



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 04:38 PM EDT

PDB ID : 6PA3  
Title : E. coli L-asparaginase II double mutant (T89V,K162T) in complex with L-Asn at pH 7.0  
Authors : Lubkowski, J.; Wlodawer, A.  
Deposited on : 2019-06-11  
Resolution : 1.65 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	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)	:	2.37.1

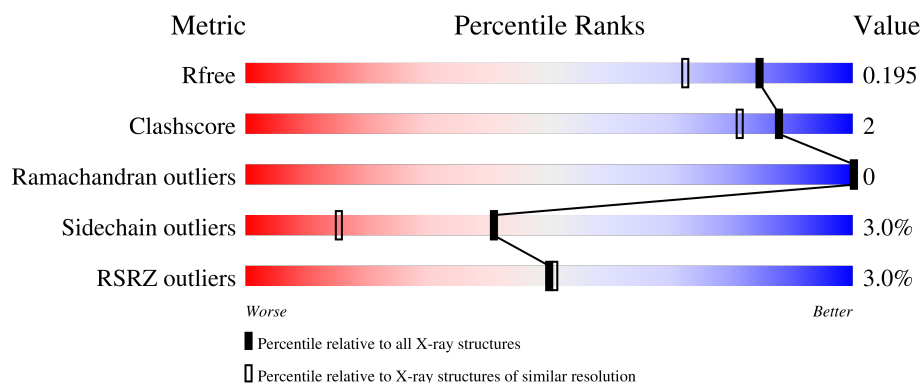
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div>3%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	B	334	<div> <div>5%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	C	334	<div> <div>%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	D	334	<div> <div>4%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11134 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 L-asparaginase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	2	0
			2511	1566	435	501	9			
1	B	328	Total	C	N	O	S	0	1	0
			2452	1530	420	494	8			
1	C	328	Total	C	N	O	S	0	0	0
			2449	1528	420	493	8			
1	D	332	Total	C	N	O	S	0	3	0
			2495	1556	430	501	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP P00805
A	-6	ASP	-	expression tag	UNP P00805
A	-5	HIS	-	expression tag	UNP P00805
A	-4	HIS	-	expression tag	UNP P00805
A	-3	HIS	-	expression tag	UNP P00805
A	-2	HIS	-	expression tag	UNP P00805
A	-1	HIS	-	expression tag	UNP P00805
A	0	HIS	-	expression tag	UNP P00805
A	89	VAL	THR	engineered mutation	UNP P00805
A	162	THR	LYS	engineered mutation	UNP P00805
B	-7	MET	-	initiating methionine	UNP P00805
B	-6	ASP	-	expression tag	UNP P00805
B	-5	HIS	-	expression tag	UNP P00805
B	-4	HIS	-	expression tag	UNP P00805
B	-3	HIS	-	expression tag	UNP P00805
B	-2	HIS	-	expression tag	UNP P00805
B	-1	HIS	-	expression tag	UNP P00805
B	0	HIS	-	expression tag	UNP P00805
B	89	VAL	THR	engineered mutation	UNP P00805
B	162	THR	LYS	engineered mutation	UNP P00805
C	-7	MET	-	initiating methionine	UNP P00805

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ASP	-	expression tag	UNP P00805
C	-5	HIS	-	expression tag	UNP P00805
C	-4	HIS	-	expression tag	UNP P00805
C	-3	HIS	-	expression tag	UNP P00805
C	-2	HIS	-	expression tag	UNP P00805
C	-1	HIS	-	expression tag	UNP P00805
C	0	HIS	-	expression tag	UNP P00805
C	89	VAL	THR	engineered mutation	UNP P00805
C	162	THR	LYS	engineered mutation	UNP P00805
D	-7	MET	-	initiating methionine	UNP P00805
D	-6	ASP	-	expression tag	UNP P00805
D	-5	HIS	-	expression tag	UNP P00805
D	-4	HIS	-	expression tag	UNP P00805
D	-3	HIS	-	expression tag	UNP P00805
D	-2	HIS	-	expression tag	UNP P00805
D	-1	HIS	-	expression tag	UNP P00805
D	0	HIS	-	expression tag	UNP P00805
D	89	VAL	THR	engineered mutation	UNP P00805
D	162	THR	LYS	engineered mutation	UNP P00805

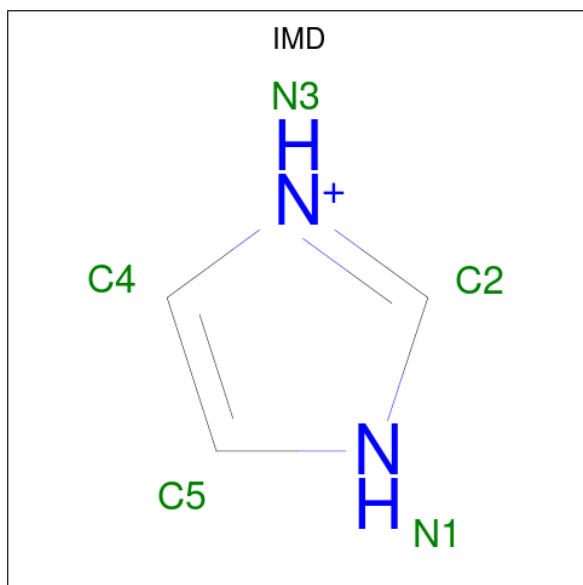
- ASN
- 
- The diagram illustrates the chemical structure of Asparagine (ASN). The central carbon atom is labeled CA(S). It is bonded to a hydrogen atom (H) and an amino group (NH<sub>2</sub>, with N labeled). The amino group is shown with a blue arrow pointing to the nitrogen atom. The CA(S) atom is also bonded to a carboxyl group (C=O, with O labeled) and an amide group (C=O, with O labeled). The amide group is further bonded to a nitrogen atom (N) which is bonded to two hydrogen atoms (H<sub>2</sub>N, with ND2 labeled). The carboxyl group is further bonded to an oxygen atom (O, with OD1 labeled). The amide group is further bonded to a carbon atom (C) which is bonded to an oxygen atom (O, with OXT labeled). The amide group is also bonded to a nitrogen atom (N, with N labeled). The carboxyl group is also bonded to a carbon atom (C, with CB labeled). The amide group is also bonded to a carbon atom (C, with CG labeled).

