



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 7, 2024 – 05:00 pm GMT

PDB ID : 6FSA
Title : Beta-Cardiac myosin post-rigor
Authors : Robert-Paganin, J.; Auguin, D.; Houdusse, A.
Deposited on : 2018-02-19
Resolution : 2.33 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

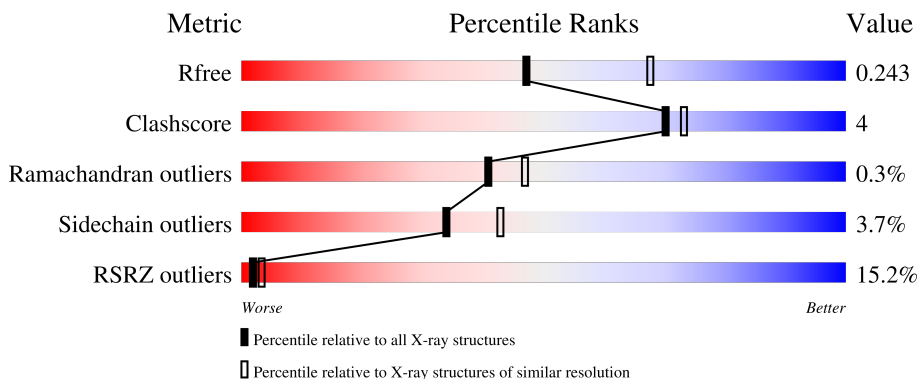
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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))
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	1935	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: grey;"></div> </div>
1	B	1935	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 35%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 61%; height: 10px; background-color: grey;"></div> </div>
2	D	199	<div style="display: flex; align-items: center;"> <div style="width: 41%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: grey;"></div> </div>
2	H	199	<div style="display: flex; align-items: center;"> <div style="width: 64%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15508 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-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	783	Total 6241	C 3978	N 1069	O 1162	S 32	0	4	0
1	B	756	Total 6021	C 3841	N 1023	O 1125	S 32	0	5	0

- Molecule 2 is a protein called Myosin light chain 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	154	Total 1215	C 766	N 201	O 240	S 8	0	0	0
2	H	150	Total 1178	C 742	N 196	O 232	S 8	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



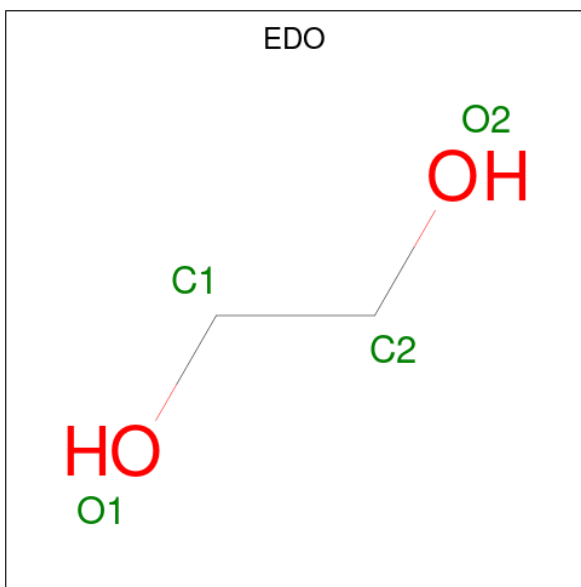
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			3	1 2		
5	A	1	Total	C O	0	0
			3	1 2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		

