Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 05:45 PM EST

PDB ID	:	1MMD
Title	:	TRUNCATED HEAD OF MYOSIN FROM DICTYOSTELIUM DISCOIDEUM COMPLEXED WITH MGADP-BEF3
Authors	:	Fisher, A.J.; Holden, H.M.; Rayment, I.
Deposited on	:	1995-03-21
Resolution	:	2.00 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 (1)) were used in the production of this report:

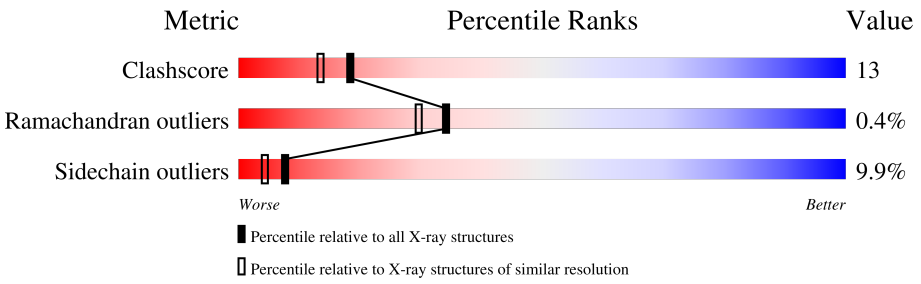
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	762	62% 28% 7% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6283 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	743	5876	3734	1012	1114	16	0	0	0

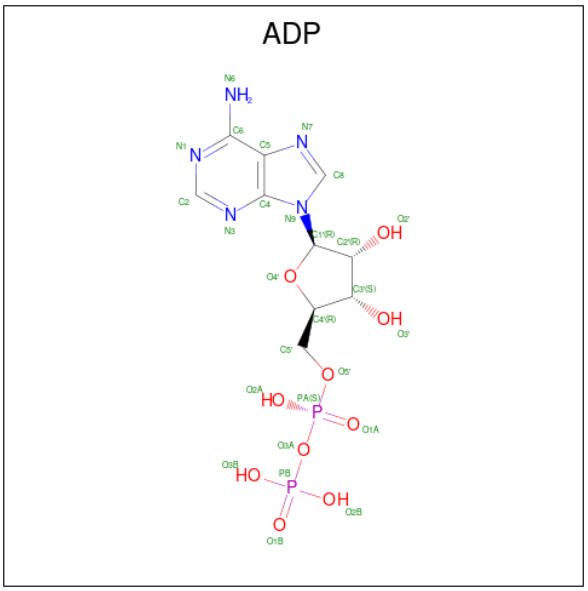
There are 7 discrepancies between the modelled and reference sequences:

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).

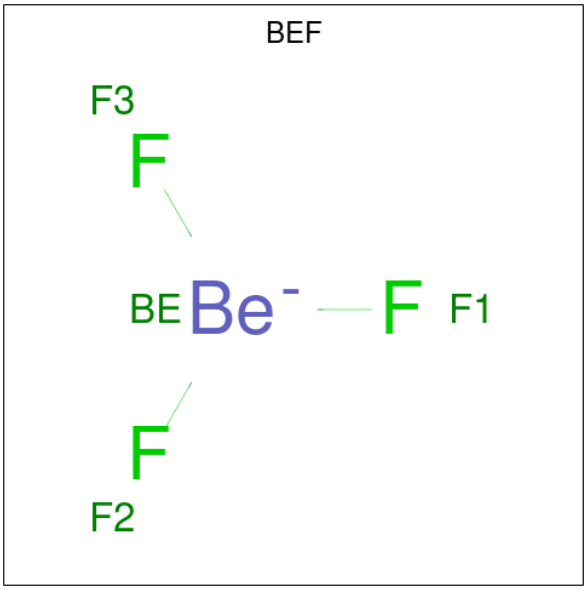
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	375	375	375	0	0

