



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 06:49 PM BST

PDB ID : 6ZHC  
Title : PROTAC6 mediated complex of VHL:EloB:EloC and Bcl-xL  
Authors : Chung, C.  
Deposited on : 2020-06-22  
Resolution : 1.92 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 : 2.13.1  
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) : 2.13.1

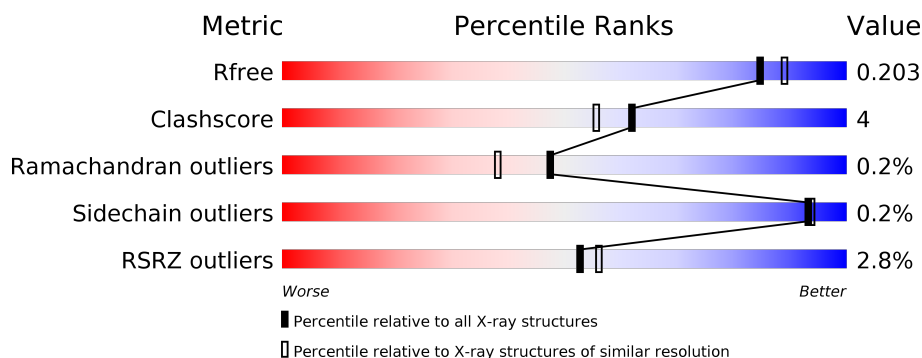
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	AAA	155	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div></div> </div> <div></div> </div>
2	BBB	107	<div> <div>%</div> <div> <div></div> <div>96%</div> <div></div> </div> <div></div> </div>
3	CCC	96	<div> <div></div> <div> <div></div> <div>86%</div> <div>6%</div> <div>7%</div> </div> <div></div> </div>
4	DDD	221	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>5%</div> <div>33%</div> </div> <div></div> </div>

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
7	GOL	DDD	307	-	-	X	-
8	IOD	CCC	207[B]	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4810 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 von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	151	Total	C	N	O	S	0	8	0
			1302	828	240	232	2			

- Molecule 2 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	105	Total	C	N	O	S	0	2	0
			841	532	140	164	5			

- Molecule 3 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	89	Total	C	N	O	S	0	2	0
			716	463	115	132	6			

- Molecule 4 is a protein called Bcl-2-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	DDD	147	Total	C	N	O	S	0	10	0
			1256	799	211	240	6			

There are 12 discrepancies between the modelled and reference sequences:

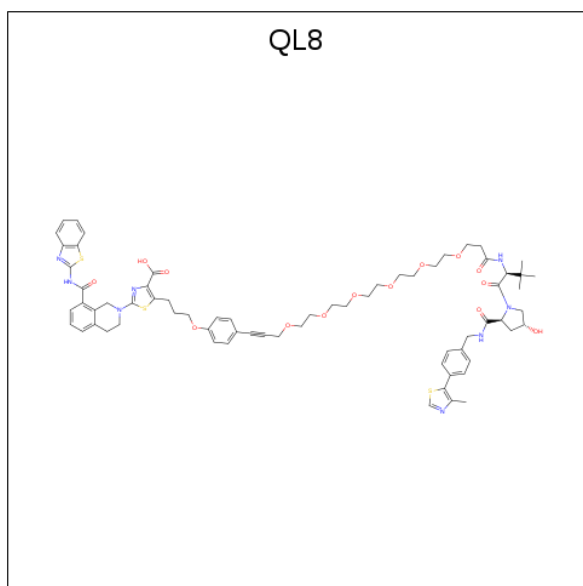
Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-3	MET	-	initiating methionine	UNP Q07817
DDD	-2	SER	-	expression tag	UNP Q07817
DDD	-1	MET	-	expression tag	UNP Q07817
DDD	0	ALA	-	expression tag	UNP Q07817
DDD	210	LEU	-	expression tag	UNP Q07817
DDD	211	GLU	-	expression tag	UNP Q07817
DDD	212	HIS	-	expression tag	UNP Q07817
DDD	213	HIS	-	expression tag	UNP Q07817

