



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:55 AM UTC

PDB ID : 8XP4 / pdb_00008xp4
Title : Crystal Structure of human lysyl-tRNA synthetase with acetyllysine
Authors : Zhang, X.; Li, N.; Guo, Y.R.; Ouyang, Z.
Deposited on : 2024-01-03
Resolution : 2.26 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

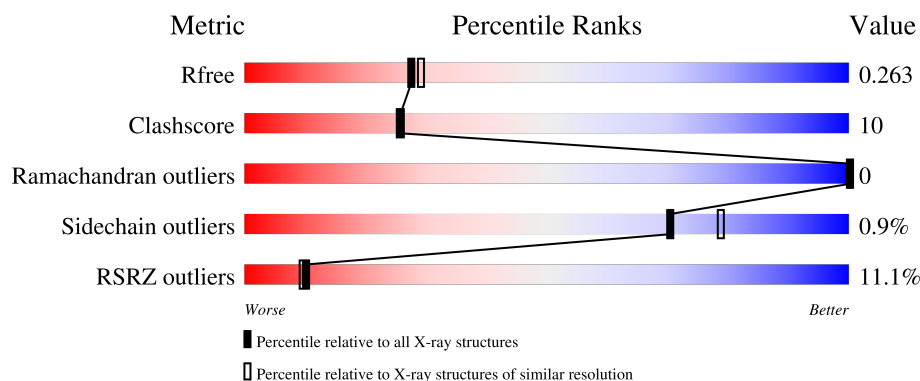
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	520	10% 77% 17% 6%
1	B	520	11% 77% 17% 6%

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	ALY	A	601	-	-	X	-
2	ALY	B	601	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16025 atoms, of which 7852 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.

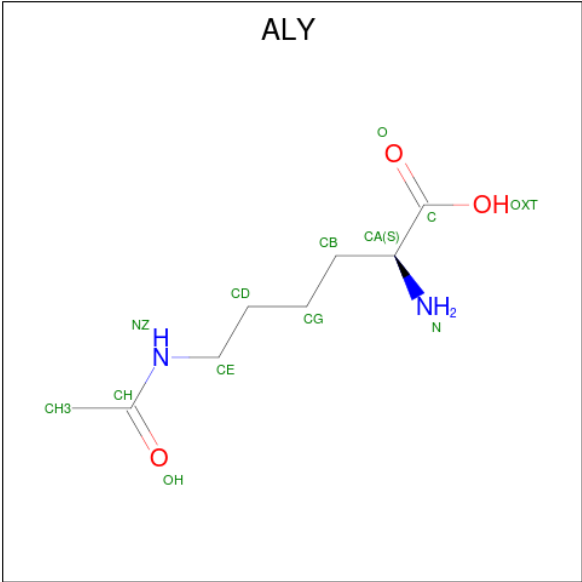
- Molecule 1 is a protein called Lysine-tRNA ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	489	Total	C	H	N	O	S	0	1	0
			7908	2552	3927	676	727	26			
1	B	490	Total	C	H	N	O	S	0	0	0
			7899	2548	3925	671	728	27			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	MET	-	initiating methionine	UNP Q15046
A	581	LEU	-	expression tag	UNP Q15046
A	582	GLU	-	expression tag	UNP Q15046
A	583	HIS	-	expression tag	UNP Q15046
A	584	HIS	-	expression tag	UNP Q15046
A	585	HIS	-	expression tag	UNP Q15046
A	586	HIS	-	expression tag	UNP Q15046
A	587	HIS	-	expression tag	UNP Q15046
A	588	HIS	-	expression tag	UNP Q15046
B	69	MET	-	initiating methionine	UNP Q15046
B	581	LEU	-	expression tag	UNP Q15046
B	582	GLU	-	expression tag	UNP Q15046
B	583	HIS	-	expression tag	UNP Q15046
B	584	HIS	-	expression tag	UNP Q15046
B	585	HIS	-	expression tag	UNP Q15046
B	586	HIS	-	expression tag	UNP Q15046
B	587	HIS	-	expression tag	UNP Q15046
B	588	HIS	-	expression tag	UNP Q15046

- Molecule 2 is N(6)-ACETYLLYSINE (CCD ID: ALY) (formula: $C_8H_{16}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	8	2	3		
2	B	1	Total	C	N	O	0	0
			13	8	2	3		

