



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:39 am BST

PDB ID : 1VOM  
Title : COMPLEX BETWEEN DICTYOSTELIUM MYOSIN AND MGADP AND  
VANADATE AT 1.9A RESOLUTION  
Authors : Rayment, I.; Smith, C.A.  
Deposited on : 1995-11-09  
Resolution : 1.90 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

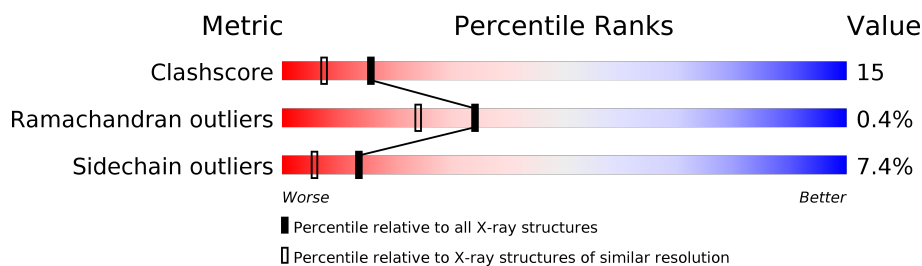
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	762	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6488 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	730	5750	3654	992	1088	16	0	0	0

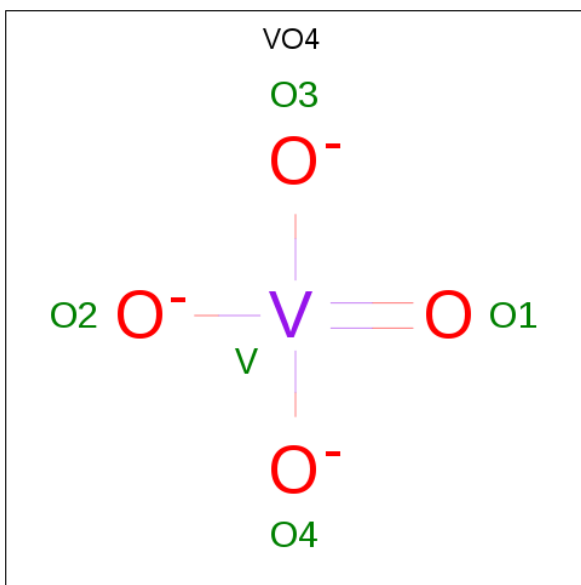
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ASP	LYS	CONFLICT	UNP P08799
A	312	CYS	TYR	CONFLICT	UNP P08799
A	321	GLU	SER	CONFLICT	UNP P08799
A	322	ASP	GLU	CONFLICT	UNP P08799
A	443	SER	GLN	CONFLICT	UNP P08799
A	446	ALA	LYS	CONFLICT	UNP P08799
A	489	VAL	LEU	CONFLICT	UNP P08799

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

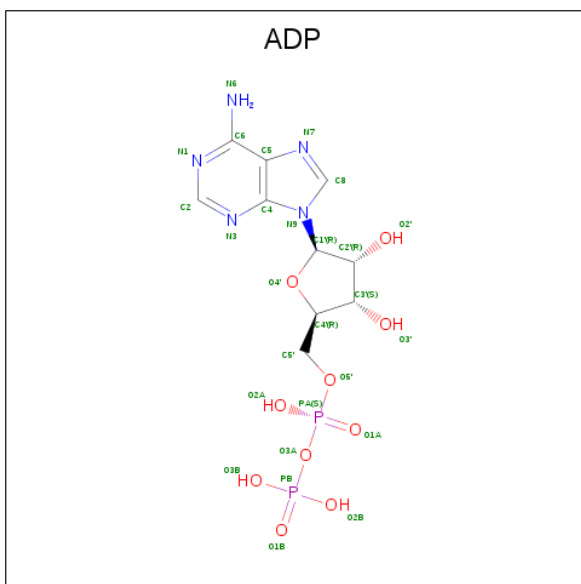
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is VANADATE ION (three-letter code: VO4) (formula: O<sub>4</sub>V).



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

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



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

- Molecule 5 is water.

