

# wwPDB X-ray Structure Validation Summary Report (i)

### Mar 3, 2024 – 01:43 AM EST

PDB ID : 6B6G

Title : Crystal Structure of GABA Aminotransferase bound to (S)-3-Amino-4-(diflu

oromethylenyl)cyclopent-1-ene-1-carboxylic acid, an Potent Inactivatorfor the

Treatment of Addiction

Authors: Mascarenhas, R.; Juncosa, J.I.; Takaya, K.; Le, L.V.; Moschitto, M.J.; Silver-

man, R.B.; Liu, D.

Deposited on : 2017-10-02

Resolution : 1.95 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

Mogul : 1.8.5 (274361), 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

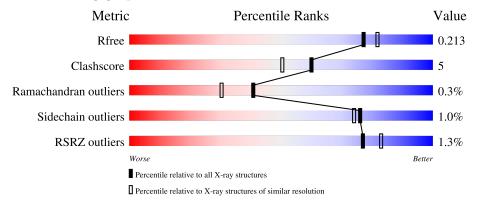


# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	462	93%	6% •		
1	В	462	86%	13%		
1	С	462	91%	8%		
1	D	462	90%	8% •		



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16396 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 4-aminobutyrate aminotransferase, mitochondrial.

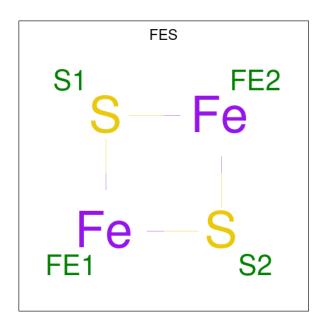
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	461	Total	С	N	О	S	0	12	0
1	A	401	3725	2379	644	677	25	0	12	0
1	В	462	Total	С	N	О	S	0	9	0
1	Б	402	3717	2368	643	681	25	U	9	0
1	C	462	Total	С	N	О	S	0	9	0
1		402	3719	2372	643	679	25	0	9	
1	D	462	Total	С	N	О	S	0	16	0
1	ע	402	3767	2404	654	683	26		10	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	GLU	GLN	conflict	UNP P80147
A	472	ALA	LYS	conflict	UNP P80147
В	158	GLU	GLN	conflict	UNP P80147
В	472	ALA	LYS	conflict	UNP P80147
С	158	GLU	GLN	conflict	UNP P80147
С	472	ALA	LYS	conflict	UNP P80147
D	158	GLU	GLN	conflict	UNP P80147
D	472	ALA	LYS	conflict	UNP P80147

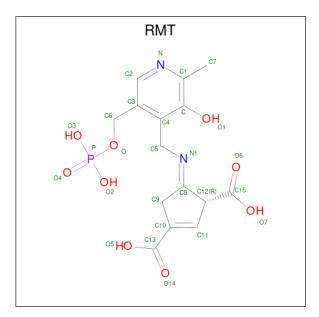
• Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 4 2 2	0	0
2	С	1	Total Fe S 4 2 2	0	0

• Molecule 3 is (3R,4E)-4-[({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyl)imino]cyclopent-1-ene-1,3-dicarboxylic acid (three-letter code: RMT) (formula:  $C_{15}H_{17}N_2O_9P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
9	Λ	1	Total	С	N	О	Р	0	0
)	A	1	27	15	2	9	1	U	0

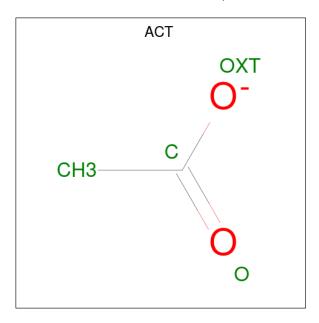
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	D	1	Total	С	N	О	Р	0	0
)	Б	1	15	8	1	5	1	U	0
2	С	1	Total	С	N	О	Р	0	0
)		1	27	15	2	9	1	U	0
2	D	1	Total	С	N	О	Р	0	0
)	D	1	27	15	2	9	1	U	

 $\bullet$  Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $\mathrm{C_2H_3O_2}).$ 



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	С	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

 $\bullet$  Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $\mathrm{C_3H_8O_3}).$ 





