



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2020 – 02:48 PM BST

PDB ID : 6WTX  
Title : Structure of VcINDY in complex with terephthalate  
Authors : Sauer, D.B.; Marden, J.J.; Wang, D.N.  
Deposited on : 2020-05-04  
Resolution : 3.92 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](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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
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) : 2.14.4.dev1

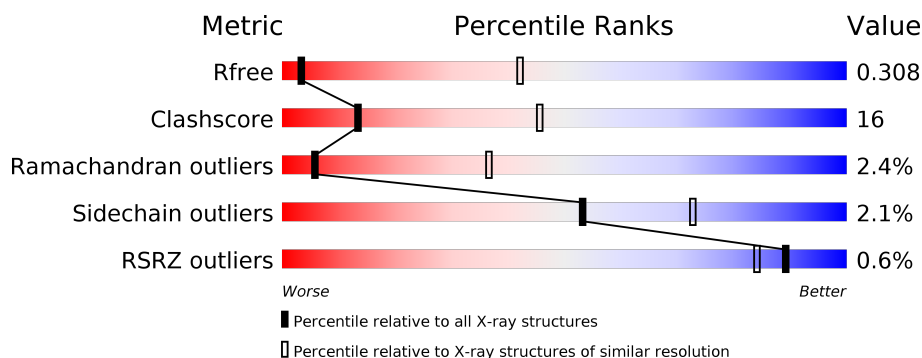
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.92 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	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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 on 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	449	 66% 30% ...
1	B	449	 69% 27% ..
1	C	449	 69% 27% ..
1	D	449	 67% 28% ...

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UB7	A	503	-	-	X	-
2	UB7	C	501	-	-	X	-

## 2 Entry composition [i](#)

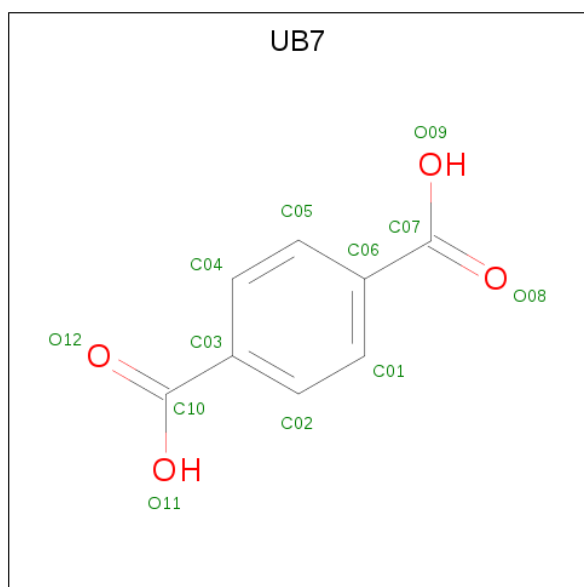
There are 3 unique types of molecules in this entry. The entry contains 27422 atoms, of which 13994 are hydrogens and 0 are deuteriums.

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 DASS family sodium-coupled anion symporter.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	445	Total	C	H	N	O	S	0	0	0
			6837	2230	3494	523	564	26			
1	D	445	Total	C	H	N	O	S	0	0	0
			6838	2230	3495	523	564	26			
1	A	445	Total	C	H	N	O	S	0	0	0
			6838	2230	3495	523	564	26			
1	B	445	Total	C	H	N	O	S	0	0	0
			6837	2230	3494	523	564	26			

- Molecule 2 is terephthalic acid (three-letter code: UB7) (formula: C<sub>8</sub>H<sub>6</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			16	8	4	4		
2	D	1	Total	C	H	O	0	0
			16	8	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			16	8	4	4		
2	B	1	Total	C	H	O	0	0
			16	8	4	4		

