



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:55 AM GMT

PDB ID : 2VAS  
Title : MYOSIN VI (MD-INSERT2-CAM, DELTA-INSERT1) POST-RIGOR STATE  
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Deposited on : 2007-09-04  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

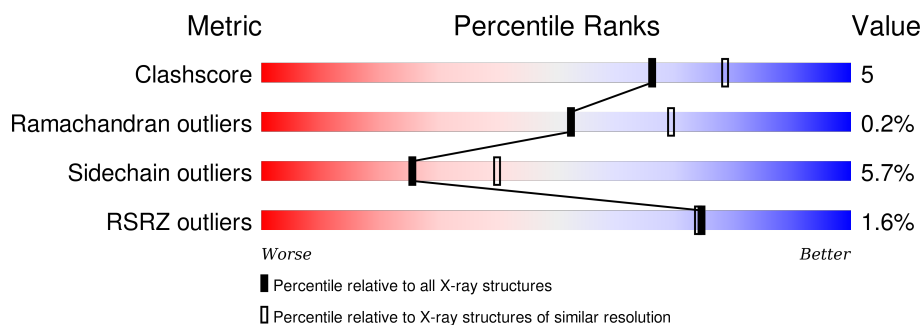
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	B	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BEF	A	999	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7213 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	732	5926	3781	1023	1094	28	132	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.

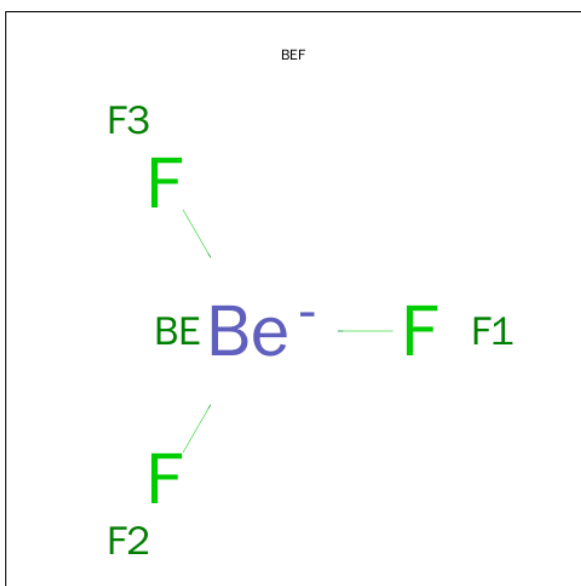
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	141	1097	674	173	242	8	46	0	0

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

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula:  $\text{BeF}_3$ ).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

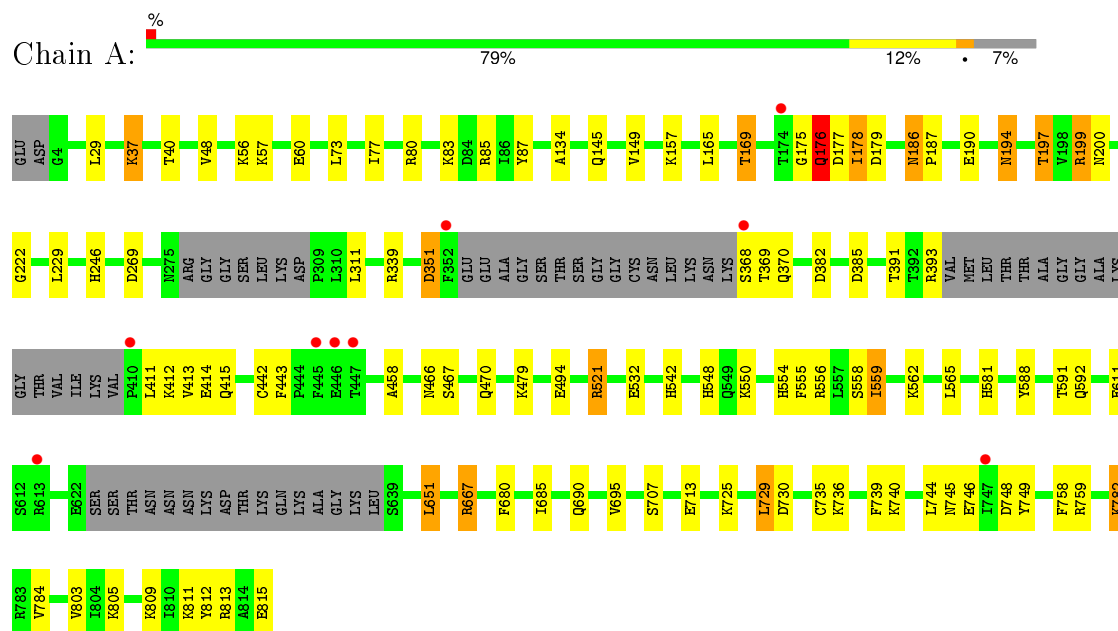
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	146	Total	O	0	0
			146	146		
7	B	8	Total	O	0	0
			8	8		

