

wwPDB X-ray Structure Validation Summary Report (i)

Dec 9, 2023 - 08:06 am GMT

PDB ID : 8QYQ

Title: Beta-cardiac myosin S1 fragment in the pre-powerstroke state complexed to

Mavacamten

Authors: Robert-Paganin, J.; Kikuti, C.; Auguin, D.; Rety, S.; David, A.; Houdusse, A.

Deposited on : 2023-10-26

Resolution : 2.61 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

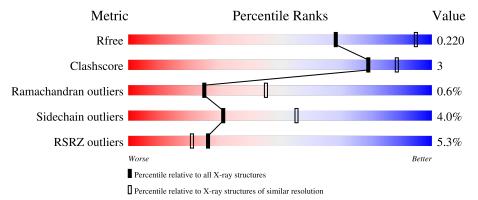
Validation Pipeline (wwPDB-VP) : 2.36

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 2.61 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length				Quality of	chain				
1	A	807	4%			87%				9%	-
1	В	807	2%			85%				10%	5%
2	С	199	4%		65%			13%	•	21%	_
3	D	199	17%	36%		7%		57%			



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14993 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					AltConf	Trace
1	A	781	Total 6323	C 4043	N 1078	O 1168	S 34	0	3	0
1	В	770	Total 6219		N 1062	O 1152	S 31	0	2	0

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

Mol	Chain	Residues		\mathbf{A}	toms			ZeroOcc	AltConf	Trace
2	С	157	Total 1240	C 781	N 205	O 244	S 10	0	0	0

• Molecule 3 is a protein called Myosin light chain 3.

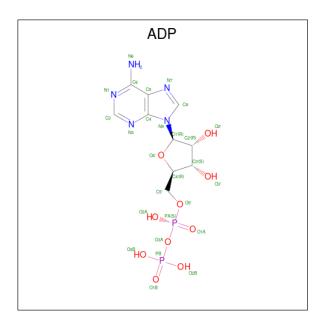
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	D	85	Total 601	C 370	N 103	O 125	S 3	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	151	VAL	THR	conflict	UNP P85100

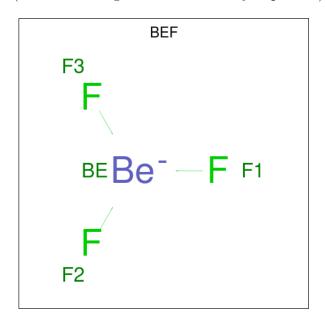
• Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf		
4	Λ	1	Total	С	N	О	Р	0	0	
4	4 A	1	27	10	5	10	2	U	0	
4	D	1	Total	С	N	О	Р	0	0	
4	Б	1	27	10	5	10	2	U	U	

• Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	At	oms		ZeroOcc	AltConf
5	A	1	Total 4	Be 1	F 3	0	0

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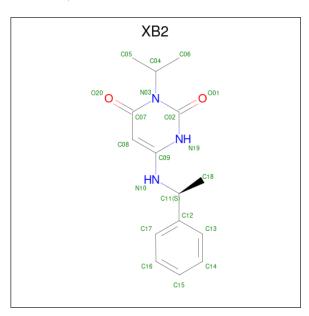
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Mol	Chain	Residues	\mathbf{At}	oms		ZeroOcc	AltConf
5	В	1	Total 4	Be 1	F 3	0	0

• Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	В	1	Total Mg 1 1	0	0

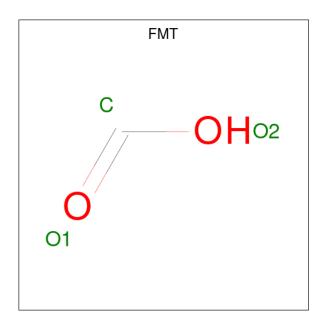
• Molecule 7 is 6-[[(1 {S})-1-phenylethyl]amino]-3-propan-2-yl-1 {H}-pyrimidine-2,4-d ione (three-letter code: XB2) (formula: $C_{15}H_{19}N_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	Δ	1	Total	С	N	О	0	0	
'	Λ	1	20	15	3	2	U		
7	D	1	Total	С	N	О	0	0	
'	Б	1	20	15	3	2	U	U	

