

Full wwPDB X-ray Structure Validation Report (i)

Apr 9, 2024 – 10:13 am BST

PDB ID : 8RHF

Title: Lytic Transglycosylase MltD of Pseudomonas aeruginosa bound to the Natural

Product Bulgecin A, with two LysM domains

Authors : Miguel-Ruano, V.; Hermoso, J.A.

Deposited on : 2023-12-15

Resolution : 1.95 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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS: 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

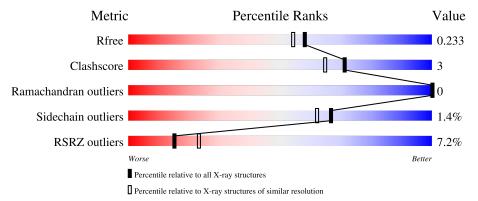
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.95 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 >=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 <=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	338	86%	10%	•	-
1	В	338	91%	69	6	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5810 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 LysM peptidoglycan-binding domain-containing protein.

\mathbf{Mol}	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace	
1	R	327	Total	С	N	О	S	0	0	0	
1	Ъ	921	2634	1660	475	491	8	0	0	U	
1	Λ	327	Total	С	N	О	S	0	2	0	
1	Λ	921	2665	1677	482	498	8		3	U	

There are 40 discrepancies between the modelled and reference sequences:

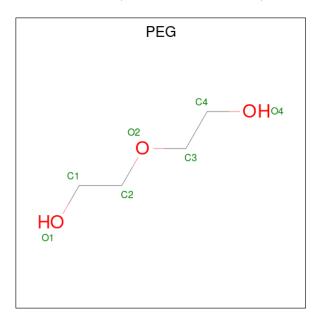
Chain	Residue	Modelled	Actual	Comment	Reference
В	56	MET	-	initiating methionine	UNP A0A0C7CWY9
В	57	GLY	-	expression tag	UNP A0A0C7CWY9
В	58	SER	-	expression tag	UNP A0A0C7CWY9
В	59	SER	-	expression tag	UNP A0A0C7CWY9
В	60	HIS	-	expression tag	UNP A0A0C7CWY9
В	61	HIS	-	expression tag	UNP A0A0C7CWY9
В	62	HIS	-	expression tag	UNP A0A0C7CWY9
В	63	HIS	-	expression tag	UNP A0A0C7CWY9
В	64	HIS	-	expression tag	UNP A0A0C7CWY9
В	65	HIS	-	expression tag	UNP A0A0C7CWY9
В	66	SER	-	expression tag	UNP A0A0C7CWY9
В	67	SER	-	expression tag	UNP A0A0C7CWY9
В	68	GLY	-	expression tag	UNP A0A0C7CWY9
В	69	GLU	-	expression tag	UNP A0A0C7CWY9
В	70	ASN	-	expression tag	UNP A0A0C7CWY9
В	71	LEU	-	expression tag	UNP A0A0C7CWY9
В	72	TYR	-	expression tag	UNP A0A0C7CWY9
В	73	PHE	-	expression tag	UNP A0A0C7CWY9
В	74	GLN	-	expression tag	UNP A0A0C7CWY9
В	75	GLY	-	expression tag	UNP A0A0C7CWY9
A	56	MET	-	initiating methionine	UNP A0A0C7CWY9
A	57	GLY	-	expression tag	UNP A0A0C7CWY9
A	58	SER	_	expression tag	UNP A0A0C7CWY9
A	59	SER	-	expression tag	UNP A0A0C7CWY9
A	60	HIS	-	expression tag	UNP A0A0C7CWY9



Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	HIS	-	expression tag	UNP A0A0C7CWY9
A	62	HIS	-	expression tag	UNP A0A0C7CWY9
A	63	HIS	-	expression tag	UNP A0A0C7CWY9
A	64	HIS	-	expression tag	UNP A0A0C7CWY9
A	65	HIS	-	expression tag	UNP A0A0C7CWY9
A	66	SER	-	expression tag	UNP A0A0C7CWY9
A	67	SER	-	expression tag	UNP A0A0C7CWY9
A	68	GLY	-	expression tag	UNP A0A0C7CWY9
A	69	GLU	-	expression tag	UNP A0A0C7CWY9
A	70	ASN	-	expression tag	UNP A0A0C7CWY9
A	71	LEU	-	expression tag	UNP A0A0C7CWY9
A	72	TYR	-	expression tag	UNP A0A0C7CWY9
A	73	PHE	-	expression tag	UNP A0A0C7CWY9
A	74	GLN	-	expression tag	UNP A0A0C7CWY9
A	75	GLY	-	expression tag	UNP A0A0C7CWY9