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			9	4	2	3		
2	C	1	Total	C	N	O	0	0
			9	4	2	3		
2	D	1	Total	C	N	O	0	0
			9	4	2	3		

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	A	1	Total	C	N	0	0
			5	3	2		
3	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

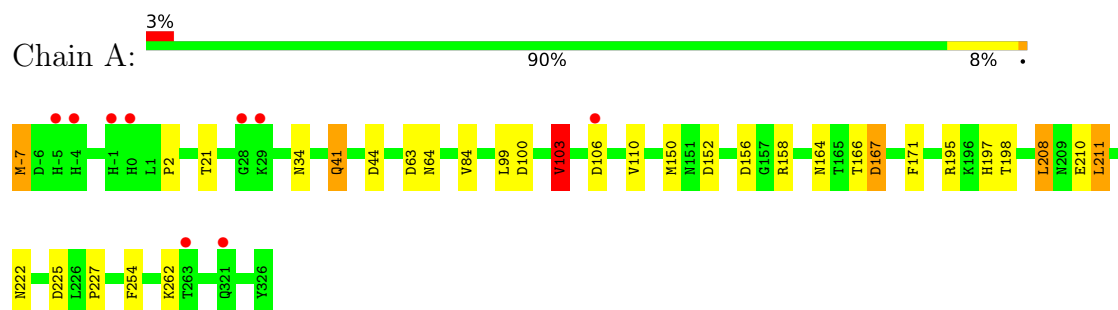
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	297	Total 297	O 297	0	0
5	B	250	Total 250	O 250	0	0
5	C	314	Total 314	O 314	0	0
5	D	314	Total 314	O 314	0	0

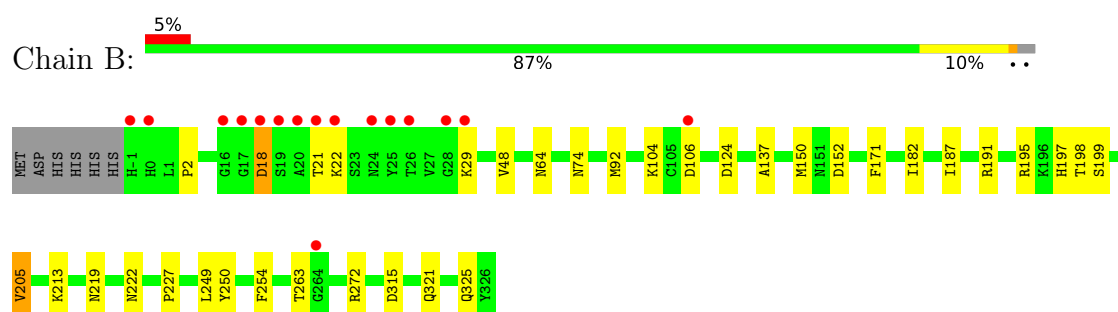
### 3 Residue-property plots [i](#)

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.

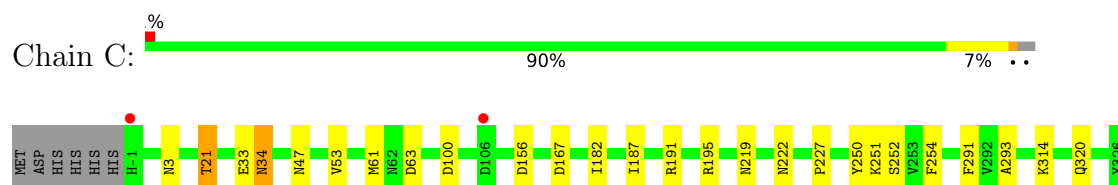
#### • Molecule 1: L-asparaginase 2



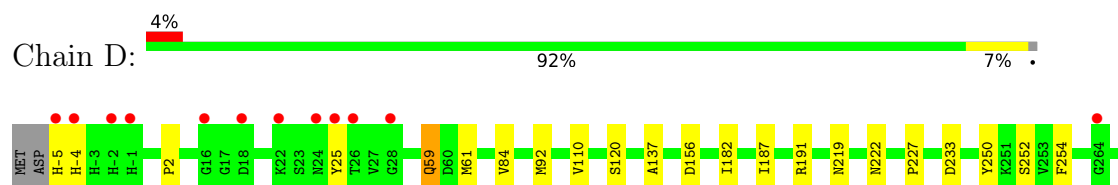
#### • Molecule 1: L-asparaginase 2



#### • Molecule 1: L-asparaginase 2



#### • Molecule 1: L-asparaginase 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.85Å 62.99Å 141.29Å 90.00° 117.83° 90.00°	Depositor
Resolution (Å)	40.00 – 1.65 34.85 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-1.65) 99.5 (34.85-1.65)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.149 , 0.184 0.163 , 0.195	Depositor DCC
$R_{free}$ test set	2723 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.4	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11134	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.91	0/2560	1.02	14/3488 (0.4%)
1	B	0.89	0/2494	0.99	11/3398 (0.3%)
1	C	0.98	2/2488 (0.1%)	1.05	14/3390 (0.4%)
1	D	0.97	2/2546 (0.1%)	0.99	7/3469 (0.2%)
All	All	0.94	4/10088 (0.0%)	1.01	46/13745 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	33	GLU	CD-OE2	6.18	1.32	1.25
1	C	252	SER	CB-OG	-6.13	1.34	1.42
1	D	252	SER	CB-OG	-5.66	1.34	1.42
1	D	25	TYR	CG-CD1	5.49	1.46	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	ASP	CB-CG-OD2	-7.86	111.22	118.30
1	C	61	MET	CG-SD-CE	7.62	112.38	100.20
1	A	100	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	A	167	ASP	CB-CG-OD1	7.44	124.99	118.30
1	D	315	ASP	CB-CG-OD1	7.42	124.98	118.30
1	C	53	VAL	CG1-CB-CG2	7.16	122.35	110.90
1	D	61	MET	CG-SD-CE	6.86	111.18	100.20
1	A	44	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	B	315	ASP	CB-CG-OD1	6.75	124.37	118.30
1	C	195	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	211	LEU	CB-CG-CD1	6.57	122.17	111.00
1	B	205	VAL	CG1-CB-CG2	6.26	120.92	110.90
1	B	272	ARG	NE-CZ-NH2	6.20	123.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	233	ASP	CB-CG-OD1	6.17	123.85	118.30
1	D	269	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	195	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	152	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	249	LEU	CB-CG-CD2	-6.02	100.76	111.00
1	A	103	VAL	CA-CB-CG2	5.94	119.80	110.90
1	B	124	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	B	272	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	C	195	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	100	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	103	VAL	CG1-CB-CG2	5.69	120.00	110.90
1	C	167	ASP	CB-CG-OD1	5.68	123.41	118.30
1	D	191	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	C	21	THR	N-CA-CB	-5.64	99.58	110.30
1	C	53	VAL	CA-CB-CG2	5.59	119.29	110.90
1	A	225	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	191	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	C	291	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	D	92	MET	CG-SD-CE	5.53	109.04	100.20
1	B	191	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	92	MET	CG-SD-CE	5.49	108.98	100.20
1	A	103	VAL	CA-CB-CG1	5.47	119.11	110.90
1	C	191	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	158	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	152	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	-7	MET	CG-SD-CE	5.18	108.48	100.20
1	C	291	PHE	CB-CG-CD1	5.17	124.42	120.80
1	D	233	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	195	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	63	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	B	48	VAL	CG1-CB-CG2	5.06	118.99	110.90
1	C	63	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	208	LEU	CB-CG-CD1	5.00	119.50	111.00

