Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2026 – 10:51 pm BST

PDB ID	:	5HMP / pdb_00005hmp
Title	:	Myosin Vc pre-powerstroke state
Authors	:	Ropars, V.; Pylypenko, O.; Sweeney, H.L.; Houdusse, A.
Deposited on	:	2016-01-16
Resolution	:	2.40 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:

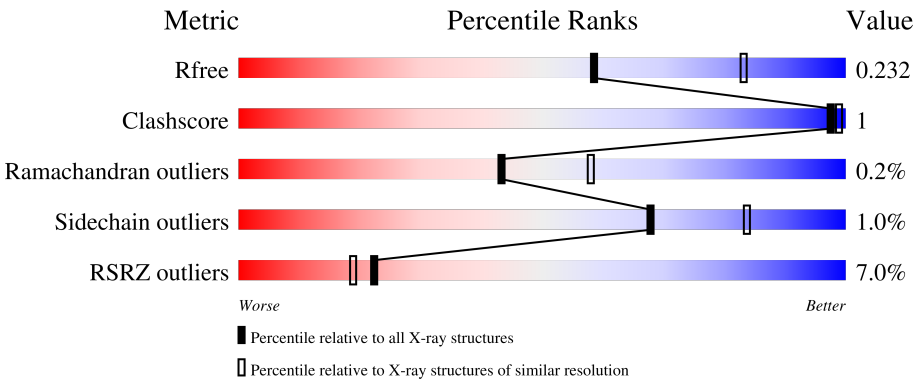
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	750	6% 91% • 7%
1	B	750	7% 92% • 5%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 22054 atoms, of which 10527 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.

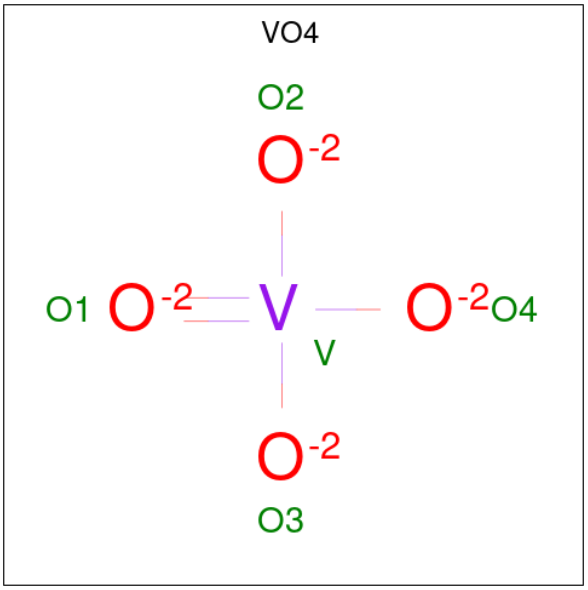
- Molecule 1 is a protein called Unconventional myosin-Vc.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	697	10580	3474	5131	926	1025	24	0	1	0
1	B	712	10972	3591	5348	954	1054	25	0	1	0

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

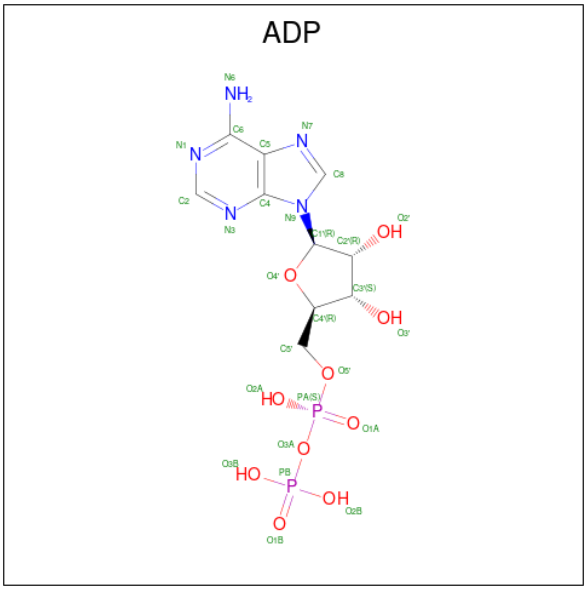
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