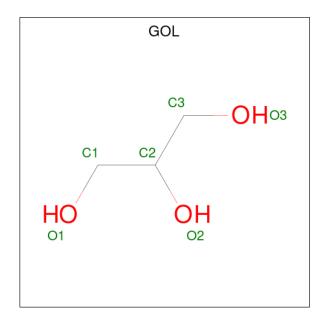
 \bullet Molecule 8 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
R	A	1	Total C O	0	0
	Λ	1	3 1 2	U	U
Q	Δ	1	Total C O	0	0
	Λ	1	3 1 2	U	U
Q	Δ	1	Total C O	0	0
	Λ	1	3 1 2	U	U
Q	В	1	Total C O	0	0
	D	1	3 1 2	U	U
R	R	1	Total C O	0	0
	ם	1	3 1 2	U	U

 \bullet Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
9	С	1	Total 6	C 3	O 3	0	0

$\bullet\,$ Molecule 10 is water.

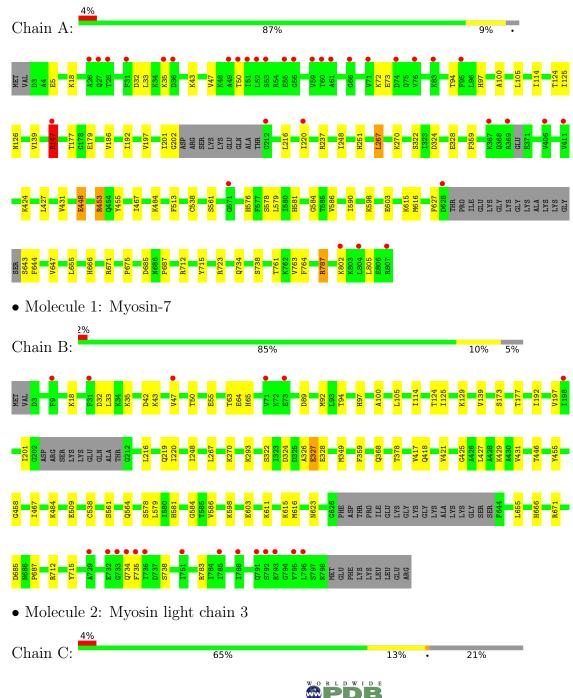
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	228	Total O 228 228	0	0
10	В	242	Total O 242 242	0	0
10	С	14	Total O 14 14	0	0
10	D	1	Total O 1 1	0	0

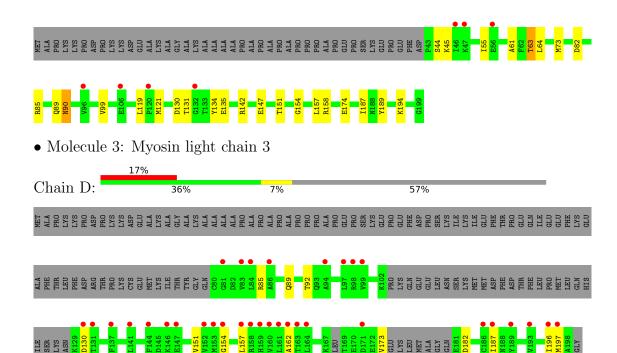


3 Residue-property plots (i)

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-7







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	102.80Å 147.98Å 116.75Å	Danagitan
a, b, c, α , β , γ	90.00° 91.62° 90.00°	Depositor
Resolution (Å)	91.64 - 2.61	Depositor
Resolution (A)	91.64 - 2.61	EDS
% Data completeness	66.0 (91.64-2.61)	Depositor
(in resolution range)	66.0 (91.64-2.61)	EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.25 (at 2.62Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
D.D.	0.178 , 0.217	Depositor
R, R_{free}	0.185 , 0.220	DCC
R_{free} test set	3478 reflections $(4.98%)$	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 73.3	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14993	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: FMT, GOL, XB2, BEF, MG, M3L, 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	0.52	0/6431	0.70	0/8662
1	В	0.51	0/6326	0.70	0/8528
2	С	0.50	0/1260	0.69	0/1690
3	D	0.44	0/605	0.67	0/813
All	All	0.51	0/14622	0.70	0/19693