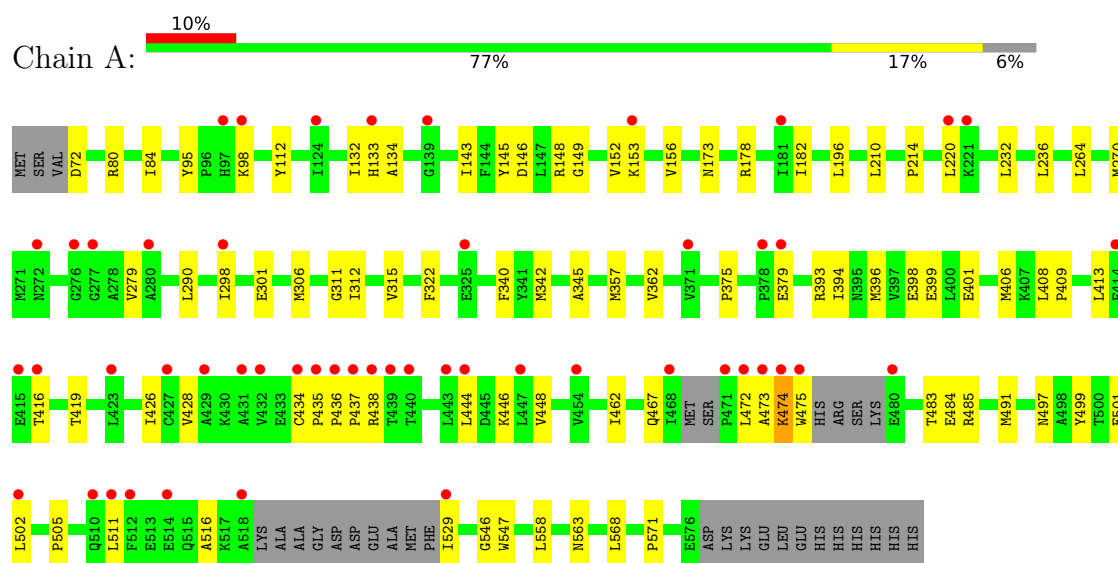
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total	O	0	0
			91	91		
3	B	101	Total	O	0	0
			101	101		

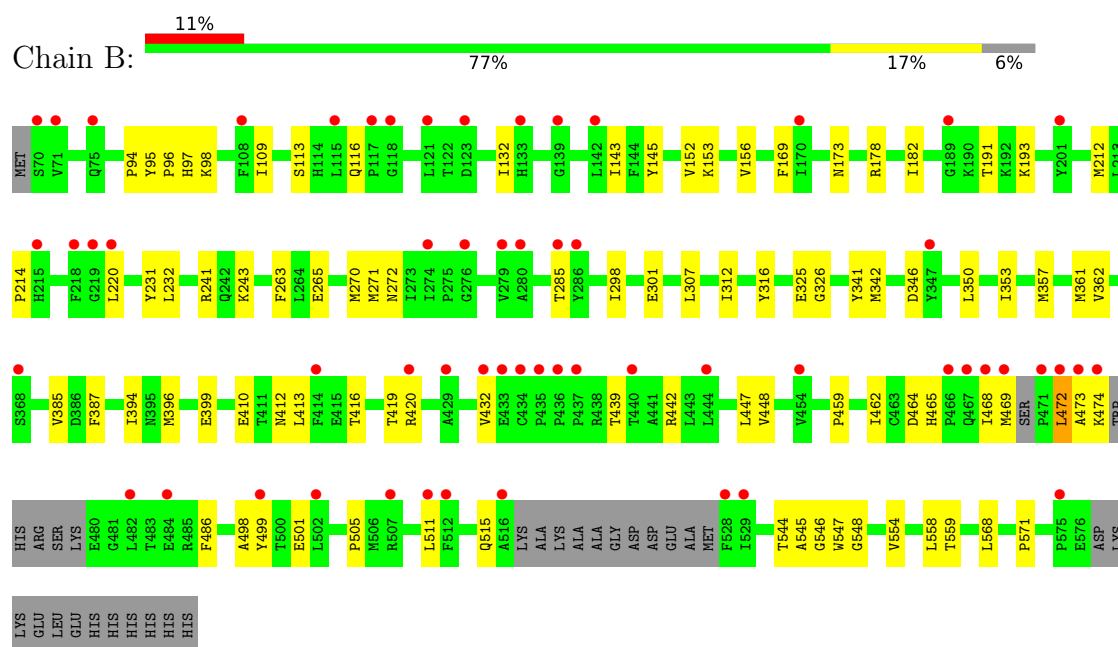
3 Residue-property plots

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: Lysine–tRNA ligase



• Molecule 1: Lysine–tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.34Å 90.47Å 107.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.44 – 2.26 23.44 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.5 (23.44-2.26) 99.6 (23.44-2.26)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.239 , 0.264 0.239 , 0.263	Depositor DCC
R_{free} test set	1999 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.816	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16025	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8614e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.14	0/4073	0.31	0/5499
1	B	0.14	0/4065	0.30	0/5488
All	All	0.14	0/8138	0.31	0/10987

There are no bond length outliers.

