



## Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 02:09 AM EDT

PDB ID : 5QR0  
Title : PanDDA analysis group deposition – Crystal Structure of human ALAS2A in complex with Z730649594  
Authors : Bezerra, G.A.; Foster, W.; Bailey, H.; Shrestha, L.; Krojer, T.; Talon, R.; Brandao-Neto, J.; Douangamath, A.; Nicola, B.B.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Brennan, P.E.; Yue, W.W.  
Deposited on : 2019-05-22  
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](#) ①) 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

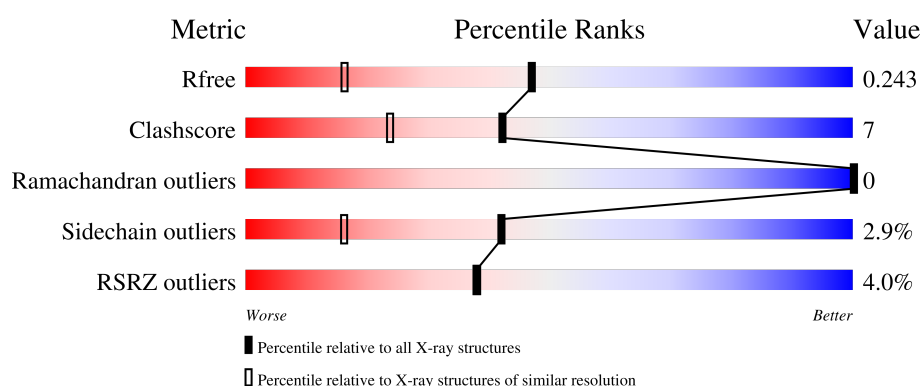
# 1 Overall quality at a glance

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	469	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	469	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	A	601	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6940 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 5-aminolevulinate synthase, erythroid-specific, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	428	Total	C	N	O	S	0	1	0
			3302	2102	577	601	22			
1	A	429	Total	C	N	O	S	0	1	0
			3322	2114	587	599	22			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	119	MET	-	initiating methionine	UNP P22557
B	120	GLY	-	expression tag	UNP P22557
B	121	HIS	-	expression tag	UNP P22557
B	122	HIS	-	expression tag	UNP P22557
B	123	HIS	-	expression tag	UNP P22557
B	124	HIS	-	expression tag	UNP P22557
B	125	HIS	-	expression tag	UNP P22557
B	126	HIS	-	expression tag	UNP P22557
B	127	SER	-	expression tag	UNP P22557
B	128	SER	-	expression tag	UNP P22557
B	129	GLY	-	expression tag	UNP P22557
B	130	VAL	-	expression tag	UNP P22557
B	131	ASP	-	expression tag	UNP P22557
B	132	LEU	-	expression tag	UNP P22557
B	133	GLY	-	expression tag	UNP P22557
B	134	THR	-	expression tag	UNP P22557
B	135	GLU	-	expression tag	UNP P22557
B	136	ASN	-	expression tag	UNP P22557
B	137	LEU	-	expression tag	UNP P22557
B	138	TYR	-	expression tag	UNP P22557
B	139	PHE	-	expression tag	UNP P22557
B	140	GLN	-	expression tag	UNP P22557
B	141	SER	-	expression tag	UNP P22557
B	142	MET	-	expression tag	UNP P22557
B	221	VAL	ALA	conflict	UNP P22557

