



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:34 PM UTC

PDB ID : 6AGT / pdb_00006agt
Title : Crystal structure of PfKRS complexed with chromone inhibitor
Authors : Yogavel, M.; Sharma, A.; Sharma, A.; Baragana, B.; Walpole, C.
Deposited on : 2018-08-14
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

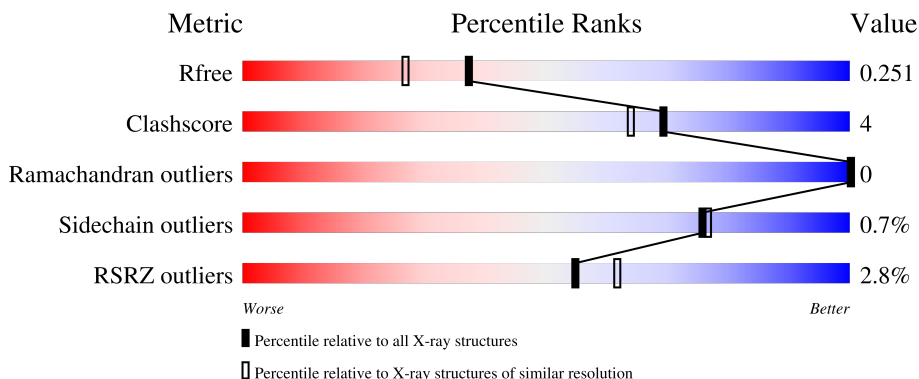
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

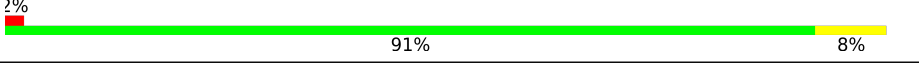
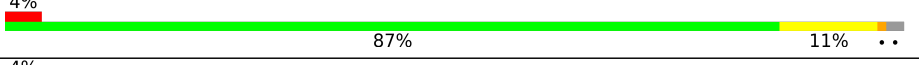
The reported resolution of this entry is 1.95 Å.

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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	507	
1	B	507	
1	C	507	
1	D	507	

2 Entry composition [i](#)

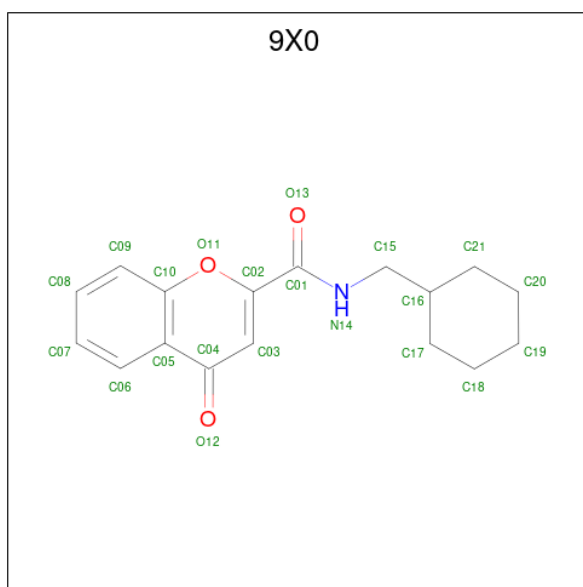
There are 7 unique types of molecules in this entry. The entry contains 16521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	4	0
			3962	2557	660	728	17			
1	B	506	Total	C	N	O	S	0	2	0
			4058	2615	680	746	17			
1	C	499	Total	C	N	O	S	0	6	0
			3966	2556	668	725	17			
1	D	485	Total	C	N	O	S	0	1	0
			3833	2480	638	699	16			

- Molecule 2 is N-(cyclohexylmethyl)-4-oxo-4H-1-benzopyran-2-carboxamide (CCD ID: 9X0) (formula: C₁₇H₁₉NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	17	1	3		
2	B	1	Total	C	N	O	0	0
			21	17	1	3		

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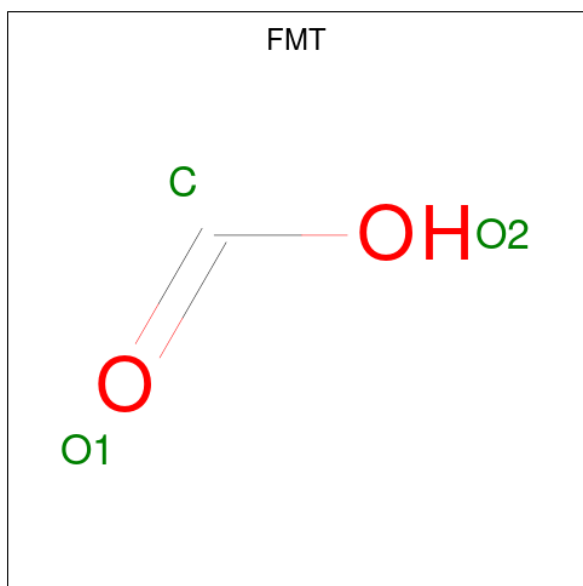
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			21	17	1	3		
2	D	1	Total	C	N	O	0	0
			21	17	1	3		

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Co	0	0
			1	1		
3	B	1	Total	Co	0	0
			1	1		
3	C	2	Total	Co	0	0
			2	2		
3	D	1	Total	Co	0	0
			1	1		

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



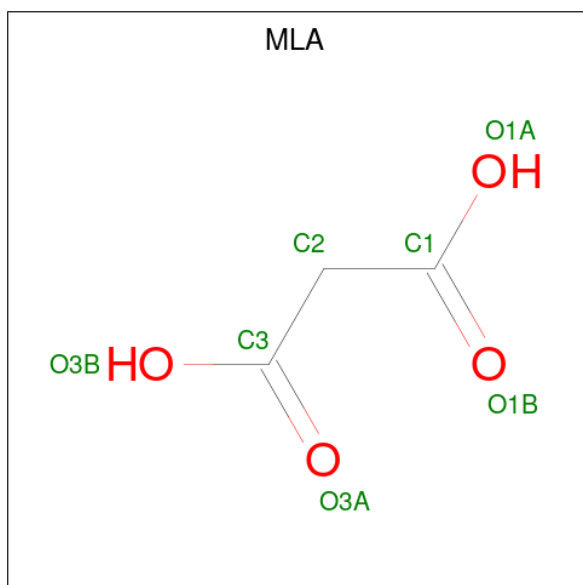
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		