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	2511	0	2486	11	0
1	B	2452	0	2439	15	0
1	C	2449	0	2434	9	0
1	D	2495	0	2471	7	0
2	A	9	0	5	0	0
2	B	9	0	5	0	0
2	C	9	0	5	0	0
2	D	9	0	5	0	0
3	A	15	0	14	0	0
4	A	1	0	0	0	0
5	A	297	0	0	2	1
5	B	250	0	0	2	2
5	C	314	0	0	2	1
5	D	314	0	0	3	1
All	All	11134	0	9864	40	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 2.

All (40) 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:D:59:GLN:H	1:D:59:GLN:HE21	1.14	0.90
1:C:293:ALA:H	1:C:320:GLN:HE22	1.22	0.87
1:A:164:ASN:HD22	1:A:167:ASP:H	1.36	0.74
1:B:74:ASN:HD21	1:B:104:LYS:H	1.43	0.67
1:B:74:ASN:ND2	1:B:104:LYS:H	2.01	0.57
1:B:197:HIS:HD2	1:B:198:THR:OG1	1.88	0.57
1:B:18:ASP:OD1	1:B:18:ASP:N	2.37	0.55
1:A:64[A]:ASN:ND2	5:A:502:HOH:O	2.40	0.55
1:C:293:ALA:H	1:C:320:GLN:NE2	2.00	0.54
1:B:219:ASN:HD22	1:B:250:TYR:H	1.57	0.53
1:A:197:HIS:HD2	1:A:198:THR:OG1	1.92	0.53
1:A:210:GLU:OE1	5:A:501:HOH:O	2.18	0.52
1:B:106:ASP:OD2	1:B:199:SER:OG	2.29	0.49
1:A:99:LEU:O	1:A:103:VAL:HG13	2.13	0.48
1:D:219:ASN:HD22	1:D:250:TYR:H	1.59	0.48
1:B:321:GLN:HG2	1:B:325:GLN:HE21	1.78	0.48
1:A:41:GLN:H	1:A:41:GLN:NE2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ASN:HD22	1:C:250:TYR:H	1.62	0.47
1:A:150:MET:HG3	1:A:171:PHE:CD2	2.50	0.47
1:B:321:GLN:HG2	1:B:325:GLN:NE2	2.29	0.47
1:A:227:PRO:HB3	1:B:227:PRO:HB3	1.98	0.46
1:C:3:ASN:HD22	1:C:47:ASN:HB2	1.80	0.45
1:D:182:ILE:HG12	1:D:187:ILE:HG12	1.98	0.45
1:A:34:ASN:HB2	5:C:706:HOH:O	2.16	0.45
1:A:164:ASN:ND2	1:A:166:THR:H	2.15	0.44
1:D:-5:HIS:N	5:D:508:HOH:O	2.51	0.44
1:C:227:PRO:HB3	1:D:227:PRO:HB3	1.99	0.43
1:A:84:VAL:HA	1:A:110:VAL:O	2.19	0.43
1:C:34:ASN:ND2	5:C:514:HOH:O	2.52	0.43
1:C:182:ILE:HG12	1:C:187:ILE:HG12	2.01	0.42
1:B:2:PRO:HG2	1:B:137:ALA:HB1	2.01	0.42
1:D:2:PRO:HG2	1:D:137:ALA:HB1	2.01	0.42
1:C:251:LYS:HD3	5:D:805:HOH:O	2.19	0.42
1:B:263:THR:HG22	1:B:263:THR:O	2.20	0.42
1:C:251:LYS:HB3	5:D:769:HOH:O	2.19	0.42
1:D:84:VAL:HA	1:D:110:VAL:O	2.20	0.41
1:B:197:HIS:HE1	5:B:566:HOH:O	2.02	0.41
1:B:182:ILE:HG12	1:B:187:ILE:HG12	2.01	0.41
1:B:64:ASN:ND2	5:B:513:HOH:O	2.54	0.41
1:B:150:MET:HG3	1:B:171:PHE:CD2	2.56	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)
5:B:610:HOH:O	5:B:610:HOH:O[2_555]	0.52	1.68
5:C:635:HOH:O	5:C:635:HOH:O[2_556]	0.67	1.53
5:D:551:HOH:O	5:D:551:HOH:O[2_556]	0.69	1.51
5:A:720:HOH:O	5:B:719:HOH:O[1_545]	2.17	0.03

## 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	334/334 (100%)	328 (98%)	6 (2%)	0	100	100
1	B	327/334 (98%)	320 (98%)	7 (2%)	0	100	100
1	C	326/334 (98%)	320 (98%)	6 (2%)	0	100	100
1	D	333/334 (100%)	328 (98%)	5 (2%)	0	100	100
All	All	1320/1336 (99%)	1296 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	275/274 (100%)	263 (96%)	12 (4%)	28	7
1	B	269/274 (98%)	261 (97%)	8 (3%)	41	15
1	C	268/274 (98%)	262 (98%)	6 (2%)	52	27
1	D	274/274 (100%)	267 (97%)	7 (3%)	46	21
All	All	1086/1096 (99%)	1053 (97%)	33 (3%)	41	15