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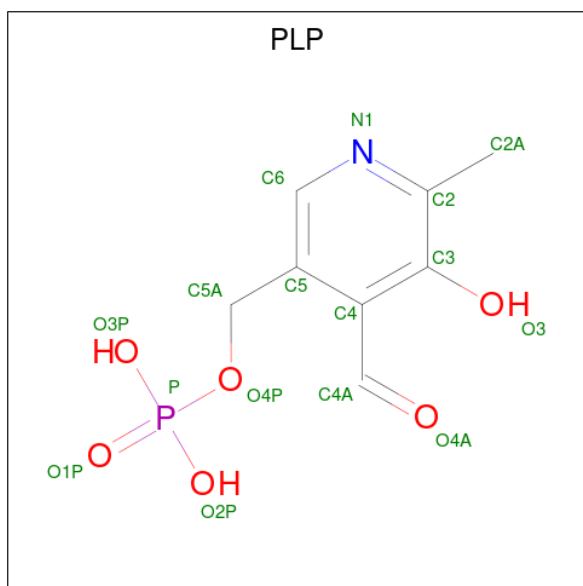
Chain	Residue	Modelled	Actual	Comment	Reference
B	579	GLY	-	expression tag	UNP P22557
B	580	PRO	-	expression tag	UNP P22557
B	581	GLN	-	expression tag	UNP P22557
B	582	TYR	-	expression tag	UNP P22557
B	583	VAL	-	expression tag	UNP P22557
B	584	THR	-	expression tag	UNP P22557
B	585	THR	-	expression tag	UNP P22557
B	586	TYR	-	expression tag	UNP P22557
B	587	ALA	-	expression tag	UNP P22557
A	119	MET	-	initiating methionine	UNP P22557
A	120	GLY	-	expression tag	UNP P22557
A	121	HIS	-	expression tag	UNP P22557
A	122	HIS	-	expression tag	UNP P22557
A	123	HIS	-	expression tag	UNP P22557
A	124	HIS	-	expression tag	UNP P22557
A	125	HIS	-	expression tag	UNP P22557
A	126	HIS	-	expression tag	UNP P22557
A	127	SER	-	expression tag	UNP P22557
A	128	SER	-	expression tag	UNP P22557
A	129	GLY	-	expression tag	UNP P22557
A	130	VAL	-	expression tag	UNP P22557
A	131	ASP	-	expression tag	UNP P22557
A	132	LEU	-	expression tag	UNP P22557
A	133	GLY	-	expression tag	UNP P22557
A	134	THR	-	expression tag	UNP P22557
A	135	GLU	-	expression tag	UNP P22557
A	136	ASN	-	expression tag	UNP P22557
A	137	LEU	-	expression tag	UNP P22557
A	138	TYR	-	expression tag	UNP P22557
A	139	PHE	-	expression tag	UNP P22557
A	140	GLN	-	expression tag	UNP P22557
A	141	SER	-	expression tag	UNP P22557
A	142	MET	-	expression tag	UNP P22557
A	221	VAL	ALA	conflict	UNP P22557
A	579	GLY	-	expression tag	UNP P22557
A	580	PRO	-	expression tag	UNP P22557
A	581	GLN	-	expression tag	UNP P22557
A	582	TYR	-	expression tag	UNP P22557
A	583	VAL	-	expression tag	UNP P22557
A	584	THR	-	expression tag	UNP P22557
A	585	THR	-	expression tag	UNP P22557
A	586	TYR	-	expression tag	UNP P22557

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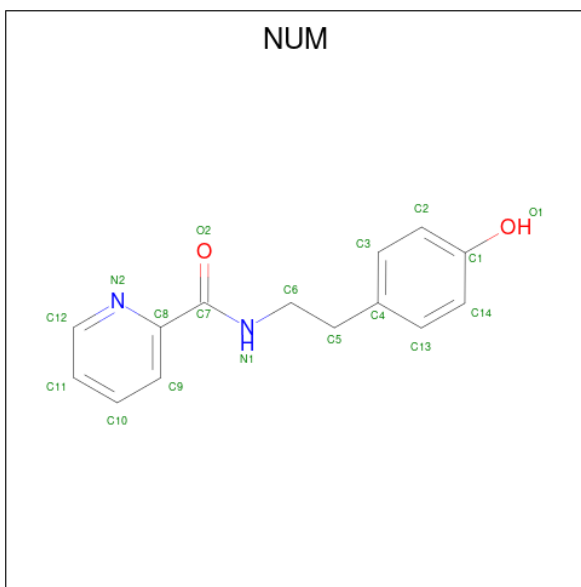
Chain	Residue	Modelled	Actual	Comment	Reference
A	587	ALA	-	expression tag	UNP P22557

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is N-[2-(4-hydroxyphenyl)ethyl]pyridine-2-carboxamide (three-letter code: NUM) (formula:  $C_{14}H_{14}N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	14	2	2		
3	A	1	Total	C	N	O	0	0
			18	14	2	2		

- Molecule 4 is water.