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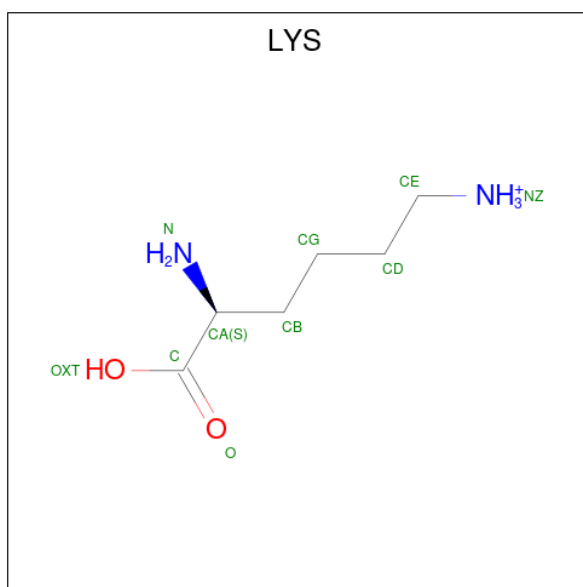
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		
5	D	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			10	6	2	2		
6	B	1	Total	C	N	O	0	0
			10	6	2	2		
6	C	1	Total	C	N	O	0	0
			10	6	2	2		
6	D	1	Total	C	N	O	0	0
			10	6	2	2		

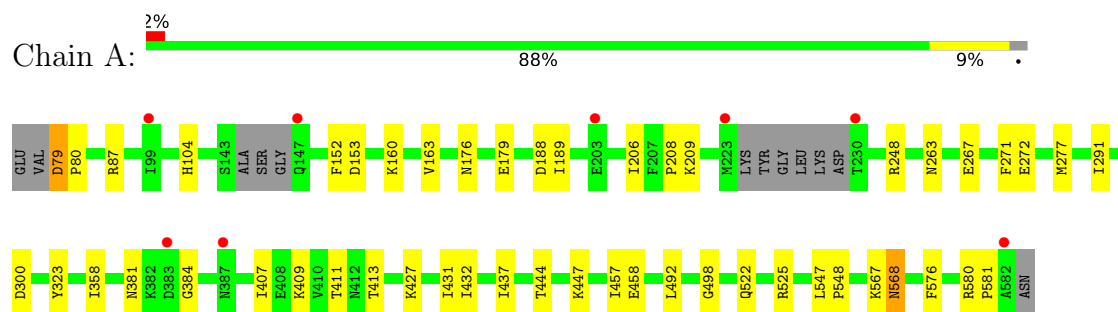
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	146	Total	O	0	0
			146	146		
7	B	169	Total	O	0	0
			169	169		
7	C	126	Total	O	0	0
			126	126		
7	D	103	Total	O	0	0
			103	103		

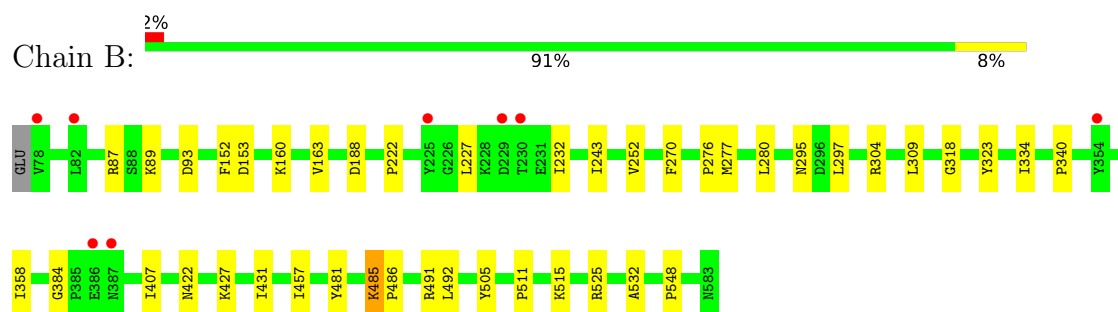
3 Residue-property plots [i](#)

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.

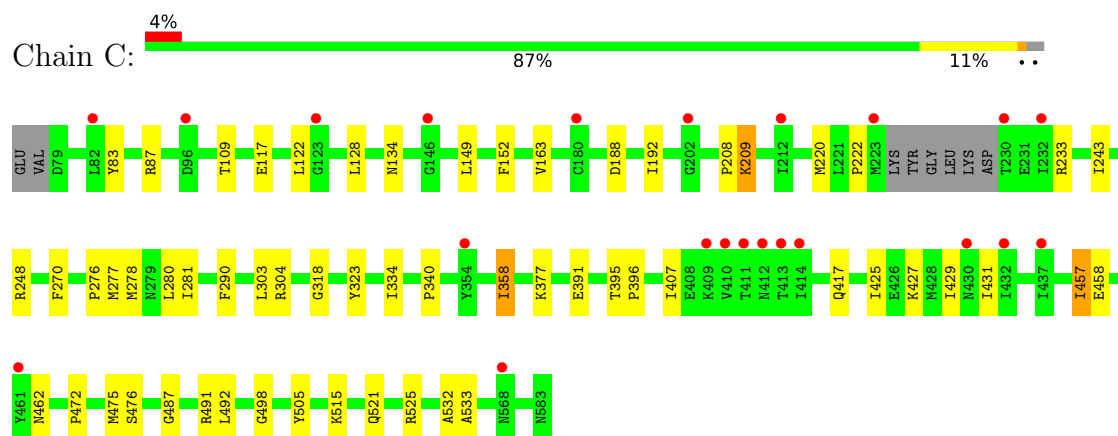
• Molecule 1: Lysine-tRNA ligase



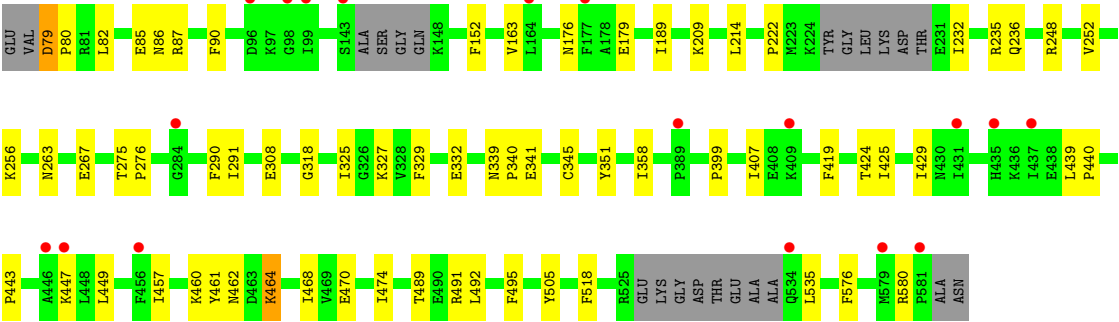
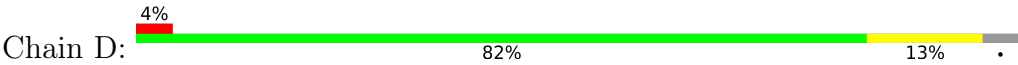
• Molecule 1: Lysine-tRNA ligase



