



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 12:10 AM UTC

PDB ID : 6FSA / pdb_00006fsa
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

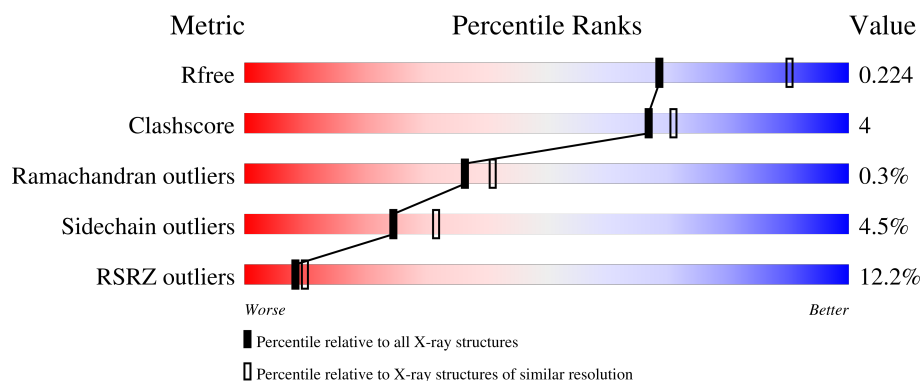
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (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	2% 35% 5% 60%
1	B	1935	3% 34% 5% 61%
2	D	199	33% 62% 14% 23%
2	H	199	31% 62% 13% 25%

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
1	A	783	Total	C	N	O	S	0	4	0
			6241	3978	1069	1162	32			
1	B	756	Total	C	N	O	S	0	5	0
			6021	3841	1023	1125	32			

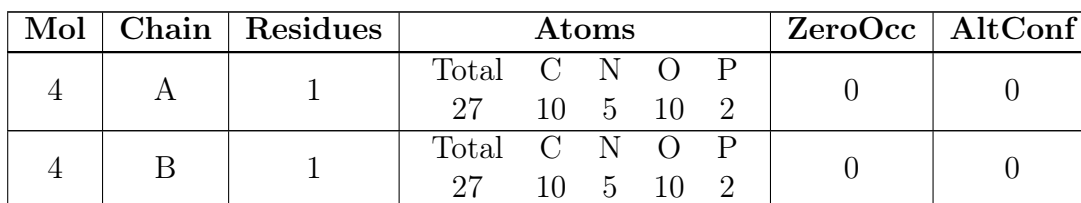
- Molecule 2 is a protein called Myosin light chain 3.

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



- FMT
- 
- The diagram shows the chemical structure of formic acid (FMT). It consists of a central carbon atom (C, green) double-bonded to an oxygen atom (O1, red) and single-bonded to a hydroxyl group (OH, red O and green H). The label O2 (green) is placed next to the hydrogen atom.

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



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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 (CCD ID: 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.

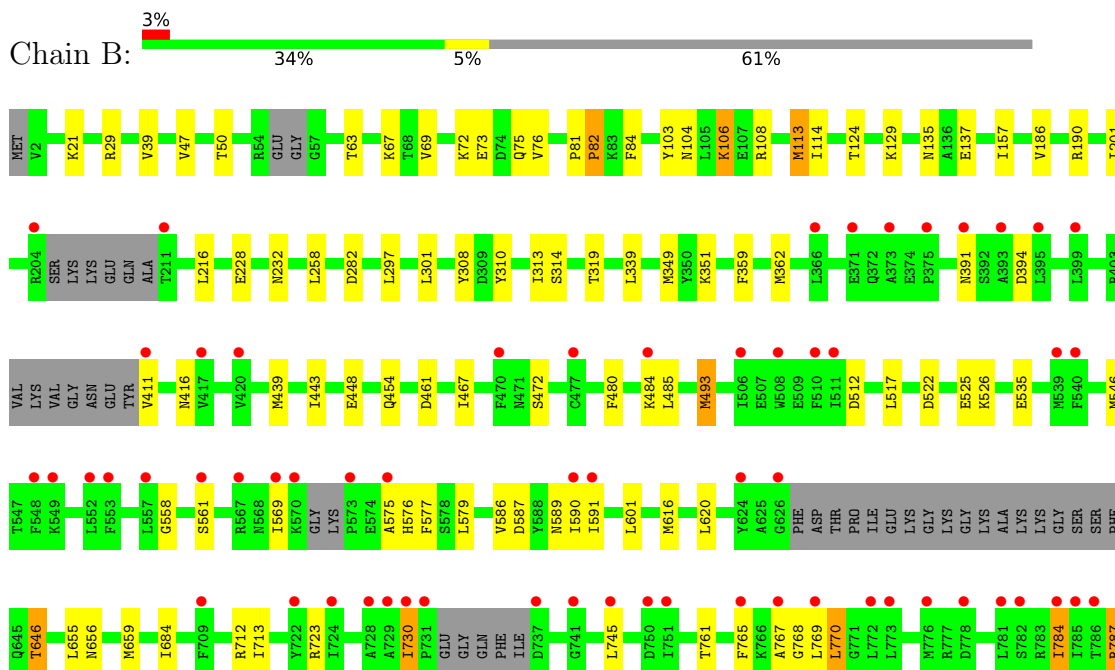
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	458	Total	O	0	0
			458	458		
7	B	314	Total	O	0	0
			314	314		
7	D	2	Total	O	0	0
			2	2		