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

# • Molecule 6 is water.

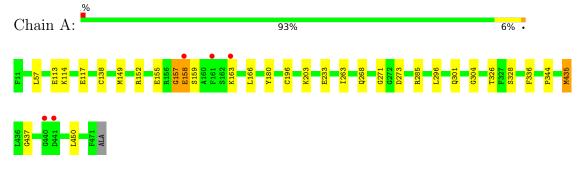
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	307	Total O 307 307	0	0
6	В	249	Total O 249 249	0	0
6	C	367	Total O 367 367	0	0
6	D	413	Total O 413 413	0	0



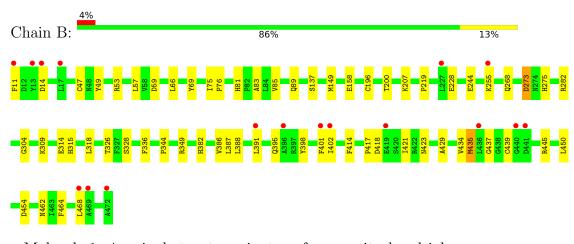
# 3 Residue-property plots (i)

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.

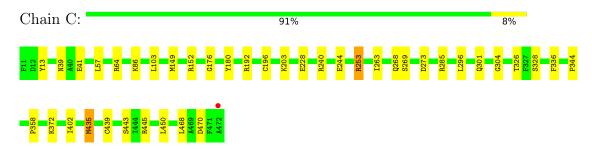
• Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial



• Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial

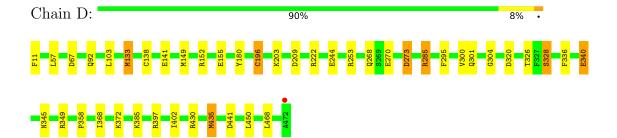


• Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial



• Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	69.63Å 228.02Å 70.82Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $109.14^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	45.71 - 1.95	Depositor
resolution (A)	66.90 - 1.95	EDS
% Data completeness	98.3 (45.71-1.95)	Depositor
(in resolution range)	98.3 (66.90-1.95)	EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.02  (at  1.95Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
$R, R_{free}$	0.168 , $0.213$	Depositor
it, it free	0.171 , $0.213$	DCC
$R_{free}$ test set	7313 reflections $(4.92%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.37, 54.6	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16396	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: FES, RMT, ACT, GOL

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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	0.39	1/3844~(0.0%)	0.55	1/5186 (0.0%)	
1	В	0.37	$1/3812 \ (0.0\%)$	0.53	0/5150	
1	С	0.44	1/3814 (0.0%)	0.58	1/5151 (0.0%)	
1	D	0.47	$1/3882 \ (0.0\%)$	0.61	1/5237 (0.0%)	
All	All	0.42	$4/15352 \ (0.0\%)$	0.57	3/20724 (0.0%)	

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
1	D	196	CYS	CB-SG	-6.48	1.71	1.82
1	С	196	CYS	CB-SG	-6.05	1.72	1.82
1	В	196	CYS	CB-SG	-5.66	1.72	1.81
1	A	196	CYS	CB-SG	-5.62	1.72	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	D	133	MET	CG-SD-CE	6.64	110.83	100.20
1	A	157	GLY	C-N-CA	6.04	136.79	121.70
1	С	192	ARG	NE-CZ-NH1	-5.44	117.58	120.30

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



. 1	, .	• 1	1 (	$\alpha$	$\alpha_1$ 1	1. /		1 , 1	1 1
the ass	zmmetric	11n1t	whereas S	Symm-	Liashes	LISTS ST	vmmetry	v-related	clashes
UIIC COD	y IIIIII OUI IO	aiii o,	WITCICOD	$\cup$ y IIIIII	CIUDIICO	110000	y IIIIIIC UI	y iciauca	CIGOTICO.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3725	0	3710	22	0
1	В	3717	0	3643	46	0
1	С	3719	0	3659	23	1
1	D	3767	0	3722	41	1
2	A	4	0	0	1	0
2	С	4	0	0	0	0
3	A	27	0	0	2	0
3	В	15	0	0	1	0
3	С	27	0	0	2	0
3	D	27	0	0	2	0
4	A	8	0	6	1	0
4	С	4	0	3	0	0
4	D	4	0	3	0	0
5	В	6	0	8	2	0
5	С	6	0	8	0	0
6	A	307	0	0	5	0
6	В	249	0	0	10	0
6	С	367	0	0	9	0
6	D	413	0	0	13	0
All	All	16396	0	14762	137	1

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 5.

