

wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2023 - 06:04 PM EDT

PDB ID	:	8ENK
Title	:	Crystal structure of UAP56 in complex with Tho1, the yeast homolog of human
		SARNP
Authors	:	Xie, Y.; Ren, Y.
Deposited on		
Resolution	:	2.50 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:

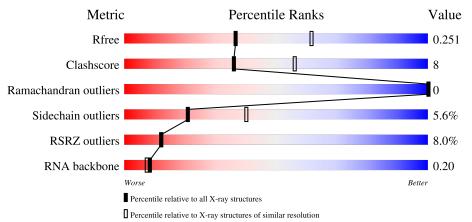
MolProbity	:	4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		
EDS	:	2.35
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range}({\rm \AA})) \end{array}$				
R _{free}	130704	4661 (2.50-2.50)				
Clashscore	141614	5346 (2.50-2.50)				
Ramachandran outliers	138981	5231 (2.50-2.50)				
Sidechain outliers	138945	5233 (2.50-2.50)				
RSRZ outliers	127900	4559 (2.50-2.50)				
RNA backbone	3102	1008 (2.84-2.16)				

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	y of chain			
1	А	390	6%		76%			19%	
1	В	390	9%		69%		2	27%	•••
2	Е	61	10%		67%		18%	·	13%
3	М	15	7% 7%	20%	13%	60'			



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Mol	Chain	Length				Quality of chain
3	N	15	13%	13%	7%	67%



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6879 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	379	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	519	3069	1956	533	558	22	0	0	
1	р	381	Total	С	Ν	0	S	0	0	0
	D	301	3081	1962	535	562	22	0	0	0

• Molecule 1 is a protein called Spliceosome RNA helicase DDX39B.

Chain	Residue	Modelled	Actual	Comment	Reference
А	39	GLY	-	expression tag	UNP Q13838
А	40	ALA	-	expression tag	UNP Q13838
А	41	MET	-	expression tag	UNP Q13838
А	42	GLY	-	expression tag	UNP Q13838
А	43	SER	-	expression tag	UNP Q13838
В	39	GLY	-	expression tag	UNP Q13838
В	40	ALA	-	expression tag	UNP Q13838
В	41	MET	-	expression tag	UNP Q13838
В	42	GLY	-	expression tag	UNP Q13838
В	43	SER	-	expression tag	UNP Q13838

There are 10 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called Protein THO1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Ε	53	Total 428	C 266	N 79	0 83	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	118	GLY	-	expression tag	UNP P40040
E	119	ALA	-	expression tag	UNP P40040
Е	120	MET	-	expression tag	UNP P40040
Е	121	GLY	-	expression tag	UNP P40040



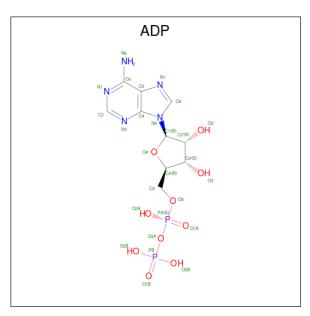
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Chain	Residue	Modelled	Actual	Comment	Reference	
E	122	SER	-	expression tag	UNP P40040	

• Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	М	6	Total	С	Ν	0	Р	Ο	0	0	
0	5 M	0	120	54	12	48	6	0	0		
3	Ν	5	Total	С	Ν	Ο	Р	0	0	0	
5	IN	5	100	45	10	40	5		U	0	

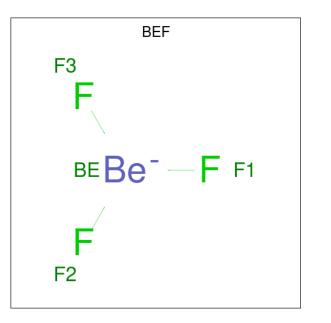
• Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	Δ	1	Total	С	Ν	Ο	Р	0	0	
4	4 A	1	27	10	5	10	2	0	0	
4	D	1	Total	С	Ν	0	Р	0	0	
4	D		27	10	5	10	2	0		

• Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Be F 4 1 3	0	0
5	В	1	Total Be F 4 1 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	А	1	Total Mg 1 1	0	0
6	В	1	Total Mg 1 1	0	0

