

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

#### Jul 17, 2024 – 03:19 pm BST

PDB ID : 8PUJ

Title: The surface-exposed lipo-protein of BtuG2 in complex with cyanocobalamin.

Authors: Whittaker, J.; Martinez-Felices, J.M.; Guskov, A.; Slotboom, D.J.

Deposited on : 2023-07-17

Resolution : 1.70 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
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 : 2.37.1

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)

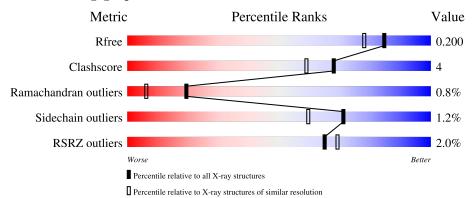
Validation Pipeline (wwPDB-VP) : 2.37.1

### 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 1.70 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	322	92%	8%			
1	С	322	92%	8%			



## 2 Entry composition (i)

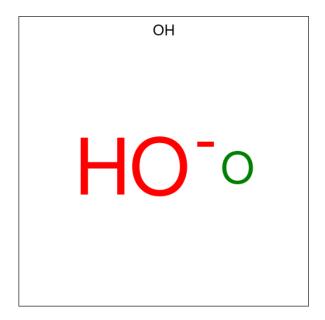
There are 5 unique types of molecules in this entry. The entry contains 5856 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 YncE family protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	322	Total 2623	C 1689	N 419	O 502	S 13	0	0	0
1	С	322	Total 2626	C 1692	N 419	O 502	S 13	0	1	0

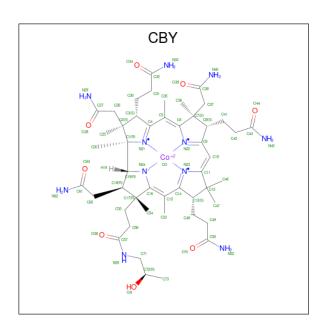
• Molecule 2 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



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

• Molecule 3 is COB(II)INAMIDE (three-letter code: CBY) (formula: C<sub>48</sub>H<sub>72</sub>CoN<sub>11</sub>O<sub>8</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
3	A	1	Total 68	C 48	Co 1	N 11	O 8	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Na 2 2	0	0
4	С	2	Total Na 2 2	0	0

 $\bullet\,$  Molecule 5 is water.

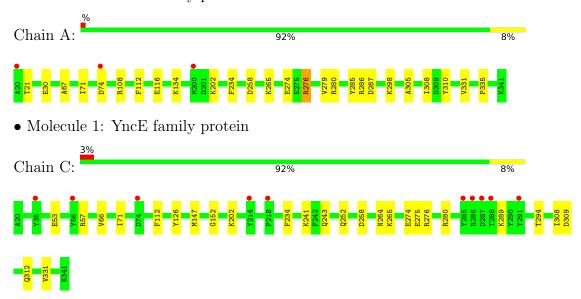
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	269	Total O 269 269	0	0
5	С	265	Total O 265 265	0	0



# 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: YncE family protein





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	107.99Å 151.99Å 45.62Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.02 - 1.70	Depositor
rtesolution (A)	44.02 - 1.70	EDS
% Data completeness	99.5 (44.02-1.70)	Depositor
(in resolution range)	99.6 (44.02-1.70)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.73 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
D D.	0.172 , 0.202	Depositor
$R, R_{free}$	0.171 , 0.200	DCC
$R_{free}$ test set	4168 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.37, 45.7	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5856	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.31% 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: CBY, NA, OH

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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.68	0/2690	0.80	0/3651	
1	С	0.64	0/2696	0.79	0/3658	
All	All	0.66	0/5386	0.80	0/7309	

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	С	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	С	276	ARG	Sidechain

