



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2023 – 10:22 am BST

PDB ID : 8COT  
Title : Complex of human soluble adenylyl cyclase 10 catalytic core with inhibitor TDI-10962  
Authors : Steegborn, C.; Fushimi, M.  
Deposited on : 2023-02-28  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.32.2  
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) : 2.32.2

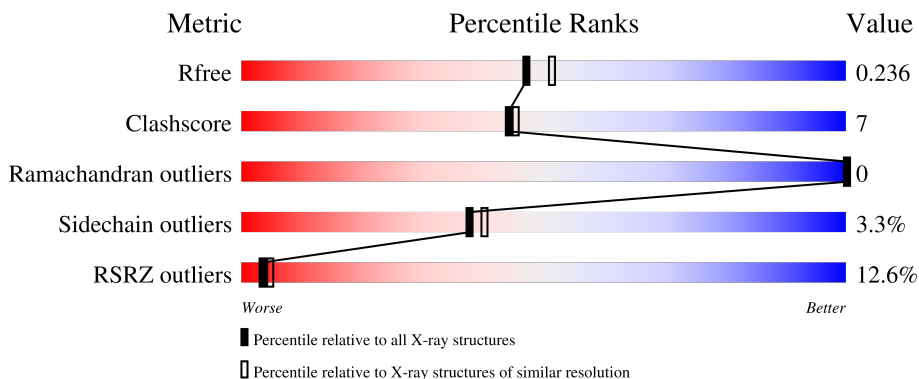
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	475	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 3849 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.

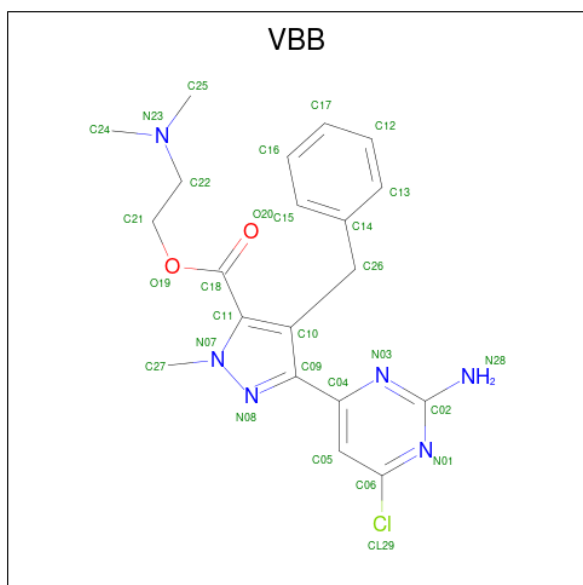
- Molecule 1 is a protein called Adenylate cyclase type 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	3644	2361	593	656	34	0	7	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	HIS	-	expression tag	UNP Q96PN6
A	471	HIS	-	expression tag	UNP Q96PN6
A	472	HIS	-	expression tag	UNP Q96PN6
A	473	HIS	-	expression tag	UNP Q96PN6
A	474	HIS	-	expression tag	UNP Q96PN6
A	475	HIS	-	expression tag	UNP Q96PN6

- Molecule 2 is 2-(dimethylamino)ethyl 5-(2-azanyl-6-chloranyl-pyrimidin-4-yl)-2-methyl-4-(phenylmethyl)pyrazole-3-carboxylate (three-letter code: VBB) (formula:  $C_{20}H_{23}ClN_6O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
2	A	1	29	20	1	6	2	0	0

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
3	A	1	4	2	1	1	0	0
3	A	1	4	2	1	1	0	0
3	A	1	4	2	1	1	0	0
3	A	1	4	2	1	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub><sup>-</sup>).



