



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:47 PM UTC

PDB ID : 1SLY / pdb_00001sly
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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

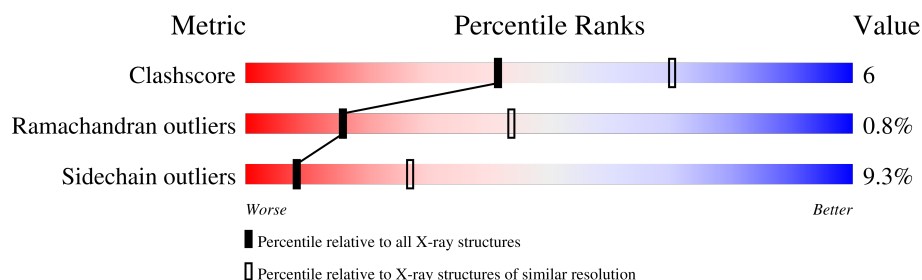
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 ≥ 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](#)

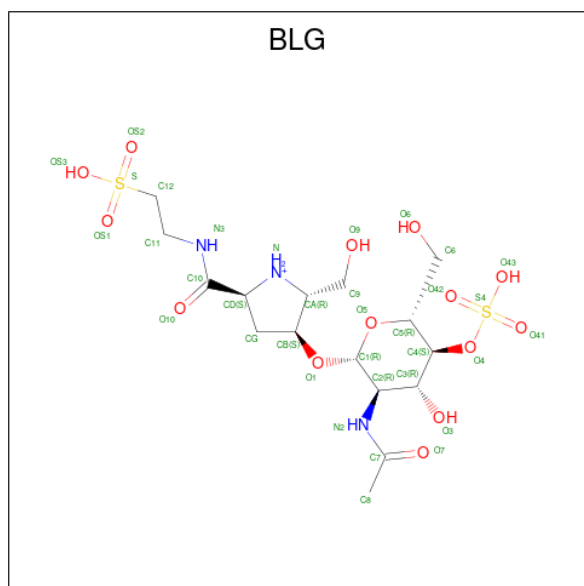
There are 2 unique types of molecules in this entry. The entry contains 5000 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	618	Total	C	N	O	S	0	0	0
			4965	3126	883	932	24			

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



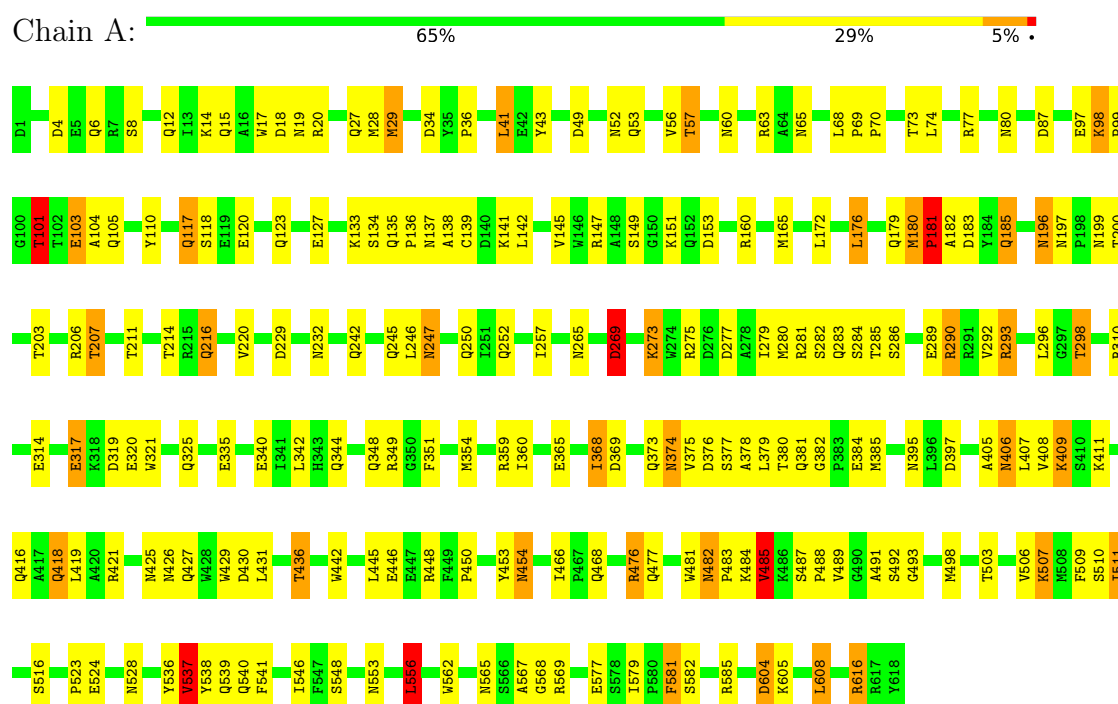
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	16	3	14	2		

