



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2024 – 09:03 PM EDT

PDB ID : 6UDC  
Title : Spectroscopic and structural characterization of a genetically encoded direct sensor for protein-ligand interactions  
Authors : Mills, J.H.; Gleason, P.R.; Simmons, C.R.; Henderson, J.N.; Kartchner, B.K.  
Deposited on : 2019-09-19  
Resolution : 2.10 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 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

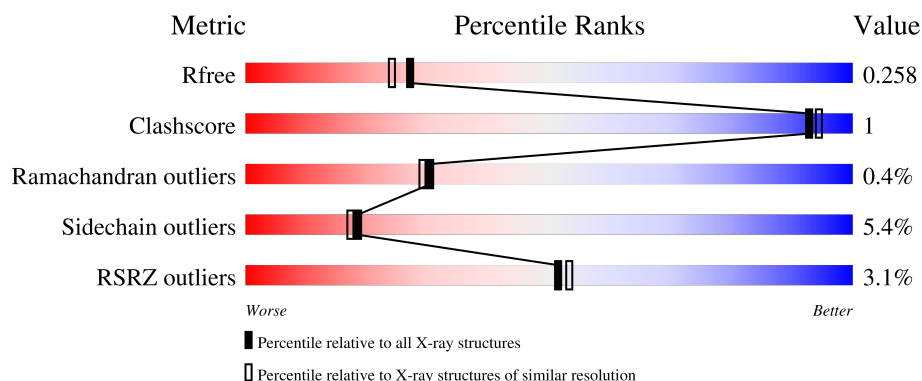
# 1 Overall quality at a glance

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))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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	136	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="width: 83%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">83%</span> </div> <div style="width: 12%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">12%</span> </div> </div>
1	B	136	<div> <div style="width: 3%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">3%</span> </div> <div style="width: 78%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">78%</span> </div> <div style="width: 10%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">10%</span> </div> <div style="width: 12%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">12%</span> </div> </div>
1	C	136	<div> <div style="width: 3%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">3%</span> </div> <div style="width: 78%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">78%</span> </div> <div style="width: 10%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">10%</span> </div> <div style="width: 12%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">12%</span> </div> </div>
1	D	136	<div> <div style="width: 4%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">4%</span> </div> <div style="width: 84%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">84%</span> </div> <div style="width: 10%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">10%</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3754 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 Streptavidin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	0	1	0
			910	569	155	186			
1	B	119	Total	C	N	O	0	0	0
			901	564	155	182			
1	C	120	Total	C	N	O	0	0	0
			906	566	155	185			
1	D	122	Total	C	N	O	0	1	0
			923	578	158	187			

There are 40 discrepancies between the modelled and reference sequences:

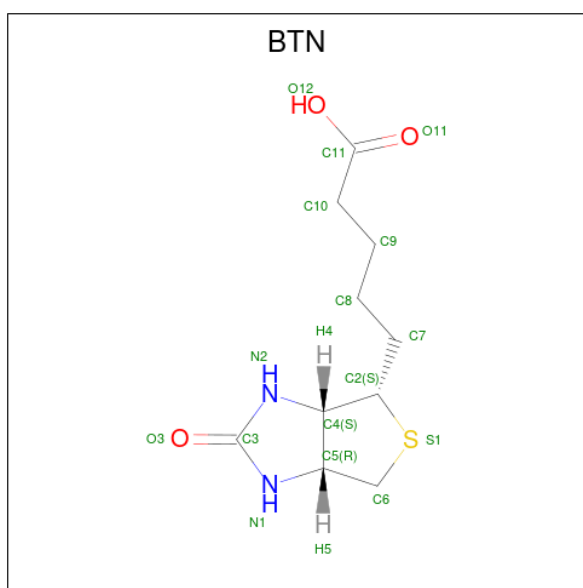
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P22629
A	110	DV7	LEU	conflict	UNP P22629
A	140	LEU	-	expression tag	UNP P22629
A	141	GLU	-	expression tag	UNP P22629
A	142	HIS	-	expression tag	UNP P22629
A	143	HIS	-	expression tag	UNP P22629
A	144	HIS	-	expression tag	UNP P22629
A	145	HIS	-	expression tag	UNP P22629
A	146	HIS	-	expression tag	UNP P22629
A	147	HIS	-	expression tag	UNP P22629
B	12	MET	-	initiating methionine	UNP P22629
B	110	DV7	LEU	conflict	UNP P22629
B	140	LEU	-	expression tag	UNP P22629
B	141	GLU	-	expression tag	UNP P22629
B	142	HIS	-	expression tag	UNP P22629
B	143	HIS	-	expression tag	UNP P22629
B	144	HIS	-	expression tag	UNP P22629
B	145	HIS	-	expression tag	UNP P22629
B	146	HIS	-	expression tag	UNP P22629
B	147	HIS	-	expression tag	UNP P22629
C	12	MET	-	initiating methionine	UNP P22629