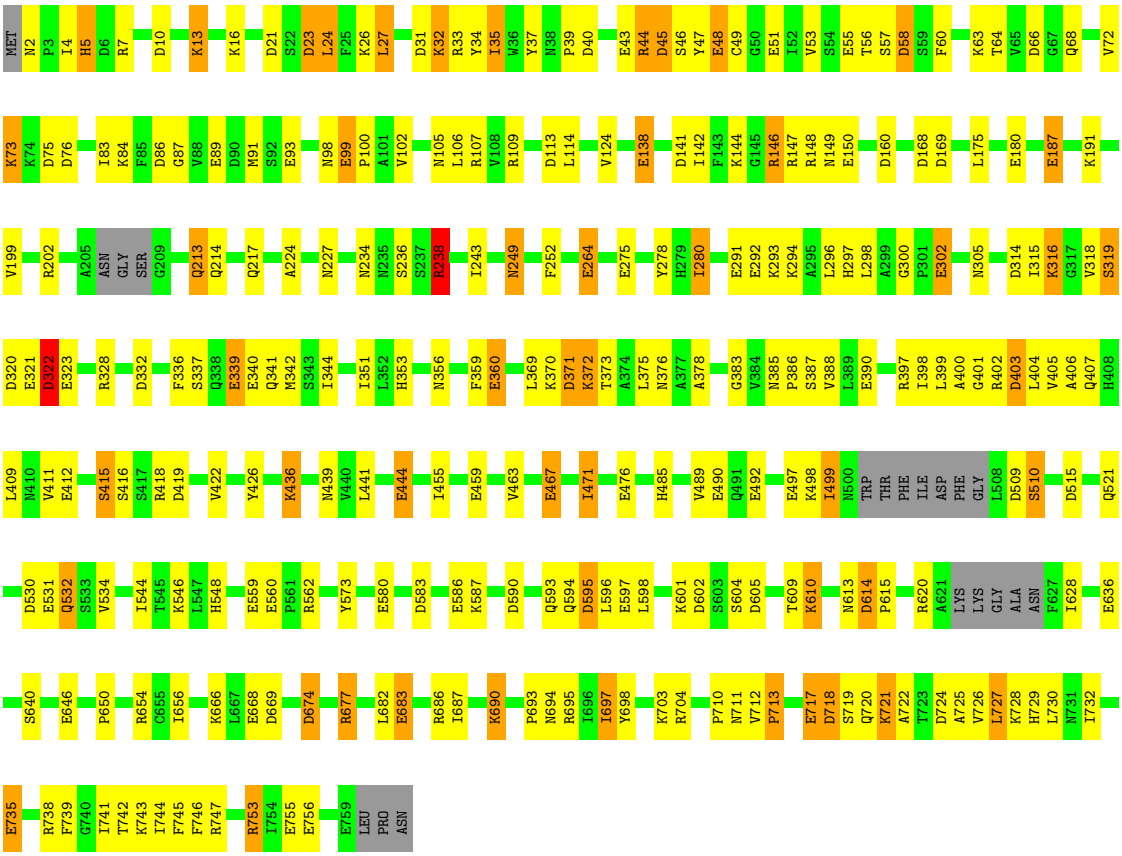
3 Residue-property plots (i)

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. 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

Chain A: 62% 28% 7% •



4 Data and refinement statistics (i)

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	105.30Å 182.60Å 54.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	88.0 (30.00-2.00)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6283	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

