Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 06:36 pm BST

PDB ID	:	2VB6
Title	:	Myosin VI (MD-insert2-CaM, Delta Insert1) Post-rigor state (crystal form 2)
Authors	:	Menetrey, J.; Llinas, P.; Cicolari, J.; Squires, G.; Liu, X.; Li, A.; Sweeney, H.L.; Houdusse, A.
Deposited on	:	2007-09-06
Resolution	:	2.30 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:

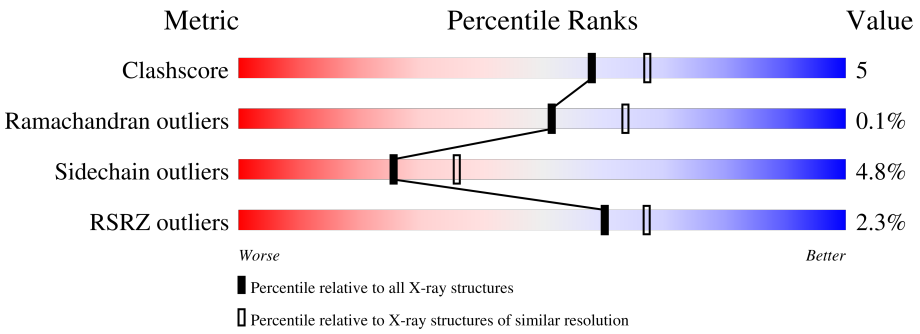
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	788	2% 80% 11% • 8%
2	B	149	% 77% 15% 5% • •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7271 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 VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	724	5857	3741	1008	1080	28	65	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	547	VAL	GLY	conflict	UNP Q29122
A	572	ARG	ALA	conflict	UNP Q29122
A	573	ASP	TYR	conflict	UNP Q29122
A	714	LEU	VAL	conflict	UNP Q29122
A	721	TYR	SER	conflict	UNP Q29122
A	722	MET	LEU	conflict	UNP Q29122

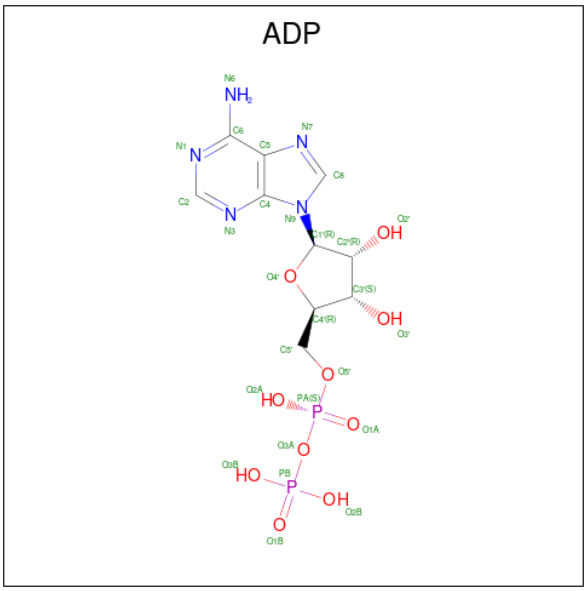
- Molecule 2 is a protein called CALMODULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	145	1141	700	183	249	9	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

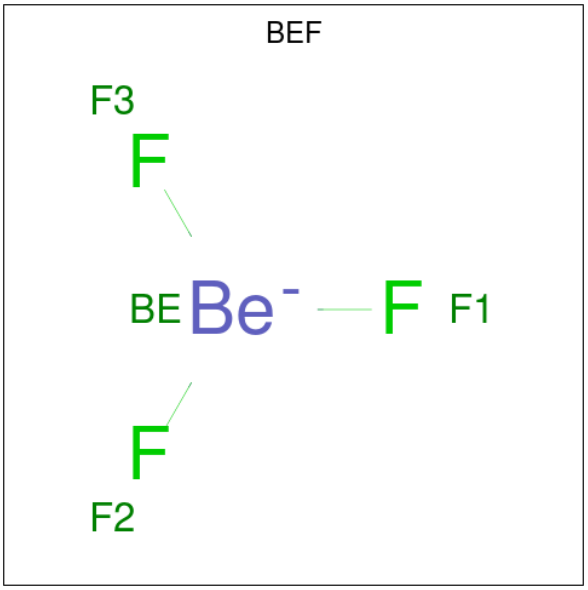
Chain	Residue	Modelled	Actual	Comment	Reference
B	99	PHE	TYR	conflict	UNP P62149
B	120	GLU	GLN	conflict	UNP P62149
B	143	THR	GLN	conflict	UNP P62149
B	147	SER	ALA	conflict	UNP P62149