• Molecule 1: Lysine-tRNA ligase



• Molecule 1: Lysine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.76Å 104.34Å 100.59Å 89.88° 69.57° 61.10°	Depositor
Resolution (Å)	31.90 – 1.95 31.90 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.1 (31.90-1.95) 96.7 (31.90-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.203 , 0.243 (Not available) , 0.251	Depositor DCC
R_{free} test set	8377 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16521	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO, 9X0, FMT, MLA

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	0.56	0/4072	0.85	6/5518 (0.1%)
1	B	0.54	0/4163	0.85	8/5632 (0.1%)
1	C	0.52	0/4082	0.82	2/5531 (0.0%)
1	D	0.56	0/3930	0.90	8/5329 (0.2%)
All	All	0.55	0/16247	0.85	24/22010 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ASP	CA-C-N	6.89	126.41	119.24
1	A	79	ASP	C-N-CA	6.89	126.41	119.24
1	D	79	ASP	CA-C-N	6.86	128.41	119.84
1	D	79	ASP	C-N-CA	6.86	128.41	119.84
1	B	295	ASN	N-CA-C	6.39	118.24	111.28
1	D	209	LYS	N-CA-C	-6.15	105.73	113.72
1	A	209	LYS	N-CA-C	-5.97	106.33	113.97
1	D	85	GLU	CA-C-N	5.95	128.54	120.38
1	D	85	GLU	C-N-CA	5.95	128.54	120.38
1	B	422	ASN	N-CA-C	-5.92	104.91	111.36
1	B	309	LEU	CA-C-N	-5.83	113.01	119.19
1	B	309	LEU	C-N-CA	-5.83	113.01	119.19
1	A	384	GLY	CA-C-N	5.80	125.48	119.56
1	A	384	GLY	C-N-CA	5.80	125.48	119.56
1	C	209	LYS	N-CA-C	-5.69	106.50	113.50
1	A	568	ASN	N-CA-C	-5.66	106.03	113.17
1	D	222	PRO	O-C-N	5.38	129.56	123.00
1	D	464	LYS	N-CA-C	5.35	113.04	108.22
1	B	384	GLY	CA-C-N	5.33	125.00	119.56
1	B	384	GLY	C-N-CA	5.33	125.00	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	457	ILE	CB-CA-C	-5.09	106.42	111.30
1	D	308	GLU	N-CA-C	5.08	117.21	111.11
1	B	485	LYS	CA-C-N	5.01	125.01	119.90
1	B	485	LYS	C-N-CA	5.01	125.01	119.90

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	3962	0	3839	31	0
1	B	4058	0	3978	25	0
1	C	3966	0	3822	32	0
1	D	3833	0	3682	36	0
2	A	21	0	0	0	0
2	B	21	0	0	0	0
2	C	21	0	0	0	0
2	D	21	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	9	0	3	0	0
4	C	6	0	2	0	0
5	A	7	0	2	0	0
5	D	7	0	2	1	0
6	A	10	0	12	0	0
6	B	10	0	12	0	0
6	C	10	0	12	0	0
6	D	10	0	12	0	0
7	A	146	0	0	1	0
7	B	169	0	0	0	0
7	C	126	0	0	0	0
7	D	103	0	0	0	0
All	All	16521	0	15378	111	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 4.