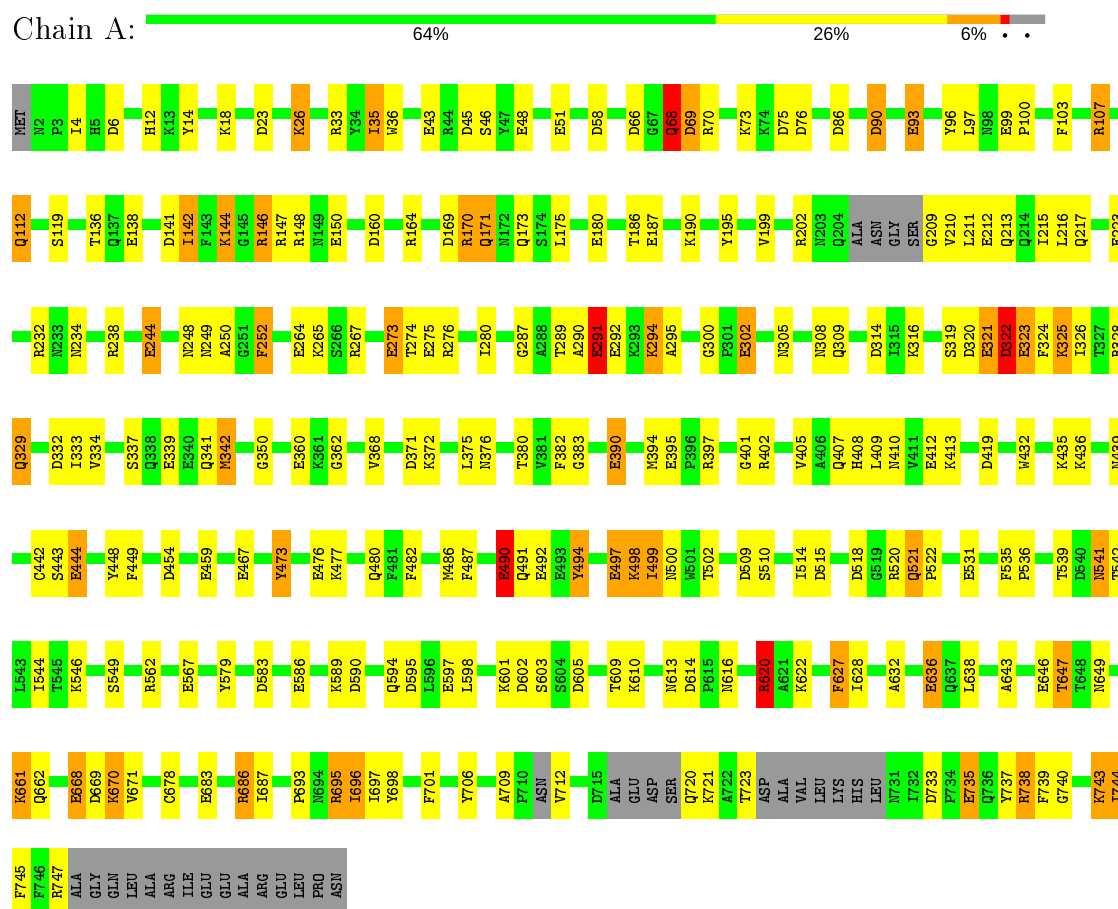
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	705	Total 705	O 705	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