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

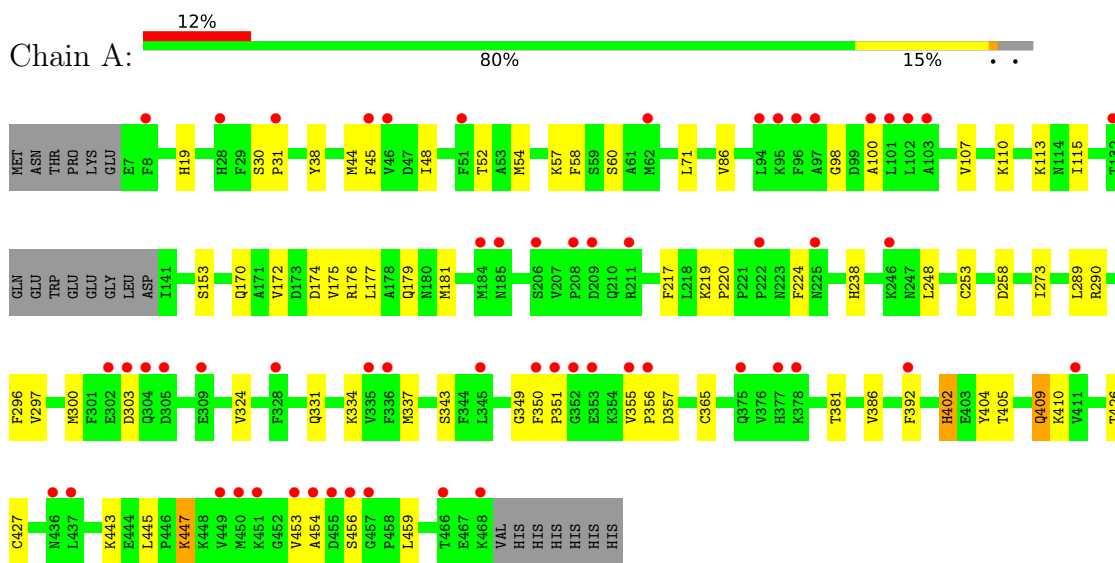
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	123	Total O 124 124	0	1

### 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: Adenylate cyclase type 10



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.31Å 99.31Å 98.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.67 – 2.10 43.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.67-2.10) 99.8 (43.00-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.192 , 0.232 0.195 , 0.236	Depositor DCC
$R_{free}$ test set	1617 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtrriage
Anisotropy	0.098	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3849	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, DMS, ACT, CME, VBB

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	0.32	0/3720	0.51	0/5035

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	456	SER	Peptide

### 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	3644	0	3605	48	0
2	A	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	16	0	24	0	0
4	A	16	0	24	3	0
5	A	20	0	15	3	0
6	A	124	0	0	4	0
All	All	3849	0	3668	49	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 7.

All (49) 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:289:LEU:HD21	1:A:392[A]:PHE:CE1	2.15	0.81
5:A:510:ACT:O	6:A:601:HOH:O	2.11	0.69
1:A:447:LYS:HD2	1:A:459:LEU:H	1.56	0.68
1:A:71:LEU:HD23	1:A:392[A]:PHE:CD2	2.31	0.64
1:A:253:CME:HE3	1:A:253:CME:HA	1.79	0.64
1:A:355:VAL:HG12	1:A:356:PRO:HD2	1.81	0.63
1:A:289:LEU:HD21	1:A:392[A]:PHE:CZ	2.33	0.63
1:A:324:VAL:HG12	1:A:365:CYS:SG	2.41	0.61
1:A:350:PHE:CB	1:A:351:PRO:HD2	2.36	0.56
1:A:289:LEU:HD11	1:A:392[A]:PHE:CZ	2.42	0.54
1:A:426:THR:HG22	1:A:445:LEU:HD11	1.90	0.53
1:A:381:THR:HA	4:A:514:EDO:C1	2.39	0.53
1:A:170:GLN:O	1:A:174:ASP:N	2.35	0.52
1:A:331:GLN:NE2	6:A:602:HOH:O	2.28	0.52
1:A:253:CME:HA	1:A:253:CME:CE	2.40	0.52
1:A:297:VAL:O	1:A:343:SER:HA	2.10	0.51
1:A:44[A]:MET:HE2	1:A:86:VAL:HG22	1.91	0.51
1:A:409:GLN:HG2	6:A:603:HOH:O	2.11	0.51
1:A:52:THR:HG21	1:A:98:GLY:O	2.10	0.50
1:A:289:LEU:HD21	1:A:392[A]:PHE:CD1	2.47	0.50
1:A:300:MET:HE1	1:A:381:THR:HG22	1.94	0.50
1:A:54:MET:O	1:A:57:LYS:N	2.44	0.50
1:A:177:LEU:O	1:A:181:MET:HG3	2.13	0.49
1:A:381:THR:HA	4:A:514:EDO:H11	1.93	0.49
1:A:30:SER:HB3	1:A:31:PRO:HD2	1.96	0.48
1:A:355:VAL:HG12	1:A:356:PRO:CD	2.44	0.48
1:A:453:VAL:HG12	1:A:454:ALA:O	2.13	0.48
1:A:217:PHE:HB3	1:A:219:LYS:HE3	1.96	0.47
1:A:172:VAL:O	1:A:175:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:TYR:HD2	1:A:153:SER:HG	1.62	0.47
1:A:409:GLN:HG2	1:A:410:LYS:N	2.30	0.46
1:A:107:VAL:HG11	1:A:115:ILE:HG13	1.96	0.46
1:A:290:ARG:NE	1:A:349:GLY:O	2.42	0.46
1:A:273:ILE:HD11	1:A:404:TYR:HB2	1.98	0.45
1:A:258:ASP:HB2	5:A:511:ACT:H2	1.99	0.44
1:A:57:LYS:O	1:A:60:SER:HB3	2.17	0.44
1:A:386:VAL:O	1:A:427:CYS:HA	2.18	0.44
1:A:289:LEU:HD11	1:A:392[A]:PHE:CE2	2.53	0.43
1:A:71:LEU:HD23	1:A:392[A]:PHE:CG	2.53	0.43
1:A:48:ILE:HG12	1:A:100:ALA:HA	2.01	0.43
1:A:19:HIS:HA	1:A:402:HIS:O	2.19	0.42
1:A:248:LEU:O	5:A:506:ACT:H3	2.20	0.41
1:A:54:MET:HE3	1:A:58:PHE:HE2	1.85	0.41
1:A:350:PHE:O	1:A:351:PRO:C	2.59	0.41
1:A:381:THR:HA	4:A:514:EDO:H12	2.03	0.41
1:A:409:GLN:HG2	1:A:410:LYS:H	1.86	0.41
1:A:220:PRO:HB2	1:A:224:PHE:HB3	2.02	0.41
1:A:45:PHE:CD2	1:A:179:GLN:HG3	2.56	0.40
1:A:405[B]:THR:HG23	6:A:612:HOH:O	2.20	0.40