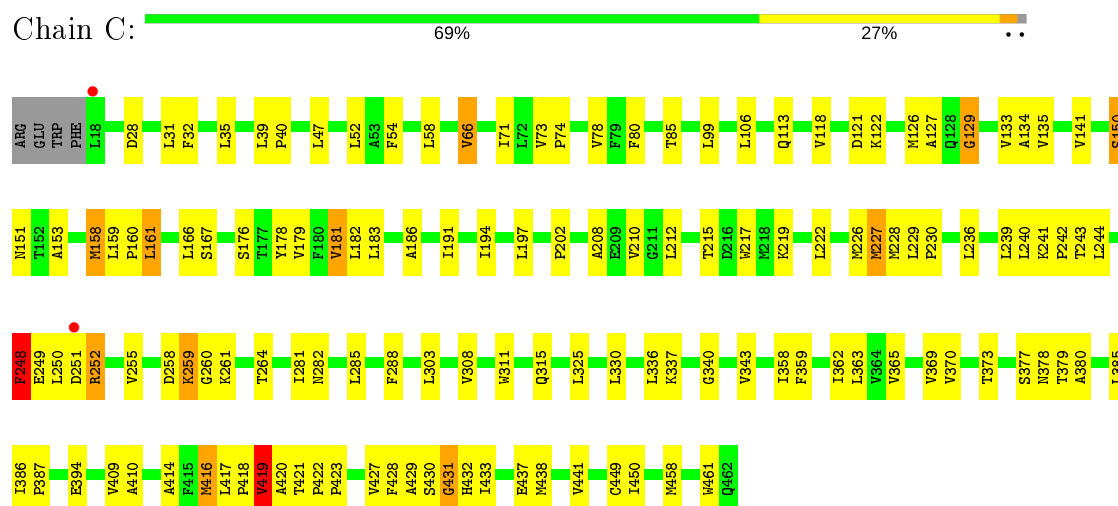
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Na	0	0
			2	2		
3	A	2	Total	Na	0	0
			2	2		
3	D	2	Total	Na	0	0
			2	2		
3	C	2	Total	Na	0	0
			2	2		

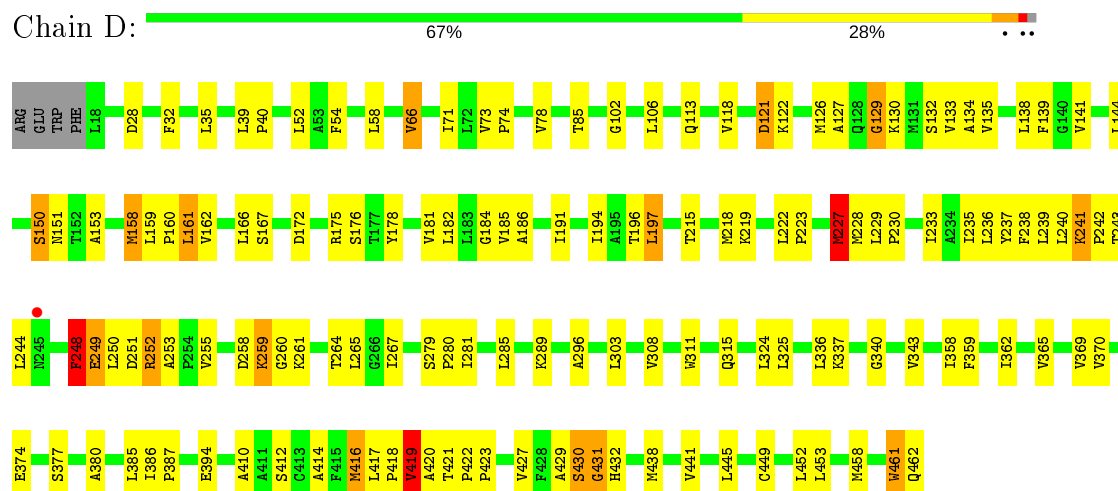
### 3 Residue-property plots [i](#)

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: DASS family sodium-coupled anion symporter

