



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:15 PM UTC

PDB ID : 6WYZ / pdb_00006wyz
Title : Crystal structure of Pseudomonas 7A Glutaminase-Asparaginase (mutant K173M) in complex with D-Glu at pH 5.5
Authors : Strzelczyk, P.; Zhang, D.; Wlodawer, A.; Lubkowski, J.
Deposited on : 2020-05-13
Resolution : 1.70 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

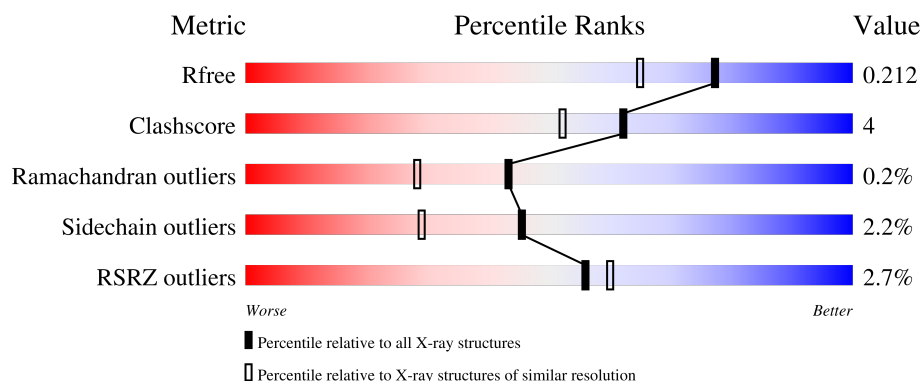
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 $\leq 5\%$. 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	337	
1	B	337	
1	C	337	
1	D	337	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10855 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.

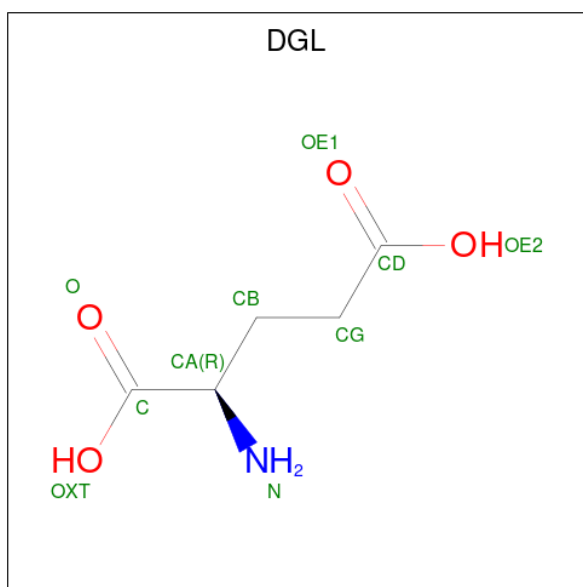
- Molecule 1 is a protein called Glutaminase-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	2	0
			2376	1488	417	460	11			
1	B	315	Total	C	N	O	S	0	2	0
			2397	1501	422	464	10			
1	C	314	Total	C	N	O	S	0	2	0
			2392	1496	422	464	10			
1	D	312	Total	C	N	O	S	0	2	0
			2376	1488	417	460	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	MET	LYS	engineered mutation	UNP Q88K39
B	173	MET	LYS	engineered mutation	UNP Q88K39
C	173	MET	LYS	engineered mutation	UNP Q88K39
D	173	MET	LYS	engineered mutation	UNP Q88K39

- Molecule 2 is D-GLUTAMIC ACID (CCD ID: DGL) (formula: C₅H₉NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		

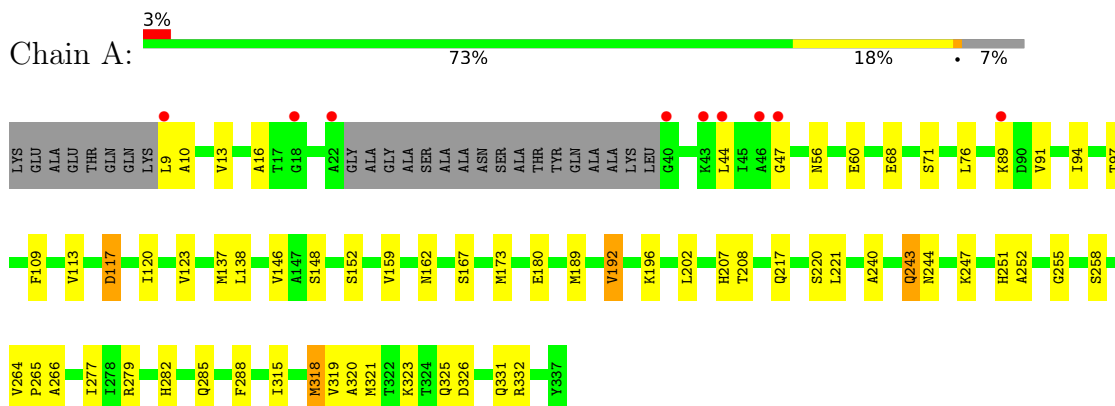
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	323	Total	O	0	0
			323	323		
3	B	324	Total	O	0	0
			324	324		
3	C	321	Total	O	0	0
			321	321		
3	D	306	Total	O	0	0
			306	306		

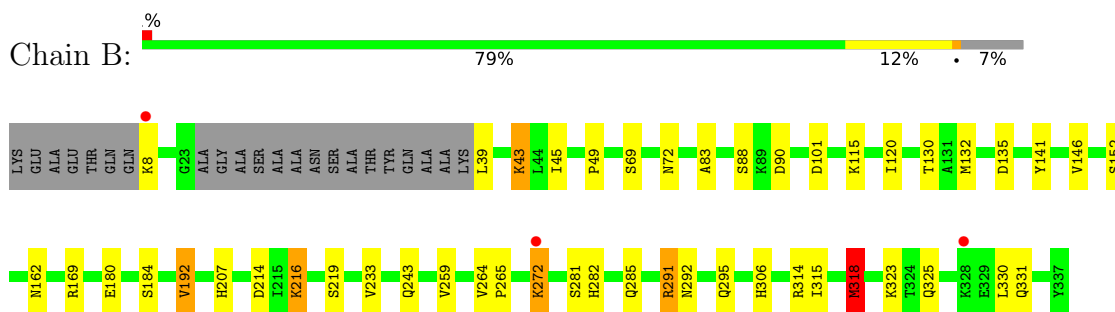
3 Residue-property plots [i](#)

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.