#### • Molecule 1: MYOSIN



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.50 Å   145.40 Å   153.80 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.90)	Depositor
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6488	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VO4, MG, 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	0.95	37/5860 (0.6%)	1.54	83/7916 (1.0%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	GLU	CD-OE2	7.54	1.33	1.25
1	A	291	GLU	CD-OE1	6.94	1.33	1.25
1	A	646	GLU	CD-OE1	6.50	1.32	1.25
1	A	292	GLU	CD-OE1	6.26	1.32	1.25
1	A	48	GLU	CD-OE1	6.15	1.32	1.25
1	A	492	GLU	CD-OE1	6.03	1.32	1.25
1	A	275	GLU	CD-OE2	6.02	1.32	1.25
1	A	273	GLU	CD-OE1	5.99	1.32	1.25
1	A	497	GLU	CD-OE2	5.98	1.32	1.25
1	A	444	GLU	CD-OE1	5.95	1.32	1.25
1	A	412	GLU	CD-OE2	5.91	1.32	1.25
1	A	360	GLU	CD-OE1	5.90	1.32	1.25
1	A	302	GLU	CD-OE2	5.84	1.32	1.25
1	A	321	GLU	CD-OE1	5.80	1.32	1.25
1	A	476	GLU	CD-OE1	5.78	1.32	1.25
1	A	490	GLU	CD-OE1	5.76	1.31	1.25
1	A	668	GLU	CD-OE2	5.75	1.31	1.25
1	A	586	GLU	CD-OE2	5.71	1.31	1.25
1	A	597	GLU	CD-OE1	5.63	1.31	1.25
1	A	531	GLU	CD-OE2	5.50	1.31	1.25
1	A	187	GLU	CD-OE1	5.50	1.31	1.25
1	A	683	GLU	CD-OE2	-5.49	1.19	1.25
1	A	323	GLU	CD-OE2	5.45	1.31	1.25
1	A	93	GLU	CD-OE1	5.42	1.31	1.25
1	A	339	GLU	CD-OE2	5.39	1.31	1.25
1	A	43	GLU	CD-OE1	5.36	1.31	1.25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	GLU	CD-OE1	5.35	1.31	1.25
1	A	636	GLU	CD-OE2	5.32	1.31	1.25
1	A	467	GLU	CD-OE2	5.32	1.31	1.25
1	A	683	GLU	CD-OE1	5.31	1.31	1.25
1	A	180	GLU	CD-OE2	5.19	1.31	1.25
1	A	223	GLU	CD-OE2	5.18	1.31	1.25
1	A	735	GLU	CD-OE2	5.18	1.31	1.25
1	A	264	GLU	CD-OE2	-5.15	1.20	1.25
1	A	390	GLU	CD-OE1	5.15	1.31	1.25
1	A	459	GLU	CD-OE1	5.12	1.31	1.25
1	A	244	GLU	CD-OE1	5.06	1.31	1.25

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ARG	NE-CZ-NH2	-16.82	111.89	120.30
1	A	620	ARG	NE-CZ-NH1	11.45	126.03	120.30
1	A	6	ASP	CB-CG-OD2	-11.13	108.28	118.30
1	A	232	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	518	ASP	CB-CG-OD1	8.90	126.31	118.30
1	A	595	ASP	CB-CG-OD1	-8.77	110.40	118.30
1	A	332	ASP	CB-CG-OD1	8.76	126.18	118.30
1	A	371	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	A	397	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	170	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	A	58	ASP	CB-CG-OD1	8.21	125.69	118.30
1	A	590	ASP	CB-CG-OD1	-8.16	110.95	118.30
1	A	332	ASP	CB-CG-OD2	-8.05	111.05	118.30
1	A	602	ASP	CB-CG-OD2	-7.91	111.19	118.30
1	A	6	ASP	CB-CG-OD1	7.81	125.33	118.30
1	A	58	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	A	267	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	A	419	ASP	CB-CG-OD1	7.65	125.18	118.30
1	A	70	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	69	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	A	494	TYR	CB-CG-CD1	-7.29	116.63	121.00
1	A	518	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	A	371	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	169	ASP	CB-CG-OD1	-7.15	111.87	118.30