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



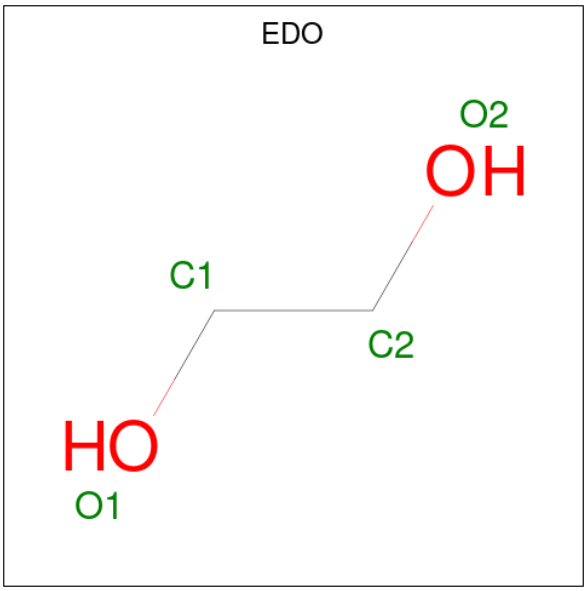
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	V		
3	A	1	5	4	1	0	0
			Total	O	V		
3	B	1	5	4	1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



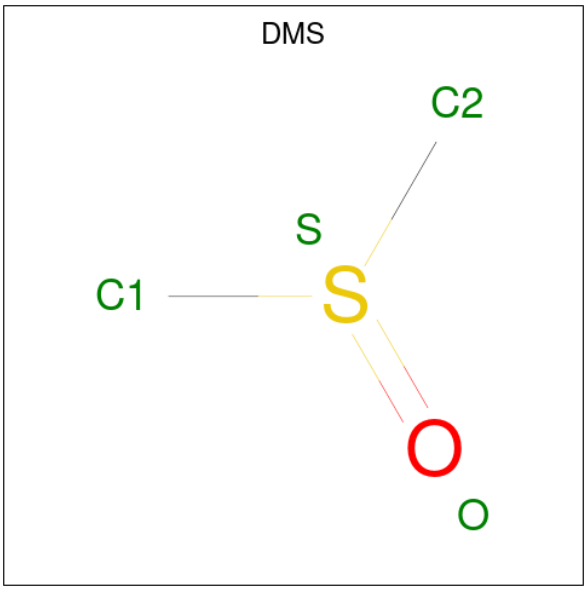
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
4	A	1	39	10	12	5	10	2	0	0
			Total	C	H	N	O	P		
4	B	1	39	10	12	5	10	2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	10	2	6	2	0	0
			Total	C	H	O		
5	B	1	10	2	6	2	0	0
			Total	C	H	O		
5	B	1	10	2	6	2	0	0

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
6	A	1	10	2	6	1	1	0	0

- Molecule 7 is water.

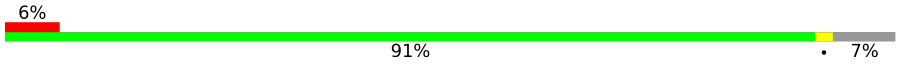
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	229	229	229	0	0
			Total	O		
7	B	143	143	143	0	0

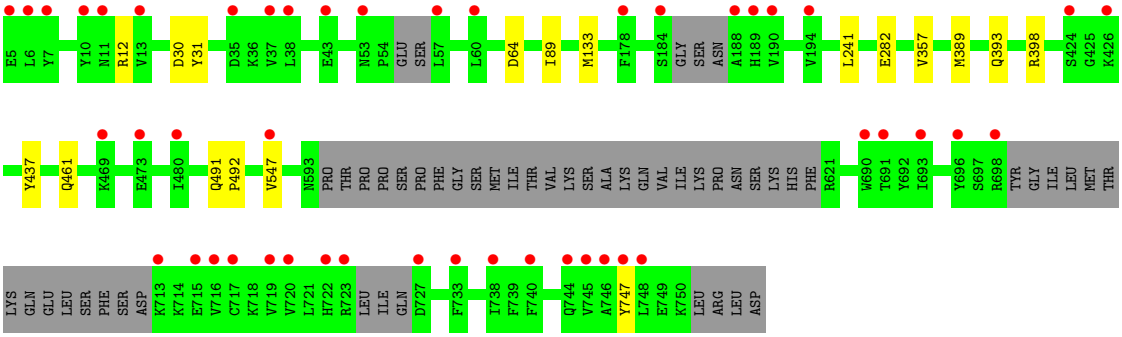
3 Residue-property plots (i)