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	456/475 (96%)	440 (96%)	16 (4%)	0	<a href="#">100</a> <a href="#">100</a>

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	397/418 (95%)	383 (96%)	14 (4%)	36 38

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LYS
1	A	113	LYS
1	A	176	ARG
1	A	238	HIS
1	A	296	PHE
1	A	303	ASP
1	A	334	LYS
1	A	337[A]	MET
1	A	337[B]	MET
1	A	357	ASP
1	A	402	HIS
1	A	409	GLN
1	A	443	LYS
1	A	447	LYS

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

Mol	Chain	Res	Type
1	A	162	HIS
1	A	223	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CME	A	253	1	8,9,10	0.99	0	5,9,11	0.76	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	CME	A	253	1	-	2/5/8/10	-

There are no bond length outliers.

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	253	CME	SD-CE-CZ-OH
1	A	253	CME	CZ-CE-SD-SG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	253	CME	2	0

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

14 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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ACT	A	510	-	3,3,3	0.93	0	3,3,3	1.45	1 (33%)
4	EDO	A	509	-	3,3,3	0.48	0	2,2,2	0.27	0
3	DMS	A	507	-	3,3,3	0.66	0	3,3,3	0.49	0
3	DMS	A	502	-	3,3,3	0.65	0	3,3,3	0.38	0
4	EDO	A	514	-	3,3,3	0.50	0	2,2,2	0.25	0
3	DMS	A	504	-	3,3,3	0.63	0	3,3,3	0.46	0
4	EDO	A	505	-	3,3,3	0.44	0	2,2,2	0.34	0
4	EDO	A	512	-	3,3,3	0.46	0	2,2,2	0.28	0
5	ACT	A	506	-	3,3,3	0.78	0	3,3,3	1.75	2 (66%)
5	ACT	A	513	-	3,3,3	1.02	0	3,3,3	1.41	0
5	ACT	A	508	-	3,3,3	0.74	0	3,3,3	1.92	2 (66%)
2	VBB	A	501	-	28,31,31	4.49	17 (60%)	33,43,43	2.49	11 (33%)
5	ACT	A	511	-	3,3,3	0.80	0	3,3,3	1.74	2 (66%)
3	DMS	A	503	-	3,3,3	0.63	0	3,3,3	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	509	-	-	0/1/1/1	-
4	EDO	A	514	-	-	1/1/1/1	-
4	EDO	A	512	-	-	0/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
2	VBB	A	501	-	-	3/16/18/18	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	VBB	C02-N03	6.96	1.47	1.35
2	A	501	VBB	C16-C15	6.88	1.53	1.38
2	A	501	VBB	C04-N03	6.80	1.45	1.34
2	A	501	VBB	C12-C13	6.66	1.52	1.38
2	A	501	VBB	C05-C06	6.54	1.49	1.38
2	A	501	VBB	C15-C14	6.45	1.52	1.38
2	A	501	VBB	C13-C14	6.38	1.52	1.38
2	A	501	VBB	C02-N01	6.36	1.46	1.35
2	A	501	VBB	C05-C04	6.18	1.49	1.39
2	A	501	VBB	C06-N01	6.16	1.43	1.33
2	A	501	VBB	C17-C12	5.57	1.52	1.38
2	A	501	VBB	C17-C16	5.56	1.52	1.38
2	A	501	VBB	C02-N28	5.43	1.44	1.33
2	A	501	VBB	C09-N08	-3.24	1.32	1.35
2	A	501	VBB	C11-C18	2.93	1.53	1.50
2	A	501	VBB	O19-C18	2.89	1.40	1.33
2	A	501	VBB	C09-C04	2.60	1.52	1.49

