



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:09 AM EDT

PDB ID : 1VOM / pdb_00001vom
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

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

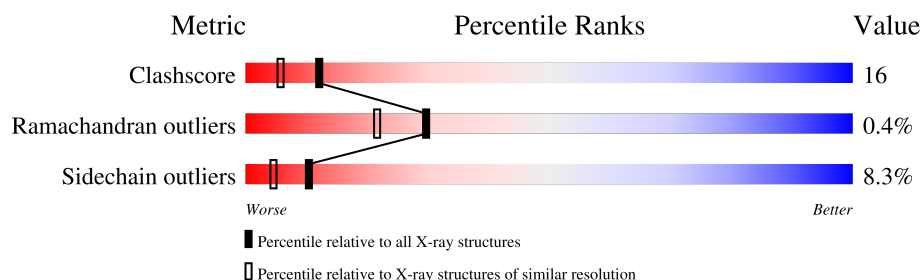
1 Overall quality at a glance

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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	762	 62% 27% 6% •

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
1	A	730	Total	C	N	O	S	0	0	0
			5750	3654	992	1088	16			

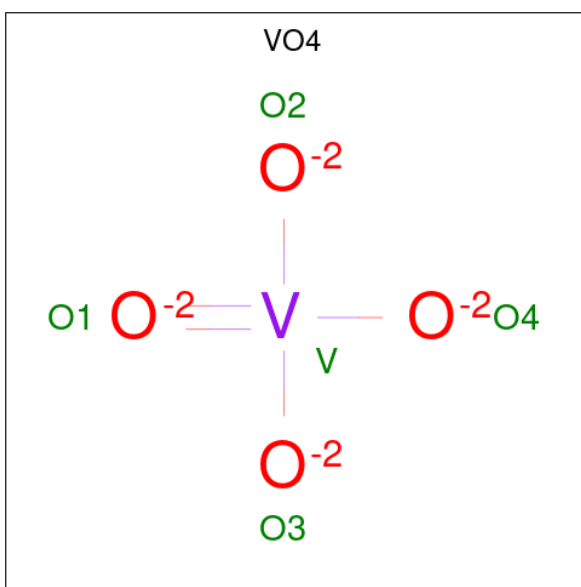
There are 7 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is VANADATE ION (CCD ID: VO4) (formula: O₄V).



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

- 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
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

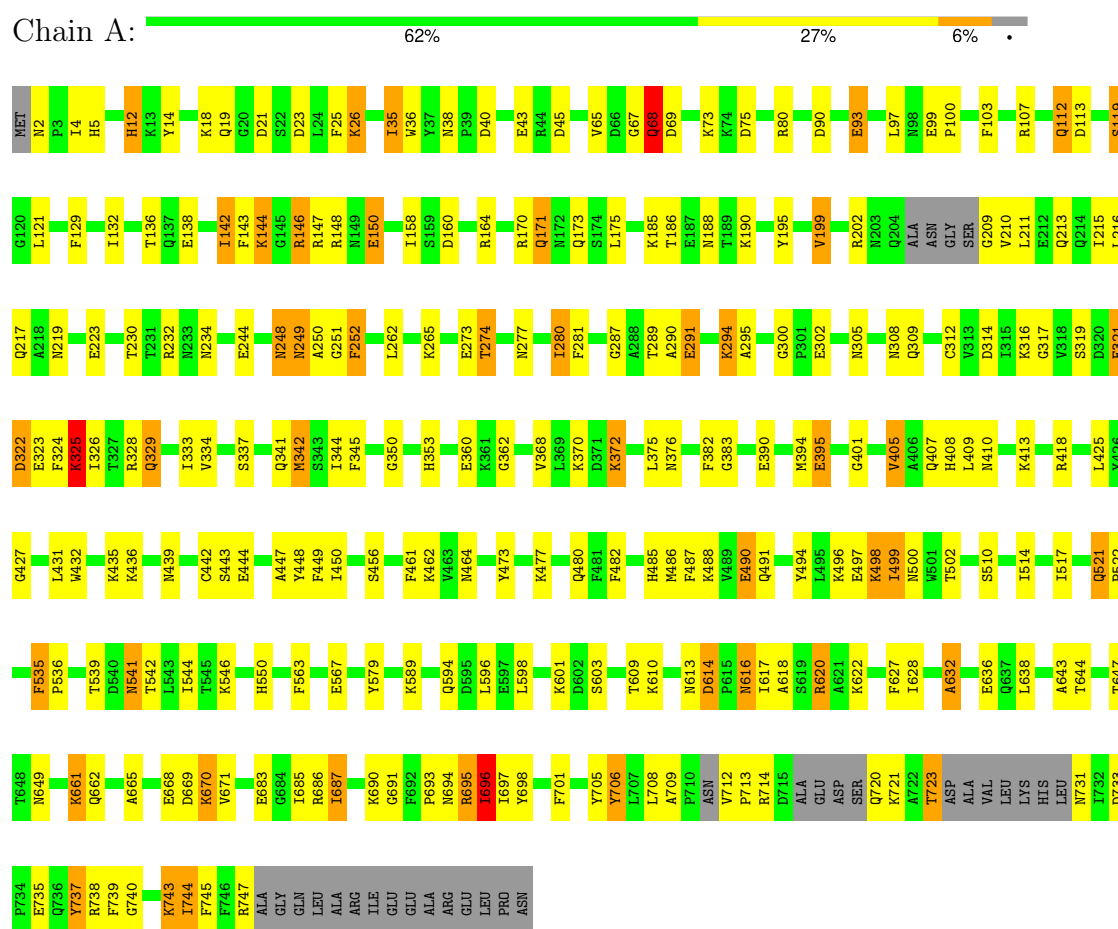
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	705	Total 705	O 705	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, 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. 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, α , β , γ	84.50Å 145.40Å 153.80Å 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 ²)	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: 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	A	1.09	0/5860	1.84	114/7916 (1.4%)