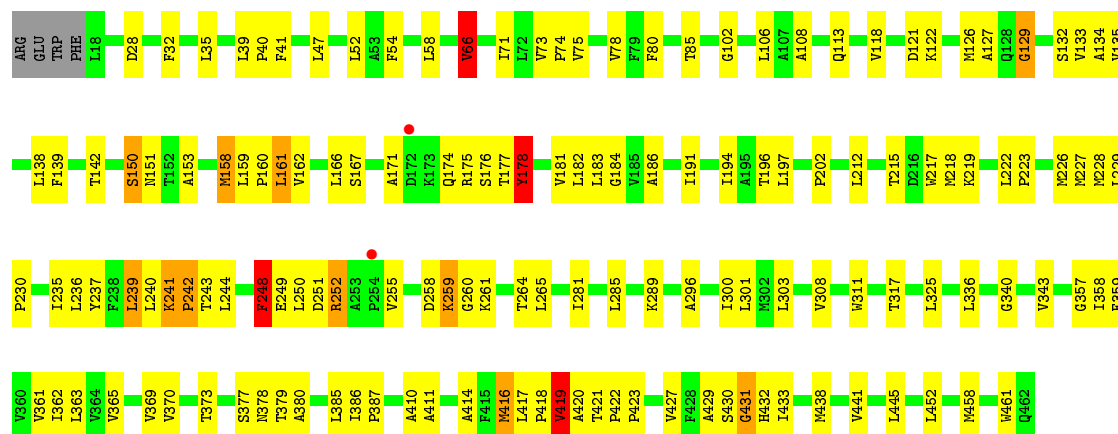


- Molecule 1: DASS family sodium-coupled anion symporter

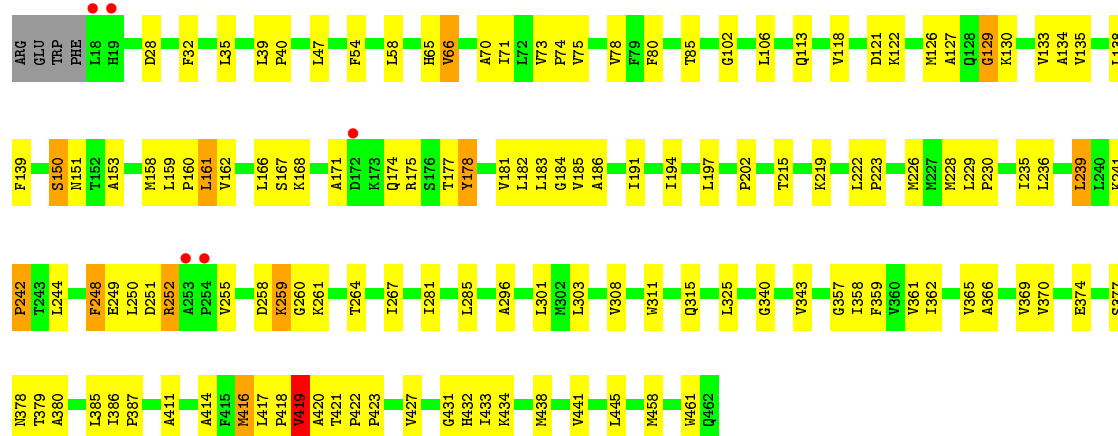


- Molecule 1: DASS family sodium-coupled anion symporter





● Molecule 1: DASS family sodium-coupled anion symporter



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.46Å 103.06Å 174.45Å 90.00° 95.85° 90.00°	Depositor
Resolution (Å)	47.80 – 3.92 47.80 – 3.92	Depositor EDS
% Data completeness (in resolution range)	82.4 (47.80-3.92) 82.4 (47.80-3.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.43 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.18 _3855	Depositor
R, $R_{free}$	0.290 , 0.308 0.290 , 0.308	Depositor DCC
$R_{free}$ test set	2000 reflections (6.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	7.1	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , -66.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.73	EDS
Total number of atoms	27422	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	5.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: NA, UB7

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	0.33	0/3422	0.65	8/4666 (0.2%)
1	B	0.36	0/3422	0.67	8/4666 (0.2%)
1	C	0.33	0/3422	0.66	9/4666 (0.2%)
1	D	0.33	0/3422	0.66	10/4666 (0.2%)
All	All	0.34	0/13688	0.66	35/18664 (0.2%)

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
1	C	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	248	PHE	CB-CG-CD1	-8.58	114.79	120.80
1	D	178	TYR	CA-CB-CG	8.53	129.61	113.40
1	B	248	PHE	CB-CG-CD2	8.00	126.40	120.80
1	D	248	PHE	CB-CG-CD2	7.99	126.39	120.80
1	C	244	LEU	CB-CG-CD1	7.97	124.55	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	TYR	Mainchain
1	C	181	VAL	Mainchain

## 5.2 Too-close contacts ⓘ

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	3343	3495	3495	124	0
1	B	3343	3494	3493	116	0
1	C	3343	3494	3494	101	0
1	D	3343	3495	3495	106	0
2	A	12	4	0	7	0
2	B	12	4	0	3	0
2	C	12	4	0	6	0
2	D	12	4	0	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
All	All	13428	13994	13977	442	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 16.