The worst 5 of 137 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:157:GLY:HA3	1:A:158:GLU:HG3	1.21	1.19
1:C:152:ARG:NH1	6:C:601:HOH:O	1.97	0.96
1:B:387:LEU:HD13	1:B:391:LEU:HD21	1.48	0.95
1:D:285[B]:ARG:NH1	1:D:320:ASP:O	2.04	0.91
1:D:152:ARG:NH1	6:D:602:HOH:O	2.04	0.90

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance}  ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap} & ( ext{Å}) \end{aligned}$
1:C:470:ASP:OD2	1:D:222[A]:ARG:NH1[1_454]	2.17	0.03



# 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	A	471/462 (102%)	449 (95%)	20 (4%)	2 (0%)	34	22
1	В	$469/462 \ (102\%)$	442 (94%)	25 (5%)	2 (0%)	34	22
1	С	$469/462 \ (102\%)$	451 (96%)	17 (4%)	1 (0%)	47	38
1	D	476/462 (103%)	456 (96%)	19 (4%)	1 (0%)	47	38
All	All	1885/1848 (102%)	1798 (95%)	81 (4%)	6 (0%)	41	30

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	SER
1	D	328	SER
1	A	158	GLU
1	С	328	SER
1	В	328	SER

### 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	409/400~(102%)	406 (99%)	3 (1%)	84 82
1	В	401/400 (100%)	396 (99%)	5 (1%)	71 68
1	С	402/400 (100%)	396 (98%)	6 (2%)	65 60
1	D	408/400 (102%)	401 (98%)	7 (2%)	60 55
All	All	1620/1600 (101%)	1599 (99%)	21 (1%)	76 65



5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	92	GLN
1	D	285[B]	ARG
1	D	435[B]	MET
1	D	340	GLU
1	D	285[A]	ARG

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

Mol	Chain	Res	Type
1	В	81	HIS
1	В	275	HIS

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

# 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

12 ligands 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	ond leng	$ ag{ths}$	В	ond angles
IVIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z  > 2	Counts	$\mid RMSZ \mid \# Z  > 2$
2	FES	С	501	1	0,4,4	-	-	-	



Mal	ol Type Chain Res Link		Tinle	Вс	ond leng	ths	Bond angles			
Mol	туре	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	RMT	С	503	-	25,28,28	2.41	4 (16%)	27,41,41	1.32	4 (14%)
3	RMT	A	502	-	25,28,28	2.61	4 (16%)	27,41,41	1.23	2 (7%)
4	ACT	D	502	-	3,3,3	1.02	0	3,3,3	1.69	1 (33%)
5	GOL	С	502	-	5,5,5	0.29	0	5,5,5	0.48	0
2	FES	A	501	1	0,4,4	-	-	-		
5	GOL	В	501	-	5,5,5	0.54	0	5,5,5	0.26	0
3	RMT	В	502	-	15,15,28	3.12	3 (20%)	20,22,41	1.27	2 (10%)
4	ACT	A	504	-	3,3,3	0.76	0	3,3,3	1.12	0
4	ACT	С	504	-	3,3,3	0.77	0	3,3,3	1.59	0
4	ACT	A	503	-	3,3,3	0.74	0	3,3,3	1.22	0
3	RMT	D	501	-	25,28,28	2.71	4 (16%)	27,41,41	1.49	3 (11%)

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
2	FES	С	501	1	-	-	0/1/1/1
3	RMT	С	503	-	-	3/18/31/31	0/2/2/2
3	RMT	A	502	-	-	3/18/31/31	0/2/2/2
5	GOL	С	502	-	-	2/4/4/4	-
2	FES	A	501	1	-	-	0/1/1/1
3	RMT	В	502	-	-	0/6/6/31	0/1/1/2
5	GOL	В	501	_	-	1/4/4/4	-
3	RMT	D	501	-	-	4/18/31/31	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
3	D	501	RMT	C-C1	9.20	1.50	1.40
3	A	502	RMT	C-C1	8.53	1.49	1.40
3	В	502	RMT	C-C1	8.17	1.49	1.40
3	С	503	RMT	C-C1	8.03	1.48	1.40
3	В	502	RMT	C3-C4	7.63	1.48	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
3	D	501	RMT	C2-C3-C4	3.42	120.54	118.12

