



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:26 PM UTC

PDB ID : 2VAS / pdb_00002vas
Title : Myosin VI (MD-insert2-CaM, Delta-Insert1) Post-rigor state
Authors : Menetrey, J.; Llinas, P.; Cicolari, J.; Squires, G.; Liu, X.; Li, A.; Sweeney, H.L.; Houdusse, A.
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

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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

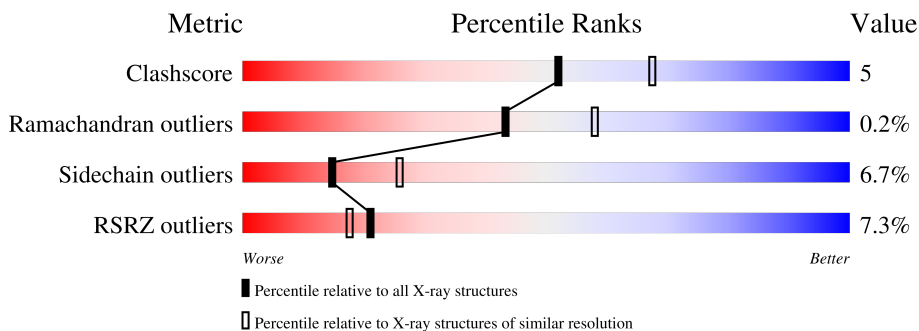
1 Overall quality at a glance

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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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 $\leq 5\%$. 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	

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.

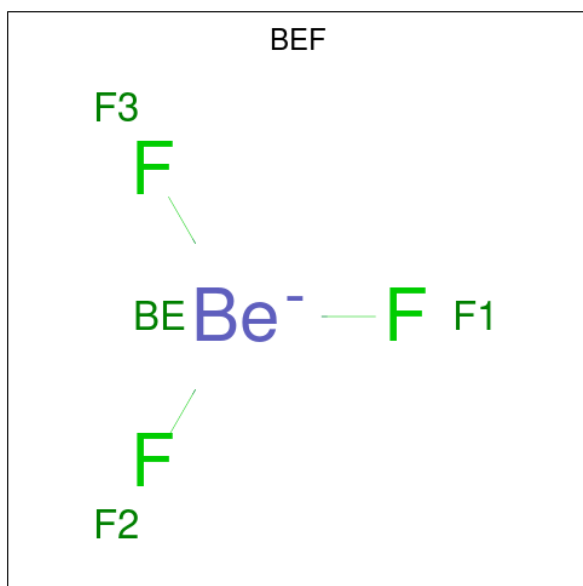
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	141	1097	674	173	242	8	46	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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 (CCD ID: BEF) (formula: BeF₃).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

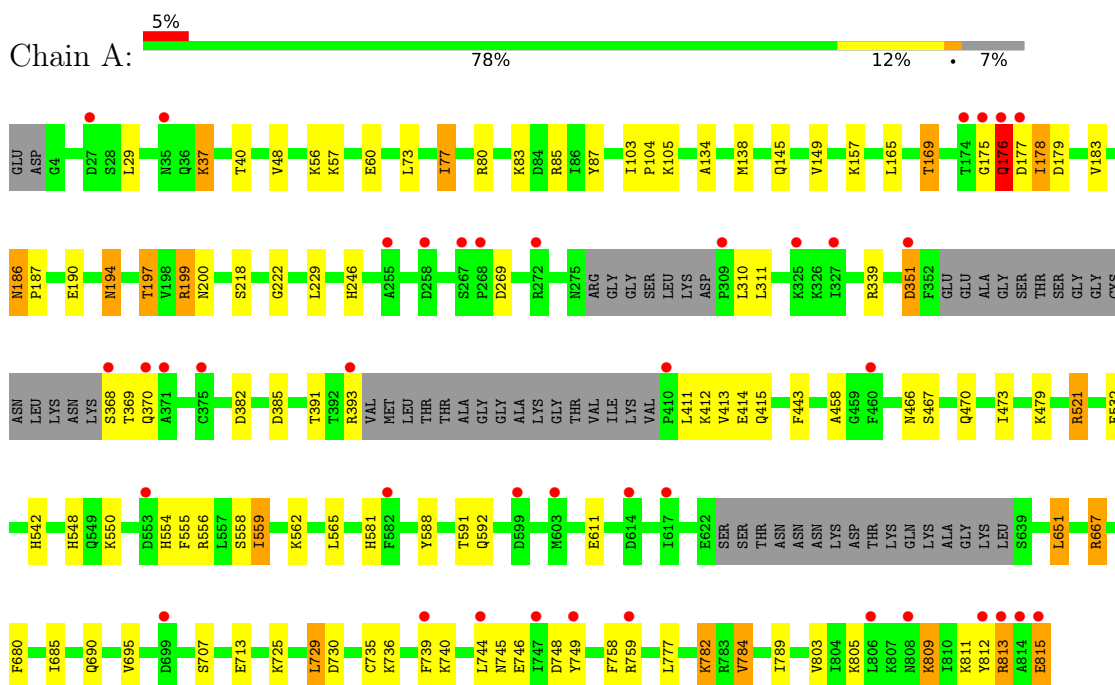
- Molecule 7 is water.

