



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 10:23 pm BST

PDB ID : 3T6A  
Title : Structure of the C-terminal domain of BCAR3  
Authors : Mace, P.D.; Robinson, H.; Riedl, S.J.  
Deposited on : 2011-07-28  
Resolution : 2.40 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.

---

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 : 2.11  
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) : 2.11

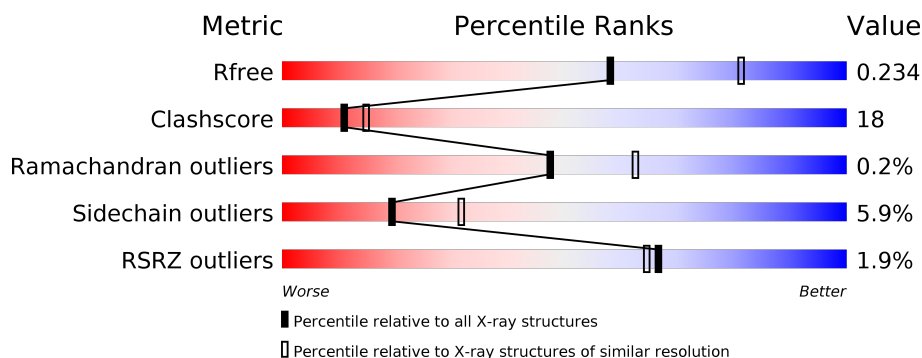
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	333	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>28%</div> <div>8%</div> </div> </div>
1	B	333	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>27%</div> <div>8%</div> </div> </div>
1	C	333	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>23%</div> <div>8%</div> </div> </div>
1	D	333	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>23%</div> <div>8%</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
3	UNX	D	841	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10297 atoms, of which 48 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 Breast cancer anti-estrogen resistance protein 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	308	Total	C	H	N	O	S	0	1	0
			2466	1545	12	427	462	20			
1	B	308	Total	C	H	N	O	S	0	3	0
			2480	1557	12	428	463	20			
1	C	308	Total	C	H	N	O	S	0	1	0
			2466	1545	12	427	462	20			
1	D	308	Total	C	H	N	O	S	0	2	0
			2471	1548	12	427	464	20			

There are 40 discrepancies between the modelled and reference sequences:

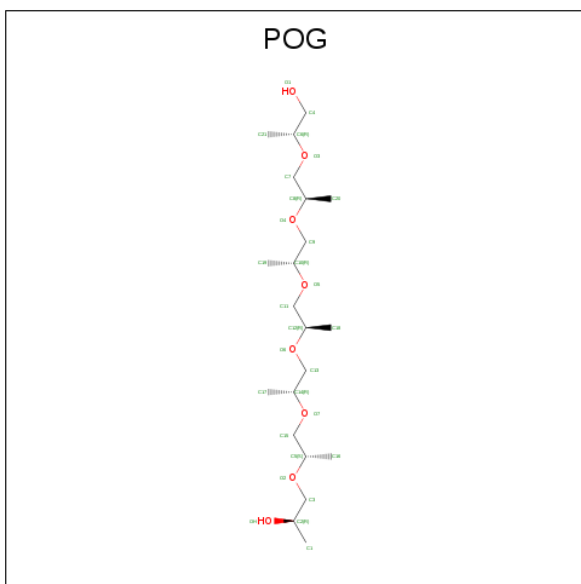
Chain	Residue	Modelled	Actual	Comment	Reference
A	501	MET	-	INITIATING METHIONINE	UNP 075815
A	536	LEU	MET	ENGINEERED MUTATION	UNP 075815
A	826	LEU	-	EXPRESSION TAG	UNP 075815
A	827	GLU	-	EXPRESSION TAG	UNP 075815
A	828	HIS	-	EXPRESSION TAG	UNP 075815
A	829	HIS	-	EXPRESSION TAG	UNP 075815
A	830	HIS	-	EXPRESSION TAG	UNP 075815
A	831	HIS	-	EXPRESSION TAG	UNP 075815
A	832	HIS	-	EXPRESSION TAG	UNP 075815
A	833	HIS	-	EXPRESSION TAG	UNP 075815
B	501	MET	-	INITIATING METHIONINE	UNP 075815
B	536	LEU	MET	ENGINEERED MUTATION	UNP 075815
B	826	LEU	-	EXPRESSION TAG	UNP 075815
B	827	GLU	-	EXPRESSION TAG	UNP 075815
B	828	HIS	-	EXPRESSION TAG	UNP 075815
B	829	HIS	-	EXPRESSION TAG	UNP 075815
B	830	HIS	-	EXPRESSION TAG	UNP 075815
B	831	HIS	-	EXPRESSION TAG	UNP 075815
B	832	HIS	-	EXPRESSION TAG	UNP 075815
B	833	HIS	-	EXPRESSION TAG	UNP 075815
C	501	MET	-	INITIATING METHIONINE	UNP 075815

