



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 11:41 PM BST

PDB ID : 6AGT
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
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) : 2.14.4.dev1

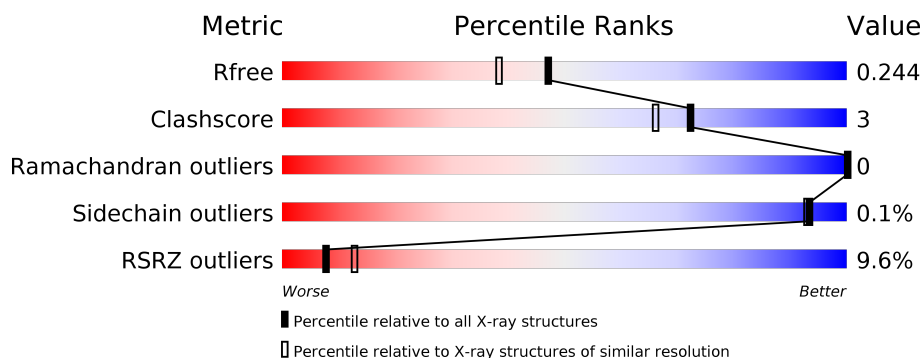
1 Overall quality at a glance

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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 on 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	<div> <div>10%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	B	507	<div> <div>7%</div> <div>93%</div> <div>7%</div> </div>
1	C	507	<div> <div>9%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	D	507	<div> <div>11%</div> <div>84%</div> <div>11%</div> <div>.</div> </div>

2 Entry composition [i](#)

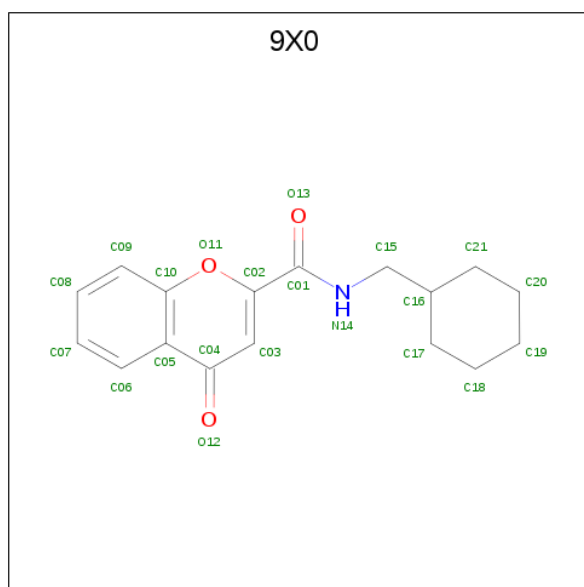
There are 7 unique types of molecules in this entry. The entry contains 16521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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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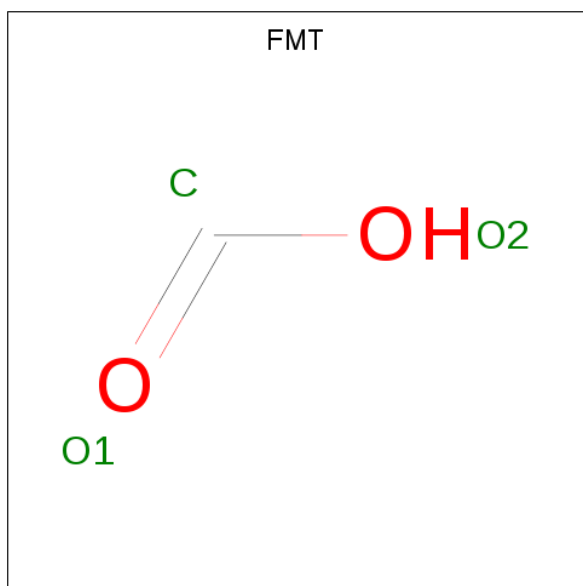
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			21	17	1	3		
2	D	1	Total	C	N	O	0	0
			21	17	1	3		

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



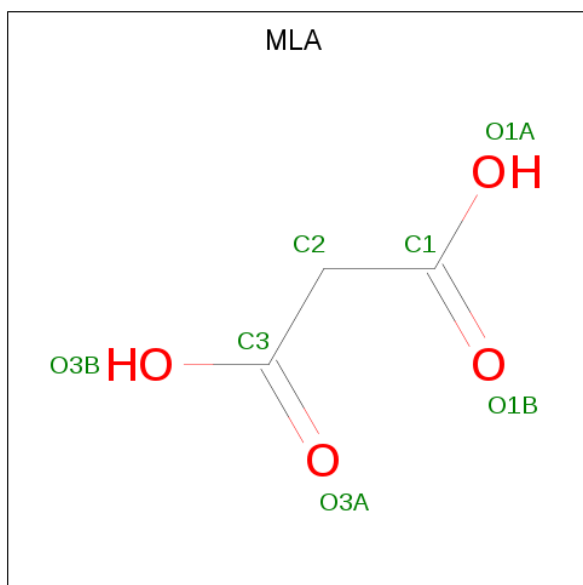
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		