There are no bond length outliers.

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ASN	CA-CB-CG	10.66	123.26	112.60
1	A	408	HIS	CA-CB-CG	-10.17	103.63	113.80
1	A	210	VAL	N-CA-C	10.01	120.01	110.30
1	A	75	ASP	CA-CB-CG	-9.64	102.96	112.60
1	A	188	ASN	CA-CB-CG	-9.11	103.49	112.60
1	A	219	ASN	CA-CB-CG	-8.91	103.69	112.60
1	A	447	ALA	N-CA-C	-8.69	102.81	113.41
1	A	5	HIS	CA-CB-CG	-8.51	105.29	113.80
1	A	345	PHE	CA-CB-CG	-8.14	105.66	113.80
1	A	232	ARG	NE-CZ-NH2	-8.12	111.89	119.20
1	A	517	ILE	N-CA-C	7.96	118.54	110.82
1	A	616	ASN	CA-CB-CG	-7.92	104.68	112.60
1	A	119	SER	CA-C-N	-7.59	111.84	120.42
1	A	119	SER	C-N-CA	-7.59	111.84	120.42
1	A	456	SER	N-CA-C	-7.35	98.07	109.76
1	A	262	LEU	N-CA-C	7.28	121.44	111.17
1	A	129	PHE	CA-CB-CG	-7.23	106.57	113.80
1	A	464	ASN	CA-CB-CG	-7.20	105.40	112.60
1	A	143	PHE	CA-CB-CG	-7.12	106.68	113.80
1	A	694	ASN	N-CA-C	7.06	121.17	109.46
1	A	618	ALA	N-CA-C	7.01	121.06	112.23
1	A	277	ASN	N-CA-C	-6.99	100.71	110.35
1	A	262	LEU	N-CA-CB	-6.94	101.16	111.71
1	A	442	CYS	CB-CA-C	6.94	121.43	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	HIS	CA-CB-CG	-6.87	106.93	113.80
1	A	334	VAL	CA-C-N	-6.76	111.55	122.30
1	A	334	VAL	C-N-CA	-6.76	111.55	122.30
1	A	395	GLU	CB-CA-C	-6.68	102.46	111.21
1	A	485	HIS	CA-CB-CG	-6.66	107.14	113.80
1	A	706	TYR	CA-C-N	6.63	131.95	120.68
1	A	706	TYR	C-N-CA	6.63	131.95	120.68
1	A	112	GLN	CB-CA-C	-6.47	100.71	111.13
1	A	2	ASN	CA-C-N	6.47	126.97	119.47
1	A	2	ASN	C-N-CA	6.47	126.97	119.47
1	A	731	ASN	CA-CB-CG	6.46	119.06	112.60
1	A	696	ILE	N-CA-C	6.45	117.59	108.17
1	A	502	THR	N-CA-CB	6.42	120.89	110.42
1	A	132	ILE	CB-CA-C	6.38	116.60	110.16
1	A	418	ARG	N-CA-C	-6.36	104.35	111.28
1	A	683	GLU	CA-C-N	-6.33	112.19	120.22
1	A	683	GLU	C-N-CA	-6.33	112.19	120.22
1	A	21	ASP	N-CA-C	6.28	120.10	110.36
1	A	252	PHE	CA-CB-CG	-6.25	107.55	113.80
1	A	121	LEU	N-CA-C	6.19	120.44	113.01
1	A	687	ILE	N-CA-CB	6.17	117.77	110.55
1	A	714	ARG	N-CA-C	-6.16	105.89	113.41
1	A	442	CYS	N-CA-CB	6.10	120.36	110.42
1	A	450	ILE	N-CA-C	-6.08	98.87	107.75
1	A	596	LEU	CA-C-O	6.05	126.83	120.42
1	A	563	PHE	CA-CB-CG	-6.04	107.76	113.80
1	A	93	GLU	CA-CB-CG	-6.03	102.03	114.10
1	A	614	ASP	CA-C-O	5.98	124.07	119.46
1	A	690	LYS	N-CA-C	5.90	118.49	111.71
1	A	616	ASN	OD1-CG-ND2	5.89	128.49	122.60
1	A	401	GLY	N-CA-C	-5.84	99.35	113.18
1	A	219	ASN	N-CA-C	5.82	122.68	109.81
1	A	708	LEU	N-CA-C	-5.74	105.77	112.89
1	A	19	GLN	CA-C-N	-5.64	113.53	120.64
1	A	19	GLN	C-N-CA	-5.64	113.53	120.64
1	A	521	GLN	CB-CG-CD	5.62	122.16	112.60