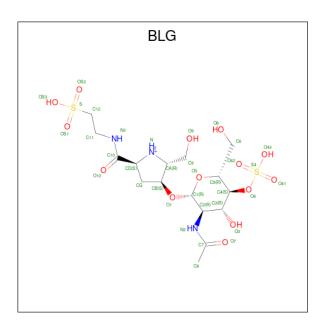
• Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total C O 7 4 3	0	0
2	A	1	Total C O 7 4 3	0	0

• Molecule 3 is 4-O-(4-O-SULFONYL-N-ACETYLGLUCOSAMININYL)-5-METHYLHYDR OXY-L-PROLINE-TAURINE (three-letter code: BLG) (formula: $C_{16}H_{30}N_3O_{14}S_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
9	D	1	Total	С	N	О	S	0	0
3	Б	1	35	16	3	14	2	U	U
9	Λ	1	Total	С	N	О	S	0	1
3	A	1	70	32	6	28	4	U	1

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mo	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
4		В	7	Total Zn 7 7	0	0
4		A	5	Total Zn 5 5	0	0

• Molecule 5 is water.

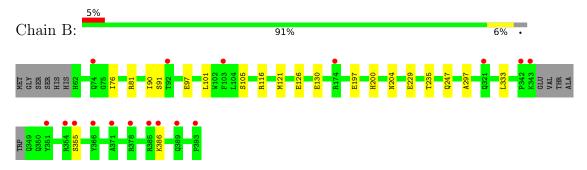
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	176	Total O 176 176	0	0
5	A	204	Total O 204 204	0	0



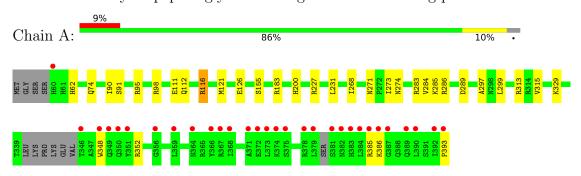
3 Residue-property plots (i)

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: LysM peptidoglycan-binding domain-containing protein



• Molecule 1: LysM peptidoglycan-binding domain-containing protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	46.75Å 116.53Å 121.10Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.62 - 1.95	Depositor
resolution (A)	60.55 - 1.95	EDS
% Data completeness	99.0 (60.62-1.95)	Depositor
(in resolution range)	99.0 (60.55-1.95)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.72 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.186 , 0.228	Depositor
it, it free	0.193 , 0.233	DCC
R_{free} test set	2375 reflections $(4.88%)$	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30, 44.3	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5810	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: ZN, PEG, 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).

Mal	Mol Chain		nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.43	0/2727	0.71	0/3699	
1	В	0.43	1/2694 (0.0%)	0.68	2/3653 (0.1%)	
All	All	0.43	1/5421 (0.0%)	0.70	$2/7352 \ (0.0\%)$	

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	В	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
1	В	197	GLU	CD-OE2	6.72	1.33	1.25

All (2) bond angle outliers are listed below:

Mo	l Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	В	81	ARG	CG-CD-NE	-6.32	98.53	111.80
1	В	81	ARG	CB-CA-C	-6.22	97.96	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	116	ARG	Sidechain
1	A	183	ARG	Sidechain
1	A	283	ARG	Sidechain
1	A	313	ARG	Sidechain
1	A	95	ARG	Sidechain
1	В	116	ARG	Sidechain