There are no bond angle outliers.

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	3981	3927	3971	80	0
1	B	3974	3925	3963	75	0
2	A	13	0	15	14	0
2	B	13	0	15	9	0
3	A	91	0	0	5	0
3	B	101	0	0	5	0
All	All	8173	7852	7964	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (152) 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:B:501:GLU:OE2	2:B:601:ALY:HG2	1.61	1.01
1:B:473:ALA:HA	2:B:601:ALY:HH32	1.53	0.91
1:B:396:MET:HE1	1:B:469:MET:HE1	1.57	0.84
1:A:546:GLY:HA3	2:A:601:ALY:HG3	1.63	0.81
1:A:132:ILE:HD11	1:A:182:ILE:HD13	1.62	0.81
1:B:394:ILE:HB	1:B:399:GLU:HG3	1.65	0.79
1:A:428:VAL:HG23	1:A:438:ARG:HH12	1.48	0.75
1:B:416:THR:HG23	1:B:419:THR:H	1.53	0.71
1:B:220:LEU:HD11	1:B:232:LEU:HD23	1.74	0.70
1:A:502:LEU:HD12	3:A:716:HOH:O	1.90	0.70
1:B:413:LEU:O	1:B:416:THR:HG22	1.92	0.68
1:A:416:THR:HG23	1:A:419:THR:H	1.57	0.68
1:A:501:GLU:OE2	2:A:601:ALY:NZ	2.28	0.67
1:A:394:ILE:HB	1:A:399:GLU:HG3	1.77	0.65
1:A:413:LEU:O	1:A:416:THR:HG22	1.97	0.65
1:A:301:GLU:CD	2:A:601:ALY:HE2	2.22	0.65
1:A:270:MET:HE1	1:B:270:MET:SD	2.37	0.64
1:A:501:GLU:OE1	2:A:601:ALY:HH31	1.98	0.63
1:A:357:MET:HE1	1:A:547:TRP:CH2	2.34	0.63
1:B:548:GLY:N	2:B:601:ALY:H2	1.97	0.63
1:B:178:ARG:NH1	1:B:214:PRO:O	2.32	0.62
1:B:396:MET:HE2	1:B:448:VAL:HG21	1.81	0.62
1:A:270:MET:HE3	1:A:322:PHE:CE1	2.35	0.62
1:A:143:ILE:HD12	1:A:173:ASN:CG	2.24	0.61
1:B:396:MET:HE1	1:B:469:MET:CE	2.29	0.60
1:A:220:LEU:HD13	1:A:236:LEU:CD1	2.32	0.60
1:B:109:ILE:HD12	1:B:152:VAL:HG21	1.82	0.59
2:A:601:ALY:C	2:A:601:ALY:HD3	2.32	0.59
1:A:394:ILE:HD11	1:A:462:ILE:HG12	1.86	0.58
1:A:342:MET:HE2	1:A:345:ALA:HB2	1.85	0.58
1:A:362:VAL:HG22	1:A:558:LEU:HD21	1.86	0.58
1:B:152:VAL:HG22	1:B:153:LYS:H	1.69	0.58
1:B:473:ALA:HA	2:B:601:ALY:CH3	2.32	0.57
1:B:396:MET:HE2	1:B:448:VAL:HG11	1.87	0.57
1:A:298:ILE:HD13	1:A:322:PHE:O	2.04	0.57
1:B:298:ILE:N	1:B:298:ILE:HD12	2.20	0.57
1:A:396:MET:HE3	1:A:448:VAL:CG2	2.35	0.56
1:A:505:PRO:HD2	1:B:95:TYR:CZ	2.39	0.56
1:A:342:MET:HE2	1:A:345:ALA:CB	2.36	0.56
1:B:341:TYR:CE2	2:B:601:ALY:HG3	2.40	0.56
1:B:243:LYS:HG2	1:B:559:THR:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:HD12	1:A:173:ASN:ND2	2.20	0.56
1:A:396:MET:HE3	1:A:448:VAL:HG21	1.87	0.56
1:A:178[B]:ARG:NH1	1:A:214:PRO:O	2.40	0.55
1:B:472:LEU:HD22	1:B:511:LEU:HB3	1.87	0.55
1:B:394:ILE:HD11	1:B:462:ILE:HG12	1.88	0.55
1:A:434:CYS:SG	1:A:435:PRO:HD2	2.48	0.54
1:B:357:MET:HE1	1:B:547:TRP:CH2	2.42	0.54