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: Unconventional myosin-Vc

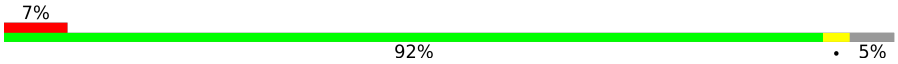
Chain A:

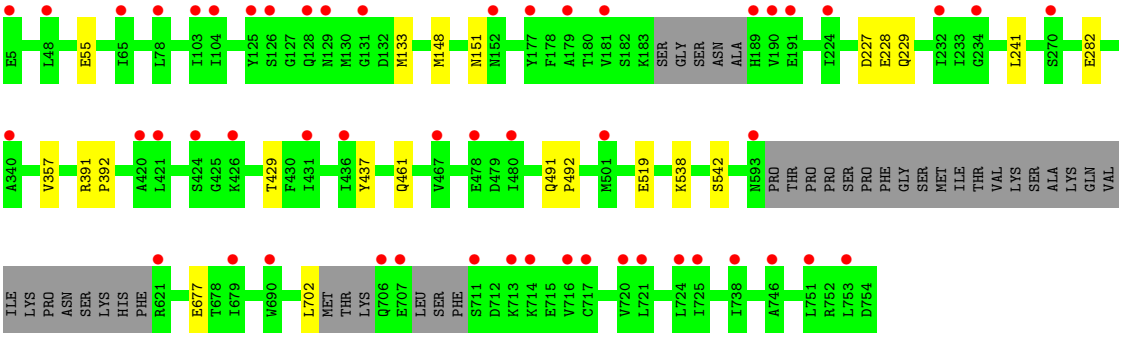




- Molecule 1: Unconventional myosin-Vc

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.78Å 66.74Å 131.26Å 90.00° 104.45° 90.00°	Depositor
Resolution (Å)	48.50 – 2.40 48.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.50-2.40) 98.3 (48.50-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.205 , 0.227 0.211 , 0.232	Depositor DCC
R_{free} test set	3380 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.1	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.7	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	0.95	EDS
Total number of atoms	22054	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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, ADP, DMS, VO4, EDO

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	0.29	0/5567	0.59	0/7543
1	B	0.28	0/5746	0.59	0/7788
All	All	0.29	0/11313	0.59	0/15331

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 (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	5449	5131	5130	7	0
1	B	5624	5348	5347	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	27	12	12	0	0
4	B	27	12	12	0	0
5	A	4	6	6	0	0
5	B	8	12	12	0	0
6	A	4	6	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	229	0	0	1	0
7	B	143	0	0	1	0
All	All	11527	10527	10525	17	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 (17) 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:461:GLN:NE2	1:A:491:GLN:OE1	2.32	0.61
1:B:461:GLN:NE2	1:B:491:GLN:OE1	2.33	0.61
1:A:282:GLU:OE1	7:A:901:HOH:O	2.16	0.60
1:B:148:MET:SD	1:B:429:THR:OG1	2.60	0.60
1:A:398:ARG:NH2	6:A:805:DMS:O	2.36	0.58
1:A:30:ASP:OD1	1:A:31:TYR:N	2.43	0.52
1:B:227:ASP:OD2	1:B:229:GLN:NE2	2.47	0.48
1:B:228:GLU:N	1:B:228:GLU:OE1	2.47	0.48
1:B:677:GLU:OE1	1:B:677:GLU:N	2.44	0.48
1:B:282:GLU:OE1	7:B:901:HOH:O	2.20	0.47
1:B:538:LYS:NZ	1:B:542:SER:O	2.45	0.47
1:A:389:MET:HE2	1:A:393:GLN:HB3	1.99	0.45
1:B:491:GLN:N	1:B:492:PRO:CD	2.79	0.45
1:B:519:GLU:OE1	1:B:519:GLU:N	2.48	0.44
1:A:491:GLN:N	1:A:492:PRO:CD	2.81	0.44
1:A:12:ARG:NH2	1:A:64:ASP:OD1	2.53	0.42
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	A	686/750 (92%)	664 (97%)	21 (3%)	1 (0%)	48	64
1	B	703/750 (94%)	679 (97%)	22 (3%)	2 (0%)	36	50
All	All	1389/1500 (93%)	1343 (97%)	43 (3%)	3 (0%)	43	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	241	LEU
1	A	241	LEU
1	B	151	ASN