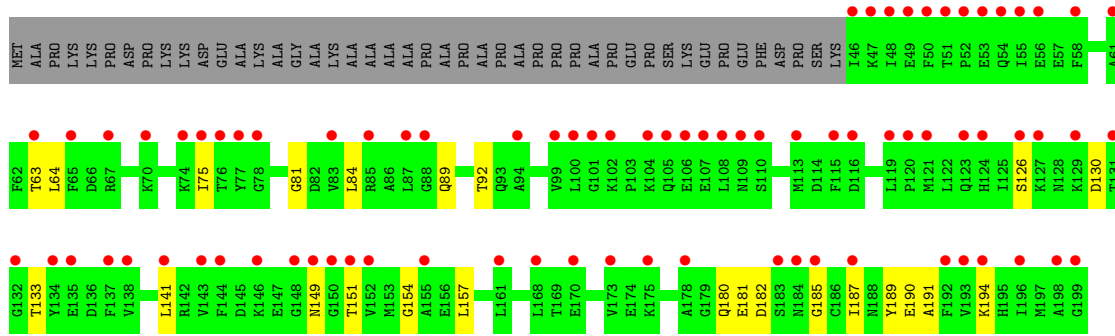
- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



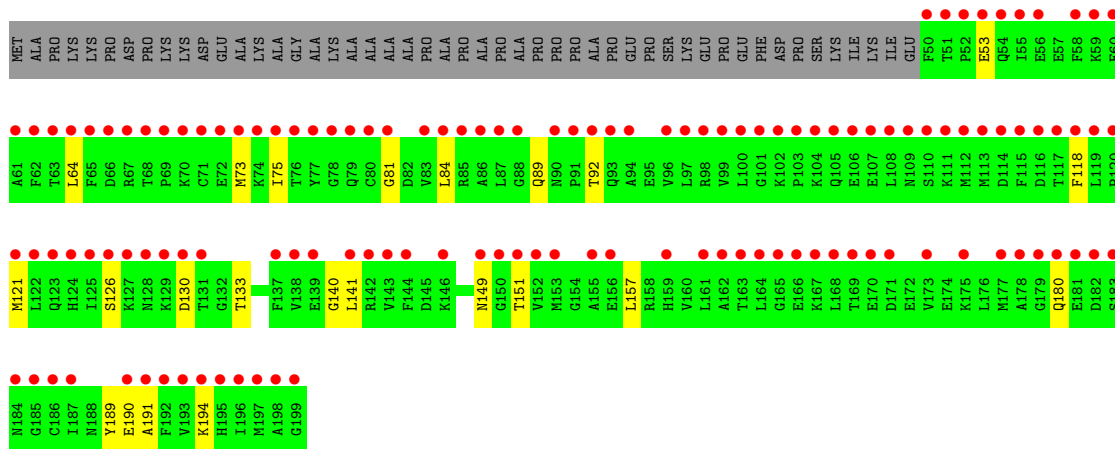
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	458	Total	O	0	0
			458	458		
7	B	314	Total	O	0	0
			314	314		
7	D	2	Total	O	0	0
			2	2		



• Molecule 2: Myosin light chain 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.12Å 94.32Å 125.41Å 104.76° 92.34° 100.06°	Depositor
Resolution (Å)	47.97 – 2.33 47.97 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.97-2.33) 98.5 (47.97-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.34Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.190 , 0.227 0.204 , 0.243	Depositor DCC
R_{free} test set	4907 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtrriage
Anisotropy	0.176	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15508	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, MG, FMT, ADP, MLY

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	0.53	1/6358 (0.0%)	0.70	0/8579
1	B	0.50	0/6130	0.68	0/8273
2	D	0.44	0/1234	0.62	0/1657
2	H	0.43	0/1197	0.59	0/1608
All	All	0.50	1/14919 (0.0%)	0.68	0/20117

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	MET	SD-CE	-5.19	1.48	1.77

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	730	ILE	Mainchain

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	6241	0	6128	47	0
1	B	6021	0	5890	44	0
2	D	1215	0	1192	10	0
2	H	1178	0	1149	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	6	0	3	0	0
5	B	9	0	4	0	0
6	A	4	0	6	0	0
6	B	4	0	6	0	0
7	A	458	0	0	4	0
7	B	314	0	0	3	0
7	D	2	0	0	0	0
All	All	15508	0	14402	105	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 4.

