



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 06:56 AM JST

PDB ID : 8X4S  
Title : The L-tryptophan specific decarboxylase PsiD covalent bonding with tryptamine  
Authors : Meng, C.Y.; Wen, Y.; Guo, W.T.; Wu, B.X.  
Deposited on : 2023-11-15  
Resolution : 2.70 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](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 : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

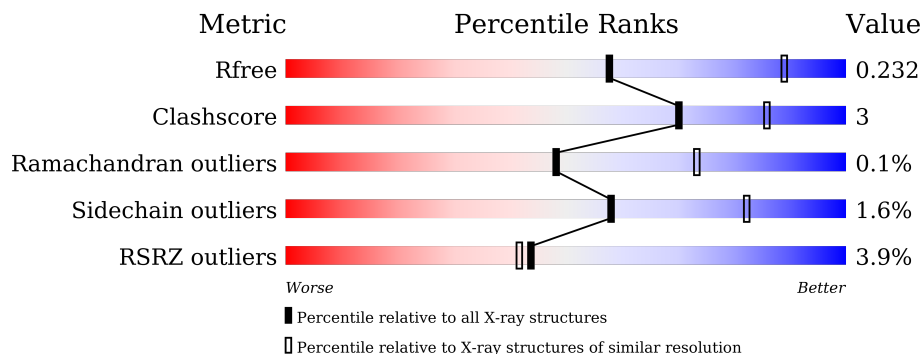
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.



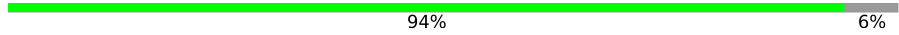
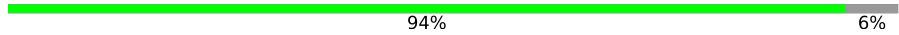
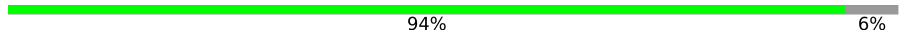
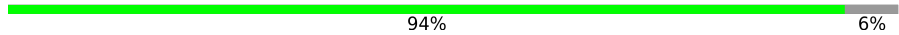
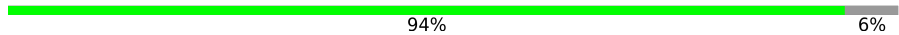
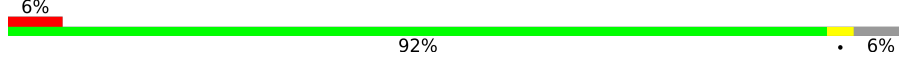
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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  $\geq 3$ , 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	402	 2% 78% 8% • 13%
1	C	402	 % 78% 7% • 14%
1	E	402	 3% 77% 8% • 14%
1	G	402	 3% 79% 6% • 14%
1	I	402	 % 79% 6% 14%
1	K	402	 12% 78% 8% 14%

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Mol	Chain	Length	Quality of chain
2	B	36	 94% 6%
2	D	36	 94% 6%
2	F	36	 94% 6%
2	H	36	 94% 6%
2	J	36	 94% 6%
2	L	36	 6% 92% 6%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18594 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.

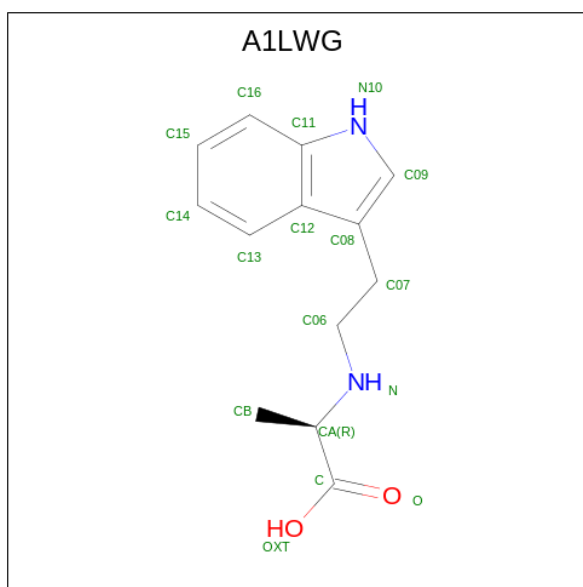
- Molecule 1 is a protein called L-tryptophan decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	I	346	2747	1766	461	505	15	0	0	0
1	G	346	2754	1768	460	511	15	0	0	0
1	A	350	2792	1792	469	516	15	0	0	0
1	C	346	2763	1776	464	508	15	0	0	0
1	E	346	2753	1769	459	510	15	0	0	0
1	K	347	2762	1773	463	511	15	0	0	0

- Molecule 2 is a protein called L-tryptophan decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	J	34	240	155	42	42	1	0	0	0
2	H	34	244	158	43	42	1	0	0	0
2	B	34	240	155	42	42	1	0	0	0
2	D	34	244	157	42	44	1	0	0	0
2	F	34	248	159	42	46	1	0	0	0
2	L	34	244	157	42	44	1	0	0	0

- Molecule 3 is (2 {R})-2-[2-(1 {H}-indol-3-yl)ethylamino]propanoic acid (three-letter code: A1LWG) (formula: C<sub>13</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	J	1	Total	C	N	O	0	0
			16	13	2	1		
3	H	1	Total	C	N	O	0	0
			16	13	2	1		
3	B	1	Total	C	N	O	0	0
			16	13	2	1		
3	D	1	Total	C	N	O	0	0
			16	13	2	1		
3	F	1	Total	C	N	O	0	0
			16	13	2	1		
3	L	1	Total	C	N	O	0	0
			16	13	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	64	Total	O	0	0
			64	64		
4	J	2	Total	O	0	0
			2	2		
4	G	99	Total	O	0	0
			99	99		
4	H	8	Total	O	0	0
			8	8		
4	A	90	Total	O	0	0
			90	90		
4	B	9	Total	O	0	0
			9	9		

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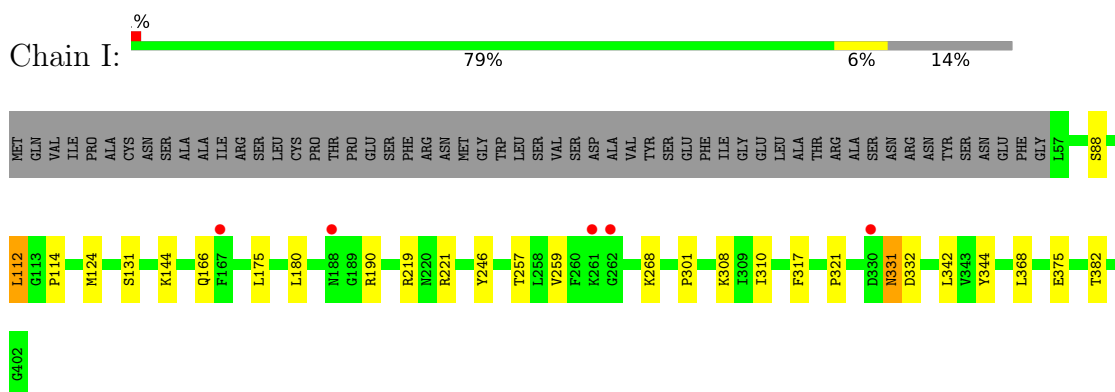
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	C	74	Total O 74 74	0	0
4	D	9	Total O 9 9	0	0
4	E	73	Total O 73 73	0	0
4	F	4	Total O 4 4	0	0
4	K	34	Total O 34 34	0	0
4	L	1	Total O 1 1	0	0

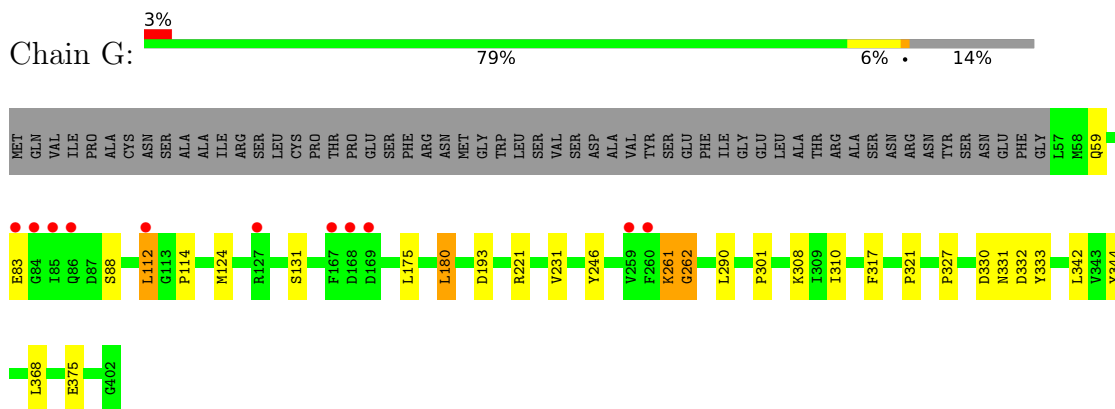
### 3 Residue-property plots [i](#)

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.