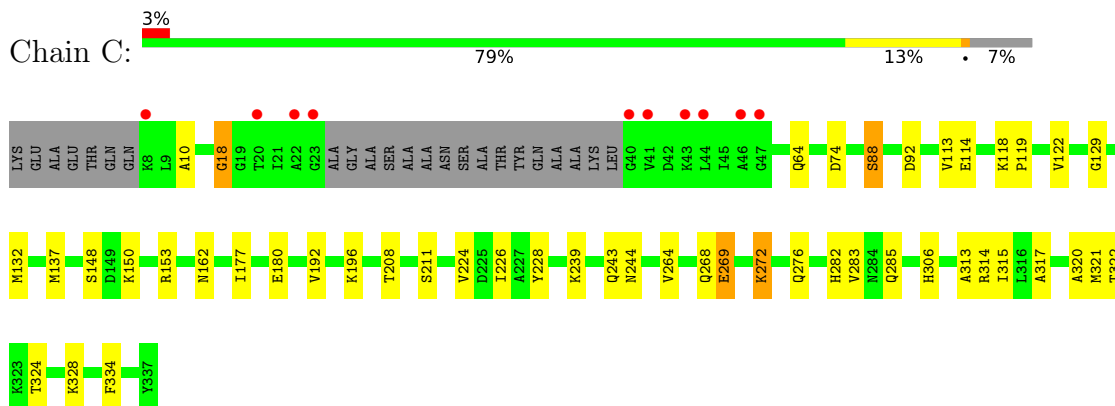
- Molecule 1: Glutaminase-asparaginase



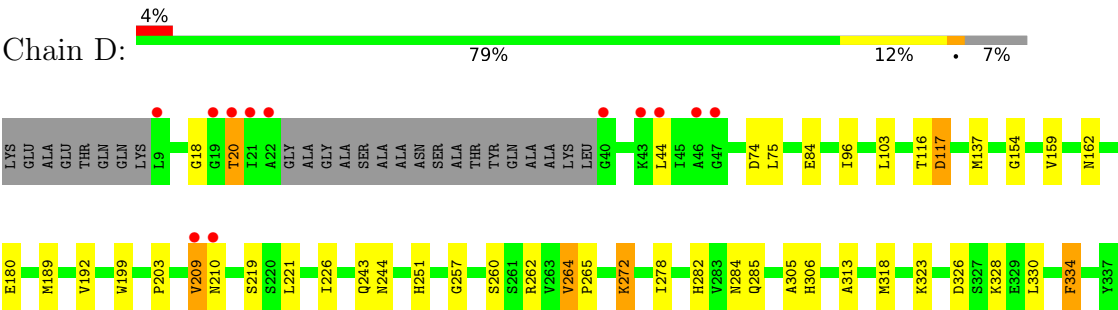
- Molecule 1: Glutaminase-asparaginase



- Molecule 1: Glutaminase-asparaginase



● Molecule 1: Glutaminase-asparaginase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	81.28Å 81.28Å 176.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.61 – 1.70 39.61 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.61-1.70) 98.2 (39.61-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.171 , 0.215 (Not available) , 0.212	Depositor DCC
R_{free} test set	3728 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.055 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10855	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.54	23/2415 (1.0%)	1.63	22/3265 (0.7%)
1	B	1.47	17/2436 (0.7%)	1.53	13/3293 (0.4%)
1	C	1.47	17/2428 (0.7%)	1.52	9/3282 (0.3%)
1	D	1.49	13/2415 (0.5%)	1.62	18/3265 (0.6%)
All	All	1.49	70/9694 (0.7%)	1.58	62/13105 (0.5%)

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	A	0	2
1	C	0	1
All	All	0	3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	HIS	CE1-NE2	10.64	1.43	1.32
1	C	282	HIS	CE1-NE2	10.60	1.43	1.32
1	A	318[A]	MET	C-O	9.44	1.34	1.24
1	A	318[B]	MET	C-O	9.44	1.34	1.24
1	D	18	GLY	C-O	9.41	1.30	1.24
1	C	315	ILE	C-O	8.60	1.33	1.24
1	C	177	ILE	C-O	8.45	1.34	1.24
1	B	306	HIS	CE1-NE2	7.99	1.40	1.32
1	B	282	HIS	CE1-NE2	7.97	1.40	1.32
1	B	146	VAL	C-O	-7.40	1.15	1.24
1	A	167	SER	CA-CB	-7.36	1.41	1.53
1	B	291	ARG	C-O	7.05	1.32	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	ILE	C-O	-6.99	1.16	1.24
1	B	169	ARG	C-O	6.91	1.32	1.24
1	A	68	GLU	C-O	-6.86	1.15	1.24
1	B	281	SER	C-O	6.60	1.31	1.23
1	A	207	HIS	CE1-NE2	6.46	1.39	1.32
1	C	313	ALA	C-O	6.39	1.31	1.24
1	A	138	LEU	C-O	-6.32	1.16	1.24
1	A	173	MET	C-O	6.25	1.31	1.23
1	C	18	GLY	C-O	6.22	1.32	1.23
1	D	251	HIS	CE1-NE2	6.21	1.38	1.32
1	A	91	VAL	C-O	-6.20	1.17	1.24
1	A	315	ILE	C-O	6.08	1.31	1.24
1	A	251	HIS	CE1-NE2	6.08	1.38	1.32
1	B	330	LEU	C-O	6.04	1.31	1.24
1	D	306	HIS	CG-ND1	-6.03	1.31	1.38
1	C	317	ALA	C-O	5.99	1.30	1.24
1	C	226	ILE	C-O	5.95	1.30	1.24
1	B	331	GLN	C-O	5.90	1.31	1.24
1	C	306	HIS	C-O	-5.88	1.19	1.24
1	A	123	VAL	C-O	5.85	1.30	1.23
1	B	184	SER	C-O	5.77	1.31	1.24
1	C	314	ARG	C-O	5.76	1.30	1.24
1	B	259	VAL	C-O	-5.73	1.18	1.24
1	C	88	SER	C-O	5.72	1.30	1.23
1	A	266	ALA	C-O	5.70	1.30	1.24
1	B	315	ILE	C-O	5.66	1.30	1.24
1	B	88	SER	CA-CB	-5.65	1.45	1.53
1	D	96	ILE	C-O	-5.52	1.18	1.24
1	D	282	HIS	CE1-NE2	5.52	1.38	1.32
1	D	260	SER	C-O	-5.51	1.17	1.23
1	C	122	VAL	C-O	5.51	1.30	1.24
1	A	252	ALA	CA-CB	-5.50	1.45	1.52
1	A	152	SER	CA-CB	-5.44	1.44	1.53
1	D	189	MET	C-O	5.44	1.31	1.24
1	B	45	ILE	C-O	5.42	1.30	1.24
1	C	272	LYS	N-CA	5.41	1.53	1.46
1	D	199	TRP	C-O	5.35	1.30	1.23
1	A	319	VAL	C-O	5.34	1.30	1.24
1	B	233	VAL	C-O	5.33	1.31	1.24
1	D	203	PRO	C-O	5.31	1.29	1.23
1	C	113	VAL	N-CA	5.30	1.51	1.46
1	A	109	PHE	N-CA	5.29	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	320	ALA	C-O	5.27	1.30	1.24
1	A	332	ARG	C-O	5.27	1.30	1.24
1	D	159	VAL	C-O	5.26	1.29	1.24
1	C	224	VAL	C-O	5.26	1.29	1.24
1	A	189	MET	C-N	-5.24	1.27	1.33
1	B	69	SER	C-O	5.22	1.31	1.24
1	B	83	ALA	C-O	-5.20	1.18	1.24
1	A	321	MET	C-O	5.18	1.30	1.24
1	A	113	VAL	N-CA	5.15	1.51	1.46
1	C	268	GLN	N-CA	5.12	1.52	1.46
1	A	240	ALA	C-O	5.11	1.30	1.24
1	D	226	ILE	C-O	5.11	1.29	1.24
1	D	278	ILE	C-O	5.09	1.29	1.24
1	D	313	ALA	CA-CB	-5.05	1.45	1.53
1	B	152	SER	CA-CB	-5.04	1.45	1.53
1	C	228	TYR	C-O	5.00	1.29	1.23