The worst 5 of 442 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:D:421:THR:HG22	1:D:423:PRO:HD2	1.32	1.11
1:B:421:THR:HG22	1:B:423:PRO:HD2	1.33	1.09
1:A:421:THR:HG22	1:A:423:PRO:HD2	1.32	1.07
1:C:421:THR:HG22	1:C:423:PRO:HD2	1.34	1.06
1:B:166:LEU:HD13	1:B:178:TYR:HB2	1.37	1.06

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	443/449 (99%)	401 (90%)	31 (7%)	11 (2%)	5	36
1	B	443/449 (99%)	404 (91%)	30 (7%)	9 (2%)	7	40
1	C	443/449 (99%)	401 (90%)	31 (7%)	11 (2%)	5	36
1	D	443/449 (99%)	403 (91%)	29 (6%)	11 (2%)	5	36
All	All	1772/1796 (99%)	1609 (91%)	121 (7%)	42 (2%)	6	36

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	242	PRO
1	C	259	LYS
1	C	419	VAL
1	D	242	PRO
1	D	259	LYS

### 5.3.2 Protein sidechains ⓘ

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	353/357 (99%)	346 (98%)	7 (2%)	55	74
1	B	353/357 (99%)	348 (99%)	5 (1%)	67	81
1	C	353/357 (99%)	346 (98%)	7 (2%)	55	74
1	D	353/357 (99%)	343 (97%)	10 (3%)	43	66
All	All	1412/1428 (99%)	1383 (98%)	29 (2%)	53	73

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	289	LYS
1	D	461	TRP
1	B	241	LYS
1	D	412	SER
1	A	121	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 12 ligands modelled in this entry, 8 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	UB7	C	501	-	8,12,12	1.50	2 (25%)	10,16,16	1.28	2 (20%)
2	UB7	B	501	-	8,12,12	1.53	2 (25%)	10,16,16	1.03	0
2	UB7	D	501	-	8,12,12	1.73	2 (25%)	10,16,16	1.12	1 (10%)
2	UB7	A	503	-	8,12,12	1.43	2 (25%)	10,16,16	1.39	2 (20%)

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	UB7	C	501	-	-	0/0/8/8	0/1/1/1
2	UB7	B	501	-	-	0/0/8/8	0/1/1/1
2	UB7	D	501	-	-	0/0/8/8	0/1/1/1
2	UB7	A	503	-	-	0/0/8/8	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	UB7	C06-C07	3.43	1.50	1.47
2	C	501	UB7	C06-C07	3.18	1.50	1.47
2	B	501	UB7	C06-C07	3.12	1.50	1.47
2	D	501	UB7	C03-C10	3.04	1.50	1.47
2	A	503	UB7	C06-C07	3.02	1.50	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	UB7	C04-C03-C10	2.99	124.39	120.37
2	C	501	UB7	C04-C03-C10	2.58	123.84	120.37
2	A	503	UB7	C05-C06-C07	2.46	123.68	120.37
2	D	501	UB7	C05-C06-C07	2.29	123.45	120.37
2	C	501	UB7	C05-C06-C07	2.12	123.22	120.37

There are no chirality outliers.

There are no torsion outliers.