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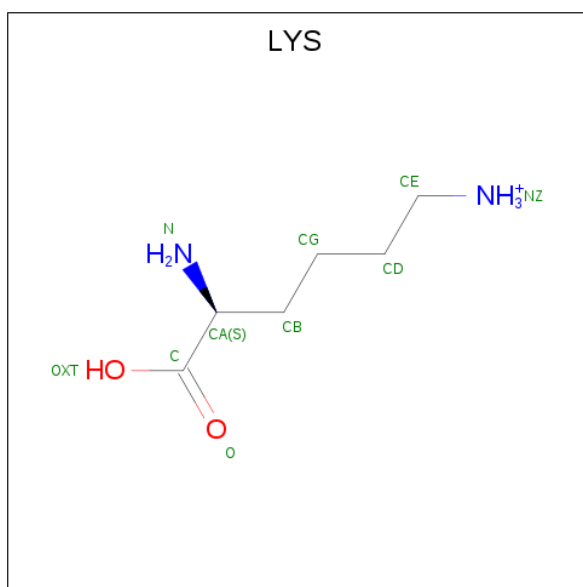
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is MALONIC ACID (three-letter code: 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 (three-letter code: 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		

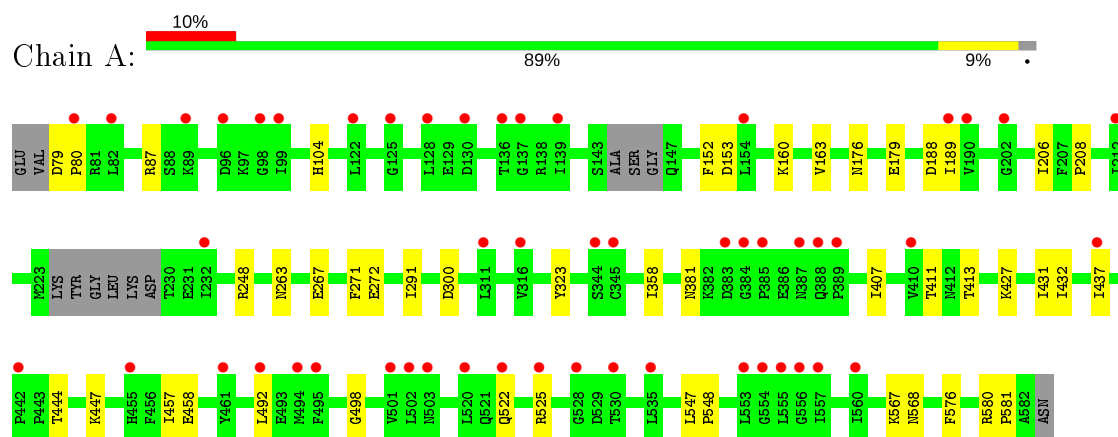
- Molecule 7 is water.

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		

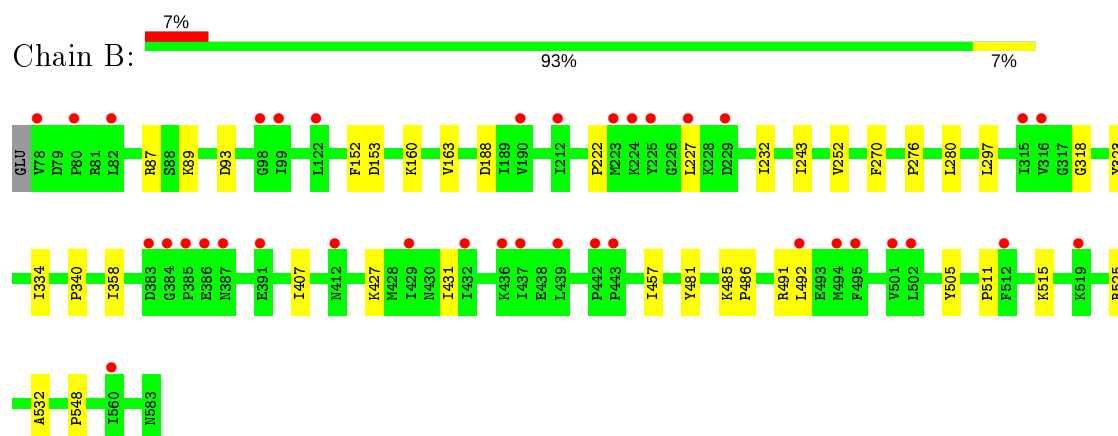
3 Residue-property plots [i](#)

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.