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ILE	O-C-N	8.21	132.06	123.20
1	D	117	ASP	CB-CA-C	7.54	123.23	111.02
1	A	94	ILE	CA-C-O	-7.29	112.63	120.36
1	D	326	ASP	CA-CB-CG	7.28	119.88	112.60
1	D	162	ASN	CA-CB-CG	7.20	119.80	112.60
1	A	162	ASN	CA-CB-CG	7.18	119.78	112.60
1	A	13	VAL	O-C-N	7.17	130.71	123.18
1	A	120	ILE	O-C-N	7.06	130.52	123.18
1	D	262	ARG	CG-CD-NE	-6.96	96.68	112.00
1	D	244	ASN	CB-CA-C	6.88	122.28	110.94
1	A	288	PHE	CA-CB-CG	6.62	120.42	113.80
1	B	162	ASN	CA-CB-CG	6.32	118.92	112.60
1	D	116	THR	CA-C-N	-6.32	112.57	122.49
1	D	116	THR	C-N-CA	-6.32	112.57	122.49
1	A	243	GLN	N-CA-C	-6.26	104.56	111.82
1	D	257	GLY	CA-C-O	-6.15	112.36	119.80
1	C	211	SER	CA-C-O	-6.12	114.89	121.56
1	B	90	ASP	CA-CB-CG	-6.10	106.50	112.60
1	D	284	ASN	CB-CA-C	6.06	119.74	109.55
1	A	320	ALA	O-C-N	6.03	128.52	122.12
1	B	120	ILE	O-C-N	5.95	129.37	123.18
1	B	318	MET	CG-SD-CE	-5.95	87.81	100.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	264	VAL	N-CA-CB	5.92	114.49	110.52
1	A	13	VAL	CA-C-O	-5.91	114.22	120.48
1	A	279	ARG	O-C-N	5.86	130.02	123.05
1	C	162	ASN	CA-CB-CG	5.79	118.39	112.60
1	B	49	PRO	CB-CA-C	5.74	120.01	111.85
1	B	207	HIS	O-C-N	5.65	129.46	123.42
1	A	255	GLY	O-C-N	5.62	129.24	122.67
1	B	43	LYS	CA-C-O	-5.62	114.59	120.55
1	C	74	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	159	VAL	CA-C-O	-5.57	114.54	120.39
1	D	334	PHE	CA-CB-CG	-5.52	108.28	113.80
1	B	45	ILE	O-C-N	5.50	127.50	121.83
1	B	141	TYR	CA-C-O	5.50	126.59	120.82
1	A	192	VAL	CB-CA-C	5.48	118.55	110.77
1	C	264	VAL	N-CA-CB	5.41	114.15	110.52
1	A	91	VAL	CA-C-O	-5.41	114.76	120.39
1	D	330	LEU	CA-C-O	-5.40	114.83	120.55
1	D	74	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	56	ASN	O-C-N	5.37	129.34	123.22
1	A	117	ASP	CA-CB-CG	5.36	117.96	112.60
1	C	269	GLU	CB-CG-CD	5.35	121.70	112.60
1	B	135	ASP	CA-CB-CG	5.33	117.94	112.60
1	B	291	ARG	O-C-N	5.31	129.54	122.95
1	C	276	GLN	CA-C-O	-5.28	115.25	121.16
1	D	272	LYS	CA-C-O	-5.28	114.14	120.10
1	D	75	LEU	CB-CA-C	-5.25	102.64	110.88
1	A	146	VAL	O-C-N	5.23	126.94	121.87
1	D	20	THR	CA-C-O	-5.22	114.36	120.20
1	A	331	GLN	N-CA-C	-5.20	105.61	111.28
1	D	210	ASN	CB-CA-C	5.18	119.31	110.56
1	C	334	PHE	CA-CB-CG	-5.17	108.63	113.80
1	B	192	VAL	CB-CA-C	5.15	118.09	110.77
1	C	322	THR	N-CA-C	-5.12	106.30	112.54
1	A	71	SER	CA-C-N	5.11	127.38	120.38
1	A	71	SER	C-N-CA	5.11	127.38	120.38
1	C	92	ASP	N-CA-C	-5.10	106.74	113.12
1	A	277	ILE	CA-C-O	-5.08	114.89	120.48
1	A	326	ASP	CA-CB-CG	5.05	117.65	112.60
1	D	326	ASP	CA-C-O	-5.04	114.85	120.54
1	B	272	LYS	CA-C-O	-5.02	115.21	120.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ASP	Mainchain
1	A	202	LEU	Mainchain
1	C	283	VAL	Peptide

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	2376	0	2404	25	0
1	B	2397	0	2428	20	0
1	C	2392	0	2416	25	0
1	D	2376	0	2404	21	0
2	A	10	0	7	0	0
2	B	10	0	7	0	0
2	C	10	0	7	0	0
2	D	10	0	7	1	0
3	A	323	0	0	10	2
3	B	324	0	0	6	2
3	C	321	0	0	12	3
3	D	306	0	0	5	1
All	All	10855	0	9680	78	4

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 4.