1:A:435:PRO:HD3	1:A:446:LYS:HD2	1.89	0.54
1:B:361:MET:HE3	1:B:558:LEU:HD11	1.90	0.54
1:B:515:GLN:N	1:B:515:GLN:OE1	2.41	0.53
1:A:473:ALA:HB2	1:A:499:TYR:HD2	1.73	0.53
1:A:473:ALA:HA	2:A:601:ALY:HH33	1.89	0.53
1:A:270:MET:HE3	1:A:322:PHE:HE1	1.73	0.52
1:A:375:PRO:HG3	1:A:491:MET:HE2	1.92	0.52
1:B:143:ILE:HD12	1:B:173:ASN:CG	2.34	0.52
1:B:350:LEU:HD23	1:B:547:TRP:HB2	1.92	0.52
1:A:473:ALA:HB2	1:A:499:TYR:CD2	2.44	0.52
2:A:601:ALY:HD3	2:A:601:ALY:O	2.10	0.51
1:A:301:GLU:OE2	2:A:601:ALY:HE2	2.10	0.51
1:B:132:ILE:HD11	1:B:182:ILE:HD13	1.93	0.51
1:B:109:ILE:HD12	1:B:152:VAL:CG2	2.41	0.51
1:A:516:ALA:HB2	1:A:529:ILE:CG2	2.41	0.51
1:B:342:MET:HE1	1:B:353:ILE:CD1	2.41	0.51
1:A:406:MET:SD	1:A:426:ILE:HD12	2.51	0.51
1:B:301:GLU:CD	2:B:601:ALY:HE2	2.36	0.50
1:B:301:GLU:HB2	1:B:341:TYR:OH	2.11	0.50
1:A:434:CYS:HA	1:A:446:LYS:HD2	1.93	0.50
1:B:432:VAL:HG21	1:B:447:LEU:HD23	1.94	0.50
1:B:473:ALA:O	1:B:474:LYS:HB2	2.12	0.50
1:A:279:VAL:HG13	1:A:279:VAL:O	2.11	0.49
1:A:467:GLN:NE2	1:A:475:TRP:HE1	2.10	0.49
1:A:98:LYS:HE2	1:B:346:ASP:HB3	1.95	0.49
1:A:311:GLY:O	1:B:241:ARG:NH2	2.46	0.49
1:B:94:PRO:O	1:B:97:HIS:HB2	2.11	0.49
1:B:301:GLU:OE2	2:B:601:ALY:HE2	2.13	0.48
1:B:361:MET:HE1	1:B:554:VAL:HG11	1.94	0.48
1:A:357:MET:HE1	1:A:547:TRP:HH2	1.76	0.48
1:B:109:ILE:O	1:B:113:SER:HB2	2.14	0.48
1:B:410:GLU:HG2	3:B:747:HOH:O	2.13	0.48
1:A:409:PRO:HG2	1:A:419:THR:HG23	1.95	0.48
1:A:220:LEU:HD13	1:A:236:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:CZ	1:A:153:LYS:HE2	2.45	0.47
1:B:109:ILE:HD11	1:B:153:LYS:O	2.15	0.47
1:A:511:LEU:C	1:A:511:LEU:HD23	2.39	0.47
1:B:472:LEU:N	1:B:472:LEU:HD23	2.31	0.46
1:B:410:GLU:OE1	1:B:412:ASN:HB2	2.15	0.46
2:B:601:ALY:C	2:B:601:ALY:HD3	2.46	0.46
1:A:436:PRO:HB2	1:A:437:PRO:HD3	1.96	0.46
1:A:516:ALA:HB2	1:A:529:ILE:HG23	1.98	0.46
1:A:134:ALA:HB3	1:A:146:ASP:HB2	1.98	0.45
1:A:306:MET:HE3	1:B:231:TYR:CE1	2.52	0.45
1:B:325:GLU:HG2	1:B:326:GLY:H	1.81	0.45
1:B:191:THR:HG23	1:B:193:LYS:H	1.81	0.45
1:A:401:GLU:HG2	1:A:408:LEU:HG	1.98	0.45
1:B:342:MET:HE1	1:B:353:ILE:HD12	1.98	0.45
1:B:473:ALA:HB1	1:B:499:TYR:HD2	1.82	0.45
1:B:116:GLN:OE1	1:B:116:GLN:N	2.50	0.45
1:B:272:ASN:HB3	3:B:746:HOH:O	2.16	0.45
1:A:112:TYR:O	1:A:196:LEU:HD13	2.17	0.44
1:A:145:TYR:HB2	1:A:156:VAL:HB	1.99	0.44
1:B:169:PHE:O	1:B:173:ASN:ND2	2.51	0.44
1:B:271:MET:CE	1:B:285:THR:HG21	2.48	0.44
1:A:497:ASN:O	2:A:601:ALY:N	2.50	0.44