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: ADP, MG, BEF

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	1.04	39/5986 (0.7%)	1.38	75/8084 (0.9%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	GLU	CD-OE2	8.16	1.34	1.25
1	A	89	GLU	CD-OE2	7.32	1.33	1.25
1	A	735	GLU	CD-OE2	7.11	1.33	1.25
1	A	412	GLU	CD-OE2	6.99	1.33	1.25
1	A	636	GLU	CD-OE2	6.95	1.33	1.25
1	A	444	GLU	CD-OE2	6.82	1.33	1.25
1	A	360	GLU	CD-OE2	6.79	1.33	1.25
1	A	339	GLU	CD-OE2	6.71	1.33	1.25
1	A	755	GLU	CD-OE2	6.71	1.33	1.25
1	A	717	GLU	CD-OE2	6.63	1.32	1.25
1	A	683	GLU	CD-OE2	6.59	1.32	1.25
1	A	48	GLU	CD-OE2	6.45	1.32	1.25
1	A	138	GLU	CD-OE2	6.41	1.32	1.25
1	A	492	GLU	CD-OE2	6.40	1.32	1.25
1	A	756	GLU	CD-OE2	6.37	1.32	1.25
1	A	459	GLU	CD-OE2	6.35	1.32	1.25
1	A	497	GLU	CD-OE2	6.26	1.32	1.25
1	A	390	GLU	CD-OE2	6.21	1.32	1.25
1	A	291	GLU	CD-OE2	6.16	1.32	1.25
1	A	597	GLU	CD-OE2	6.16	1.32	1.25
1	A	187	GLU	CD-OE2	6.14	1.32	1.25
1	A	264	GLU	CD-OE1	-6.04	1.19	1.25
1	A	43	GLU	CD-OE2	6.00	1.32	1.25
1	A	531	GLU	CD-OE2	5.98	1.32	1.25
1	A	321	GLU	CD-OE2	5.98	1.32	1.25
1	A	150	GLU	CD-OE2	5.96	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	GLU	CD-OE2	5.93	1.32	1.25
1	A	586	GLU	CD-OE2	5.85	1.32	1.25
1	A	292	GLU	CD-OE2	5.84	1.32	1.25
1	A	668	GLU	CD-OE2	5.80	1.32	1.25
1	A	646	GLU	CD-OE2	5.79	1.32	1.25
1	A	302	GLU	CD-OE2	5.64	1.31	1.25
1	A	93	GLU	CD-OE2	5.57	1.31	1.25
1	A	99	GLU	CD-OE2	5.51	1.31	1.25
1	A	559	GLU	CD-OE2	5.37	1.31	1.25
1	A	476	GLU	CD-OE2	5.33	1.31	1.25
1	A	467	GLU	CD-OE2	5.29	1.31	1.25
1	A	580	GLU	CD-OE2	5.16	1.31	1.25
1	A	275	GLU	CD-OE1	-5.06	1.20	1.25

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	238	ARG	NE-CZ-NH1	20.67	130.64	120.30
1	A	238	ARG	NE-CZ-NH2	-15.76	112.42	120.30
1	A	146	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	A	45	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	A	674	ASP	CB-CG-OD2	-8.16	110.95	118.30
1	A	322	ASP	CB-CG-OD2	-8.12	111.00	118.30
1	A	753	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	A	595	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	A	590	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	A	419	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	A	419	ASP	CB-CG-OD1	7.66	125.20	118.30
1	A	238	ARG	CD-NE-CZ	7.51	134.12	123.60
1	A	322	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	595	ASP	CB-CG-OD1	7.23	124.81	118.30
1	A	148	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	A	58	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	66	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	278	TYR	CB-CG-CD1	-6.98	116.81	121.00
1	A	168	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	A	160	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	A	403	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	A	314	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	76	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	A	7	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	583	ASP	CB-CG-OD2	-6.42	112.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	509	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	169	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	573	TYR	CB-CG-CD1	-6.26	117.24	121.00
1	A	113	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	7	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	573	TYR	CB-CG-CD2	6.13	124.68	121.00
1	A	605	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	583	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	590	ASP	CB-CG-OD1	5.98	123.69	118.30
1	A	278	TYR	CB-CG-CD2	5.94	124.57	121.00
1	A	40	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	33	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	160	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	753	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	31	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	605	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	75	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	A	371	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	169	ASP	CB-CG-OD1	5.68	123.42	118.30
1	A	718	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	509	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	724	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	A	332	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	A	21	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	45	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	620	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	10	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	168	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	86	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	180	GLU	CB-CA-C	-5.42	99.55	110.40
1	A	530	ASP	CB-CG-OD1	5.38	123.15	118.30
1	A	515	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	21	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	602	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	314	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	23	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	320	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	23	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	147	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	614	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	669	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	677	ARG	NE-CZ-NH1	5.15	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	489	VAL	CB-CA-C	5.08	121.06	111.40
1	A	141	ASP	CB-CG-OD1	5.07	122.87	118.30
1	A	75	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	44	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	31	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	297	HIS	CA-CB-CG	-5.03	105.06	113.60
1	A	403	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	371	ASP	CB-CG-OD2	-5.00	113.80	118.30