All (111) 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:C:358:ILE:HG13	1:C:492:LEU:HD22	1.63	0.79
1:D:358:ILE:HG13	1:D:492:LEU:HD22	1.77	0.66
1:D:351:TYR:HB2	5:D:603:MLA:HC21	1.78	0.66
1:D:439:LEU:HD11	1:D:443:PRO:HB3	1.76	0.65
1:C:407:ILE:HG13	1:C:457:ILE:HD11	1.78	0.64
1:A:358:ILE:HG13	1:A:492:LEU:HD22	1.78	0.64
1:A:153:ASP:HB3	1:A:160:LYS:HD2	1.79	0.63
1:B:358:ILE:HG13	1:B:492:LEU:HD22	1.83	0.59
1:A:152:PHE:HB2	1:A:163:VAL:HB	1.83	0.59
1:B:334:ILE:HG12	1:B:340:PRO:HD3	1.85	0.59
1:D:176:ASN:HB3	1:D:179:GLU:HB3	1.85	0.58
1:C:152:PHE:HB2	1:C:163:VAL:HB	1.84	0.58
1:C:277:MET:HE2	1:C:304:ARG:NH2	2.19	0.58
1:D:82:LEU:O	1:D:86:ASN:HB2	2.03	0.58
1:B:511:PRO:O	1:B:515:LYS:HG3	2.05	0.56
1:C:458:GLU:O	1:C:498:GLY:HA2	2.07	0.55
1:D:152:PHE:HB2	1:D:163:VAL:HB	1.89	0.54
1:A:522:GLN:NE2	1:A:522:GLN:HA	2.23	0.54
1:C:192:ILE:HG23	1:C:208:PRO:HB3	1.89	0.53
1:A:407:ILE:HG13	1:A:457:ILE:HD11	1.91	0.53
1:A:291:ILE:HD11	1:A:300:ASP:HB3	1.92	0.52
1:C:122:LEU:HD21	1:C:128:LEU:HD11	1.92	0.52
1:B:152:PHE:HB2	1:B:163:VAL:HB	1.91	0.52
1:B:153:ASP:HB3	1:B:160:LYS:HD2	1.92	0.52
1:D:263[B]:ASN:ND2	1:D:267:GLU:OE2	2.38	0.51
1:A:381:ASN:O	1:A:568:ASN:OD1	2.30	0.50
1:B:277:MET:HE2	1:B:304:ARG:NH2	2.27	0.50
1:D:449:LEU:HD12	1:D:474:ILE:HD11	1.93	0.50
1:C:278:MET:HE3	1:D:329:PHE:CD2	2.46	0.50
1:B:491:ARG:HA	1:B:505:TYR:HB3	1.94	0.50
1:A:104[A]:HIS:HE1	1:B:481:TYR:O	1.94	0.50
1:A:432:ILE:HG12	1:A:437:ILE:HD11	1.94	0.50
1:B:87:ARG:NH2	1:B:188:ASP:OD1	2.45	0.49
1:B:407:ILE:HG13	1:B:457:ILE:HD11	1.94	0.49
1:D:407:ILE:HG13	1:D:457:ILE:HD11	1.94	0.49
1:D:425:ILE:O	1:D:429:ILE:HG13	2.12	0.49
1:A:272:GLU:HB2	1:A:323:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:THR:HG23	1:C:134:ASN:HB2	1.94	0.49
1:C:248:ARG:NH2	1:D:318:GLY:O	2.47	0.48
1:A:580:ARG:NH2	1:B:297:LEU:O	2.47	0.48
1:A:432:ILE:HG23	1:A:437:ILE:HG13	1.94	0.48
1:B:525:ARG:HB2	1:B:532:ALA:HB3	1.96	0.48
1:C:334:ILE:HG12	1:C:340:PRO:HD3	1.96	0.48
1:C:525:ARG:NH1	1:C:532:ALA:O	2.40	0.48
1:D:460:LYS:HG2	1:D:461:TYR:CD2	2.50	0.47
1:D:252:VAL:HG12	1:D:256:LYS:HE2	1.96	0.47
1:A:87:ARG:NH2	1:A:188:ASP:OD1	2.48	0.47
1:C:525:ARG:HB2	1:C:532:ALA:HB3	1.95	0.47
1:D:468:ILE:HD12	1:D:495:PHE:CE1	2.49	0.47
1:D:439:LEU:HD12	1:D:440:PRO:HD2	1.96	0.47
1:A:271:PHE:CZ	1:B:252:VAL:HA	2.49	0.46
1:A:277:MET:HE1	1:B:277:MET:HE1	1.97	0.46
1:B:485:LYS:HA	1:B:486:PRO:HD2	1.76	0.46
1:C:515:LYS:HA	1:C:515:LYS:HD2	1.65	0.46
1:D:327:LYS:NZ	1:D:341:GLU:OE1	2.40	0.46
1:B:427:LYS:O	1:B:431:ILE:HG13	2.16	0.46
1:C:491:ARG:HA	1:C:505:TYR:HB3	1.97	0.46
1:C:276:PRO:HD3	1:D:576:PHE:HB2	1.97	0.46
1:D:460:LYS:HG2	1:D:461:TYR:CE2	2.51	0.46
1:A:444:THR:OG1	1:A:447:LYS:HG3	2.16	0.46
1:C:377:LYS:HD3	1:C:391[B]:GLU:CD	2.41	0.45
1:C:87:ARG:NH2	1:C:188:ASP:OD1	2.50	0.45
1:B:270:PHE:HB3	1:B:323:TYR:HD1	1.82	0.45
1:D:518:PHE:CB	1:D:535:LEU:HD13	2.47	0.45
1:A:576:PHE:HB2	1:B:276:PRO:HD3	1.98	0.44
1:A:176:ASN:HB3	1:A:179:GLU:HB3	1.98	0.44
1:A:581:PRO:HG3	1:B:280:LEU:HD22	2.00	0.44
1:C:318:GLY:O	1:D:248:ARG:NH2	2.50	0.44
1:A:411:THR:O	1:A:413:THR:HG23	2.17	0.44
1:D:79:ASP:HA	1:D:80:PRO:HD2	1.69	0.44
1:D:235:ARG:NH2	1:D:580:ARG:O	2.27	0.44
1:D:275:THR:HB	1:D:276:PRO:HD2	2.01	0.43
1:A:248:ARG:NH2	1:B:318:GLY:O	2.51	0.43
1:C:427:LYS:O	1:C:431:ILE:HG13	2.18	0.43
1:D:470:GLU:HA	1:D:489:THR:O	2.19	0.43
1:C:222:PRO:HG2	1:C:243:ILE:CD1	2.48	0.43
1:C:290:PHE:HB2	1:C:303:LEU:HD22	2.01	0.43
1:C:270:PHE:HB3	1:C:323:TYR:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:ILE:O	1:C:429:ILE:HG13	2.18	0.43
1:C:395:THR:HA	1:C:396:PRO:HD3	1.89	0.43
1:A:547:LEU:HD12	1:A:548:PRO:HD2	2.01	0.42
1:D:325:ILE:HG12	1:D:345:CYS:HB2	2.01	0.42
1:A:189:ILE:HD13	1:B:548:PRO:HB3	2.01	0.42
1:A:263[B]:ASN:ND2	1:A:267:GLU:OE2	2.42	0.42
1:D:491:ARG:HA	1:D:505:TYR:HB3	2.01	0.42
1:A:458:GLU:O	1:A:498:GLY:HA2	2.18	0.42
1:A:427:LYS:O	1:A:431:ILE:HG13	2.20	0.42
1:D:232:ILE:O	1:D:236:GLN:N	2.48	0.42
1:C:521:GLN:HG3	1:C:533:ALA:HB3	2.01	0.42
1:B:222:PRO:HG2	1:B:243:ILE:HD13	2.02	0.41
1:C:472:PRO:HD2	1:C:475:MET:SD	2.60	0.41
1:C:278:MET:HE1	1:D:290:PHE:CD1	2.56	0.41
1:A:522:GLN:OE1	1:A:525:ARG:HD2	2.20	0.41
1:C:417:GLN:OE1	1:C:487:GLY:HA3	2.20	0.41
1:D:339:ASN:HA	1:D:340:PRO:HD3	1.95	0.41
1:A:104[A]:HIS:HD2	7:A:779:HOH:O	2.03	0.41
1:A:206:ILE:O	1:A:208:PRO:HD3	2.21	0.41
1:B:227:LEU:HD11	1:B:232:ILE:HG21	2.03	0.41
1:C:222:PRO:HG2	1:C:243:ILE:HD13	2.03	0.41
1:D:419:PHE:HA	1:D:424:THR:HG21	2.01	0.41
1:B:270:PHE:HB3	1:B:323:TYR:CD1	2.56	0.40
1:C:83:TYR:CG	1:C:220:MET:HG3	2.56	0.40
1:D:399:PRO:HG2	1:D:464:LYS:CE	2.51	0.40
1:D:518:PHE:HB3	1:D:535:LEU:HD13	2.02	0.40
1:B:89:LYS:NZ	1:B:93:ASP:OD2	2.55	0.40
1:D:82:LEU:HD23	1:D:82:LEU:HA	1.66	0.40
1:D:189:ILE:HG22	1:D:214:LEU:HB2	2.03	0.40
1:A:79:ASP:HA	1:A:80:PRO:HD2	1.72	0.40
1:A:567:LYS:HA	1:A:567:LYS:HD3	1.93	0.40
1:C:280:LEU:C	1:C:281:ILE:HD12	2.46	0.40
1:D:87:ARG:O	1:D:90:PHE:HB3	2.22	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	493/507 (97%)	488 (99%)	5 (1%)	0	100	100
1	B	506/507 (100%)	501 (99%)	5 (1%)	0	100	100
1	C	501/507 (99%)	494 (99%)	7 (1%)	0	100	100
1	D	478/507 (94%)	469 (98%)	9 (2%)	0	100	100
All	All	1978/2028 (98%)	1952 (99%)	26 (1%)	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	423/457 (93%)	422 (100%)	1 (0%)	87	89
1	B	436/457 (95%)	436 (100%)	0	100	100
1	C	416/457 (91%)	409 (98%)	7 (2%)	53	49
1	D	401/457 (88%)	397 (99%)	4 (1%)	68	67
All	All	1676/1828 (92%)	1664 (99%)	12 (1%)	76	76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	409	LYS
1	C	117	GLU