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-7	MET
1	A	2	PRO
1	A	21	THR
1	A	41	GLN
1	A	103	VAL
1	A	106	ASP
1	A	156	ASP
1	A	208	LEU
1	A	211	LEU
1	A	222	ASN

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Mol	Chain	Res	Type
1	A	254	PHE
1	A	262	LYS
1	B	18	ASP
1	B	21	THR
1	B	22	LYS
1	B	29	LYS
1	B	205	VAL
1	B	213	LYS
1	B	222	ASN
1	B	254	PHE
1	C	21	THR
1	C	34	ASN
1	C	156	ASP
1	C	222	ASN
1	C	254	PHE
1	C	314	LYS
1	D	-4	HIS
1	D	59	GLN
1	D	120[A]	SER
1	D	120[B]	SER
1	D	156	ASP
1	D	222	ASN
1	D	254	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	164	ASN
1	A	190	GLN
1	A	197	HIS
1	A	321	GLN
1	B	24	ASN
1	B	34	ASN
1	B	37	ASN
1	B	64	ASN
1	B	74	ASN
1	B	143	ASN
1	B	151	ASN
1	B	197	HIS
1	B	219	ASN
1	B	325	GLN

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Mol	Chain	Res	Type
1	C	3	ASN
1	C	34	ASN
1	C	219	ASN
1	C	318	GLN
1	C	320	GLN
1	C	324	ASN
1	C	325	GLN
1	D	59	GLN
1	D	151	ASN
1	D	184	ASN
1	D	190	GLN
1	D	219	ASN
1	D	312	GLN
1	D	317	GLN
1	D	318	GLN
1	D	324	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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	IMD	A	402	4	3,5,5	0.21	0	4,5,5	0.52	0
2	ASN	B	401	-	6,8,8	1.38	1 (16%)	8,10,10	0.89	0
3	IMD	A	403	4	3,5,5	0.21	0	4,5,5	0.69	0
2	ASN	C	401	-	6,8,8	1.32	1 (16%)	8,10,10	0.92	0
2	ASN	A	401	-	6,8,8	0.75	0	8,10,10	0.43	0
2	ASN	D	401	-	6,8,8	0.99	0	8,10,10	0.47	0
3	IMD	A	404	4	3,5,5	0.43	0	4,5,5	0.53	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	IMD	A	402	4	-	-	0/1/1/1
2	ASN	B	401	-	-	2/8/8/8	-
3	IMD	A	403	4	-	-	0/1/1/1
2	ASN	C	401	-	-	2/8/8/8	-
2	ASN	A	401	-	-	4/8/8/8	-
2	ASN	D	401	-	-	4/8/8/8	-
3	IMD	A	404	4	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ASN	OXT-C	-2.50	1.22	1.30
2	C	401	ASN	O-C	2.22	1.28	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ASN	O-C-CA-N
2	B	401	ASN	O-C-CA-N
2	C	401	ASN	O-C-CA-N
2	D	401	ASN	O-C-CA-N
2	A	401	ASN	OXT-C-CA-N
2	D	401	ASN	OXT-C-CA-N
2	B	401	ASN	OXT-C-CA-N