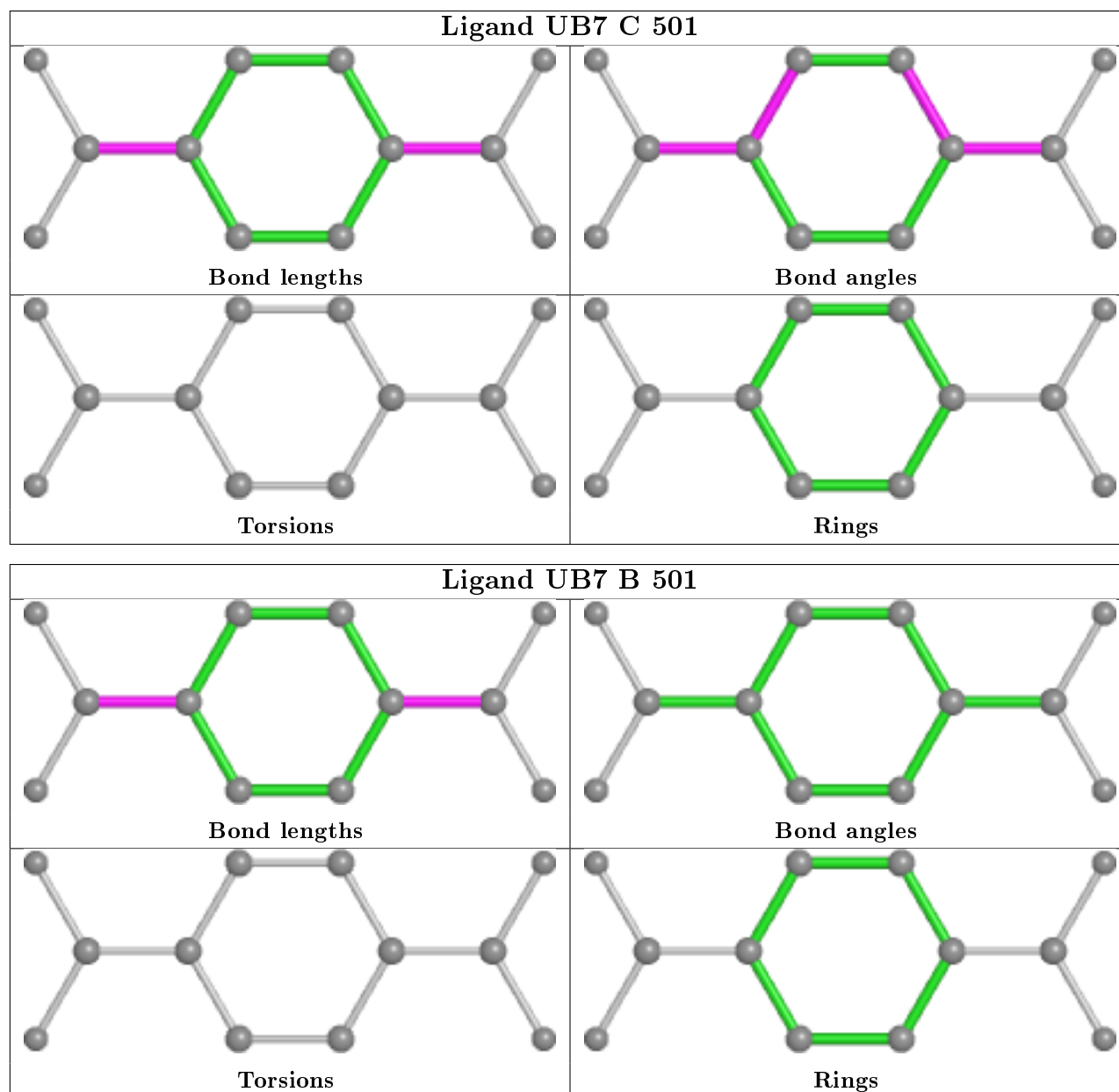
There are no ring outliers.

