



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 01:42 AM EDT

PDB ID : 1SLY  
Title : COMPLEX OF THE 70-KDA SOLUBLE LYTIC TRANSGLYCOSYLASE  
WITH BULGECIN A  
Authors : Thunnissen, A.M.W.H.; Kalk, K.H.; Rozeboom, H.J.; Dijkstra, B.W.  
Deposited on : 1995-08-02  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

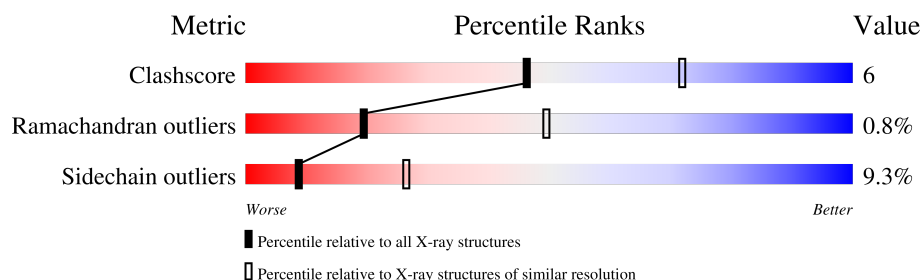
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	618	

## 2 Entry composition [i](#)

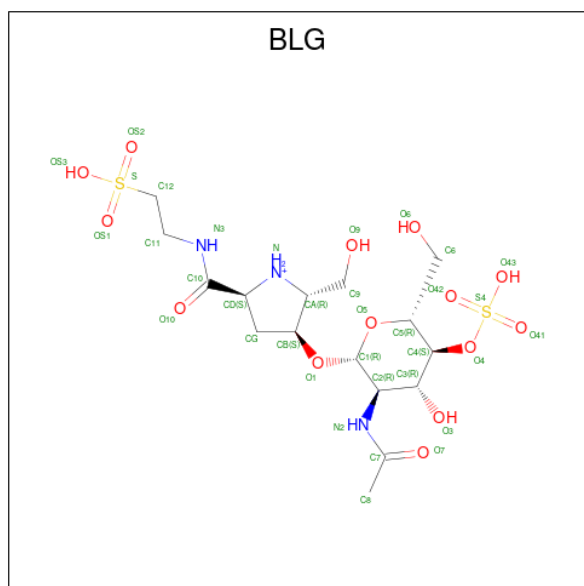
There are 2 unique types of molecules in this entry. The entry contains 5000 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 70-KDA SOLUBLE LYTIC TRANSGLYCOSYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	618	4965	3126	883	932	24	0	0	0

- Molecule 2 is 4-O-(4-O-SULFONYL-N-ACETYLGLUCOSAMININYL)-5-METHYLHYDROXY-L-PROLINE-TAURINE (three-letter code: BLG) (formula:  $C_{16}H_{30}N_3O_{14}S_2$ ).



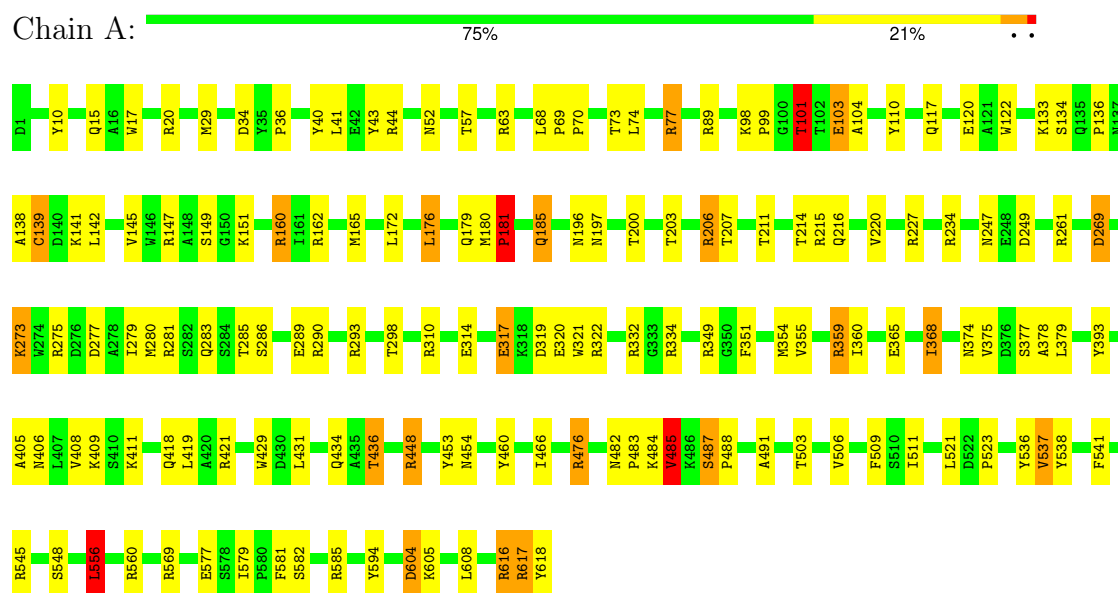
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	35	16	3	14	2	0	0