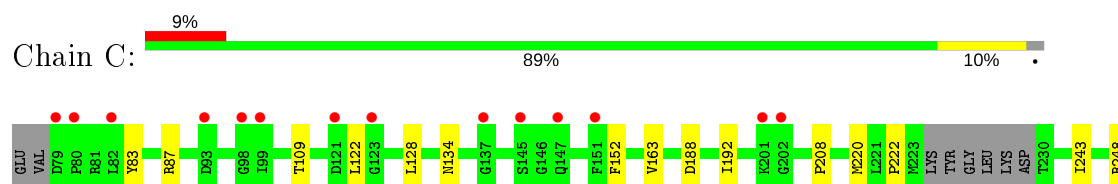
• Molecule 1: Lysine–tRNA ligase

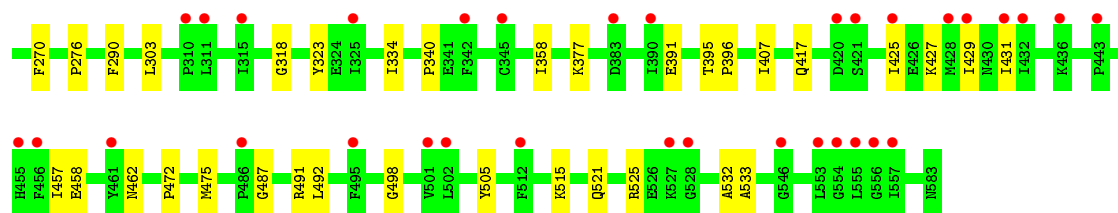


• Molecule 1: Lysine–tRNA ligase

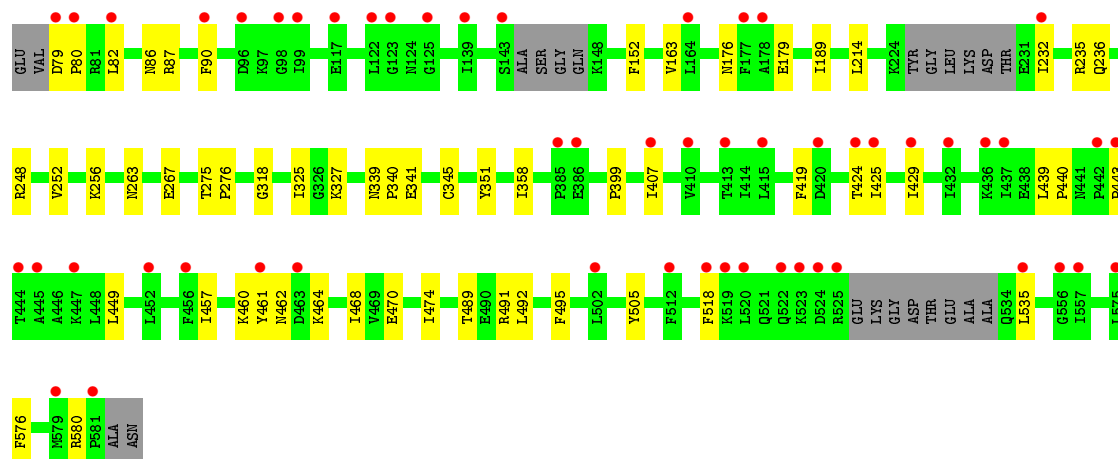
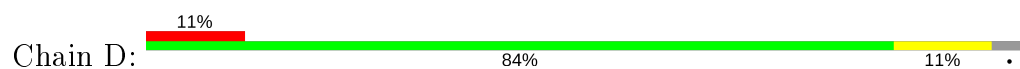


• Molecule 1: Lysine–tRNA ligase





● 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 0.207 , 0.244	Depositor DCC
R_{free} test set	8375 reflections (5.02%)	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 , 51.4	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	0.95	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/4072	0.57	0/5518
1	B	0.44	0/4163	0.57	0/5632
1	C	0.43	0/4082	0.55	0/5531
1	D	0.45	0/3930	0.58	0/5329
All	All	0.44	0/16247	0.57	0/22010

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 [i](#)

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	30	0
1	B	4058	0	3978	23	0
1	C	3966	0	3822	28	0
1	D	3833	0	3682	34	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	105	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 3.