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	VBB	C04-N03-C02	7.80	120.79	116.34
2	A	501	VBB	C06-N01-C02	5.84	120.50	114.43
2	A	501	VBB	C09-C04-N03	4.74	122.25	116.61
2	A	501	VBB	C05-C06-N01	-4.34	120.74	125.50
2	A	501	VBB	N03-C02-N01	-3.62	119.74	125.42
2	A	501	VBB	N28-C02-N03	3.37	122.49	117.25
2	A	501	VBB	C05-C06-CL29	2.72	122.27	118.88
5	A	508	ACT	O-C-CH3	-2.49	112.63	122.33
2	A	501	VBB	O19-C18-O20	-2.49	118.62	123.67
2	A	501	VBB	C05-C04-N03	-2.41	119.49	122.35
5	A	506	ACT	O-C-CH3	-2.20	113.77	122.33
5	A	511	ACT	O-C-CH3	-2.17	113.86	122.33
5	A	508	ACT	OXT-C-O	2.14	129.96	122.05
2	A	501	VBB	C05-C04-C09	-2.09	118.25	120.98
5	A	510	ACT	OXT-C-O	2.08	129.72	122.05
5	A	511	ACT	OXT-C-O	2.07	129.68	122.05
5	A	506	ACT	OXT-C-O	2.06	129.66	122.05
2	A	501	VBB	C10-C26-C14	-2.03	109.39	114.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	VBB	C11-C18-O19-C21
2	A	501	VBB	O20-C18-O19-C21
2	A	501	VBB	O19-C21-C22-N23
4	A	514	EDO	O1-C1-C2-O2