The worst 5 of 105 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:B:784:ILE:HD11	2:H:140:GLY:HA3	1.41	1.02
1:A:152:PRO:HD2	7:A:2143:HOH:O	1.77	0.84
1:A:493:MET:HE1	7:A:2300:HOH:O	1.87	0.75
1:A:493:MET:CE	7:A:2300:HOH:O	2.35	0.74
1:A:45:GLU:HG2	1:A:690:MET:HG3	1.69	0.73

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	780/1935 (40%)	757 (97%)	21 (3%)	2 (0%)	41	47
1	B	746/1935 (39%)	730 (98%)	15 (2%)	1 (0%)	51	62
2	D	152/199 (76%)	142 (93%)	8 (5%)	2 (1%)	12	9
2	H	148/199 (74%)	140 (95%)	8 (5%)	0	100	100
All	All	1826/4268 (43%)	1769 (97%)	52 (3%)	5 (0%)	41	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	561	SER
2	D	185	GLY
2	D	180	GLN
1	B	767	ALA
1	A	558	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	657/1696 (39%)	629 (96%)	28 (4%)	29	36
1	B	634/1696 (37%)	617 (97%)	17 (3%)	44	55
2	D	131/165 (79%)	125 (95%)	6 (5%)	27	33
2	H	126/165 (76%)	119 (94%)	7 (6%)	21	24
All	All	1548/3722 (42%)	1490 (96%)	58 (4%)	34	43

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	VAL
2	H	130	ASP
1	B	546	MET
2	H	75	ILE
2	D	133	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	149	ASN
2	H	149	ASN
1	A	753	HIS
1	B	391	ASN
1	B	451	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	MLY	B	129	1	9,10,11	1.13	1 (11%)	6,11,13	1.98	2 (33%)
1	MLY	A	129	1	9,10,11	1.01	1 (11%)	6,11,13	2.27	2 (33%)

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
1	MLY	B	129	1	-	2/8/9/11	-
1	MLY	A	129	1	-	2/8/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	MLY	CB-CA	2.89	1.57	1.53
1	A	129	MLY	CB-CA	2.53	1.56	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	MLY	CH2-NZ-CH1	-3.91	99.62	109.73
1	B	129	MLY	CH2-NZ-CH1	-3.34	101.09	109.73
1	A	129	MLY	CH2-NZ-CE	-2.68	100.11	110.74
1	B	129	MLY	CH2-NZ-CE	-2.39	101.25	110.74

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	129	MLY	CD-CE-NZ-CH1
1	A	129	MLY	CD-CE-NZ-CH2
1	B	129	MLY	CD-CE-NZ-CH1
1	B	129	MLY	CD-CE-NZ-CH2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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
6	EDO	A	2005	-	3,3,3	0.12	0	2,2,2	0.38	0
5	FMT	B	2005	-	2,2,2	1.14	0	1,1,1	1.08	0
5	FMT	A	2004	-	2,2,2	1.33	0	1,1,1	1.01	0
5	FMT	B	2004	-	2,2,2	1.18	0	1,1,1	1.05	0
5	FMT	A	2003	-	2,2,2	1.23	0	1,1,1	1.12	0
4	ADP	A	2002	3	24,29,29	0.77	0	29,45,45	0.85	2 (6%)
4	ADP	B	2002	3	24,29,29	0.59	0	29,45,45	0.73	1 (3%)
5	FMT	B	2003	-	2,2,2	1.51	1 (50%)	1,1,1	1.02	0
6	EDO	B	2006	-	3,3,3	0.44	0	2,2,2	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	2002	3	-	3/12/32/32	0/3/3/3
6	EDO	B	2006	-	-	0/1/1/1	-
4	ADP	B	2002	3	-	3/12/32/32	0/3/3/3
6	EDO	A	2005	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2003	FMT	O2-C	2.10	1.39	1.28

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2002	ADP	C5-C6-N6	2.35	123.93	120.35
4	A	2002	ADP	C5-C6-N6	2.15	123.62	120.35
4	A	2002	ADP	PA-O3A-PB	2.02	139.77	132.83

There are no chirality outliers.