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

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	B	4	4	4	0	0

- Molecule 7 is water.

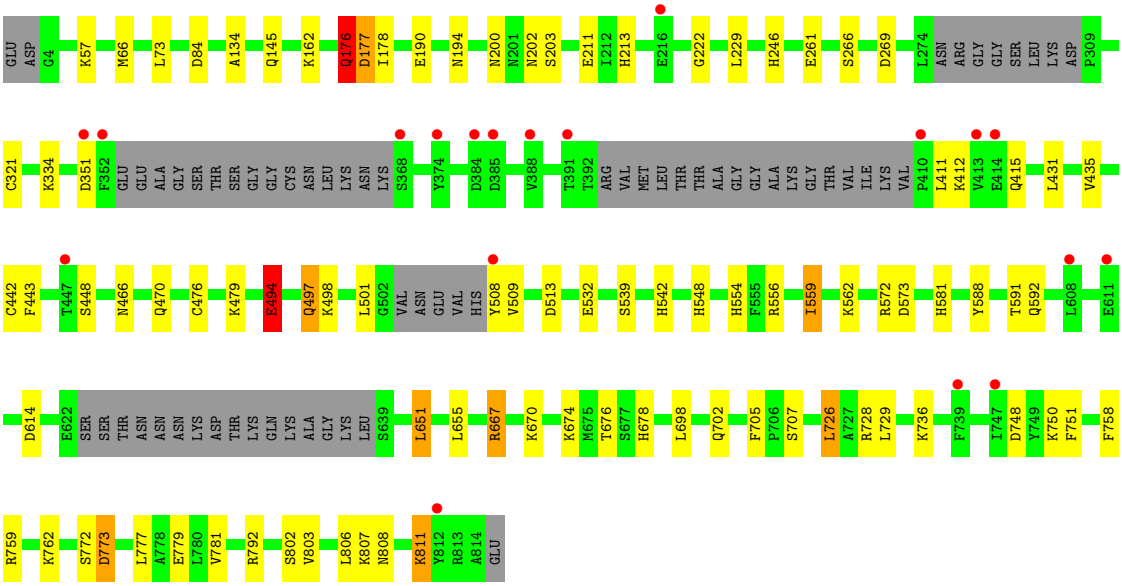
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	211	211	211	0	0
			Total	O		
7	B	26	26	26	0	0

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: MYOSIN VI

Chain A:



• Molecule 2: CALMODULIN

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.31Å 107.59Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.18 – 2.30 46.17 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.18-2.30) 99.1 (46.17-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.91 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.253 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7271	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: ADP, MG, BEF, CA

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	0.56	3/5980 (0.1%)	0.63	2/8052 (0.0%)
2	B	0.56	1/1153 (0.1%)	0.73	3/1548 (0.2%)
All	All	0.56	4/7133 (0.1%)	0.65	5/9600 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	1	2
All	All	1	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	494	GLU	CB-CG	7.55	1.66	1.52
1	A	412	LYS	CA-CB	-6.95	1.38	1.53
2	B	78	ASP	CA-CB	6.91	1.69	1.53
1	A	261	GLU	CA-CB	-5.01	1.43	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	773	ASP	N-CA-C	-7.97	89.49	111.00
2	B	24	ASP	N-CA-C	6.20	127.74	111.00
2	B	78	ASP	CB-CA-C	-5.75	98.89	110.40
1	A	177	ASP	N-CA-C	-5.62	95.81	111.00
2	B	23	GLY	N-CA-C	5.02	125.65	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	24	ASP	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	GLN	Peptide
1	A	729	LEU	Peptide
1	A	772	SER	Peptide
2	B	23	GLY	Peptide
2	B	57	ALA	Peptide

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	5857	0	5813	49	3
2	B	1141	0	1067	19	0
3	A	27	0	12	0	0
4	A	4	0	0	0	0
5	A	1	0	0	0	0
6	B	4	0	0	0	0
7	A	211	0	0	3	0
7	B	26	0	0	2	0
All	All	7271	0	6892	66	3

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 5.