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

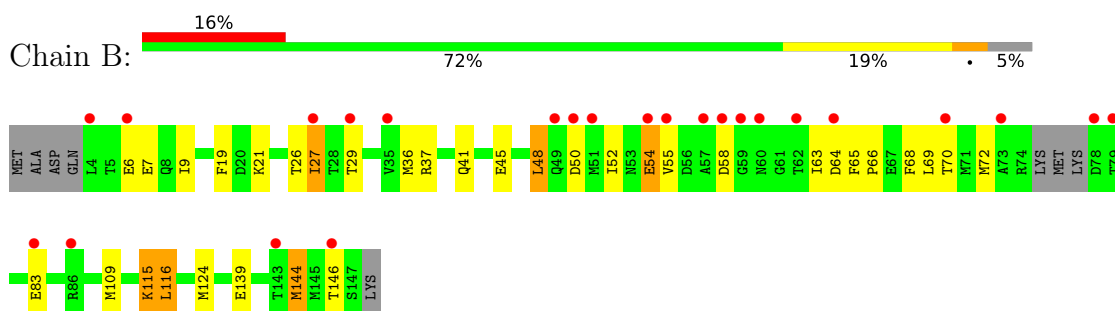
3 Residue-property plots i

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



• Molecule 2: CALMODULIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.42Å 100.47Å 174.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.28 – 2.40 48.28 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.28-2.40) 100.0 (48.28-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.63 (at 2.39Å)	Xtrriage
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.	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtrriage
Anisotropy	0.417	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7213	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, ADP, 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	0.90	14/6051 (0.2%)	1.07	29/8150 (0.4%)
2	B	0.87	4/1108 (0.4%)	1.30	8/1490 (0.5%)
All	All	0.90	18/7159 (0.3%)	1.11	37/9640 (0.4%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	812	TYR	CA-CB	-27.61	1.09	1.53
1	A	393	ARG	CA-CB	-25.48	1.02	1.53
1	A	351	ASP	CB-CG	-21.75	0.97	1.52
2	B	48	LEU	CA-CB	-12.88	1.33	1.53
1	A	809	LYS	CA-CB	-12.52	1.33	1.53
1	A	740	LYS	CG-CD	-10.82	1.20	1.52
2	B	64	ASP	CB-CG	-10.79	1.25	1.52
1	A	414	GLU	CA-CB	-10.32	1.36	1.53
2	B	21	LYS	CG-CD	-10.07	1.22	1.52
1	A	782	LYS	CG-CD	8.98	1.79	1.52
1	A	412	LYS	CA-CB	-8.91	1.40	1.53
1	A	269	ASP	CA-CB	-7.95	1.39	1.53
2	B	45	GLU	CA-CB	-7.45	1.41	1.53
1	A	177	ASP	N-CA	6.93	1.55	1.46
1	A	310	LEU	CA-CB	6.23	1.61	1.53
1	A	413	VAL	CA-CB	-5.77	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	370	GLN	CB-CG	-5.51	1.35	1.52
1	A	745	ASN	CB-CG	5.16	1.65	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	64	ASP	CA-CB-CG	22.51	135.11	112.60
1	A	351	ASP	CA-CB-CG	21.95	134.55	112.60
1	A	812	TYR	CB-CA-C	-20.29	76.19	110.68
1	A	393	ARG	N-CA-CB	16.03	137.75	110.50
2	B	50	ASP	N-CA-CB	15.91	133.51	110.12
1	A	413	VAL	N-CA-CB	14.26	127.23	110.55
1	A	611	GLU	CB-CA-C	13.19	127.44	111.22
1	A	611	GLU	N-CA-CB	-9.75	94.33	110.22
1	A	815	GLU	N-CA-CB	-9.61	94.16	110.50
1	A	745	ASN	CA-CB-CG	-9.14	103.45	112.60
1	A	393	ARG	CA-CB-CG	8.91	131.92	114.10
1	A	369	THR	N-CA-CB	8.88	122.95	110.07
1	A	740	LYS	CB-CG-CD	8.80	131.54	111.30
1	A	103	ILE	CA-C-N	8.73	130.76	119.84
1	A	103	ILE	C-N-CA	8.73	130.76	119.84
2	B	7	GLU	N-CA-CB	-8.48	97.71	110.01
1	A	811	LYS	N-CA-CB	-8.22	98.15	110.07
2	B	7	GLU	CB-CA-C	8.10	123.59	110.88
1	A	811	LYS	CB-CA-C	7.92	123.42	110.90
2	B	45	GLU	CB-CA-C	7.83	123.33	110.81
1	A	269	ASP	CA-CB-CG	-7.28	105.32	112.60