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	536	LEU	MET	ENGINEERED MUTATION	UNP O75815
C	826	LEU	-	EXPRESSION TAG	UNP O75815
C	827	GLU	-	EXPRESSION TAG	UNP O75815
C	828	HIS	-	EXPRESSION TAG	UNP O75815
C	829	HIS	-	EXPRESSION TAG	UNP O75815
C	830	HIS	-	EXPRESSION TAG	UNP O75815
C	831	HIS	-	EXPRESSION TAG	UNP O75815
C	832	HIS	-	EXPRESSION TAG	UNP O75815
C	833	HIS	-	EXPRESSION TAG	UNP O75815
D	501	MET	-	INITIATING METHIONINE	UNP O75815
D	536	LEU	MET	ENGINEERED MUTATION	UNP O75815
D	826	LEU	-	EXPRESSION TAG	UNP O75815
D	827	GLU	-	EXPRESSION TAG	UNP O75815
D	828	HIS	-	EXPRESSION TAG	UNP O75815
D	829	HIS	-	EXPRESSION TAG	UNP O75815
D	830	HIS	-	EXPRESSION TAG	UNP O75815
D	831	HIS	-	EXPRESSION TAG	UNP O75815
D	832	HIS	-	EXPRESSION TAG	UNP O75815
D	833	HIS	-	EXPRESSION TAG	UNP O75815

- Molecule 2 is (20S)-2,5,8,11,14,17-HEXAMETHYL-3,6,9,12,15,18-HEXAOXAHENICOSAN E-1,20-DIOL (three-letter code: POG) (formula: C<sub>21</sub>H<sub>44</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	12	4		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			17	12	5		

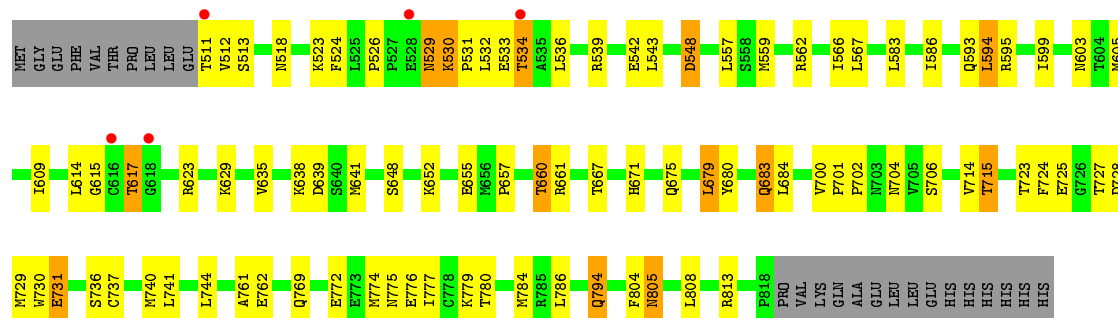
- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	8	Total	X	0	0
			8	8		