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	214	HIS	-	expression tag	UNP Q07817
DDD	215	HIS	-	expression tag	UNP Q07817
DDD	216	HIS	-	expression tag	UNP Q07817
DDD	217	HIS	-	expression tag	UNP Q07817

- Molecule 5 is 2-[8-(1,3-benzothiazol-2-ylcarbamoyl)-3,4-dihydro-1 {H}-isoquinolin-2-yl]-5-[3-[4-[3-[2-[2-[2-[2-[3-[(2 {S})-3,3-dimethyl-1-[(2 {S}),4 {R})-2-[[4-(4-methyl-1,3-thiazol-5-yl) phenyl]methylcarbamoyl]-4-oxidanyl-pyrrolidin-1-yl]-1-oxidanylidene-butan-2-yl]amino]-3-oxidanylidene-propoxy]ethoxy]ethoxy]ethoxy]ethoxy]prop-1-ynyl]phenoxy]propyl]-1,3-thiazole-4-carboxylic acid (three-letter code: QL8) (formula: C<sub>68</sub>H<sub>80</sub>N<sub>8</sub>O<sub>14</sub>S<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	AAA	1	Total	C	N	O	S	0	0
			93	68	8	14	3		

- Molecule 6 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
6	AAA	1	Total	C	O	0	0
			4	2	2		
6	AAA	1	Total	C	O	0	0
			4	2	2		
6	AAA	1	Total	C	O	0	0
			4	2	2		
6	AAA	1	Total	C	O	0	0
			4	2	2		
6	BBB	1	Total	C	O	0	0
			4	2	2		
6	BBB	1	Total	C	O	0	0
			4	2	2		
6	BBB	1	Total	C	O	0	0
			4	2	2		
6	BBB	1	Total	C	O	0	0
			4	2	2		
6	BBB	1	Total	C	O	0	0
			4	2	2		
6	CCC	1	Total	C	O	0	0
			4	2	2		
6	CCC	1	Total	C	O	0	0
			4	2	2		
6	CCC	1	Total	C	O	0	0
			4	2	2		
6	CCC	1	Total	C	O	0	0
			4	2	2		
6	DDD	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	DDD	1	Total	C	O	0	0
			4	2	2		
6	DDD	1	Total	C	O	0	0
			4	2	2		
6	DDD	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	C	O	0	0
			6	3	3		
7	AAA	1	Total	C	O	0	0
			6	3	3		
7	AAA	1	Total	C	O	0	0
			6	3	3		
7	AAA	1	Total	C	O	0	0
			6	3	3		
7	AAA	1	Total	C	O	0	0
			6	3	3		
7	CCC	1	Total	C	O	0	0
			6	3	3		
7	DDD	1	Total	C	O	0	0
			6	3	3		
7	DDD	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	DDD	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	CCC	3	Total	I	0	2
			5	5		
8	BBB	2	Total	I	0	1
			3	3		
8	DDD	2	Total	I	0	0
			2	2		
8	AAA	5	Total	I	0	2
			7	7		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	141	Total	O	0	4
			143	143		
9	BBB	103	Total	O	0	0
			103	103		
9	CCC	99	Total	O	0	2
			100	100		
9	DDD	117	Total	O	0	4
			117	117		

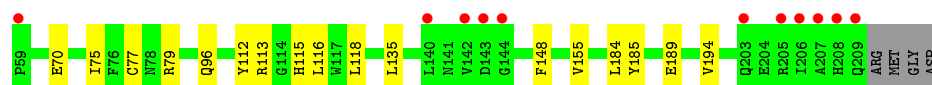


### 3 Residue-property plots

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.