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	A	556/669 (83%)	550 (99%)	6 (1%)	65	82
1	B	581/669 (87%)	576 (99%)	5 (1%)	70	85
All	All	1137/1338 (85%)	1126 (99%)	11 (1%)	68	84

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ILE
1	A	133	MET
1	A	357	VAL
1	A	437	TYR
1	A	547	VAL
1	A	747	TYR
1	B	55	GLU
1	B	133	MET
1	B	357	VAL
1	B	437	TYR
1	B	702	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	307	GLN
1	A	591	GLN
1	B	85	HIS
1	B	123	HIS
1	B	154	ASN
1	B	320	GLN
1	B	527	ASN
1	B	730	GLN
1	B	744	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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	B	805	-	3,3,3	0.47	0	2,2,2	0.28	0
5	EDO	B	804	-	3,3,3	0.48	0	2,2,2	0.28	0
3	VO4	B	802	4,2	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	VO4	A	802	4,2	0,4,4	-	-	-		
4	ADP	A	803	2,3	27,29,29	1.31	4 (14%)	42,45,45	1.96	10 (23%)
5	EDO	A	804	-	3,3,3	0.47	0	2,2,2	0.29	0
6	DMS	A	805	-	3,3,3	0.66	0	3,3,3	0.43	0
4	ADP	B	803	2,3	27,29,29	1.33	4 (14%)	42,45,45	2.01	10 (23%)

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	805	-	-	0/1/1/1	-
5	EDO	B	804	-	-	0/1/1/1	-
4	ADP	A	803	2,3	-	1/16/32/32	0/3/3/3
5	EDO	A	804	-	-	0/1/1/1	-
4	ADP	B	803	2,3	-	1/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803	ADP	C5-C4	4.37	1.47	1.39
4	A	803	ADP	C5-C4	4.28	1.47	1.39
4	B	803	ADP	C5-C6	2.61	1.48	1.41
4	A	803	ADP	C5-C6	2.54	1.48	1.41
4	B	803	ADP	C8-N7	2.32	1.36	1.31
4	A	803	ADP	C8-N7	2.31	1.36	1.31
4	A	803	ADP	C5-N7	-2.26	1.34	1.39
4	B	803	ADP	C5-N7	-2.25	1.34	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	803	ADP	C5-C4-N3	-6.36	118.45	126.75
4	A	803	ADP	C5-C4-N3	-6.00	118.92	126.75
4	B	803	ADP	N3-C4-N9	5.16	135.58	127.08
4	A	803	ADP	N3-C4-N9	4.96	135.25	127.08
4	B	803	ADP	C2-N3-C4	4.09	121.42	111.75
4	A	803	ADP	C2-N3-C4	3.99	121.17	111.75
4	B	803	ADP	N3-C2-N1	-3.63	122.93	128.60
4	A	803	ADP	N3-C2-N1	-3.62	122.94	128.60
4	B	803	ADP	PA-O3A-PB	-3.17	121.96	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	ADP	C4-N9-C8	3.12	109.11	105.73
4	B	803	ADP	C4-C5-N7	-3.10	106.84	110.62
4	A	803	ADP	C4-C5-N7	-2.98	106.99	110.62
4	B	803	ADP	C5-N7-C8	2.95	107.70	103.51
4	A	803	ADP	C5-N7-C8	2.89	107.61	103.51
4	B	803	ADP	C4-N9-C8	2.82	108.78	105.73
4	A	803	ADP	PA-O3A-PB	-2.73	123.47	132.83
4	A	803	ADP	N9-C8-N7	-2.52	110.47	113.91
4	B	803	ADP	N9-C8-N7	-2.35	110.71	113.91
4	A	803	ADP	C6-C5-N7	2.20	136.12	132.02
4	B	803	ADP	C6-C5-N7	2.05	135.85	132.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	ADP	PA-O3A-PB-O2B
4	B	803	ADP	PA-O3A-PB-O2B