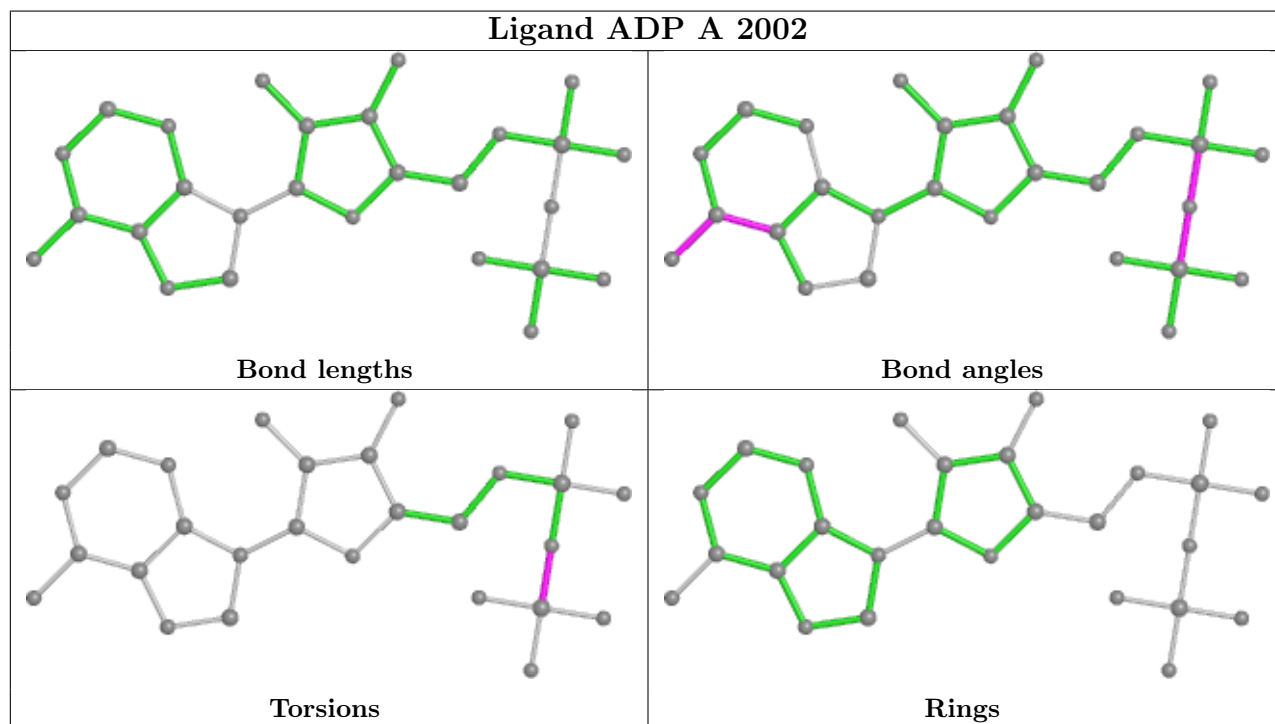
5 of 6 torsion outliers are listed below:

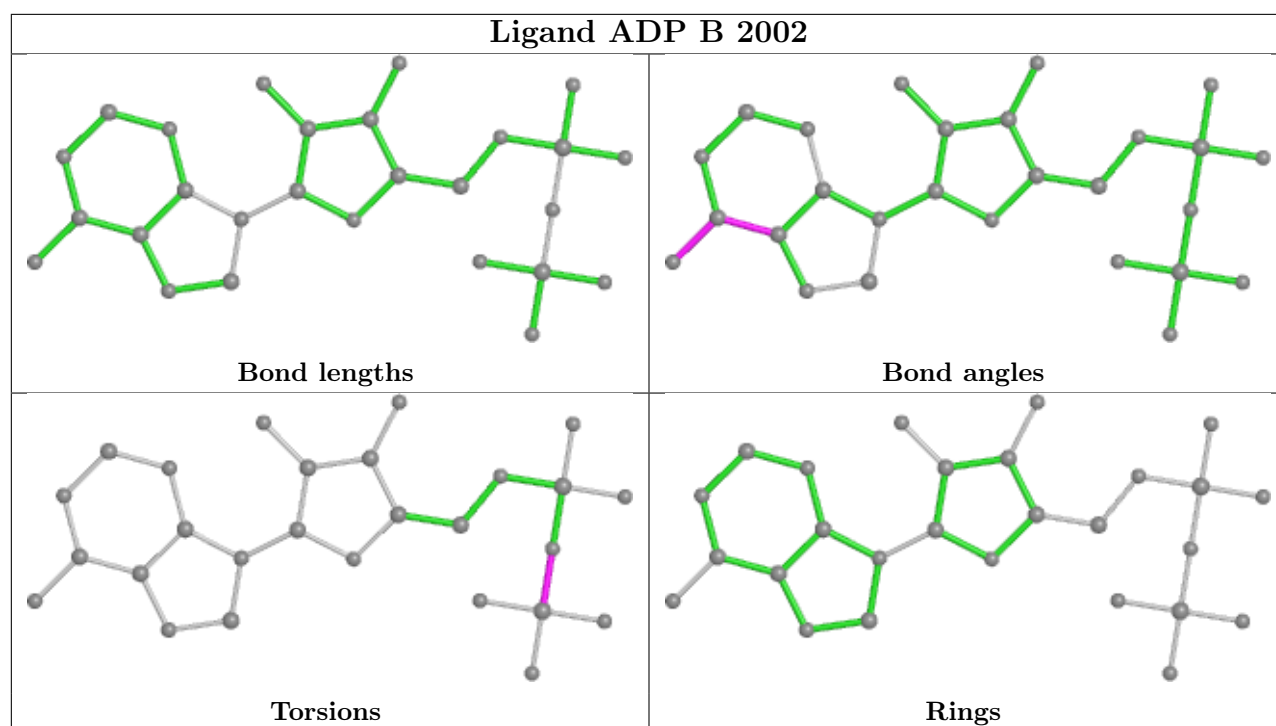
Mol	Chain	Res	Type	Atoms
4	B	2002	ADP	PA-O3A-PB-O3B
4	A	2002	ADP	PA-O3A-PB-O2B
4	A	2002	ADP	PA-O3A-PB-O3B
4	B	2002	ADP	PA-O3A-PB-O2B
4	A	2002	ADP	PA-O3A-PB-O1B

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 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 [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	782/1935 (40%)	0.29	28 (3%) 42 53	22, 42, 94, 129	0
1	B	755/1935 (39%)	0.40	43 (5%) 23 33	25, 55, 103, 135	0
2	D	154/199 (77%)	2.51	81 (52%) 0 0	88, 130, 159, 167	0
2	H	150/199 (75%)	5.14	128 (85%) 0 0	121, 162, 191, 198	0
All	All	1841/4268 (43%)	0.91	280 (15%) 2 3	22, 56, 160, 198	0

The worst 5 of 280 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	65	PHE	20.9
2	H	75	ILE	14.0
2	H	119	LEU	12.5
2	H	50	PHE	12.0
2	H	69	PRO	11.3

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	MLY	A	129	11/12	0.97	0.14	35,37,40,41	0
1	MLY	B	129	11/12	0.97	0.13	41,41,47,48	0