All (78) 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)
3:B:527:HOH:O	1:D:180:GLU:HG2	1.42	1.19
1:A:323:LYS:HB2	3:A:783:HOH:O	1.66	0.94
1:C:285[B]:GLN:NE2	3:C:501:HOH:O	1.92	0.90
1:D:318[A]:MET:SD	3:D:506:HOH:O	2.29	0.89
1:A:285[A]:GLN:HG2	1:B:285[A]:GLN:NE2	1.96	0.79
1:B:314:ARG:NH2	1:B:318:MET:HE1	2.00	0.77
1:B:39:LEU:HD22	1:B:43:LYS:HD2	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:THR:HG23	3:B:589:HOH:O	1.90	0.71
1:A:217:GLN:HG3	3:A:807:HOH:O	1.93	0.68
1:C:272:LYS:O	3:C:502:HOH:O	2.12	0.67
1:A:247:LYS:HE3	3:A:791:HOH:O	1.93	0.67
1:B:72:ASN:HD21	1:B:318:MET:CE	2.09	0.65
1:B:180:GLU:OE1	1:D:180:GLU:OE2	2.15	0.65
1:B:72:ASN:HD21	1:B:318:MET:HE1	1.63	0.64
1:B:132:MET:HG2	1:D:137:MET:HE2	1.84	0.59
1:A:243:GLN:HG3	3:A:625:HOH:O	2.02	0.59
1:C:285[A]:GLN:NE2	1:D:285[A]:GLN:HG2	2.17	0.59
1:D:323:LYS:HD2	3:D:733:HOH:O	2.04	0.57
1:A:137:MET:CE	1:C:132:MET:HG2	2.35	0.57
1:A:60:GLU:OE2	3:A:502:HOH:O	2.17	0.57
1:C:196:LYS:HE3	3:C:777:HOH:O	2.04	0.57
1:B:132:MET:HG2	1:D:137:MET:CE	2.35	0.56
1:B:285[B]:GLN:NE2	3:B:503:HOH:O	2.38	0.56
1:C:285[B]:GLN:HG2	3:C:501:HOH:O	2.04	0.56
1:C:244[B]:ASN:ND2	3:C:508:HOH:O	2.37	0.56
3:B:527:HOH:O	1:D:180:GLU:CG	2.20	0.54
1:C:10:ALA:HB3	1:C:148:SER:HB2	1.90	0.54
1:A:325:GLN:NE2	3:A:503:HOH:O	2.31	0.54
1:A:9:LEU:N	3:A:511:HOH:O	2.41	0.53
1:A:247:LYS:NZ	3:A:513:HOH:O	2.43	0.52
1:C:137:MET:CB	3:C:799:HOH:O	2.59	0.51
1:C:153:ARG:O	3:C:503:HOH:O	2.19	0.51
1:A:285[A]:GLN:NE2	1:B:285[A]:GLN:HG2	2.25	0.51
1:C:137:MET:HG2	3:C:799:HOH:O	2.11	0.51
1:A:247:LYS:CE	3:A:791:HOH:O	2.56	0.50
1:A:76:LEU:HD11	1:A:220:SER:HA	1.94	0.50
1:C:285[B]:GLN:CG	3:C:501:HOH:O	2.59	0.50
1:D:243:GLN:HG3	3:D:605:HOH:O	2.09	0.50
1:A:285[A]:GLN:HG2	1:B:285[A]:GLN:CD	2.36	0.50
1:D:117:ASP:HB3	1:D:209:VAL:CG1	2.42	0.50
1:C:285[A]:GLN:HG2	1:D:285[A]:GLN:NE2	2.27	0.50
1:D:84:GLU:HG2	3:D:532:HOH:O	2.12	0.49
1:C:18:GLY:HA2	1:C:64:GLN:OE1	2.13	0.49
1:D:305:ALA:HA	1:D:334:PHE:CD2	2.48	0.49
1:C:129:GLY:O	1:C:137:MET:HE1	2.13	0.48
1:B:243:GLN:HG2	3:B:807:HOH:O	2.13	0.48
1:D:221:LEU:HD13	1:D:318[B]:MET:SD	2.54	0.48
1:A:258:SER:CB	1:B:101:ASP:OD2	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ASN:HA	1:B:295:GLN:O	2.15	0.47
1:A:137:MET:HE2	1:C:132:MET:HG2	1.97	0.46
1:A:16:ALA:HA	1:A:97:THR:HG1	1.81	0.45
1:D:221:LEU:HD22	1:D:318[B]:MET:HG2	1.97	0.45
1:C:137:MET:HG2	3:C:519:HOH:O	2.15	0.45
1:D:328:LYS:HE2	3:D:735:HOH:O	2.17	0.45
1:A:10:ALA:HB3	1:A:148:SER:HB2	1.99	0.45
1:A:180:GLU:OE2	1:C:180:GLU:OE1	2.35	0.45
1:D:117:ASP:HB2	1:D:154:GLY:HA2	2.00	0.44
1:D:264:VAL:HB	1:D:265:PRO:HD3	2.00	0.44
1:D:117:ASP:HB3	1:D:209:VAL:HG13	2.00	0.43
1:A:221:LEU:HD13	1:A:318[A]:MET:CE	2.49	0.43
1:C:88:SER:O	1:C:118:LYS:NZ	2.51	0.43
1:C:137:MET:HB3	3:C:799:HOH:O	2.17	0.43
1:D:20:THR:OG1	2:D:401:DGL:CD	2.67	0.42
1:C:129:GLY:HA2	1:C:137:MET:HE1	2.02	0.42
1:A:258:SER:OG	1:B:101:ASP:OD2	2.28	0.42
1:C:321:MET:HA	1:C:324:THR:O	2.20	0.42
1:C:239:LYS:O	1:C:243:GLN:HG3	2.20	0.42
1:A:16:ALA:HA	1:A:97:THR:OG1	2.20	0.41
1:A:323:LYS:CB	3:A:783:HOH:O	2.44	0.41
1:C:119:PRO:HA	3:C:582:HOH:O	2.19	0.41
1:B:264:VAL:N	1:B:265:PRO:CD	2.84	0.41
1:C:114:GLU:O	1:C:208:THR:HA	2.19	0.41
1:B:72:ASN:HD21	1:B:318:MET:HE2	1.82	0.41
1:A:264:VAL:N	1:A:265:PRO:CD	2.84	0.41
1:B:214:ASP:OD1	1:B:216:LYS:CG	2.68	0.41
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.91	0.41
1:B:291:ARG:HD3	3:B:782:HOH:O	2.21	0.41
1:D:103:LEU:C	1:D:103:LEU:HD23	2.46	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:527:HOH:O	3:C:502:HOH:O[1_455]	1.20	1.00
3:B:760:HOH:O	3:C:664:HOH:O[2_545]	1.71	0.49
3:A:791:HOH:O	3:C:771:HOH:O[1_455]	2.13	0.07
3:B:778:HOH:O	3:D:720:HOH:O[2_545]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	310/337 (92%)	300 (97%)	8 (3%)	2 (1%)	21	9
1	B	313/337 (93%)	304 (97%)	9 (3%)	0	100	100
1	C	312/337 (93%)	305 (98%)	7 (2%)	0	100	100
1	D	310/337 (92%)	298 (96%)	12 (4%)	0	100	100
All	All	1245/1348 (92%)	1207 (97%)	36 (3%)	2 (0%)	43	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	THR
1	A	47	GLY