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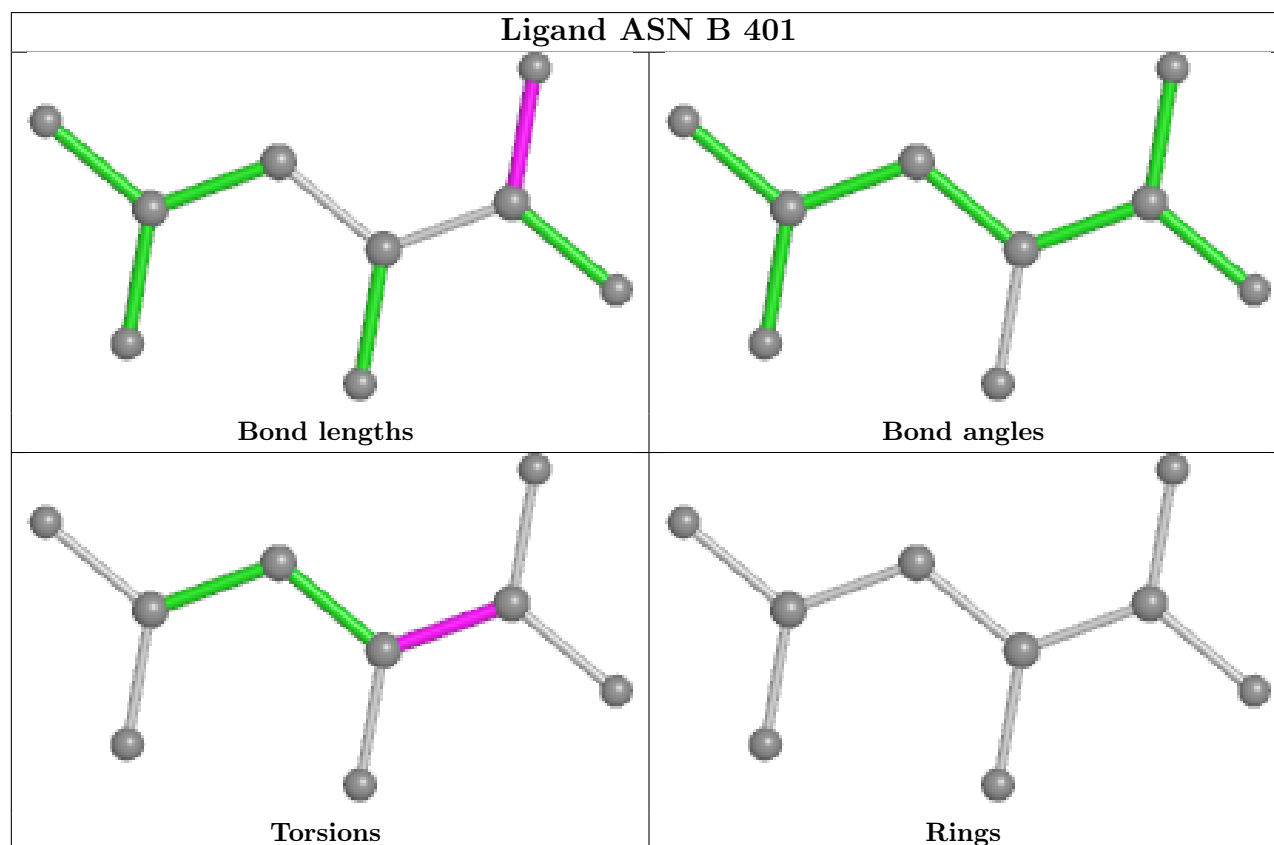
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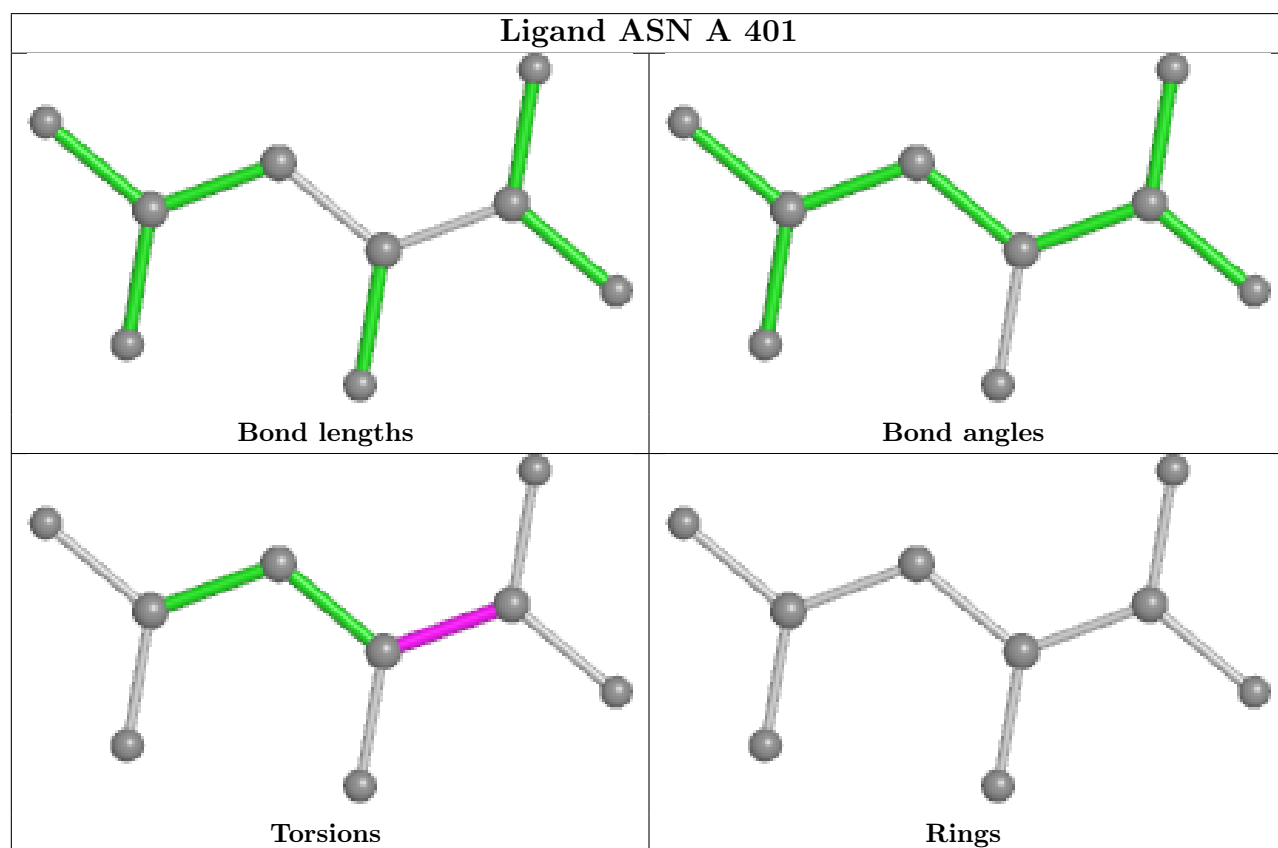
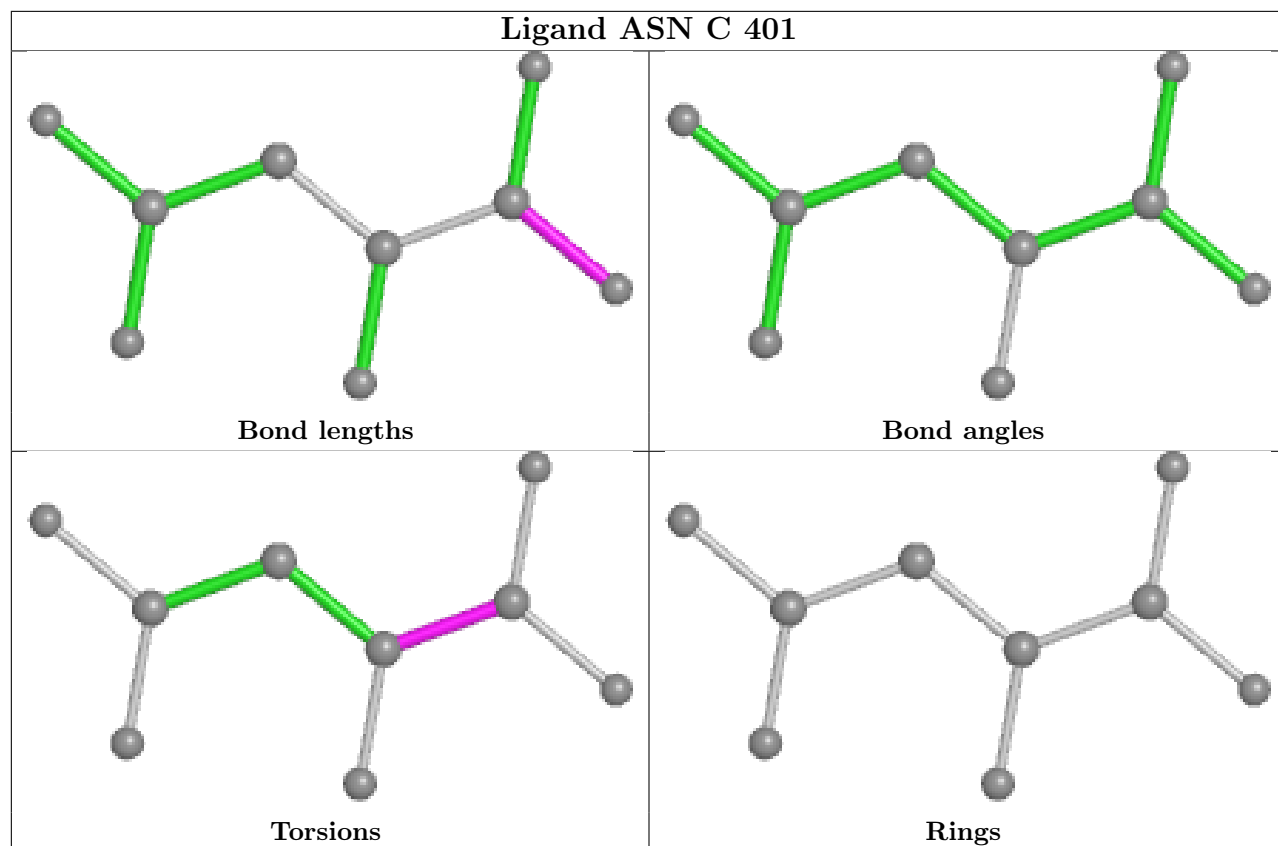
Mol	Chain	Res	Type	Atoms
2	C	401	ASN	OXT-C-CA-N
2	A	401	ASN	OXT-C-CA-CB
2	D	401	ASN	O-C-CA-CB
2	D	401	ASN	OXT-C-CA-CB
2	A	401	ASN	O-C-CA-CB