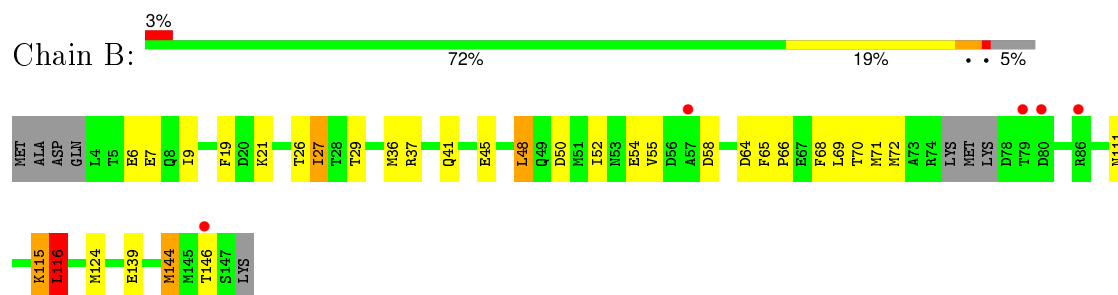
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



#### • Molecule 2: CALMODULIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.42Å 100.47Å 174.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.28 – 2.40 48.27 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.28-2.40) 100.0 (48.27-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.63 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.217 , 0.256 0.213 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 51151 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7213	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BEF, 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	0.77	11/6051 (0.2%)	0.75	19/8150 (0.2%)
2	B	0.75	4/1108 (0.4%)	0.93	9/1490 (0.6%)
All	All	0.77	15/7159 (0.2%)	0.78	28/9640 (0.3%)

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	2	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	351	ASP	CB-CG	-25.75	0.97	1.51
1	A	393	ARG	CA-CB	-23.39	1.02	1.53
1	A	812	TYR	CA-CB	-20.09	1.09	1.53
2	B	64	ASP	CB-CG	-12.71	1.25	1.51
1	A	740	LYS	CG-CD	-9.54	1.20	1.52
1	A	809	LYS	CA-CB	-9.17	1.33	1.53
2	B	21	LYS	CG-CD	-8.89	1.22	1.52
2	B	48	LEU	CA-CB	-8.86	1.33	1.53
1	A	782	LYS	CG-CD	7.92	1.79	1.52
1	A	414	GLU	CA-CB	-7.77	1.36	1.53
1	A	269	ASP	CA-CB	-6.55	1.39	1.53
1	A	412	LYS	CA-CB	-6.20	1.40	1.53
1	A	370	GLN	CB-CG	-6.16	1.35	1.52
1	A	745	ASN	CB-CG	6.04	1.65	1.51
2	B	45	GLU	CA-CB	-5.53	1.41	1.53