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Mol	Chain	Res	Type
1	C	149	LEU
1	C	209	LYS
1	C	233	ARG
1	C	358	ILE
1	C	462	ASN
1	C	476	SER
1	D	291	ILE
1	D	332	GLU
1	D	447	LYS
1	D	462	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	459	ASN
1	C	387	ASN
1	D	86	ASN
1	D	92	GLN
1	D	162	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](#)

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	9X0	D	601	-	23,23,23	2.41	6 (26%)	30,31,31	1.32	3 (10%)
2	9X0	C	601	-	23,23,23	2.24	7 (30%)	30,31,31	1.54	6 (20%)
4	FMT	C	604	-	2,2,2	0.66	0	1,1,1	0.26	0
6	LYS	C	606	-	8,9,9	0.88	1 (12%)	7,10,10	0.83	0
4	FMT	C	605	-	2,2,2	0.73	0	1,1,1	0.28	0
6	LYS	B	603	-	8,9,9	0.82	0	7,10,10	0.81	0
6	LYS	A	607	-	8,9,9	0.76	0	7,10,10	0.76	0
6	LYS	D	604	-	8,9,9	0.79	0	7,10,10	0.80	0
4	FMT	A	604	-	2,2,2	0.62	0	1,1,1	0.20	0
2	9X0	A	601	-	23,23,23	2.48	9 (39%)	30,31,31	1.69	7 (23%)
5	MLA	D	603	-	6,6,6	0.97	0	7,7,7	1.40	1 (14%)
4	FMT	A	603	-	2,2,2	0.59	0	1,1,1	0.26	0
4	FMT	A	605	-	2,2,2	0.67	0	1,1,1	0.17	0
5	MLA	A	606	-	6,6,6	1.33	0	7,7,7	1.54	1 (14%)
2	9X0	B	601	-	23,23,23	2.13	6 (26%)	30,31,31	1.44	6 (20%)

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	9X0	D	601	-	-	0/9/17/17	0/3/3/3
2	9X0	C	601	-	-	0/9/17/17	0/3/3/3
6	LYS	C	606	-	-	0/9/9/9	-
6	LYS	B	603	-	-	1/9/9/9	-
6	LYS	A	607	-	-	1/9/9/9	-
6	LYS	D	604	-	-	0/9/9/9	-
2	9X0	A	601	-	-	0/9/17/17	0/3/3/3
5	MLA	D	603	-	-	0/4/4/4	-
5	MLA	A	606	-	-	0/4/4/4	-
2	9X0	B	601	-	-	0/9/17/17	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	9X0	C05-C04	-6.75	1.36	1.48
2	B	601	9X0	C05-C04	-6.74	1.36	1.48
2	A	601	9X0	C05-C04	-6.57	1.37	1.48
2	C	601	9X0	C05-C04	-6.56	1.37	1.48
2	A	601	9X0	O11-C10	-4.96	1.31	1.38
2	D	601	9X0	O11-C10	-4.88	1.31	1.38
2	C	601	9X0	O11-C10	-4.45	1.31	1.38
2	D	601	9X0	C02-C01	-3.61	1.40	1.47
2	A	601	9X0	C03-C04	-3.49	1.37	1.44
2	A	601	9X0	C02-C01	-3.36	1.40	1.47
2	D	601	9X0	C03-C04	-3.24	1.37	1.44
2	C	601	9X0	C02-C01	-3.24	1.41	1.47
2	B	601	9X0	C03-C04	-3.17	1.38	1.44
2	B	601	9X0	C02-C01	-3.05	1.41	1.47
2	C	601	9X0	C03-C04	-2.86	1.38	1.44
2	C	601	9X0	C20-C21	-2.83	1.46	1.53
2	A	601	9X0	C17-C16	-2.52	1.45	1.52
2	A	601	9X0	C06-C05	-2.51	1.36	1.39
2	A	601	9X0	C18-C17	-2.49	1.46	1.53
2	D	601	9X0	C06-C05	-2.49	1.36	1.39
2	B	601	9X0	O11-C10	-2.41	1.34	1.38
2	D	601	9X0	C20-C21	-2.37	1.47	1.53
2	B	601	9X0	C18-C17	-2.34	1.47	1.53
2	A	601	9X0	C05-C10	-2.25	1.36	1.40
6	C	606	LYS	OXT-C	-2.21	1.23	1.30
2	B	601	9X0	O13-C01	-2.07	1.19	1.23
2	C	601	9X0	O13-C01	-2.06	1.19	1.23
2	C	601	9X0	C05-C10	-2.02	1.37	1.40
2	A	601	9X0	O13-C01	-2.01	1.19	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	9X0	C16-C15-N14	-4.26	105.38	112.77
2	D	601	9X0	C16-C15-N14	-3.85	106.10	112.77
2	C	601	9X0	C15-N14-C01	3.44	127.24	122.06
2	C	601	9X0	O11-C02-C03	-3.36	119.11	123.84
2	A	601	9X0	O11-C02-C03	-3.32	119.16	123.84
2	B	601	9X0	C15-N14-C01	3.21	126.89	122.06
2	C	601	9X0	C16-C15-N14	-3.20	107.22	112.77
2	B	601	9X0	O11-C02-C03	-3.13	119.43	123.84
2	A	601	9X0	C15-N14-C01	3.10	126.72	122.06
2	B	601	9X0	O11-C10-C09	3.06	120.33	116.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	9X0	O11-C10-C05	-2.87	118.96	121.57
2	D	601	9X0	O11-C02-C03	-2.77	119.94	123.84
2	B	601	9X0	C16-C15-N14	-2.75	108.00	112.77
2	A	601	9X0	O11-C10-C05	-2.72	119.09	121.57
2	A	601	9X0	O11-C02-C01	2.67	119.11	113.12
2	A	601	9X0	C18-C17-C16	-2.67	106.47	112.08
2	B	601	9X0	O11-C02-C01	2.52	118.77	113.12
2	D	601	9X0	O11-C02-C01	2.51	118.74	113.12
2	C	601	9X0	O11-C02-C01	2.48	118.67	113.12
2	B	601	9X0	O11-C10-C05	-2.31	119.47	121.57
5	A	606	MLA	C3-C2-C1	-2.24	105.04	112.95
2	A	601	9X0	O11-C10-C09	2.16	119.13	116.25
5	D	603	MLA	O3B-C3-C2	2.10	121.02	114.51
2	C	601	9X0	O11-C10-C09	2.02	118.94	116.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	603	LYS	CG-CD-CE-NZ
6	A	607	LYS	CG-CD-CE-NZ