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	5876	0	5754	155	1
2	A	1	0	0	0	0
3	A	27	0	12	0	0
4	A	4	0	0	0	0
5	A	375	0	0	13	1
All	All	6283	0	5766	155	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (155) 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:727:LEU:HD12	1:A:732:ILE:HD13	1.23	1.19
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.24	1.15
1:A:398:ILE:HD13	1:A:407:GLN:HG3	1.33	1.07
1:A:628:ILE:CB	1:A:628:ILE:CD1	2.42	0.96
1:A:397:ARG:HA	1:A:406:ALA:HA	1.50	0.92
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.53	0.88
1:A:727:LEU:HD12	1:A:732:ILE:CD1	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.04	0.87
1:A:735:GLU:HA	1:A:738:ARG:HH21	1.42	0.82
1:A:674:ASP:HB3	5:A:1049:HOH:O	1.79	0.81
1:A:727:LEU:HA	1:A:732:ILE:HD12	1.60	0.81
1:A:398:ILE:CD1	1:A:407:GLN:HG3	2.10	0.81
1:A:4:ILE:HD11	1:A:142:ILE:CG2	2.11	0.78
1:A:64:THR:HG23	1:A:68:GLN:O	1.83	0.78
1:A:697:ILE:HD12	1:A:742:THR:HG22	1.65	0.78
1:A:727:LEU:HA	1:A:732:ILE:CD1	2.14	0.77
1:A:144:LYS:HE2	1:A:199:VAL:HG12	1.66	0.76
1:A:124:VAL:HG13	1:A:656:ILE:HD12	1.70	0.73
1:A:710:PRO:HD2	1:A:729:HIS:CE1	2.24	0.72
1:A:224:ALA:O	1:A:280:ILE:HG13	1.89	0.72
1:A:628:ILE:CD1	1:A:628:ILE:CA	2.70	0.70
1:A:53:VAL:HG21	1:A:63:LYS:HD2	1.72	0.69
1:A:91:MET:CE	1:A:106:LEU:HD13	2.22	0.69
1:A:614:ASP:OD1	1:A:615:PRO:HD2	1.94	0.68
1:A:39:PRO:HD2	5:A:1294:HOH:O	1.94	0.68
1:A:697:ILE:HD13	1:A:743:LYS:HG2	1.75	0.67
1:A:735:GLU:HA	1:A:738:ARG:NH2	2.08	0.67
1:A:238:ARG:HD3	1:A:264:GLU:OE2	1.94	0.67
1:A:372:LYS:O	1:A:376:ASN:ND2	2.29	0.65
1:A:628:ILE:CD1	1:A:628:ILE:HA	2.25	0.65
1:A:32:LYS:N	1:A:32:LYS:HD2	2.10	0.65
1:A:300:GLY:HA3	1:A:302:GLU:OE2	1.96	0.65
1:A:722:ALA:O	1:A:725:ALA:HB3	1.97	0.65
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.28	0.64
1:A:305:ASN:HD22	1:A:356:ASN:HA	1.63	0.64
1:A:45:ASP:CG	1:A:677:ARG:HH22	2.02	0.64
1:A:249:ASN:ND2	5:A:1355:HOH:O	2.29	0.64
1:A:439:ASN:ND2	5:A:1317:HOH:O	2.31	0.63
1:A:4:ILE:HD13	1:A:146:ARG:NH2	2.13	0.63
1:A:337:SER:O	1:A:341:GLN:HG3	1.99	0.63
1:A:72:VAL:HG22	1:A:73:LYS:O	1.98	0.63
1:A:727:LEU:CA	1:A:732:ILE:HD12	2.28	0.62
1:A:718:ASP:CG	1:A:721:LYS:HB2	2.19	0.62
1:A:87:GLY:H	1:A:105:ASN:ND2	1.98	0.61
1:A:697:ILE:CD1	1:A:742:THR:HG22	2.30	0.61
1:A:404:LEU:O	1:A:404:LEU:HD23	2.01	0.61
1:A:213:GLN:O	1:A:217:GLN:HG2	2.01	0.61
1:A:710:PRO:HG2	1:A:729:HIS:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:HD23	1:A:404:LEU:C	2.22	0.59