1:B:145:TYR:HB2	1:B:156:VAL:HB	1.99	0.44
1:A:95:TYR:CZ	1:B:505:PRO:HD2	2.53	0.43
1:A:467:GLN:HE21	1:A:475:TRP:HE1	1.67	0.43
1:A:499:TYR:HD1	2:A:601:ALY:HB3	1.84	0.43
1:B:212:MET:HA	3:B:728:HOH:O	2.18	0.43
1:B:362:VAL:HG22	1:B:558:LEU:HD21	2.01	0.43
1:A:80:ARG:O	1:A:84:ILE:HG12	2.19	0.43
1:B:546:GLY:HA3	2:B:601:ALY:HG3	2.00	0.43
1:A:501:GLU:CD	2:A:601:ALY:HZ	2.24	0.42
1:B:396:MET:HE3	1:B:465:HIS:ND1	2.34	0.42
1:A:434:CYS:HB3	1:A:438:ARG:HG2	2.02	0.42
1:B:263:PHE:HB3	1:B:316:TYR:HD1	1.83	0.42
1:A:148:ARG:HD3	1:A:153:LYS:HG2	2.02	0.42
1:A:398:GLU:HG3	3:A:782:HOH:O	2.19	0.42
1:B:568:LEU:O	1:B:571:PRO:HD3	2.19	0.42
1:A:72:ASP:OD1	3:A:702:HOH:O	2.22	0.42
1:A:84:ILE:HG13	1:A:210:LEU:HD21	2.01	0.42
1:A:444:LEU:O	1:A:448:VAL:HG23	2.19	0.41
1:B:307:LEU:HD22	1:B:312:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LYS:NZ	3:A:701:HOH:O	2.22	0.41
1:B:265:GLU:HB2	1:B:316:TYR:CZ	2.55	0.41
1:A:133:HIS:CG	1:A:148:ARG:HG3	2.55	0.41
1:A:133:HIS:ND1	1:A:148:ARG:HG3	2.35	0.41
1:A:264:LEU:HD23	1:A:312:ILE:HG21	2.02	0.41
1:A:568:LEU:O	1:A:571:PRO:HD3	2.21	0.41
1:A:315:VAL:O	1:A:340:PHE:HA	2.20	0.41
1:B:385:VAL:O	1:B:385:VAL:HG23	2.20	0.41
1:A:379:GLU:OE1	1:A:379:GLU:N	2.30	0.41
1:B:439:THR:HG23	1:B:442:ARG:H	1.85	0.41
1:A:270:MET:HE3	1:A:322:PHE:CZ	2.55	0.41
1:A:563:ASN:OD1	1:A:563:ASN:C	2.64	0.41
1:A:473:ALA:CB	1:A:483:THR:CG2	2.99	0.41
1:B:95:TYR:N	1:B:96:PRO:HD2	2.36	0.41
1:B:152:VAL:HG22	1:B:153:LYS:N	2.34	0.41
1:B:361:MET:HE3	1:B:558:LEU:CD1	2.50	0.41
1:A:301:GLU:OE1	2:A:601:ALY:HE2	2.21	0.41
1:B:464:ASP:O	3:B:701:HOH:O	2.22	0.41
1:B:439:THR:CG2	1:B:442:ARG:HG3	2.51	0.40
1:B:486:PHE:CE2	1:B:498:ALA:HB3	2.55	0.40
1:A:393:ARG:HH11	1:A:393:ARG:HG2	1.86	0.40
1:A:484:GLU:OE1	1:B:98:LYS:NZ	2.36	0.40
1:A:546:GLY:HA3	2:A:601:ALY:CG	2.43	0.40
2:A:601:ALY:CH3	3:A:716:HOH:O	2.69	0.40
1:B:387:PHE:CD2	1:B:459:PRO:HG3	2.56	0.40
1:A:148:ARG:CD	1:A:153:LYS:HG2	2.51	0.40
1:B:272:ASN:ND2	3:B:715:HOH:O	2.51	0.40
1:A:149:GLY:O	1:A:152:VAL:HG22	2.22	0.40
1:B:544:THR:HG22	1:B:545:ALA:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/520 (93%)	464 (96%)	18 (4%)	0	100	100
1	B	482/520 (93%)	469 (97%)	13 (3%)	0	100	100
All	All	964/1040 (93%)	933 (97%)	31 (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	436/462 (94%)	431 (99%)	5 (1%)	65	75
1	B	437/462 (95%)	434 (99%)	3 (1%)	76	82
All	All	873/924 (94%)	865 (99%)	8 (1%)	70	79