All (105) 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: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:HA	1:A:522:GLN:NE2	2.23	0.54
1:C:192:ILE:HG23	1:C:208:PRO:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:153:ASP:HB3	1:B:160:LYS:HD2	1.92	0.52
1:B:152:PHE:HB2	1:B:163:VAL:HB	1.91	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:D:449:LEU:HD12	1:D:474:ILE:HD11	1.93	0.50
1:B:491:ARG:HA	1:B:505:TYR:HB3	1.94	0.50
1:A:432:ILE:HG12	1:A:437:ILE:HD11	1.94	0.50
1:A:104[A]:HIS:HE1	1:B:481:TYR:O	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:377:LYS:HD3	1:C:391[B]:GLU:CD	2.41	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ILE:HG22	1:D:214:LEU:HB2	2.03	0.40
1:D:82:LEU:HA	1:D:82:LEU:HD23	1.66	0.40
1:A:567:LYS:HD3	1:A:567:LYS:HA	1.93	0.40
1:A:79:ASP:HA	1:A:80:PRO:HD2	1.72	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 [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	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 [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	423/457 (93%)	423 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	436/457 (95%)	436 (100%)	0	100	100
1	C	416/457 (91%)	415 (100%)	1 (0%)	93	93
1	D	401/457 (88%)	400 (100%)	1 (0%)	93	93
All	All	1676/1828 (92%)	1674 (100%)	2 (0%)	93	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	462	ASN
1	D	462	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
4	FMT	A	603	-	0,2,2	0.00	-	0,1,1	0.00	-
2	9X0	A	601	-	20,23,23	2.12	6 (30%)	20,31,31	1.83	6 (30%)
6	LYS	C	606	-	5,9,9	0.36	0	4,10,10	0.47	0
4	FMT	C	605	-	0,2,2	0.00	-	0,1,1	0.00	-
2	9X0	D	601	-	20,23,23	1.99	5 (25%)	20,31,31	1.70	3 (15%)
5	MLA	D	603	-	0,6,6	0.00	-	0,7,7	0.00	-
5	MLA	A	606	-	0,6,6	0.00	-	0,7,7	0.00	-
2	9X0	C	601	-	20,23,23	1.94	4 (20%)	20,31,31	1.48	4 (20%)
6	LYS	A	607	-	5,9,9	0.46	0	4,10,10	0.29	0
4	FMT	A	605	-	0,2,2	0.00	-	0,1,1	0.00	-
6	LYS	B	603	-	5,9,9	0.54	0	4,10,10	0.39	0
4	FMT	A	604	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	604	-	0,2,2	0.00	-	0,1,1	0.00	-
2	9X0	B	601	-	20,23,23	1.75	3 (15%)	20,31,31	1.61	4 (20%)
6	LYS	D	604	-	5,9,9	0.37	0	4,10,10	0.42	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	9X0	A	601	-	-	0/7/17/17	0/3/3/3
6	LYS	C	606	-	-	0/5/9/9	-
6	LYS	B	603	-	-	1/5/9/9	-
2	9X0	D	601	-	-	0/7/17/17	0/3/3/3
5	MLA	D	603	-	-	0/0/4/4	-
5	MLA	A	606	-	-	0/0/4/4	-
2	9X0	C	601	-	-	0/7/17/17	0/3/3/3
6	LYS	A	607	-	-	1/5/9/9	-
2	9X0	B	601	-	-	0/7/17/17	0/3/3/3
6	LYS	D	604	-	-	0/5/9/9	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	9X0	C02-C01	-6.20	1.40	1.49
2	A	601	9X0	C02-C01	-5.88	1.40	1.49
2	C	601	9X0	C02-C01	-5.72	1.41	1.49
2	B	601	9X0	C02-C01	-5.48	1.41	1.49
2	A	601	9X0	C05-C10	-3.44	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	9X0	O11-C10	-3.24	1.31	1.36
2	D	601	9X0	O11-C10	-3.17	1.31	1.36
2	C	601	9X0	C05-C10	-3.15	1.37	1.41
2	D	601	9X0	C05-C10	-2.88	1.37	1.41
2	C	601	9X0	O11-C10	-2.81	1.31	1.36
2	C	601	9X0	C20-C21	-2.70	1.46	1.53
2	A	601	9X0	C17-C16	-2.61	1.45	1.52
2	B	601	9X0	C05-C10	-2.44	1.38	1.41
2	A	601	9X0	C06-C05	-2.40	1.36	1.41
2	D	601	9X0	C06-C05	-2.39	1.36	1.41
2	A	601	9X0	C18-C17	-2.38	1.46	1.53
2	D	601	9X0	C20-C21	-2.26	1.47	1.53
2	B	601	9X0	C18-C17	-2.23	1.47	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	9X0	C03-C04-C05	-4.78	117.76	123.05
2	B	601	9X0	C03-C04-C05	-4.71	117.83	123.05
2	A	601	9X0	C03-C04-C05	-4.34	118.25	123.05
2	A	601	9X0	C16-C15-N14	-3.90	105.38	112.73
2	C	601	9X0	C03-C04-C05	-3.71	118.94	123.05
2	D	601	9X0	C16-C15-N14	-3.52	106.10	112.73
2	A	601	9X0	C18-C17-C16	-3.01	106.47	112.15
2	C	601	9X0	C16-C15-N14	-2.92	107.22	112.73
2	C	601	9X0	C15-N14-C01	2.62	127.24	122.33
2	B	601	9X0	C16-C15-N14	-2.51	108.00	112.73
2	D	601	9X0	C02-C01-N14	2.50	119.08	115.59
2	B	601	9X0	C15-N14-C01	2.43	126.89	122.33
2	B	601	9X0	C02-C01-N14	2.35	118.87	115.59
2	A	601	9X0	C15-N14-C01	2.34	126.72	122.33
2	C	601	9X0	O11-C10-C05	-2.32	118.96	121.20
2	A	601	9X0	O11-C10-C05	-2.18	119.09	121.20
2	A	601	9X0	C02-C01-N14	2.01	118.40	115.59