### 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. 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. 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.

Note EDS was not executed.

#### • Molecule 1: 70-KDA SOLUBLE LYTIC TRANSGLYCOSYLASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.31 Å 88.47 Å 133.06 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	88.1 (8.00-2.80)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.185 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5000	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

## 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: BLG

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	0.71	1/5079 (0.0%)	1.52	48/6888 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	ILE	CA-CB	5.49	1.67	1.54

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	616	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	A	359	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	A	354	MET	CG-SD-CE	-7.82	87.69	100.20
1	A	234	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	A	179	GLN	CA-CB-CG	7.64	130.20	113.40
1	A	15	GLN	CA-CB-CG	7.48	129.86	113.40
1	A	569	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	322	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	A	215	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	29	MET	CA-CB-CG	-7.02	101.36	113.30
1	A	545	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	206	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	332	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	A	448	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	63	ARG	CA-CB-CG	6.50	127.70	113.40
1	A	594	TYR	CB-CG-CD2	-6.34	117.19	121.00
1	A	485	VAL	CB-CA-C	-6.33	99.38	111.40
1	A	393	TYR	CB-CG-CD1	-6.29	117.23	121.00
1	A	476	ARG	CG-CD-NE	-6.19	98.79	111.80
1	A	460	TYR	CB-CG-CD1	-6.16	117.30	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	A	537	VAL	N-CA-CB	-6.00	98.31	111.50
1	A	521	LEU	CB-CG-CD1	-5.99	100.82	111.00
1	A	349	ARG	CA-CB-CG	5.92	126.42	113.40
1	A	616	ARG	CD-NE-CZ	5.68	131.55	123.60
1	A	560	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	40	TYR	CB-CG-CD1	-5.61	117.63	121.00
1	A	89	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	298	THR	CA-CB-CG2	5.60	120.24	112.40
1	A	379	LEU	CA-C-N	-5.56	104.97	117.20
1	A	234	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	355	VAL	CG1-CB-CG2	-5.50	102.10	110.90
1	A	160	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	101	THR	CA-CB-CG2	5.45	120.03	112.40
1	A	185	GLN	CA-CB-CG	5.41	125.31	113.40
1	A	617	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	10	TYR	CB-CG-CD2	-5.34	117.79	121.00
1	A	44	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	139	CYS	CA-CB-SG	-5.33	104.42	114.00
1	A	429	TRP	CG-CD2-CE3	-5.26	129.17	133.90
1	A	368	ILE	CA-C-N	-5.23	105.69	117.20
1	A	604	ASP	CA-CB-CG	5.22	124.88	113.40
1	A	460	TYR	CB-CG-CD2	5.18	124.11	121.00
1	A	283	GLN	CA-CB-CG	5.16	124.74	113.40
1	A	290	ARG	CA-CB-CG	5.14	124.72	113.40
1	A	476	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	227	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	618	TYR	CB-CG-CD1	5.01	124.00	121.00

There are no chirality outliers.

There are no planarity outliers.

## 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	4965	0	4852	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	35	0	29	0	0
All	All	5000	0	4881	62	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 6.