- Molecule 1: Myosin-7



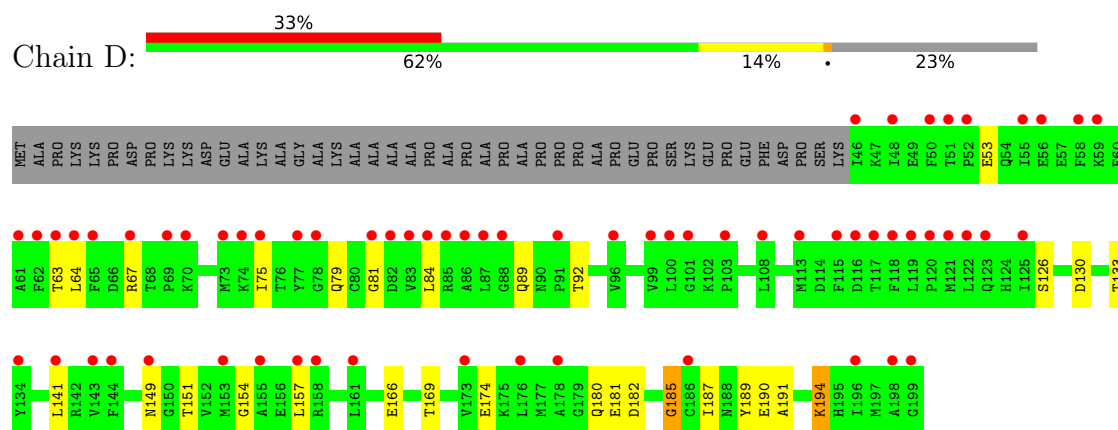
GLY THR LYS GLY LEU ASN GLU GLU	VAL	GLY	CYS	LEU	GLN	ILE	GLU	ASN	GLU	ALA	ARG
	LYS	LYS	ARG	ARG	LEU	ALA	ILE	PHE	ALA	LEU	SER
	LYS	GLN	ASN	ALA	HIS	ASP	SER	ASP	LYS	ALA	VAL
	LEU	VAL	GLU	VAL	MET	GLU	ASP	LYS	LYS	HIS	ASN
	LEU	GLN	GLU	GLU	GLU	THR	THR	LEU	LEU	LEU	THR
	LYS	LYS	LYS	GLN	ARG	GLU	GLU	ALA	ALA	GLN	LYS
	VAL	LEU	ALA	THR	LYS	ARG	GLN	GLN	GLN	SER	GLN
	LYS	GLU	LYS	GLU	ALA	LYS	GLY	LYS	ARG	ALA	GLN
	ALA	ALA	LYS	ARG	ALA	ALA	GLY	LEU	LEU	ARG	ALA
	THR	ARG	ALA	SER	GLU	GLU	SER	SER	GLN	HIS	LYS
GLY THR LYS GLY LEU ASN GLU GLU	VAL	GLY	CYS	LEU	GLN	ILE	GLU	ASN	GLU	ALA	ARG
	LYS	LYS	ARG	ARG	LEU	ALA	ILE	PHE	ALA	LEU	SER
	LYS	GLN	ASN	ALA	ALA	HIS	ASP	ASP	LYS	ALA	VAL
	LEU	VAL	GLU	VAL	MET	GLU	GLU	ILE	LYS	LYS	HIS
	LEU	GLN	GLU	GLU	GLU	THR	THR	LEU	LEU	LEU	THR
	LYS	LYS	LYS	GLN	ARG	GLU	GLU	ALA	ALA	GLN	LYS
	VAL	ARG	ALA	THR	LYS	LYS	GLY	THR	ALA	GLN	GLN
	LYS	ARG	ALA	SER	GLU	GLU	SER	GLN	GLN	GLN	GLN
	ALA	GLU	LYS	GLU	ALA	ALA	GLY	GLU	GLU	GLU	GLU