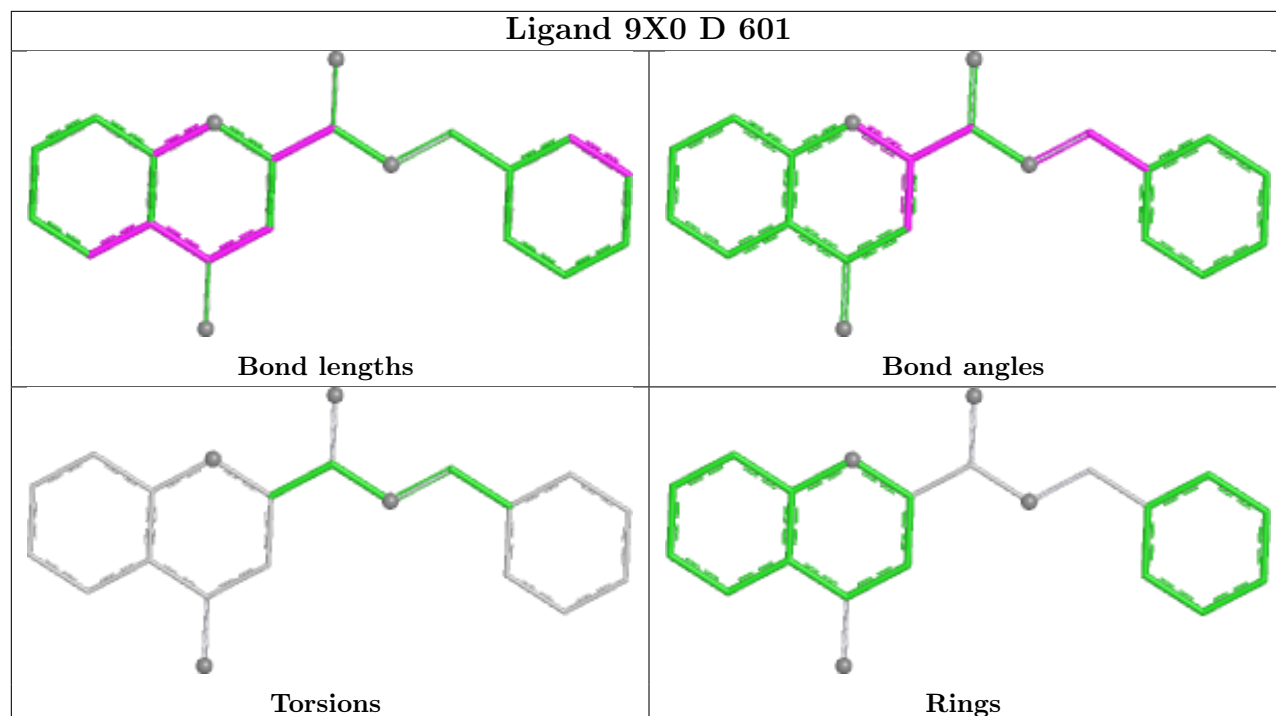
There are no ring outliers.

1 monomer is involved in 1 short contact:

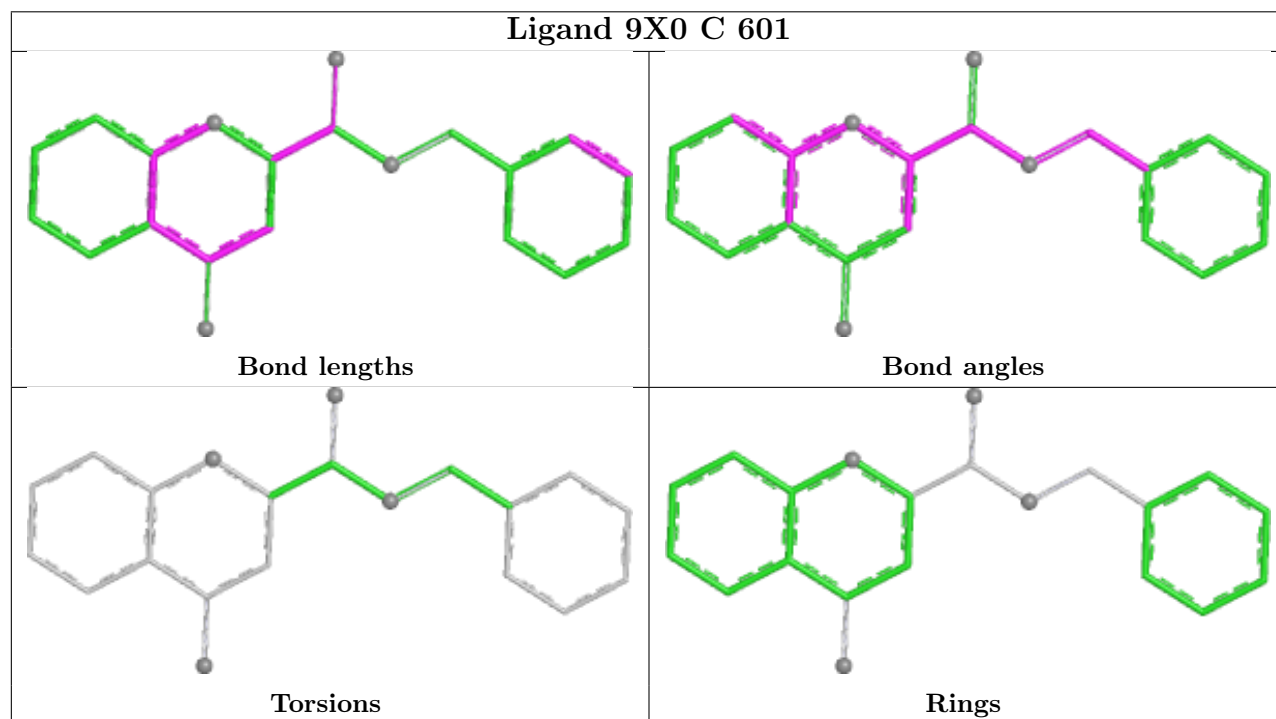
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	603	MLA	1	0