1	A	488	LYS	N-CA-CB	5.61	118.10	109.91
1	A	317	GLY	CA-C-N	-5.61	115.32	123.06
1	A	317	GLY	C-N-CA	-5.61	115.32	123.06
1	A	312	CYS	N-CA-C	5.60	117.52	108.34
1	A	75	ASP	N-CA-C	5.57	118.28	111.82
1	A	223	GLU	CG-CD-OE2	-5.55	105.64	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ASN	OD1-CG-ND2	-5.50	117.11	122.60
1	A	113	ASP	N-CA-C	5.49	119.27	112.24
1	A	251	GLY	N-CA-C	-5.47	107.48	115.63
1	A	249	ASN	N-CA-C	-5.45	104.57	111.11
1	A	705	TYR	CA-C-N	5.44	130.92	122.49
1	A	705	TYR	C-N-CA	5.44	130.92	122.49
1	A	632	ALA	CA-C-N	-5.39	113.11	120.44
1	A	632	ALA	C-N-CA	-5.39	113.11	120.44
1	A	353	HIS	CA-CB-CG	-5.38	108.42	113.80
1	A	344	ILE	N-CA-CB	5.35	116.81	110.55
1	A	40	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	521	GLN	N-CA-CB	5.26	119.73	110.37
1	A	535	PHE	CB-CA-C	5.26	116.20	110.15
1	A	370	LYS	CA-C-N	-5.25	115.59	122.99
1	A	370	LYS	C-N-CA	-5.25	115.59	122.99
1	A	38	ASN	CA-C-O	5.24	123.76	119.36
1	A	80	ARG	O-C-N	-5.24	116.90	123.04
1	A	683	GLU	N-CA-C	-5.22	105.59	111.28
1	A	45	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	325	LYS	N-CA-CB	5.22	117.88	110.16
1	A	280	ILE	N-CA-C	5.21	116.56	110.62
1	A	550	HIS	ND1-CG-CD2	5.20	111.30	106.10
1	A	617	ILE	N-CA-CB	-5.19	105.70	111.41
1	A	685	ILE	N-CA-C	-5.19	105.65	110.53
1	A	112	GLN	N-CA-CB	5.19	119.68	111.17
1	A	431	LEU	CB-CA-C	-5.18	102.19	110.79
1	A	14	TYR	N-CA-C	5.18	119.65	113.23
1	A	281	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	723	THR	CA-CB-CG2	5.17	119.29	110.50
1	A	665	ALA	CB-CA-C	-5.17	104.26	111.80
1	A	314	ASP	CA-CB-CG	-5.15	107.45	112.60
1	A	425	LEU	N-CA-C	-5.12	105.60	111.07
1	A	691	GLY	CA-C-N	5.11	129.98	122.98
1	A	691	GLY	C-N-CA	5.11	129.98	122.98
1	A	439	ASN	N-CA-CB	5.10	118.18	110.28
1	A	21	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	713	PRO	N-CA-CB	5.09	108.59	103.25
1	A	427	GLY	CA-C-N	-5.07	112.61	120.31
1	A	427	GLY	C-N-CA	-5.07	112.61	120.31
1	A	230	THR	N-CA-CB	5.07	118.25	110.70
1	A	75	ASP	CB-CA-C	5.06	120.39	110.67
1	A	158	ILE	CB-CA-C	5.06	119.20	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ASN	CA-C-N	5.05	127.36	120.54
1	A	248	ASN	C-N-CA	5.05	127.36	120.54
1	A	12	HIS	ND1-CG-CD2	5.05	111.15	106.10
1	A	25	PHE	N-CA-CB	5.05	117.64	110.06
1	A	185	LYS	CB-CA-C	-5.05	102.95	110.88
1	A	461	PHE	CA-CB-CG	-5.01	108.78	113.80

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	177	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	14	1
All	All	6488	0	5581	177	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 16.