	THR	ARG	ALA	SER	GLU	GLU	SER	HIS	VAL	VAL	GLY
GLY THR LYS GLY LEU ASN GLU GLU	VAL	GLY	CYS	LEU	GLN	ILE	GLU	ASN	GLU	ALA	ARG
	LYS	LYS	ARG	ARG	LEU	ALA	ILE	PHE	ALA	LEU	SER
	LYS	GLN	ASN	ALA	ALA	HIS	ASP	ASP	LYS	ALA	VAL
	LEU	VAL	GLU	VAL	MET	GLU	GLU	ILE	LYS	LYS	HIS
	LEU	GLN	GLU	GLU	GLU	THR	THR	LEU	LEU	LEU	THR
	LYS	LYS	LYS	GLN	ARG	GLU	GLU	ALA	ALA	GLN	LYS
	VAL	ARG	ALA	THR	LYS	LYS	GLY	THR	ALA	GLN	GLN
	LYS	ARG	ALA	SER	GLU	GLU	SER	GLN	GLN	GLN	GLN
	ALA	GLU	LYS	GLU	ALA	ALA	GLY	GLU	GLU	GLU	GLU
	THR	ARG	ALA	SER	GLU	GLU	SER	HIS	VAL	VAL	GLY
GLY THR LYS GLY LEU ASN GLU GLU	VAL	GLY	CYS	LEU	GLN	ILE	GLU	ASN	GLU	ALA	ARG
	LYS	LYS	ARG	ARG	LEU	ALA	ILE	PHE	ALA	LEU	SER
	LYS	GLN	ASN	ALA	ALA	HIS	ASP	ASP	LYS	ALA	VAL
	LEU	VAL	GLU	VAL	MET	GLU	GLU	ILE	LYS	LYS	HIS
	LEU	GLN	GLU	GLU	GLU	THR	THR	LEU	LEU	LEU	THR
	LYS	LYS	LYS	GLN	ARG	GLU	GLU	ALA	ALA	GLN	LYS
	VAL	ARG	ALA	THR	LYS	LYS	GLY	THR	ALA	GLN	GLN
	LYS	ARG	ALA	SER	GLU	GLU	SER	GLN	GLN	GLN	GLN
	ALA	GLU	LYS	GLU	ALA	ALA	GLY	GLU	GLU	GLU	GLU
	THR	ARG	ALA	SER	GLU	GLU	SER	HIS	VAL	VAL	GLY