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Chain	Residue	Modelled	Actual	Comment	Reference
C	110	DV7	LEU	conflict	UNP P22629
C	140	LEU	-	expression tag	UNP P22629
C	141	GLU	-	expression tag	UNP P22629
C	142	HIS	-	expression tag	UNP P22629
C	143	HIS	-	expression tag	UNP P22629
C	144	HIS	-	expression tag	UNP P22629
C	145	HIS	-	expression tag	UNP P22629
C	146	HIS	-	expression tag	UNP P22629
C	147	HIS	-	expression tag	UNP P22629
D	12	MET	-	initiating methionine	UNP P22629
D	110	DV7	LEU	conflict	UNP P22629
D	140	LEU	-	expression tag	UNP P22629
D	141	GLU	-	expression tag	UNP P22629
D	142	HIS	-	expression tag	UNP P22629
D	143	HIS	-	expression tag	UNP P22629
D	144	HIS	-	expression tag	UNP P22629
D	145	HIS	-	expression tag	UNP P22629
D	146	HIS	-	expression tag	UNP P22629
D	147	HIS	-	expression tag	UNP P22629

- Molecule 2 is BIOTIN (three-letter code: BTN) (formula:  $C_{10}H_{16}N_2O_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	B	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	D	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

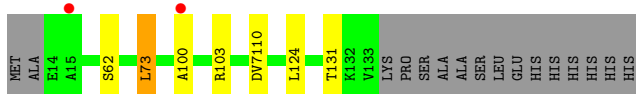
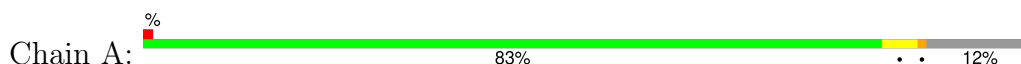
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	11	Total	O	0	0
			11	11		
3	C	13	Total	O	0	0
			13	13		
3	D	16	Total	O	0	0
			16	16		

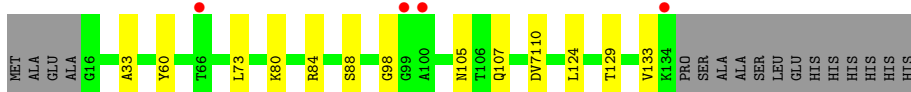
### 3 Residue-property plots [i](#)

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.

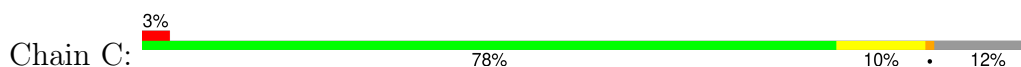
- Molecule 1: Streptavidin



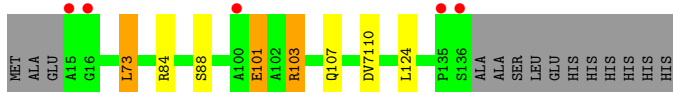
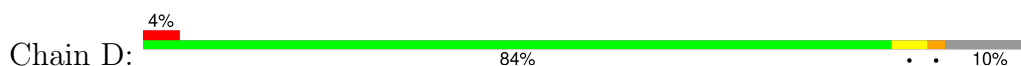
- Molecule 1: Streptavidin