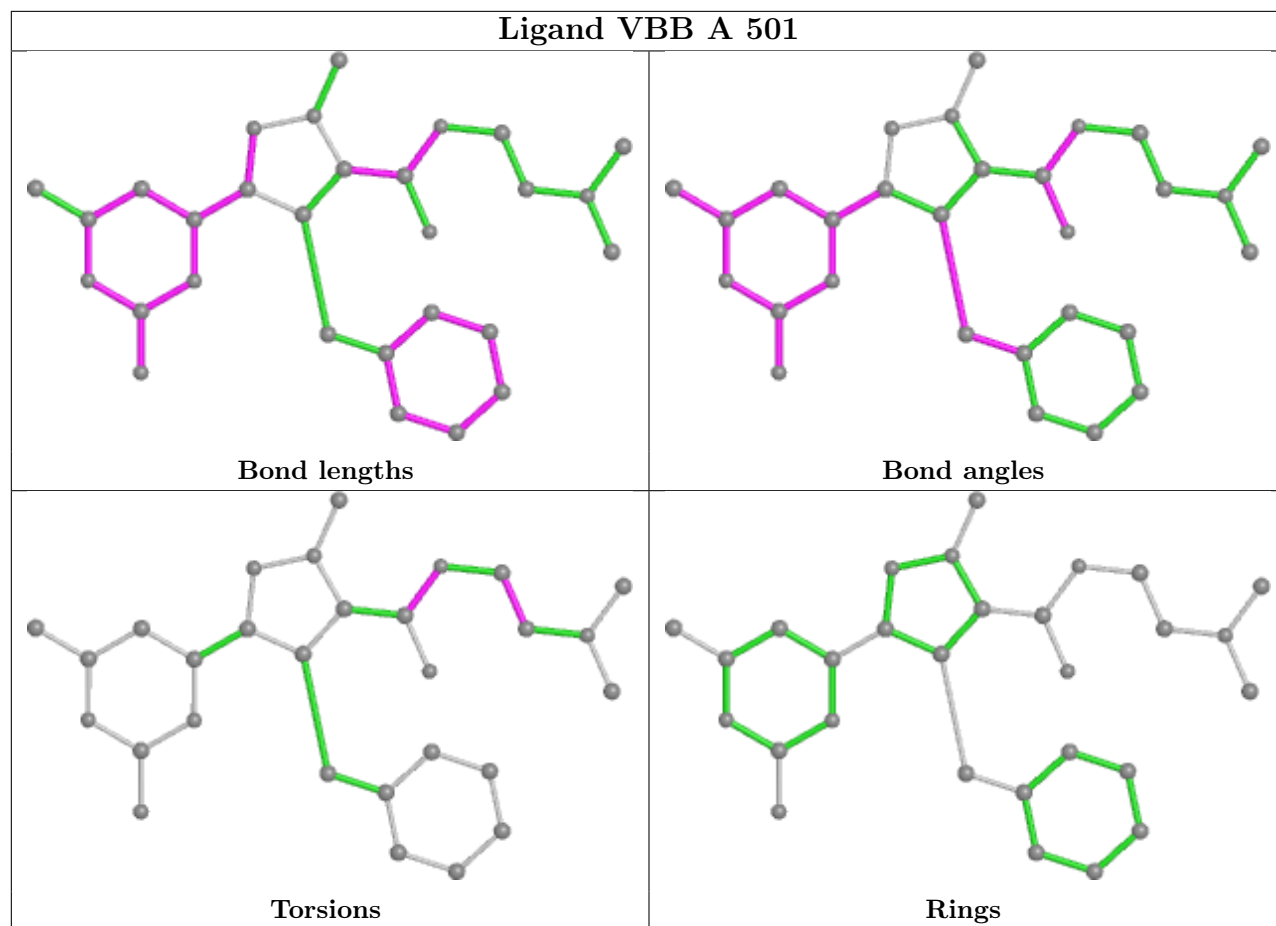
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	510	ACT	1	0
4	A	514	EDO	3	0
5	A	506	ACT	1	0
5	A	511	ACT	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	453/475 (95%)	0.65	57 (12%) <b>3</b> <b>5</b>	27, 49, 99, 140	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	PHE	6.9
1	A	449	VAL	6.4
1	A	51	PHE	5.5
1	A	304	GLN	5.5
1	A	351	PRO	5.2
1	A	356	PRO	5.1
1	A	303	ASP	5.0
1	A	352	GLY	4.9
1	A	209	ASP	4.7
1	A	453	VAL	4.3
1	A	454	ALA	4.1
1	A	132	THR	3.8
1	A	100	ALA	3.8
1	A	211	ARG	3.7
1	A	451	LYS	3.6
1	A	305	ASP	3.5
1	A	208	PRO	3.4
1	A	101	LEU	3.4
1	A	355	VAL	3.3
1	A	102	LEU	3.2
1	A	457	GLY	3.2
1	A	28[A]	HIS	3.1
1	A	46	VAL	3.1
1	A	436	ASN	3.0
1	A	45	PHE	3.0
1	A	336	PHE	3.0
1	A	184	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	222	PRO	2.9
1	A	62	MET	2.8
1	A	31	PRO	2.7
1	A	455	ASP	2.7
1	A	246	LYS	2.7
1	A	377	HIS	2.7
1	A	456	SER	2.7
1	A	302	GLU	2.6
1	A	96	PHE	2.6
1	A	103	ALA	2.5
1	A	328	PHE	2.5
1	A	345	LEU	2.4
1	A	225	ASN	2.4
1	A	353	GLU	2.4
1	A	335	VAL	2.4
1	A	375	GLN	2.3
1	A	466	THR	2.3
1	A	437	LEU	2.3
1	A	392[A]	PHE	2.3
1	A	94	LEU	2.2
1	A	378	LYS	2.2
1	A	206	SER	2.2
1	A	185	ASN	2.1
1	A	411	VAL	2.1
1	A	468	LYS	2.1
1	A	8	PHE	2.1
1	A	309	GLU	2.1
1	A	95	LYS	2.0
1	A	450	MET	2.0
1	A	97	ALA	2.0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CME	A	253	10/11	0.91	0.13	33,44,101,108	0