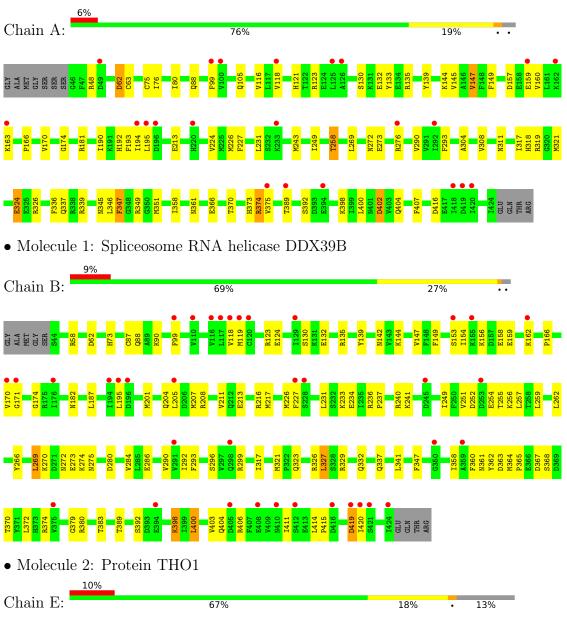
• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	8	Total O 8 8	0	0
7	В	9	Total O 9 9	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: Spliceosome RNA helicase DDX39B



CLY ALA ALA ALA CLY CLY CL3 E124 E124 E124 E123 E124 H136	K142 K142 0145 0147	A148 D149 D151 D151 E161 L167	L171 L175 GLY VAL	
• Molecule 3: RNA	ł			
Chain M: 7%	20%	13%	60%	
<mark>. 28 2 8 8</mark> 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9	n			
• Molecule 3: RNA	ł			
Chain N: 13%	13%	7%	67%	
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	,			



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	88.53Å 96.79Å 126.18Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 - 2.50	Depositor
Resolution (A)	29.72 - 2.50	EDS
% Data completeness	99.8 (29.72-2.50)	Depositor
(in resolution range)	99.8 (29.72-2.50)	EDS
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.44 (at 2.51\AA)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
D D.	0.224 , 0.253	Depositor
R, R_{free}	0.223 , 0.251	DCC
R_{free} test set	1993 reflections (5.23%)	wwPDB-VP
Wilson B-factor $(Å^2)$	57.2	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 41.8	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6879	wwPDB-VP
Average B, all atoms $(Å^2)$	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: ADP, BEF, MG

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).

Mal	Mol Chain		lengths	Bond angles	
			# Z > 5	RMSZ	# Z > 5
1	А	0.27	0/3124	0.52	0/4205
1	В	0.27	0/3136	0.52	0/4221
2	Е	0.24	0/430	0.45	0/572
3	М	0.28	0/131	0.98	0/200
3	Ν	0.24	0/109	0.74	0/166
All	All	0.27	0/6930	0.53	0/9364

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	А	3069	0	3113	46	0
1	В	3081	0	3123	63	0
2	Е	428	0	440	2	0
3	М	120	0	61	4	0
3	N	100	0	51	2	0
4	А	27	0	12	0	0
4	В	27	0	12	0	0
5	А	4	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	В	4	0	0	0	0
6	А	1	0	0	0	0
6	В	1	0	0	0	0
7	А	8	0	0	0	0
7	В	9	0	0	0	0
All	All	6879	0	6812	110	0

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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 8.

The worst 5 of 110 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:63:CYS:HB2	1:A:135:ARG:HH21	1.49	0.77
1:A:345:ASN:ND2	1:A:366:GLU:OE2	2.24	0.70
1:B:174:GLY:HA3	3:N:5:U:H5"	1.75	0.69
1:A:132:GLU:OE2	1:A:135:ARG:NH1	2.29	0.66
1:A:174:GLY:HA3	3:M:5:U:H5"	1.79	0.65

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	Perce	ntiles
1	А	377/390~(97%)	372~(99%)	5 (1%)	0	100	100
1	В	379/390~(97%)	371 (98%)	8 (2%)	0	100	100
2	Е	51/61~(84%)	49 (96%)	2(4%)	0	100	100
All	All	807/841~(96%)	792 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	342/350~(98%)	327~(96%)	15~(4%)	28 52
1	В	344/350~(98%)	328~(95%)	16 (5%)	26 49
2	Е	46/50~(92%)	36~(78%)	10 (22%)	1 1
All	All	732/750~(98%)	691 (94%)	41 (6%)	21 40

5 of 41 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	400	LEU
2	Е	145	GLN
1	В	404	GLN
2	Е	124	GLU
2	Е	147	GLN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
1	В	88	GLN
1	В	121	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	М	5/15~(33%)	3~(60%)	0
3	N	4/15~(26%)	2(50%)	0
All	All	9/30~(30%)	5~(55%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	М	4	U