There are no chirality outliers.

All (2) torsion outliers are listed below:

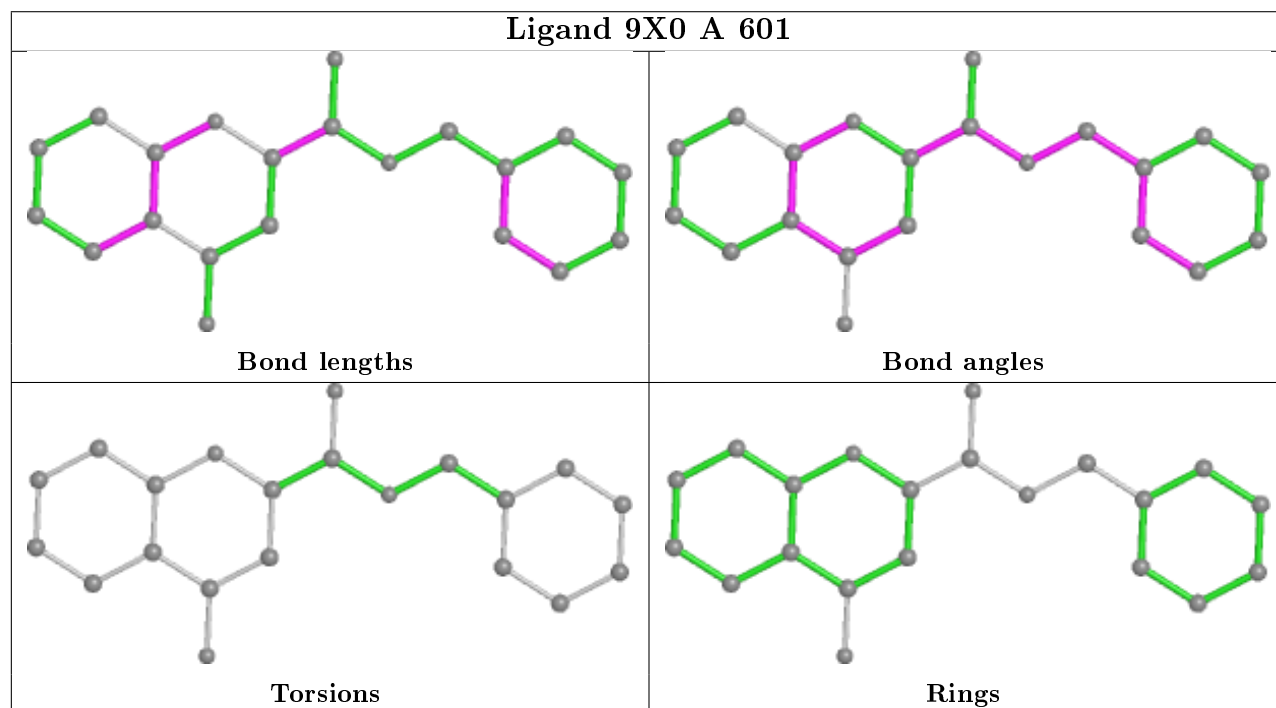
Mol	Chain	Res	Type	Atoms
6	B	603	LYS	CG-CD-CE-NZ
6	A	607	LYS	CG-CD-CE-NZ

There are no ring outliers.