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	D	501	RMT	O7-C15-C12	3.36	122.50	114.22
3	D	501	RMT	C-C4-C3	-3.26	115.60	118.72
3	С	503	RMT	C2-N-C1	2.79	124.33	119.17
3	A	502	RMT	C2-C3-C4	2.72	120.05	118.12

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	RMT	C-C4-C5-N1
3	A	502	RMT	C3-C4-C5-N1
3	С	503	RMT	C-C4-C5-N1
3	С	503	RMT	C3-C4-C5-N1
3	D	501	RMT	C-C4-C5-N1

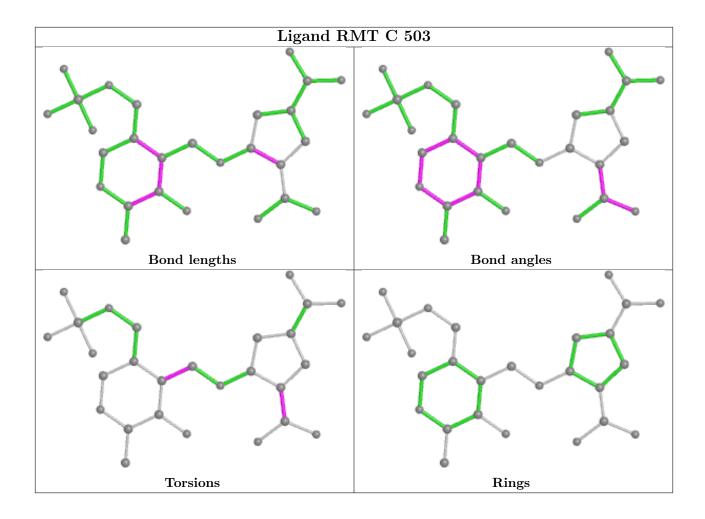
There are no ring outliers.

7 monomers are involved in 11 short contacts:

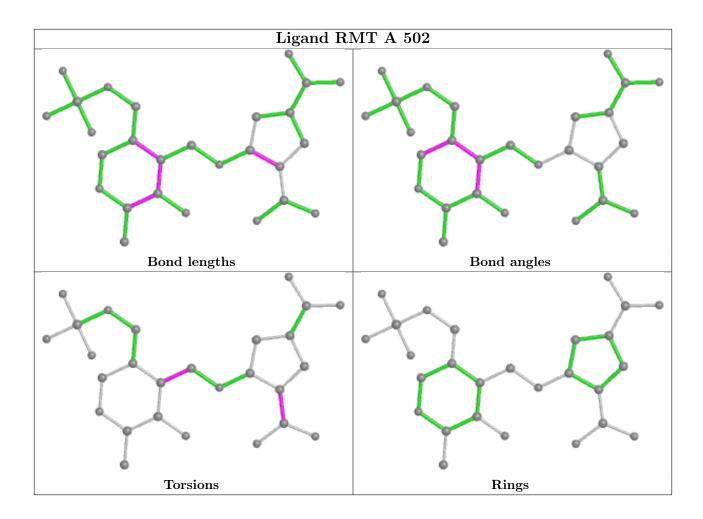
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	503	RMT	2	0
3	A	502	RMT	2	0
2	A	501	FES	1	0
5	В	501	GOL	2	0
3	В	502	RMT	1	0
4	A	504	ACT	1	0
3	D	501	RMT	2	0

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.