1	A	419	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	A	627	PHE	CB-CG-CD2	-7.04	115.87	120.80
1	A	66	ASP	CB-CG-OD2	6.81	124.43	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	320	ASP	CB-CG-OD1	-6.78	112.20	118.30
1	A	322	ASP	CB-CG-OD1	6.65	124.29	118.30
1	A	314	ASP	CB-CG-OD1	-6.64	112.32	118.30
1	A	75	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	A	70	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	69	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	238	ARG	NE-CZ-NH2	6.41	123.51	120.30
1	A	583	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	A	595	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	33	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	141	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	A	223	GLU	CG-CD-OE2	-6.33	105.64	118.30
1	A	107	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	A	90	ASP	CB-CG-OD2	6.18	123.87	118.30
1	A	90	ASP	CB-CG-OD1	-6.16	112.76	118.30
1	A	75	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	473	TYR	CB-CG-CD1	5.89	124.53	121.00
1	A	408	HIS	CA-CB-CG	-5.87	103.63	113.60
1	A	583	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	562	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	509	ASP	CB-CG-OD1	-5.76	113.11	118.30
1	A	33	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	590	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	314	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	454	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	A	66	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	A	502	THR	N-CA-CB	5.57	120.89	110.30
1	A	442	CYS	CB-CA-C	5.51	121.43	110.40
1	A	605	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	401	GLY	N-CA-C	-5.50	99.35	113.10
1	A	515	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	454	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	45	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	442	CYS	N-CA-CB	5.42	120.36	110.60
1	A	210	VAL	CA-CB-CG2	-5.42	102.77	110.90
1	A	602	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	509	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	647	THR	CA-CB-CG2	-5.34	104.92	112.40
1	A	322	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	380	THR	CA-CB-CG2	-5.33	104.94	112.40
1	A	402	ARG	NE-CZ-NH1	5.28	122.94	120.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	402	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	14	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	A	252	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	A	276	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	A	93	GLU	CA-CB-CG	-5.17	102.03	113.40
1	A	515	ASP	CB-CG-OD1	-5.17	113.65	118.30
1	A	686	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	334	VAL	C-N-CA	-5.12	111.55	122.30
1	A	521	GLN	N-CA-CB	5.08	119.73	110.60
1	A	112	GLN	N-CA-CB	5.05	119.68	110.60
1	A	141	ASP	CB-CG-OD2	5.03	122.82	118.30
1	A	86	ASP	CB-CG-OD1	-5.00	113.80	118.30
1	A	96	TYR	CB-CG-CD1	-5.00	118.00	121.00