All (62) 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:A:280:MET:SD	1:A:310:ARG:HD2	2.12	0.90
1:A:556:LEU:H	1:A:556:LEU:HD22	1.49	0.78
1:A:436:THR:HG21	1:A:448:ARG:HG2	1.66	0.77
1:A:375:VAL:HG13	1:A:418:GLN:HB3	1.67	0.75
1:A:101:THR:HG22	1:A:104:ALA:H	1.51	0.75
1:A:103:GLU:HG2	1:A:136:PRO:HB3	1.69	0.75
1:A:68:LEU:HG	1:A:70:PRO:HD2	1.69	0.74
1:A:506:VAL:HG23	1:A:511:ILE:HB	1.71	0.70
1:A:149:SER:OG	1:A:151:LYS:HB2	1.96	0.65
1:A:436:THR:CG2	1:A:448:ARG:HG2	2.26	0.64
1:A:411:LYS:N	1:A:411:LYS:HD2	2.16	0.61
1:A:43:TYR:HE1	1:A:74:LEU:HG	1.70	0.55
1:A:293:ARG:HD3	1:A:577:GLU:O	2.08	0.54
1:A:172:LEU:O	1:A:176:LEU:HB2	2.08	0.54
1:A:537:VAL:HG22	1:A:556:LEU:HD11	1.90	0.54
1:A:103:GLU:HG2	1:A:136:PRO:CB	2.39	0.53
1:A:172:LEU:HG	1:A:176:LEU:HD22	1.91	0.53
1:A:99:PRO:HG2	1:A:104:ALA:HB1	1.91	0.52
1:A:503:THR:O	1:A:506:VAL:HG12	2.09	0.52
1:A:43:TYR:CE1	1:A:74:LEU:HG	2.44	0.51
1:A:197:ASN:ND2	1:A:200:THR:HG23	2.26	0.50
1:A:537:VAL:CG2	1:A:556:LEU:HD11	2.43	0.49
1:A:277:ASP:HB3	1:A:281:ARG:HH12	1.78	0.49
1:A:216:GLN:O	1:A:220:VAL:HG23	2.13	0.48
1:A:405:ALA:O	1:A:409:LYS:HB2	2.14	0.48
1:A:73:THR:O	1:A:77:ARG:HB2	2.13	0.47
1:A:556:LEU:H	1:A:556:LEU:CD2	2.23	0.47
1:A:160:ARG:HG2	1:A:176:LEU:HD21	1.97	0.47
1:A:141:LYS:O	1:A:145:VAL:HG22	2.15	0.47
1:A:110:TYR:CE2	1:A:141:LYS:HD2	2.50	0.46
1:A:117:GLN:O	1:A:120:GLU:HB2	2.15	0.46
1:A:147:ARG:HH12	1:A:181:PRO:HD3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:THR:O	1:A:289:GLU:HG3	2.15	0.46
1:A:482:ASN:O	1:A:485:VAL:HG22	2.16	0.46
1:A:483:PRO:HB2	1:A:484:LYS:HE2	1.97	0.46
1:A:421:ARG:HA	1:A:421:ARG:HD2	1.75	0.45
1:A:133:LYS:HE2	1:A:134:SER:O	2.17	0.45
1:A:453:TYR:OH	1:A:483:PRO:HG3	2.15	0.45
1:A:541:PHE:HE2	1:A:556:LEU:HD12	1.82	0.45
1:A:314:GLU:O	1:A:317:GLU:HB2	2.16	0.45
1:A:69:PRO:HG3	1:A:406:ASN:ND2	2.33	0.44
1:A:579:ILE:HG22	1:A:581:PHE:H	1.83	0.43
1:A:506:VAL:HA	1:A:511:ILE:HD12	1.99	0.43
1:A:293:ARG:NH1	1:A:577:GLU:OE2	2.51	0.43
1:A:487:SER:HB3	1:A:491:ALA:HB3	2.01	0.42
1:A:138:ALA:O	1:A:141:LYS:HG2	2.18	0.42
1:A:360:ILE:HD13	1:A:360:ILE:HG21	1.82	0.42
1:A:408:VAL:HG12	1:A:419:LEU:HD13	2.02	0.42
1:A:506:VAL:CG2	1:A:511:ILE:HB	2.44	0.42
1:A:538:TYR:HA	1:A:548:SER:HB3	2.02	0.42
1:A:275:ARG:O	1:A:279:ILE:HG13	2.20	0.41
1:A:269:ASP:O	1:A:273:LYS:HG2	2.20	0.41
1:A:277:ASP:HB3	1:A:281:ARG:NH1	2.35	0.41
1:A:351:PHE:CE1	1:A:608:LEU:HD21	2.56	0.41
1:A:448:ARG:HG2	1:A:448:ARG:HH11	1.85	0.41
1:A:203:THR:O	1:A:207:THR:HB	2.21	0.41
1:A:320:GLU:HG2	1:A:321:TRP:N	2.36	0.41
1:A:509:PHE:CZ	1:A:536:TYR:HB2	2.56	0.41
1:A:556:LEU:HD22	1:A:556:LEU:N	2.27	0.41
1:A:17:TRP:O	1:A:20:ARG:NH1	2.54	0.40
1:A:579:ILE:O	1:A:585:ARG:NH1	2.55	0.40
1:A:466:ILE:HG13	1:A:466:ILE:O	2.21	0.40