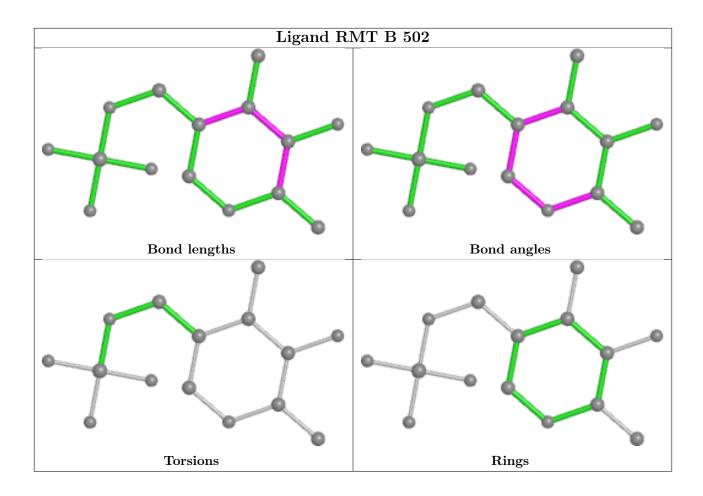




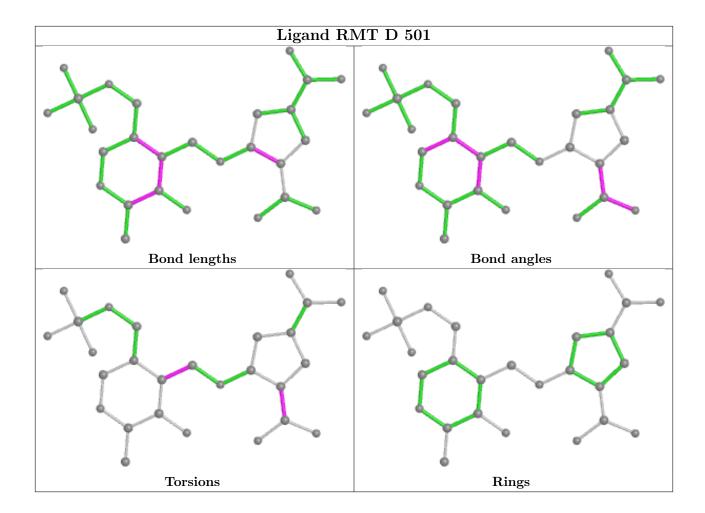












# 5.7 Other polymers (i)

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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	461/462 (99%)	-0.24	5 (1%) 80 85	18, 32, 54, 84	0
1	В	$462/462 \ (100\%)$	0.12	17 (3%) 41 51	21, 41, 70, 87	0
1	С	462/462 (100%)	-0.38	1 (0%) 95 97	14, 24, 42, 70	0
1	D	$462/462 \ (100\%)$	-0.37	1 (0%) 95 97	13, 21, 35, 65	0
All	All	1847/1848 (99%)	-0.22	24 (1%) 77 83	13, 28, 57, 87	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	472	ALA	5.7
1	В	469	ALA	5.6
1	В	440	GLY	4.6
1	В	396	ALA	4.5
1	В	17	LEU	4.1

### 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)

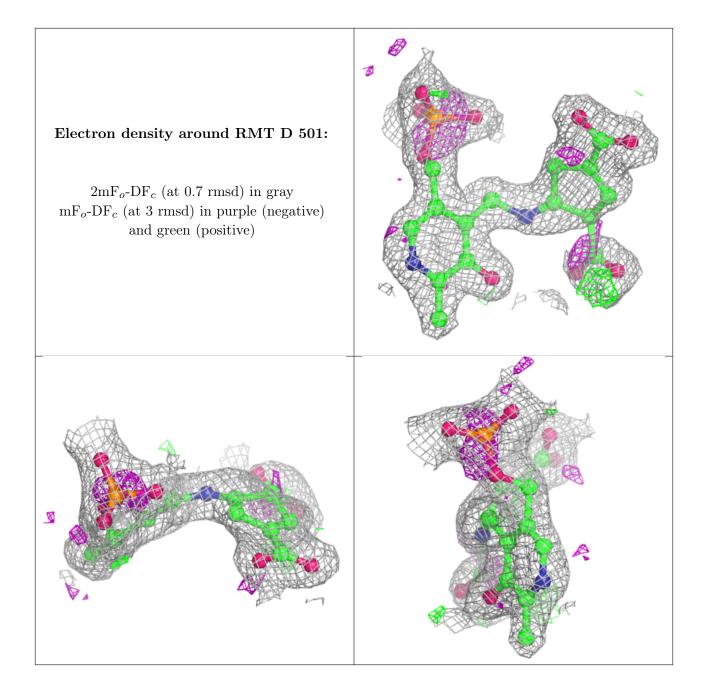
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathrm{A}}^2)$	Q < 0.9
4	ACT	D	502	4/4	0.69	0.20	26,37,47,56	0
4	ACT	A	503	4/4	0.75	0.15	27,40,43,46	0
5	GOL	В	501	6/6	0.79	0.31	38,51,57,65	0
4	ACT	С	504	4/4	0.84	0.12	27,35,49,56	0
4	ACT	A	504	4/4	0.88	0.11	39,41,52,55	0
3	RMT	D	501	27/27	0.93	0.15	23,33,53,54	0
3	RMT	В	502	15/27	0.93	0.16	23,37,42,46	15
3	RMT	С	503	27/27	0.94	0.17	23,31,57,59	0
5	GOL	С	502	6/6	0.94	0.13	32,44,46,46	0
3	RMT	A	502	27/27	0.95	0.16	25,35,53,57	0
2	FES	A	501	4/4	0.99	0.09	24,25,25,26	0
2	FES	С	501	4/4	0.99	0.10	19,19,20,23	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.