All (66) 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)
2:B:116:LEU:HD21	2:B:124:MET:HE1	1.54	0.89
1:A:811:LYS:NZ	1:A:811:LYS:HB3	1.98	0.77
1:A:811:LYS:HB3	1:A:811:LYS:HZ2	1.50	0.74
1:A:811:LYS:NZ	1:A:811:LYS:CB	2.48	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:HIS:HD2	1:A:556:ARG:H	1.37	0.70
1:A:532:GLU:OE2	1:A:542:HIS:HD2	1.75	0.70
1:A:548:HIS:CE1	1:A:559:ILE:HD12	2.33	0.63
1:A:667:ARG:NH2	7:A:2180:HOH:O	2.27	0.63
1:A:811:LYS:HZ2	1:A:811:LYS:CB	2.07	0.63
1:A:554:HIS:HE1	7:A:2123:HOH:O	1.83	0.61
1:A:559:ILE:HG22	1:A:562:LYS:HG3	1.81	0.61
2:B:135:GLN:NE2	7:B:2026:HOH:O	2.33	0.60
1:A:748:ASP:HA	1:A:759:ARG:HG3	1.85	0.59
2:B:20:ASP:OD2	2:B:23:GLY:HA2	2.03	0.58
1:A:211:GLU:OE1	1:A:213:HIS:HE1	1.87	0.57
1:A:73:LEU:HD22	1:A:698:LEU:HD11	1.86	0.57
1:A:707:SER:HB2	1:A:758:PHE:HB2	1.87	0.57
1:A:466:ASN:HD22	1:A:470:GLN:HG2	1.69	0.56
1:A:190:GLU:O	1:A:194:ASN:HB2	2.05	0.56
2:B:63:ILE:HD12	2:B:67:GLU:HB3	1.86	0.55
1:A:581:HIS:HE1	1:A:588:TYR:OH	1.90	0.55
1:A:581:HIS:CE1	1:A:588:TYR:OH	2.61	0.54
1:A:178:ILE:HD11	1:A:222:GLY:HA2	1.89	0.54
2:B:52:ILE:HA	2:B:71:MET:CE	2.39	0.53
1:A:807:LYS:HE3	1:A:808:ASN:OD1	2.10	0.52
2:B:64:ASP:OD1	2:B:66:PRO:HD2	2.10	0.51
1:A:726:LEU:HD13	1:A:781:VAL:HG11	1.93	0.50
1:A:213:HIS:HD2	1:A:448:SER:OG	1.95	0.50
2:B:52:ILE:HG12	2:B:71:MET:HE1	1.93	0.50
2:B:27:ILE:HD12	2:B:32:LEU:HD13	1.94	0.49
2:B:28:THR:HG22	2:B:62:THR:HG22	1.94	0.49
1:A:202:ASN:OD1	1:A:246:HIS:HE1	1.95	0.49
1:A:476:CYS:HA	1:A:651:LEU:HD11	1.95	0.48
1:A:513:ASP:OD2	1:A:556:ARG:HD3	2.12	0.48
2:B:52:ILE:HA	2:B:71:MET:HE2	1.95	0.48
1:A:501:LEU:HD23	1:A:750:LYS:HG2	1.96	0.47
1:A:705:PHE:CZ	1:A:750:LYS:HD3	2.50	0.47
1:A:211:GLU:OE1	1:A:213:HIS:CE1	2.67	0.47
1:A:802:SER:O	1:A:806:LEU:HG	2.15	0.46
2:B:24:ASP:OD2	2:B:24:ASP:C	2.54	0.46
1:A:803:VAL:HG13	2:B:36:MET:HG2	1.98	0.46
1:A:674:LYS:O	1:A:676:THR:HG23	2.16	0.45
2:B:116:LEU:CD2	2:B:124:MET:HE1	2.36	0.45
1:A:811:LYS:HB3	1:A:811:LYS:HZ3	1.80	0.45
2:B:90:ARG:HA	2:B:90:ARG:HD2	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:HIS:CD2	1:A:556:ARG:HG2	2.52	0.45
1:A:411:LEU:HD22	1:A:415:GLN:HB3	1.99	0.45
2:B:105:LEU:HD21	2:B:124:MET:HE3	1.97	0.45
1:A:479:LYS:HB3	1:A:655:LEU:HD11	1.99	0.44
1:A:497:GLN:HG3	1:A:498:LYS:N	2.28	0.44
2:B:37:ARG:HA	2:B:41:GLN:O	2.16	0.44
2:B:126:ARG:NH2	7:B:2024:HOH:O	2.48	0.44
1:A:736:LYS:HG2	1:A:751:PHE:CZ	2.52	0.44
1:A:509:VAL:O	1:A:509:VAL:HG23	2.18	0.44
2:B:115:LYS:HB2	2:B:115:LYS:HE3	1.88	0.44
1:A:176:GLN:H	1:A:176:GLN:HG2	1.55	0.43
1:A:84:ASP:OD1	1:A:678:HIS:HE1	2.02	0.43
1:A:762:LYS:HA	1:A:762:LYS:HD3	1.85	0.42
1:A:200:ASN:HB3	1:A:203:SER:HB2	2.01	0.42
1:A:321:CYS:SG	1:A:334:LYS:HE3	2.60	0.41
1:A:431:LEU:O	1:A:435:VAL:HG23	2.20	0.41
1:A:134:ALA:O	1:A:145:GLN:HG3	2.21	0.41
1:A:591:THR:O	1:A:592:GLN:HB2	2.20	0.41
1:A:702:GLN:HG2	7:A:2189:HOH:O	2.21	0.41
1:A:728:ARG:HB3	2:B:115:LYS:O	2.21	0.41
1:A:559:ILE:HD11	1:A:573:ASP:HB3	2.04	0.40