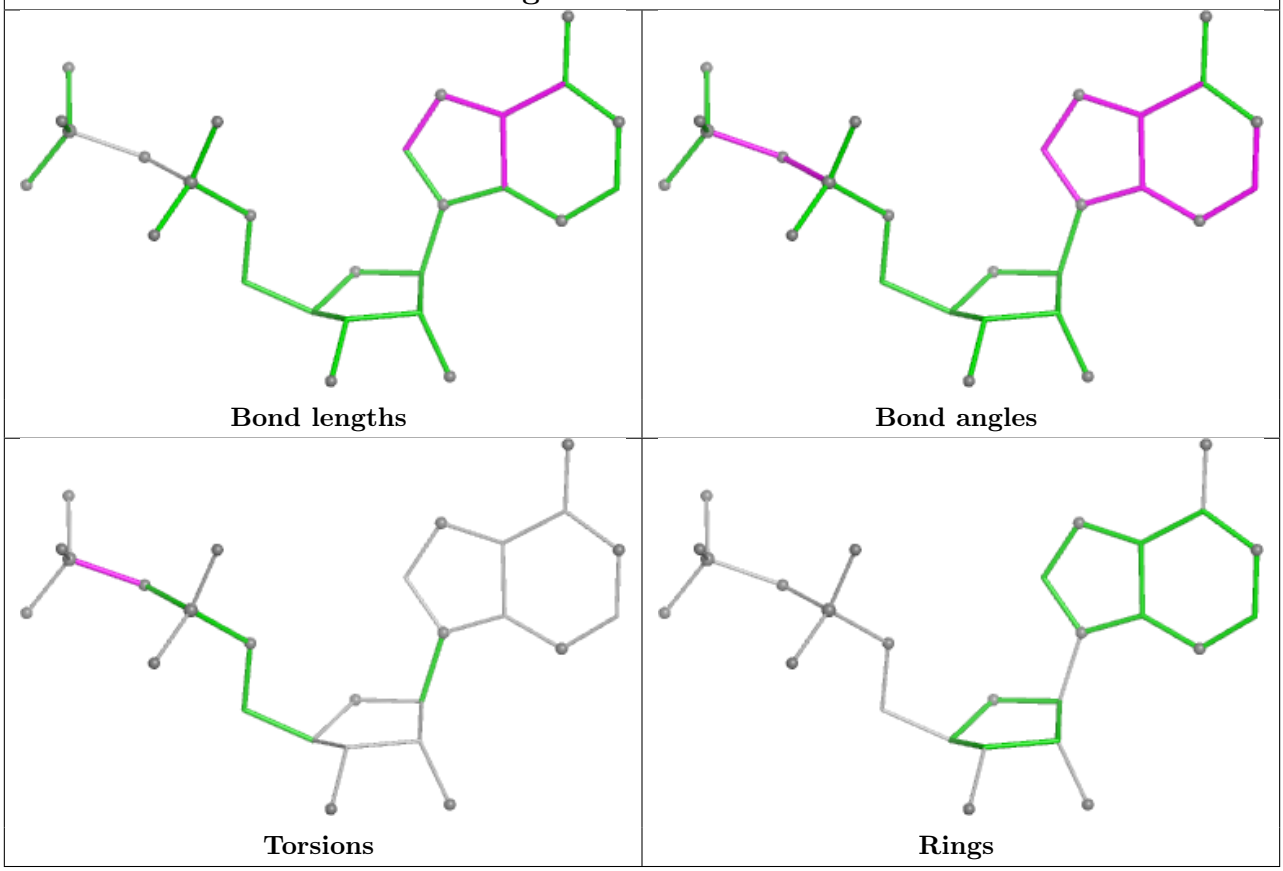
There are no ring outliers.