2	B	48	LEU	N-CA-CB	6.88	119.99	110.01
1	A	413	VAL	CA-CB-CG1	6.84	122.04	110.40
1	A	177	ASP	N-CA-C	-6.80	96.32	110.80
1	A	812	TYR	CA-CB-CG	-6.69	101.85	113.90
1	A	809	LYS	N-CA-CB	6.40	119.52	110.12
1	A	611	GLU	CA-CB-CG	6.22	126.53	114.10
2	B	21	LYS	CB-CG-CD	6.07	125.27	111.30
1	A	178	ILE	CG1-CB-CG2	6.03	128.78	110.70
1	A	813	ARG	N-CA-CB	5.83	119.53	110.44
1	A	412	LYS	N-CA-CB	5.78	118.11	110.25
1	A	176	GLN	CB-CA-C	-5.73	99.21	110.10
1	A	269	ASP	N-CA-CB	5.65	119.77	110.39
2	B	83	GLU	N-CA-CB	5.61	118.86	110.22
1	A	176	GLN	CA-C-N	-5.54	110.95	121.54
1	A	176	GLN	C-N-CA	-5.54	110.95	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	PRO	N-CA-C	5.41	123.61	112.47

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 [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	5926	0	5876	51	0
2	B	1097	0	1013	20	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	69	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 (69) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:115:LYS:HB3	2:B:115:LYS:HZ3	1.45	0.82
1:A:532:GLU:OE2	1:A:542:HIS:HD2	1.74	0.70
2:B:144:MET:HE3	2:B:144:MET:HA	1.75	0.67
1:A:521:ARG:HH11	1:A:521:ARG:CG	2.05	0.66
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:HG2	1:A:521:ARG:NH1	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
2:B:116:LEU:HD21	2:B:124:MET:HE2	1.87	0.55
1:A:479:LYS:HD3	1:A:651:LEU:HD13	1.88	0.55
1:A:729:LEU:HB3	1:A:730:ASP:HB3	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
1:A:134:ALA:O	1:A:145:GLN:HG3	2.14	0.48
2:B:55:VAL:HG11	2:B:70:THR:OG1	2.13	0.48
2:B:68:PHE:CZ	2:B:72:MET:HE1	2.48	0.48
1:A:532:GLU:OE2	1:A:542:HIS:CD2	2.61	0.48
2:B:116:LEU:CD2	2:B:124:MET:HE2	2.44	0.47
1:A:194:ASN:N	1:A:194:ASN:HD22	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:HA	2:B:144:MET:CE	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:115:LYS:HB3	2:B:115:LYS:HZ2	1.73	0.44
1:A:186:ASN:HB2	1:A:187:PRO:HD3	2.00	0.44
1:A:555:PHE:CD1	1:A:556:ARG:HD2	2.53	0.44
1:A:559:ILE:HG22	1:A:562:LYS:HG3	1.99	0.44
1:A:382:ASP:HB3	1:A:385:ASP:HB2	1.99	0.44
1:A:470:GLN:NE2	1:A:470:GLN:H	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:138:MET:HE3	1:A:218:SER:HB2	2.02	0.42
2:B:109:MET:SD	2:B:124:MET:HE1	2.60	0.41
1:A:197:THR:HG22	1:A:199:ARG:N	2.35	0.41
1:A:784:VAL:HG13	1:A:784:VAL:O	2.20	0.41
1:A:190:GLU:O	1:A:194:ASN:HB2	2.21	0.41
1:A:581:HIS:HE1	1:A:588:TYR:OH	2.03	0.41
2:B:146:THR:O	2:B:146:THR:CG2	2.69	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%)	36	50
2	B	137/149 (92%)	135 (98%)	2 (2%)	0	100	100
All	All	859/937 (92%)	840 (98%)	17 (2%)	2 (0%)	43	58