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	2665	0	2585	24	0
1	В	2634	0	2583	12	0
2	A	7	0	10	1	0
2	В	7	0	10	0	0
3	A	70	0	56	1	0
3	В	35	0	28	0	0
4	A	5	0	0	0	0
4	В	7	0	0	0	0
5	A	204	0	0	11	0
5	В	176	0	0	5	0
All	All	5810	0	5272	37	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 3.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	$egin{array}{c} { m Clash} \\ { m overlap} \ ({ m \AA}) \end{array}$
1:A:297:ALA:HB3	1:A:299:LEU:HD13	1.57	0.86
1:A:155:SER:OG	3:A:402[A]:BLG:OS1	1.95	0.85
1:A:274:ASN:HB3	5:A:681:HOH:O	1.77	0.84
1:B:126:GLU:OE1	5:B:501:HOH:O	2.00	0.77
1:A:126:GLU:OE1	5:A:501:HOH:O	2.04	0.74
1:A:227:ARG:O	1:A:231:LEU:HD13	1.97	0.64
1:A:289:ASP:HB3	1:A:315:VAL:HG12	1.82	0.62
1:A:352:ARG:NH2	5:A:504:HOH:O	2.34	0.60



Continued from previous page...

Continued from prediction		Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	overlap (Å)
1:B:91:SER:CB	5:B:514:HOH:O	2.50	0.58
1:A:121:MET:HE3	1:A:273:ILE:HD13	1.86	0.58
1:A:98:ARG:NH1	5:A:507:HOH:O	2.37	0.57
1:A:386:LYS:NZ	5:A:504:HOH:O	2.38	0.57
1:A:111[B]:GLU:CD	1:A:271:ASN:OD1	2.43	0.57
1:A:121:MET:CE	1:A:273:ILE:HD13	2.36	0.56
1:B:229:GLU:HG3	1:B:235:THR:HG21	1.89	0.54
1:A:299:LEU:HD11	1:A:329:LYS:HG3	1.89	0.54
1:A:297:ALA:CB	1:A:299:LEU:HD13	2.33	0.54
1:B:247:GLN:NE2	5:B:509:HOH:O	2.39	0.51
1:B:90:ILE:HG22	1:B:91:SER:N	2.25	0.50
1:A:393:PRO:HB2	5:A:696:HOH:O	2.12	0.50
1:B:91:SER:HB3	5:B:514:HOH:O	2.13	0.49
1:B:90:ILE:CG2	1:B:91:SER:N	2.78	0.47
1:B:76:ILE:HG21	1:B:121:MET:HE2	1.97	0.46
1:A:90:ILE:HG22	1:A:91:SER:N	2.31	0.45
1:A:116:ARG:HD3	5:A:687:HOH:O	2.16	0.44
1:B:355:SER:HB2	1:B:386:LYS:HE2	2.00	0.44
1:A:284:VAL:HG12	1:A:285:LYS:O	2.18	0.43
2:A:401:PEG:H12	5:A:690:HOH:O	2.17	0.43
1:A:62:HIS:HD2	5:A:672:HOH:O	2.02	0.42
1:B:297:ALA:HB2	1:B:333:LEU:HD21	2.01	0.42
1:A:289:ASP:CB	1:A:315:VAL:HG12	2.47	0.42
1:A:90:ILE:CG2	1:A:91:SER:N	2.84	0.41
1:A:286:ARG:HD3	5:A:668:HOH:O	2.20	0.41
1:B:97:GLU:O	1:B:101:LEU:HG	2.21	0.41
1:B:130:GLU:OE2	5:B:502:HOH:O	2.22	0.41
1:A:348:TRP:HB3	5:A:650:HOH:O	2.21	0.40
1:A:121:MET:CE	1:A:273:ILE:CD1	3.00	0.40

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	sed Favoured Allowed		Outliers	Percentiles		
1	A	$324/338 \ (96\%)$	320 (99%)	4 (1%)	0	100	100	
1	В	323/338 (96%)	318 (98%)	5 (2%)	0	100	100	
All	All	647/676 (96%)	638 (99%)	9 (1%)	0	100	100	

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	284/291 (98%)	279 (98%)	5 (2%)	59 53		
1	В	282/291 (97%)	279 (99%)	3 (1%)	73 71		
All	All	$566/582 \ (97\%)$	558 (99%)	8 (1%)	67 62		

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	105	SER
1	В	200	HIS
1	В	204	ASN
1	A	74	GLN
1	A	112	GLN
1	A	200	HIS
1	A	268	ILE
1	A	385	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	В	112	GLN
1	В	200	HIS
1	В	247	GLN
1	В	389	GLN
1	A	74	GLN



Continued from previous page...