1:A:359:PHE:HB3	1:A:411:VAL:HG22	1.83	0.59
1:A:727:LEU:O	1:A:732:ILE:HD12	2.02	0.58
1:A:385:ASN:OD1	1:A:386:PRO:HD2	2.03	0.58
1:A:467:GLU:OE2	1:A:587:LYS:HE2	2.05	0.57
1:A:726:VAL:O	1:A:730:LEU:HG	2.04	0.57
1:A:280:ILE:HD12	1:A:280:ILE:N	2.19	0.57
1:A:693:PRO:HD2	1:A:746:PHE:O	2.05	0.57
1:A:403:ASP:HB3	1:A:405:VAL:HG23	1.87	0.57
1:A:730:LEU:HB2	1:A:732:ILE:HD11	1.87	0.57
1:A:409:LEU:HA	5:A:1076:HOH:O	2.04	0.56
1:A:683:GLU:HB2	1:A:686:ARG:NH1	2.20	0.56
1:A:359:PHE:CB	1:A:411:VAL:HG22	2.36	0.55
1:A:403:ASP:HB3	1:A:405:VAL:CG2	2.37	0.55
1:A:319:SER:OG	1:A:322:ASP:HB2	2.08	0.54
1:A:371:ASP:OD2	1:A:372:LYS:N	2.41	0.54
1:A:687:ILE:O	1:A:690:LYS:HB2	2.07	0.54
1:A:39:PRO:HG3	1:A:48:GLU:CG	2.38	0.53
1:A:532:GLN:HE21	1:A:532:GLN:HA	1.73	0.53
1:A:397:ARG:HD2	1:A:404:LEU:HD21	1.91	0.53
1:A:124:VAL:CG1	1:A:656:ILE:HD12	2.37	0.52
1:A:510:SER:OG	5:A:1094:HOH:O	2.19	0.51
1:A:296:LEU:CB	1:A:298:LEU:HG	2.31	0.51
1:A:32:LYS:HG3	1:A:51:GLU:OE1	2.10	0.51
1:A:56:THR:OG1	1:A:58:ASP:OD2	2.26	0.51
1:A:677:ARG:HG3	1:A:682:LEU:HD12	1.92	0.51
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.93	0.50
1:A:683:GLU:HB2	1:A:686:ARG:HH12	1.76	0.50
1:A:710:PRO:HD2	1:A:729:HIS:NE2	2.25	0.50
1:A:718:ASP:OD2	1:A:721:LYS:HD3	2.11	0.50
1:A:234:ASN:ND2	5:A:1060:HOH:O	2.43	0.50
1:A:353:HIS:HB2	1:A:378:ALA:HB2	1.95	0.49
1:A:84:LYS:HD2	1:A:704:ARG:NE	2.27	0.48
1:A:341:GLN:HA	1:A:344:ILE:HD12	1.95	0.48
1:A:601:LYS:HG2	1:A:613:ASN:HD21	1.78	0.48
1:A:109:ARG:HB3	1:A:114:LEU:HB2	1.95	0.48
1:A:730:LEU:HD12	1:A:732:ILE:HD11	1.95	0.48
1:A:84:LYS:HD2	1:A:704:ARG:CZ	2.43	0.48
1:A:397:ARG:HG2	1:A:406:ALA:HB2	1.94	0.48
1:A:718:ASP:OD2	1:A:721:LYS:HB2	2.13	0.47
1:A:698:TYR:OH	1:A:739:PHE:HD2	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:TYR:CE1	1:A:51:GLU:HB2	2.49	0.47
1:A:398:ILE:CG2	1:A:399:LEU:N	2.78	0.47
1:A:373:THR:O	1:A:376:ASN:HB2	2.14	0.47
1:A:463:VAL:HA	5:A:1117:HOH:O	2.14	0.47
1:A:99:GLU:N	1:A:100:PRO:HD2	2.30	0.47
1:A:2:ASN:HB3	1:A:5:HIS:HD2	1.79	0.47
1:A:694:ASN:C	1:A:695:ARG:HG3	2.35	0.46
1:A:72:VAL:CG2	1:A:73:LYS:N	2.77	0.46
1:A:202:ARG:HH11	1:A:252:PHE:HB2	1.79	0.46
1:A:719:SER:O	1:A:722:ALA:HB3	2.15	0.46
1:A:471:ILE:HG23	1:A:471:ILE:HD12	1.37	0.46
1:A:485:HIS:CE1	1:A:650:PRO:HD2	2.50	0.46
1:A:39:PRO:HG3	1:A:48:GLU:HG2	1.97	0.46
1:A:316:LYS:HB2	1:A:316:LYS:HE3	1.56	0.46
1:A:601:LYS:HG2	1:A:613:ASN:ND2	2.30	0.45
1:A:415:SER:OG	1:A:418:ARG:NH2	2.49	0.45