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	A	5750	0	5569	167	10
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	27	0	12	0	0
5	A	705	0	0	13	1
All	All	6488	0	5581	167	10

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 15.

All (167) 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:289:THR:HG22	1:A:291:GLU:H	1.17	1.07

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:LYS:HE2	1:A:671:VAL:HG23	1.39	1.02
1:A:620:ARG:HH11	1:A:620:ARG:HG3	1.23	1.00
1:A:342:MET:HA	1:A:342:MET:HE2	1.45	0.98
1:A:480:GLN:HE21	1:A:510:SER:HB2	1.25	0.98
1:A:480:GLN:HE22	1:A:510:SER:H	1.05	0.96
1:A:541:ASN:HD22	1:A:541:ASN:H	1.07	0.93
1:A:628:ILE:CD1	1:A:628:ILE:CB	2.46	0.93
1:A:97:LEU:HD23	1:A:686:ARG:HG2	1.50	0.91
1:A:480:GLN:NE2	1:A:510:SER:H	1.67	0.91
1:A:499:ILE:HG12	1:A:738:ARG:HB3	1.54	0.90
1:A:289:THR:HG22	1:A:291:GLU:N	1.86	0.89
1:A:541:ASN:N	1:A:541:ASN:HD22	1.77	0.81
1:A:480:GLN:NE2	1:A:510:SER:HB2	1.95	0.80
1:A:322:ASP:O	1:A:326:ILE:HD12	1.83	0.79
1:A:490:GLU:HG2	5:A:1456:HOH:O	1.82	0.79
1:A:171:GLN:HG2	1:A:173:GLN:NE2	1.97	0.79
1:A:628:ILE:CD1	1:A:628:ILE:CA	2.61	0.78
1:A:706:TYR:O	1:A:709:ALA:HB3	1.83	0.78
1:A:628:ILE:CD1	1:A:628:ILE:HA	2.13	0.78
1:A:325:LYS:O	1:A:329:GLN:HG2	1.83	0.78
1:A:720:GLN:O	1:A:723:THR:HB	1.83	0.77
1:A:90:ASP:O	1:A:93:GLU:HG3	1.84	0.76
1:A:265:LYS:HE2	5:A:1647:HOH:O	1.85	0.76
1:A:68:GLN:HG3	1:A:69:ASP:N	2.01	0.75
1:A:535:PHE:CD1	1:A:536:PRO:HD2	2.22	0.74
1:A:697:ILE:HA	1:A:743:LYS:HB3	1.70	0.74
1:A:601:LYS:HG2	1:A:613:ASN:ND2	2.04	0.72
1:A:589:LYS:O	1:A:620:ARG:NH2	2.22	0.71
1:A:701:PHE:CE2	1:A:723:THR:HG23	2.26	0.71
1:A:4:ILE:HD12	1:A:146:ARG:NH2	2.07	0.69
1:A:541:ASN:HB2	5:A:1591:HOH:O	1.92	0.69
1:A:390:GLU:HG2	1:A:394:MET:CE	2.23	0.69
1:A:614:ASP:OD1	1:A:616:ASN:HB2	1.93	0.68
1:A:308:ASN:OD1	1:A:309:GLN:NE2	2.26	0.68
1:A:541:ASN:H	1:A:541:ASN:ND2	1.88	0.68
1:A:138:GLU:O	1:A:142:ILE:HD12	1.94	0.67
1:A:747:ARG:HG2	5:A:1339:HOH:O	1.93	0.67
1:A:97:LEU:HD23	1:A:686:ARG:CG	2.24	0.67
1:A:432:TRP:CZ2	1:A:436:LYS:HE2	2.29	0.67
1:A:695:ARG:HB2	1:A:743:LYS:HD2	1.78	0.66
1:A:701:PHE:HE2	1:A:723:THR:HG23	1.60	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LYS:HG2	5:A:1681:HOH:O	1.95	0.65
1:A:696:ILE:H	1:A:696:ILE:HD12	1.60	0.65
1:A:300:GLY:HA3	1:A:302:GLU:OE2	1.97	0.64
1:A:620:ARG:NH1	1:A:620:ARG:HG3	1.97	0.63
1:A:209:GLY:O	1:A:213:GLN:HB2	1.99	0.62
1:A:160:ASP:O	1:A:164:ARG:HG2	1.99	0.62
1:A:287:GLY:HA3	1:A:324:PHE:HD2	1.65	0.62
1:A:329:GLN:O	1:A:333:ILE:HD12	2.00	0.61