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	256/269 (95%)	252 (98%)	4 (2%)	55	41
1	B	258/269 (96%)	249 (96%)	9 (4%)	32	15
1	C	257/269 (96%)	253 (98%)	4 (2%)	55	41
1	D	256/269 (95%)	251 (98%)	5 (2%)	48	32
All	All	1027/1076 (95%)	1005 (98%)	22 (2%)	45	30

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LYS
1	A	192	VAL
1	A	196	LYS
1	A	244	ASN
1	B	8	LYS
1	B	115	LYS
1	B	192	VAL
1	B	216	LYS
1	B	219	SER
1	B	272	LYS
1	B	318	MET
1	B	323	LYS
1	B	325	GLN
1	C	150	LYS
1	C	192	VAL
1	C	269	GLU
1	C	328	LYS
1	D	44	LEU
1	D	192	VAL
1	D	209	VAL
1	D	219	SER
1	D	272	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	GLN
1	A	295	GLN
1	B	72	ASN
1	B	325	GLN
1	C	217	GLN
1	D	295	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 [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	DGL	B	401	-	8,9,9	1.99	1 (12%)	8,11,11	1.32	1 (12%)
2	DGL	A	401	-	8,9,9	1.39	2 (25%)	8,11,11	1.07	0
2	DGL	D	401	-	8,9,9	1.97	3 (37%)	8,11,11	1.10	0
2	DGL	C	401	-	8,9,9	1.68	2 (25%)	8,11,11	1.66	2 (25%)

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	DGL	B	401	-	-	4/9/9/9	-
2	DGL	A	401	-	-	5/9/9/9	-
2	DGL	D	401	-	-	6/9/9/9	-
2	DGL	C	401	-	-	5/9/9/9	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	DGL	OE1-CD	5.40	1.39	1.22
2	C	401	DGL	OE1-CD	3.63	1.34	1.22
2	D	401	DGL	OXT-C	-3.38	1.19	1.30
2	D	401	DGL	OE1-CD	3.00	1.31	1.22
2	D	401	DGL	O-C	2.87	1.30	1.22
2	A	401	DGL	OE1-CD	2.72	1.31	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	DGL	O-C	2.19	1.28	1.22
2	C	401	DGL	O-C	2.04	1.28	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	DGL	CB-CG-CD	2.47	119.08	112.49
2	B	401	DGL	OE1-CD-CG	-2.28	115.85	123.09
2	C	401	DGL	OE1-CD-CG	-2.02	116.70	123.09

There are no chirality outliers.

All (20) torsion outliers are listed below:

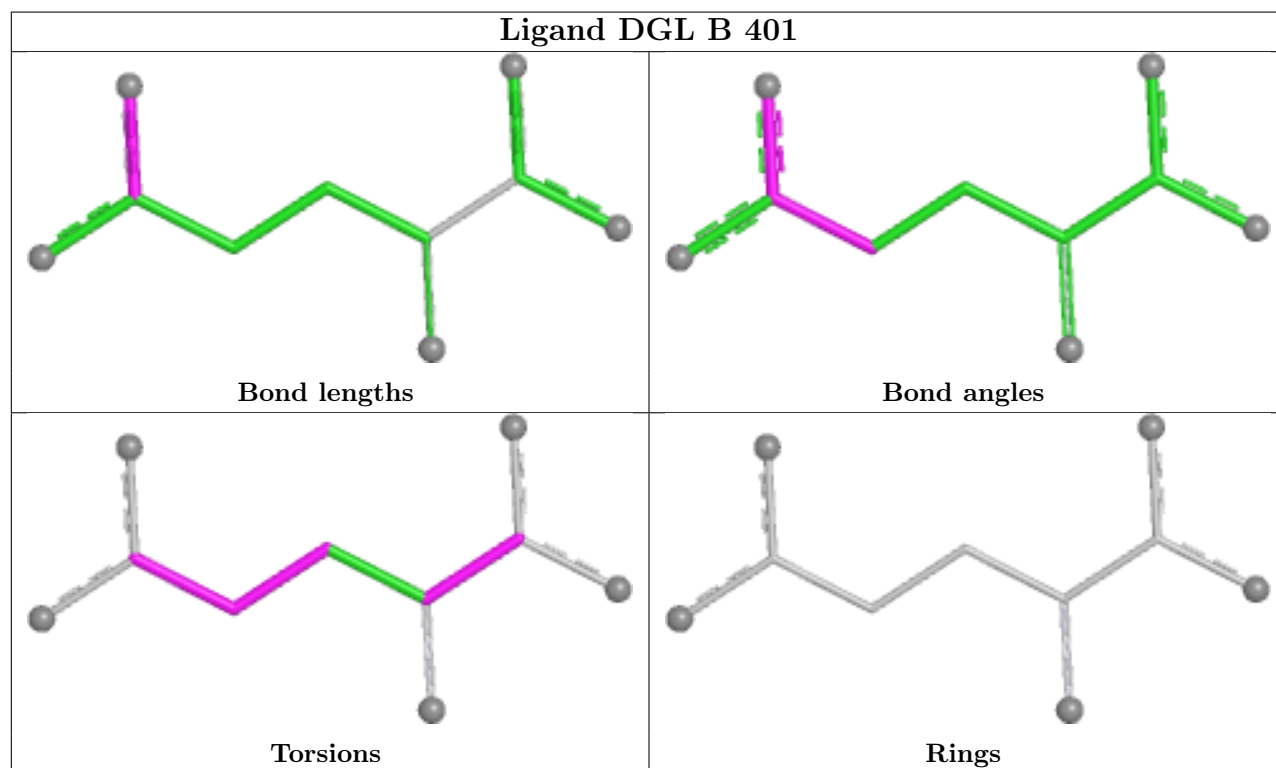
Mol	Chain	Res	Type	Atoms
2	A	401	DGL	N-CA-CB-CG
2	A	401	DGL	OXT-C-CA-N
2	A	401	DGL	CA-CB-CG-CD
2	A	401	DGL	C-CA-CB-CG
2	B	401	DGL	CA-CB-CG-CD
2	D	401	DGL	CA-CB-CG-CD
2	D	401	DGL	N-CA-CB-CG
2	C	401	DGL	CA-CB-CG-CD
2	C	401	DGL	OXT-C-CA-N
2	D	401	DGL	OXT-C-CA-N
2	C	401	DGL	O-C-CA-N
2	D	401	DGL	O-C-CA-N
2	C	401	DGL	OE1-CD-CG-CB
2	C	401	DGL	OE2-CD-CG-CB
2	B	401	DGL	OE2-CD-CG-CB
2	D	401	DGL	OE2-CD-CG-CB
2	B	401	DGL	OXT-C-CA-N
2	B	401	DGL	OE1-CD-CG-CB
2	D	401	DGL	OE1-CD-CG-CB
2	A	401	DGL	O-C-CA-N