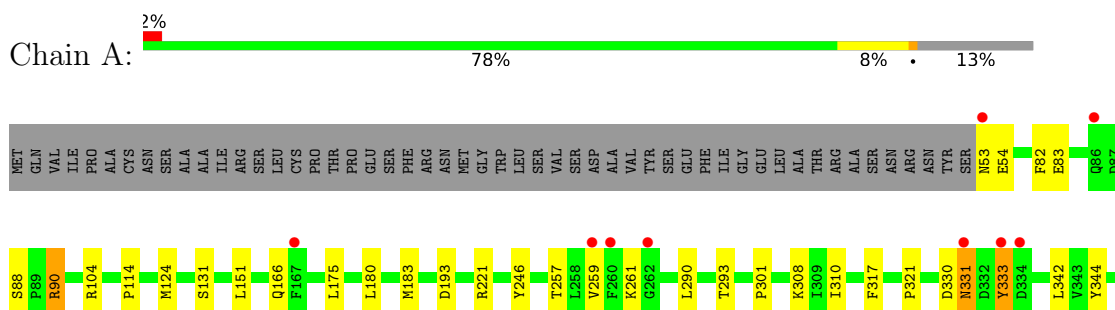
- Molecule 1: L-tryptophan decarboxylase



- Molecule 1: L-tryptophan decarboxylase

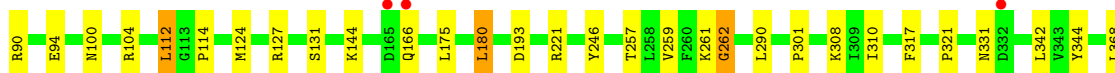
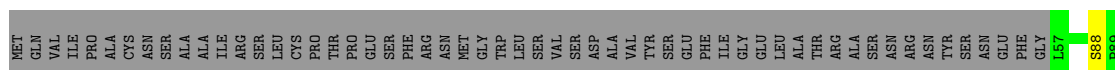
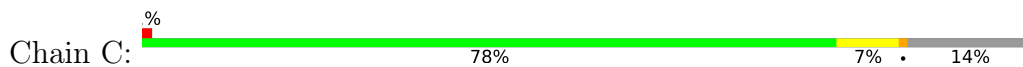


- Molecule 1: L-tryptophan decarboxylase

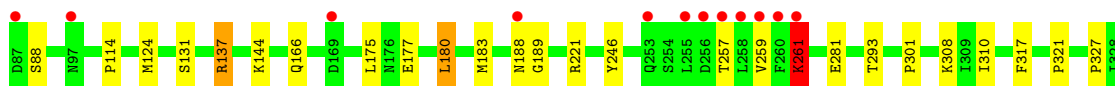
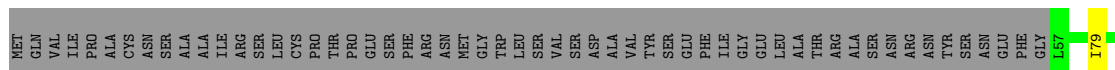
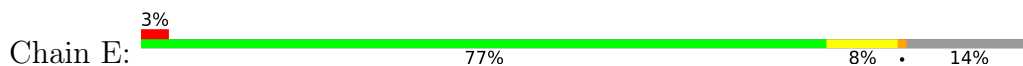




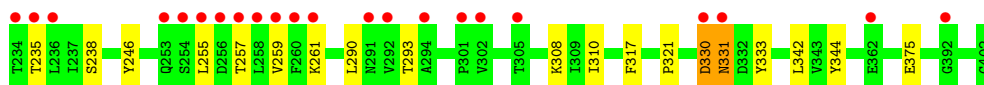
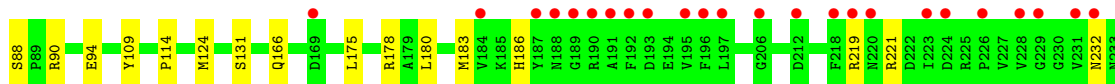
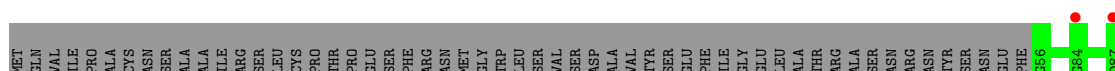
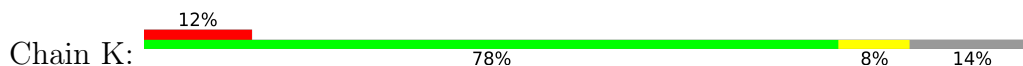
- Molecule 1: L-tryptophan decarboxylase



- Molecule 1: L-tryptophan decarboxylase



- Molecule 1: L-tryptophan decarboxylase



- Molecule 2: L-tryptophan decarboxylase







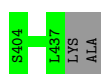
- Molecule 2: L-tryptophan decarboxylase

Chain H: 94% 6%



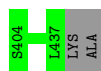
- Molecule 2: L-tryptophan decarboxylase

Chain B: 94% 6%



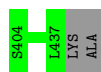
- Molecule 2: L-tryptophan decarboxylase

Chain D: 94% 6%



- Molecule 2: L-tryptophan decarboxylase

Chain F: 94% 6%



- Molecule 2: L-tryptophan decarboxylase

Chain L: 6% 92% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.68Å 122.50Å 128.72Å 90.00° 99.77° 90.00°	Depositor
Resolution (Å)	29.77 – 2.70 29.77 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.77-2.70) 99.6 (29.77-2.70)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.68Å)	Xtrriage
Refinement program	PHENIX 1.21rc1_5156	Depositor
R, $R_{free}$	0.198 , 0.233 0.200 , 0.232	Depositor DCC
$R_{free}$ test set	3493 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtrriage
Anisotropy	0.372	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18594	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: A1LWG

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	0.52	2/2870 (0.1%)	0.68	2/3896 (0.1%)
1	C	0.47	0/2840	0.67	1/3854 (0.0%)
1	E	0.51	2/2830 (0.1%)	0.67	1/3844 (0.0%)
1	G	0.49	1/2831 (0.0%)	0.68	3/3846 (0.1%)
1	I	0.48	0/2824	0.67	1/3836 (0.0%)
1	K	0.51	1/2839 (0.0%)	0.69	1/3855 (0.0%)
2	B	0.44	0/242	0.66	0/329
2	D	0.45	0/246	0.68	0/334
2	F	0.53	0/250	0.69	0/339
2	H	0.46	0/246	0.65	0/333
2	J	0.44	0/242	0.66	0/329
2	L	0.46	0/246	0.66	0/334
All	All	0.49	6/18506 (0.0%)	0.68	9/25129 (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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	I	0	1
1	K	0	2
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	330	ASP	CB-CG	8.46	1.69	1.51
1	A	83	GLU	CG-CD	7.80	1.63	1.51
1	E	177	GLU	CG-CD	6.58	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	177	GLU	CB-CG	5.85	1.63	1.52
1	A	333	TYR	C-N	5.71	1.47	1.34
1	G	83	GLU	CB-CG	5.43	1.62	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	83	GLU	CA-CB-CG	-8.76	94.14	113.40
1	K	330	ASP	CB-CG-OD2	8.46	125.91	118.30
1	I	112	LEU	CB-CG-CD2	-7.00	99.10	111.00
1	G	112	LEU	CB-CG-CD2	-6.75	99.52	111.00
1	A	330	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	G	330	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	330	ASP	CB-CG-OD1	5.28	123.05	118.30
1	C	112	LEU	CB-CG-CD2	-5.14	102.27	111.00
1	E	261	LYS	CA-CB-CG	5.03	124.46	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	ASN	Mainchain
1	A	90	ARG	Sidechain
1	I	331	ASN	Mainchain
1	K	178	ARG	Sidechain
1	K	331	ASN	Peptide

## 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	2792	0	2643	18	2
1	C	2763	0	2631	18	0
1	E	2753	0	2602	27	2
1	G	2754	0	2601	17	0
1	I	2747	0	2602	18	1
1	K	2762	0	2617	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	240	0	241	0	0
2	D	244	0	245	0	0
2	F	248	0	249	0	0
2	H	244	0	252	0	0
2	J	240	0	241	0	0
2	L	244	0	245	1	0
3	B	16	0	0	1	0
3	D	16	0	0	1	0
3	F	16	0	0	0	0
3	H	16	0	0	1	0
3	J	16	0	0	0	0
3	L	16	0	0	1	0
4	A	90	0	0	1	1
4	B	9	0	0	0	0
4	C	74	0	0	2	0
4	D	9	0	0	0	0
4	E	73	0	0	6	0
4	F	4	0	0	0	0
4	G	99	0	0	3	0
4	H	8	0	0	0	0
4	I	64	0	0	1	0
4	J	2	0	0	0	0
4	K	34	0	0	2	0
4	L	1	0	0	0	0
All	All	18594	0	17169	118	3