1 monomer is involved in 1 short contact:

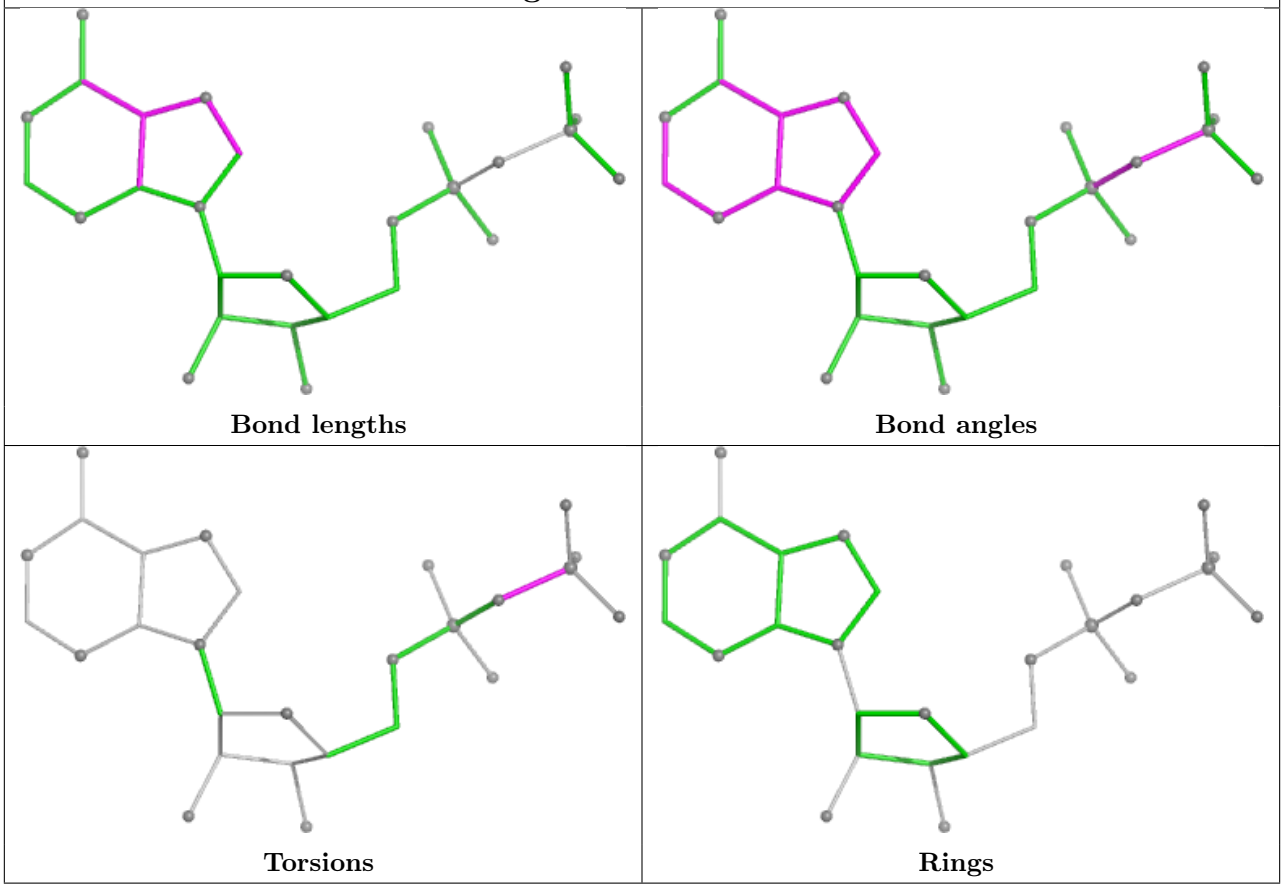
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	805	DMS	1	0