All (3) 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:494:GLU:CD	1:A:572:ARG:NH1[4_556]	1.58	0.62
1:A:494:GLU:OE2	1:A:572:ARG:NH1[4_556]	1.66	0.54
1:A:494:GLU:OE1	1:A:572:ARG:NH1[4_556]	1.67	0.53

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	712/788 (90%)	692 (97%)	20 (3%)	0	100	100
2	B	143/149 (96%)	138 (96%)	4 (3%)	1 (1%)	22	26
All	All	855/937 (91%)	830 (97%)	24 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	58	ASP

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	646/697 (93%)	620 (96%)	26 (4%)	31	44
2	B	125/129 (97%)	114 (91%)	11 (9%)	10	12
All	All	771/826 (93%)	734 (95%)	37 (5%)	25	36

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	66	MET
1	A	162	LYS
1	A	176	GLN
1	A	177	ASP
1	A	229	LEU
1	A	266	SER
1	A	269	ASP
1	A	351	ASP
1	A	442	CYS
1	A	443	PHE
1	A	494	GLU
1	A	497	GLN
1	A	508	TYR
1	A	539	SER

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Mol	Chain	Res	Type
1	A	559	ILE
1	A	614	ASP
1	A	651	LEU
1	A	667	ARG
1	A	670	LYS
1	A	726	LEU
1	A	773	ASP
1	A	777	LEU
1	A	779	GLU
1	A	792	ARG
1	A	811	LYS
2	B	29	THR
2	B	32	LEU
2	B	42	ASN
2	B	52	ILE
2	B	58	ASP
2	B	63	ILE
2	B	90	ARG
2	B	94	LYS
2	B	111	ASN
2	B	116	LEU
2	B	146	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	75	HIS
1	A	116	GLN
1	A	194	ASN
1	A	213	HIS
1	A	246	HIS
1	A	383	GLN
1	A	415	GLN
1	A	466	ASN
1	A	481	GLN
1	A	485	ASN
1	A	537	GLN
1	A	542	HIS
1	A	554	HIS
1	A	581	HIS
1	A	678	HIS