Mol	Chain	Res	Type
1	A	244	GLN
1	A	382	ASN

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 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 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	Trunc	Type Chain	Chain Res	Res Link		Bond lengths			Bond angles		
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	BLG	В	402	4	36,36,36	0.86	3 (8%)	41,53,53	1.08	3 (7%)	
3	BLG	A	402[A]	4	36,36,36	0.80	2 (5%)	41,53,53	0.77	0	
3	BLG	A	402[B]	4	36,36,36	0.88	2 (5%)	41,53,53	0.77	0	
2	PEG	В	401	-	6,6,6	0.17	0	5,5,5	0.10	0	
2	PEG	A	401	-	6,6,6	0.20	0	5,5,5	0.22	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
3	BLG	В	402	4	-	6/28/60/60	0/2/2/2
3	BLG	A	402[A]	4	-	6/28/60/60	0/2/2/2
3	BLG	A	402[B]	4	-	6/28/60/60	0/2/2/2
2	PEG	В	401	-	-	2/4/4/4	-
2	PEG	A	401	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
3	A	402[B]	BLG	OS3-S	2.92	1.58	1.47
3	В	402	BLG	OS3-S	2.89	1.57	1.47
3	A	402[A]	BLG	CA-N	2.61	1.52	1.48
3	A	402[B]	BLG	CA-N	2.55	1.52	1.48
3	В	402	BLG	CA-N	2.52	1.52	1.48
3	В	402	BLG	CD-N	2.38	1.51	1.46
3	A	402[A]	BLG	OS3-S	2.30	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
3	В	402	BLG	OS3-S-C12	-3.49	100.13	105.77
3	В	402	BLG	C1-O1-CB	2.35	118.96	115.33
3	В	402	BLG	O43-S4-O42	2.19	116.09	108.49

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	402	BLG	C4-O4-S4-O41
3	В	402	BLG	C4-O4-S4-O42
3	В	402	BLG	C4-O4-S4-O43
3	В	402	BLG	C11-C12-S-OS2
3	A	402[A]	BLG	C4-O4-S4-O41
3	A	402[A]	BLG	C4-O4-S4-O42
3	A	402[A]	BLG	C4-O4-S4-O43
3	A	402[A]	BLG	O9-C9-CA-N
3	A	402[A]	BLG	N3-C11-C12-S
3	A	402[B]	BLG	C11-C12-S-OS1
3	A	402[B]	BLG	C11-C12-S-OS2
3	В	402	BLG	C11-C12-S-OS3
2	В	401	PEG	O2-C3-C4-O4



Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	402[B]	BLG	C11-C12-S-OS3
2	A	401	PEG	O1-C1-C2-O2
2	В	401	PEG	O1-C1-C2-O2
3	A	402[B]	BLG	C4-C5-C6-O6
3	A	402[B]	BLG	O9-C9-CA-N
3	A	402[B]	BLG	O5-C5-C6-O6
2	A	401	PEG	O2-C3-C4-O4
3	В	402	BLG	C11-C12-S-OS1
3	A	402[A]	BLG	C11-C12-S-OS2

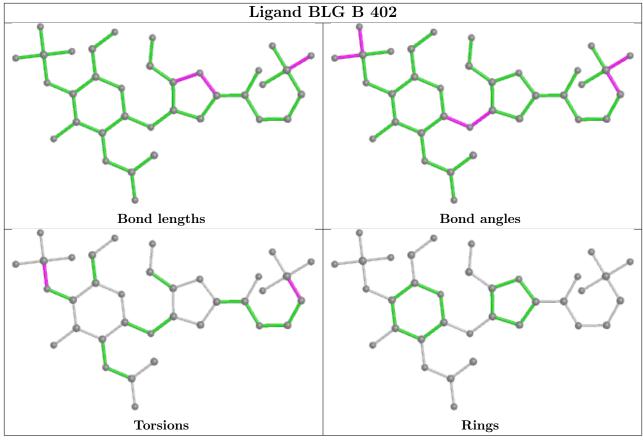
There are no ring outliers.