1:A:103:PHE:CE2	1:A:669:ASP:HB3	2.34	0.61
1:A:147:ARG:HB2	1:A:150:GLU:CG	2.30	0.61
1:A:342:MET:CE	1:A:342:MET:HA	2.26	0.61
1:A:211:LEU:O	1:A:215:ILE:HG13	2.01	0.61
1:A:497:GLU:HG3	1:A:745:PHE:CZ	2.36	0.61
1:A:521:GLN:HA	1:A:522:PRO:C	2.21	0.61
1:A:698:TYR:CE1	1:A:744:ILE:HB	2.36	0.61
1:A:620:ARG:HD2	1:A:627:PHE:HB3	1.83	0.61
1:A:670:LYS:H	1:A:670:LYS:HD3	1.66	0.59
1:A:443:SER:O	1:A:444:GLU:HG2	2.02	0.59
1:A:337:SER:O	1:A:341:GLN:HG3	2.02	0.59
1:A:164:ARG:HG3	5:A:1106:HOH:O	2.03	0.59
1:A:435:LYS:HE2	1:A:616:ASN:HB3	1.84	0.59
1:A:147:ARG:HB2	1:A:150:GLU:HG3	1.85	0.59
1:A:202:ARG:HG3	1:A:252:PHE:CD1	2.38	0.58
1:A:601:LYS:HG2	1:A:613:ASN:HD21	1.69	0.58
1:A:698:TYR:O	1:A:701:PHE:HB3	2.04	0.57
1:A:209:GLY:O	1:A:213:GLN:N	2.35	0.57
1:A:480:GLN:NE2	1:A:510:SER:N	2.48	0.57
1:A:97:LEU:CD2	1:A:686:ARG:HG2	2.28	0.57
1:A:372:LYS:HG3	1:A:375:LEU:HD23	1.87	0.57
1:A:541:ASN:N	1:A:541:ASN:ND2	2.47	0.57
1:A:234:ASN:H	1:A:662:GLN:HE22	1.53	0.57
1:A:372:LYS:HB3	1:A:376:ASN:ND2	2.20	0.56
1:A:302:GLU:H	1:A:302:GLU:CD	2.09	0.56
1:A:490:GLU:CD	1:A:695:ARG:HH22	2.09	0.56
1:A:670:LYS:HB2	5:A:1580:HOH:O	2.05	0.55
1:A:287:GLY:HA3	1:A:324:PHE:CD2	2.41	0.55
1:A:636:GLU:HG3	5:A:1461:HOH:O	2.06	0.55
1:A:697:ILE:CA	1:A:743:LYS:HB3	2.35	0.54
1:A:23:ASP:HA	1:A:26:LYS:HE3	1.90	0.54
1:A:217:GLN:HG3	1:A:333:ILE:HD13	1.90	0.53
1:A:609:THR:HG22	5:A:1506:HOH:O	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ILE:HD12	1:A:740:GLY:CA	2.39	0.53
1:A:696:ILE:HD12	1:A:696:ILE:N	2.22	0.53
1:A:248:ASN:OD1	1:A:250:ALA:HB3	2.09	0.52
1:A:289:THR:HG22	1:A:290:ALA:N	2.23	0.52
1:A:234:ASN:ND2	5:A:1062:HOH:O	2.41	0.52
1:A:609:THR:HG23	1:A:613:ASN:OD1	2.10	0.52
1:A:138:GLU:CD	1:A:138:GLU:H	2.13	0.52
1:A:35:ILE:HG12	1:A:36:TRP:N	2.24	0.52
1:A:497:GLU:HG3	1:A:745:PHE:CE1	2.45	0.51
1:A:35:ILE:HD11	5:A:1063:HOH:O	2.09	0.51
1:A:668:GLU:HB3	1:A:670:LYS:HZ3	1.76	0.51
1:A:409:LEU:HB3	1:A:413:LYS:HB2	1.93	0.51
1:A:319:SER:OG	1:A:321:GLU:HG2	2.10	0.51
1:A:383:GLY:O	1:A:603:SER:HA	2.11	0.51
1:A:499:ILE:HD12	1:A:740:GLY:HA2	1.92	0.51
1:A:90:ASP:OD2	1:A:148:ARG:NH2	2.43	0.50
1:A:99:GLU:N	1:A:100:PRO:HD2	2.25	0.50
1:A:610:LYS:HD3	1:A:614:ASP:HB2	1.93	0.50
1:A:668:GLU:CD	1:A:670:LYS:HZ1	2.14	0.50
1:A:709:ALA:HB1	1:A:712:VAL:CB	2.42	0.50
1:A:499:ILE:CG1	1:A:738:ARG:HB3	2.33	0.50
1:A:482:PHE:CE1	1:A:486:MET:HG3	2.47	0.50
1:A:186:THR:O	1:A:190:LYS:HG3	2.12	0.50
1:A:668:GLU:HB3	1:A:670:LYS:NZ	2.27	0.49
1:A:291:GLU:O	1:A:294:LYS:HD2	2.12	0.49
1:A:698:TYR:HD1	1:A:723:THR:HG21	1.77	0.49