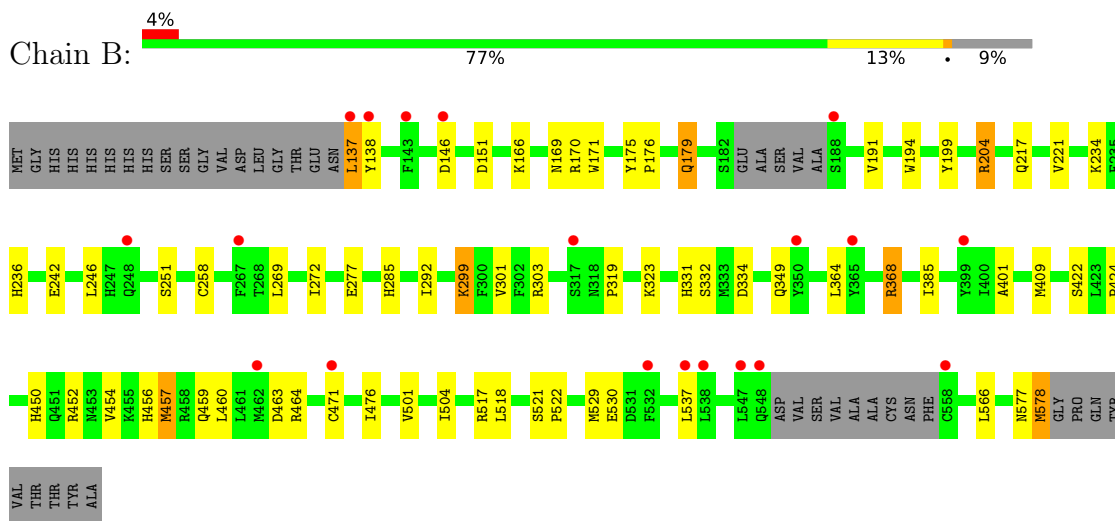
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	134	Total	O	0	0
			134	134		
4	A	114	Total	O	0	0
			114	114		



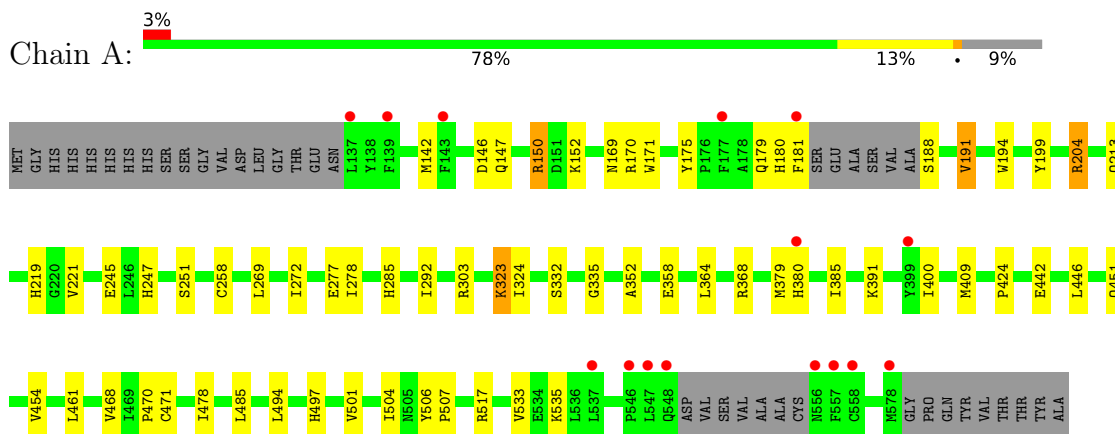
### 3 Residue-property plots [i](#)

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: 5-aminolevulinate synthase, erythroid-specific, mitochondrial



- Molecule 1: 5-aminolevulinate synthase, erythroid-specific, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.67Å 108.58Å 75.83Å 90.00° 109.17° 90.00°	Depositor
Resolution (Å)	80.12 – 1.65 80.12 – 1.65	Depositor EDS
% Data completeness (in resolution range)	70.7 (80.12-1.65) 70.7 (80.12-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.208 , 0.236 0.220 , 0.243	Depositor DCC
$R_{free}$ test set	4059 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: NUM, PLP