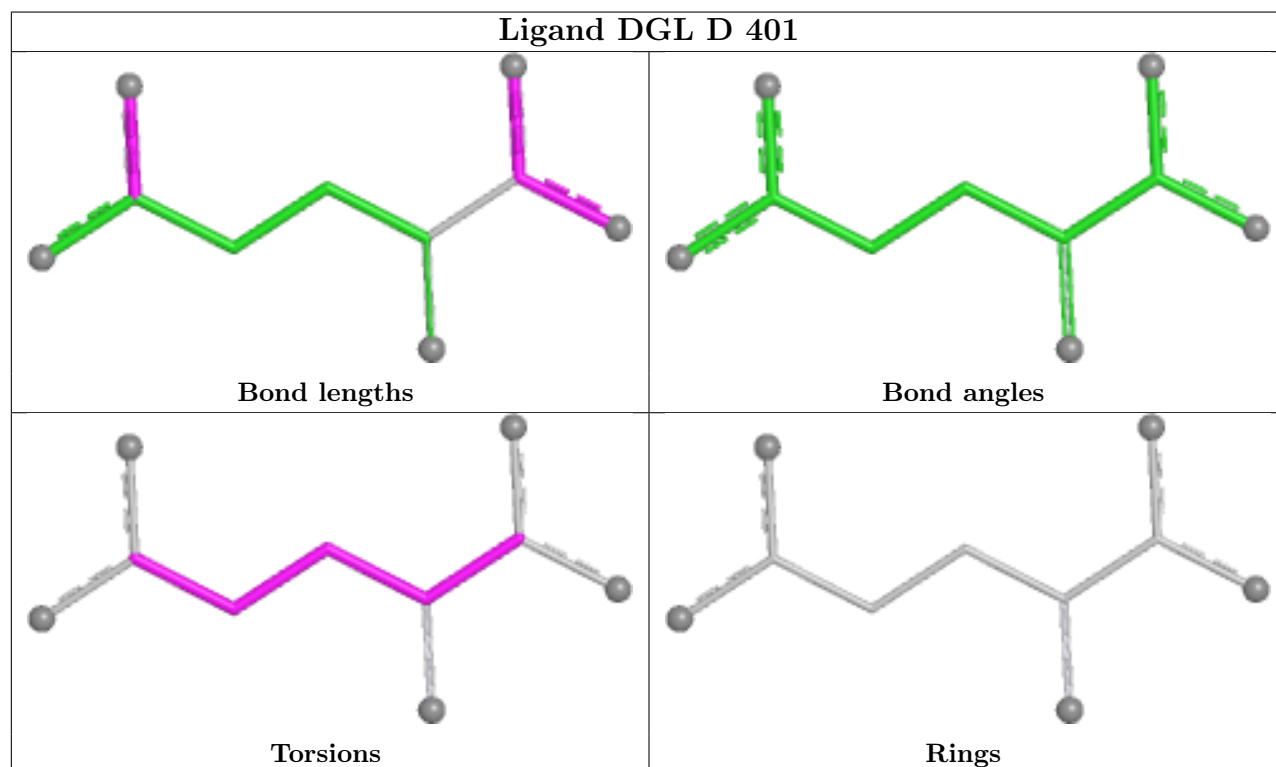
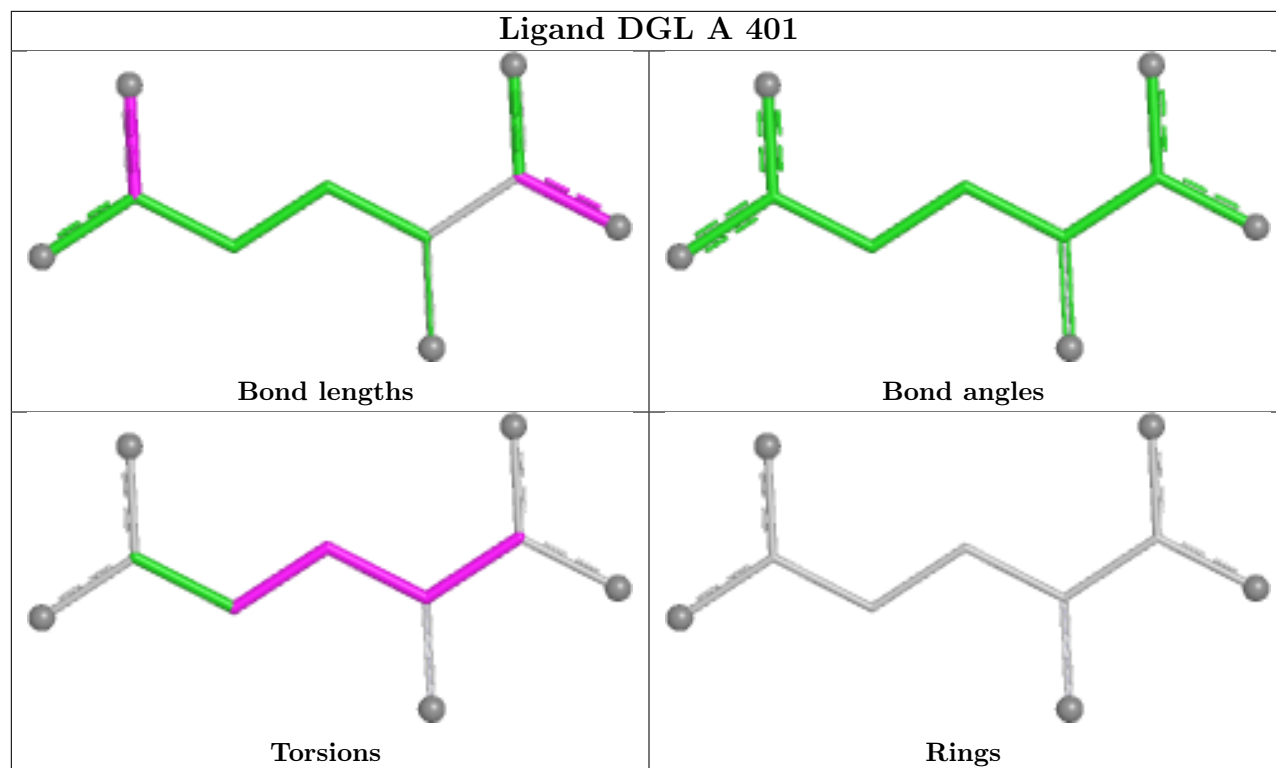
There are no ring outliers.