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 (118) 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:K:331:ASN:OD1	1:K:333:TYR:N	2.13	0.81
1:K:186:HIS:O	4:K:501:HOH:O	1.99	0.79
1:C:388:HIS:O	4:C:501:HOH:O	2.02	0.78
1:E:166:GLN:HB3	1:K:232:ASN:CG	2.07	0.75
1:A:53:ASN:O	1:A:104:ARG:NH1	2.22	0.72
1:G:261:LYS:O	1:G:262:GLY:O	2.08	0.72
1:E:327:PRO:O	4:E:501:HOH:O	2.09	0.71
1:E:166:GLN:HB3	1:K:232:ASN:OD1	1.91	0.70
1:I:112:LEU:HD12	1:I:112:LEU:H	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:190:ARG:O	4:I:501:HOH:O	2.11	0.69
1:E:281:GLU:OE1	4:E:502:HOH:O	2.11	0.68
1:E:333:TYR:CD1	1:K:219:ARG:HD3	2.28	0.68
1:G:112:LEU:H	1:G:112:LEU:HD12	1.61	0.66
1:K:255:LEU:HD13	1:K:261:LYS:HD3	1.79	0.66
1:A:331:ASN:HB2	1:A:333:TYR:CE2	2.32	0.64
1:E:334:ASP:O	4:E:503:HOH:O	2.15	0.63
1:K:255:LEU:HD13	1:K:261:LYS:CD	2.29	0.63
1:A:193:ASP:OD1	4:A:501:HOH:O	2.16	0.63
1:E:259:VAL:O	1:E:261:LYS:HG2	2.02	0.59
1:C:261:LYS:O	1:C:262:GLY:O	2.22	0.57
1:K:238:SER:HA	4:K:502:HOH:O	2.04	0.56
1:E:259:VAL:C	1:E:261:LYS:H	2.08	0.56
1:E:333:TYR:CE1	1:K:219:ARG:HD3	2.41	0.56
1:G:59:GLN:HG2	1:E:79:ILE:HD11	1.87	0.56
1:A:331:ASN:HB2	1:A:333:TYR:CZ	2.41	0.55
1:E:144:LYS:HD2	4:E:547:HOH:O	2.06	0.55
1:K:90:ARG:HG2	1:K:94:GLU:OE2	2.08	0.54
1:C:90:ARG:CZ	1:C:94:GLU:OE2	2.57	0.53
1:G:231:VAL:HG12	4:G:570:HOH:O	2.09	0.53
1:G:112:LEU:HD21	1:G:331:ASN:O	2.09	0.52
1:K:255:LEU:HD22	1:K:261:LYS:HE2	1.91	0.52
1:G:193:ASP:OD1	4:G:501:HOH:O	2.18	0.51
1:I:112:LEU:HD21	1:I:331:ASN:O	2.10	0.51
1:E:308:LYS:HD3	1:E:310:ILE:HD11	1.94	0.50
1:G:308:LYS:HD3	1:G:310:ILE:HD11	1.94	0.50
1:E:329:PRO:O	4:E:504:HOH:O	2.18	0.50
1:A:308:LYS:HD3	1:A:310:ILE:HD11	1.94	0.50
1:C:100:ASN:O	1:C:104:ARG:HG3	2.12	0.50
1:C:90:ARG:NH2	1:C:94:GLU:OE2	2.44	0.49
1:K:308:LYS:HD3	1:K:310:ILE:HD11	1.94	0.49
1:C:308:LYS:HD3	1:C:310:ILE:HD11	1.94	0.49
1:I:308:LYS:HD3	1:I:310:ILE:HD11	1.94	0.49
1:E:166:GLN:HB3	1:K:232:ASN:ND2	2.27	0.49
1:I:175:LEU:HA	1:I:180:LEU:HD13	1.96	0.47
1:C:144:LYS:HB3	1:C:144:LYS:HE3	1.73	0.47
1:K:175:LEU:HA	1:K:180:LEU:HD13	1.96	0.47
1:A:175:LEU:HA	1:A:180:LEU:HD13	1.96	0.47
1:C:114:PRO:HB2	1:C:375:GLU:OE2	2.15	0.47
1:K:114:PRO:HB2	1:K:375:GLU:OE2	2.15	0.47
1:I:124:MET:HG2	1:I:317:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:TYR:CZ	1:C:342:LEU:HB2	2.51	0.46
1:I:246:TYR:CZ	1:I:342:LEU:HB2	2.51	0.46
1:G:246:TYR:CZ	1:G:342:LEU:HB2	2.51	0.46
1:E:114:PRO:HB2	1:E:375:GLU:OE2	2.15	0.46
1:I:112:LEU:H	1:I:112:LEU:CD1	2.27	0.46
1:E:246:TYR:CZ	1:E:342:LEU:HB2	2.51	0.46
1:A:124:MET:HG2	1:A:317:PHE:HB3	1.97	0.46
1:A:246:TYR:CZ	1:A:342:LEU:HB2	2.51	0.46
1:K:246:TYR:CZ	1:K:342:LEU:HB2	2.51	0.46
1:K:255:LEU:HD13	1:K:261:LYS:HD2	1.98	0.46
1:I:114:PRO:HB2	1:I:375:GLU:OE2	2.15	0.46
1:A:114:PRO:HB2	1:A:375:GLU:OE2	2.15	0.46
1:I:382:THR:HB	1:G:333:TYR:CE2	2.51	0.46
1:G:114:PRO:HB2	1:G:375:GLU:OE2	2.15	0.46
1:C:124:MET:HG2	1:C:317:PHE:HB3	1.97	0.46
1:G:124:MET:HG2	1:G:317:PHE:HB3	1.97	0.45
1:I:166:GLN:HE21	1:I:166:GLN:HB2	1.60	0.45
1:A:321:PRO:HD3	1:A:344:TYR:CZ	2.52	0.45
1:G:290:LEU:HD13	3:H:501:A1LWG:C	2.46	0.45
1:E:124:MET:HG2	1:E:317:PHE:HB3	1.97	0.45
1:A:166:GLN:HE21	1:A:166:GLN:HB2	1.60	0.45
1:C:112:LEU:HD21	1:C:331:ASN:O	2.17	0.45
1:C:193:ASP:HB2	4:C:508:HOH:O	2.17	0.45
1:E:166:GLN:O	1:K:232:ASN:ND2	2.50	0.45
1:K:124:MET:HG2	1:K:317:PHE:HB3	1.97	0.45
1:E:189:GLY:N	4:E:512:HOH:O	2.51	0.44
1:C:321:PRO:HD3	1:C:344:TYR:CZ	2.52	0.44
1:K:321:PRO:HD3	1:K:344:TYR:CZ	2.52	0.44
1:G:321:PRO:HD3	1:G:344:TYR:CZ	2.52	0.44
1:I:321:PRO:HD3	1:I:344:TYR:CZ	2.52	0.44
1:E:321:PRO:HD3	1:E:344:TYR:CZ	2.52	0.44
1:E:333:TYR:CE1	1:K:219:ARG:CD	3.00	0.44
1:K:331:ASN:CG	1:K:333:TYR:H	2.22	0.43
1:K:90:ARG:HG2	1:K:94:GLU:CD	2.38	0.43
1:K:235:THR:HB	2:L:437:LEU:HD12	2.01	0.43
1:I:219:ARG:O	1:G:327:PRO:HD3	2.18	0.42
1:E:175:LEU:HA	1:E:180:LEU:HD13	2.02	0.42
1:G:262:GLY:HA3	4:G:508:HOH:O	2.19	0.42
1:I:331:ASN:OD1	1:I:332:ASP:N	2.52	0.42
1:K:331:ASN:CG	1:K:333:TYR:HB3	2.40	0.42
1:G:175:LEU:HA	1:G:180:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:GLN:HE21	1:C:166:GLN:HB2	1.60	0.42
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.84	0.42
1:A:175:LEU:HA	1:A:180:LEU:CD1	2.50	0.42
1:C:175:LEU:HA	1:C:180:LEU:HD13	2.02	0.42
1:C:290:LEU:HD13	3:D:501:A1LWG:C	2.50	0.41
1:K:166:GLN:HE21	1:K:166:GLN:HB2	1.60	0.41
1:E:334:ASP:HA	1:E:335:PRO:HD3	1.92	0.41
1:A:290:LEU:HD13	3:B:501:A1LWG:C	2.51	0.41
1:A:257:THR:HB	1:A:259:VAL:HG23	2.03	0.41
1:E:137:ARG:HD2	1:E:137:ARG:HA	1.71	0.41
1:E:257:THR:HB	1:E:259:VAL:HG23	2.03	0.41
1:K:257:THR:HB	1:K:259:VAL:HG23	2.03	0.41
1:I:175:LEU:HA	1:I:180:LEU:CD1	2.50	0.41
1:I:257:THR:HB	1:I:259:VAL:HG23	2.03	0.41
1:A:301:PRO:HG3	1:A:368:LEU:HD11	2.03	0.41
1:C:257:THR:HB	1:C:259:VAL:HG23	2.03	0.41
1:C:301:PRO:HG3	1:C:368:LEU:HD11	2.03	0.41
1:K:175:LEU:HA	1:K:180:LEU:CD1	2.50	0.41
1:K:290:LEU:HD13	3:L:501:A1LWG:C	2.51	0.41
1:G:301:PRO:HG3	1:G:368:LEU:HD11	2.03	0.40
1:E:301:PRO:HG3	1:E:368:LEU:HD11	2.03	0.40
1:E:183:MET:HG2	1:E:293:THR:HB	2.04	0.40
1:K:183:MET:HG2	1:K:293:THR:HB	2.04	0.40
1:I:112:LEU:HD12	1:I:112:LEU:N	2.30	0.40
1:I:301:PRO:HG3	1:I:368:LEU:HD11	2.03	0.40
1:A:54:GLU:OE1	1:K:109:TYR:OH	2.24	0.40
1:A:183:MET:HG2	1:A:293:THR:HB	2.04	0.40