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	0.72	0/3403	0.87	4/4608 (0.1%)
1	B	0.73	0/3381	0.87	4/4580 (0.1%)
All	All	0.72	0/6784	0.87	8/9188 (0.1%)

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	B	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	170	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	B	170	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	368	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	A	368	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	B	368	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	170	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	179	GLN	CB-CA-C	-5.09	100.22	110.40
1	A	170	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	137	LEU	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	3322	0	3215	49	0
1	B	3302	0	3192	45	1
2	A	16	0	7	6	0
2	B	16	0	8	4	0
3	A	36	0	0	0	0
4	A	114	0	0	3	0
4	B	134	0	0	7	0
All	All	6940	0	6422	91	1

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 7.

All (91) 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)
2:B:601:PLP:O3P	4:B:701:HOH:O	1.89	0.90
1:A:147:GLN:OE1	1:A:150:ARG:NH1	2.13	0.82
1:B:242:GLU:OE2	4:B:702:HOH:O	2.04	0.76
1:A:497:HIS:ND1	1:A:535:LYS:HE2	2.01	0.76
1:B:303:ARG:NH1	4:B:704:HOH:O	2.14	0.75
1:B:175:TYR:HB2	1:B:204:ARG:HD2	1.69	0.74
1:B:175:TYR:CB	1:B:204:ARG:HD2	2.18	0.73
1:B:194:TRP:HB2	1:B:501:VAL:CG1	2.20	0.71
1:B:319:PRO:O	1:A:142:MET:HB3	1.90	0.71
2:A:601:PLP:O2P	4:A:701:HOH:O	2.08	0.70
1:B:217:GLN:NE2	1:A:213:GLN:OE1	2.23	0.70
1:A:169:ASN:HD21	1:A:181:PHE:HE2	1.37	0.69
1:A:146:ASP:O	1:A:150:ARG:HG2	1.92	0.69
1:B:349:GLN:OE1	4:B:703:HOH:O	2.13	0.67
1:B:460:LEU:O	1:B:464:ARG:HG2	1.95	0.67
1:A:470:PRO:O	1:A:471:CYS:SG	2.58	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ARG:HB3	1:B:537:LEU:HD11	1.82	0.60
1:B:194:TRP:HB2	1:B:501:VAL:HG12	1.82	0.60
1:B:258:CYS:HB3	2:B:601:PLP:O4P	2.02	0.59
1:A:451:GLN:O	1:A:454:VAL:HG12	2.02	0.59
1:B:504:ILE:HD12	1:B:517:ARG:HB2	1.84	0.59
1:B:236:HIS:NE2	1:B:422:SER:OG	2.38	0.57
1:A:504:ILE:CD1	1:A:517:ARG:HB2	2.34	0.57
1:A:391:LYS:CE	2:A:601:PLP:H4A	2.34	0.57
1:A:323:LYS:HG3	1:A:352:ALA:HB2	1.87	0.57
1:A:461:LEU:HD21	1:A:478:ILE:HD11	1.87	0.56
1:A:461:LEU:HD12	1:A:533:VAL:HG12	1.87	0.56
1:B:459:GLN:NE2	4:B:705:HOH:O	2.38	0.56
1:B:452:ARG:NH1	4:B:706:HOH:O	2.38	0.55
1:B:175:TYR:HB3	1:B:204:ARG:HD2	1.89	0.54
1:B:171:TRP:CZ2	1:B:179:GLN:HG3	2.42	0.54
1:A:258:CYS:HB3	2:A:601:PLP:O4P	2.08	0.54
1:A:221:VAL:O	1:A:424:PRO:HB3	2.08	0.53