- Molecule 1: Streptavidin



- Molecule 1: Streptavidin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.81Å 98.28Å 52.65Å 90.00° 112.26° 90.00°	Depositor
Resolution (Å)	49.14 – 2.10 49.14 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.7 (49.14-2.10) 96.8 (49.14-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.194 , 0.256 0.202 , 0.258	Depositor DCC
$R_{free}$ test set	2916 reflections (7.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 28.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.198 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BTN, DV7

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	0.83	0/916	0.92	2/1253 (0.2%)
1	B	0.81	0/904	0.91	0/1235
1	C	0.81	0/909	0.90	0/1243
1	D	0.85	0/930	0.91	2/1272 (0.2%)
All	All	0.82	0/3659	0.91	4/5003 (0.1%)

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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	124	LEU	CA-CB-CG	6.47	130.17	115.30
1	D	124	LEU	CA-CB-CG	5.89	128.86	115.30
1	D	73	LEU	CA-CB-CG	5.14	127.13	115.30
1	A	73	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	98	GLY	Peptide



## 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	910	0	830	2	0
1	B	901	0	825	4	0
1	C	906	0	823	5	0
1	D	923	0	849	1	0
2	A	16	0	15	0	0
2	B	16	0	15	0	0
2	C	16	0	15	0	0
2	D	16	0	15	0	0
3	A	10	0	0	0	0
3	B	11	0	0	0	0
3	C	13	0	0	0	0
3	D	16	0	0	0	0
All	All	3754	0	3387	10	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 1.

The worst 5 of 10 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:C:22:TYR:HE1	1:C:133:VAL:HG22	1.66	0.59
1:B:105:ASN:OD1	1:B:129:THR:HG23	2.04	0.57
1:A:62:SER:OG	1:B:80:LYS:HE3	2.14	0.47
1:C:132:LYS:C	1:C:133:VAL:HG23	2.37	0.45
1:C:37:GLY:O	1:C:59:ARG:HA	2.16	0.44

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	118/136 (87%)	111 (94%)	6 (5%)	1 (1%)	16	13
1	B	116/136 (85%)	111 (96%)	5 (4%)	0	100	100
1	C	117/136 (86%)	110 (94%)	6 (5%)	1 (1%)	14	11
1	D	120/136 (88%)	116 (97%)	4 (3%)	0	100	100
All	All	471/544 (87%)	448 (95%)	21 (4%)	2 (0%)	30	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ALA
1	C	68	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	88/100 (88%)	87 (99%)	1 (1%)	70	77
1	B	87/100 (87%)	82 (94%)	5 (6%)	17	15
1	C	87/100 (87%)	80 (92%)	7 (8%)	10	7
1	D	90/100 (90%)	84 (93%)	6 (7%)	13	11
All	All	352/400 (88%)	333 (95%)	19 (5%)	18	17

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	84	ARG
1	D	103	ARG
1	D	107	GLN
1	D	101	GLU
1	C	57	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	C	107	GLN
1	C	127	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	DV7	D	110	1	18,19,20	1.01	1 (5%)	21,26,28	1.62	4 (19%)
1	DV7	C	110	1	18,19,20	0.75	1 (5%)	21,26,28	1.61	5 (23%)
1	DV7	B	110	1	18,19,20	0.98	0	21,26,28	1.54	4 (19%)
1	DV7	A	110	1	18,19,20	0.79	0	21,26,28	1.52	5 (23%)

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	DV7	D	110	1	-	1/6/7/9	0/2/2/2
1	DV7	C	110	1	-	1/6/7/9	0/2/2/2
1	DV7	B	110	1	-	2/6/7/9	0/2/2/2
1	DV7	A	110	1	-	2/6/7/9	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	110	DV7	CB-CA	-2.33	1.50	1.53
1	D	110	DV7	OH1-CZ1	-2.27	1.34	1.38