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	LEU
1	A	290	LEU
1	A	472	LEU
1	A	474	LYS
1	A	485	ARG
1	B	420	ARG
1	B	468	ILE
1	B	472	LEU

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

Mol	Chain	Res	Type
1	A	75	GLN
1	A	171	HIS
1	A	217	HIS
1	A	465	HIS
1	A	467	GLN

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Mol	Chain	Res	Type
1	B	100	HIS
1	B	133	HIS
1	B	173	ASN
1	B	187	ASN
1	B	321	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 [i](#)

2 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	ALY	A	601	-	11,12,12	0.99	0	11,14,14	1.34	1 (9%)
2	ALY	B	601	-	11,12,12	1.06	1 (9%)	11,14,14	1.14	1 (9%)

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	ALY	A	601	-	-	4/12/12/12	-
2	ALY	B	601	-	-	7/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ALY	CH-NZ	2.20	1.40	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ALY	OXT-C-O	-2.69	117.97	124.08
2	A	601	ALY	OXT-C-O	-2.68	118.01	124.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ALY	O-C-CA-N
2	B	601	ALY	OXT-C-CA-N
2	A	601	ALY	OXT-C-CA-N
2	B	601	ALY	N-CA-CB-CG
2	B	601	ALY	CG-CD-CE-NZ
2	B	601	ALY	O-C-CA-CB
2	B	601	ALY	C-CA-CB-CG
2	A	601	ALY	O-C-CA-CB
2	B	601	ALY	OXT-C-CA-CB
2	A	601	ALY	OXT-C-CA-CB
2	B	601	ALY	O-C-CA-N