1:A:269:LEU:HB3	1:A:324:ILE:HD11	1.91	0.53
1:B:269:LEU:HD23	1:B:409:MET:HE1	1.91	0.53
1:A:191:VAL:HG21	1:A:494:LEU:HD12	1.92	0.52
1:A:194:TRP:HB2	1:A:501:VAL:HG12	1.92	0.51
1:A:332:SER:HB3	2:A:601:PLP:H2A1	1.91	0.51
1:A:504:ILE:CD1	1:A:517:ARG:CB	2.88	0.51
1:B:456:HIS:HE1	4:B:766:HOH:O	1.93	0.51
1:B:194:TRP:HB2	1:B:501:VAL:HG13	1.90	0.51
1:A:191:VAL:HG21	1:A:494:LEU:CD1	2.42	0.50
1:B:137:LEU:HD12	1:B:137:LEU:N	2.27	0.50
1:A:171:TRP:CZ2	1:A:179:GLN:HB2	2.47	0.49
1:A:442:GLU:O	1:A:446:LEU:HD23	2.13	0.49
1:A:303:ARG:NH1	4:A:702:HOH:O	2.46	0.48
1:B:456:HIS:ND1	1:B:529:MET:HE2	2.28	0.48
1:A:461:LEU:HD12	1:A:533:VAL:CG1	2.43	0.48
1:A:380[B]:HIS:HE1	4:A:738:HOH:O	1.97	0.48
1:B:234:LYS:HG2	1:A:169:ASN:ND2	2.29	0.48
1:B:331:HIS:HB3	1:B:334:ASP:OD1	2.14	0.47
1:B:171:TRP:CZ2	1:B:179:GLN:CG	2.97	0.47
1:B:504:ILE:HD12	1:B:517:ARG:CB	2.45	0.47
1:B:285:HIS:HB2	2:B:601:PLP:H2A3	1.97	0.47
1:A:285:HIS:HB2	2:A:601:PLP:H2A3	1.97	0.47
1:B:521:SER:HB2	1:B:522:PRO:HD2	1.98	0.46
1:A:272:ILE:HG21	1:A:409:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:PRO:C	1:A:471:CYS:SG	2.93	0.46
1:A:175:TYR:HB2	1:A:204:ARG:HD2	1.96	0.46
1:A:194:TRP:HB2	1:A:501:VAL:CG1	2.45	0.45
1:A:175:TYR:CB	1:A:204:ARG:HD2	2.47	0.45
1:B:459:GLN:NE2	1:B:463:ASP:OD1	2.51	0.44
1:B:457:MET:HB2	1:B:529:MET:HE3	1.99	0.44
1:A:180:HIS:O	1:A:188:SER:HA	2.17	0.44
1:A:335:GLY:O	1:A:471:CYS:HB3	2.18	0.44
1:B:221:VAL:O	1:B:424:PRO:HB3	2.17	0.44
1:B:272:ILE:HD11	1:A:152:LYS:HE2	1.99	0.44
1:A:277:GLU:O	1:A:323:LYS:HA	2.18	0.43
1:A:451:GLN:HA	1:A:454:VAL:HG12	1.99	0.43
1:B:476:ILE:HB	1:B:518:LEU:HB2	2.00	0.43
1:A:461:LEU:CD2	1:A:478:ILE:HD11	2.48	0.43
1:A:391:LYS:HE3	2:A:601:PLP:H4A	2.01	0.43
1:B:301:VAL:HG11	1:B:566:LEU:O	2.19	0.42
1:B:199:TYR:CD2	1:B:364:LEU:HD11	2.54	0.42
1:A:278:ILE:HG21	1:A:292:ILE:HG12	2.02	0.42
1:B:277:GLU:O	1:B:323:LYS:HA	2.20	0.42
1:B:385:ILE:CG2	1:B:401:ALA:HB3	2.49	0.42
1:A:385:ILE:O	1:A:400:ILE:HA	2.18	0.42
1:B:277:GLU:OE1	1:B:323:LYS:HE3	2.20	0.42
1:A:451:GLN:O	1:A:454:VAL:CG1	2.68	0.42
1:A:501:VAL:HG23	1:A:501:VAL:O	2.20	0.42
1:A:247:HIS:HA	1:A:379:MET:CE	2.50	0.41
1:B:450:HIS:O	1:B:454:VAL:HG23	2.20	0.41
1:A:506:TYR:CG	1:A:507:PRO:HA	2.55	0.41
1:A:358:GLU:HG3	1:A:385:ILE:HD11	2.03	0.41
1:B:246:LEU:O	1:B:368:ARG:NH2	2.54	0.41
1:B:332:SER:HB3	2:B:601:PLP:H2A1	2.02	0.41
1:A:199:TYR:CD2	1:A:364:LEU:HD11	2.56	0.41
1:B:169:ASN:HB3	1:A:219:HIS:CE1	2.57	0.40
1:B:577:ASN:OD1	1:B:578:MET:N	2.54	0.40
1:B:292:ILE:CG2	1:B:299:LYS:HG3	2.51	0.40