### 6.3 Carbohydrates [i](#)

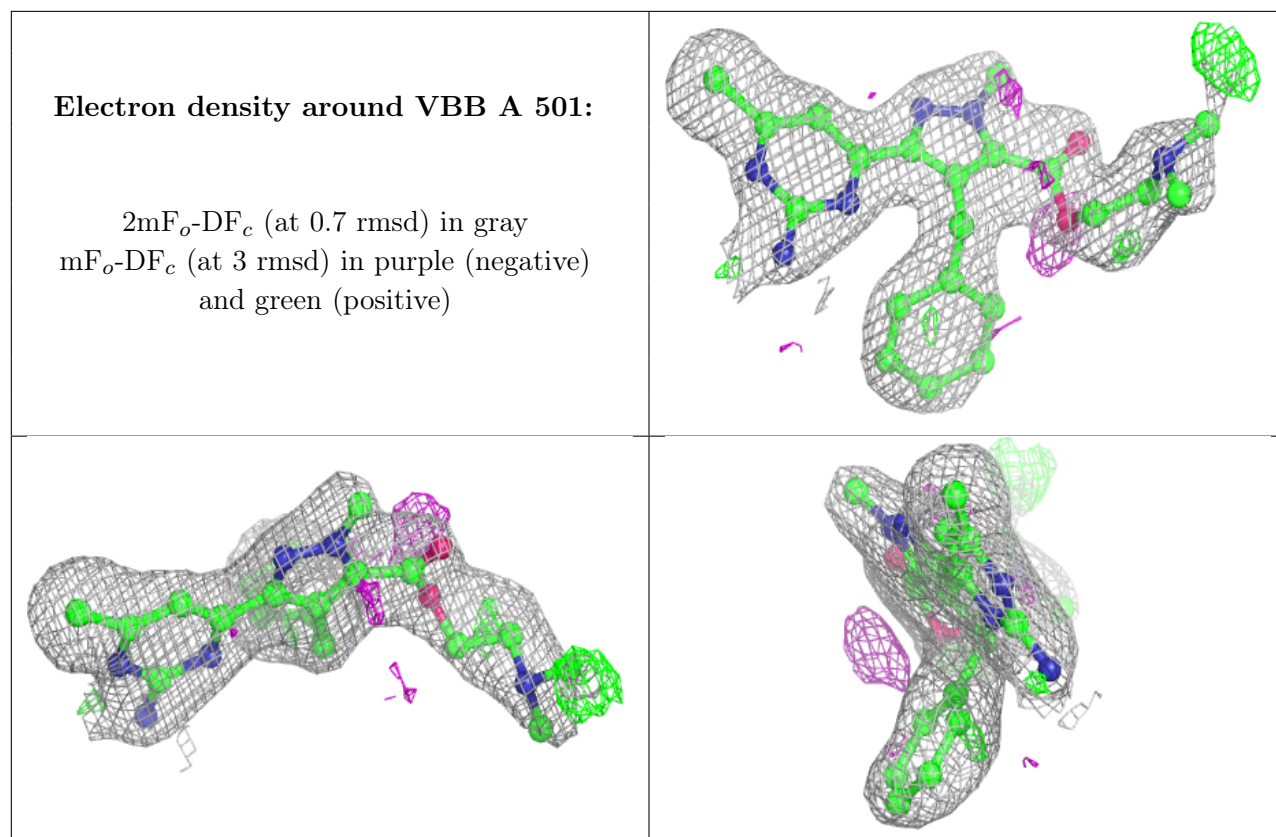
There are no monosaccharides in this entry.

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	EDO	A	514	4/4	0.75	0.35	44,46,48,53	0
5	ACT	A	506	4/4	0.84	0.20	60,62,64,64	0
5	ACT	A	510	4/4	0.87	0.43	103,110,112,112	0
5	ACT	A	511	4/4	0.87	0.34	124,124,124,124	0
4	EDO	A	512	4/4	0.88	0.24	81,81,82,82	0
4	EDO	A	505	4/4	0.89	0.23	71,73,75,77	0
2	VBB	A	501	29/29	0.91	0.27	36,50,80,83	0
5	ACT	A	508	4/4	0.93	0.23	52,60,61,63	0
3	DMS	A	504	4/4	0.94	0.15	73,76,76,78	0
4	EDO	A	509	4/4	0.94	0.15	46,47,49,51	0
3	DMS	A	503	4/4	0.96	0.16	58,58,58,59	0
5	ACT	A	513	4/4	0.96	0.08	44,48,50,53	0
3	DMS	A	507	4/4	0.97	0.22	105,105,105,106	0
3	DMS	A	502	4/4	0.98	0.15	47,50,51,56	0

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.