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%)	614 (94%)	40 (6%)	17	30
2	B	119/128 (93%)	107 (90%)	12 (10%)	7	11
All	All	773/825 (94%)	721 (93%)	52 (7%)	15	26

All (52) 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	77	ILE
1	A	105	LYS
1	A	149	VAL
1	A	169	THR
1	A	176	GLN
1	A	183	VAL
1	A	186	ASN
1	A	194	ASN
1	A	197	THR
1	A	199	ARG

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Mol	Chain	Res	Type
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	443	PHE
1	A	473	ILE
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	777	LEU
1	A	782	LYS
1	A	784	VAL
1	A	789	ILE
1	A	809	LYS
1	A	813	ARG
1	A	815	GLU
2	B	6	GLU
2	B	9	ILE
2	B	26	THR
2	B	27	ILE
2	B	29	THR
2	B	54	GLU
2	B	58	ASP
2	B	63	ILE
2	B	115	LYS
2	B	116	LEU
2	B	139	GLU
2	B	144	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	36	GLN
1	A	116	GLN
1	A	160	ASN
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	470	GLN
1	A	481	GLN
1	A	482	GLN
1	A	485	ASN
1	A	493	GLN
1	A	497	GLN
1	A	512	GLN
1	A	542	HIS
1	A	554	HIS
1	A	568	HIS
1	A	581	HIS
1	A	597	ASN
1	A	650	GLN
1	A	679	HIS
1	A	690	GLN
1	A	786	HIS
2	B	53	ASN
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 oligosaccharides 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	28,29,29	1.35	3 (10%)	43,45,45	1.91	10 (23%)
4	BEF	A	999	5,3	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	5,4	-	1/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	998	ADP	C5-C4	4.29	1.46	1.39
3	A	998	ADP	C5-C6	2.95	1.49	1.41
3	A	998	ADP	C8-N7	2.32	1.36	1.31

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	998	ADP	C5-C4-N3	-6.14	118.27	126.72
3	A	998	ADP	N3-C4-N9	4.80	135.34	127.17
3	A	998	ADP	C2-N3-C4	4.12	121.90	111.83
3	A	998	ADP	N3-C2-N1	-3.67	123.03	128.58
3	A	998	ADP	C4-C5-N7	-3.65	106.41	110.58
3	A	998	ADP	C4-N9-C8	2.80	108.68	105.74
3	A	998	ADP	C5-N7-C8	2.77	107.81	103.45
3	A	998	ADP	O4'-C1'-N9	2.55	112.99	108.09
3	A	998	ADP	C6-C5-N7	2.30	136.52	132.09
3	A	998	ADP	N9-C8-N7	-2.26	110.72	113.94

There are no chirality outliers.