1:A:195:TYR:O	1:A:199:VAL:HG13	2.14	0.48
1:A:170:ARG:HG2	1:A:448:TYR:OH	2.14	0.48
1:A:567:GLU:HA	1:A:579:TYR:O	2.14	0.48
1:A:616:ASN:ND2	5:A:1330:HOH:O	2.29	0.48
1:A:390:GLU:HG2	1:A:394:MET:HE3	1.95	0.47
1:A:539:THR:H	1:A:542:THR:HG1	1.63	0.47
1:A:499:ILE:HD13	1:A:745:PHE:CD1	2.50	0.47
1:A:491:GLN:O	1:A:494:TYR:HB2	2.16	0.46
1:A:273:GLU:C	1:A:274:THR:HG23	2.36	0.46
1:A:693:PRO:HD2	1:A:747:ARG:HA	1.98	0.46
1:A:643:ALA:O	1:A:647:THR:HG23	2.15	0.46
1:A:362:GLY:HA3	1:A:368:VAL:HG13	1.97	0.46
1:A:670:LYS:N	1:A:670:LYS:HD3	2.29	0.46
1:A:171:GLN:CG	1:A:173:GLN:NE2	2.76	0.46
1:A:350:GLY:HA3	1:A:382:PHE:CZ	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:SER:O	1:A:323:GLU:HG2	2.16	0.45
1:A:324:PHE:O	1:A:328:ARG:HG3	2.16	0.45
1:A:698:TYR:HE1	1:A:744:ILE:HB	1.79	0.45
1:A:195:TYR:CZ	1:A:199:VAL:HG11	2.52	0.45
1:A:490:GLU:OE2	1:A:695:ARG:NH1	2.50	0.45
1:A:497:GLU:HG3	1:A:745:PHE:HZ	1.79	0.45
1:A:372:LYS:HG3	1:A:375:LEU:CD2	2.46	0.45
1:A:171:GLN:HG2	1:A:173:GLN:HE21	1.77	0.44
1:A:594:GLN:O	1:A:598:LEU:HG	2.17	0.44
1:A:342:MET:HE2	1:A:342:MET:CA	2.32	0.44
1:A:173:GLN:OE1	1:A:649:ASN:HB3	2.18	0.44
1:A:473:TYR:CE2	1:A:638:LEU:HD23	2.53	0.44
1:A:289:THR:CG2	1:A:290:ALA:N	2.80	0.44
1:A:26:LYS:HE3	1:A:26:LYS:HB2	1.39	0.43
1:A:490:GLU:OE1	1:A:490:GLU:HA	2.18	0.43
1:A:280:ILE:HG13	1:A:280:ILE:O	2.17	0.43
1:A:709:ALA:CB	1:A:712:VAL:CB	2.97	0.43
1:A:146:ARG:HD2	1:A:146:ARG:HA	1.83	0.43
1:A:305:ASN:O	1:A:309:GLN:HG2	2.19	0.43
1:A:487:PHE:O	1:A:491:GLN:HG3	2.19	0.43
1:A:171:GLN:HG2	1:A:173:GLN:HE22	1.79	0.43
1:A:622:LYS:HA	1:A:627:PHE:HA	2.00	0.43
1:A:294:LYS:HD3	1:A:295:ALA:N	2.34	0.43
1:A:432:TRP:HZ2	1:A:436:LYS:HE2	1.77	0.43
1:A:661:LYS:O	1:A:662:GLN:HB2	2.19	0.43
1:A:739:PHE:HA	1:A:744:ILE:HG12	2.01	0.43
1:A:697:ILE:N	1:A:743:LYS:HB3	2.34	0.43
1:A:248:ASN:HD21	1:A:252:PHE:HB2	1.84	0.42
1:A:410:ASN:OD1	1:A:413:LYS:HG3	2.18	0.42
1:A:514:ILE:HD13	5:A:1287:HOH:O	2.18	0.42
1:A:696:ILE:C	1:A:743:LYS:HB3	2.40	0.42
1:A:499:ILE:CD1	1:A:740:GLY:CA	2.97	0.42
1:A:477:LYS:HB3	1:A:477:LYS:HE3	1.85	0.42
1:A:738:ARG:O	1:A:744:ILE:HG12	2.18	0.42
1:A:405:VAL:HG23	1:A:405:VAL:O	2.19	0.42
1:A:628:ILE:CD1	1:A:632:ALA:HB3	2.50	0.41
1:A:244:GLU:HG2	1:A:449:PHE:CD2	2.54	0.41
1:A:136:THR:HB	1:A:138:GLU:OE1	2.21	0.41
1:A:499:ILE:HD11	1:A:740:GLY:N	2.37	0.40
1:A:395:GLU:HA	1:A:407:GLN:O	2.21	0.40
1:A:443:SER:C	1:A:444:GLU:HG2	2.42	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:GLN:NE2	1:A:510:SER:CB	2.78	0.40
1:A:614:ASP:CG	1:A:616:ASN:HB2	2.42	0.40