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	6323	0	6298	36	0
1	В	6219	0	6190	31	0
2	С	1240	0	1226	15	0
3	D	601	0	522	4	0
4	A	27	0	12	1	0
4	В	27	0	12	0	0
5	A	4	0	0	0	0
5	В	4	0	0	0	0
6	A	1	0	0	0	0

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Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	В	1	0	0	0	0
7	A	20	0	0	0	0
7	В	20	0	0	0	0
8	A	9	0	6	1	0
8	В	6	0	4	0	0
9	С	6	0	8	0	0
10	A	228	0	0	2	0
10	В	242	0	0	0	0
10	С	14	0	0	0	0
10	D	1	0	0	0	0
All	All	14993	0	14278	81	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 3.

The worst 5 of 81 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\mathring{\mathbf{A}}) \end{aligned}$
2:C:154:GLY:HA2	2:C:187:ILE:HD12	1.71	0.72
1:A:513:PHE:H	8:A:1005:FMT:H	1.55	0.72
3:D:154:GLY:HA2	3:D:187:ILE:HD12	1.73	0.70
1:A:251:HIS:HB3	1:A:453:ARG:HG2	1.73	0.69
2:C:61:ALA:HA	2:C:64:LEU:HD12	1.79	0.62

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	774/807~(96%)	742 (96%)	28 (4%)	4 (0%)	29 50
1	В	764/807~(95%)	736 (96%)	23 (3%)	5 (1%)	22 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
2	\mathbf{C}	155/199 (78%)	148 (96%)	6 (4%)	1 (1%)	25	45
3	D	77/199 (39%)	76 (99%)	1 (1%)	0	100	100
All	All	1770/2012 (88%)	1702 (96%)	58 (3%)	10 (1%)	25	45

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ILE
1	A	267	LEU
1	В	55	GLU
1	В	267	LEU
1	A	72	LYS

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	677/695 (97%)	651 (96%)	26 (4%)	33 57
1	В	665/695~(96%)	642 (96%)	23 (4%)	36 60
2	С	136/165 (82%)	130 (96%)	6 (4%)	28 52
3	D	54/165 (33%)	48 (89%)	6 (11%)	6 10
All	All	1532/1720 (89%)	1471 (96%)	61 (4%)	31 55

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	42	ASP
3	D	92	THR
1	В	368	GLN
2	С	151	THR
3	D	196	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:



Mol	Chain	Res	Type
2	С	54	GLN
2	С	105	GLN
2	С	109	ASN
1	В	160	ASN
1	В	75	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)

4 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	Bo	Bond lengths			Bond angles		
WIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
1	M3L	A	129	1	10,11,12	0.64	0	9,14,16	0.79	0	
1	M3L	A	549	1	10,11,12	0.46	0	9,14,16	0.42	0	
1	M3L	В	549	1	10,11,12	0.43	0	9,14,16	0.44	0	
1	M3L	В	129	1	10,11,12	0.84	1 (10%)	9,14,16	0.78	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
1	M3L	A	129	1	-	0/9/10/12	-
1	M3L	A	549	1	-	1/9/10/12	-
1	M3L	В	549	1	-	1/9/10/12	-
1	M3L	В	129	1	-	0/9/10/12	-

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$	
1	В	129	M3L	CB-CA	2.20	1.56	1.53	

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	549	M3L	CA-CB-CG-CD
1	В	549	M3L	CA-CB-CG-CD

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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	Во	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BEF	В	1002	4	0,3,3	-	-	-		
7	XB2	A	1004	-	19,21,21	4.15	6 (31%)	23,29,29	2.02	6 (26%)
8	FMT	A	1005	-	2,2,2	1.32	0	1,1,1	1.06	0
8	FMT	В	1004	-	2,2,2	1.24	0	1,1,1	1.03	0
5	BEF	A	1002	4	0,3,3	-	-	-		
4	ADP	В	1001	6,5	24,29,29	0.84	1 (4%)	29,45,45	0.70	0
8	FMT	A	1006	-	2,2,2	1.44	1 (50%)	1,1,1	1.09	0
8	FMT	A	1007	-	2,2,2	1.48	1 (50%)	1,1,1	0.79	0
7	XB2	В	1003	-	19,21,21	4.12	6 (31%)	23,29,29	2.08	7 (30%)