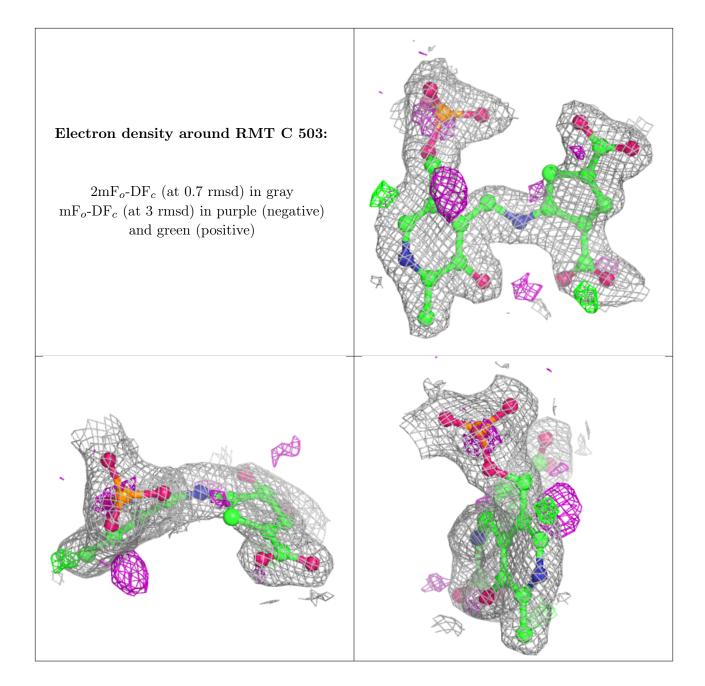




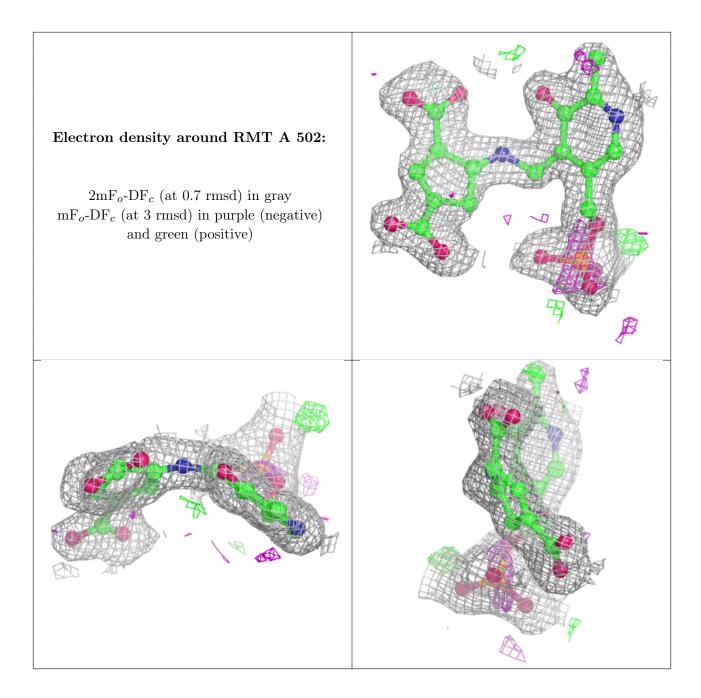


# Electron density around RMT B 502: 2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)









# 6.5 Other polymers (i)

There are no such residues in this entry.