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Mol	Chain	Res	Type
3	М	5	U
3	М	6	U
3	Ν	5	U
3	Ν	6	U

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	Tune	Chain	Chain Res	Res Link	Bo	Bond lengths			Bond angles		
IVIOI	Type	Unam			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	ADP	А	1000	6,5	24,29,29	0.95	1 (4%)	$29,\!45,\!45$	1.34	3 (10%)	
5	BEF	В	1001	4	0,3,3	-	-	-			
5	BEF	А	1001	4	0,3,3	-	-	-			
4	ADP	В	1000	6,5	$24,\!29,\!29$	0.94	1 (4%)	$29,\!45,\!45$	1.36	4 (13%)	

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	А	1000	6,5	-	2/12/32/32	0/3/3/3
4	ADP	В	1000	6,5	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	В	1000	ADP	C5-C4	2.40	1.47	1.40
4	А	1000	ADP	C5-C4	2.33	1.47	1.40

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	В	1000	ADP	N3-C2-N1	-3.51	123.20	128.68
4	А	1000	ADP	N3-C2-N1	-3.28	123.55	128.68
4	В	1000	ADP	C4-C5-N7	-2.94	106.34	109.40
4	А	1000	ADP	C4-C5-N7	-2.81	106.47	109.40
4	А	1000	ADP	PA-O3A-PB	-2.79	123.27	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

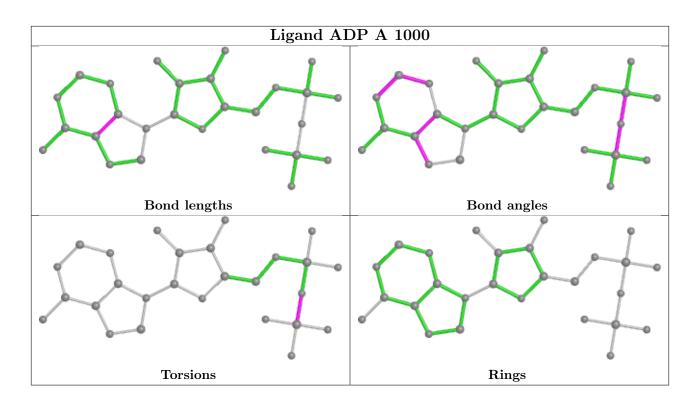
Mol	Chain	Res	Type	Atoms
4	А	1000	ADP	PA-O3A-PB-O2B
4	В	1000	ADP	PA-O3A-PB-O1B
4	А	1000	ADP	PA-O3A-PB-O3B
4	В	1000	ADP	PA-O3A-PB-O3B

There are no ring outliers.

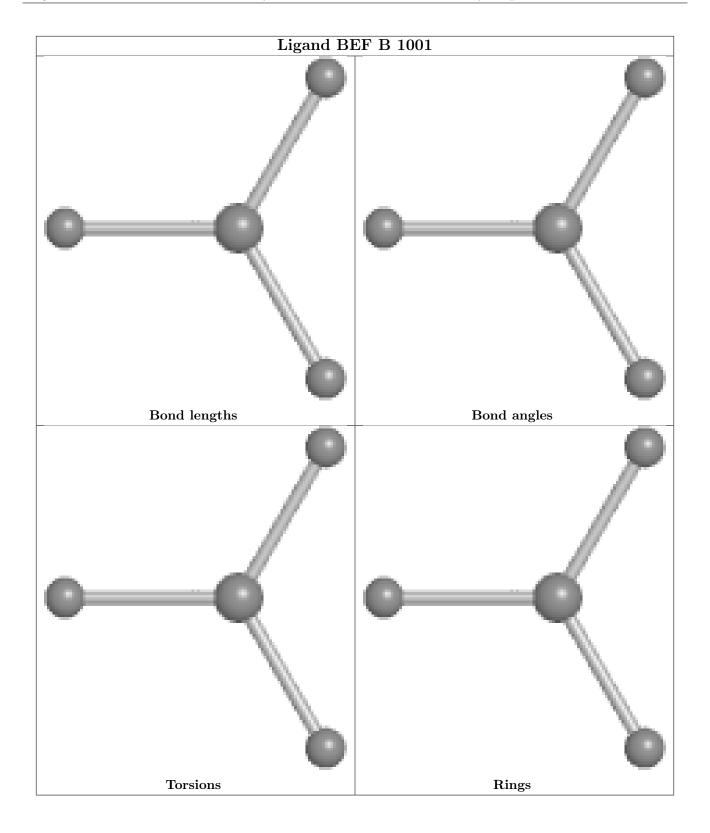
No monomer is involved in short contacts.