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. 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, α , β , γ	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 ²)	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	0.96	2/5079 (0.0%)	1.96	159/6888 (2.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	ILE	CA-CB	10.49	1.67	1.53
1	A	546	ILE	CA-CB	5.25	1.61	1.54

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	604	ASP	CA-CB-CG	12.28	124.88	112.60
1	A	247	ASN	CA-CB-CG	10.90	123.50	112.60
1	A	49	ASP	CA-CB-CG	10.60	123.20	112.60
1	A	183	ASP	CA-CB-CG	9.38	121.98	112.60
1	A	481	TRP	N-CA-C	9.20	124.01	112.24
1	A	537	VAL	N-CA-CB	-8.99	98.31	110.54
1	A	325	GLN	OE1-CD-NE2	-8.86	113.74	122.60
1	A	406	ASN	OD1-CG-ND2	-8.77	113.83	122.60
1	A	284	SER	N-CA-C	8.73	123.24	108.23
1	A	179	GLN	CA-CB-CG	8.05	130.20	114.10
1	A	454	ASN	OD1-CG-ND2	-7.90	114.70	122.60
1	A	29	MET	N-CA-C	7.89	123.48	112.75
1	A	381	GLN	OE1-CD-NE2	-7.89	114.71	122.60
1	A	15	GLN	CA-CB-CG	7.88	129.86	114.10
1	A	12	GLN	OE1-CD-NE2	-7.88	114.72	122.60
1	A	539	GLN	OE1-CD-NE2	-7.73	114.87	122.60
1	A	442	TRP	N-CA-C	7.70	122.35	112.34
1	A	445	LEU	N-CA-C	7.70	119.67	111.28
1	A	28	MET	N-CA-C	7.64	121.86	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	GLU	N-CA-C	-7.63	102.90	111.14
1	A	430	ASP	CA-CB-CG	7.41	120.01	112.60
1	A	429	TRP	N-CA-C	7.34	119.28	111.28
1	A	485	VAL	CB-CA-C	-7.32	99.38	111.32
1	A	15	GLN	OE1-CD-NE2	-7.27	115.33	122.60
1	A	540	GLN	OE1-CD-NE2	-7.25	115.35	122.60
1	A	6	GLN	OE1-CD-NE2	-7.24	115.36	122.60
1	A	608	LEU	N-CA-C	7.24	119.17	111.28
1	A	581	PHE	CA-CB-CG	7.01	120.81	113.80
1	A	395	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	A	252	GLN	OE1-CD-NE2	-6.98	115.62	122.60
1	A	80	ASN	OD1-CG-ND2	-6.93	115.67	122.60
1	A	123	GLN	OE1-CD-NE2	-6.92	115.68	122.60
1	A	153	ASP	CA-CB-CG	6.92	119.52	112.60
1	A	454	ASN	CB-CG-ND2	6.91	126.77	116.40
1	A	416	GLN	OE1-CD-NE2	-6.81	115.79	122.60
1	A	468	GLN	OE1-CD-NE2	-6.80	115.80	122.60
1	A	63	ARG	CA-CB-CG	6.80	127.70	114.10
1	A	426	ASN	OD1-CG-ND2	-6.75	115.85	122.60
1	A	127	GLU	CB-CG-CD	6.73	124.04	112.60
1	A	379	LEU	CA-C-O	6.73	128.06	121.00
1	A	265	ASN	OD1-CG-ND2	-6.65	115.95	122.60
1	A	369	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	269	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	245	GLN	OE1-CD-NE2	-6.50	116.10	122.60
1	A	56	VAL	CB-CA-C	-6.48	103.68	111.97
1	A	87	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	137	ASN	CB-CG-ND2	6.47	126.10	116.40
1	A	477	GLN	OE1-CD-NE2	-6.46	116.14	122.60
1	A	257	ILE	CA-C-O	-6.45	114.56	121.27
1	A	397	ASP	N-CA-C	6.44	117.96	111.07
1	A	468	GLN	CG-CD-NE2	6.41	126.01	116.40
1	A	29	MET	CA-CB-CG	-6.37	101.36	114.10
1	A	137	ASN	OD1-CG-ND2	-6.35	116.25	122.60
1	A	247	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	A	409	LYS	N-CA-C	6.28	120.51	112.34
1	A	395	ASN	CB-CG-ND2	6.26	125.80	116.40
1	A	185	GLN	OE1-CD-NE2	-6.26	116.34	122.60
1	A	15	GLN	CB-CA-C	-6.24	101.34	110.96
1	A	199	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	A	65	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	A	335	GLU	N-CA-C	6.21	118.57	111.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	ASN	N-CA-C	6.20	119.32	111.69
1	A	349	ARG	CA-CB-CG	6.16	126.42	114.10
1	A	492	SER	N-CA-C	6.15	119.50	109.59
1	A	344	GLN	OE1-CD-NE2	-6.11	116.49	122.60
1	A	567	ALA	N-CA-C	6.10	119.81	111.39
1	A	182	ALA	N-CA-C	6.08	119.53	111.75
1	A	373	GLN	OE1-CD-NE2	-6.06	116.54	122.60
1	A	101	THR	CA-CB-OG1	-6.04	100.54	109.60
1	A	374	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	A	354	MET	CG-SD-CE	-6.00	87.69	100.90
1	A	476	ARG	CG-CD-NE	-6.00	98.79	112.00
1	A	426	ASN	CB-CG-ND2	6.00	125.40	116.40
1	A	180	MET	N-CA-C	5.99	119.37	110.32
1	A	8	SER	CB-CA-C	-5.99	101.48	110.88