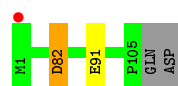
- Molecule 1: von Hippel-Lindau disease tumor suppressor

Chain AAA: 



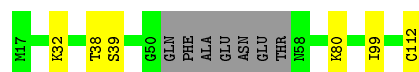
- Molecule 2: Elongin-B

Chain BBB: 



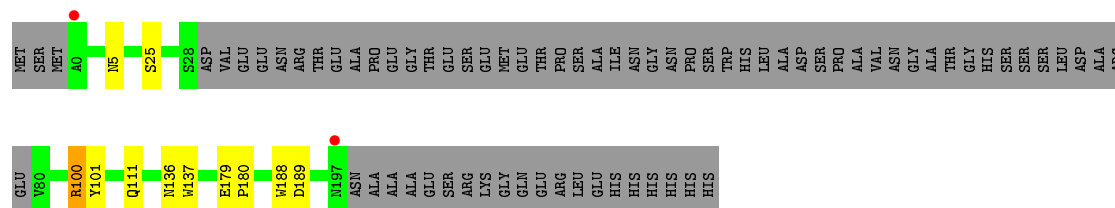
- Molecule 3: Elongin-C

Chain CCC: 



- Molecule 4: Bcl-2-like protein 1

Chain DDD: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.99Å 101.18Å 106.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.27 – 1.92 47.27 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.27-1.92) 99.8 (47.27-1.92)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.169 , 0.196 0.179 , 0.203	Depositor DCC
$R_{free}$ test set	2910 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4810	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: GOL, IOD, EDO, QL8

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	AAA	0.61	0/1341	0.71	0/1829
2	BBB	0.62	0/861	0.74	0/1165
3	CCC	0.64	0/734	0.69	0/989
4	DDD	0.65	0/1291	0.70	2/1745 (0.1%)
All	All	0.63	0/4227	0.71	2/5728 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	DDD	100[A]	ARG	NE-CZ-NH1	5.55	123.08	120.30
4	DDD	100[B]	ARG	NE-CZ-NH1	5.55	123.08	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 the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1302	0	1310	16	0
2	BBB	841	0	841	1	0
3	CCC	716	0	724	7	0
4	DDD	1256	0	1191	12	0
5	AAA	93	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AAA	16	0	24	0	0
6	BBB	20	0	30	0	0
6	CCC	16	0	24	0	0
6	DDD	16	0	24	0	0
7	AAA	30	0	40	3	0
7	CCC	6	0	8	1	0
7	DDD	18	0	24	4	0
8	AAA	7	0	0	2	0
8	BBB	3	0	0	0	0
8	CCC	5	0	0	3	0
8	DDD	2	0	0	1	0
9	AAA	143	0	0	3	0
9	BBB	103	0	0	2	0
9	CCC	100	0	0	1	0
9	DDD	117	0	0	4	0
All	All	4810	0	4240	38	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.

The worst 5 of 38 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)
9:AAA:452:HOH:O	8:DDD:309:IOD:I	2.48	1.00
3:CCC:99[B]:ILE:CG2	8:CCC:207[B]:IOD:I	3.00	0.79
3:CCC:99[B]:ILE:HG21	8:CCC:207[B]:IOD:I	2.53	0.79
1:AAA:194:VAL:HG23	8:AAA:311[A]:IOD:I	2.54	0.77
4:DDD:100[B]:ARG:NH1	9:DDD:401:HOH:O	2.20	0.74

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	AAA	157/155 (101%)	152 (97%)	5 (3%)	0	100	100
2	BBB	105/107 (98%)	101 (96%)	3 (3%)	1 (1%)	15	6
3	CCC	87/96 (91%)	87 (100%)	0	0	100	100
4	DDD	153/221 (69%)	152 (99%)	1 (1%)	0	100	100
All	All	502/579 (87%)	492 (98%)	9 (2%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BBB	82	ASP

### 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	AAA	149/144 (104%)	149 (100%)	0	100	100
2	BBB	95/95 (100%)	94 (99%)	1 (1%)	73	72
3	CCC	81/85 (95%)	81 (100%)	0	100	100
4	DDD	135/185 (73%)	135 (100%)	0	100	100
All	All	460/509 (90%)	459 (100%)	1 (0%)	93	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BBB	82	ASP