All (3) 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)
1:A:82:PHE:O	1:E:188:ASN:ND2[2_656]	2.03	0.17
1:I:268:LYS:NZ	4:A:588:HOH:O[2_645]	2.04	0.16
1:A:90:ARG:O	1:E:188:ASN:OD1[2_656]	2.07	0.13



## 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	348/402 (87%)	335 (96%)	13 (4%)	0	100	100
1	C	344/402 (86%)	331 (96%)	12 (4%)	1 (0%)	37	61
1	E	344/402 (86%)	331 (96%)	13 (4%)	0	100	100
1	G	344/402 (86%)	331 (96%)	12 (4%)	1 (0%)	37	61
1	I	344/402 (86%)	330 (96%)	14 (4%)	0	100	100
1	K	345/402 (86%)	332 (96%)	13 (4%)	0	100	100
2	B	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
2	D	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
2	F	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
2	H	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
2	J	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
2	L	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
All	All	2261/2628 (86%)	2176 (96%)	83 (4%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	262	GLY
1	C	262	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	299/350 (85%)	295 (99%)	4 (1%)	65	85
1	C	296/350 (85%)	291 (98%)	5 (2%)	56	81
1	E	294/350 (84%)	287 (98%)	7 (2%)	44	73
1	G	295/350 (84%)	289 (98%)	6 (2%)	50	78
1	I	293/350 (84%)	289 (99%)	4 (1%)	62	84
1	K	296/350 (85%)	292 (99%)	4 (1%)	62	84
2	B	23/29 (79%)	23 (100%)	0	100	100
2	D	24/29 (83%)	24 (100%)	0	100	100
2	F	25/29 (86%)	25 (100%)	0	100	100
2	H	24/29 (83%)	24 (100%)	0	100	100
2	J	23/29 (79%)	23 (100%)	0	100	100
2	L	24/29 (83%)	24 (100%)	0	100	100
All	All	1916/2274 (84%)	1886 (98%)	30 (2%)	58	82

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	88	SER
1	I	131	SER
1	I	144	LYS
1	I	221	ARG
1	G	88	SER
1	G	131	SER
1	G	180	LEU
1	G	221	ARG
1	G	261	LYS
1	G	332	ASP
1	A	88	SER
1	A	131	SER
1	A	221	ARG
1	A	261	LYS
1	C	88	SER
1	C	127	ARG
1	C	131	SER
1	C	180	LEU
1	C	221	ARG
1	E	88	SER
1	E	131	SER
1	E	137	ARG

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Mol	Chain	Res	Type
1	E	180	LEU
1	E	221	ARG
1	E	261	LYS
1	E	333	TYR
1	K	88	SER
1	K	131	SER
1	K	221	ARG
1	K	330	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	166	GLN
1	I	253	GLN
1	G	166	GLN
1	G	253	GLN
1	A	166	GLN
1	A	253	GLN
1	C	166	GLN
1	C	186	HIS
1	C	253	GLN
1	E	86	GLN
1	E	166	GLN
1	E	253	GLN
1	K	166	GLN
1	K	253	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

6 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
3	A1LWG	J	501	2	15,17,18	1.82	5 (33%)	12,22,24	1.38	1 (8%)
3	A1LWG	D	501	2	15,17,18	1.81	4 (26%)	12,22,24	1.54	1 (8%)
3	A1LWG	L	501	2	15,17,18	1.70	5 (33%)	12,22,24	0.88	0
3	A1LWG	B	501	2	15,17,18	1.66	4 (26%)	12,22,24	1.79	2 (16%)
3	A1LWG	F	501	2	15,17,18	1.72	4 (26%)	12,22,24	1.30	1 (8%)
3	A1LWG	H	501	2	15,17,18	1.87	5 (33%)	12,22,24	1.02	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	A1LWG	J	501	2	-	2/5/8/10	0/2/2/2
3	A1LWG	D	501	2	-	2/5/8/10	0/2/2/2
3	A1LWG	L	501	2	-	3/5/8/10	0/2/2/2
3	A1LWG	B	501	2	-	3/5/8/10	0/2/2/2
3	A1LWG	F	501	2	-	3/5/8/10	0/2/2/2
3	A1LWG	H	501	2	-	2/5/8/10	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	A1LWG	CA-N	4.09	1.54	1.47
3	J	501	A1LWG	CA-N	3.91	1.54	1.47
3	H	501	A1LWG	CA-N	3.57	1.53	1.47
3	B	501	A1LWG	CA-N	3.47	1.53	1.47
3	D	501	A1LWG	CA-N	3.29	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	501	A1LWG	C06-N	3.22	1.54	1.47
3	L	501	A1LWG	CA-N	3.20	1.53	1.47
3	J	501	A1LWG	C06-N	3.17	1.53	1.47
3	D	501	A1LWG	C06-N	2.80	1.53	1.47
3	D	501	A1LWG	C14-C13	2.77	1.43	1.36
3	B	501	A1LWG	C14-C13	2.61	1.42	1.36
3	L	501	A1LWG	C15-C16	2.54	1.42	1.36
3	H	501	A1LWG	C07-C08	2.48	1.59	1.51
3	L	501	A1LWG	C14-C13	2.45	1.42	1.36
3	B	501	A1LWG	C15-C16	2.39	1.42	1.36
3	F	501	A1LWG	C06-N	2.39	1.52	1.47
3	H	501	A1LWG	C14-C13	2.38	1.42	1.36
3	L	501	A1LWG	C06-N	2.34	1.52	1.47
3	J	501	A1LWG	C14-C13	2.33	1.42	1.36
3	L	501	A1LWG	CB-CA	2.29	1.58	1.51
3	B	501	A1LWG	C06-N	2.27	1.51	1.47
3	F	501	A1LWG	C14-C13	2.22	1.41	1.36
3	F	501	A1LWG	CB-CA	2.20	1.57	1.51
3	D	501	A1LWG	C15-C16	2.18	1.41	1.36
3	J	501	A1LWG	C15-C16	2.09	1.41	1.36
3	H	501	A1LWG	C15-C16	2.08	1.41	1.36
3	J	501	A1LWG	C07-C08	2.07	1.58	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	A1LWG	C06-C07-C08	5.00	120.93	111.28
3	B	501	A1LWG	CB-CA-N	4.78	117.51	108.76
3	J	501	A1LWG	C06-C07-C08	4.59	120.14	111.28
3	F	501	A1LWG	CB-CA-N	3.80	115.72	108.76
3	B	501	A1LWG	C06-C07-C08	3.30	117.64	111.28

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	501	A1LWG	CB-CA-N-C06
3	J	501	A1LWG	C06-C07-C08-C12
3	H	501	A1LWG	CB-CA-N-C06
3	B	501	A1LWG	C06-C07-C08-C12
3	D	501	A1LWG	CB-CA-N-C06
3	D	501	A1LWG	C06-C07-C08-C12