1	A	537	VAL	CB-CA-C	5.94	120.16	112.14
1	A	516	SER	CA-C-N	5.91	125.79	119.28
1	A	516	SER	C-N-CA	5.91	125.79	119.28
1	A	298	THR	CA-CB-OG1	-5.90	100.75	109.60
1	A	196	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	A	537	VAL	O-C-N	-5.89	116.16	121.87
1	A	250	GLN	OE1-CD-NE2	-5.88	116.72	122.60
1	A	196	ASN	CA-CB-CG	5.87	118.47	112.60
1	A	384	GLU	CB-CG-CD	5.85	122.54	112.60
1	A	60	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	A	4	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	57	THR	CB-CA-C	-5.80	101.74	110.90
1	A	498	MET	CA-C-N	5.79	125.27	119.24
1	A	498	MET	C-N-CA	5.79	125.27	119.24
1	A	569	ARG	N-CA-C	5.74	118.47	111.82
1	A	298	THR	CA-CB-CG2	5.73	120.24	110.50
1	A	242	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	A	117	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	A	27	GLN	N-CA-C	5.66	117.91	111.11
1	A	65	ASN	CA-C-N	5.66	125.02	118.85
1	A	65	ASN	C-N-CA	5.66	125.02	118.85
1	A	229	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	562	TRP	CA-C-O	-5.63	114.91	120.82
1	A	507	LYS	N-CA-C	5.62	117.49	111.36
1	A	406	ASN	CB-CG-ND2	5.62	124.83	116.40
1	A	427	GLN	CA-CB-CG	-5.61	102.89	114.10
1	A	185	GLN	CA-CB-CG	5.60	125.31	114.10
1	A	101	THR	CA-CB-CG2	5.60	120.03	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	539	GLN	CG-CD-NE2	5.60	124.80	116.40
1	A	516	SER	N-CA-C	5.59	118.82	109.09
1	A	477	GLN	CG-CD-NE2	5.58	124.78	116.40
1	A	292	VAL	CB-CA-C	-5.57	104.62	112.14
1	A	135	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	A	528	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	A	60	ASN	CB-CG-ND2	5.50	124.65	116.40
1	A	376	ASP	N-CA-C	5.49	118.24	110.50
1	A	296	LEU	N-CA-C	5.46	116.91	111.07
1	A	510	SER	N-CA-C	5.45	118.91	111.39
1	A	511	ILE	N-CA-C	5.42	113.30	108.63
1	A	180	MET	CA-C-N	5.41	126.60	119.84
1	A	180	MET	C-N-CA	5.41	126.60	119.84
1	A	123	GLN	N-CA-C	-5.38	105.49	111.36
1	A	382	GLY	N-CA-C	5.38	123.32	112.34
1	A	446	GLU	N-CA-C	5.38	117.57	111.11
1	A	283	GLN	CA-CB-CG	5.32	124.74	114.10
1	A	450	PRO	O-C-N	-5.32	116.52	123.06
1	A	568	GLY	CA-C-O	5.32	124.68	119.04
1	A	97	GLU	CA-C-O	-5.31	115.01	121.28
1	A	290	ARG	CA-CB-CG	5.31	124.72	114.10
1	A	348	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	A	293	ARG	CA-C-O	-5.30	114.93	120.55
1	A	380	THR	CA-CB-OG1	-5.30	101.66	109.60
1	A	429	TRP	CE2-CD2-CE3	5.30	124.10	118.80
1	A	282	SER	N-CA-C	5.28	118.42	109.76
1	A	216	GLN	CA-CB-CG	-5.27	103.56	114.10
1	A	18	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	395	ASN	CA-CB-CG	-5.25	107.35	112.60
1	A	53	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	A	153	ASP	CA-C-N	5.24	125.05	119.28
1	A	153	ASP	C-N-CA	5.24	125.05	119.28
1	A	382	GLY	CA-C-N	5.23	124.68	119.24
1	A	382	GLY	C-N-CA	5.23	124.68	119.24
1	A	482	ASN	CA-C-N	5.22	125.53	119.47
1	A	482	ASN	C-N-CA	5.22	125.53	119.47
1	A	246	LEU	N-CA-C	5.22	118.06	109.76
1	A	105	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	A	14	LYS	CA-C-O	-5.17	115.07	120.55
1	A	118	SER	CB-CA-C	-5.15	102.28	110.84
1	A	425	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	98	LYS	N-CA-C	5.15	115.52	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	THR	N-CA-CB	-5.14	102.03	110.41
1	A	41	LEU	N-CA-CB	-5.14	102.55	110.16
1	A	368	ILE	CA-C-O	5.12	126.11	120.48
1	A	489	VAL	N-CA-CB	-5.11	102.80	111.23
1	A	493	GLY	N-CA-C	5.11	122.18	112.62
1	A	616	ARG	CD-NE-CZ	5.11	131.55	124.40
1	A	546	ILE	N-CA-C	-5.10	105.87	110.82
1	A	425	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	A	19	ASN	CA-CB-CG	5.07	117.67	112.60
1	A	418	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	A	482	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	53	GLN	O-C-N	-5.04	116.92	121.66
1	A	342	LEU	O-C-N	-5.03	116.79	122.12
1	A	524	GLU	N-CA-C	5.01	117.47	111.71