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 44 ligands modelled in this entry, 17 are monoatomic - leaving 27 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	$\# Z  > 2$
6	EDO	DDD	302	-	3,3,3	0.10	0	2,2,2	0.43	0
7	GOL	DDD	305	-	5,5,5	0.09	0	5,5,5	0.28	0
6	EDO	AAA	303	-	3,3,3	0.11	0	2,2,2	0.35	0
6	EDO	DDD	301	-	3,3,3	0.11	0	2,2,2	0.29	0
7	GOL	AAA	310	-	5,5,5	0.13	0	5,5,5	0.29	0
7	GOL	CCC	205	-	5,5,5	0.13	0	5,5,5	0.37	0
6	EDO	AAA	302	-	3,3,3	0.04	0	2,2,2	0.21	0
6	EDO	DDD	303	-	3,3,3	0.10	0	2,2,2	0.28	0
6	EDO	BBB	203	-	3,3,3	0.06	0	2,2,2	0.17	0
7	GOL	AAA	307	-	5,5,5	0.10	0	5,5,5	0.27	0
7	GOL	DDD	306	-	5,5,5	0.10	0	5,5,5	0.25	0
6	EDO	AAA	304	-	3,3,3	0.08	0	2,2,2	0.26	0
5	QL8	AAA	301	-	87,101,101	0.95	4 (4%)	102,137,137	1.30	13 (12%)
6	EDO	CCC	204	-	3,3,3	0.08	0	2,2,2	0.20	0
7	GOL	AAA	309	-	5,5,5	0.11	0	5,5,5	0.33	0
6	EDO	CCC	202	-	3,3,3	0.11	0	2,2,2	0.34	0
6	EDO	CCC	201	-	3,3,3	0.24	0	2,2,2	0.55	0
7	GOL	AAA	308	-	5,5,5	0.10	0	5,5,5	0.28	0
6	EDO	BBB	202	-	3,3,3	0.11	0	2,2,2	0.14	0
6	EDO	CCC	203	-	3,3,3	0.06	0	2,2,2	0.22	0
7	GOL	AAA	306	-	5,5,5	0.10	0	5,5,5	0.29	0
7	GOL	DDD	307	-	5,5,5	0.10	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	BBB	201	-	3,3,3	0.10	0	2,2,2	0.11	0
6	EDO	BBB	204	-	3,3,3	0.07	0	2,2,2	0.35	0
6	EDO	BBB	205	-	3,3,3	0.07	0	2,2,2	0.21	0
6	EDO	AAA	305	-	3,3,3	0.05	0	2,2,2	0.18	0
6	EDO	DDD	304	-	3,3,3	0.06	0	2,2,2	0.25	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
6	EDO	DDD	302	-	-	1/1/1/1	-
7	GOL	DDD	305	-	-	2/4/4/4	-
6	EDO	AAA	303	-	-	0/1/1/1	-
6	EDO	DDD	301	-	-	0/1/1/1	-
7	GOL	AAA	310	-	-	4/4/4/4	-
7	GOL	CCC	205	-	-	2/4/4/4	-
6	EDO	AAA	302	-	-	1/1/1/1	-
6	EDO	DDD	303	-	-	1/1/1/1	-
6	EDO	BBB	203	-	-	1/1/1/1	-
7	GOL	AAA	307	-	-	2/4/4/4	-
7	GOL	DDD	306	-	-	2/4/4/4	-
6	EDO	AAA	304	-	-	1/1/1/1	-
5	QL8	AAA	301	-	-	5/68/99/99	0/9/9/9
6	EDO	CCC	204	-	-	1/1/1/1	-
7	GOL	AAA	309	-	-	1/4/4/4	-
6	EDO	CCC	202	-	-	1/1/1/1	-
6	EDO	CCC	201	-	-	1/1/1/1	-
7	GOL	AAA	308	-	-	0/4/4/4	-
6	EDO	BBB	202	-	-	1/1/1/1	-
6	EDO	CCC	203	-	-	0/1/1/1	-
7	GOL	AAA	306	-	-	2/4/4/4	-
7	GOL	DDD	307	-	-	2/4/4/4	-
6	EDO	BBB	201	-	-	0/1/1/1	-
6	EDO	BBB	204	-	-	0/1/1/1	-
6	EDO	BBB	205	-	-	1/1/1/1	-
6	EDO	AAA	305	-	-	0/1/1/1	-
6	EDO	DDD	304	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AAA	301	QL8	C61-N46	3.94	1.38	1.32
5	AAA	301	QL8	C66-C63	-2.80	1.49	1.50
5	AAA	301	QL8	C6-C2	-2.09	1.46	1.48
5	AAA	301	QL8	O23-C21	2.02	1.26	1.22