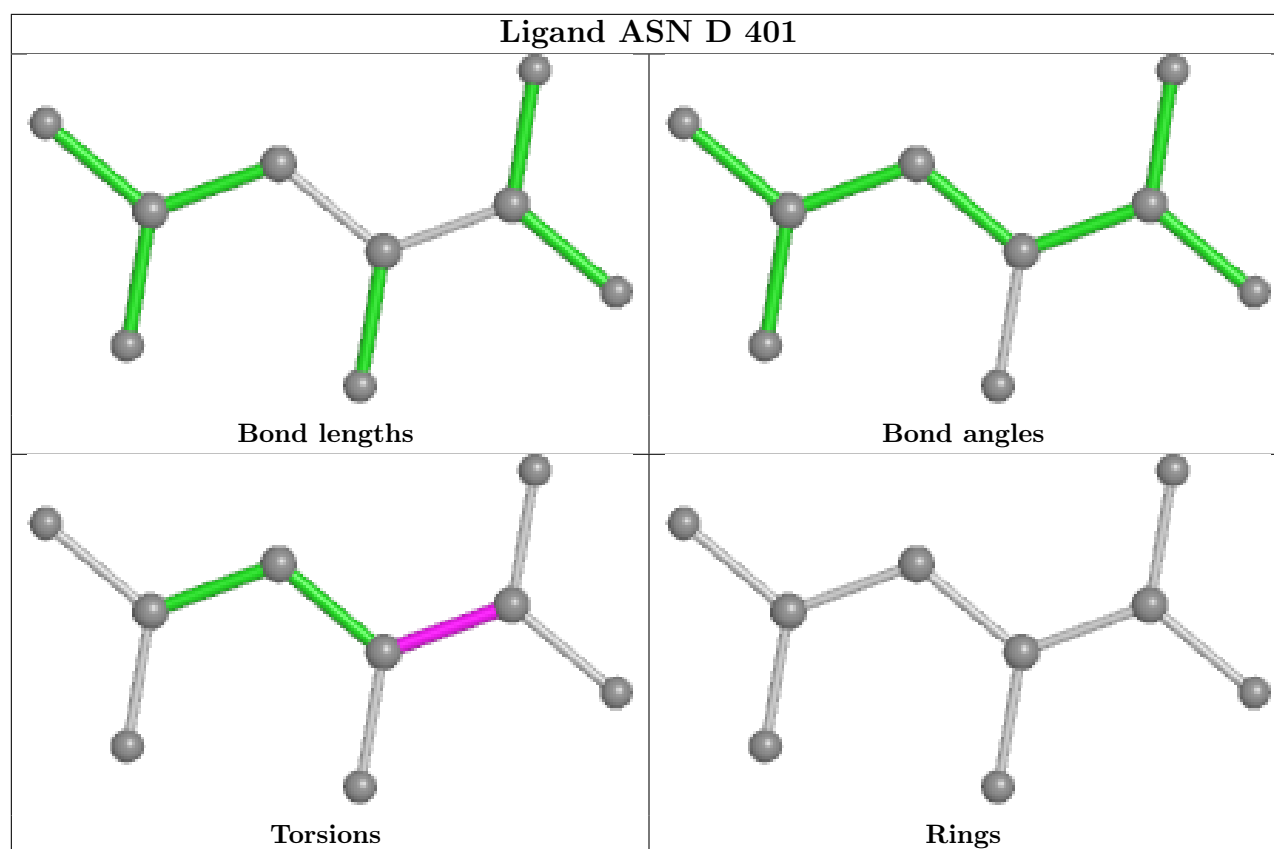
There are no ring outliers.