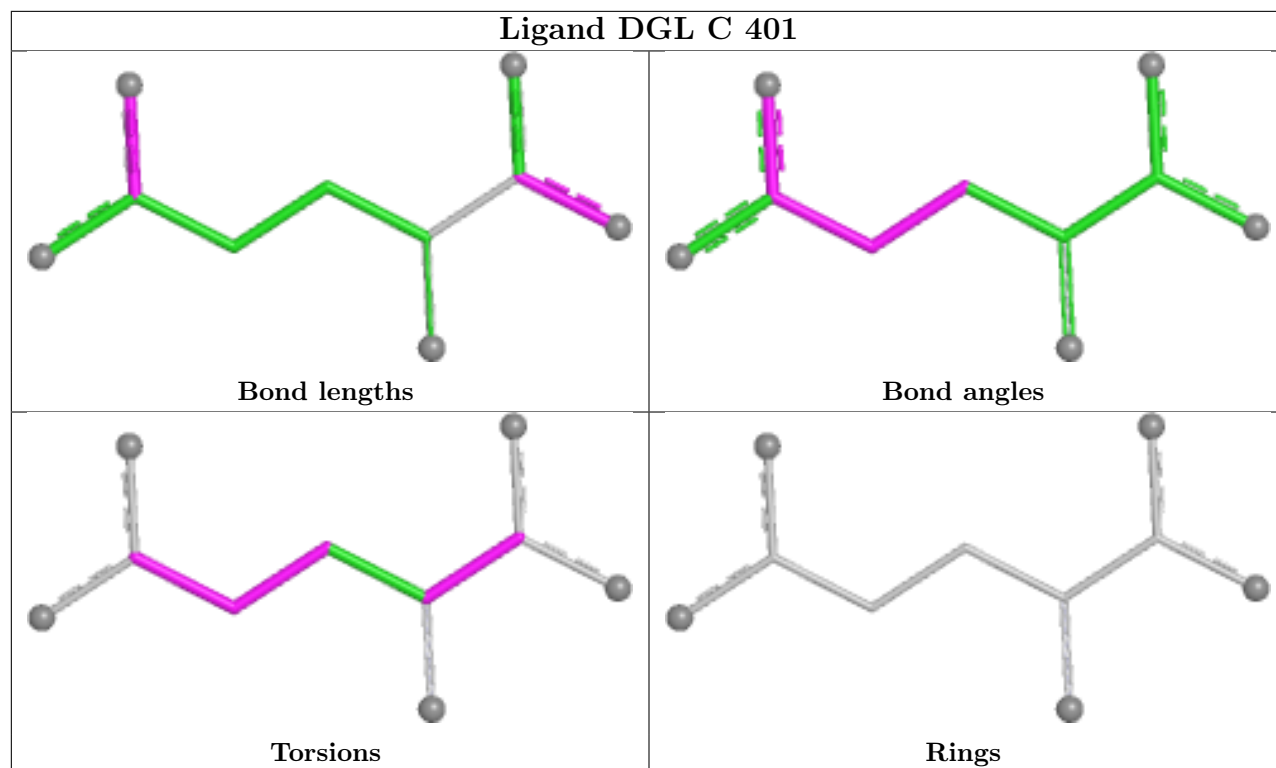
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	DGL	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	312/337 (92%)	0.16	9 (2%) 53 58	6, 17, 39, 63	2 (0%)
1	B	315/337 (93%)	-0.13	3 (0%) 79 82	6, 15, 31, 54	2 (0%)
1	C	314/337 (93%)	-0.03	10 (3%) 50 54	5, 16, 40, 76	2 (0%)
1	D	312/337 (92%)	-0.01	12 (3%) 44 48	5, 14, 39, 71	2 (0%)
All	All	1253/1348 (92%)	-0.00	34 (2%) 56 60	5, 15, 37, 76	8 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	44	LEU	6.1
1	D	22	ALA	4.1
1	D	21	ILE	3.6
1	D	40	GLY	3.6
1	D	47	GLY	3.4
1	A	9	LEU	3.3
1	D	9	LEU	3.2
1	D	46	ALA	3.2
1	C	22	ALA	3.1
1	C	40	GLY	3.0
1	A	22	ALA	2.8
1	D	209	VAL	2.8
1	D	20	THR	2.7
1	A	47	GLY	2.6
1	C	20	THR	2.6
1	D	19	GLY	2.6
1	C	44	LEU	2.6
1	D	43	LYS	2.6
1	A	46	ALA	2.5
1	A	43	LYS	2.5
1	C	8	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	18	GLY	2.3
1	B	8	LYS	2.3
1	B	328	LYS	2.3
1	A	40	GLY	2.3
1	C	46	ALA	2.3
1	C	47	GLY	2.3
1	C	41	VAL	2.2
1	C	43	LYS	2.2
1	A	89	LYS	2.2
1	D	210	ASN	2.2
1	C	23	GLY	2.1
1	B	272	LYS	2.1
1	A	44	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

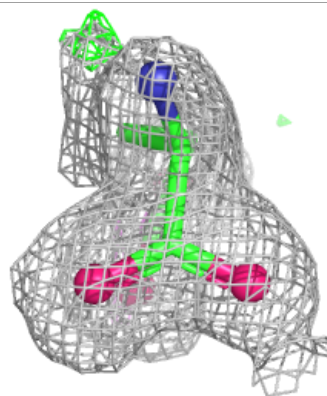
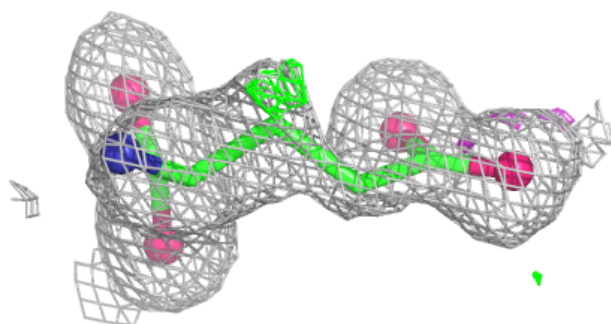
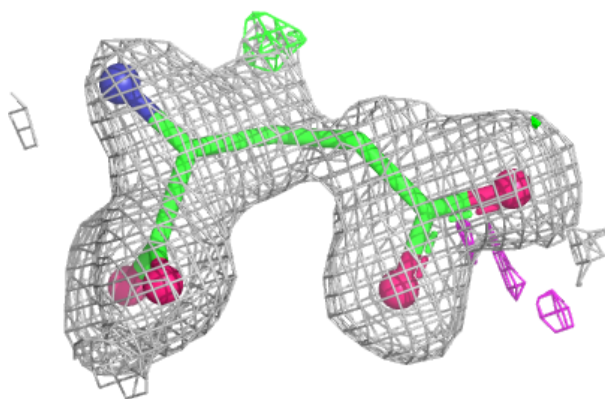
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	DGL	A	401	10/10	0.92	0.10	19,26,35,37	0
2	DGL	C	401	10/10	0.92	0.11	21,28,35,37	0
2	DGL	D	401	10/10	0.92	0.11	16,26,35,36	0
2	DGL	B	401	10/10	0.94	0.08	12,18,25,25	0