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 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 sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

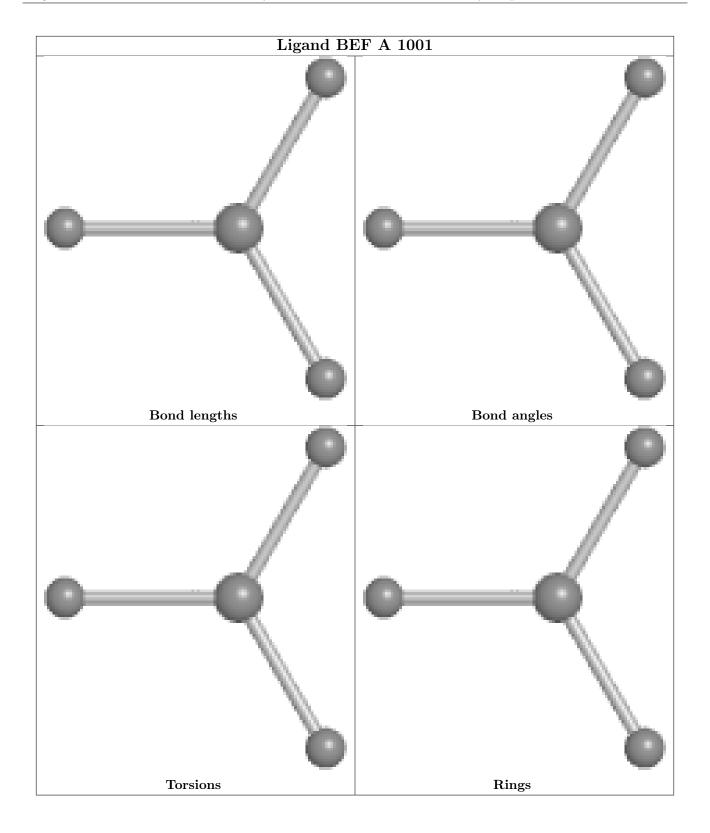




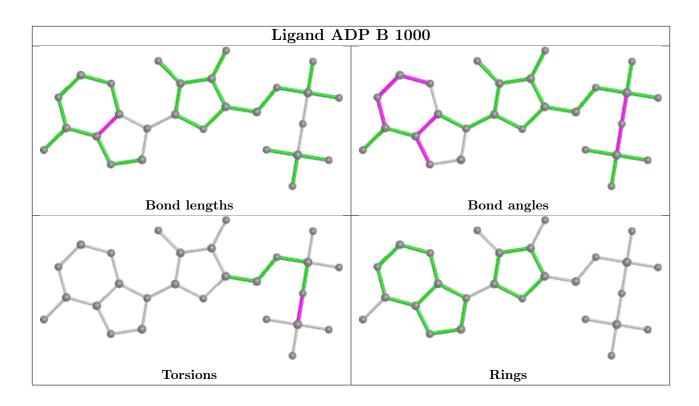












5.7 Other polymers (i)

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, 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	379/390~(97%)	0.29	22 (5%) 23 24	43, 64, 95, 128	0
1	В	381/390~(97%)	0.45	37 (9%) 7 7	46, 71, 105, 130	0
2	Ε	53/61~(86%)	0.64	6 (11%) 5 4	68, 81, 103, 110	0
3	М	6/15~(40%)	0.06	1 (16%) 1 1	56, 63, 77, 109	0
3	Ν	5/15~(33%)	-0.11	0 100 100	77, 78, 86, 99	0
All	All	824/871~(94%)	0.38	66 (8%) 12 12	43, 69, 100, 130	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	118	VAL	4.6
1	В	410	ASN	4.2
1	В	205	LEU	4.0
1	В	194	ILE	3.7
1	А	420	ILE	3.7

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 monosaccharides in this entry.