#### 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	2623	0	2529	17	0
1	С	2626	0	2534	14	0
2	A	1	0	0	0	0
3	A	68	0	72	13	0
4	A	2	0	0	0	0
4	С	2	0	0	0	0
5	A	269	0	0	2	0
5	С	265	0	0	4	0
All	All	5856	0	5135	40	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
1:C:280:ARG:NH1	5:C:501:HOH:O	2.21	0.73
1:A:265:LYS:NZ	5:A:502:HOH:O	2.22	0.72
1:A:202:LYS:HE3	1:A:258:ASP:HB3	1.72	0.70
3:A:402:CBY:H3	3:A:402:CBY:HN29	1.57	0.70
1:C:53:GLU:O	1:C:57:ARG:HG3	1.96	0.66
1:A:71:ILE:HD11	1:A:112:PHE:CE1	2.36	0.60
1:C:309:ASP:OD2	1:C:312:GLN:HG2	2.01	0.60
1:C:280:ARG:NH1	5:C:502:HOH:O	2.35	0.58
1:A:108:ARG:HH12	3:A:402:CBY:HN2A	1.51	0.58
3:A:402:CBY:H3	3:A:402:CBY:N29	2.19	0.57
1:A:310:TYR:HB2	3:A:402:CBY:H68	1.87	0.54
1:C:147:MET:HG2	1:C:152:GLY:HA2	1.90	0.53
1:A:274:GLU:HG3	1:A:276:ARG:O	2.09	0.53
1:A:310:TYR:CD2	3:A:402:CBY:H68	2.45	0.52
3:A:402:CBY:H26A	3:A:402:CBY:H60	1.92	0.52
1:A:74:ASP:HB2	5:A:503:HOH:O	2.11	0.51
1:C:126:TYR:HB2	1:C:147:MET:HB3	1.92	0.51
3:A:402:CBY:H49A	3:A:402:CBY:C15	2.42	0.50
1:C:71:ILE:HD11	1:C:112:PHE:CE1	2.47	0.49
1:C:252:GLN:OE1	1:C:294:THR:HA	2.14	0.48
3:A:402:CBY:H35A	3:A:402:CBY:H36	1.98	0.46
1:C:202:LYS:HD2	1:C:258:ASP:HB3	1.98	0.46
1:C:241:LYS:HB3	1:C:241:LYS:HE3	1.69	0.45
1:A:310:TYR:HD2	3:A:402:CBY:H68	1.82	0.45
3:A:402:CBY:H25	3:A:402:CBY:C61	2.47	0.45
1:A:305:ALA:HB1	1:A:335:PRO:O	2.17	0.45

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Atom-1	Atom-2	Interatomic	Clash
		${ m distance}({ m \AA})$	overlap (Å)
1:C:280:ARG:NH2	5:C:502:HOH:O	2.49	0.45
1:A:30:GLU:HG2	1:A:67:ALA:O	2.17	0.44
1:C:71:ILE:HD11	1:C:112:PHE:HE1	1.81	0.44
1:A:116:GLU:HG2	1:A:134:LYS:HD2	1.99	0.44
1:A:71:ILE:HD11	1:A:112:PHE:HE1	1.81	0.44
1:C:280:ARG:CZ	5:C:502:HOH:O	2.64	0.44
1:A:21:THR:O	1:A:298:LYS:HD2	2.18	0.43
1:A:285:TYR:CZ	1:A:287:ASP:HA	2.53	0.43
3:A:402:CBY:H36A	3:A:402:CBY:H41A	1.69	0.43
1:C:264:ASN:O	1:C:265:LYS:HB2	2.19	0.43
1:A:286:ARG:O	1:A:286:ARG:HG3	2.20	0.42
3:A:402:CBY:H18	3:A:402:CBY:H56	1.86	0.41
1:A:279:VAL:HG23	1:A:280:ARG:HG3	2.03	0.41
3:A:402:CBY:H13	3:A:402:CBY:H53	1.89	0.41