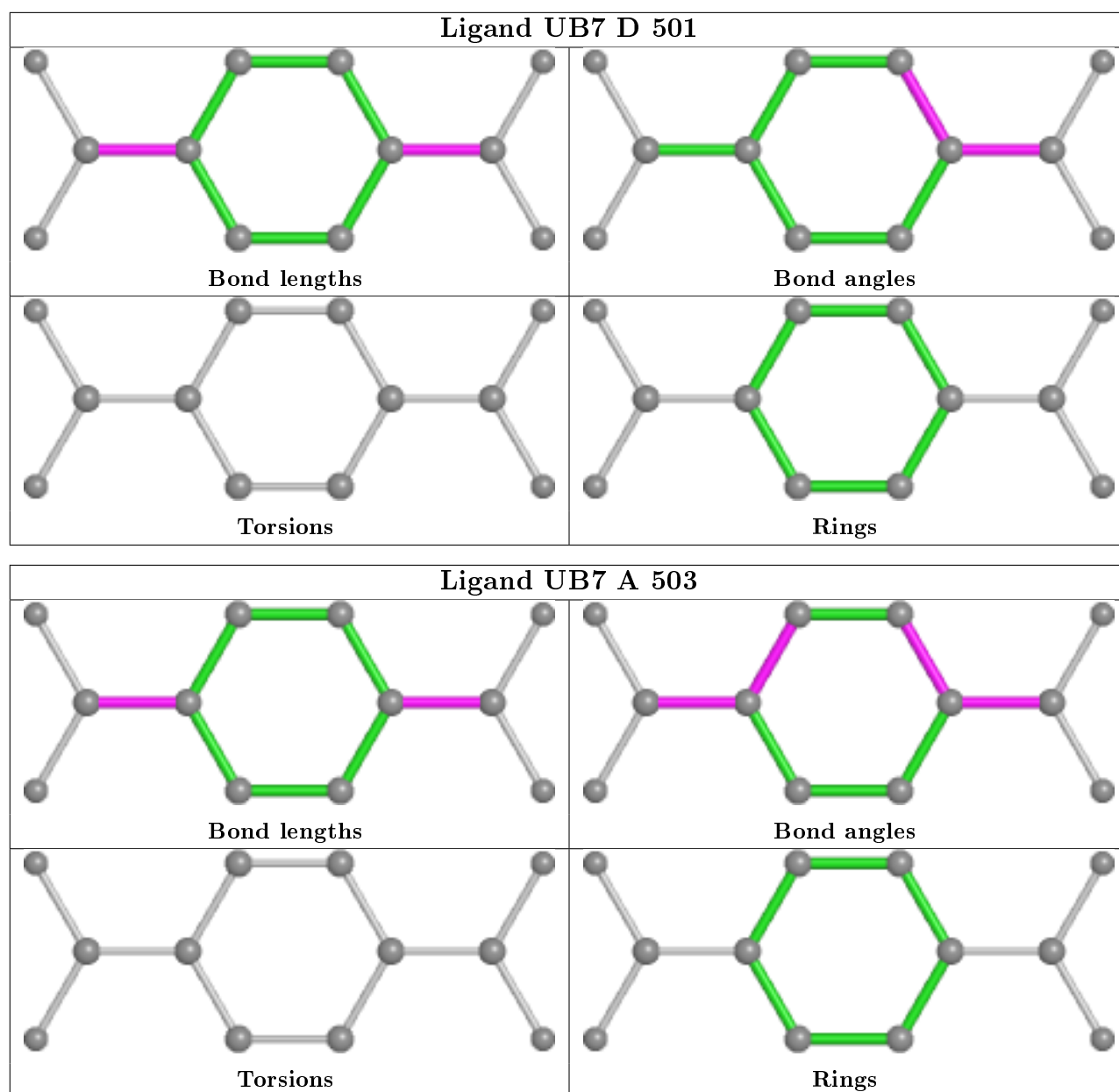
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	UB7	6	0
2	B	501	UB7	3	0
2	D	501	UB7	3	0
2	A	503	UB7	7	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 [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<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	445/449 (99%)	-0.24	2 (0%) 92 87	5, 6, 6, 7	0
1	B	445/449 (99%)	-0.22	5 (1%) 80 73	5, 6, 6, 6	0
1	C	445/449 (99%)	-0.21	2 (0%) 92 87	5, 6, 6, 7	0
1	D	445/449 (99%)	-0.22	1 (0%) 95 93	5, 6, 6, 6	0
All	All	1780/1796 (99%)	-0.22	10 (0%) 89 84	5, 6, 6, 7	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	ALA	3.1
1	B	18	LEU	2.9
1	C	251	ASP	2.8
1	B	254	PRO	2.5
1	B	19	HIS	2.3