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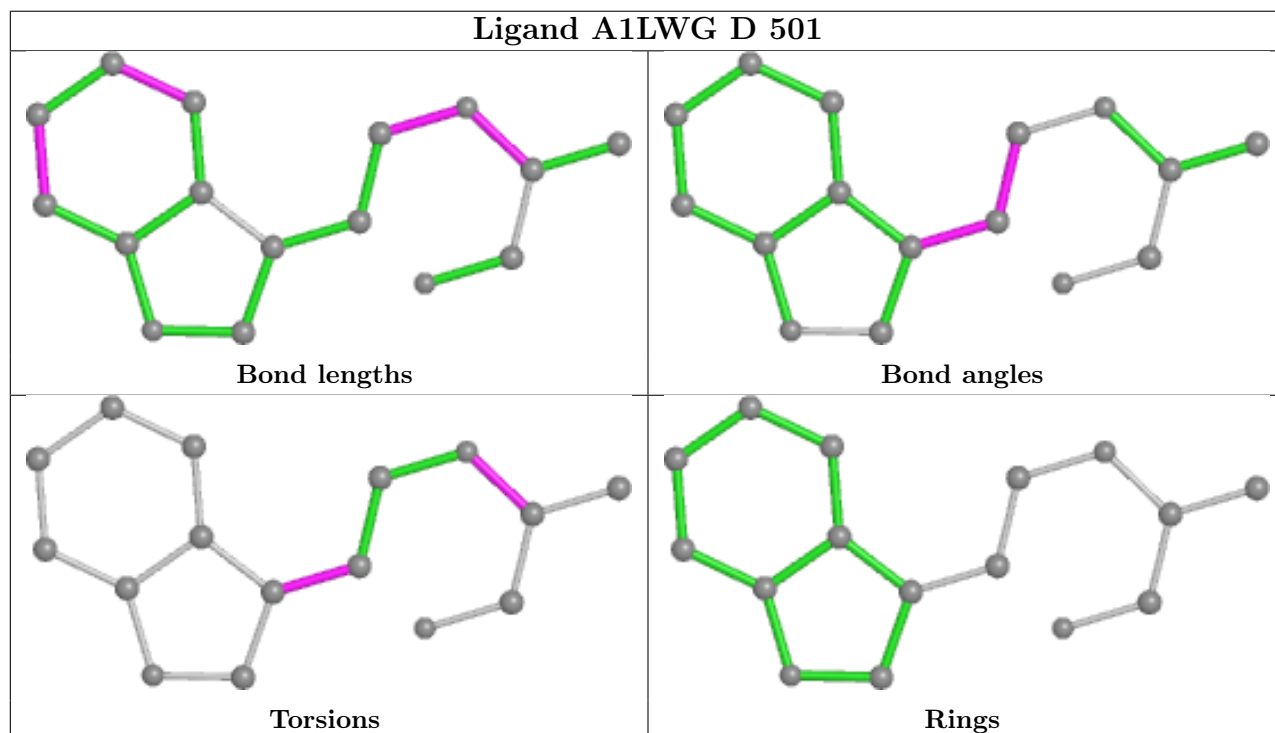
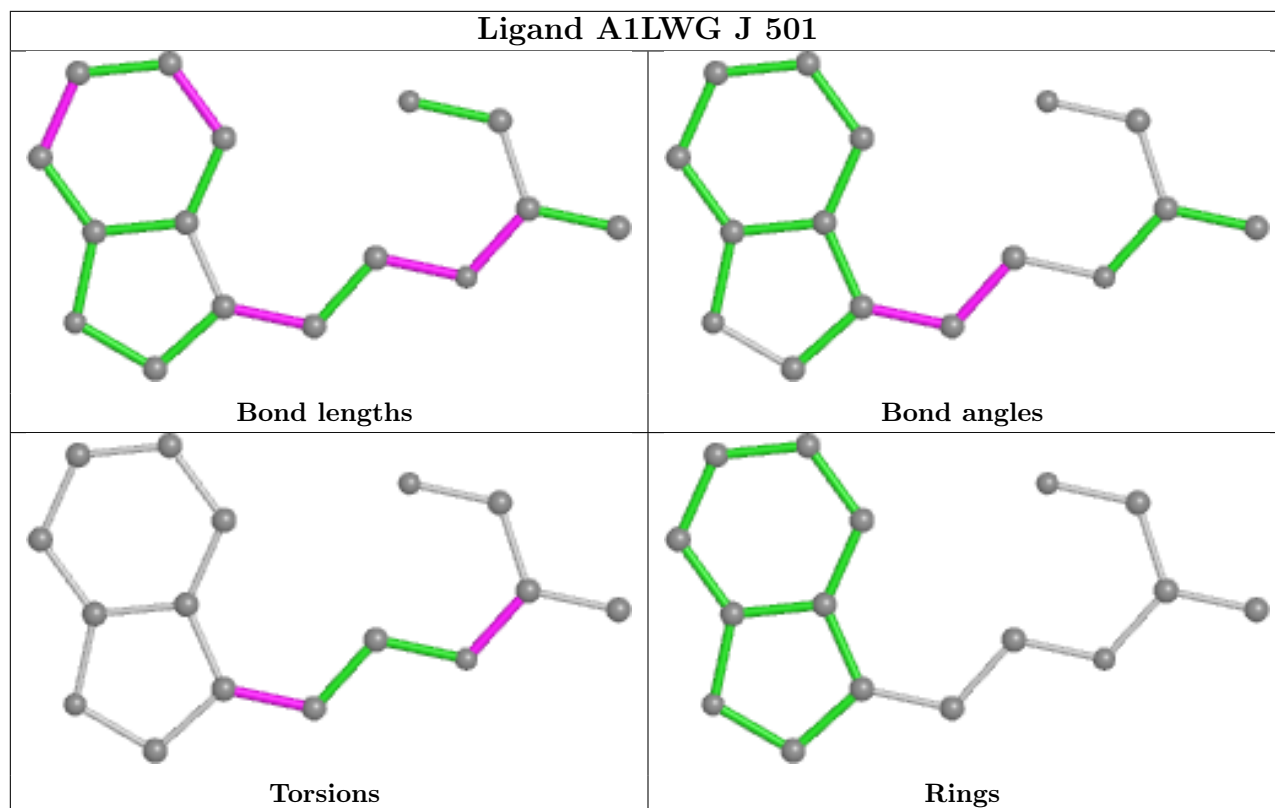
Mol	Chain	Res	Type	Atoms
3	F	501	A1LWG	CB-CA-N-C06
3	F	501	A1LWG	N-C06-C07-C08
3	L	501	A1LWG	N-C06-C07-C08
3	B	501	A1LWG	N-C06-C07-C08
3	H	501	A1LWG	C06-C07-C08-C12
3	F	501	A1LWG	C06-C07-C08-C12
3	L	501	A1LWG	C06-C07-C08-C12
3	B	501	A1LWG	CB-CA-N-C06
3	L	501	A1LWG	CB-CA-N-C06