All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	812	TYR	CB-CA-C	-17.11	76.19	110.40
1	A	393	ARG	N-CA-CB	15.09	137.75	110.60
2	B	50	ASP	N-CA-CB	12.73	133.51	110.60
2	B	64	ASP	CB-CG-OD2	11.76	128.88	118.30
2	B	64	ASP	CB-CG-OD1	-10.29	109.03	118.30
2	B	64	ASP	CA-CB-CG	9.87	135.11	113.40
1	A	351	ASP	CA-CB-CG	9.61	134.55	113.40
1	A	815	GLU	N-CA-CB	-9.13	94.16	110.60
1	A	611	GLU	N-CA-CB	-9.04	94.33	110.60
1	A	611	GLU	CB-CA-C	8.52	127.44	110.40
1	A	393	ARG	CA-CB-CG	8.42	131.92	113.40
1	A	178	ILE	CG1-CB-CG2	7.90	128.78	111.40
1	A	740	LYS	CB-CG-CD	7.67	131.54	111.60
1	A	413	VAL	CA-CB-CG1	7.42	122.04	110.90
2	B	7	GLU	N-CA-CB	-7.16	97.71	110.60
1	A	413	VAL	N-CA-CB	7.15	127.23	111.50
1	A	811	LYS	N-CA-CB	-6.92	98.15	110.60
1	A	369	THR	N-CA-CB	6.66	122.95	110.30
2	B	7	GLU	CB-CA-C	6.60	123.59	110.40
1	A	811	LYS	CB-CA-C	6.51	123.42	110.40
2	B	45	GLU	CB-CA-C	6.46	123.33	110.40
1	A	812	TYR	CA-CB-CG	-6.08	101.85	113.40
1	A	611	GLU	CA-CB-CG	5.97	126.53	113.40
2	B	116	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	176	GLN	CB-CA-C	-5.60	99.21	110.40
1	A	177	ASP	N-CA-C	-5.44	96.32	111.00
2	B	21	LYS	CB-CG-CD	5.26	125.27	111.60
1	A	269	ASP	N-CA-CB	5.09	119.77	110.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	178	ILE	CB
1	A	393	ARG	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	GLN	Peptide
1	A	729	LEU	Peptide