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/334 (100%)	-0.26	9 (2%) 54 55	11, 18, 31, 46	0
1	B	328/334 (98%)	-0.13	16 (4%) 29 28	12, 19, 40, 68	0
1	C	328/334 (98%)	-0.36	2 (0%) 89 90	9, 16, 28, 52	0
1	D	332/334 (99%)	-0.22	12 (3%) 42 43	10, 16, 35, 58	0
All	All	1322/1336 (98%)	-0.25	39 (2%) 50 51	9, 17, 34, 68	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	THR	7.6
1	B	18	ASP	6.2
1	B	25	TYR	5.9
1	D	-4	HIS	5.2
1	D	-1	HIS	5.2
1	B	21	THR	5.1
1	A	-5	HIS	4.9
1	B	22	LYS	4.6
1	D	26	THR	4.4
1	B	16	GLY	4.4
1	B	24	ASN	4.2
1	D	-5	HIS	4.1
1	B	19	SER	4.0
1	B	-1	HIS	3.8
1	D	18	ASP	3.8
1	B	17	GLY	3.7
1	D	25	TYR	3.6
1	A	-1	HIS	3.6
1	A	106	ASP	3.5
1	C	-1	HIS	3.5
1	D	16	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	20	ALA	3.3
1	A	0	HIS	3.1
1	D	22	LYS	2.9
1	A	28	GLY	2.9
1	C	106	ASP	2.9
1	B	0	HIS	2.7
1	B	28	GLY	2.6
1	D	24	ASN	2.5
1	A	263	THR	2.5
1	D	264	GLY	2.4
1	D	28	GLY	2.3
1	B	106	ASP	2.2
1	B	29	LYS	2.2
1	D	-2	HIS	2.2
1	A	321	GLN	2.1
1	B	264	GLY	2.1
1	A	-4	HIS	2.1
1	A	29	LYS	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	IMD	A	402	5/5	0.71	0.23	40,42,43,45	0
3	IMD	A	404	5/5	0.85	0.25	32,33,34,35	0
3	IMD	A	403	5/5	0.86	0.32	44,44,44,45	0
2	ASN	B	401	9/9	0.97	0.07	15,16,17,17	0
2	ASN	A	401	9/9	0.98	0.06	12,13,13,14	0

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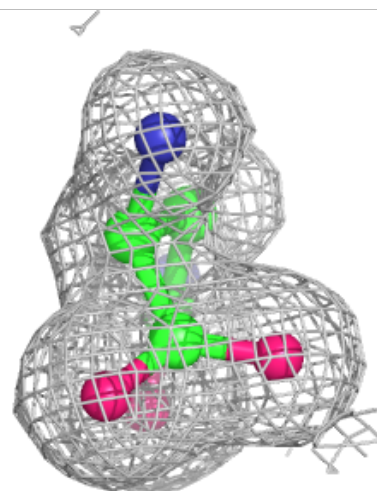
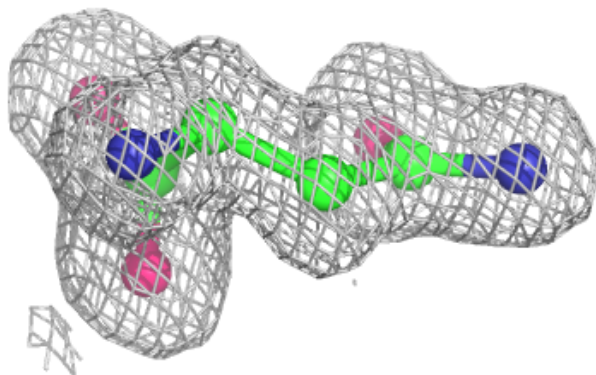
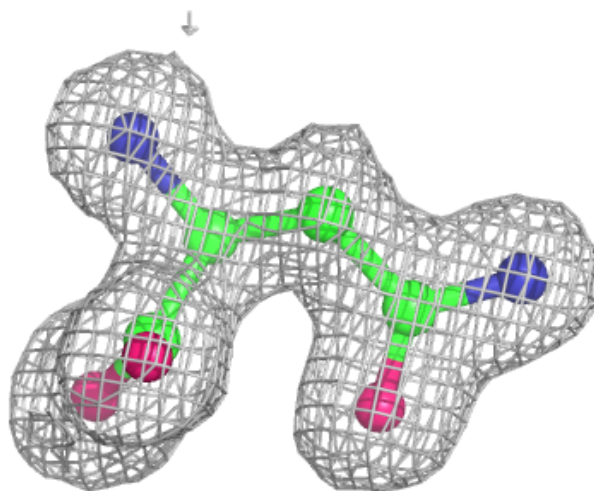
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ASN	C	401	9/9	0.98	0.05	11,12,12,12	0
2	ASN	D	401	9/9	0.98	0.07	13,13,14,14	0
4	MG	A	405	1/1	0.98	0.08	13,13,13,13	0

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.

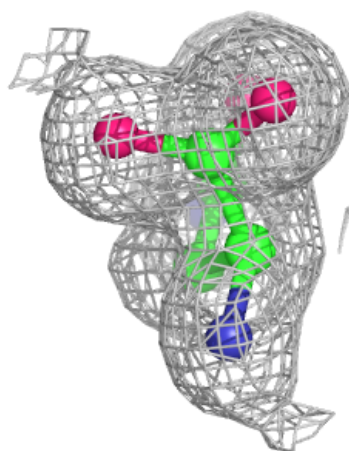
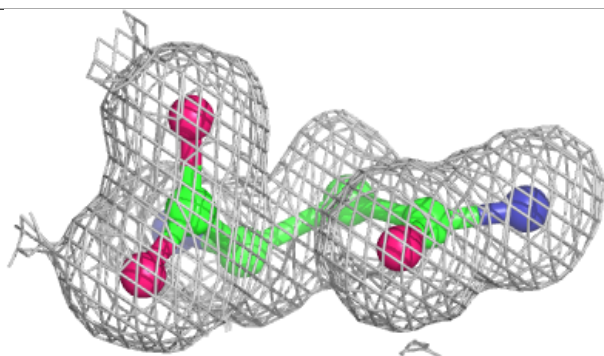
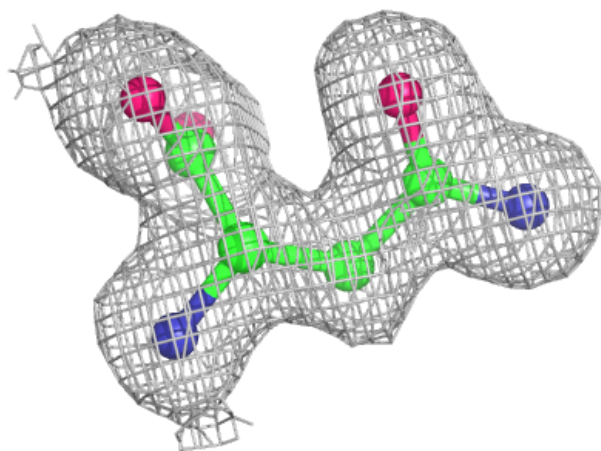
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2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ASN A 401:**