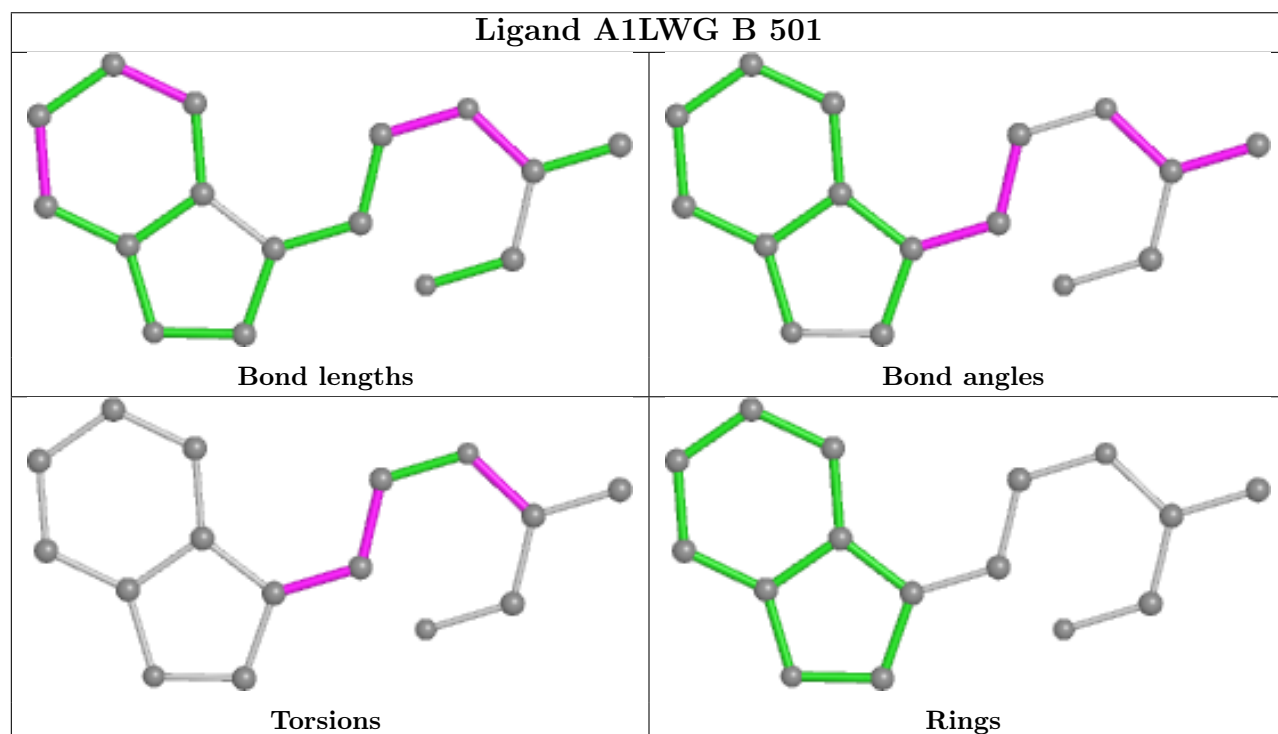
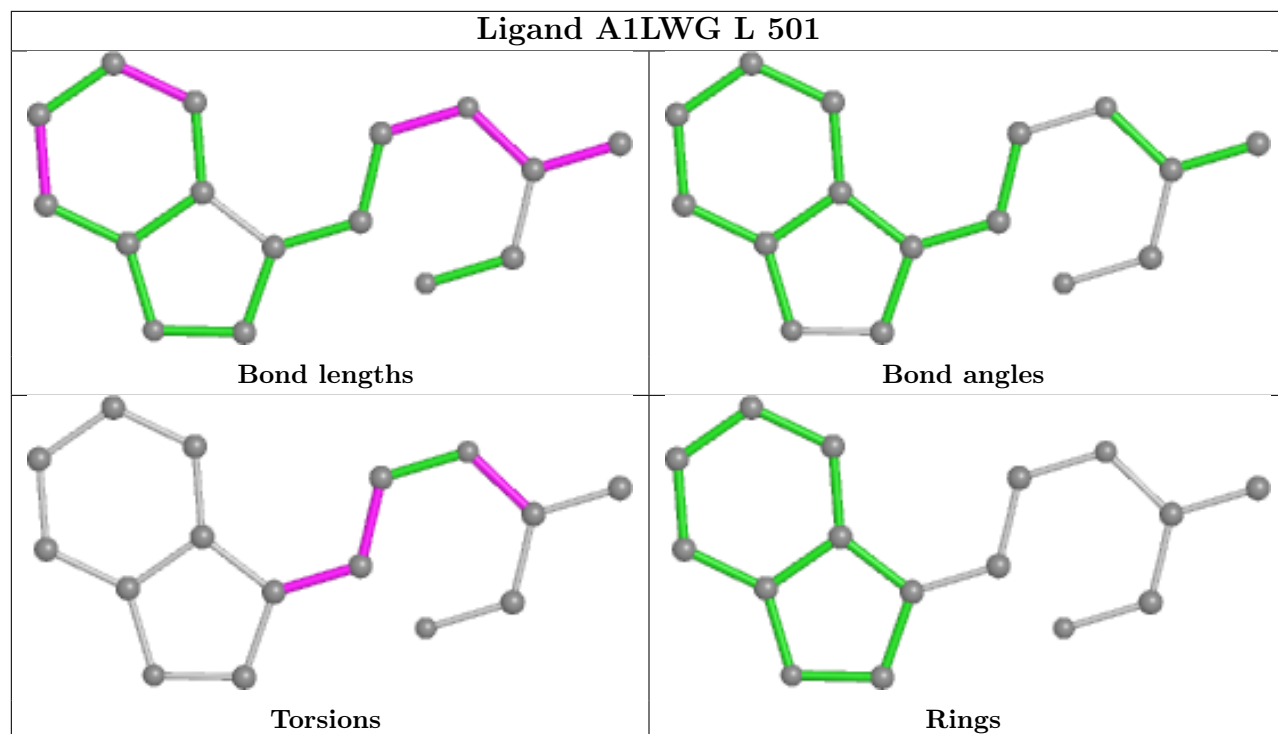
There are no ring outliers.

4 monomers are involved in 4 short contacts:

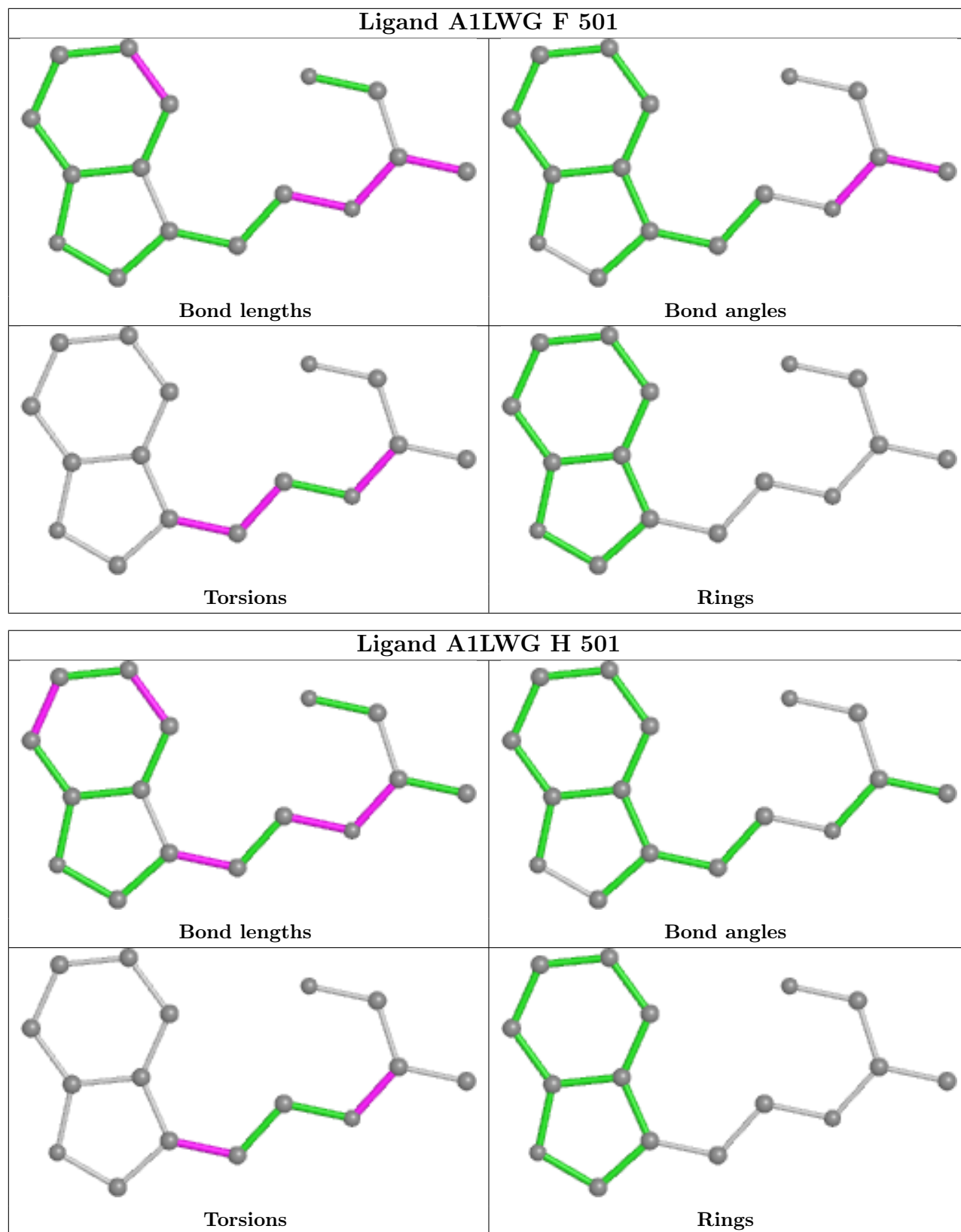
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	A1LWG	1	0
3	L	501	A1LWG	1	0
3	B	501	A1LWG	1	0
3	H	501	A1LWG	1	0