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 803



Ligand ADP B 803



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	697/750 (92%)	0.34	47 (6%)	24	20	42, 71, 171, 210	1 (0%)
1	B	712/750 (94%)	0.57	52 (7%)	21	17	45, 95, 155, 198	1 (0%)
All	All	1409/1500 (93%)	0.46	99 (7%)	22	19	42, 81, 159, 210	2 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	SER	5.6
1	B	234	GLY	5.3
1	B	724	LEU	5.3
1	B	129	ASN	5.1
1	B	720	VAL	4.8
1	B	189	HIS	4.3
1	B	706	GLN	4.2
1	B	5	GLU	4.0
1	B	707	GLU	4.0
1	B	128	GLN	3.9
1	A	716	VAL	3.8
1	A	188	ALA	3.8
1	B	593	ASN	3.7
1	A	696	TYR	3.7
1	A	693	ILE	3.6
1	A	7	TYR	3.6
1	B	725	ILE	3.5
1	A	424	SER	3.4
1	A	5	GLU	3.4
1	A	690	TRP	3.4
1	B	270	SER	3.3
1	A	53	ASN	3.3
1	B	717	CYS	3.2
1	A	35	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	721	LEU	3.2
1	B	711	SER	3.1
1	A	744	GLN	3.1
1	B	753	LEU	3.1
1	A	57	LEU	3.1
1	B	78	LEU	3.0
1	B	501	MET	3.0
1	B	104	ILE	3.0
1	B	103	ILE	3.0
1	B	65	ILE	2.9
1	A	717	CYS	2.9
1	A	480	ILE	2.9
1	A	748	LEU	2.9
1	A	719	VAL	2.9
1	A	715	GLU	2.9
1	B	424	SER	2.9
1	B	713	LYS	2.8
1	A	698	ARG	2.8
1	A	720	VAL	2.8
1	B	480	ILE	2.8
1	A	60	LEU	2.8
1	A	722	HIS	2.7
1	A	713	LYS	2.7
1	A	723	ARG	2.7
1	A	691	THR	2.7
1	B	478	GLU	2.7
1	B	421	LEU	2.6
1	B	190	VAL	2.6
1	A	13	VAL	2.6
1	A	745	VAL	2.6
1	B	716	VAL	2.6
1	A	426	LYS	2.6
1	B	679	ILE	2.5
1	A	194	VAL	2.5
1	B	126	SER	2.5
1	B	181	VAL	2.5
1	B	431	ILE	2.5
1	B	738	ILE	2.5
1	B	179	ALA	2.5
1	A	43	GLU	2.5
1	B	232	ILE	2.5
1	B	621	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	38	LEU	2.4
1	A	727	ASP	2.4
1	A	189	HIS	2.4
1	B	152	ASN	2.4
1	A	10	TYR	2.3
1	B	714	LYS	2.3
1	A	547	VAL	2.3
1	A	733	PHE	2.3
1	A	6	LEU	2.3
1	A	473	GLU	2.3
1	B	467	VAL	2.3
1	B	48	LEU	2.3
1	A	469	LYS	2.3
1	A	190	VAL	2.3
1	B	224	ILE	2.2
1	B	436	ILE	2.2
1	B	426	LYS	2.2
1	A	747	TYR	2.2
1	B	340	ALA	2.2
1	B	746	ALA	2.2
1	B	690	TRP	2.1
1	A	37	VAL	2.1
1	B	420	ALA	2.1
1	A	11	ASN	2.1
1	B	191	GLU	2.1
1	A	178	PHE	2.1
1	A	740	PHE	2.1
1	B	125	TYR	2.0
1	B	177	TYR	2.0
1	B	131	GLY	2.0
1	A	746	ALA	2.0
1	B	751	LEU	2.0
1	A	738	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 oligosaccharides in this entry.

6.4 Ligands (i)

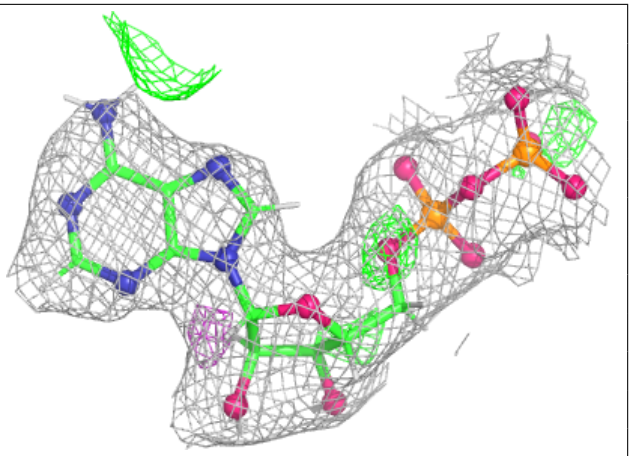
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