All (1) 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:B:137:LEU:CD1	1:B:151:ASP:OD2[2_656]	2.15	0.05

## 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	424/469 (90%)	413 (97%)	11 (3%)	0	100	100
1	B	423/469 (90%)	409 (97%)	14 (3%)	0	100	100
All	All	847/938 (90%)	822 (97%)	25 (3%)	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	347/396 (88%)	339 (98%)	8 (2%)	50	25
1	B	345/396 (87%)	333 (96%)	12 (4%)	36	11
All	All	692/792 (87%)	672 (97%)	20 (3%)	42	16

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	138	TYR
1	B	146	ASP
1	B	166	LYS
1	B	176	PRO
1	B	191	VAL
1	B	204	ARG
1	B	251	SER
1	B	299	LYS

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Mol	Chain	Res	Type
1	B	457	MET
1	B	471	CYS
1	B	530	GLU
1	B	578	MET
1	A	150	ARG
1	A	191	VAL
1	A	204	ARG
1	A	245	GLU
1	A	251	SER
1	A	323	LYS
1	A	468	VAL
1	A	485	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	180	HIS

### 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](#)

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	PLP	A	601	-	16,16,16	0.79	1 (6%)	20,23,23	0.93	1 (5%)
3	NUM	A	602	-	19,19,19	0.21	0	24,24,24	0.34	0
2	PLP	B	601	-	16,16,16	1.00	1 (6%)	20,23,23	1.29	2 (10%)
3	NUM	A	603	-	19,19,19	0.19	0	24,24,24	0.30	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
2	PLP	A	601	-	-	2/8/8/8	0/1/1/1
3	NUM	A	602	-	-	8/10/10/10	0/2/2/2
2	PLP	B	601	-	-	2/8/8/8	0/1/1/1
3	NUM	A	603	-	-	0/10/10/10	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	PLP	P-O4P	2.61	1.68	1.60
2	A	601	PLP	P-O4P	2.10	1.67	1.60

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	PLP	O4P-C5A-C5	3.08	115.22	109.35
2	B	601	PLP	C3-C4-C4A	-2.69	116.08	119.90
2	A	601	PLP	O4P-C5A-C5	2.20	113.54	109.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	PLP	C5A-O4P-P-O1P
2	A	601	PLP	C3-C4-C4A-O4A
3	A	602	NUM	O2-C7-C8-N2
3	A	602	NUM	O2-C7-C8-C9