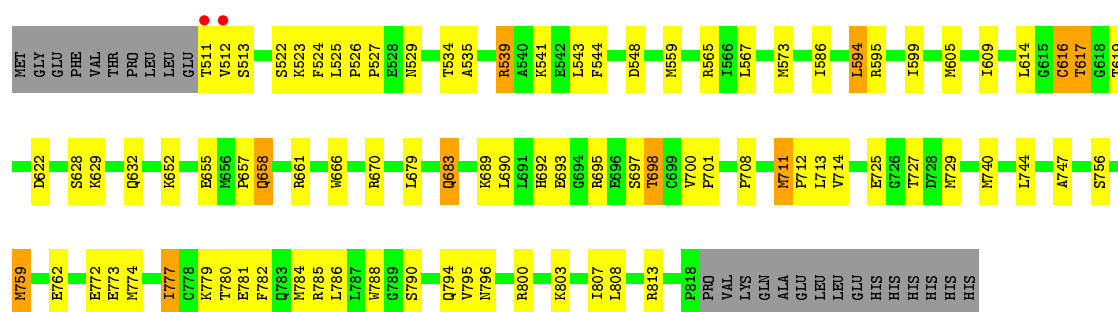
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		
4	B	105	Total	O	0	0
			105	105		
4	C	87	Total	O	0	0
			87	87		
4	D	88	Total	O	0	0
			88	88		





● Molecule 1: Breast cancer anti-estrogen resistance protein 3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.23 Å   151.89 Å   196.50 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.76 – 2.40 19.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (19.76-2.40) 98.6 (19.76-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.41 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.174   ,   0.244 0.169   ,   0.234	Depositor DCC
$R_{free}$ test set	2942 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.4	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	0.96	EDS
Total number of atoms	10297	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2527e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: UNX, POG

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	0.38	0/2500	0.52	0/3376
1	B	0.39	0/2521	0.52	0/3404
1	C	0.39	0/2500	0.54	0/3376
1	D	0.38	0/2508	0.53	0/3387
All	All	0.38	0/10029	0.53	0/13543

There are no bond length outliers.

There are no bond angle outliers.

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	A	2454	12	2484	94	0
1	B	2468	12	2501	108	0
1	C	2454	12	2484	84	0
1	D	2459	12	2488	88	0
2	A	16	0	23	0	0
2	B	17	0	24	7	0
3	D	8	0	0	0	0
4	A	93	0	0	6	0
4	B	105	0	0	13	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	87	0	0	6	0
4	D	88	0	0	7	0
All	All	10249	48	10004	360	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 18.

The worst 5 of 360 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:619:THR:HG23	1:D:622[B]:ASP:H	1.04	1.16
1:D:619:THR:HG23	1:D:622[A]:ASP:H	1.05	1.16
1:C:744:LEU:HD12	1:D:744:LEU:HD12	1.19	1.15
1:A:744:LEU:HD12	1:B:744:LEU:HD12	1.29	1.15
1:D:813:ARG:HH11	1:D:813:ARG:HG2	1.11	1.15

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	307/333 (92%)	292 (95%)	14 (5%)	1 (0%)	41	55
1	B	309/333 (93%)	295 (96%)	14 (4%)	0	100	100
1	C	307/333 (92%)	291 (95%)	15 (5%)	1 (0%)	41	55
1	D	308/333 (92%)	293 (95%)	14 (4%)	1 (0%)	41	55
All	All	1231/1332 (92%)	1171 (95%)	57 (5%)	3 (0%)	47	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	616	CYS
1	A	732	LYS
1	C	615	GLY

### 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	273/295 (92%)	258 (94%)	15 (6%)	21	35
1	B	275/295 (93%)	257 (94%)	18 (6%)	17	27
1	C	273/295 (92%)	255 (93%)	18 (7%)	16	26
1	D	274/295 (93%)	259 (94%)	15 (6%)	21	35
All	All	1095/1180 (93%)	1029 (94%)	66 (6%)	19	31

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	741	LEU
1	C	548	ASP
1	D	711	MET
1	B	748	ARG
1	C	529	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	593	GLN
1	B	733	ASN
1	D	658	GLN
1	B	658	GLN
1	B	683	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 8 are unknown - leaving 2 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	POG	B	834	-	12,16,28	1.32	2 (16%)	14,19,34	2.34	6 (42%)
2	POG	A	834	-	12,15,28	1.08	0	13,17,34	2.51	6 (46%)

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	POG	B	834	-	-	7/17/17/32	-
2	POG	A	834	-	-	8/16/16/32	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	834	POG	C9-C10	2.50	1.55	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	834	POG	C13-C14	2.13	1.55	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	834	POG	C11-O5-C10	5.44	123.14	115.02
2	B	834	POG	O4-C9-C10	4.04	122.49	111.78
2	B	834	POG	O7-C15-C5	3.89	116.40	108.86
2	A	834	POG	C9-O4-C8	3.49	120.24	115.02
2	A	834	POG	O5-C11-C12	3.35	118.98	110.90