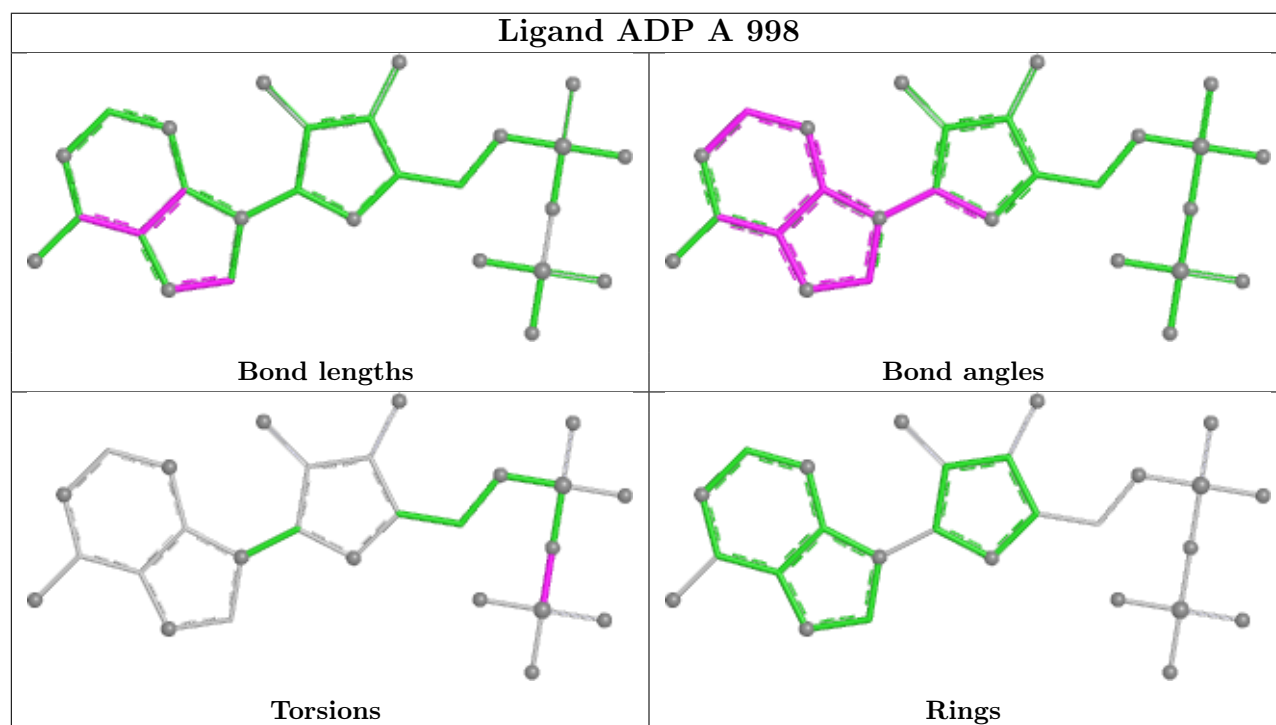
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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 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 [\(i\)](#)

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

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	732/788 (92%)	0.31	40 (5%) 30 27	10, 27, 53, 66	29 (3%)
2	B	141/149 (94%)	1.02	24 (17%) 4 3	23, 42, 66, 68	11 (7%)
All	All	873/937 (93%)	0.43	64 (7%) 21 17	10, 30, 55, 68	40 (4%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	78	ASP	4.4
1	A	368	SER	4.3
1	A	176	GLN	3.7
2	B	27	ILE	3.6
2	B	57	ALA	3.4
1	A	174	THR	3.3
1	A	327	ILE	3.1
1	A	410	PRO	3.1
1	A	175	GLY	3.0
1	A	617	ILE	2.9
2	B	70	THR	2.9
1	A	27	ASP	2.9
2	B	79	THR	2.8
1	A	815	GLU	2.8
1	A	747	ILE	2.8
1	A	814	ALA	2.7
1	A	393	ARG	2.7
1	A	813	ARG	2.7
2	B	49	GLN	2.7
2	B	59	GLY	2.7
2	B	51	MET	2.7
2	B	62	THR	2.7
1	A	699	ASP	2.6
1	A	35	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	50	ASP	2.6
1	A	812	TYR	2.6
1	A	351	ASP	2.5
2	B	54	GLU	2.5
1	A	759	ARG	2.5
2	B	64	ASP	2.4
1	A	806	LEU	2.4
1	A	272	ARG	2.4
1	A	614	ASP	2.4
1	A	371	ALA	2.4
1	A	744	LEU	2.4
2	B	4	LEU	2.4
1	A	749	TYR	2.4
2	B	55	VAL	2.3
2	B	58	ASP	2.3
1	A	808	ASN	2.3
2	B	29	THR	2.2
2	B	60	ASN	2.2
1	A	370	GLN	2.2
2	B	146	THR	2.2
2	B	83	GLU	2.2
2	B	86	ARG	2.2
1	A	268	PRO	2.2
1	A	325	LYS	2.2
1	A	603	MET	2.2
1	A	177	ASP	2.2
1	A	553	ASP	2.2
2	B	6	GLU	2.2
1	A	582	PHE	2.2
2	B	35	VAL	2.1
1	A	255	ALA	2.1
1	A	599	ASP	2.1
1	A	309	PRO	2.1
1	A	739	PHE	2.1
1	A	258	ASP	2.1
1	A	460	PHE	2.1
2	B	143	THR	2.1
1	A	375	CYS	2.1
2	B	73	ALA	2.0
1	A	267	SER	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](#)