All (177) 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
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: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:H	1:A:541:ASN:HD22	1.07	0.93
1:A:628:ILE:CB	1:A:628:ILE:CD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	1:A:541:ASN:N	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:342:MET:HA	1:A:342:MET:HE2	1.67	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:97:LEU:HD23	1:A:686:ARG:CG	2.24	0.67
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: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:521:GLN:HA	1:A:522:PRO:C	2.21	0.65
1:A:701:PHE:HE2	1:A:723:THR:HG23	1.60	0.65
1:A:325:LYS:HG2	5:A:1681:HOH:O	1.95	0.65
1:A:342:MET:HA	1:A:342:MET:CE	2.26	0.65
1:A:342:MET:HE2	1:A:342:MET:O	1.97	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:HG3	1:A:620:ARG:NH1	1.97	0.63
1:A:209:GLY:O	1:A:213:GLN:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:103:PHE:CE2	1:A:669:ASP:HB3	2.34	0.61
1:A:329:GLN:O	1:A:333:ILE:HD12	2.00	0.61
1:A:147:ARG:HB2	1:A:150:GLU:CG	2.30	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:302:GLU:H	1:A:302:GLU:CD	2.09	0.61
1:A:490:GLU:CD	1:A:695:ARG:HH22	2.09	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:342:MET:HE2	1:A:342:MET:CA	2.32	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:97:LEU:CD2	1:A:686:ARG:HG2	2.28	0.57
1:A:480:GLN:NE2	1:A:510:SER:N	2.48	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:138:GLU:H	1:A:138:GLU:CD	2.13	0.56
1:A:372:LYS:HB3	1:A:376:ASN:ND2	2.20	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:668:GLU:HB3	1:A:670:LYS:HZ3	1.72	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
1:A:668:GLU:CD	1:A:670:LYS:HZ1	2.16	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:273:GLU:C	1:A:274:THR:HG23	2.36	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:499:ILE:CG1	1:A:738:ARG:HB3	2.33	0.50
1:A:709:ALA:HB1	1:A:712:VAL:CB	2.42	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:390:GLU:HG2	1:A:394:MET:HE3	1.95	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:696:ILE:C	1:A:743:LYS:HB3	2.40	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: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:321:GLU:CD	1:A:321:GLU:H	2.18	0.46
1:A:362:GLY:HA3	1:A:368:VAL:HG13	1.97	0.46
1:A:670:LYS:HD3	1:A:670:LYS:N	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:443:SER:C	1:A:444:GLU:HG2	2.42	0.45
1:A:614:ASP:CG	1:A:616:ASN:HB2	2.42	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:737:TYR:C	1:A:737:TYR:CD1	2.95	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:342:MET:HE2	1:A:342:MET:C	2.43	0.44
1:A:496:LYS:C	1:A:498:LYS:H	2.26	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:737:TYR:C	1:A:737:TYR:HD1	2.25	0.43
1:A:280:ILE:O	1:A:280:ILE:HG13	2.17	0.43
1:A:709:ALA:CB	1:A:712:VAL:CB	2.97	0.43
1:A:146:ARG:HA	1:A:146:ARG:HD2	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: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:499:ILE:CD1	1:A:740:GLY:CA	2.97	0.42
1:A:661:LYS:O	1:A:662:GLN:HB2	2.19	0.42
1:A:477:LYS:HE3	1:A:477:LYS:HB3	1.85	0.42
1:A:738:ARG:O	1:A:744:ILE:HG12	2.18	0.42
1:A:405:VAL:O	1:A:405:VAL:HG23	2.19	0.42
1:A:628:ILE:CD1	1:A:632:ALA:HB3	2.50	0.41
1:A:486:MET:HE3	1:A:486:MET:HB3	1.72	0.41
1:A:265:LYS:NZ	5:A:1211:HOH:O	2.54	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:138:GLU:CD	1:A:138:GLU:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:VAL:C	1:A:67:GLY:N	2.77	0.40
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:480:GLN:NE2	1:A:510:SER:CB	2.78	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