- Molecule 1: Myosin-7

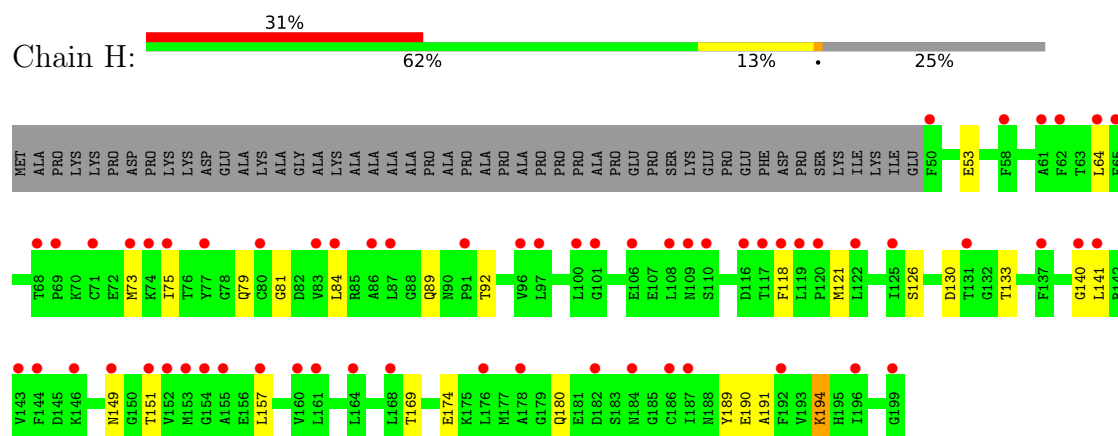




- Molecule 2: Myosin light chain 3



- 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)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.190 , 0.227 (Not available) , 0.224	Depositor DCC
R_{free} test set	4907 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.92	4/6358 (0.1%)	1.40	20/8579 (0.2%)
1	B	0.88	2/6130 (0.0%)	1.38	21/8273 (0.3%)
2	D	0.81	0/1234	1.42	8/1657 (0.5%)
2	H	0.81	0/1197	1.41	4/1608 (0.2%)
All	All	0.88	6/14919 (0.0%)	1.39	53/20117 (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	B	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	MET	SD-CE	-12.31	1.48	1.79
1	B	113	MET	SD-CE	-11.67	1.50	1.79
1	A	493	MET	SD-CE	-7.71	1.60	1.79
1	B	493	MET	SD-CE	-6.99	1.62	1.79
1	A	674	ILE	CA-C	6.33	1.58	1.53

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	685	ASP	CA-CB-CG	9.43	122.03	112.60
1	A	560[A]	SER	CA-C-N	9.28	139.26	121.54
1	A	560[A]	SER	C-N-CA	9.28	139.26	121.54
1	A	560[B]	SER	CA-C-N	9.28	139.26	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	560[B]	SER	C-N-CA	9.28	139.26	121.54

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 [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	6241	0	6128	47	0
1	B	6021	0	5890	46	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	107	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 107 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PRO:HD2	7:A:2143:HOH:O	1.77	0.84
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
1:A:493:MET:HE1	7:A:2300:HOH:O	1.93	0.68

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%)	36	41
1	B	746/1935 (39%)	730 (98%)	15 (2%)	1 (0%)	48	57
2	D	152/199 (76%)	142 (93%)	8 (5%)	2 (1%)	9	7
2	H	148/199 (74%)	140 (95%)	8 (5%)	0	100	100
All	All	1826/4268 (43%)	1769 (97%)	52 (3%)	5 (0%)	36	41

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%)	627 (95%)	30 (5%)	24	31
1	B	634/1696 (37%)	612 (96%)	22 (4%)	32	41
2	D	131/165 (79%)	121 (92%)	10 (8%)	12	13
2	H	126/165 (76%)	117 (93%)	9 (7%)	13	14
All	All	1548/3722 (42%)	1477 (95%)	71 (5%)	24	31

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	130	ASP
2	D	169	THR
2	H	75	ILE
1	A	745	LEU
1	A	738	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	128	ASN
2	H	188	ASN
2	D	149	ASN
2	H	123	GLN
1	B	163	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	1.04	1 (11%)	6,11,13	1.98	2 (33%)
1	MLY	A	129	1	9,10,11	0.93	1 (11%)	6,11,13	2.28	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	2.53	1.57	1.53
1	A	129	MLY	CB-CA	2.22	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	-3.94	99.62	109.72
1	B	129	MLY	CH2-NZ-CH1	-3.37	101.09	109.72
1	A	129	MLY	CH2-NZ-CE	-2.68	100.11	110.75
1	B	129	MLY	CH2-NZ-CE	-2.40	101.25	110.75

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	B	129	MLY	CD-CE-NZ-CH1
1	A	129	MLY	CD-CE-NZ-CH2
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 oligosaccharides 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	$\# Z > 2$
5	FMT	A	2004	-	2,2,2	1.31	0	1,1,1	1.01	0
4	ADP	A	2002	3	28,29,29	0.55	0	43,45,45	0.59	1 (2%)
5	FMT	B	2003	-	2,2,2	1.48	1 (50%)	1,1,1	1.02	0
6	EDO	A	2005	-	3,3,3	0.12	0	2,2,2	0.41	0
5	FMT	A	2003	-	2,2,2	1.20	0	1,1,1	1.13	0
4	ADP	B	2002	3	28,29,29	0.33	0	43,45,45	0.42	0
5	FMT	B	2005	-	2,2,2	1.11	0	1,1,1	1.09	0
5	FMT	B	2004	-	2,2,2	1.15	0	1,1,1	1.06	0
6	EDO	B	2006	-	3,3,3	0.40	0	2,2,2	0.57	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
6	EDO	A	2005	-	-	0/1/1/1	-
4	ADP	B	2002	3	-	3/16/32/32	0/3/3/3
6	EDO	B	2006	-	-	0/1/1/1	-
4	ADP	A	2002	3	-	3/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2003	FMT	O2-C	2.07	1.39	1.28