## 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	5926	0	5876	50	0
2	B	1097	0	1013	18	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	146	0	0	2	0
7	B	8	0	0	0	0
All	All	7213	0	6901	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 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)
1:A:197:THR:HG21	7:A:2045:HOH:O	1.62	0.99
1:A:521:ARG:HG2	1:A:521:ARG:HH11	1.26	0.97
2:B:115:LYS:HB3	2:B:115:LYS:NZ	1.77	0.96
1:A:554:HIS:HD2	1:A:556:ARG:H	1.19	0.89
2:B:144:MET:HE3	2:B:144:MET:HA	1.71	0.71
2:B:115:LYS:HB3	2:B:115:LYS:HZ3	1.56	0.71
1:A:532:GLU:OE2	1:A:542:HIS:HD2	1.74	0.70
1:A:521:ARG:CG	1:A:521:ARG:HH11	2.05	0.66
2:B:115:LYS:HZ2	2:B:115:LYS:HB3	1.62	0.65
1:A:554:HIS:CD2	1:A:556:ARG:H	2.08	0.64
1:A:466:ASN:HD22	1:A:470:GLN:HG2	1.65	0.61
1:A:60:GLU:HG2	1:A:80:ARG:NH2	2.15	0.61
2:B:19:PHE:HB3	2:B:27:ILE:HD11	1.85	0.59
1:A:165:LEU:O	1:A:169:THR:HB	2.05	0.57
1:A:690:GLN:HG2	1:A:695:VAL:HG21	1.87	0.56
1:A:521:ARG:NH1	1:A:521:ARG:HG2	2.06	0.56
2:B:37:ARG:HA	2:B:41:GLN:O	2.05	0.56
1:A:178:ILE:HD11	1:A:222:GLY:HA2	1.86	0.56
1:A:479:LYS:HD3	1:A:651:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:LEU:HB3	1:A:730:ASP:HB3	1.89	0.54
2:B:116:LEU:HD21	2:B:124:MET:HE1	1.89	0.54
1:A:197:THR:HG22	1:A:199:ARG:H	1.74	0.53
1:A:707:SER:HB2	1:A:758:PHE:HB2	1.91	0.53
1:A:467:SER:H	1:A:470:GLN:NE2	2.06	0.52
1:A:176:GLN:O	1:A:179:ASP:HB2	2.11	0.51
1:A:748:ASP:HA	1:A:759:ARG:HG3	1.93	0.50
1:A:591:THR:O	1:A:592:GLN:HB2	2.12	0.49
2:B:55:VAL:HG11	2:B:70:THR:OG1	2.13	0.48
1:A:134:ALA:O	1:A:145:GLN:HG3	2.14	0.48
1:A:532:GLU:OE2	1:A:542:HIS:CD2	2.61	0.48
1:A:194:ASN:HD22	1:A:194:ASN:N	2.12	0.47
1:A:29:LEU:HD12	1:A:48:VAL:HG21	1.95	0.47
2:B:146:THR:O	2:B:146:THR:HG22	2.13	0.47
1:A:197:THR:HG22	1:A:200:ASN:H	1.80	0.47
1:A:744:LEU:HB3	1:A:749:TYR:CD1	2.50	0.47
1:A:411:LEU:HD22	1:A:415:GLN:HB3	1.96	0.46
2:B:144:MET:CE	2:B:144:MET:HA	2.42	0.46
1:A:467:SER:H	1:A:470:GLN:HE21	1.63	0.46
2:B:66:PRO:HA	2:B:69:LEU:HD12	1.97	0.46
1:A:197:THR:CG2	1:A:199:ARG:H	2.28	0.46
1:A:803:VAL:HG13	2:B:36:MET:HG2	1.97	0.46
1:A:667:ARG:HA	1:A:667:ARG:HD2	1.75	0.46
1:A:735:CYS:O	1:A:739:PHE:HD1	1.99	0.46
1:A:83:LYS:HD3	1:A:85:ARG:HH11	1.81	0.45
2:B:65:PHE:O	2:B:68:PHE:HB3	2.17	0.45
1:A:555:PHE:CD1	1:A:556:ARG:HD2	2.53	0.44
1:A:186:ASN:HB2	1:A:187:PRO:HD3	2.00	0.44
1:A:559:ILE:HG22	1:A:562:LYS:HG3	1.99	0.44
2:B:52:ILE:HD13	2:B:71:MET:HE1	2.00	0.44
1:A:382:ASP:HB3	1:A:385:ASP:HB2	1.99	0.44
1:A:470:GLN:H	1:A:470:GLN:NE2	2.15	0.44
2:B:48:LEU:O	2:B:52:ILE:HG12	2.18	0.43
1:A:73:LEU:HD12	1:A:77:ILE:HD13	2.00	0.43
1:A:37:LYS:HE3	1:A:37:LYS:HB2	1.85	0.43
1:A:80:ARG:NH1	1:A:87:TYR:O	2.52	0.43
1:A:246:HIS:HD2	7:A:2061:HOH:O	2.01	0.43
1:A:548:HIS:CE1	1:A:559:ILE:HD12	2.55	0.42
1:A:805:LYS:HB3	2:B:72:MET:HG3	2.02	0.42
1:A:197:THR:HG22	1:A:199:ARG:N	2.35	0.41
1:A:784:VAL:O	1:A:784:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLU:O	1:A:194:ASN:HB2	2.21	0.41
2:B:146:THR:CG2	2:B:146:THR:O	2.69	0.41
1:A:581:HIS:HE1	1:A:588:TYR:OH	2.03	0.41
1:A:680:PHE:CE1	1:A:685:ILE:HD13	2.56	0.40
1:A:157:LYS:HE3	1:A:458:ALA:HA	2.04	0.40
2:B:54:GLU:HG3	2:B:55:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	722/788 (92%)	705 (98%)	15 (2%)	2 (0%)	46	63
2	B	137/149 (92%)	135 (98%)	2 (2%)	0	100	100
All	All	859/937 (92%)	840 (98%)	17 (2%)	2 (0%)	52	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	175	GLY