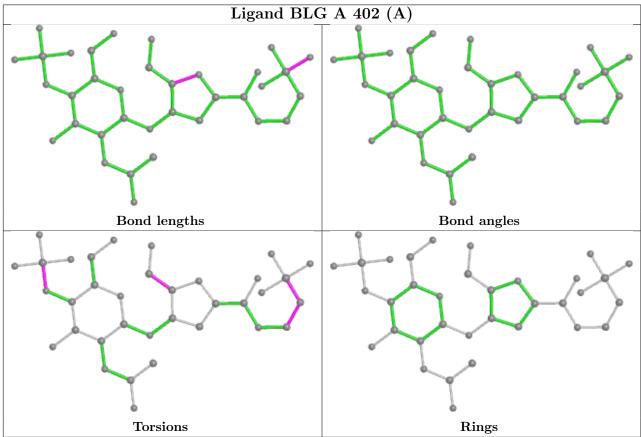
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402[A]	BLG	1	0
2	A	401	PEG	1	0

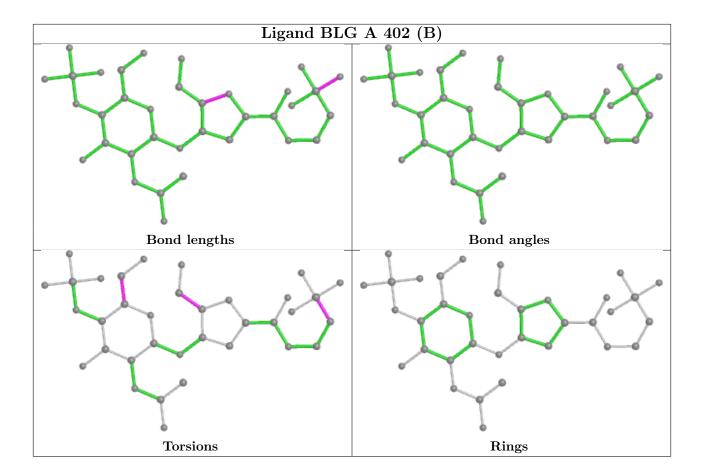
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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^{th} 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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	327/338~(96%)	0.35	30 (9%) 9 14	16, 32, 83, 118	0
1	В	327/338~(96%)	0.17	17 (5%) 27 37	18, 36, 68, 101	0
All	All	654/676 (96%)	0.26	47 (7%) 15 23	16, 34, 78, 118	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	LEU	8.2
1	В	343	LYS	5.9
1	A	375	SER	5.6
1	A	378	ARG	4.8
1	В	378	ARG	4.7
1	A	393	PRO	4.4
1	A	382	ASN	4.3
1	В	371	ALA	4.2
1	A	351	TYR	4.2
1	A	348	TRP	4.2
1	A	367	ARG	4.1
1	A	386	LYS	3.8
1	A	381	SER	3.6
1	A	60	HIS	3.6
1	A	346	THR	3.5
1	В	366	TYR	3.4
1	A	390	LEU	3.4
1	A	392	ILE	3.3
1	В	386	LYS	3.2
1	A	384	LEU	3.1
1	В	342	PRO	3.1
1	A	359	LEU	2.9
1	В	351	TYR	2.9
1	A	373	LEU	2.9



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	383	HIS	2.8
1	В	355	SER	2.8
1	A	350	GLN	2.7
1	A	356	GLY	2.7
1	A	349	GLN	2.7
1	A	371	ALA	2.6
1	A	389	GLN	2.5
1	A	366	TYR	2.5
1	A	372	GLU	2.5
1	В	385	ARG	2.4
1	В	389	GLN	2.2
1	В	103	PHE	2.2
1	В	393	PRO	2.1
1	A	385	ARG	2.1
1	A	387	GLY	2.1
1	В	354	ARG	2.1
1	В	74	GLN	2.1
1	В	321	GLN	2.1
1	В	92	THR	2.1
1	A	368	ILE	2.1
1	A	374	LYS	2.0
1	A	364	ASN	2.0
1	В	174	ARG	2.0

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^{th} 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.