1:A:39:PRO:HG3	1:A:48:GLU:HG3	1.98	0.45
1:A:72:VAL:HG22	1:A:73:LYS:N	2.29	0.45
1:A:187:GLU:O	1:A:191:LYS:HG2	2.16	0.45
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.72	0.45
1:A:280:ILE:HD11	1:A:426:TYR:OH	2.17	0.45
1:A:682:LEU:HD23	1:A:682:LEU:HA	1.77	0.45
1:A:249:ASN:ND2	1:A:249:ASN:H	2.13	0.45
1:A:227:ASN:HA	1:A:236:SER:O	2.17	0.44
1:A:534:VAL:O	1:A:534:VAL:HG12	2.17	0.44
1:A:214:GLN:HB3	1:A:441:LEU:HD21	1.99	0.44
1:A:499:ILE:HD12	1:A:745:PHE:CG	2.52	0.44
1:A:16:LYS:NZ	5:A:1285:HOH:O	2.49	0.44
1:A:730:LEU:HB2	1:A:732:ILE:CD1	2.47	0.44
1:A:593:GLN:HB2	1:A:596:LEU:HD12	1.98	0.44
1:A:397:ARG:HB3	1:A:404:LEU:HD21	1.98	0.44
1:A:35:ILE:HD11	5:A:1156:HOH:O	2.18	0.43
1:A:315:ILE:HB	1:A:318:VAL:HB	2.00	0.43
1:A:498:LYS:HE2	1:A:498:LYS:HB3	1.83	0.43
1:A:595:ASP:HA	1:A:598:LEU:HD12	1.99	0.43
1:A:610:LYS:HB3	1:A:610:LYS:HE2	1.81	0.43
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.72	0.43
1:A:383:GLY:HA3	1:A:604:SER:OG	2.19	0.42
1:A:400:ALA:O	1:A:402:ARG:N	2.52	0.42
1:A:191:LYS:HA	1:A:191:LYS:HD3	1.86	0.42
1:A:712:VAL:HG12	1:A:713:PRO:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASN:HB3	1:A:388:VAL:CG2	2.49	0.42
1:A:683:GLU:CB	1:A:686:ARG:NH1	2.81	0.42
1:A:56:THR:HG23	5:A:1168:HOH:O	2.19	0.42
1:A:58:ASP:OD2	1:A:58:ASP:N	2.53	0.42
1:A:548:HIS:CE1	1:A:560:GLU:HG3	2.55	0.42
1:A:293:LYS:HA	1:A:298:LEU:HD12	2.02	0.41
1:A:98:ASN:O	1:A:102:VAL:HG23	2.20	0.41
1:A:654:ARG:HH11	1:A:654:ARG:HD3	1.64	0.41
1:A:2:ASN:HB3	1:A:5:HIS:CD2	2.55	0.41
1:A:13:LYS:HB2	1:A:13:LYS:HE2	1.80	0.41
1:A:37:TYR:O	1:A:47:TYR:HA	2.21	0.41
1:A:323:GLU:OE1	1:A:323:GLU:HA	2.20	0.41
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.61	0.41
1:A:710:PRO:CD	1:A:729:HIS:CE1	2.99	0.41
1:A:35:ILE:HG21	1:A:35:ILE:HD12	1.70	0.41
1:A:107:ARG:HD3	5:A:1340:HOH:O	2.19	0.41
1:A:336:PHE:CE2	1:A:436:LYS:HG2	2.56	0.41
1:A:698:TYR:CZ	1:A:720:GLN:HG2	2.56	0.41
1:A:697:ILE:HD12	1:A:742:THR:CG2	2.45	0.40
1:A:60:PHE:HB2	1:A:72:VAL:HG13	2.04	0.40
1:A:87:GLY:H	1:A:105:ASN:HD21	1.66	0.40
1:A:727:LEU:HD12	1:A:727:LEU:HA	1.80	0.40
1:A:27:LEU:HA	1:A:27:LEU:HD12	1.77	0.40
1:A:654:ARG:NH1	5:A:1174:HOH:O	2.51	0.40
1:A:698:TYR:OH	1:A:739:PHE:CD2	2.75	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:GLN:OE1	5:A:1280:HOH:O[4_555]	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	735/762 (96%)	708 (96%)	24 (3%)	3 (0%)	34 30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ASN
1	A	401	GLY
1	A	713	PRO