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	63	0
2	A	35	0	29	0	0
All	All	5000	0	4881	63	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 (63) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:385:MET:HE2	1:A:407:LEU:HD21	1.80	0.63
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	16 44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	SER
1	A	319	ASP
1	A	378	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	8 27

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

Mol	Chain	Res	Type
1	A	29	MET
1	A	34	ASP
1	A	36	PRO
1	A	41	LEU
1	A	52	ASN
1	A	57	THR
1	A	98	LYS
1	A	101	THR
1	A	103	GLU
1	A	139	CYS
1	A	142	LEU
1	A	165	MET
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	207	THR
1	A	211	THR
1	A	214	THR
1	A	232	ASN
1	A	247	ASN
1	A	269	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	273	LYS
1	A	286	SER
1	A	290	ARG
1	A	298	THR
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	436	THR
1	A	454	ASN
1	A	476	ARG
1	A	485	VAL
1	A	488	PRO
1	A	507	LYS
1	A	523	PRO
1	A	537	VAL
1	A	556	LEU
1	A	565	ASN
1	A	582	SER
1	A	604	ASP
1	A	605	LYS
1	A	616	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	15	GLN
1	A	19	ASN
1	A	53	GLN
1	A	152	GLN
1	A	232	ASN
1	A	325	GLN
1	A	416	GLN
1	A	454	ASN
1	A	468	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 oligosaccharides 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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.