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

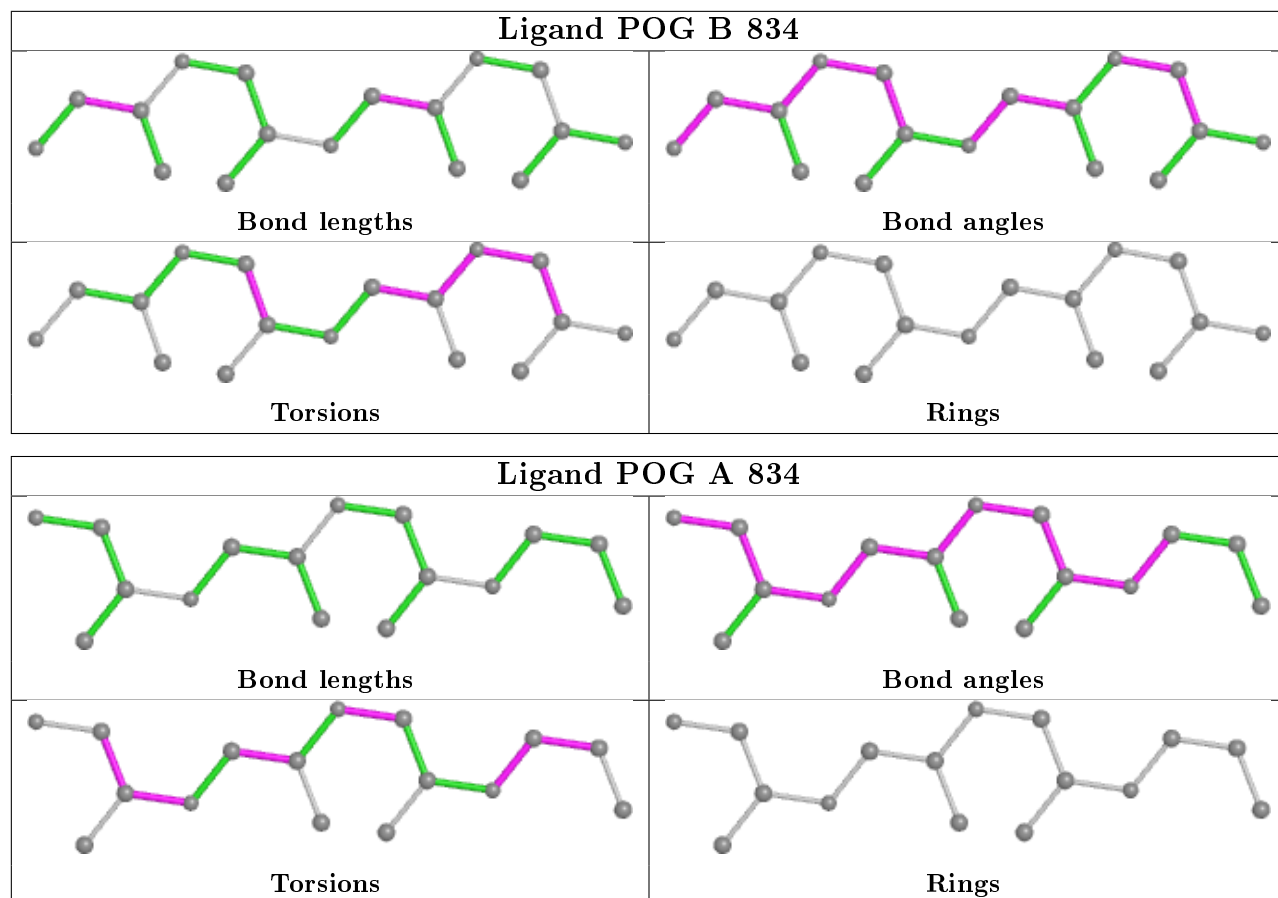
Mol	Chain	Res	Type	Atoms
2	B	834	POG	O5-C11-C12-O6
2	B	834	POG	O5-C11-C12-C18
2	B	834	POG	O6-C13-C14-O7
2	B	834	POG	O6-C13-C14-C17
2	B	834	POG	C17-C14-O7-C15