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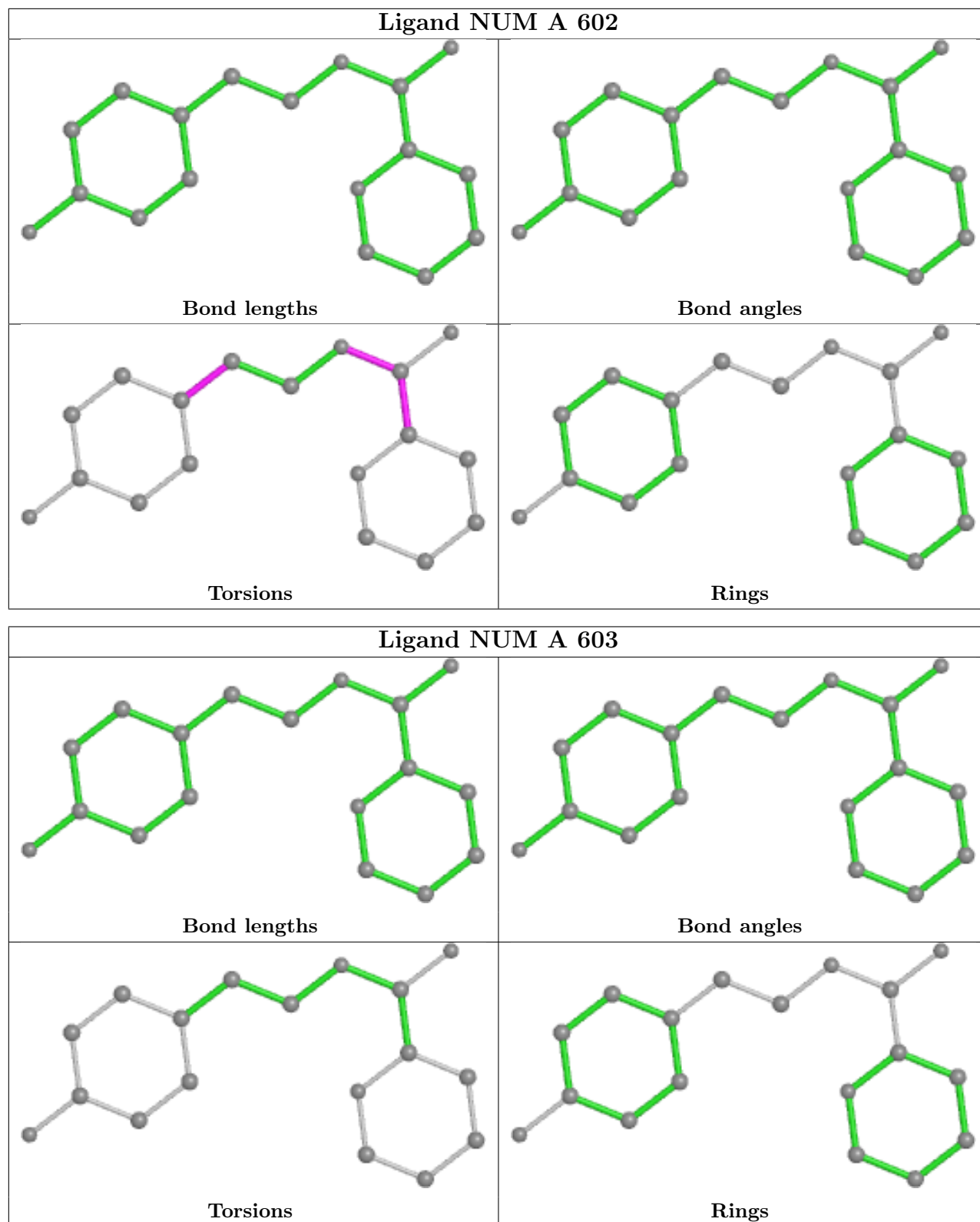
Mol	Chain	Res	Type	Atoms
3	A	602	NUM	N1-C7-C8-N2
3	A	602	NUM	N1-C7-C8-C9
2	A	601	PLP	C5-C4-C4A-O4A
3	A	602	NUM	C3-C4-C5-C6
3	A	602	NUM	C13-C4-C5-C6
3	A	602	NUM	C8-C7-N1-C6
2	B	601	PLP	C5A-O4P-P-O3P
3	A	602	NUM	O2-C7-N1-C6

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PLP	6	0
2	B	601	PLP	4	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 ⓘ

### 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	429/469 (91%)	-0.02	15 (3%)	44 45	10, 19, 40, 63	5 (1%)
1	B	428/469 (91%)	0.03	19 (4%)	34 34	10, 19, 38, 68	7 (1%)
All	All	857/938 (91%)	0.00	34 (3%)	38 38	10, 19, 39, 68	12 (1%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	PHE	8.3
1	A	143	PHE	8.2
1	B	143	PHE	8.0
1	B	399	TYR	8.0
1	A	399	TYR	7.9
1	A	557	PHE	7.6
1	B	365	TYR	7.4
1	B	532	PHE	7.2
1	A	177	PHE	7.2
1	B	350	TYR	6.5
1	A	380[A]	HIS	6.2
1	B	547	LEU	6.1
1	A	181	PHE	6.0
1	B	548	GLN	4.7
1	B	558	CYS	4.5
1	B	248[A]	GLN	4.5
1	A	547	LEU	4.3
1	B	137	LEU	3.7
1	B	138	TYR	3.6
1	A	137	LEU	3.5
1	A	578	MET	3.4
1	B	537	LEU	3.4
1	A	537	LEU	3.1
1	A	556	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	146	ASP	2.8
1	A	558	CYS	2.8
1	A	548	GLN	2.7
1	A	139	PHE	2.5
1	B	188	SER	2.5
1	B	462	MET	2.3
1	B	538	LEU	2.2
1	B	317	SER	2.1
1	A	546	PRO	2.1
1	B	471	CYS	2.1