### 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<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.

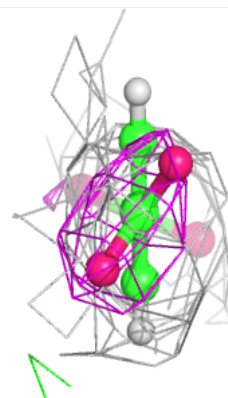
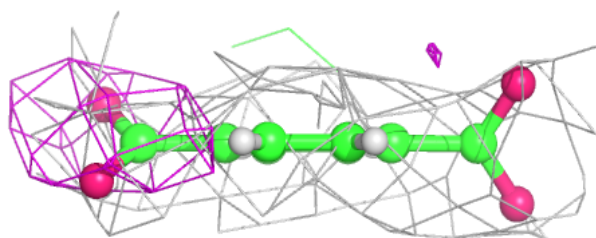
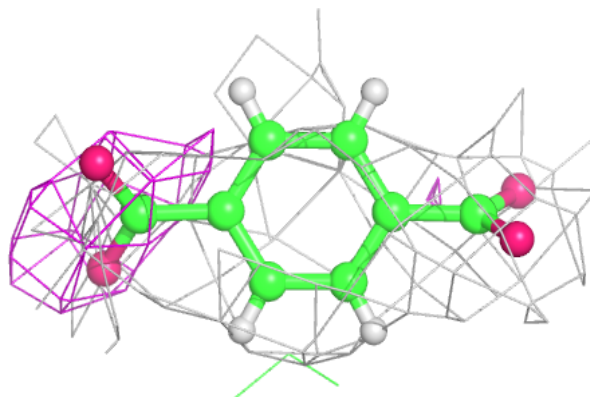


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	B	503	1/1	0.85	0.18	5,5,5,5	0
2	UB7	C	501	12/12	0.86	0.42	5,6,6,6	0
2	UB7	A	503	12/12	0.87	0.24	5,5,5,5	0
2	UB7	D	501	12/12	0.87	0.37	5,5,5,5	0
3	NA	C	502	1/1	0.91	0.18	5,5,5,5	0
2	UB7	B	501	12/12	0.93	0.23	5,5,5,5	0
3	NA	C	503	1/1	0.93	0.23	5,5,5,5	0
3	NA	B	502	1/1	0.96	0.13	5,5,5,5	0
3	NA	A	502	1/1	0.97	0.12	5,5,5,5	0
3	NA	D	502	1/1	0.97	0.12	5,5,5,5	0
3	NA	D	503	1/1	0.97	0.34	5,5,5,5	0
3	NA	A	501	1/1	0.98	0.15	5,5,5,5	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.

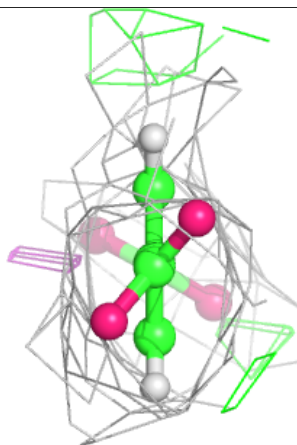
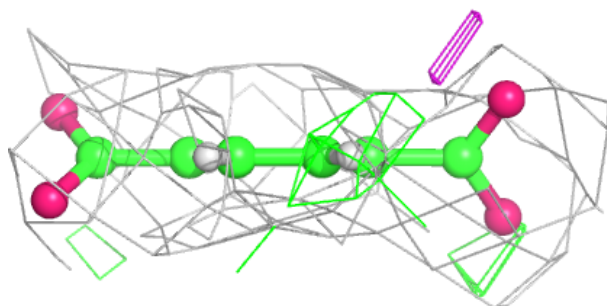
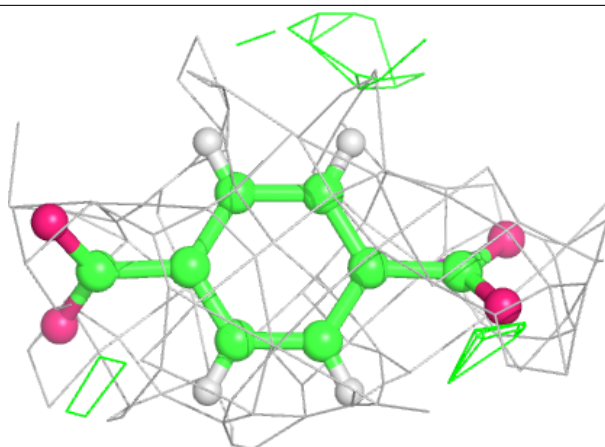
**Electron density around UB7 C 501:**