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2002	ADP	O2A-PA-O3A	2.03	112.75	107.27

There are no chirality outliers.

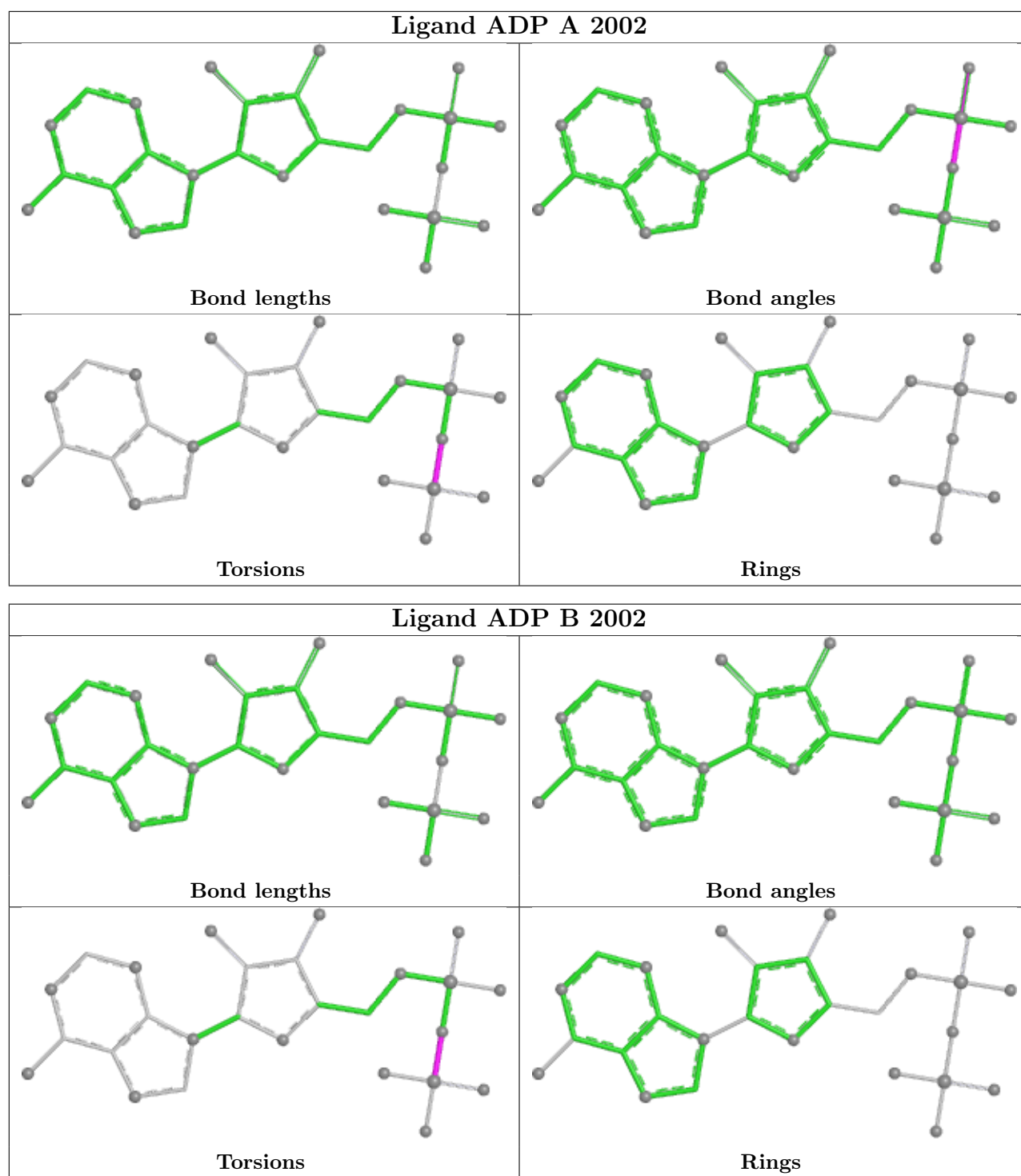
5 of 6 torsion outliers are listed below:

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 ⓘ

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 [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%)	0.18	34 (4%)	40 46	12, 42, 94, 129	4 (0%)
1	B	755/1935 (39%)	0.59	64 (8%)	16 20	15, 55, 103, 135	5 (0%)
2	D	154/199 (77%)	1.95	65 (42%)	0 0	88, 130, 159, 167	0
2	H	150/199 (75%)	2.00	61 (40%)	0 0	121, 162, 191, 198	0
All	All	1841/4268 (43%)	0.65	224 (12%)	8 10	12, 55, 160, 198	9 (0%)

The worst 5 of 224 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	65	PHE	6.2
1	B	784	ILE	5.9
1	B	731	PRO	5.3
2	D	58	PHE	5.2
1	A	735	PHE	4.9

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	0.96	0.07	35,37,40,41	0
1	MLY	B	129	11/12	0.96	0.07	41,41,47,48	0

6.3 Carbohydrates [i](#)

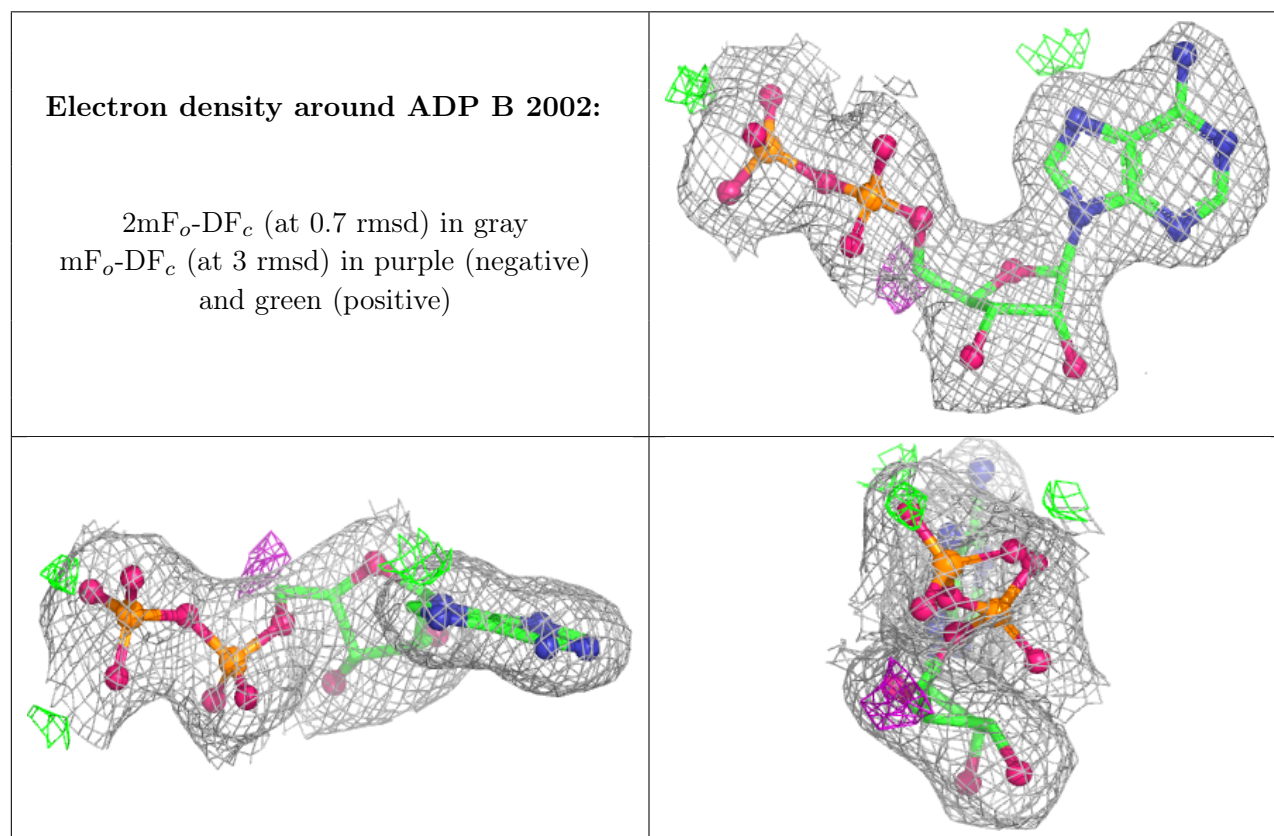
There are no oligosaccharides in this entry.