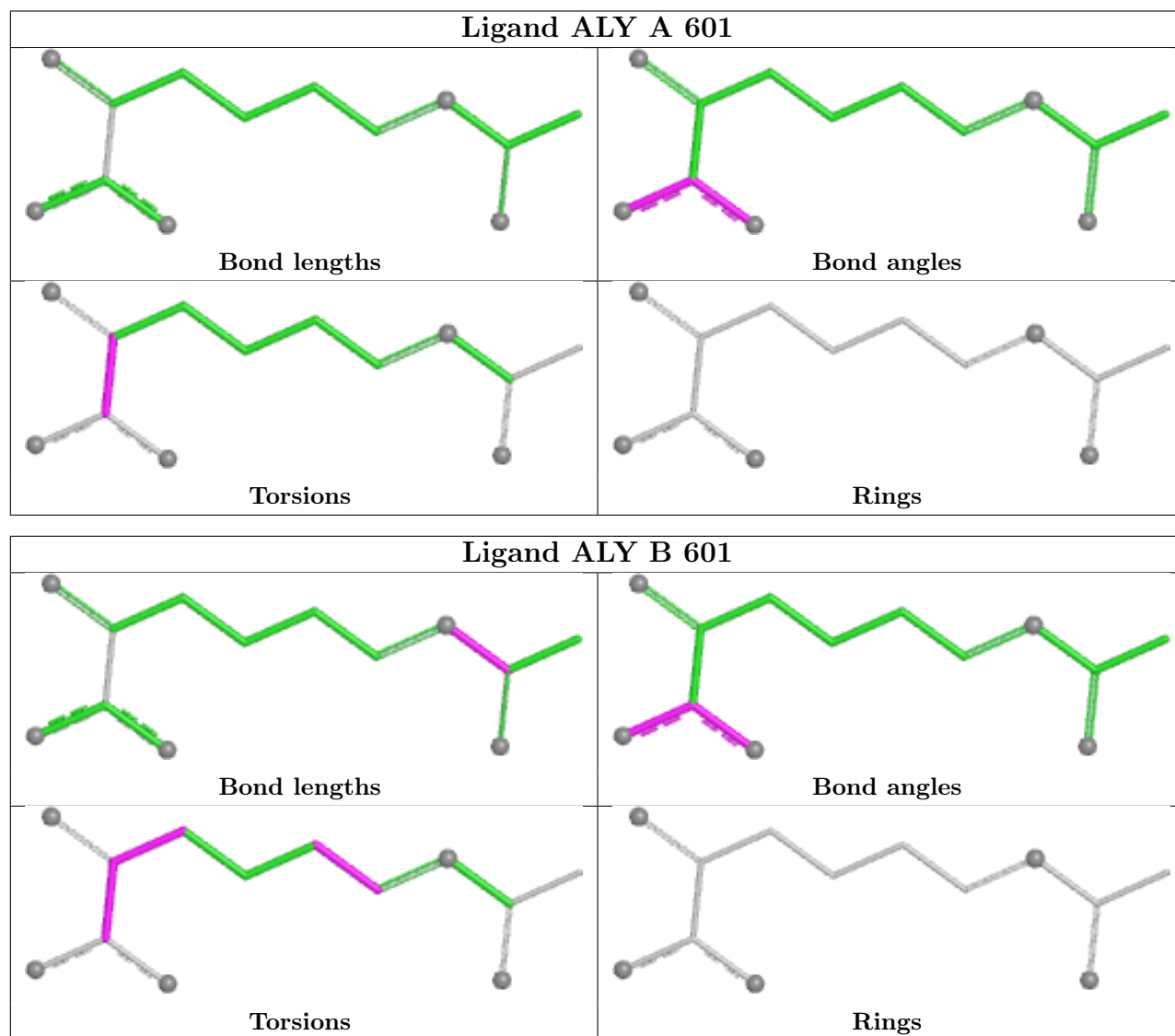
There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	ALY	14	0
2	B	601	ALY	9	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	489/520 (94%)	1.02	51 (10%)	11 11	23, 52, 91, 126	1 (0%)
1	B	490/520 (94%)	0.88	58 (11%)	9 8	23, 48, 83, 101	0
All	All	979/1040 (94%)	0.95	109 (11%)	10 9	23, 50, 89, 126	1 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	473	ALA	7.1
1	A	475	TRP	6.6
1	A	220	LEU	6.4
1	B	473	ALA	6.1
1	A	472	LEU	5.9
1	A	443	LEU	5.7
1	A	471	PRO	5.7
1	A	512	PHE	5.7
1	B	516	ALA	5.2
1	A	434	CYS	4.8
1	B	280	ALA	4.6
1	A	432	VAL	4.6
1	A	437	PRO	4.2
1	A	440	THR	4.2
1	A	277	GLY	4.1
1	A	98	LYS	4.1
1	B	189	GLY	4.0
1	B	502	LEU	4.0
1	B	512	PHE	4.0
1	A	468	ILE	4.0
1	A	518	ALA	3.9
1	B	511	LEU	3.9
1	A	436	PRO	3.6
1	B	471	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	528	PHE	3.6
1	A	454	VAL	3.4
1	B	468	ILE	3.4
1	B	472	LEU	3.4
1	B	507	ARG	3.4
1	A	435	PRO	3.4
1	B	71	VAL	3.3
1	B	279	VAL	3.3
1	A	276	GLY	3.2
1	B	437	PRO	3.2
1	A	429	ALA	3.2
1	A	379	GLU	3.2
1	A	153	LYS	3.2
1	A	439	THR	3.1
1	B	529	ILE	3.1
1	A	444	LEU	3.1
1	A	298	ILE	3.0
1	B	434	CYS	3.0
1	B	435	PRO	3.0
1	B	474	LYS	3.0
1	B	220	LEU	2.9
1	B	432	VAL	2.8
1	A	474	LYS	2.8
1	B	276	GLY	2.8
1	B	467	GLN	2.8
1	B	414	PHE	2.8
1	B	469	MET	2.8
1	A	431	ALA	2.8
1	A	371	VAL	2.8
1	A	480	GLU	2.7
1	B	201	TYR	2.7
1	B	108	PHE	2.7
1	A	325	GLU	2.7
1	B	436	PRO	2.7
1	A	427	CYS	2.7
1	B	368	SER	2.6
1	B	123	ASP	2.6
1	A	139	GLY	2.6
1	B	285	THR	2.6
1	B	219	GLY	2.5
1	A	423	LEU	2.5
1	A	280	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	529	ILE	2.5
1	A	502	LEU	2.5
1	A	415	GLU	2.5
1	B	433	GLU	2.5
1	B	121	LEU	2.5
1	A	414	PHE	2.4
1	B	75	GLN	2.4
1	B	115	LEU	2.4
1	B	499	TYR	2.4
1	A	514	GLU	2.4
1	A	511	LEU	2.4
1	B	440	THR	2.3
1	B	118	GLY	2.3
1	B	133	HIS	2.3
1	B	454	VAL	2.3
1	A	378	PRO	2.3
1	B	139	GLY	2.3
1	A	416	THR	2.3
1	A	438	ARG	2.3
1	B	170	ILE	2.3
1	B	420	ARG	2.3
1	A	272	ASN	2.2
1	A	221	LYS	2.2
1	B	444	LEU	2.2
1	B	70	SER	2.2
1	B	347	TYR	2.2
1	B	466	PRO	2.2
1	B	575	PRO	2.2
1	B	429	ALA	2.2
1	B	484	GLU	2.1
1	A	510	GLN	2.1
1	B	274	ILE	2.1
1	A	124	ILE	2.1
1	A	447	LEU	2.1
1	B	482	LEU	2.1
1	B	286	TYR	2.1
1	B	215	HIS	2.1
1	B	117	PRO	2.1
1	A	133	HIS	2.1
1	B	218	PHE	2.1
1	B	142	LEU	2.0
1	A	181	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	97	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