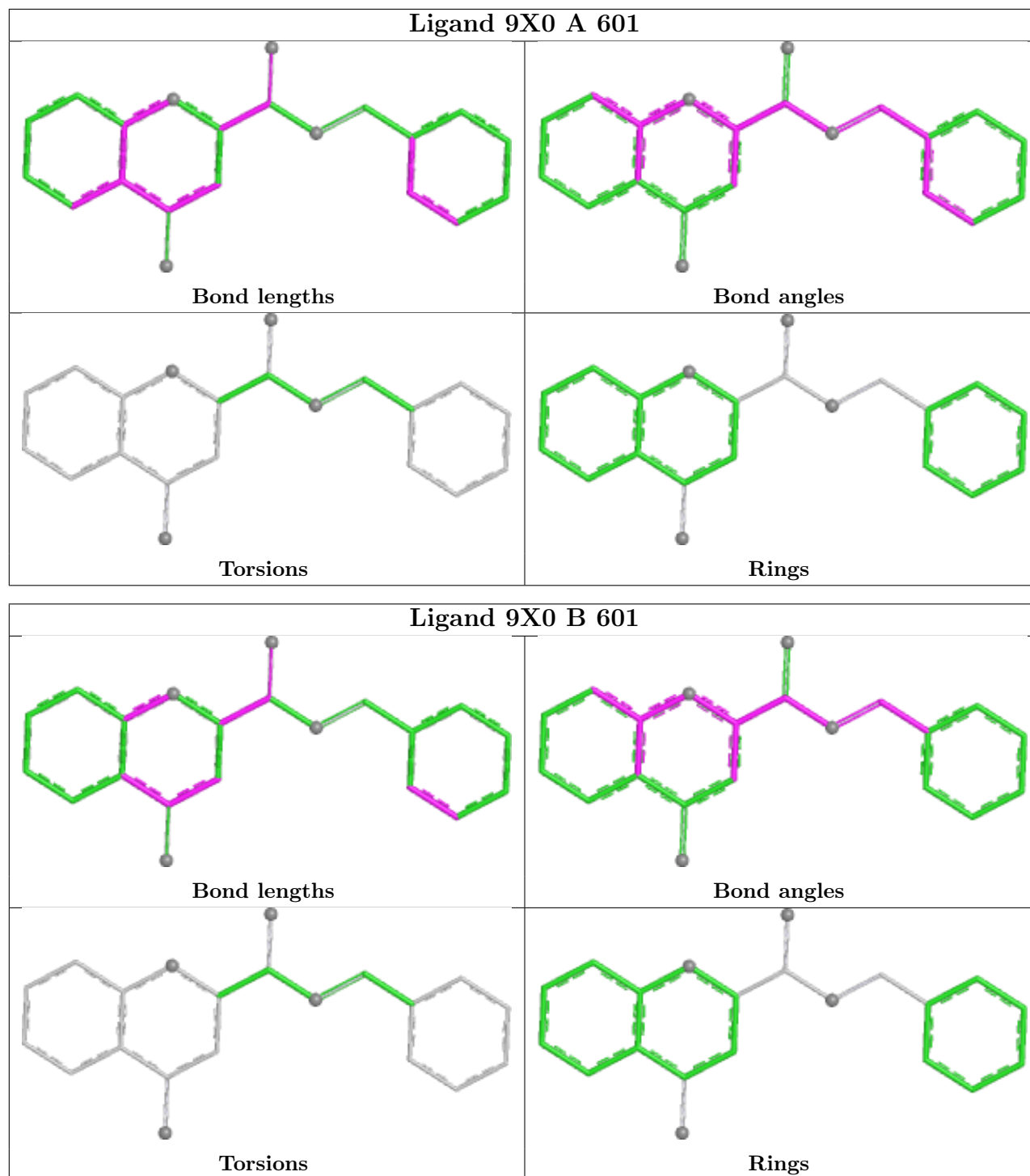
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 9X0 D 601



Ligand 9X0 C 601





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	495/507 (97%)	0.05	8 (1%) 70 77	16, 39, 74, 101	4 (0%)
1	B	506/507 (99%)	-0.03	8 (1%) 70 77	18, 39, 67, 108	2 (0%)
1	C	499/507 (98%)	0.19	22 (4%) 39 45	21, 44, 79, 97	6 (1%)
1	D	485/507 (95%)	0.23	18 (3%) 45 52	17, 45, 83, 106	1 (0%)
All	All	1985/2028 (97%)	0.11	56 (2%) 55 62	16, 42, 79, 108	13 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	THR	4.6
1	C	230	THR	4.5
1	C	223	MET	4.3
1	B	78	VAL	3.9
1	A	223	MET	3.6
1	D	99	ILE	3.5
1	D	431	ILE	3.4
1	A	99	ILE	3.3
1	D	143	SER	3.3
1	D	534	GLN	3.1
1	A	383	ASP	3.0
1	C	437	ILE	3.0
1	B	230	THR	2.9
1	C	414	ILE	2.9
1	C	432	ILE	2.8
1	C	354	TYR	2.7
1	B	387	ASN	2.6
1	B	354	TYR	2.6
1	C	412	ASN	2.6
1	D	456	PHE	2.5
1	C	82	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	146	GLY	2.5
1	D	98	GLY	2.5
1	A	147	GLN	2.5
1	B	225	TYR	2.5
1	C	410	VAL	2.4
1	D	435	HIS	2.4
1	D	409	LYS	2.4
1	D	437	ILE	2.4
1	D	177	PHE	2.3
1	C	212	ILE	2.3
1	C	202	GLY	2.3
1	C	430	ASN	2.3
1	C	96	ASP	2.3
1	B	82	LEU	2.3
1	C	461	TYR	2.2
1	C	413	THR	2.2
1	D	164	LEU	2.2
1	C	123	GLY	2.2
1	D	284	GLY	2.2
1	D	389	PRO	2.2
1	C	232	ILE	2.2
1	C	180	CYS	2.2
1	D	581	PRO	2.2
1	A	387	ASN	2.1
1	D	96	ASP	2.1
1	A	582	ALA	2.1
1	B	386	GLU	2.1
1	C	411	THR	2.1
1	D	447	LYS	2.1
1	D	446	ALA	2.1
1	A	203	GLU	2.0
1	C	568	ASN	2.0
1	B	229	ASP	2.0
1	C	409	LYS	2.0
1	D	579	MET	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

There are no oligosaccharides in this entry.