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	320/322 (99%)	304 (95%)	14 (4%)	2 (1%)	25 11
1	С	321/322 (100%)	306 (95%)	12 (4%)	3 (1%)	17 5
All	All	641/644 (100%)	610 (95%)	26 (4%)	5 (1%)	19 6

#### All (5) Ramachandran outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	A	308	ILE
1	С	308	ILE
1	A	331	VAL
1	С	331	VAL

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Mol	Chain	Res	Type
1	С	66	VAL

#### 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	Analysed Rotameric Outliers		Percentiles		
1	A	284/284 (100%)	282 (99%)	2 (1%)	84 77		
1	С	285/284 (100%)	280 (98%)	5 (2%)	59 43		
All	All	569/568~(100%)	562 (99%)	7 (1%)	71 59		

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	PHE
1	A	276	ARG
1	С	234	PHE
1	С	243	GLN
1	С	274	GLU
1	С	275	GLU
1	С	289	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	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)

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, 1 is modelled with single atom and 4 are monoatomic - leaving 1 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	Dec	Tiple	Во	ond leng	ths	Bo	nd angle	es
$ig  \operatorname{Mol} ig  \operatorname{Ty}$	туре	Chain	$\operatorname{ain} \mid \operatorname{Res} \mid$	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CBY	A	402	2	65,75,75	1.04	3 (4%)	106,125,125	1.84	16 (15%)

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
3	CBY	A	402	2	-	15/40/191/191	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$Ideal(\AA)$
3	A	402	CBY	C14-N23	4.79	1.43	1.30
3	A	402	CBY	C9-N22	4.11	1.41	1.30
3	A	402	CBY	C10-C9	2.75	1.47	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\mathbf{Ideal}(^o)$
3	A	402	CBY	C11-N23-C14	-10.98	102.15	106.31
3	A	402	CBY	C12-C11-C10	-4.93	119.04	123.54
3	A	402	CBY	C20-C1-N21	-4.78	102.43	110.27
3	A	402	CBY	C19-C1-N21	4.69	107.63	101.67
3	A	402	CBY	C9-C10-C11	-3.94	120.06	125.88

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
3	A	402	CBY	C19-N24-C16	-3.54	106.23	111.96
3	A	402	CBY	C2-C1-N21	3.53	106.69	101.77
3	A	402	CBY	C36-C7-C37	-2.76	106.26	110.80
3	A	402	CBY	C25-C2-C1	-2.64	109.80	113.78
3	A	402	CBY	C30-C3-C2	-2.59	113.61	119.09
3	A	402	CBY	C10-C11-N23	2.52	129.06	124.93
3	A	402	CBY	C47-C12-C46	2.49	113.56	109.35
3	A	402	CBY	C1-C2-C3	2.29	104.52	101.60
3	A	402	CBY	C1-C19-N24	-2.27	102.75	106.33
3	A	402	CBY	C13-C14-N23	2.15	114.00	109.39
3	A	402	CBY	C48-C13-C12	-2.04	110.92	116.63

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	CBY	C38-C37-C7-C8
3	A	402	CBY	C42-C41-C8-C9
3	A	402	CBY	C42-C41-C8-C7
3	A	402	CBY	C38-C37-C7-C36
3	A	402	CBY	N59-C71-C72-C73
3	A	402	CBY	C2-C26-C27-N29
3	A	402	CBY	C2-C26-C27-O28
3	A	402	CBY	C41-C42-C43-N45
3	A	402	CBY	C13-C48-C49-C50
3	A	402	CBY	C55-C56-C57-O58
3	A	402	CBY	C38-C37-C7-C6
3	A	402	CBY	C41-C42-C43-O44
3	A	402	CBY	C55-C56-C57-N59
3	A	402	CBY	C48-C49-C50-N52
3	A	402	CBY	C48-C49-C50-O51

There are no ring outliers.