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	616/618 (100%)	579 (94%)	32 (5%)	5 (1%)	19	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	SER
1	A	319	ASP
1	A	378	ALA
1	A	556	LEU
1	A	181	PRO

### 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	514/514 (100%)	466 (91%)	48 (9%)	9	26

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	36	PRO
1	A	41	LEU
1	A	52	ASN
1	A	57	THR
1	A	77	ARG
1	A	98	LYS
1	A	101	THR
1	A	103	GLU
1	A	122	TRP
1	A	139	CYS
1	A	142	LEU
1	A	162	ARG
1	A	165	MET

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Mol	Chain	Res	Type
1	A	176	LEU
1	A	180	MET
1	A	181	PRO
1	A	185	GLN
1	A	196	ASN
1	A	206	ARG
1	A	211	THR
1	A	214	THR
1	A	247	ASN
1	A	249	ASP
1	A	261	ARG
1	A	269	ASP
1	A	273	LYS
1	A	286	SER
1	A	317	GLU
1	A	359	ARG
1	A	365	GLU
1	A	368	ILE
1	A	374	ASN
1	A	431	LEU
1	A	434	GLN
1	A	436	THR
1	A	454	ASN
1	A	476	ARG
1	A	485	VAL
1	A	487	SER
1	A	488	PRO
1	A	523	PRO
1	A	556	LEU
1	A	582	SER
1	A	604	ASP
1	A	605	LYS
1	A	616	ARG
1	A	617	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	325	GLN
1	A	416	GLN
1	A	454	ASN

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Mol	Chain	Res	Type
1	A	468	GLN
1	A	477	GLN
1	A	590	ASN

### 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 ⓘ

1 ligand is 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	BLG	A	619	-	36,36,36	1.47	5 (13%)	43,53,53	1.55	9 (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	BLG	A	619	-	-	6/28/60/60	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	619	BLG	O1-CB	-5.44	1.34	1.44
2	A	619	BLG	C12-S	3.28	1.82	1.77
2	A	619	BLG	OS1-S	2.75	1.52	1.45
2	A	619	BLG	CD-N	2.71	1.52	1.46
2	A	619	BLG	OS2-S	2.42	1.51	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	619	BLG	CD-C10-N3	-3.72	108.55	116.54
2	A	619	BLG	O9-C9-CA	-3.50	102.62	111.10
2	A	619	BLG	O10-C10-CD	3.33	127.45	120.48
2	A	619	BLG	CG-CD-C10	3.09	116.17	111.38
2	A	619	BLG	OS3-S-OS2	-2.95	104.03	111.40
2	A	619	BLG	C9-CA-N	2.47	115.83	111.47
2	A	619	BLG	CG-CB-CA	-2.25	100.64	103.88
2	A	619	BLG	OS3-S-C12	2.03	109.98	106.00
2	A	619	BLG	OS2-S-C12	2.01	109.77	106.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