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AAA	301	QL8	C45-N46-C47	4.82	124.40	112.91
5	AAA	301	QL8	C55-C54-N53	3.31	115.73	108.04
5	AAA	301	QL8	C66-C63-C64	2.89	131.25	127.66
5	AAA	301	QL8	C47-C48-C43	2.80	116.32	111.35
5	AAA	301	QL8	C21-C24-N26	-2.59	104.51	107.34

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	DDD	305	GOL	O1-C1-C2-C3
7	AAA	310	GOL	O1-C1-C2-C3
7	AAA	310	GOL	C1-C2-C3-O3
7	CCC	205	GOL	C1-C2-C3-O3
7	CCC	205	GOL	O2-C2-C3-O3

There are no ring outliers.

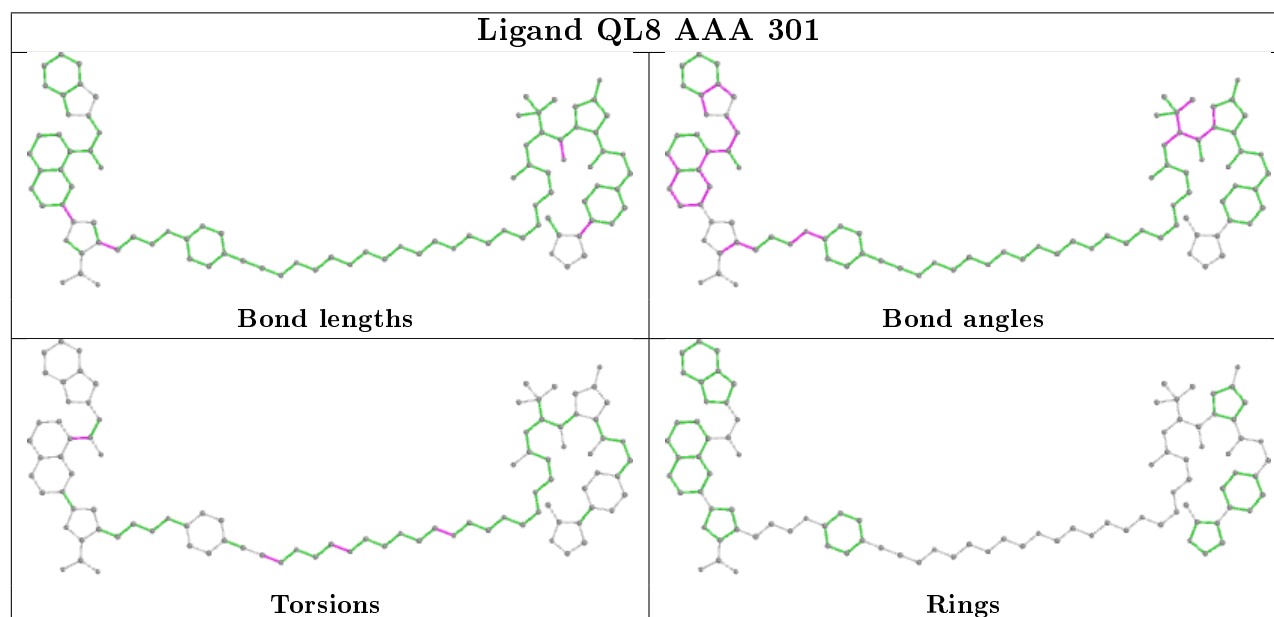
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	CCC	205	GOL	1	0
5	AAA	301	QL8	1	0
7	AAA	309	GOL	3	0
7	DDD	307	GOL	4	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	AAA	151/155 (97%)	0.19	11 (7%) 15 17	22, 30, 68, 104	0
2	BBB	105/107 (98%)	-0.14	1 (0%) 82 84	24, 35, 57, 74	0
3	CCC	89/96 (92%)	0.11	0 100 100	22, 27, 58, 65	0
4	DDD	147/221 (66%)	-0.09	2 (1%) 75 77	22, 31, 51, 88	1 (0%)
All	All	492/579 (84%)	0.02	14 (2%) 53 56	22, 31, 59, 104	1 (0%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	DDD	0	ALA	6.1
1	AAA	209	GLN	5.8
1	AAA	208	HIS	5.8
1	AAA	59	PRO	4.4
2	BBB	1	MET	4.2