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	834	POG	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	308/333 (92%)	-0.41	7 (2%) 60 58	16, 37, 80, 125	0
1	B	308/333 (92%)	-0.36	9 (2%) 51 50	15, 38, 76, 125	0
1	C	308/333 (92%)	-0.45	5 (1%) 72 70	17, 37, 69, 129	0
1	D	308/333 (92%)	-0.44	2 (0%) 89 88	16, 39, 75, 123	0
All	All	1232/1332 (92%)	-0.41	23 (1%) 66 64	15, 38, 76, 129	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	511	THR	7.2
1	D	511	THR	6.6
1	B	733	ASN	5.9
1	C	616	CYS	4.8
1	B	732	LYS	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 carbohydrates in this entry.

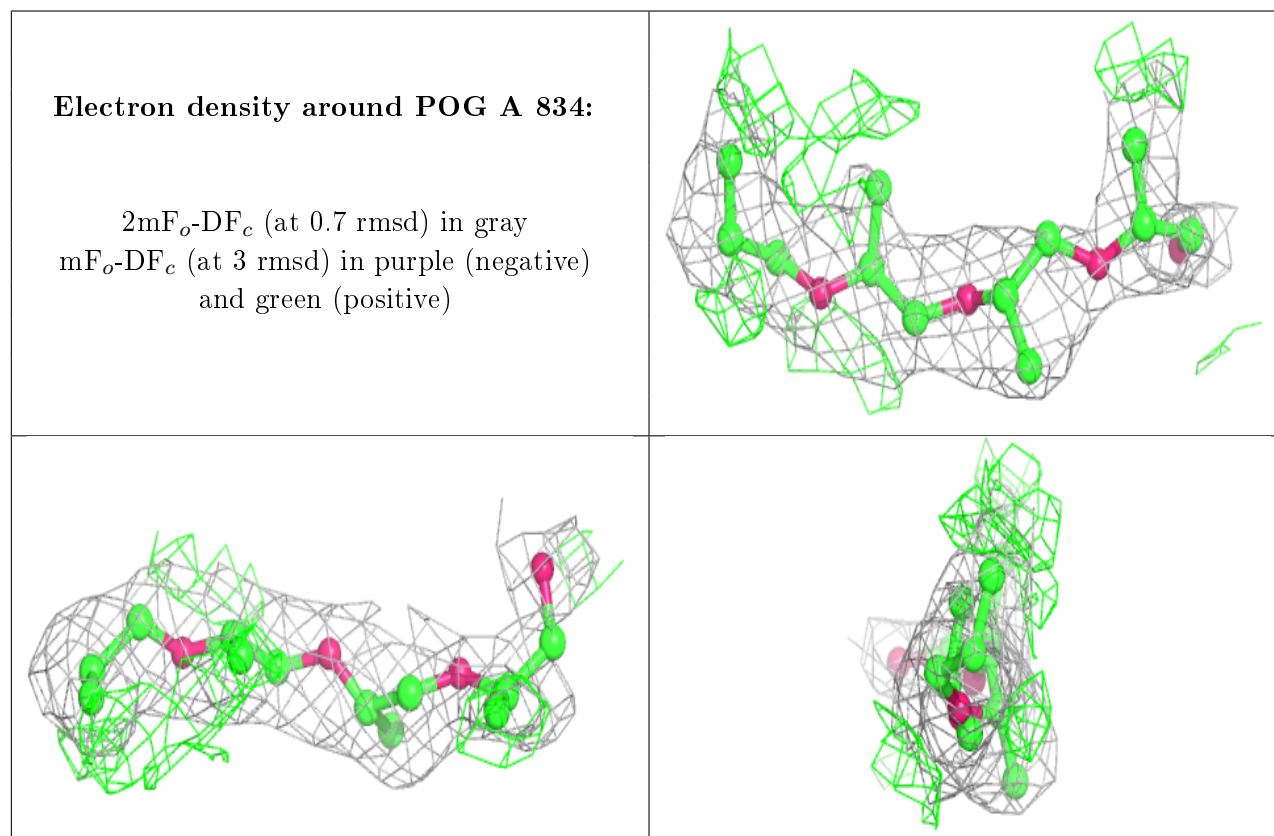
### 6.4 Ligands [i](#)