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	626/665 (94%)	564 (90%)	62 (10%)	8 4

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	13	LYS
1	A	23	ASP
1	A	24	LEU
1	A	26	LYS
1	A	27	LEU
1	A	32	LYS
1	A	35	ILE
1	A	44	ARG
1	A	46	SER
1	A	57	SER
1	A	73	LYS
1	A	83	ILE
1	A	138	GLU
1	A	149	ASN
1	A	175	LEU

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Mol	Chain	Res	Type
1	A	213	GLN
1	A	238	ARG
1	A	243	ILE
1	A	249	ASN
1	A	280	ILE
1	A	294	LYS
1	A	316	LYS
1	A	319	SER
1	A	322	ASP
1	A	328	ARG
1	A	339	GLU
1	A	342	MET
1	A	360	GLU
1	A	370	LYS
1	A	372	LYS
1	A	375	LEU
1	A	387	SER
1	A	415	SER
1	A	416	SER
1	A	436	LYS
1	A	444	GLU
1	A	455	ILE
1	A	471	ILE
1	A	490	GLU
1	A	499	ILE
1	A	510	SER
1	A	532	GLN
1	A	544	ILE
1	A	546	LYS
1	A	562	ARG
1	A	594	GLN
1	A	609	THR
1	A	610	LYS
1	A	640	SER
1	A	666	LYS
1	A	690	LYS
1	A	697	ILE
1	A	703	LYS
1	A	717	GLU
1	A	721	LYS
1	A	727	LEU
1	A	728	LYS