Mol	Type	Chain	Res	Link	Bond lengths			В	ond ang	les
IVIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	С	201	-	5,5,5	0.13	0	5, 5, 5	0.33	0
8	FMT	В	1005	-	2,2,2	1.43	0	1,1,1	1.02	0
4	ADP	A	1001	6,5	24,29,29	0.63	0	29,45,45	0.85	2 (6%)

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
7	XB2	A	1004	-	-	0/10/12/12	0/2/2/2
4	ADP	В	1001	6,5	-	2/12/32/32	0/3/3/3
7	XB2	В	1003	-	-	0/10/12/12	0/2/2/2
9	GOL	С	201	-	-	1/4/4/4	-
4	ADP	A	1001	6,5	-	2/12/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\mathring{\mathrm{A}})$	Ideal(Å)
7	В	1003	XB2	O01-C02	14.01	1.48	1.23
7	A	1004	XB2	O01-C02	13.60	1.47	1.23
7	A	1004	XB2	O20-C07	7.67	1.40	1.23
7	В	1003	XB2	O20-C07	7.30	1.39	1.23
7	A	1004	XB2	C02-N03	-5.78	1.32	1.39

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
7	A	1004	XB2	C07-C08-C09	-5.27	116.62	121.47
7	В	1003	XB2	N19-C02-N03	4.88	121.22	115.54
7	В	1003	XB2	C07-C08-C09	-4.78	117.07	121.47
7	A	1004	XB2	N19-C02-N03	4.69	120.99	115.54
7	В	1003	XB2	C08-C07-N03	3.24	120.92	115.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	ADP	PA-O3A-PB-O3B
4	В	1001	ADP	PA-O3A-PB-O3B
4	A	1001	ADP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
9	С	201	GOL	C1-C2-C3-O3
4	В	1001	ADP	PA-O3A-PB-O1B

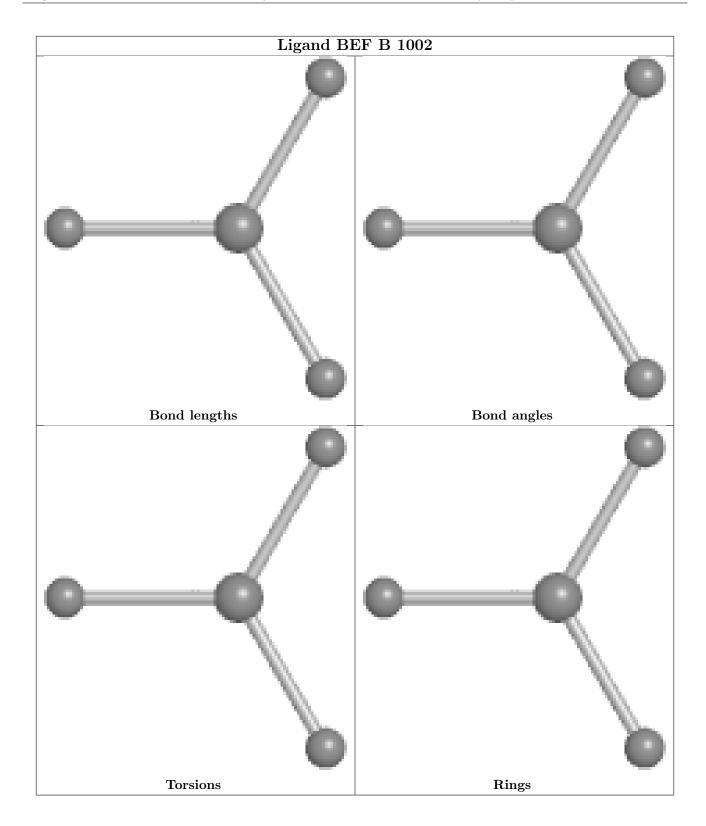
There are no ring outliers.