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

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<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	350/402 (87%)	-0.23	9 (2%) 57 56	20, 35, 70, 102	0
1	C	346/402 (86%)	-0.23	3 (0%) 81 80	20, 40, 71, 111	0
1	E	346/402 (86%)	-0.01	12 (3%) 47 45	24, 41, 76, 113	0
1	G	346/402 (86%)	-0.18	11 (3%) 50 48	19, 34, 69, 108	0
1	I	346/402 (86%)	0.00	5 (1%) 73 73	23, 43, 75, 97	0
1	K	347/402 (86%)	0.68	48 (13%) 8 7	25, 57, 97, 132	0
2	B	34/36 (94%)	-0.49	0 100 100	20, 37, 62, 78	0
2	D	34/36 (94%)	-0.44	0 100 100	23, 36, 61, 73	0
2	F	34/36 (94%)	-0.28	0 100 100	23, 37, 55, 69	0
2	H	34/36 (94%)	-0.59	0 100 100	23, 33, 58, 70	0
2	J	34/36 (94%)	-0.24	0 100 100	26, 39, 68, 75	0
2	L	34/36 (94%)	1.13	2 (5%) 29 27	37, 69, 94, 111	0
All	All	2285/2628 (86%)	-0.01	90 (3%) 44 42	19, 40, 83, 132	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	256	ASP	5.5
1	G	259	VAL	5.4
1	G	167	PHE	4.8
1	E	188	ASN	4.6
1	K	257	THR	4.1
1	E	260	PHE	3.9
1	K	260	PHE	3.8
1	K	259	VAL	3.8
1	K	254	SER	3.5
1	G	86	GLN	3.5
1	E	258	LEU	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	259	VAL	3.4
1	K	87	ASP	3.4
1	K	331	ASN	3.4
1	K	392	GLY	3.4
1	K	232	ASN	3.3
1	K	302	VAL	3.3
1	K	220	ASN	3.2
1	K	258	LEU	3.1
2	L	433	VAL	3.1
1	I	262	GLY	3.1
1	I	330	ASP	3.0
1	G	168	ASP	3.0
2	L	436	ALA	3.0
1	K	229	GLY	3.0
1	K	219	ARG	3.0
1	K	226	PRO	3.0
1	K	253	GLN	2.9
1	K	255	LEU	2.9
1	K	261	LYS	2.9
1	K	231	VAL	2.9
1	E	259	VAL	2.8
1	G	169	ASP	2.8
1	A	260	PHE	2.8
1	K	197	LEU	2.7
1	A	334	ASP	2.7
1	K	188	ASN	2.7
1	K	224	ASP	2.6
1	K	187	TYR	2.6
1	G	84	GLY	2.6
1	K	84	GLY	2.6
1	K	169	ASP	2.6
1	K	234	THR	2.6
1	G	260	PHE	2.5
1	G	83	GLU	2.5
1	K	184	VAL	2.5
1	E	256	ASP	2.5
1	K	189	GLY	2.5
1	G	85	ILE	2.5
1	K	223	ILE	2.5
1	A	86	GLN	2.4
1	K	195	VAL	2.4
1	A	331	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	166	GLN	2.3
1	A	333	TYR	2.3
1	I	261	LYS	2.3
1	A	262	GLY	2.3
1	K	236	LEU	2.3
1	K	305	THR	2.2
1	K	330	ASP	2.2
1	K	196	PHE	2.2
1	C	332	ASP	2.2
1	K	218	PHE	2.2
1	K	301	PRO	2.2
1	K	291	ASN	2.2
1	E	97	ASN	2.2
1	E	261	LYS	2.2
1	G	112	LEU	2.2
1	K	206	GLY	2.1
1	I	167	PHE	2.1
1	K	190	ARG	2.1
1	E	253	GLN	2.1
1	K	292	VAL	2.1
1	K	212	ASP	2.1
1	K	235	THR	2.1
1	A	167	PHE	2.1
1	K	294	ALA	2.1
1	K	362	GLU	2.0
1	E	257	THR	2.0
1	G	127	ARG	2.0
1	E	87	ASP	2.0
1	E	169	ASP	2.0
1	K	191	ALA	2.0
1	E	255	LEU	2.0
1	K	192	PHE	2.0
1	K	228	VAL	2.0
1	I	188	ASN	2.0
1	A	53	ASN	2.0
1	C	165	ASP	2.0
1	K	193	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

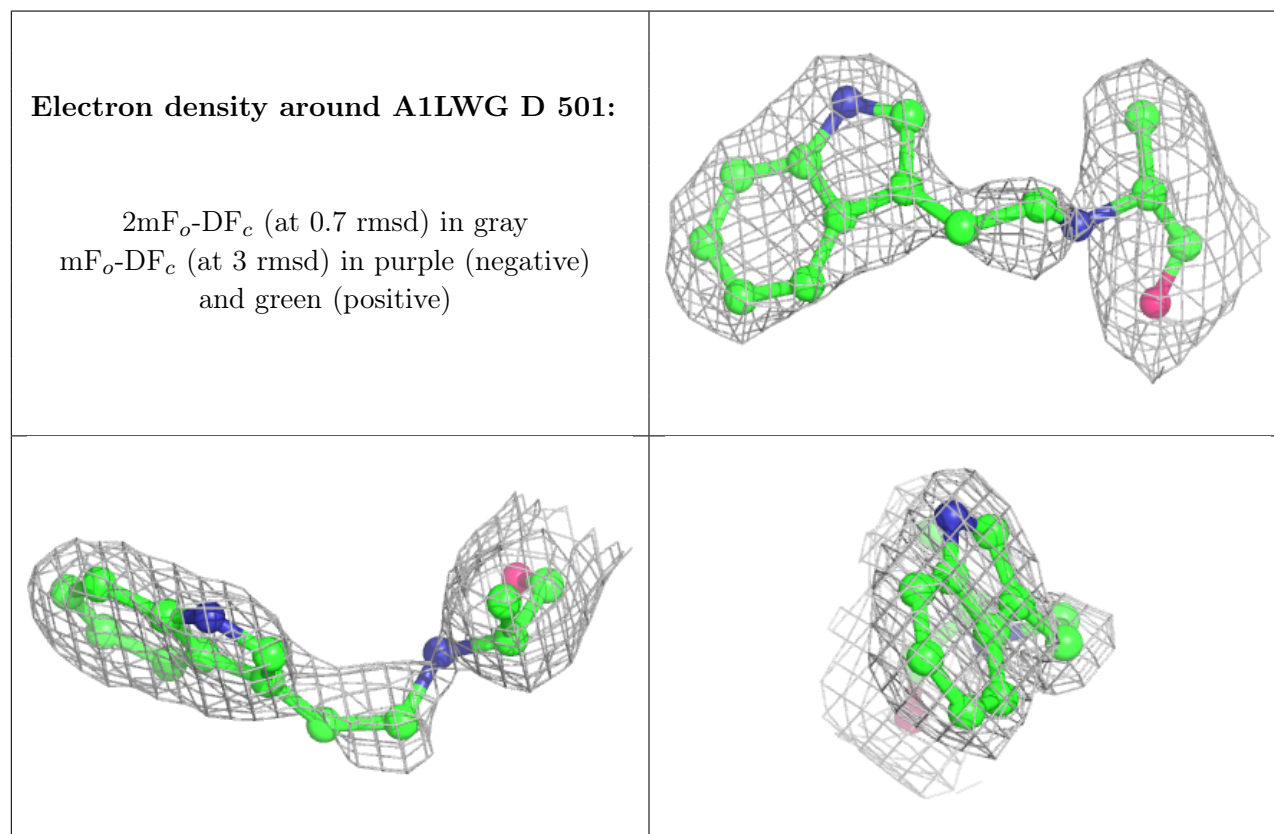
There are no monosaccharides in this entry.

### 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.

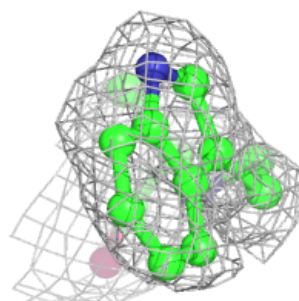
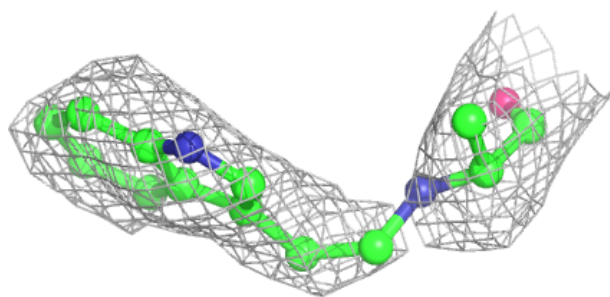
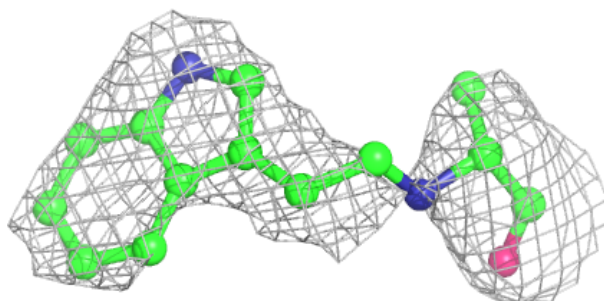
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	A1LWG	D	501	16/17	0.93	0.14	17,48,123,128	0
3	A1LWG	L	501	16/17	0.94	0.14	23,59,127,130	0
3	A1LWG	B	501	16/17	0.95	0.14	16,60,122,124	0
3	A1LWG	J	501	16/17	0.95	0.10	17,54,92,96	0
3	A1LWG	H	501	16/17	0.95	0.10	16,39,89,90	0
3	A1LWG	F	501	16/17	0.96	0.10	24,38,126,146	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.