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Mol	Chain	Res	Type
1	A	741	ILE
1	A	744	ILE
1	A	747	ARG
1	A	753	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	105	ASN
1	A	234	ASN
1	A	249	ASN
1	A	283	GLN
1	A	305	ASN
1	A	329	GLN
1	A	439	ASN
1	A	485	HIS
1	A	532	GLN
1	A	594	GLN
1	A	613	ASN
1	A	633	GLN
1	A	662	GLN
1	A	729	HIS
1	A	731	ASN

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 monosaccharides 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	ADP	A	999	4,2	24,29,29	1.20	3 (12%)	29,45,45	1.39	3 (10%)
4	BEF	A	1000	3,2	0,3,3	-	-	-		

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	ADP	C2'-C1'	-3.41	1.48	1.53
3	A	999	ADP	C2-N1	2.42	1.38	1.33
3	A	999	ADP	O4'-C1'	-2.15	1.38	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	999	ADP	C5-C6-N6	5.24	128.31	120.35
3	A	999	ADP	N6-C6-N1	-2.71	112.94	118.57
3	A	999	ADP	C1'-N9-C4	-2.38	122.46	126.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

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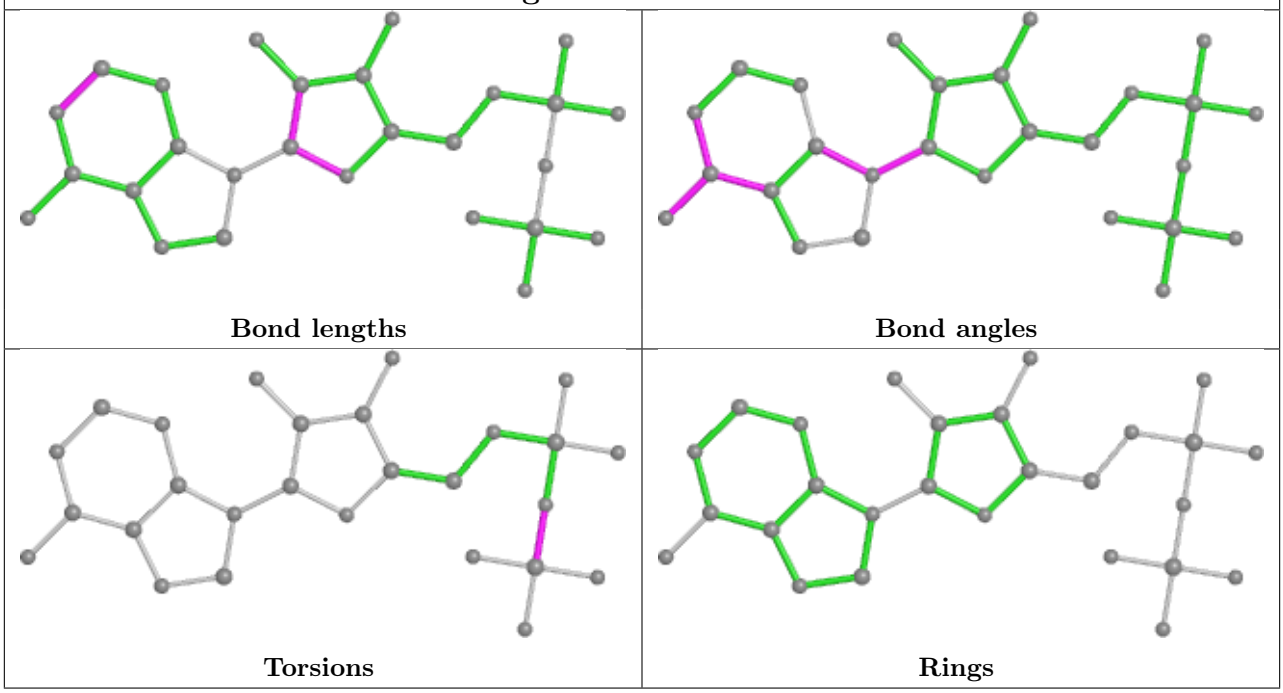
Mol	Chain	Res	Type	Atoms
3	A	999	ADP	PA-O3A-PB-O1B

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 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 999



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.