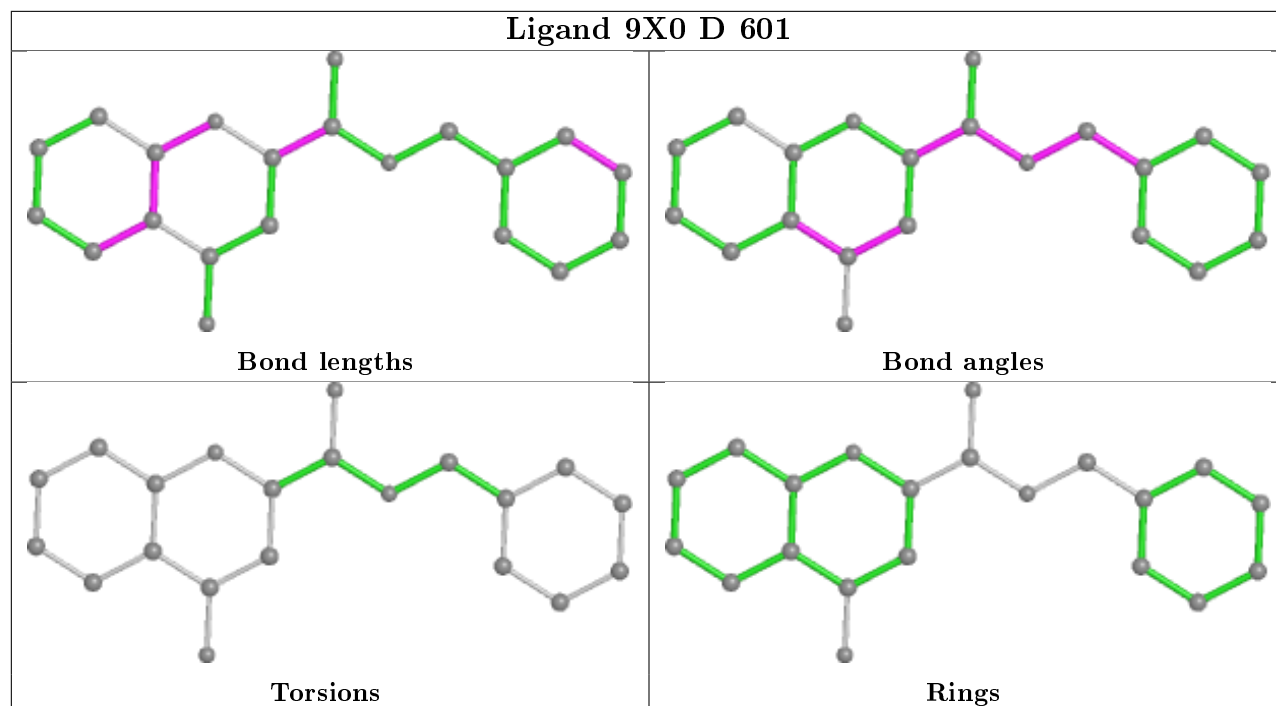
1 monomer is involved in 1 short contact:

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

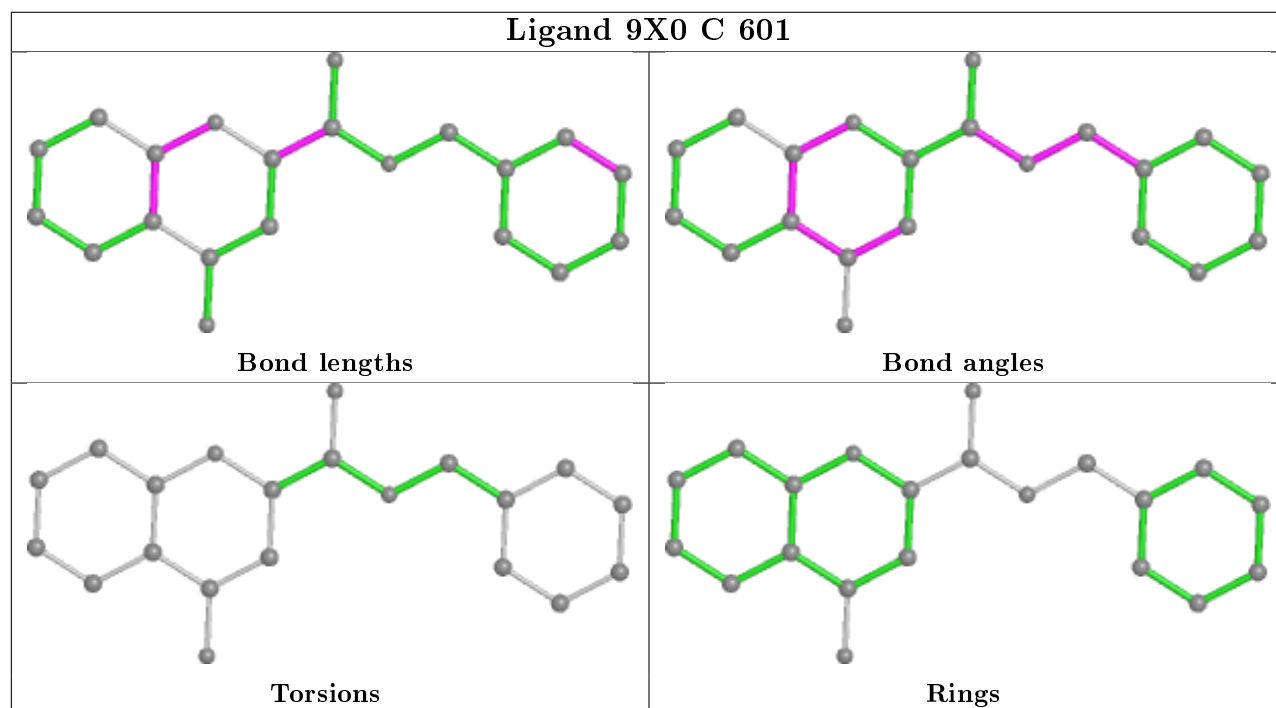
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