All (10) 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:498:LYS:CG	1:A:498:LYS:NZ[2_755]	0.67	1.53
1:A:498:LYS:CD	1:A:498:LYS:CE[2_755]	0.74	1.46
1:A:498:LYS:CG	1:A:498:LYS:CE[2_755]	0.99	1.21
1:A:498:LYS:CD	1:A:498:LYS:CD[2_755]	1.16	1.04
1:A:498:LYS:CB	1:A:498:LYS:NZ[2_755]	1.60	0.60
1:A:500:ASN:OD1	5:A:1464:HOH:O[2_755]	1.66	0.54
1:A:498:LYS:CG	1:A:498:LYS:CD[2_755]	1.92	0.28
1:A:498:LYS:CE	1:A:498:LYS:CE[2_755]	2.08	0.12
1:A:498:LYS:CD	1:A:498:LYS:NZ[2_755]	2.11	0.09
1:A:498:LYS:CB	1:A:498:LYS:CE[2_755]	2.18	0.02

## 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	720/762 (94%)	693 (96%)	24 (3%)	3 (0%)	34 24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	144	LYS
1	A	733	ASP



### 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	605/665 (91%)	560 (93%)	45 (7%)	13 6

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	18	LYS
1	A	26	LYS
1	A	35	ILE
1	A	46	SER
1	A	68	GLN
1	A	73	LYS
1	A	107	ARG
1	A	112	GLN
1	A	119	SER
1	A	142	ILE
1	A	144	LYS
1	A	171	GLN
1	A	175	LEU
1	A	216	LEU
1	A	249	ASN
1	A	291	GLU
1	A	294	LYS
1	A	316	LYS
1	A	322	ASP
1	A	325	LYS
1	A	329	GLN
1	A	342	MET
1	A	439	ASN
1	A	490	GLU
1	A	498	LYS
1	A	499	ILE
1	A	520	ARG
1	A	541	ASN
1	A	544	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	546	LYS
1	A	549	SER
1	A	620	ARG
1	A	661	LYS
1	A	670	LYS
1	A	678	CYS
1	A	687	ILE
1	A	695	ARG
1	A	696	ILE
1	A	721	LYS
1	A	735	GLU
1	A	737	TYR
1	A	738	ARG
1	A	743	LYS
1	A	744	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	79	GLN
1	A	234	ASN
1	A	283	GLN
1	A	338	GLN
1	A	407	GLN
1	A	408	HIS
1	A	480	GLN
1	A	500	ASN
1	A	532	GLN
1	A	541	ASN
1	A	606	ASN
1	A	662	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	A	998	2,4	1,4,4	0.71	0	-		
4	ADP	A	999	3,2	24,29,29	0.91	0	29,45,45	1.21	3 (10%)

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
4	ADP	A	999	3,2	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	ADP	C5-C6-N6	3.05	124.99	120.35
4	A	999	ADP	C4-C5-N7	2.71	112.22	109.40
4	A	999	ADP	C2'-C3'-C4'	-2.13	98.51	102.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	999	ADP	PA-O3A-PB-O1B
4	A	999	ADP	PA-O3A-PB-O2B

*Continued on next page...*

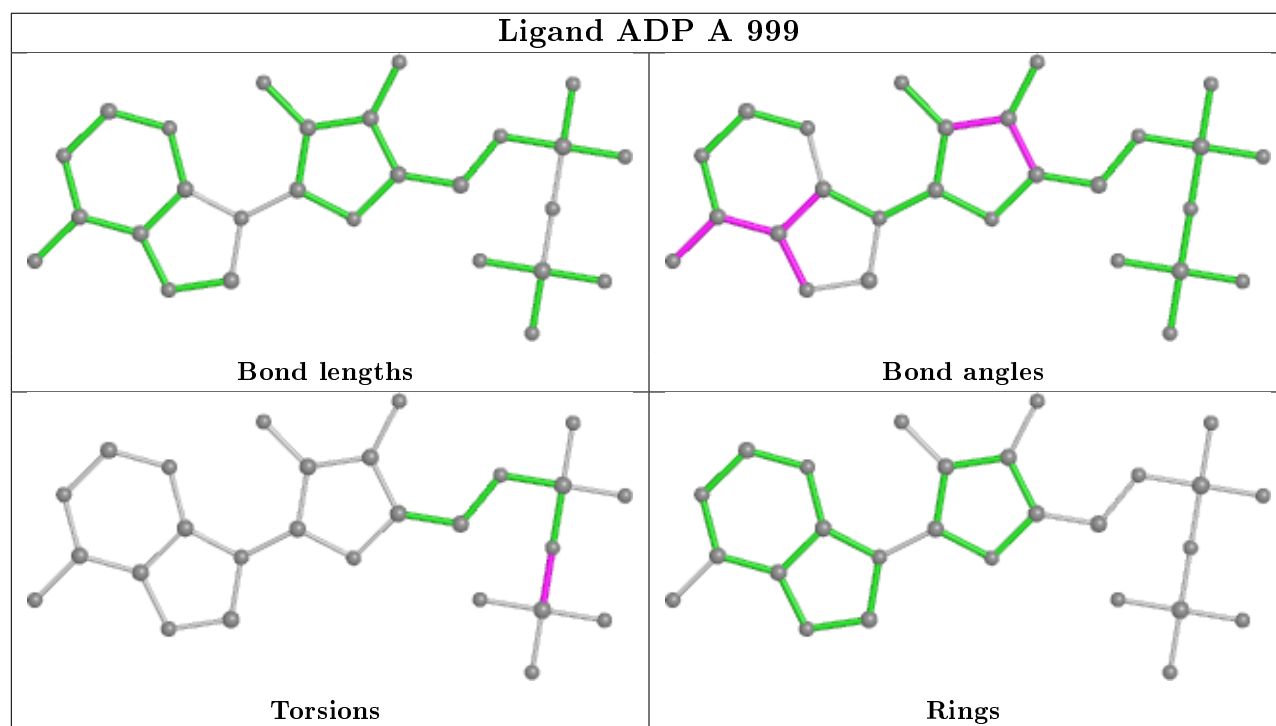
*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	A	999	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 ⓘ

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 ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.