5.3.1 Protein backbone

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%)	30 22

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%)	555 (92%)	50 (8%)	10 4

All (50) 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	43	GLU
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	146	ARG
1	A	150	GLU
1	A	171	GLN
1	A	175	LEU
1	A	199	VAL
1	A	216	LEU
1	A	249	ASN
1	A	274	THR
1	A	291	GLU
1	A	294	LYS
1	A	316	LYS
1	A	321	GLU
1	A	322	ASP
1	A	325	LYS
1	A	329	GLN
1	A	342	MET
1	A	360	GLU
1	A	372	LYS

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Mol	Chain	Res	Type
1	A	405	VAL
1	A	462	LYS
1	A	490	GLU
1	A	498	LYS
1	A	499	ILE
1	A	541	ASN
1	A	544	ILE
1	A	546	LYS
1	A	620	ARG
1	A	644	THR
1	A	661	LYS
1	A	670	LYS
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	743	LYS
1	A	744	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	149	ASN
1	A	188	ASN
1	A	234	ASN
1	A	246	GLN
1	A	283	GLN
1	A	407	GLN
1	A	408	HIS
1	A	439	ASN
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 [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 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	0,4,4	-	-	-		
4	ADP	A	999	3,2	28,29,29	0.94	0	43,45,45	0.84	1 (2%)

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	-	3/16/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	ADP	C2'-C3'-C4'	-2.12	98.51	102.61

There are no chirality outliers.

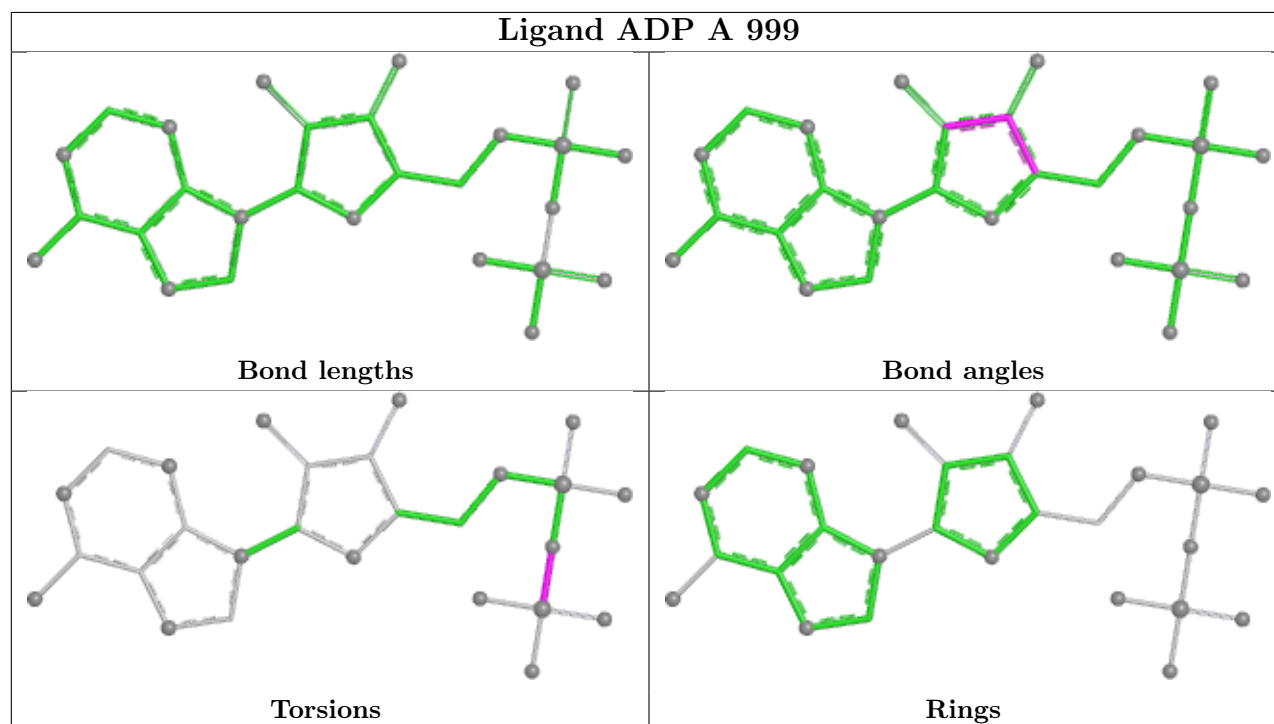
All (3) torsion outliers are listed below:

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