6.4 Ligands (i)

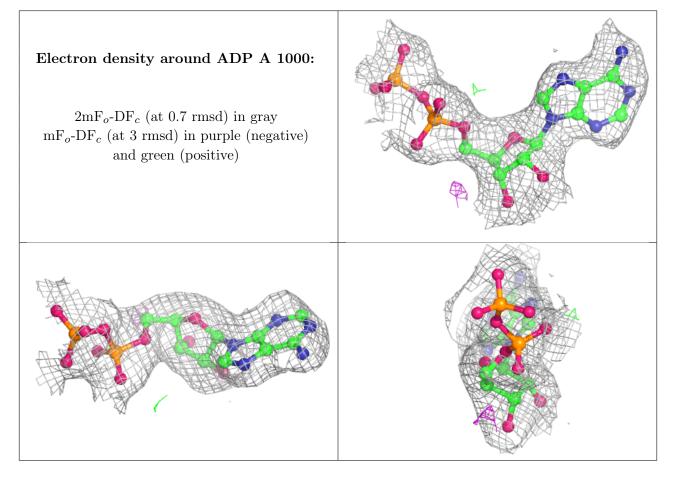
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



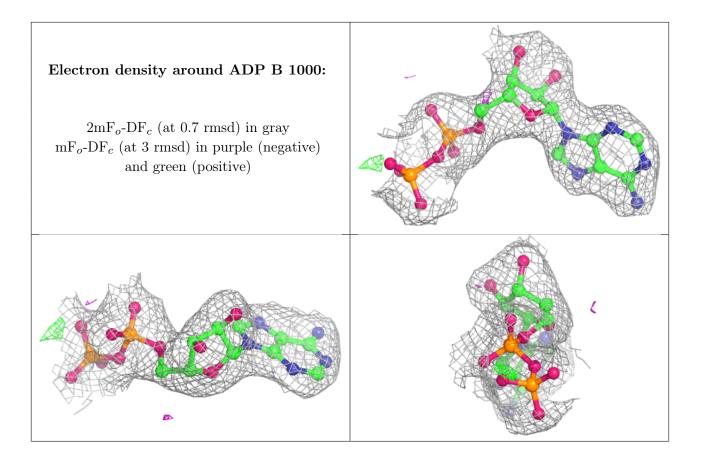
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	$\mathbf{Q} \!\!<\!\! 0.9$
4	ADP	А	1000	27/27	0.93	0.15	47,55,66,68	0
4	ADP	В	1000	27/27	0.94	0.14	47,52,57,57	0
6	MG	В	1002	1/1	0.96	0.22	$54,\!54,\!54,\!54$	0
5	BEF	В	1001	4/4	0.97	0.28	$51,\!53,\!53,\!54$	0
6	MG	А	1002	1/1	0.97	0.20	50,50,50,50	0
5	BEF	А	1001	4/4	0.97	0.22	49,49,50,51	0

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.

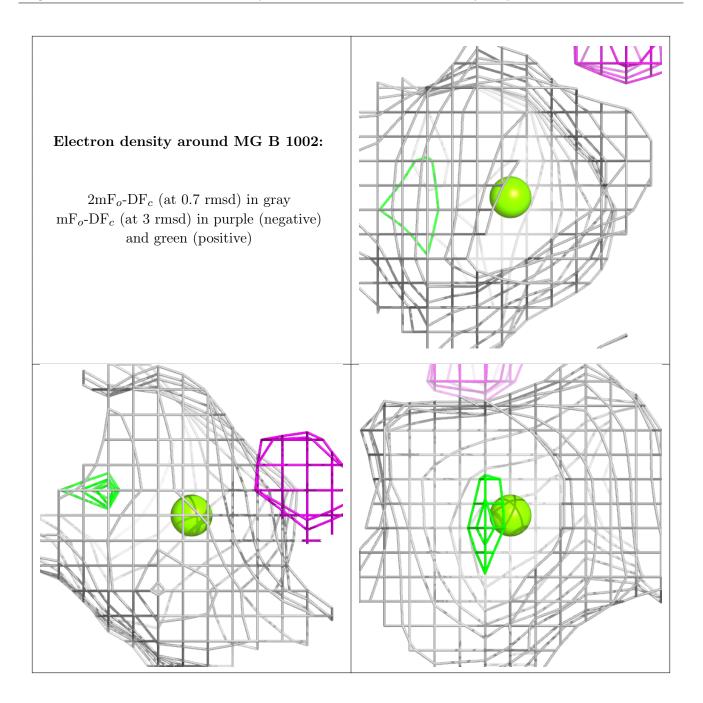
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