2 monomers are involved in 2 short contacts:

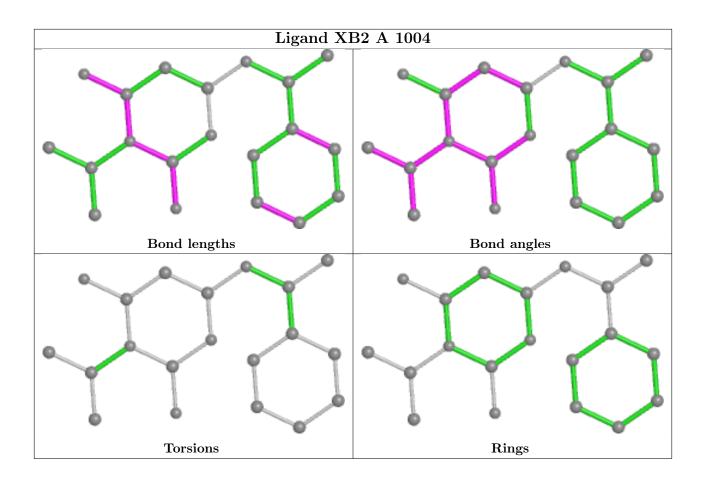
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1005	FMT	1	0
4	A	1001	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

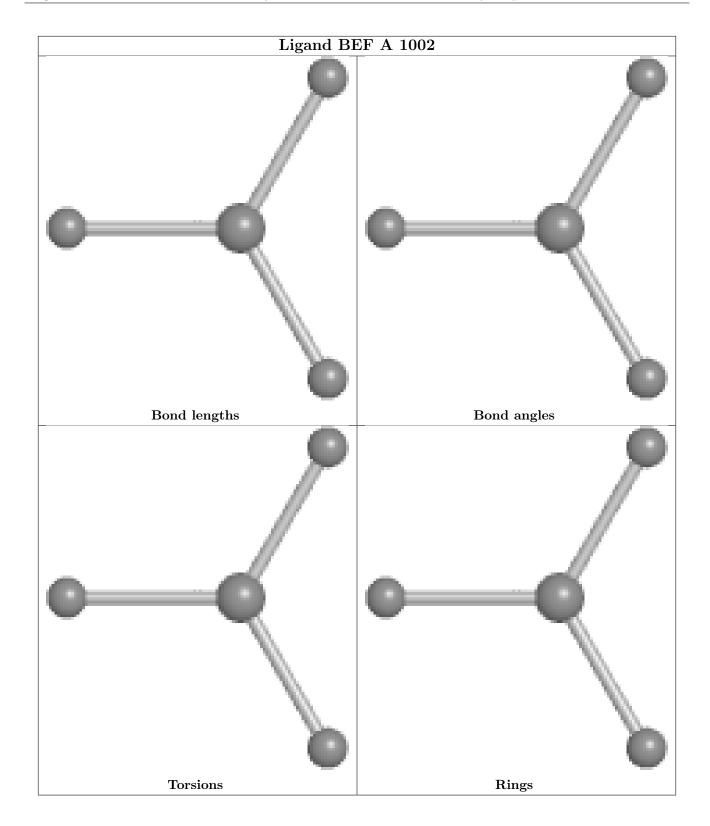




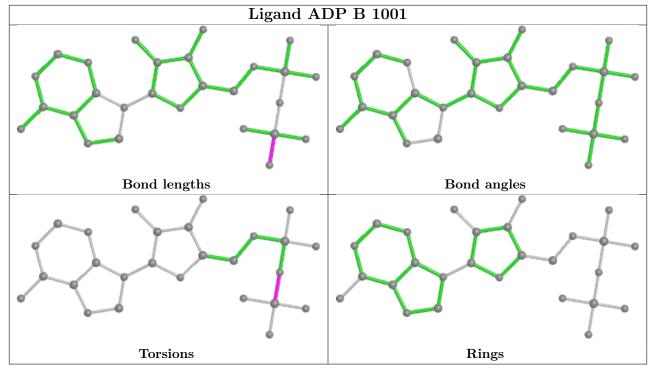


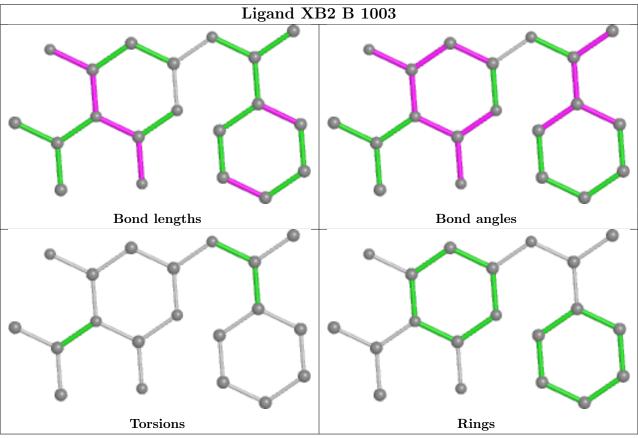






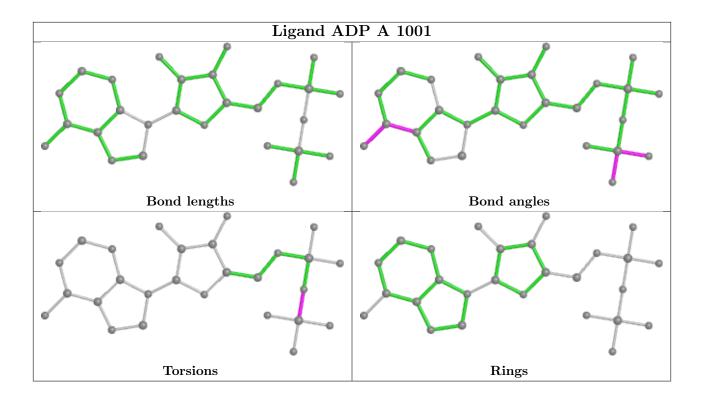








8QYQ



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, 95^{th} 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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	779/807~(96%)	0.43	34 (4%) 34 28	24, 51, 117, 163	0
1	В	768/807~(95%)	0.40	20 (2%) 56 50	20, 49, 108, 200	0
2	С	157/199~(78%)	0.43	7 (4%) 33 27	42, 79, 127, 163	0