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	110	DV7	CG-CD-CE2	4.18	123.29	118.68
1	C	110	DV7	CZ3-CE2-CZ2	-3.24	113.95	118.21
1	B	110	DV7	CG-CD-CE2	3.11	122.12	118.68
1	C	110	DV7	CG-CD-CE2	3.00	121.99	118.68
1	A	110	DV7	OH1-CZ1-OH2	-2.95	112.57	116.40

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	110	DV7	CA-CB-CG-CD
1	B	110	DV7	CA-CB-CG-CD
1	C	110	DV7	CA-CB-CG-CD
1	D	110	DV7	CA-CB-CG-CD
1	A	110	DV7	CE2-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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
2	BTN	C	5001	-	17,17,17	0.94	1 (5%)	23,23,23	2.02	3 (13%)
2	BTN	D	5001	-	17,17,17	1.21	3 (17%)	23,23,23	1.31	1 (4%)
2	BTN	B	5001	-	17,17,17	0.89	0	23,23,23	2.06	3 (13%)
2	BTN	A	5001	-	17,17,17	1.14	2 (11%)	23,23,23	1.33	2 (8%)

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	BTN	C	5001	-	-	0/7/28/28	0/2/2/2
2	BTN	D	5001	-	-	1/7/28/28	0/2/2/2
2	BTN	B	5001	-	-	2/7/28/28	0/2/2/2
2	BTN	A	5001	-	-	0/7/28/28	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5001	BTN	C5-N1	-2.55	1.42	1.46
2	A	5001	BTN	C6-S1	-2.35	1.74	1.81
2	C	5001	BTN	C2-S1	-2.19	1.79	1.82
2	D	5001	BTN	C2-S1	-2.16	1.79	1.82
2	A	5001	BTN	C2-S1	-2.02	1.79	1.82

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5001	BTN	C2-C4-N2	7.58	121.37	113.34
2	C	5001	BTN	C4-C2-S1	5.45	111.22	105.03
2	C	5001	BTN	C5-C6-S1	4.94	112.86	106.06
2	D	5001	BTN	C6-C5-N1	-4.31	107.63	113.18
2	C	5001	BTN	C2-C4-N2	4.24	117.83	113.34

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5001	BTN	C9-C10-C11-O11
2	B	5001	BTN	C9-C10-C11-O12

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
2	D	5001	BTN	C9-C10-C11-O11

There are no ring outliers.

No monomer is involved in short contacts.

## 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	119/136 (87%)	0.17	2 (1%) 69 70	21, 36, 62, 98	1 (0%)
1	B	118/136 (86%)	0.28	4 (3%) 48 50	25, 39, 64, 90	0
1	C	119/136 (87%)	0.21	4 (3%) 48 50	24, 38, 61, 122	0
1	D	121/136 (88%)	0.18	5 (4%) 42 44	21, 36, 63, 110	1 (0%)
All	All	477/544 (87%)	0.21	15 (3%) 51 53	21, 37, 63, 122	2 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	ALA	4.5
1	C	133	VAL	4.4
1	D	15	ALA	4.3
1	D	100	ALA	4.2
1	D	135	PRO	3.9

### 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	DV7	C	110	18/19	0.92	0.10	26,38,43,47	0
1	DV7	A	110	18/19	0.93	0.10	24,35,43,44	0
1	DV7	B	110	18/19	0.94	0.10	26,41,51,53	0
1	DV7	D	110	18/19	0.95	0.09	27,32,38,40	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( $\text{\AA}^2$ )	Q<0.9
2	BTN	C	5001	16/16	0.95	0.08	32,34,40,40	0
2	BTN	B	5001	16/16	0.96	0.08	24,32,38,40	0
2	BTN	D	5001	16/16	0.96	0.07	27,30,35,36	0
2	BTN	A	5001	16/16	0.97	0.07	29,32,37,39	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.