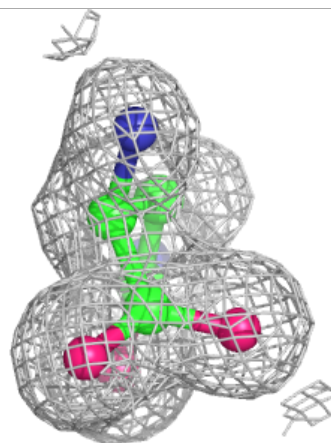
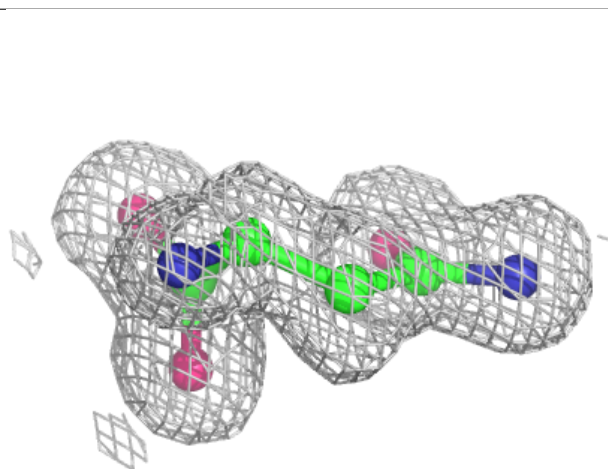
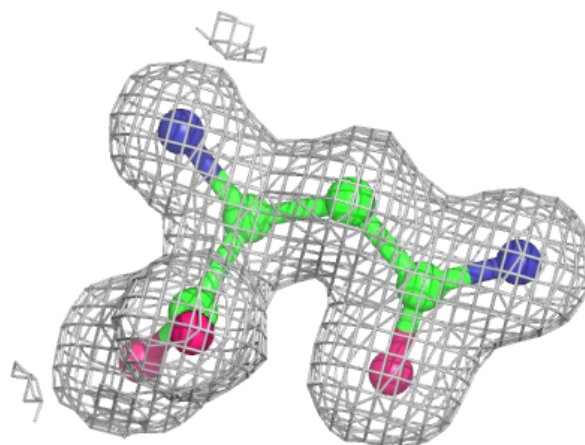
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

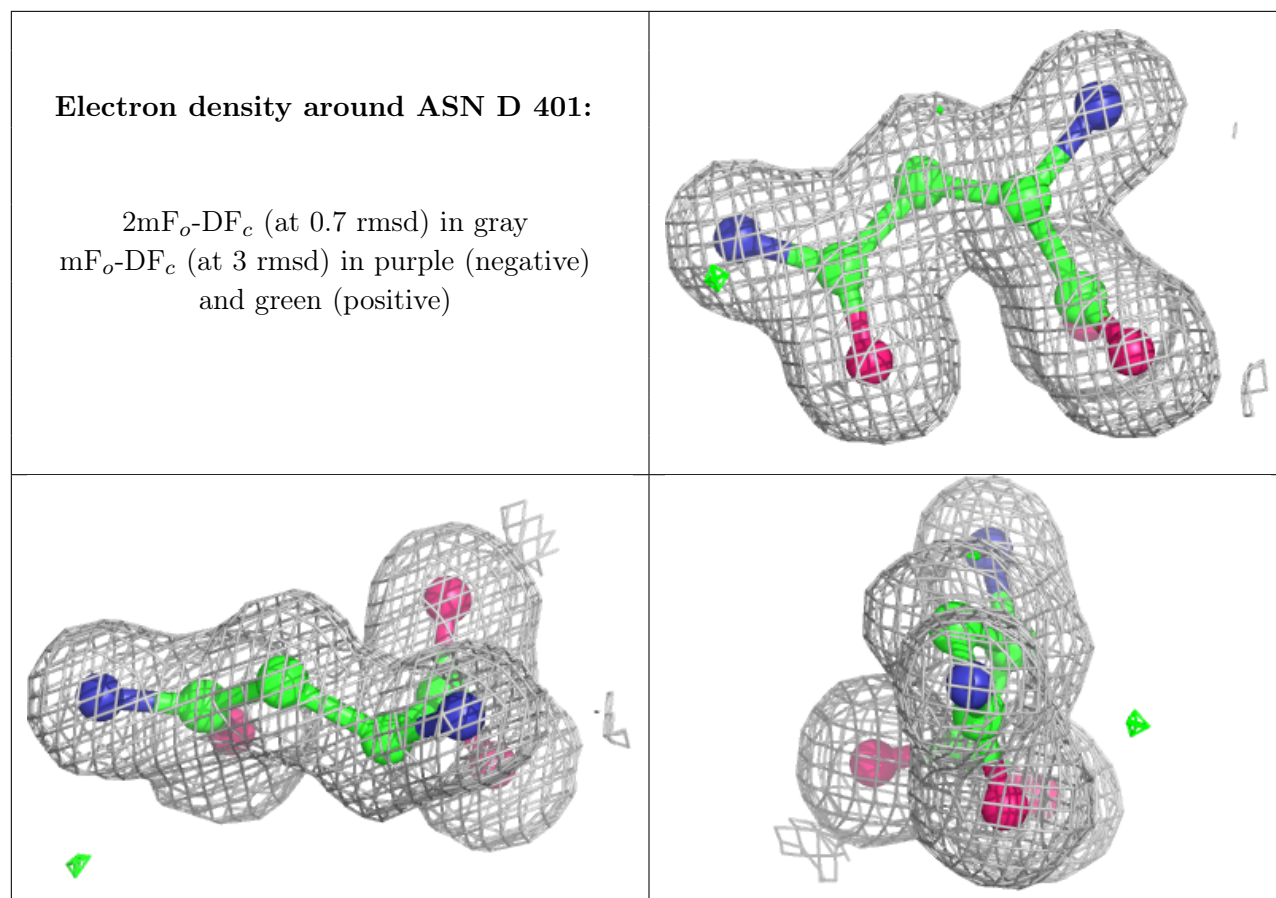




**Electron density around ASN C 401:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.