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Mol	Chain	Res	Type
2	B	3	GLN
2	B	49	GLN
2	B	111	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 7 ligands modelled in this entry, 5 are 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	998	4,5	24,29,29	1.10	2 (8%)	29,45,45	1.22	3 (10%)
4	BEF	A	999	3,5	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	998	4,5	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	998	ADP	C2-N3	2.54	1.36	1.32
3	A	998	ADP	C5-C4	2.46	1.47	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	998	ADP	N3-C2-N1	-3.69	122.90	128.68
3	A	998	ADP	C4-C5-N7	-2.34	106.97	109.40
3	A	998	ADP	C3'-C2'-C1'	2.02	104.02	100.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

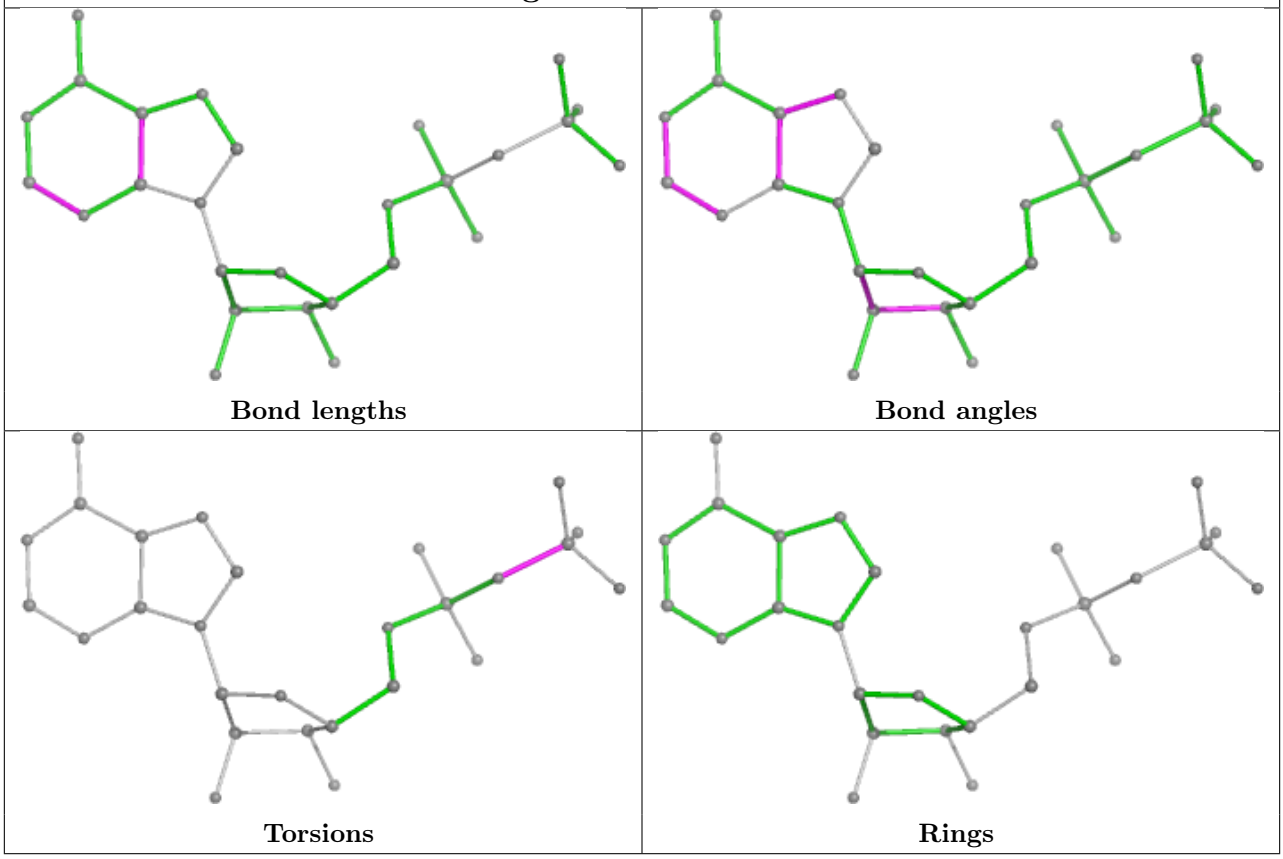
Mol	Chain	Res	Type	Atoms
3	A	998	ADP	PA-O3A-PB-O1B
3	A	998	ADP	PA-O3A-PB-O2B
3	A	998	ADP	PA-O3A-PB-O3B