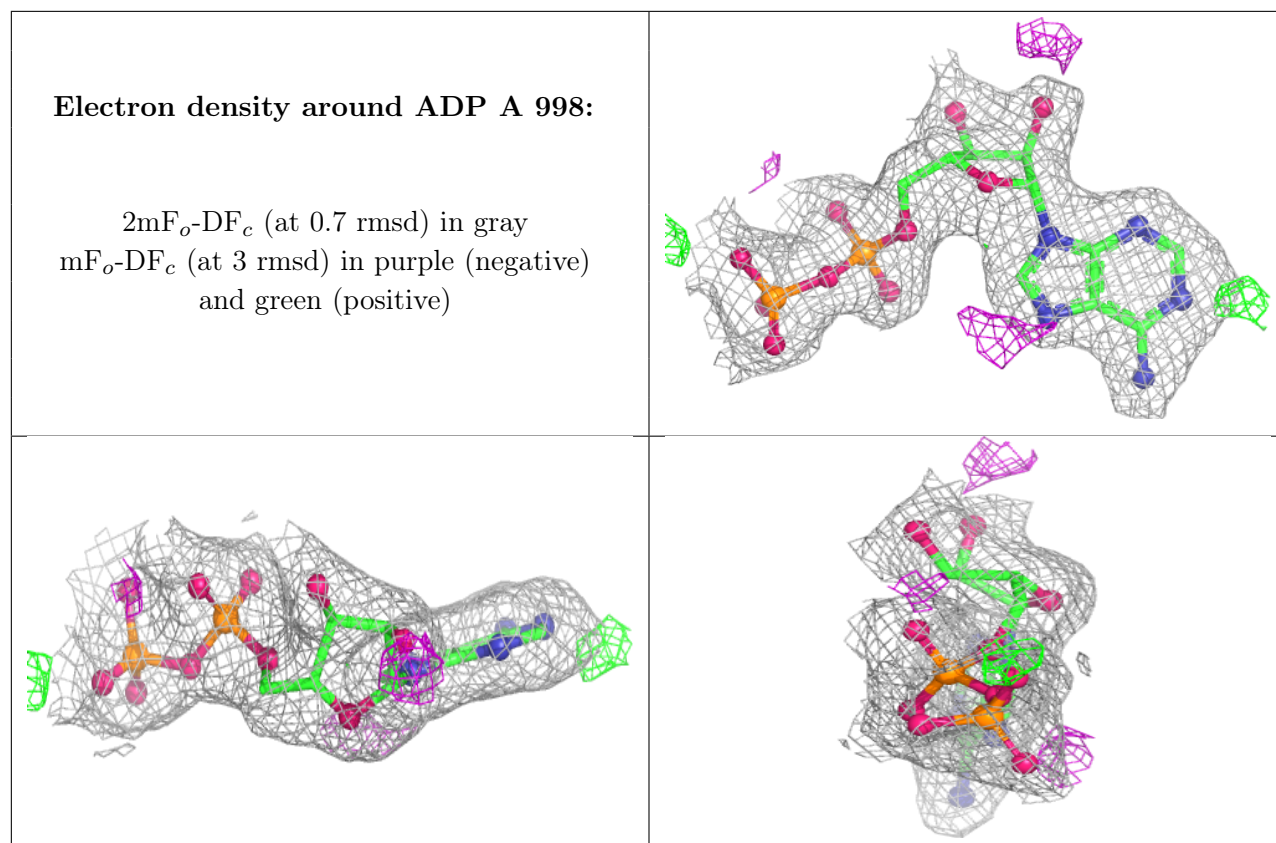
There are no oligosaccharides in this entry.

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(\AA^2)	Q<0.9
6	CA	B	1149	1/1	0.69	0.19	101,101,101,101	0
4	BEF	A	999	4/4	0.89	0.11	17,17,17,19	0
6	CA	B	1148	1/1	0.90	0.09	62,62,62,62	0
6	CA	B	1151	1/1	0.94	0.06	37,37,37,37	0
6	CA	B	1150	1/1	0.97	0.05	27,27,27,27	0
3	ADP	A	998	27/27	0.98	0.06	10,16,19,19	0
5	MG	A	1000	1/1	0.99	0.07	16,16,16,16	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.