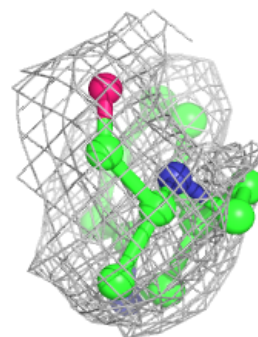
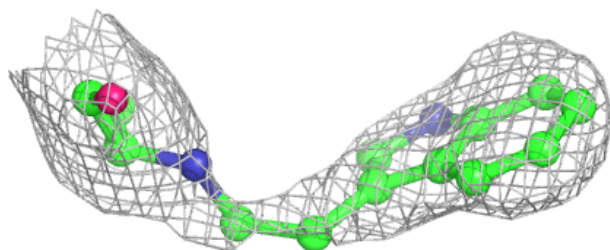
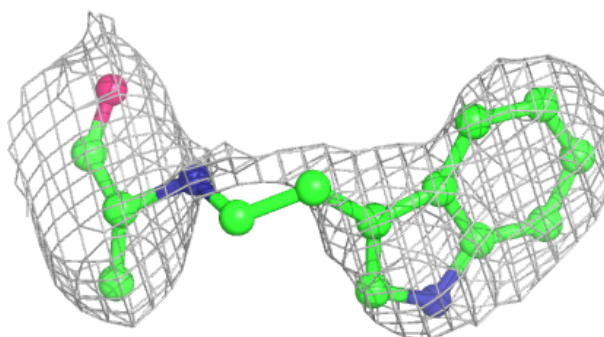


**Electron density around A1LWG L 501:**

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

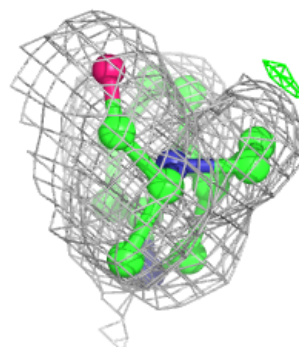
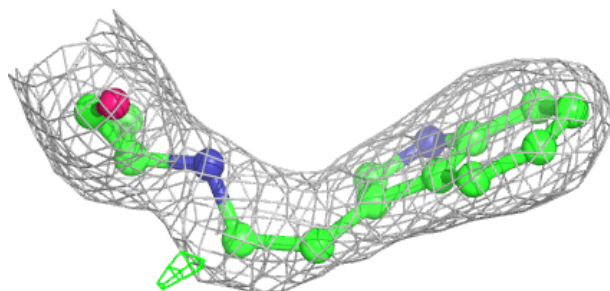
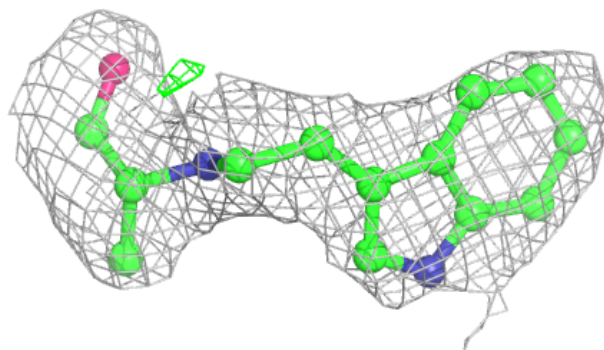
**Electron density around A1LWG B 501:**

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

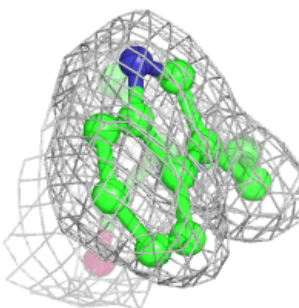
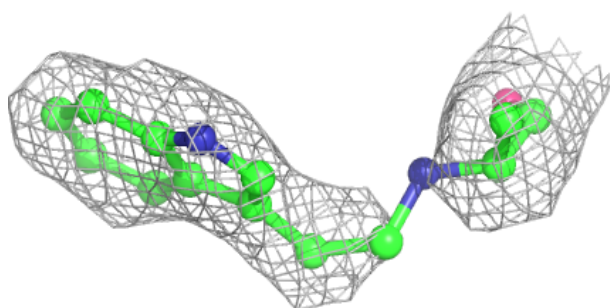
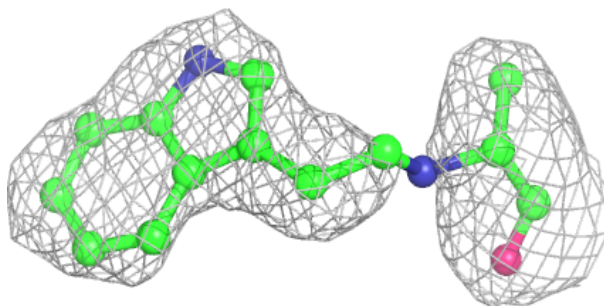


**Electron density around A1LWG J 501:**

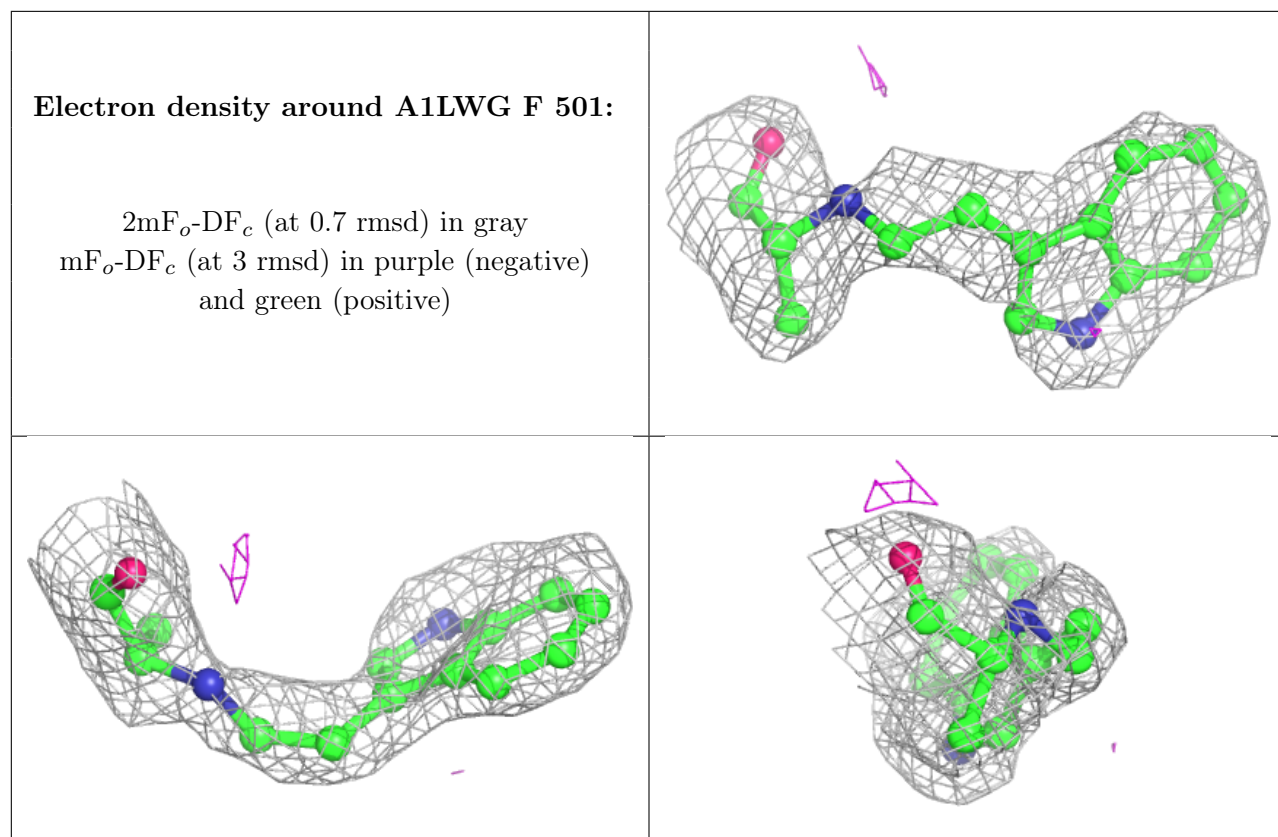
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around A1LWG H 501:**

$2mF_o-DF_c$  (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.