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 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 998



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	724/788 (91%)	-0.14	19 (2%)	56	63	16, 31, 61, 75	14 (1%)
2	B	145/149 (97%)	-0.15	1 (0%)	87	91	25, 38, 56, 65	2 (1%)
All	All	869/937 (92%)	-0.14	20 (2%)	60	67	16, 33, 60, 75	16 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	PHE	4.6
1	A	413	VAL	3.4
1	A	388	VAL	3.2
1	A	608	LEU	2.8
1	A	747	ILE	2.7
1	A	391	THR	2.7
1	A	368	SER	2.4
1	A	351	ASP	2.4
1	A	447	THR	2.3
1	A	812	TYR	2.3
1	A	384	ASP	2.2
1	A	739	PHE	2.2
1	A	611	GLU	2.2
2	B	75	LYS	2.2
1	A	414	GLU	2.2
1	A	374	TYR	2.1
1	A	508	TYR	2.1
1	A	410	PRO	2.1
1	A	216	GLU	2.1
1	A	385	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

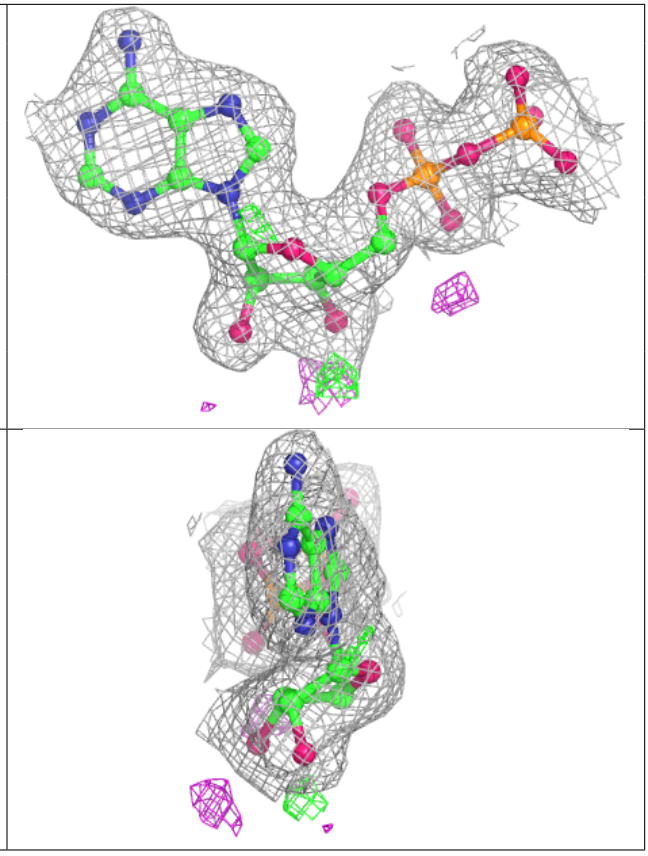
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CA	B	1149	1/1	0.86	0.05	72,72,72,72	0
4	BEF	A	999	4/4	0.93	0.18	22,22,24,25	0
6	CA	B	1148	1/1	0.96	0.05	64,64,64,64	0
5	MG	A	1000	1/1	0.96	0.13	24,24,24,24	0
6	CA	B	1150	1/1	0.98	0.09	31,31,31,31	0
3	ADP	A	998	27/27	0.99	0.15	17,20,22,26	0
6	CA	B	1151	1/1	0.99	0.06	41,41,41,41	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 A 998:

$2mF_o$-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.