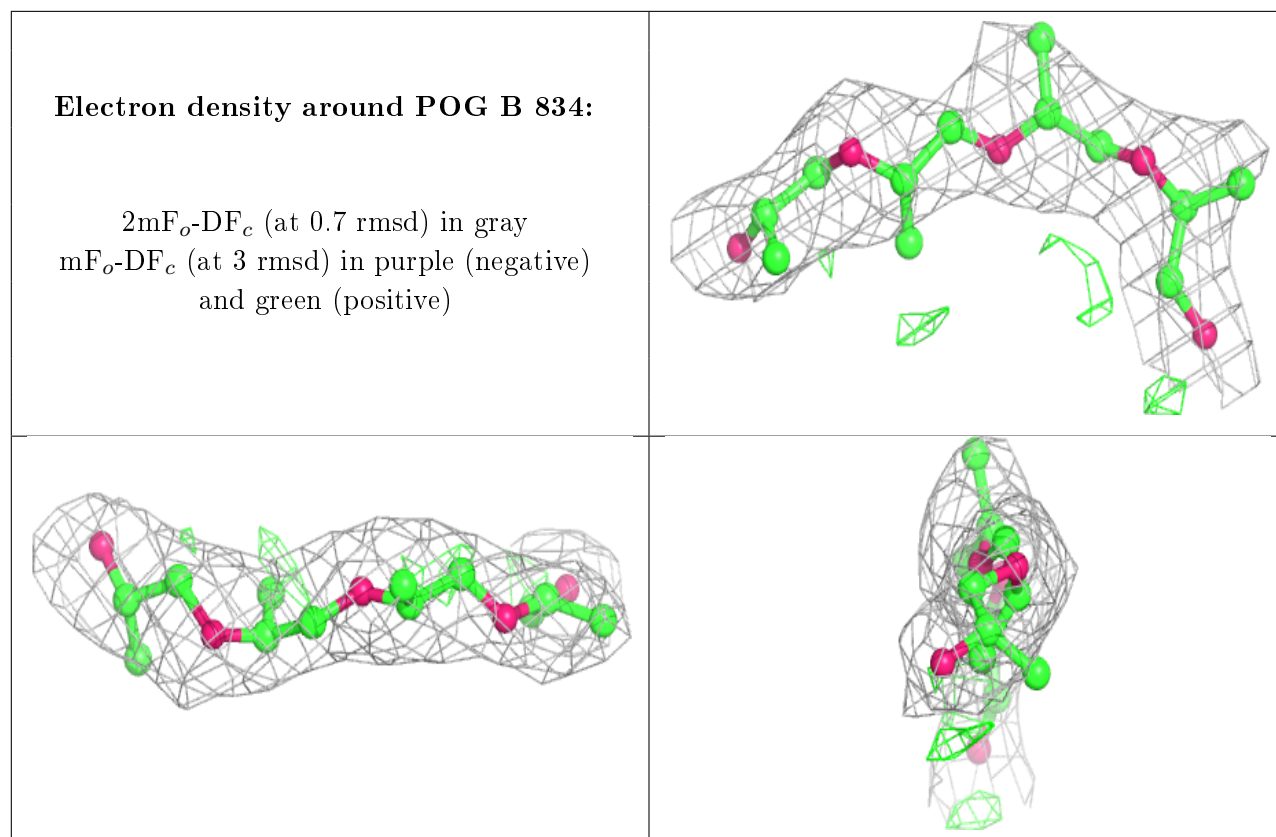
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	UNX	D	841	1/1	0.77	0.69	47,47,47,47	0
3	UNX	D	836	1/1	0.82	0.52	39,39,39,39	0
2	POG	A	834	16/29	0.83	0.19	23,54,74,75	0
3	UNX	D	840	1/1	0.84	0.63	41,41,41,41	0
3	UNX	D	839	1/1	0.87	0.42	33,33,33,33	0
2	POG	B	834	17/29	0.91	0.16	37,54,64,67	0
3	UNX	D	835	1/1	0.91	0.49	42,42,42,42	0
3	UNX	D	834	1/1	0.92	0.51	51,51,51,51	0
3	UNX	D	838	1/1	0.92	0.45	35,35,35,35	0
3	UNX	D	837	1/1	0.93	0.46	43,43,43,43	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.