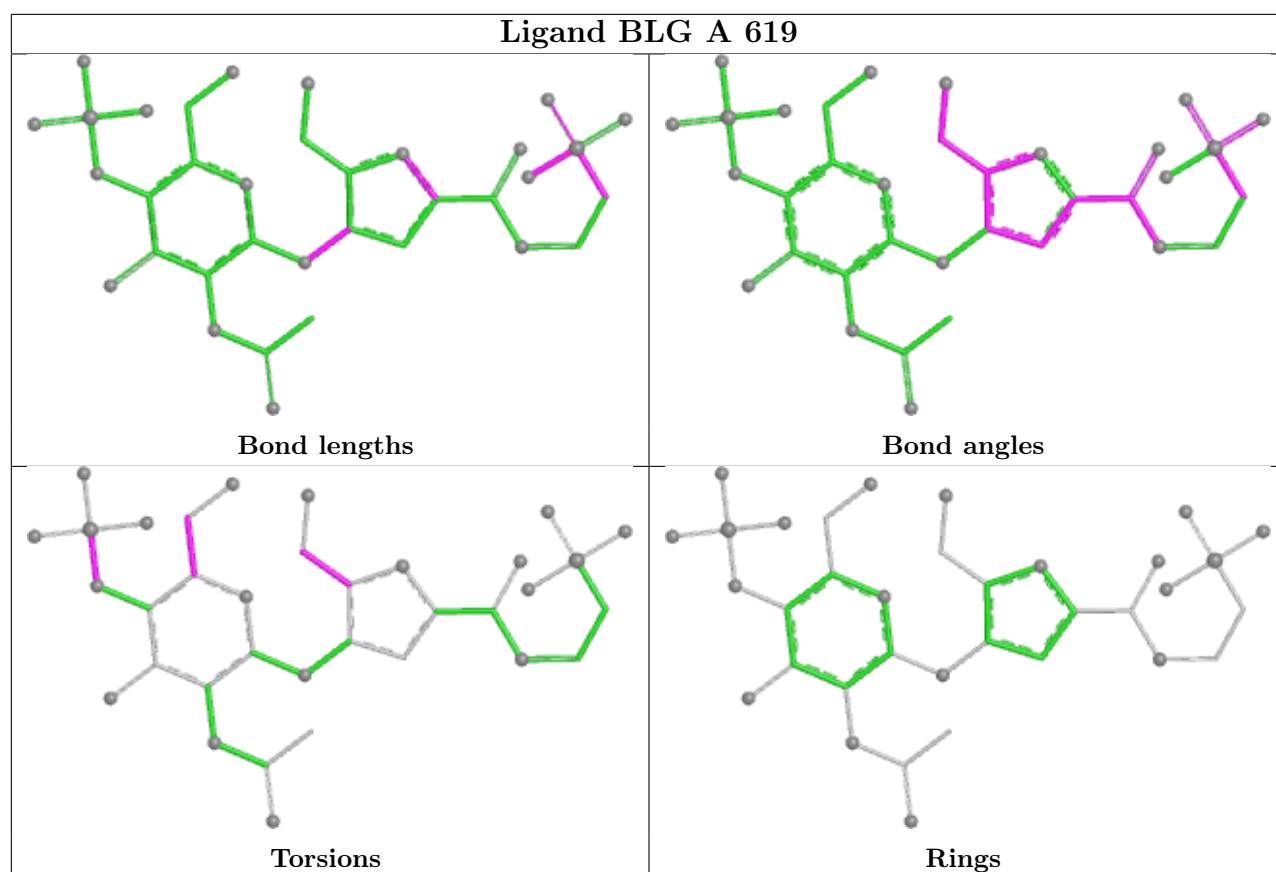
All (6) torsion outliers are listed below:

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.