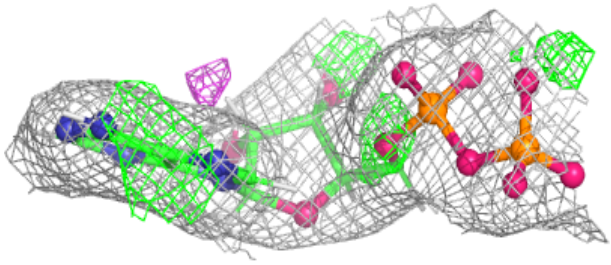
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	DMS	A	805	4/4	0.85	0.28	84,115,162,162	0
5	EDO	B	805	4/4	0.88	0.15	76,91,92,93	0
5	EDO	B	804	4/4	0.88	0.21	80,96,99,100	0
4	ADP	B	803	27/27	0.95	0.10	47,64,77,81	0
5	EDO	A	804	4/4	0.96	0.12	57,68,69,70	0
4	ADP	A	803	27/27	0.97	0.07	40,52,63,64	0
2	MG	B	801	1/1	0.98	0.10	58,58,58,58	0
3	VO4	B	802	5/5	0.98	0.07	39,52,61,64	0
3	VO4	A	802	5/5	0.99	0.06	32,44,45,53	0
2	MG	A	801	1/1	1.00	0.10	43,43,43,43	0

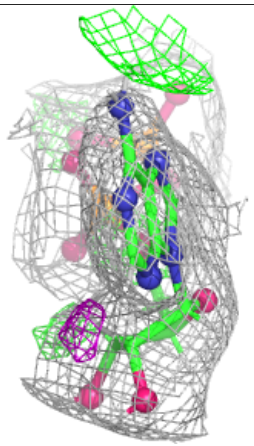
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

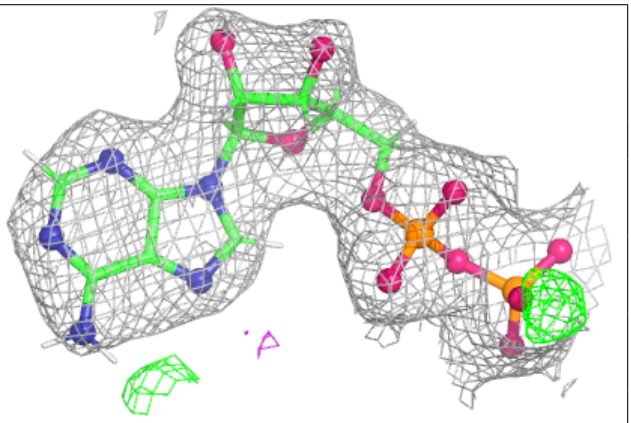


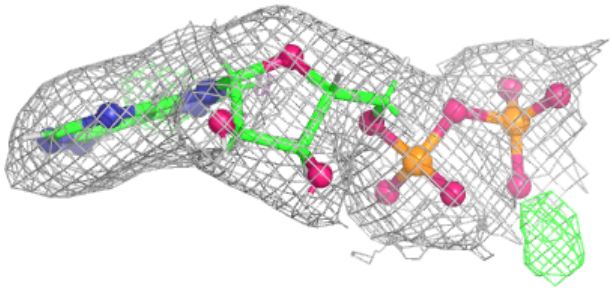


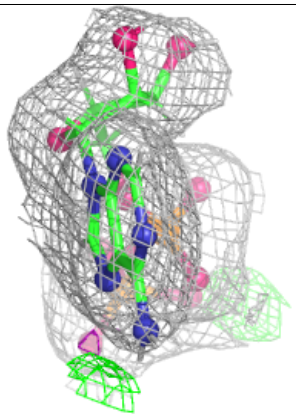


Electron density around ADP A 803:

$2mF_o$-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.