6.4 Ligands

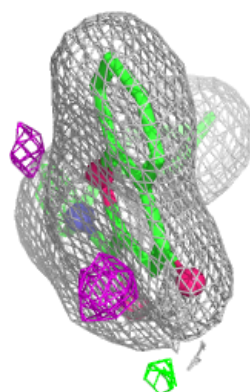
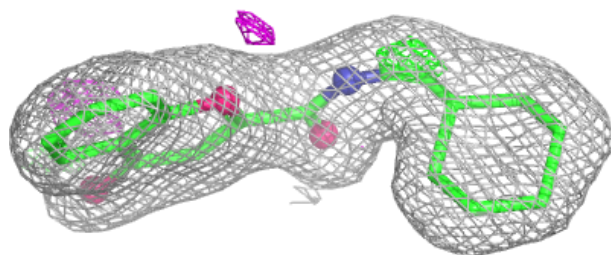
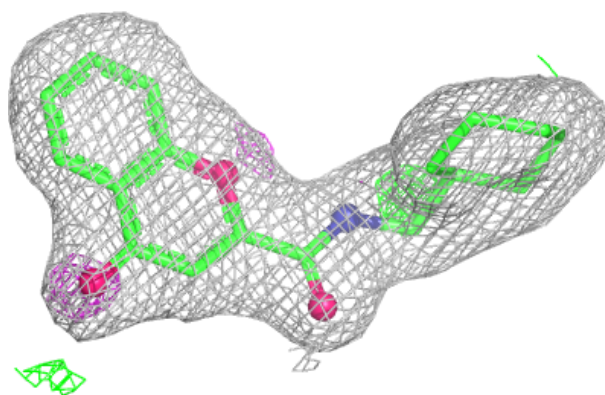
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	MLA	D	603	7/7	0.78	0.16	41,50,52,62	7
4	FMT	A	605	3/3	0.82	0.11	45,45,46,50	0
5	MLA	A	606	7/7	0.85	0.15	41,44,48,49	0
4	FMT	A	603	3/3	0.85	0.12	35,35,39,42	0
4	FMT	C	604	3/3	0.88	0.10	47,47,47,53	0
3	CO	C	602	1/1	0.89	0.08	80,80,80,80	1
4	FMT	A	604	3/3	0.91	0.08	40,40,49,58	0
4	FMT	C	605	3/3	0.92	0.07	32,32,34,39	3
2	9X0	B	601	21/21	0.95	0.06	25,31,33,38	0
6	LYS	A	607	10/10	0.95	0.06	23,27,31,35	0
6	LYS	D	604	10/10	0.95	0.07	28,33,42,43	0
2	9X0	A	601	21/21	0.96	0.05	26,31,35,42	0
6	LYS	B	603	10/10	0.96	0.06	24,28,35,36	0
6	LYS	C	606	10/10	0.96	0.07	25,28,34,35	0
2	9X0	C	601	21/21	0.96	0.05	27,30,35,36	0
2	9X0	D	601	21/21	0.97	0.04	30,33,37,38	0
3	CO	C	603	1/1	0.98	0.03	66,66,66,66	0
3	CO	B	602	1/1	0.98	0.04	53,53,53,53	1
3	CO	D	602	1/1	0.99	0.04	67,67,67,67	1
3	CO	A	602	1/1	1.00	0.02	59,59,59,59	1

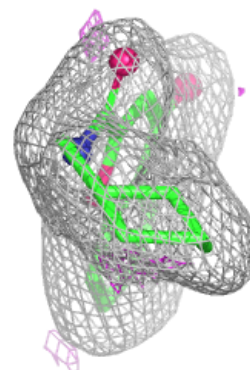
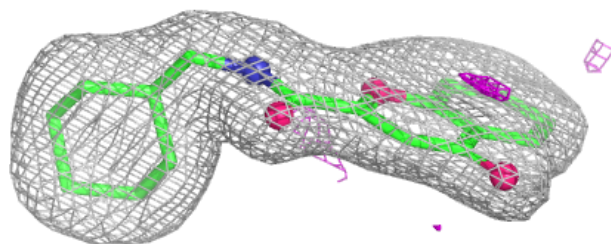
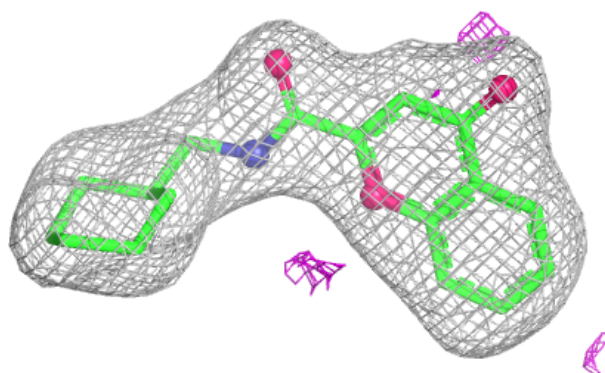
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9X0 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)

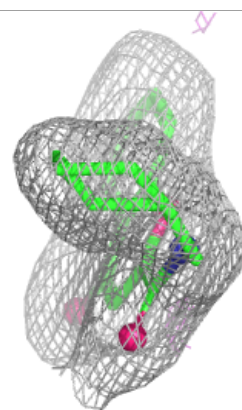
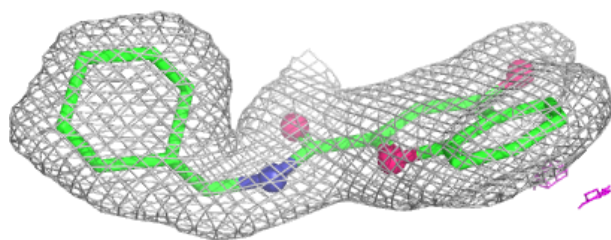
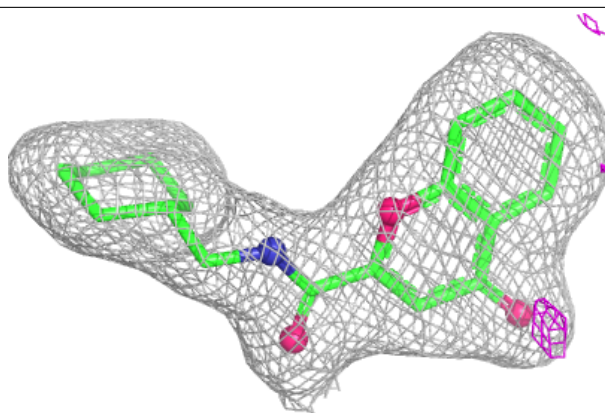
**Electron density around 9X0 A 601:**

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

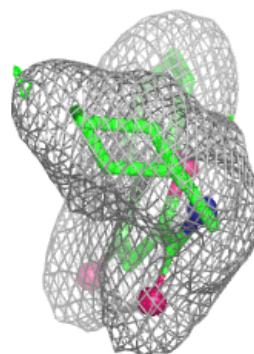
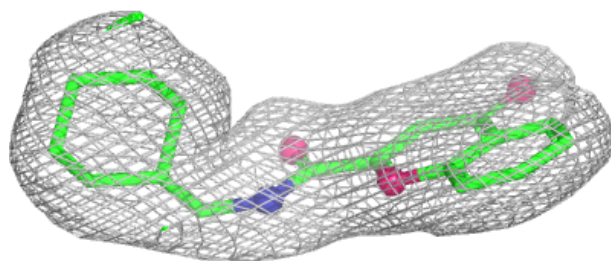
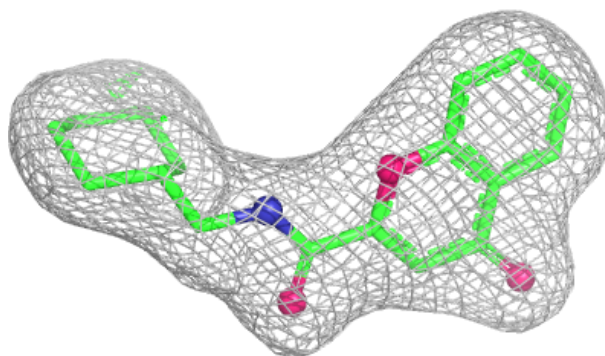


Electron density around 9X0 C 601:

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

**Electron density around 9X0 D 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.