### 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	654/697 (94%)	621 (95%)	33 (5%)	30	48
2	B	119/128 (93%)	108 (91%)	11 (9%)	11	16
All	All	773/825 (94%)	729 (94%)	44 (6%)	25	40

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	40	THR
1	A	56	LYS
1	A	57	LYS
1	A	149	VAL
1	A	169	THR
1	A	176	GLN
1	A	186	ASN
1	A	194	ASN
1	A	197	THR
1	A	199	ARG
1	A	229	LEU
1	A	311	LEU
1	A	339	ARG
1	A	351	ASP
1	A	368	SER
1	A	391	THR
1	A	442	CYS
1	A	443	PHE
1	A	494	GLU
1	A	521	ARG
1	A	550	LYS
1	A	558	SER
1	A	559	ILE
1	A	565	LEU
1	A	651	LEU
1	A	667	ARG
1	A	713	GLU
1	A	725	LYS
1	A	736	LYS
1	A	746	GLU
1	A	782	LYS
1	A	813	ARG
2	B	6	GLU
2	B	9	ILE

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Mol	Chain	Res	Type
2	B	26	THR
2	B	27	ILE
2	B	29	THR
2	B	58	ASP
2	B	111	ASN
2	B	115	LYS
2	B	116	LEU
2	B	139	GLU
2	B	144	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	116	GLN
1	A	194	ASN
1	A	213	HIS
1	A	246	HIS
1	A	383	GLN
1	A	430	HIS
1	A	466	ASN
1	A	470	GLN
1	A	481	GLN
1	A	485	ASN
1	A	493	GLN
1	A	497	GLN
1	A	542	HIS
1	A	554	HIS
1	A	581	HIS
1	A	678	HIS
1	A	679	HIS
1	A	684	GLN
2	B	53	ASN
2	B	111	ASN

### 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 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	5,4	22,29,29	1.03	2 (9%)	27,45,45	1.90	3 (11%)
4	BEF	A	999	3,5	0,3,3	0.00	-	0,3,3	0.00	-

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	5,4	-	0/12/32/32	0/3/3/3
4	BEF	A	999	3,5	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	998	ADP	O4'-C1'	2.19	1.44	1.41
3	A	998	ADP	C5-C4	2.77	1.46	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	998	ADP	N3-C2-N1	-7.66	123.03	128.89
3	A	998	ADP	C4-C5-N7	-3.34	106.41	109.48
3	A	998	ADP	O4'-C1'-N9	2.34	112.99	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	732/788 (92%)	-0.23	9 (1%) 81 81	10, 28, 54, 67	29 (3%)
2	B	141/149 (94%)	0.05	5 (3%) 48 48	25, 45, 66, 68	11 (7%)
All	All	873/937 (93%)	-0.19	14 (1%) 74 74	10, 32, 58, 68	40 (4%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	747	ILE	3.3
2	B	57	ALA	3.2
1	A	352	PHE	3.2
1	A	446	GLU	3.1
1	A	174	THR	2.9
1	A	447	THR	2.9
1	A	368	SER	2.7
2	B	80	ASP	2.5
2	B	79	THR	2.5
1	A	410	PRO	2.4
1	A	613	ARG	2.1
2	B	86	ARG	2.1
1	A	445	PHE	2.1
2	B	146	THR	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	BEF	A	999	4/4	0.93	0.18	2.41	17,17,17,19	0
5	MG	A	1000	1/1	0.99	0.16	1.69	16,16,16,16	0
3	ADP	A	998	27/27	0.98	0.12	-0.02	10,16,19,19	0
6	CA	B	1148	1/1	0.89	0.09	-0.89	62,62,62,62	0
6	CA	B	1150	1/1	0.97	0.09	-1.12	27,27,27,27	0
6	CA	B	1149	1/1	0.80	0.11	-2.42	101,101,101,101	0
6	CA	B	1151	1/1	0.98	0.05	-2.93	37,37,37,37	0

## 6.5 Other polymers

There are no such residues in this entry.