## 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](#)

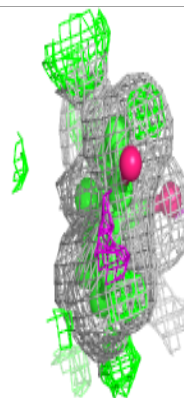
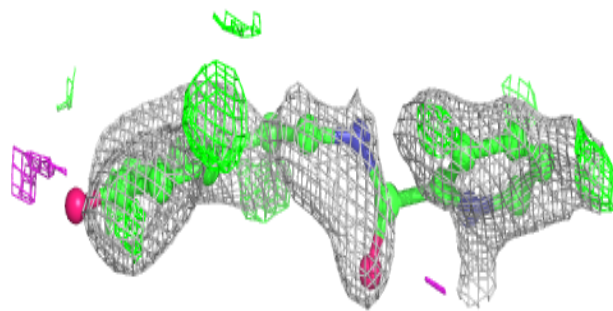
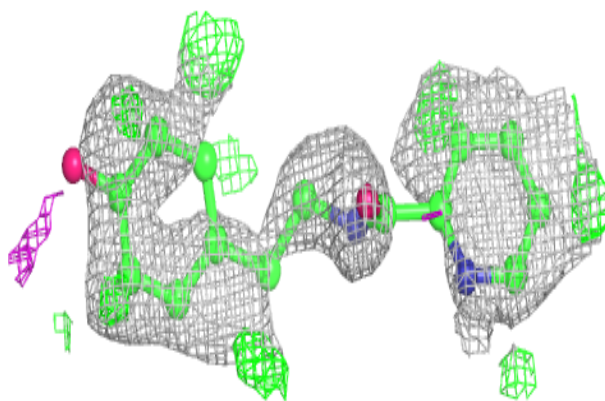
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	NUM	A	602	18/18	0.46	0.28	52,60,64,64	0
3	NUM	A	603	18/18	0.79	0.15	41,46,52,54	0
2	PLP	B	601	16/16	0.88	0.15	18,24,28,38	0
2	PLP	A	601	16/16	0.92	0.12	20,25,30,39	0

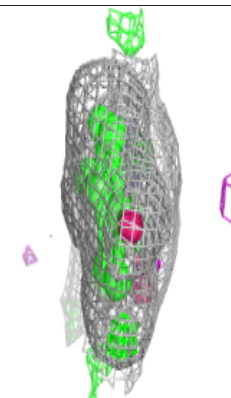
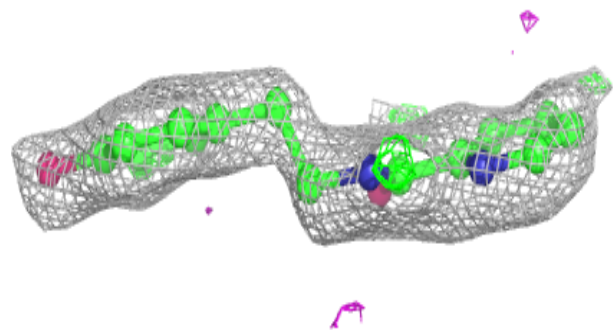
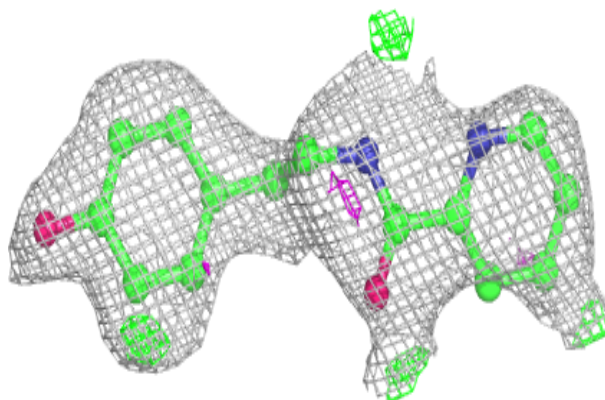
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NUM A 602:**

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

**Electron density around NUM A 603:**

$2mF_o-DF_c$  (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.