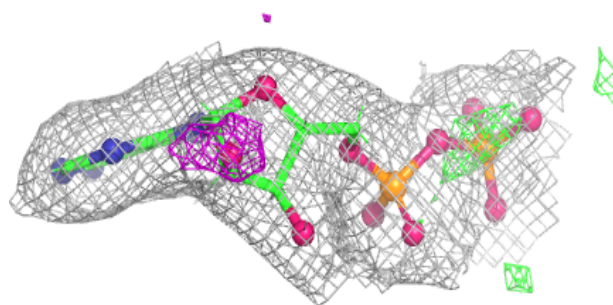
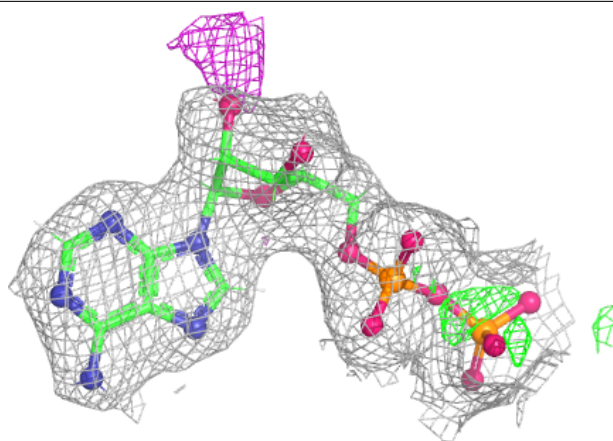
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	B	804	4/4	0.87	0.15	74,88,98,110	0
4	ADP	E	803	27/27	0.97	0.07	46,56,66,78	0
4	ADP	B	803	27/27	0.97	0.07	35,48,59,63	0
3	VO4	E	802	5/5	0.99	0.04	45,50,51,55	0
2	MG	B	801	1/1	0.99	0.08	44,44,44,44	0
2	MG	E	801	1/1	0.99	0.04	53,53,53,53	0
3	VO4	B	802	5/5	0.99	0.06	41,42,47,54	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 B 803:

$2mF_o-DF_c$ (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.