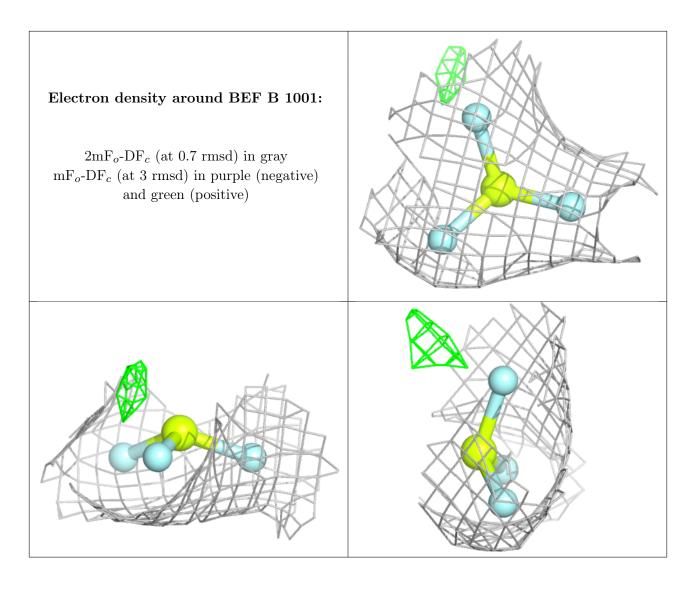




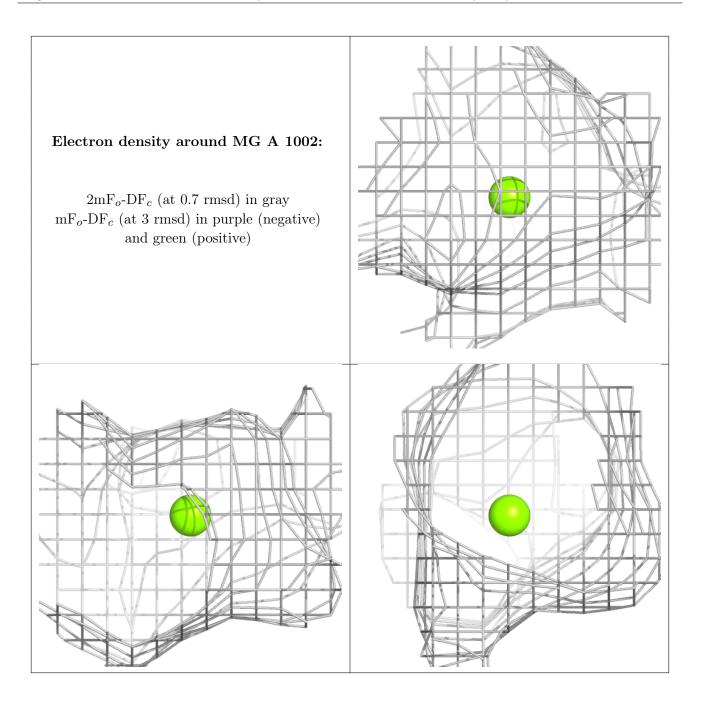




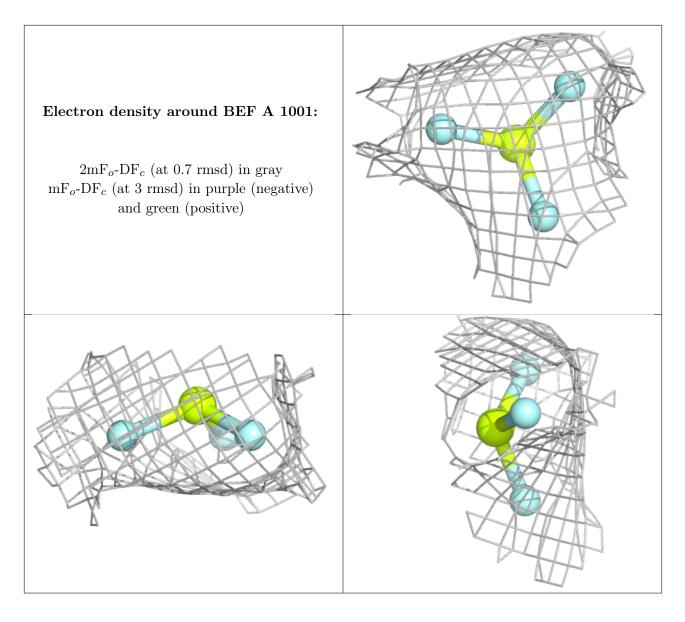












6.5 Other polymers (i)

There are no such residues in this entry.