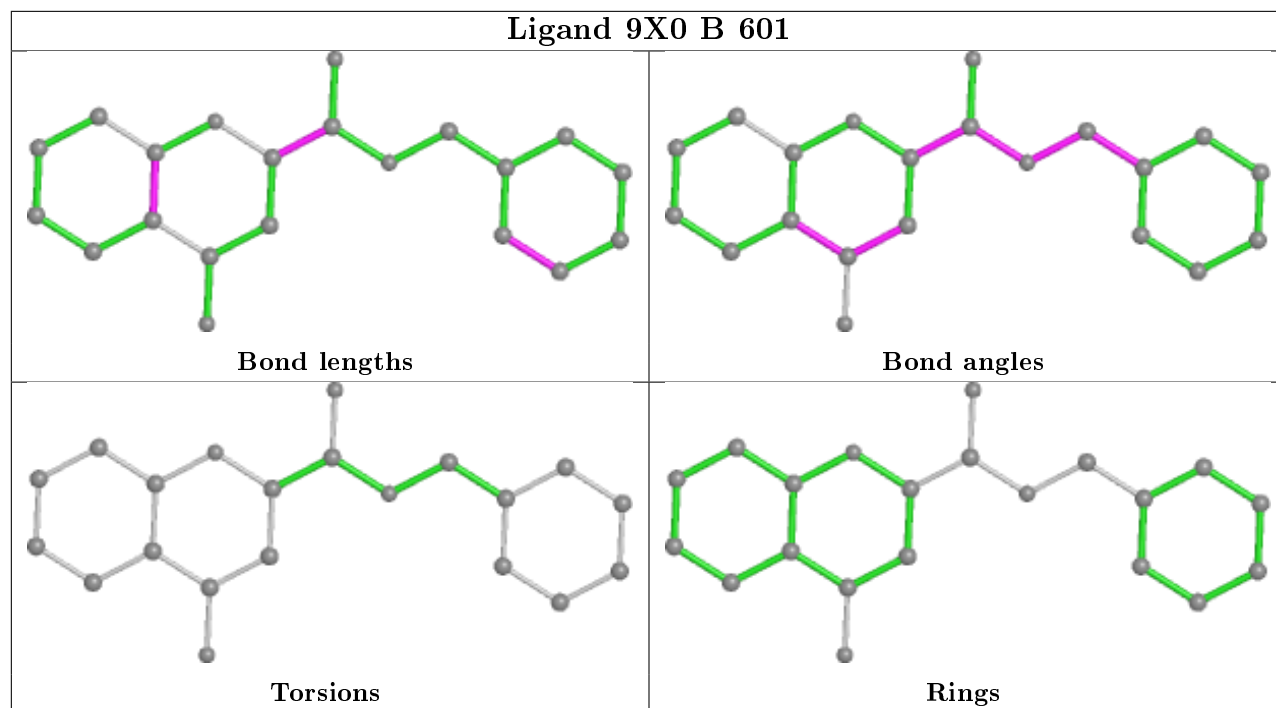


Ligand 9X0 D 601



Ligand 9X0 C 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.55	52 (10%) 6 10	20, 39, 74, 101	0
1	B	506/507 (99%)	0.51	37 (7%) 15 23	22, 39, 67, 108	0
1	C	499/507 (98%)	0.63	47 (9%) 8 13	23, 44, 79, 97	0
1	D	485/507 (95%)	0.66	54 (11%) 5 8	23, 45, 83, 106	0
All	All	1985/2028 (97%)	0.59	190 (9%) 8 13	20, 42, 79, 108	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	TYR	8.4
1	D	432	ILE	5.3
1	D	82	LEU	5.0
1	B	384	GLY	5.0
1	A	385	PRO	4.8
1	D	385	PRO	4.8
1	D	436	LYS	4.7
1	C	82	LEU	4.7
1	D	98	GLY	4.7
1	D	442	PRO	4.6
1	C	98	GLY	4.5
1	A	528	GLY	4.4
1	A	383	ASP	4.4
1	A	82	LEU	4.4
1	C	502	LEU	4.3
1	B	385	PRO	4.3
1	C	123	GLY	4.3
1	B	432	ILE	4.3
1	C	121[A]	ASP	4.2
1	D	456	PHE	4.1
1	B	82	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	425	ILE	4.0
1	D	535	LEU	4.0
1	A	520	LEU	4.0
1	C	555	LEU	4.0
1	A	502	LEU	3.9
1	A	437	ILE	3.8
1	C	80	PRO	3.8
1	B	78	VAL	3.8
1	A	555	LEU	3.8
1	B	229	ASP	3.7
1	D	424	THR	3.7
1	D	80	PRO	3.7
1	D	96	ASP	3.5
1	C	147	GLN	3.5
1	A	122	LEU	3.4
1	A	345	CYS	3.4
1	C	501	VAL	3.4
1	A	455	HIS	3.4
1	A	501	VAL	3.4
1	B	437	ILE	3.4
1	C	432	ILE	3.4
1	D	429	ILE	3.4
1	D	522	GLN	3.3
1	D	444	THR	3.3
1	C	431	ILE	3.3
1	D	232	ILE	3.3
1	A	535	LEU	3.3
1	B	99	ILE	3.2
1	B	315	ILE	3.2
1	D	437	ILE	3.1
1	D	139	ILE	3.1
1	B	386	GLU	3.1
1	D	461	TYR	3.1
1	A	189	ILE	3.0
1	C	512	PHE	3.0
1	A	461	TYR	3.0
1	B	519	LYS	3.0
1	C	456	PHE	2.9
1	B	122	LEU	2.9
1	D	407	ILE	2.9
1	A	554	GLY	2.9