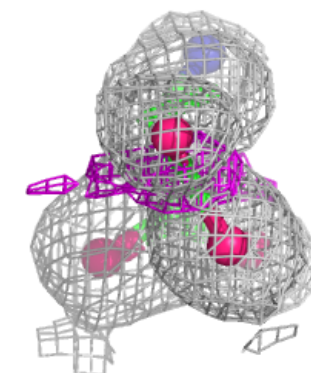
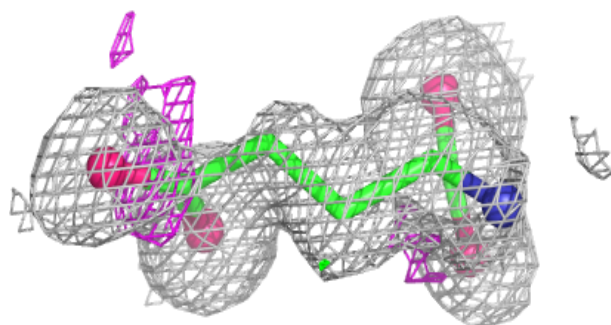
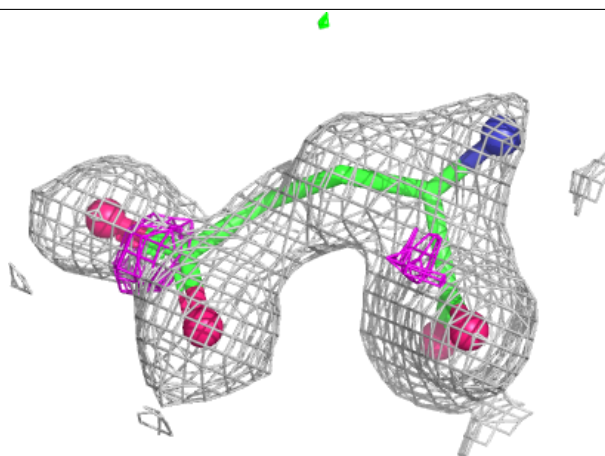
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGL A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

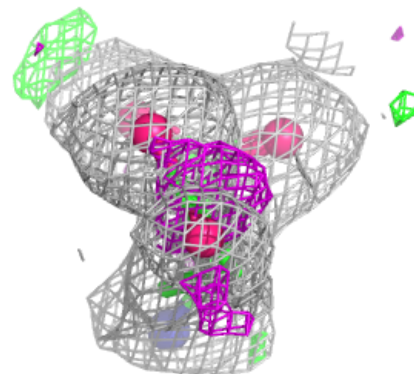
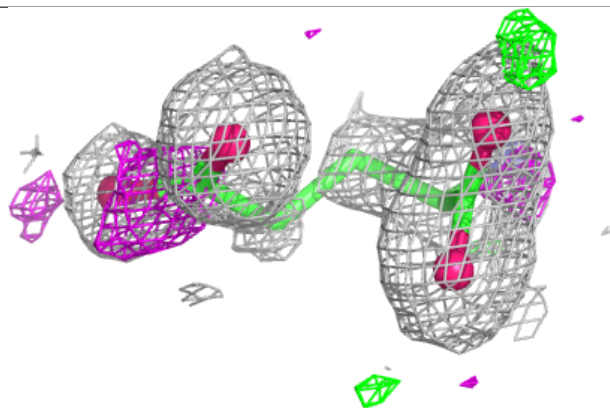
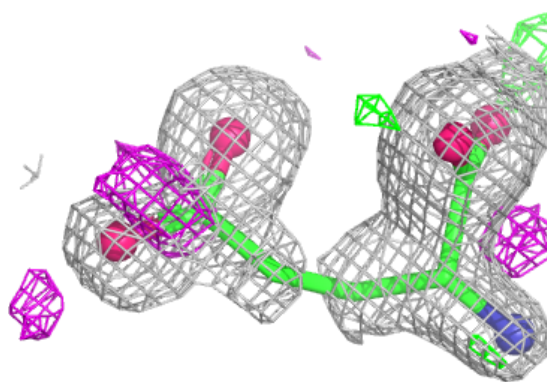
**Electron density around DGL C 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

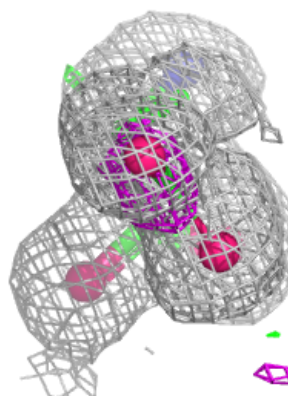
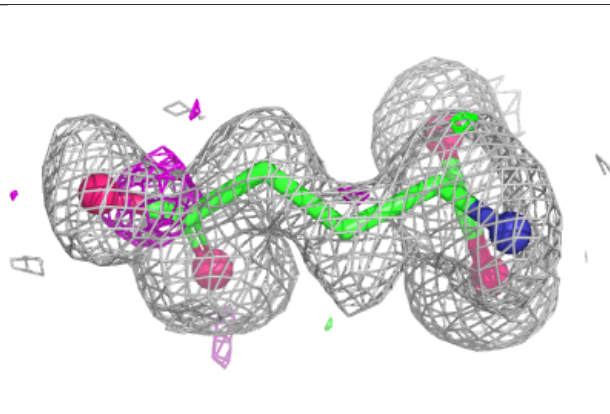
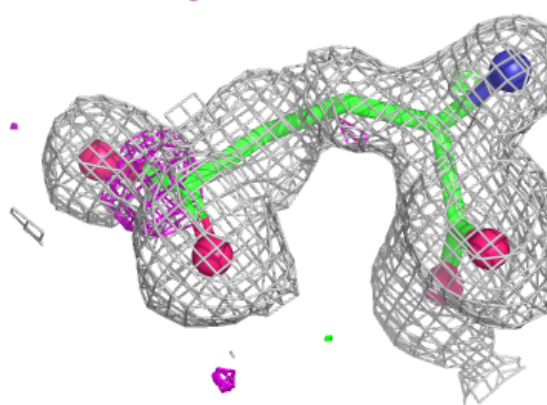


Electron density around DGL D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around DGL B 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.