### 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.

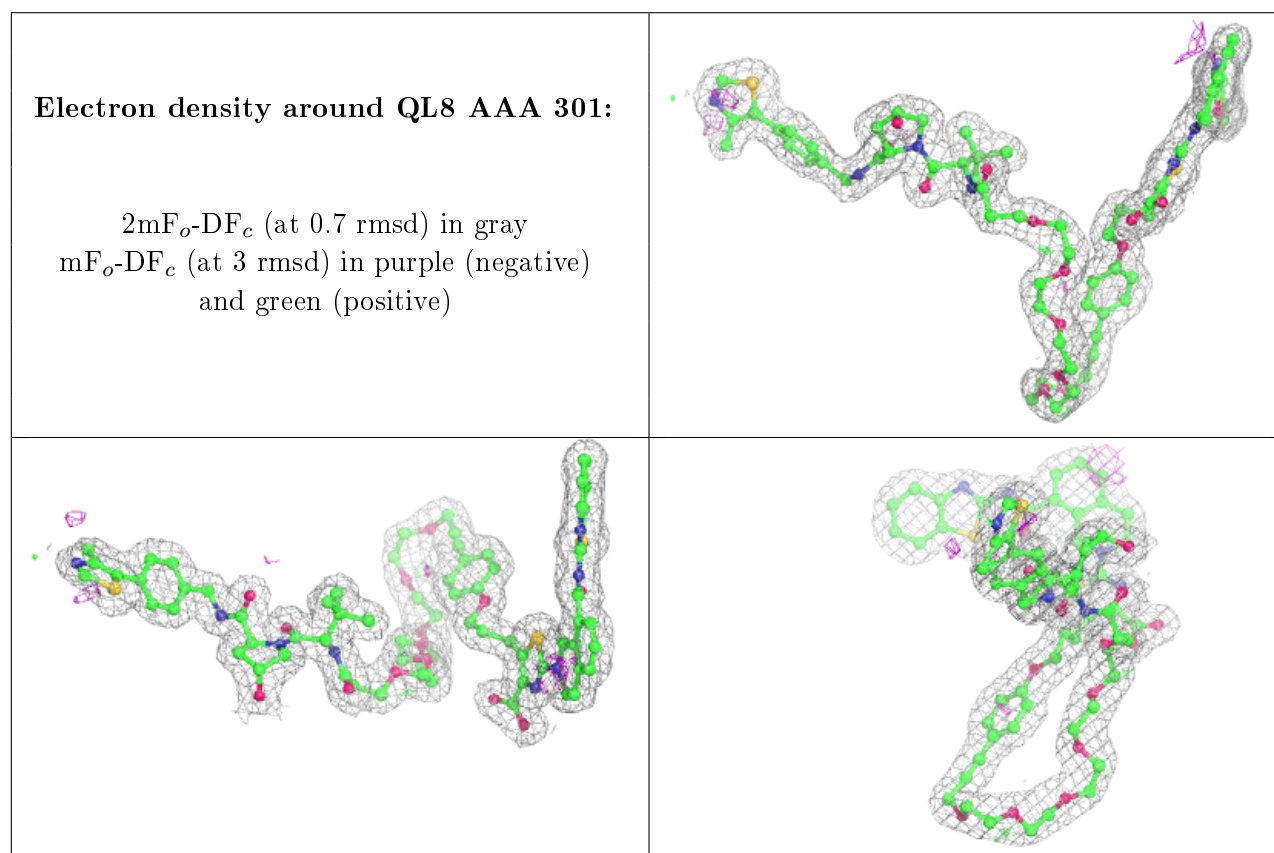
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	DDD	304	4/4	0.67	0.26	79,80,84,88	0
6	EDO	BBB	204	4/4	0.73	0.32	55,63,63,69	0
7	GOL	DDD	307	6/6	0.73	0.20	46,51,58,66	0
7	GOL	AAA	309	6/6	0.74	0.20	67,70,71,75	0
6	EDO	DDD	302	4/4	0.74	0.30	60,61,63,64	0
7	GOL	DDD	305	6/6	0.75	0.28	66,69,70,71	0
6	EDO	AAA	303	4/4	0.80	0.15	62,63,63,65	0
7	GOL	CCC	205	6/6	0.80	0.26	44,60,68,68	0
7	GOL	AAA	310	6/6	0.81	0.25	47,61,65,69	0
6	EDO	BBB	203	4/4	0.81	0.34	49,60,65,69	0
6	EDO	AAA	305	4/4	0.82	0.13	58,64,66,70	0
7	GOL	DDD	306	6/6	0.82	0.22	64,69,72,75	0
6	EDO	CCC	204	4/4	0.83	0.25	60,61,69,71	0
6	EDO	AAA	304	4/4	0.83	0.12	67,67,68,69	0
6	EDO	DDD	303	4/4	0.84	0.14	57,67,70,76	0
6	EDO	BBB	205	4/4	0.85	0.19	63,64,68,69	0
6	EDO	AAA	302	4/4	0.87	0.19	55,60,63,66	0
6	EDO	CCC	202	4/4	0.88	0.16	37,49,50,51	0
6	EDO	DDD	301	4/4	0.89	0.18	45,51,54,57	0
6	EDO	BBB	201	4/4	0.89	0.14	51,52,54,61	0
7	GOL	AAA	306	6/6	0.90	0.25	41,45,50,52	0
6	EDO	CCC	203	4/4	0.91	0.16	61,62,62,68	0