3	D	85/199 (42%)	1.82	33 (38%) 0 0	101, 149, 178, 196	0
All	All	1789/2012 (88%)	0.49	94 (5%) 26 21	20, 54, 138, 200	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	628	ASP	7.1
3	D	171	ASP	6.1
3	D	160	VAL	6.0
2	С	46	ILE	5.9
1	В	733	GLY	5.5

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	M3L	В	549	12/13	0.97	0.21	50,56,61,63	0
1	M3L	A	549	12/13	0.98	0.17	53,58,65,65	0
1	M3L	В	129	12/13	0.98	0.21	47,50,54,58	0
1	M3L	A	129	12/13	0.98	0.24	47,50,53,54	0



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

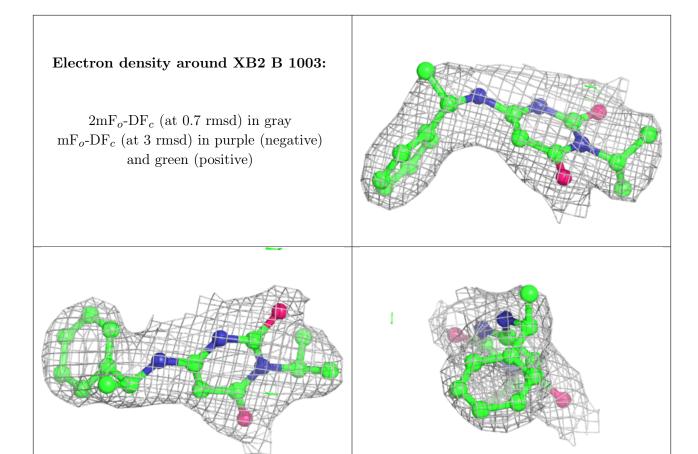
6.4 Ligands (i)

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, 95^{th} 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.