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.

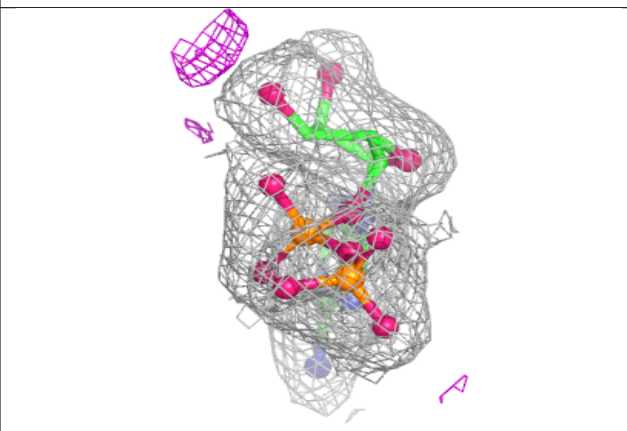
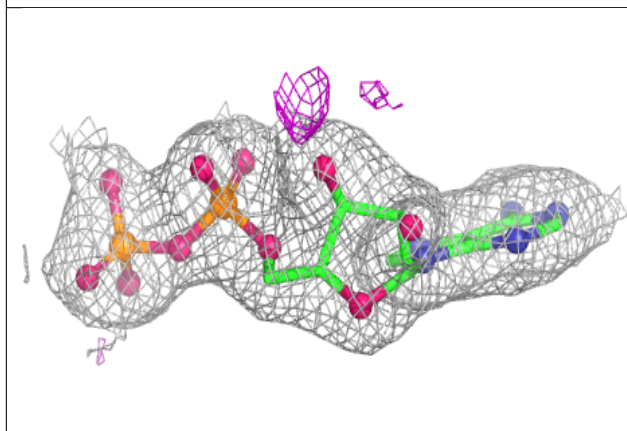
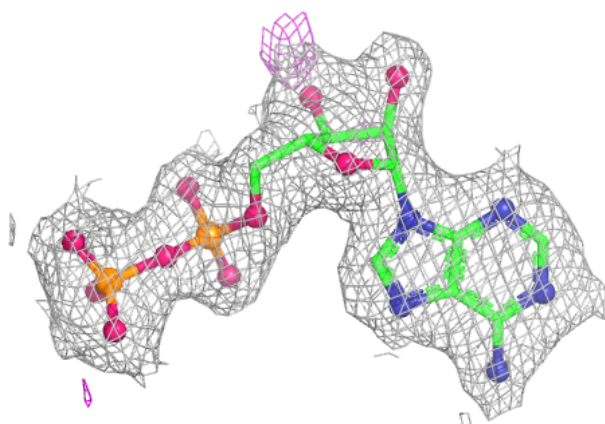
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	B	2005	3/3	0.87	0.16	58,58,59,60	0
5	FMT	B	2003	3/3	0.88	0.15	48,48,49,49	0
3	MG	B	2001	1/1	0.88	0.12	65,65,65,65	0
5	FMT	B	2004	3/3	0.89	0.15	42,42,48,52	0
6	EDO	B	2006	4/4	0.90	0.12	42,44,44,47	0
5	FMT	A	2003	3/3	0.91	0.11	36,36,43,49	0
6	EDO	A	2005	4/4	0.93	0.10	32,33,33,39	0
5	FMT	A	2004	3/3	0.94	0.15	44,44,46,46	0
4	ADP	B	2002	27/27	0.97	0.06	35,39,47,52	0
3	MG	A	2001	1/1	0.97	0.07	39,39,39,39	0
4	ADP	A	2002	27/27	0.99	0.04	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.



Electron density around ADP A 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.