6	EDO	BBB	202	4/4	0.91	0.28	56,58,61,63	0
7	GOL	AAA	307	6/6	0.93	0.25	36,45,50,55	0
8	IOD	CCC	208	1/1	0.94	0.08	59,59,59,59	1
7	GOL	AAA	308	6/6	0.94	0.21	39,43,46,46	0
8	IOD	AAA	313	1/1	0.96	0.07	58,58,58,58	1
8	IOD	DDD	308	1/1	0.96	0.04	58,58,58,58	1
6	EDO	CCC	201	4/4	0.96	0.22	31,31,32,33	0
8	IOD	CCC	207[B]	1/1	0.97	0.06	51,51,51,51	1
5	QL8	AAA	301	93/93	0.97	0.09	21,25,50,54	0
8	IOD	CCC	207[A]	1/1	0.97	0.06	48,48,48,48	1
8	IOD	DDD	309	1/1	0.97	0.31	60,60,60,60	0
8	IOD	AAA	315[B]	1/1	0.99	0.07	62,62,62,62	1
8	IOD	AAA	311[A]	1/1	0.99	0.08	28,28,28,28	1
8	IOD	AAA	314	1/1	0.99	0.05	34,34,34,34	1
8	IOD	AAA	311[B]	1/1	0.99	0.08	30,30,30,30	1
8	IOD	AAA	315[A]	1/1	0.99	0.07	37,37,37,37	1
8	IOD	BBB	207	1/1	0.99	0.05	51,51,51,51	1
8	IOD	BBB	206[A]	1/1	1.00	0.06	29,29,29,29	1
8	IOD	BBB	206[B]	1/1	1.00	0.06	31,31,31,31	1
8	IOD	CCC	206[A]	1/1	1.00	0.11	28,28,28,28	1
8	IOD	AAA	312	1/1	1.00	0.07	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	IOD	CCC	206[B]	1/1	1.00	0.11	30,30,30,30	1

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.