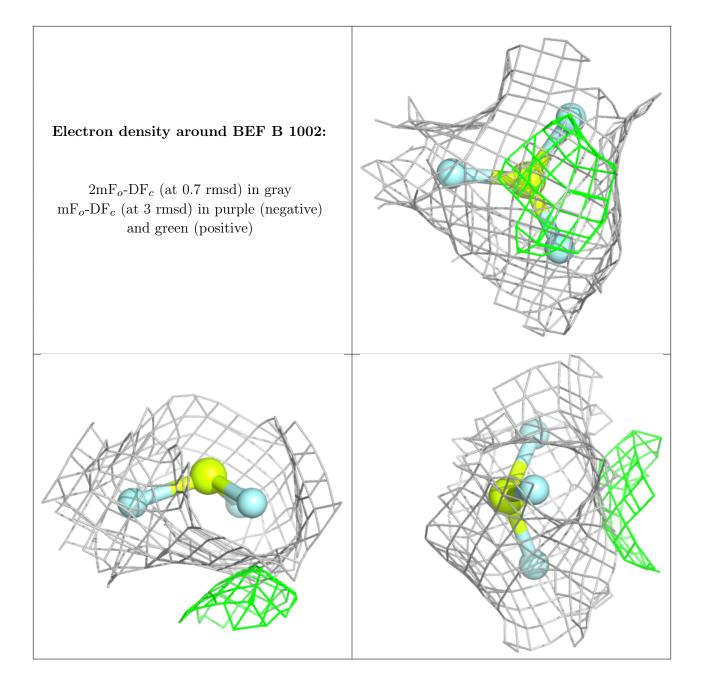
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B ext{-}factors}({f \AA}^2)$	Q < 0.9
9	GOL	С	201	6/6	0.91	0.17	70,78,80,82	0
8	FMT	A	1007	3/3	0.92	0.18	69,69,72,75	0
8	FMT	В	1005	3/3	0.95	0.19	60,60,60,61	0
8	FMT	A	1006	3/3	0.96	0.23	50,50,52,54	0
8	FMT	В	1004	3/3	0.97	0.19	51,51,53,55	0
7	XB2	В	1003	20/20	0.98	0.28	33,42,49,51	0
5	BEF	В	1002	4/4	0.98	0.12	34,37,38,41	0
8	FMT	A	1005	3/3	0.99	0.20	42,42,43,43	0
5	BEF	A	1002	4/4	0.99	0.15	31,32,34,38	0
4	ADP	A	1001	27/27	0.99	0.18	35,41,45,52	0
6	MG	В	1006	1/1	0.99	0.12	35,35,35,35	0
7	XB2	A	1004	20/20	0.99	0.23	20,29,44,45	0
4	ADP	В	1001	27/27	0.99	0.20	35,40,45,48	0
6	MG	A	1003	1/1	1.00	0.17	27,27,27,27	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.