6.3 Carbohydrates [i](#)

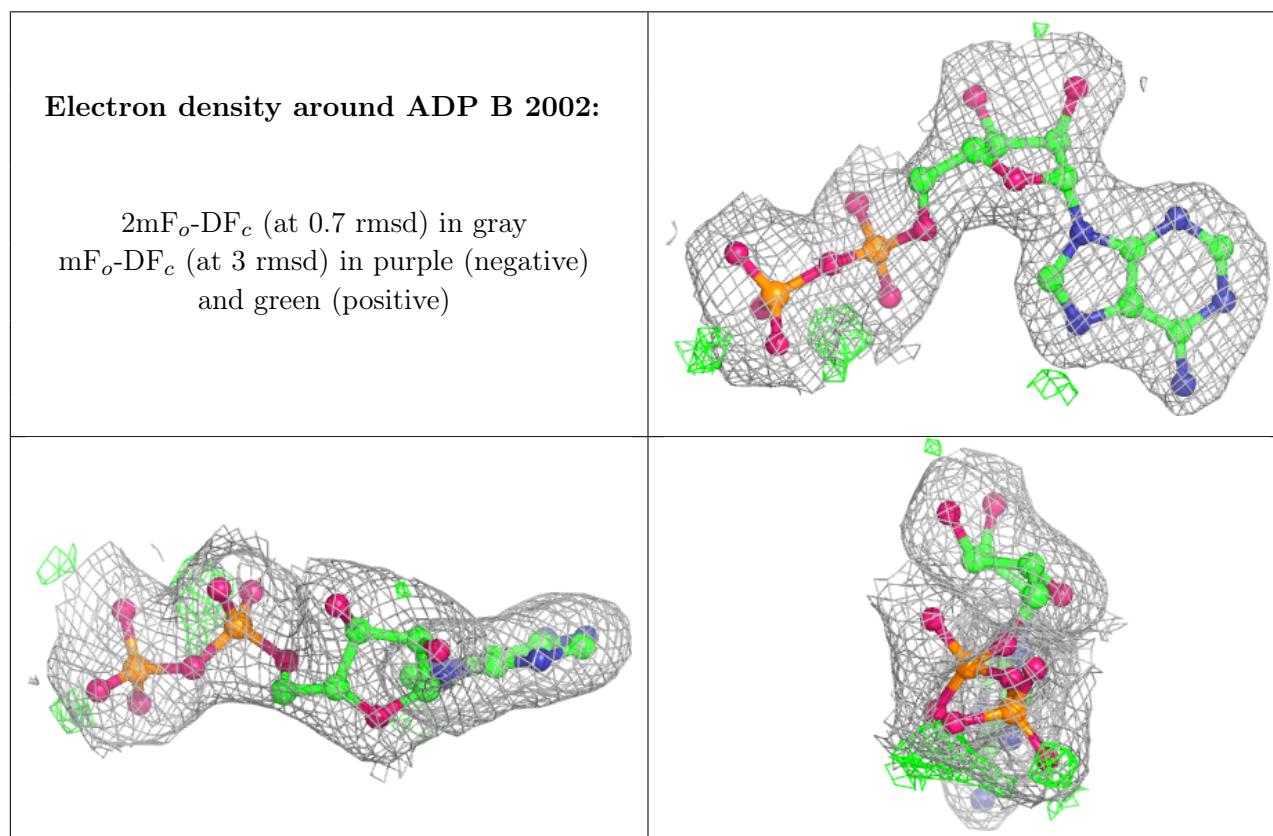
There are no monosaccharides in this entry.