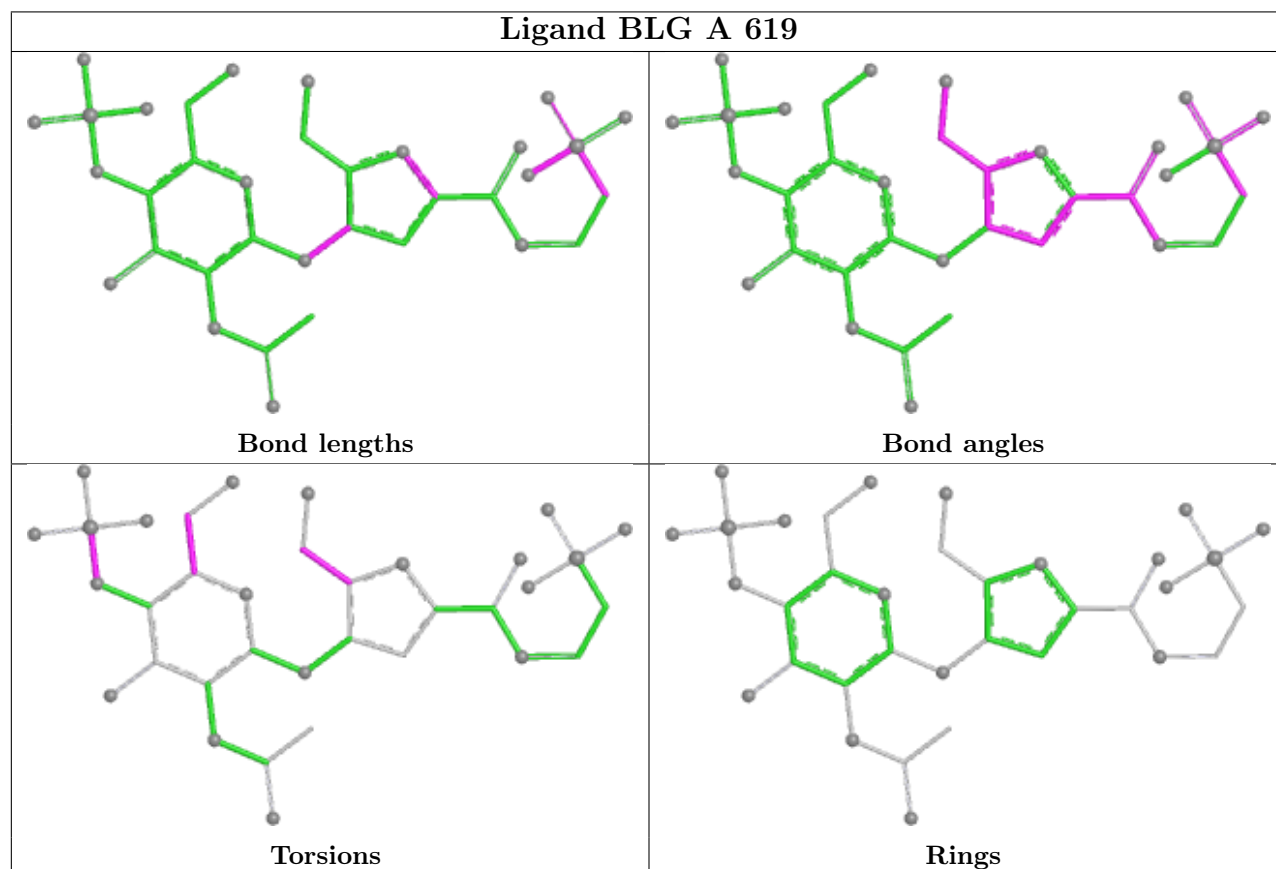
Mol	Chain	Res	Type	Atoms
2	A	619	BLG	C4-O4-S4-O43
2	A	619	BLG	O9-C9-CA-N
2	A	619	BLG	C4-C5-C6-O6
2	A	619	BLG	O5-C5-C6-O6
2	A	619	BLG	C4-O4-S4-O42
2	A	619	BLG	C4-O4-S4-O41

There are no ring outliers.

No monomer is involved in short contacts.

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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.