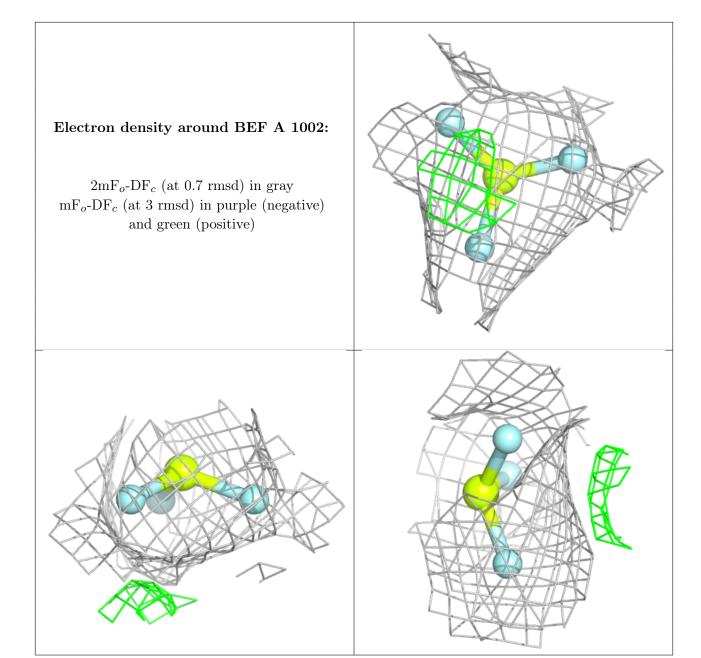




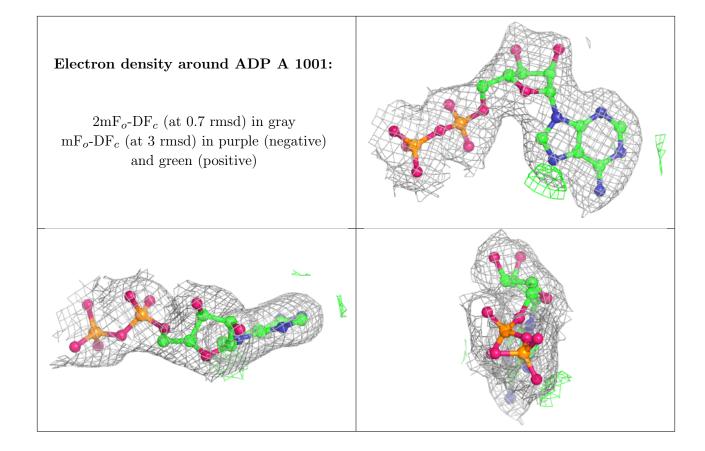




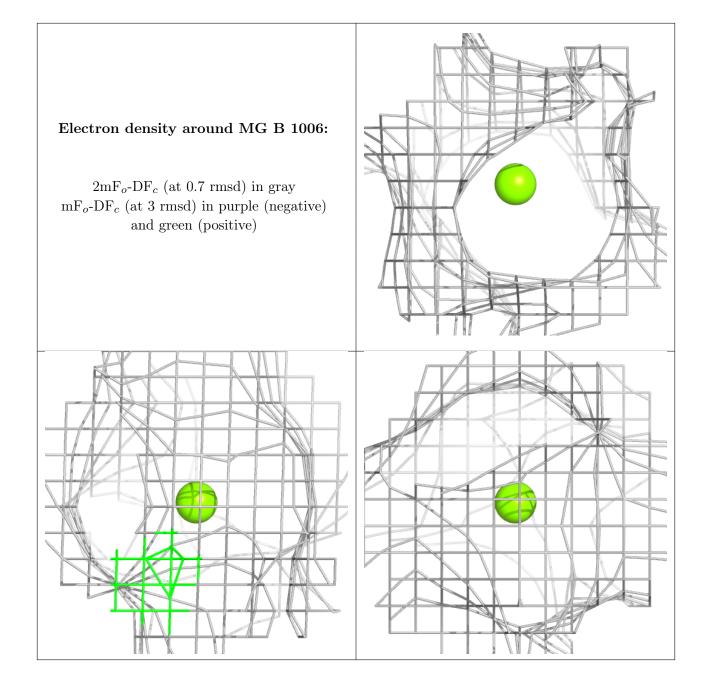








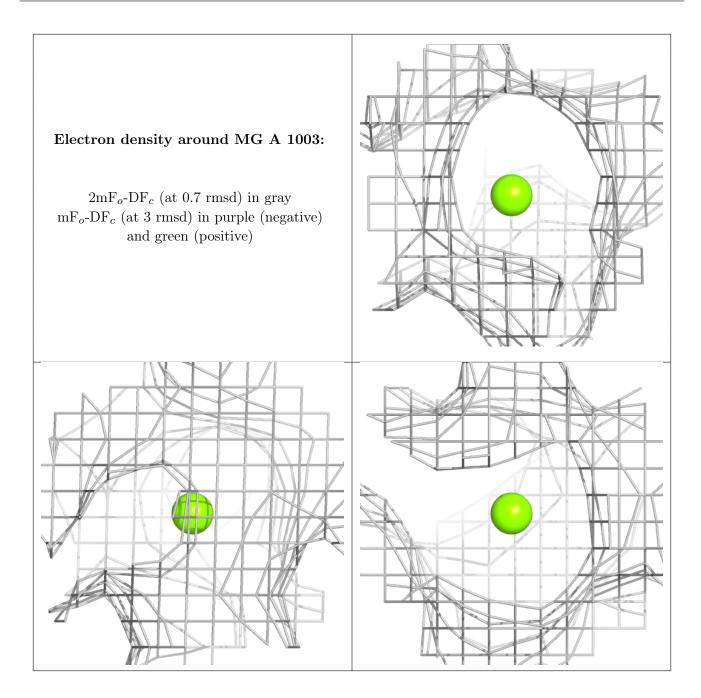






Electron density around XB2 A 1004: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive) Electron density around ADP B 1001: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.