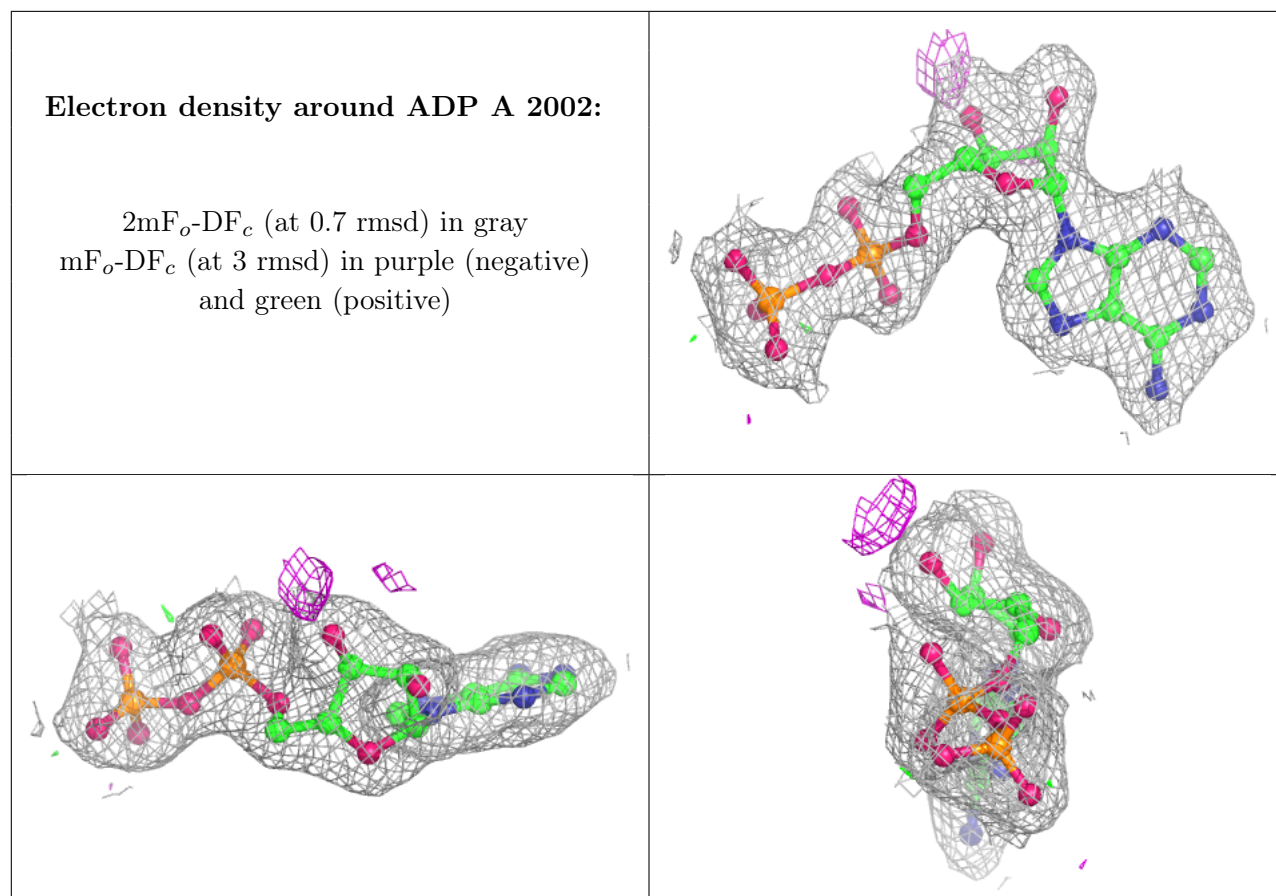
6.4 Ligands [i](#)

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
5	FMT	B	2003	3/3	0.82	0.17	48,48,49,49	0
3	MG	B	2001	1/1	0.90	0.10	65,65,65,65	0
5	FMT	B	2005	3/3	0.91	0.16	58,58,59,60	0
5	FMT	B	2004	3/3	0.92	0.15	42,42,48,52	0
5	FMT	A	2003	3/3	0.93	0.11	36,36,43,49	0
6	EDO	B	2006	4/4	0.94	0.17	42,44,44,47	0
6	EDO	A	2005	4/4	0.95	0.20	32,33,33,39	0
5	FMT	A	2004	3/3	0.96	0.18	44,44,46,46	0
3	MG	A	2001	1/1	0.97	0.08	39,39,39,39	0
4	ADP	B	2002	27/27	0.98	0.14	35,39,47,52	0
4	ADP	A	2002	27/27	0.99	0.14	24,28,35,42	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.