 $Continued\ from\ previous\ page...$

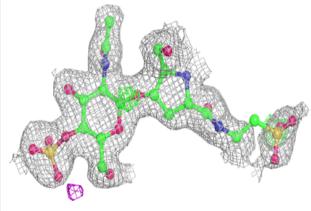
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{ ilde{A}}^2)$	Q<0.9
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-}factors}({f A}^2)$	\mid Q<0.9 \mid
2	PEG	В	401	7/7	0.88	0.16	54,54,59,60	0
2	PEG	A	401	7/7	0.90	0.15	52,54,61,70	0
4	ZN	A	407	1/1	0.94	0.13	66,66,66,66	0
3	BLG	A	402[B]	35/35	0.96	0.12	20,25,34,37	35
3	BLG	A	402[A]	35/35	0.96	0.12	24,30,59,63	35
4	ZN	В	405	1/1	0.97	0.03	53,53,53,53	0
4	ZN	В	408	1/1	0.97	0.04	32,32,32,32	1
3	BLG	В	402	35/35	0.97	0.08	23,30,51,55	0
4	ZN	В	404	1/1	0.98	0.06	32,32,32,32	0
4	ZN	В	406	1/1	0.99	0.05	29,29,29,29	1
4	ZN	В	409	1/1	0.99	0.04	59,59,59,59	0
4	ZN	В	407	1/1	0.99	0.03	32,32,32,32	1
4	ZN	A	408	1/1	0.99	0.11	27,27,27,27	1
4	ZN	A	405	1/1	1.00	0.08	29,29,29,29	0
4	ZN	A	406	1/1	1.00	0.09	25,25,25,25	0
4	ZN	В	403	1/1	1.00	0.07	27,27,27,27	0
4	ZN	A	404	1/1	1.00	0.06	20,20,20,20	0

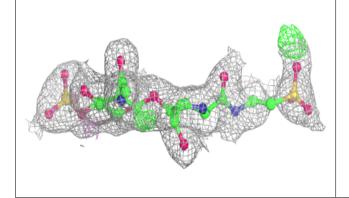
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

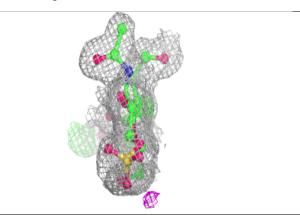


Electron density around BLG A 402 (B):

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

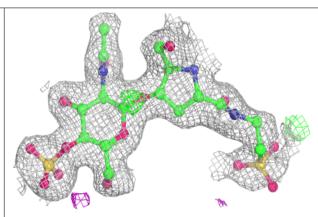


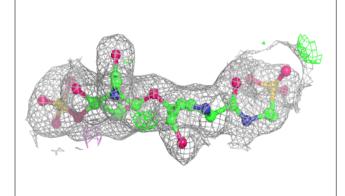


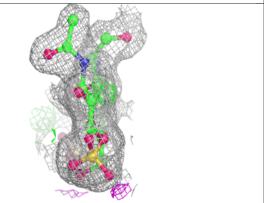


Electron density around BLG A 402 (A):

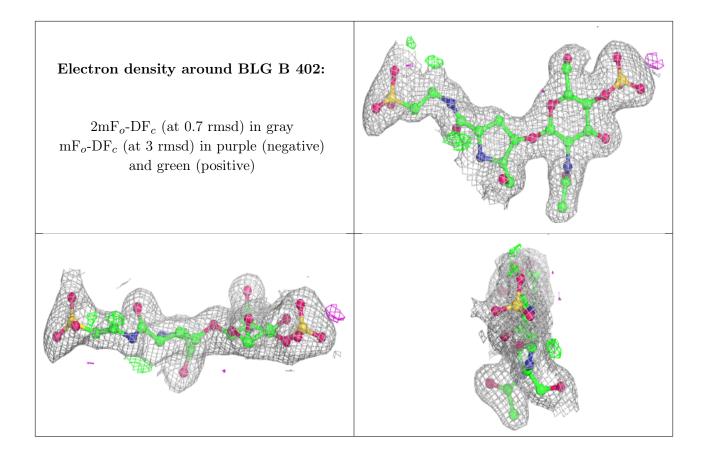
 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