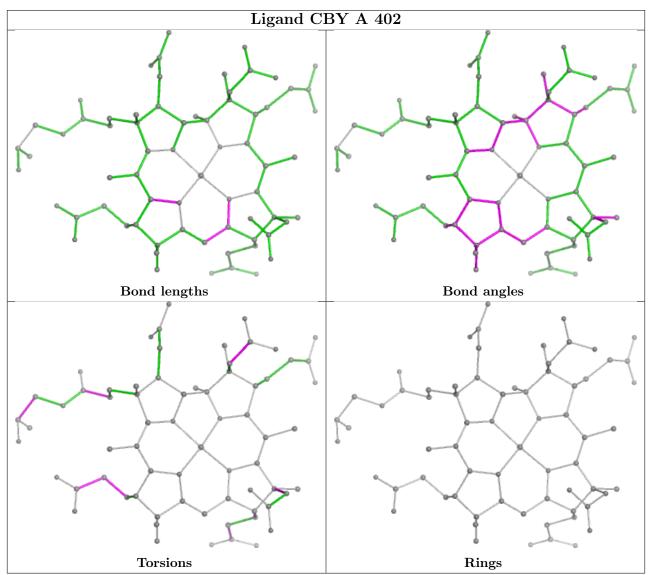
1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	CBY	13	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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(\AA^2)$	Q<0.9
1	A	322/322 (100%)	-0.40	3 (0%) 84 87	9, 16, 31, 50	0
1	C	322/322 (100%)	-0.20	10 (3%) 49 53	10, 18, 35, 67	0
All	All	644/644 (100%)	-0.30	13 (2%) 65 69	9, 17, 34, 67	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	287	ASP	4.6
1	С	286	ARG	4.5
1	С	291	TYR	3.3
1	С	285	TYR	3.2
1	A	74	ASP	2.7
1	С	214	TYR	2.5
1	A	20	ALA	2.5
1	С	218	PRO	2.4
1	A	200	MET	2.4
1	С	56	TYR	2.3
1	С	288	THR	2.2
1	С	74	ASP	2.2
1	С	35	TYR	2.0

### 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.



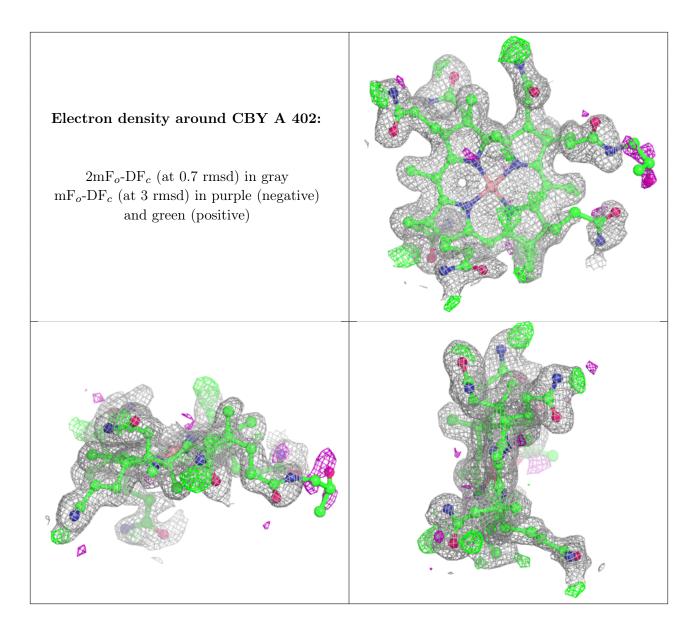
### 6.4 Ligands (i)

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	ОН	A	401	1/1	0.87	0.14	31,31,31,31	0
3	CBY	A	402	68/68	0.93	0.13	19,28,56,69	0
4	NA	A	403	1/1	0.94	0.15	37,37,37,37	0
4	NA	С	402	1/1	0.94	0.09	44,44,44,44	0
4	NA	С	401	1/1	0.98	0.06	24,24,24,24	0
4	NA	A	404	1/1	0.99	0.05	23,23,23,23	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.





## 6.5 Other polymers (i)

There are no such residues in this entry.