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)

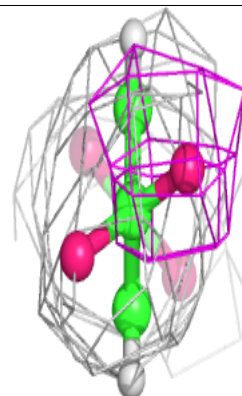
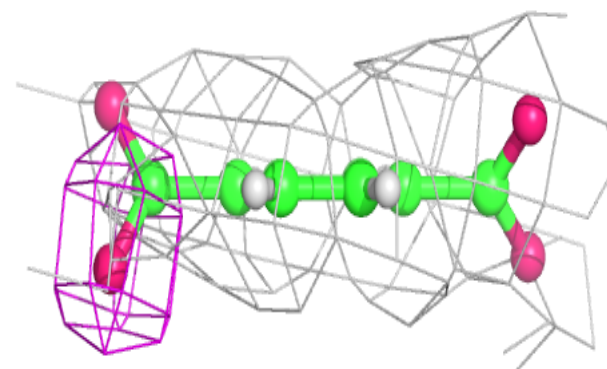
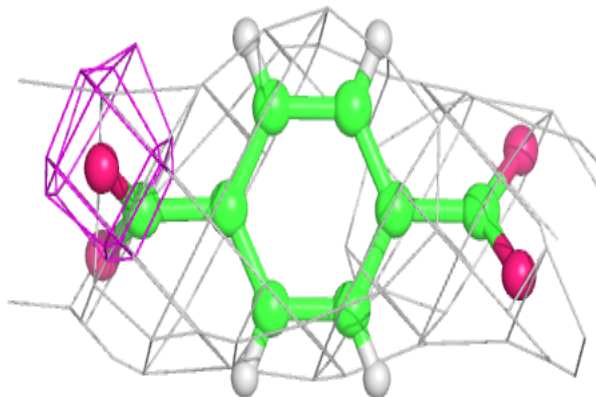


**Electron density around UB7 A 503:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

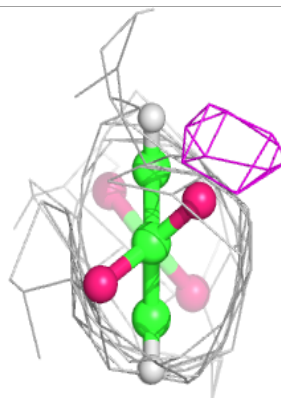
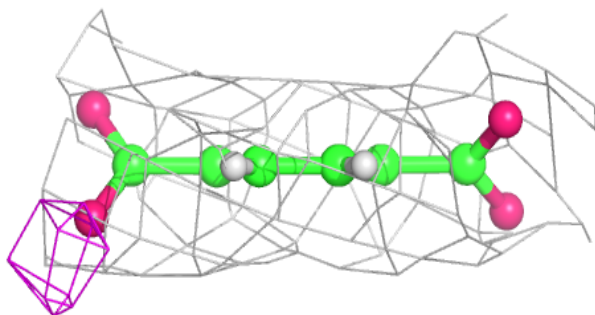
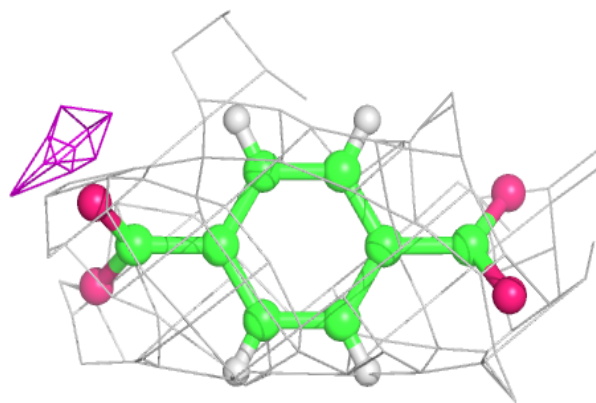
**Electron density around UB7 D 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around UB7 B 501:**

$2mF_o - DF_c$  (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.