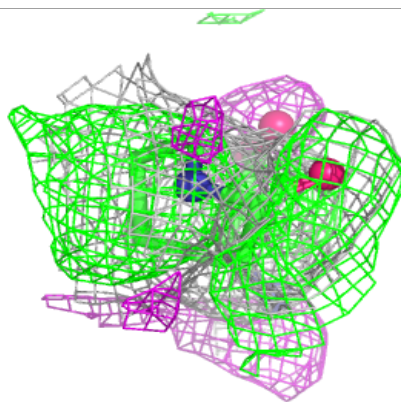
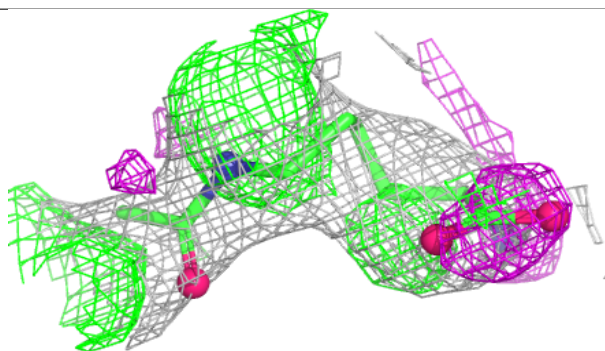
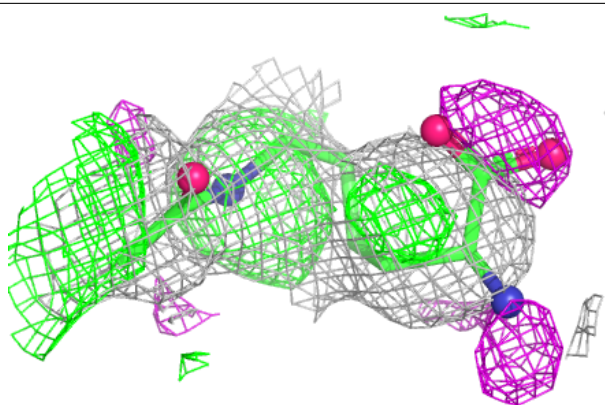
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ALY	B	601	13/13	0.53	0.37	46,56,70,77	0
2	ALY	A	601	13/13	0.73	0.31	29,59,67,71	0

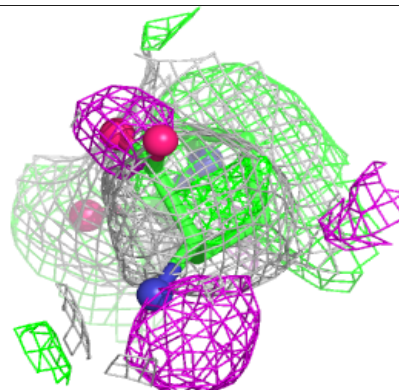
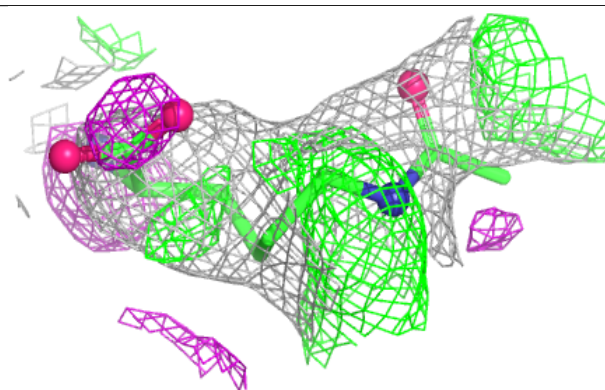
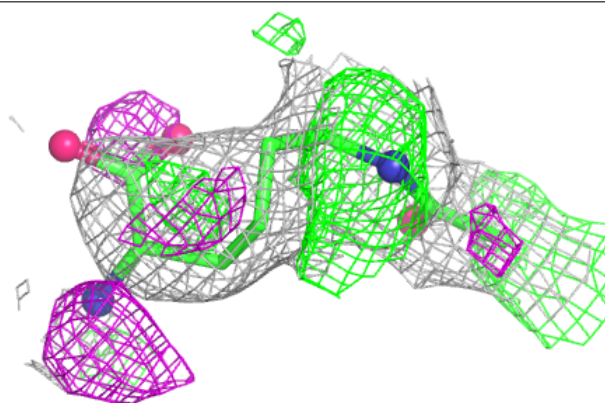
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ALY B 601:

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

**Electron density around ALY A 601:**

$2mF_o-DF_c$ (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.