1	B	227	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	145	SER	2.9
1	C	345	CYS	2.9
1	A	128	LEU	2.9
1	A	556	GLY	2.9
1	D	164	LEU	2.8
1	B	224	LYS	2.8
1	C	486	PRO	2.8
1	C	201	LYS	2.8
1	B	495	PHE	2.8
1	C	461	TYR	2.8
1	A	96	ASP	2.7
1	C	429	ILE	2.7
1	C	383	ASP	2.7
1	D	122	LEU	2.7
1	D	123	GLY	2.7
1	D	447	LYS	2.7
1	C	553	LEU	2.7
1	A	389	PRO	2.7
1	D	581	PRO	2.7
1	D	90	PHE	2.6
1	D	410	VAL	2.6
1	A	154	LEU	2.6
1	C	425	ILE	2.6
1	C	557	ILE	2.6
1	B	316	VAL	2.6
1	B	429	ILE	2.6
1	B	443	PRO	2.6
1	A	492	LEU	2.6
1	D	386	GLU	2.6
1	B	190	VAL	2.6
1	D	177	PHE	2.6
1	C	79	ASP	2.6
1	A	525	ARG	2.6
1	A	202	GLY	2.6
1	C	202	GLY	2.6
1	C	421	SER	2.5
1	A	442	PRO	2.5
1	D	463	ASP	2.5
1	A	232	ILE	2.5
1	D	556	GLY	2.5
1	A	137	GLY	2.5
1	D	557	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	503	ASN	2.5
1	D	79	ASP	2.5
1	B	512	PHE	2.5
1	C	528	GLY	2.5
1	A	80	PRO	2.5
1	C	151	PHE	2.5
1	C	428	MET	2.5
1	D	520	LEU	2.5
1	A	522	GLN	2.5
1	B	436	LYS	2.5
1	D	413	THR	2.5
1	B	98	GLY	2.4
1	C	527	LYS	2.4
1	A	410	VAL	2.4
1	C	455	HIS	2.4
1	B	560	ILE	2.4
1	C	311	LEU	2.4
1	D	525	ARG	2.4
1	C	443	PRO	2.4
1	B	223	MET	2.4
1	D	178	ALA	2.4
1	D	579	MET	2.4
1	C	315	ILE	2.4
1	B	502	LEU	2.4
1	D	512	PHE	2.4
1	D	524	ASP	2.4
1	B	492	LEU	2.3
1	D	445	ALA	2.3
1	A	495	PHE	2.3
1	A	125	GLY	2.3
1	A	388	GLN	2.3
1	C	93	ASP	2.3
1	C	420	ASP	2.3
1	A	560	ILE	2.3
1	A	89	LYS	2.3
1	D	420	ASP	2.3
1	A	136	THR	2.3
1	B	442	PRO	2.3
1	D	415	LEU	2.3
1	A	98	GLY	2.3
1	B	387	ASN	2.2
1	B	501	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	139	ILE	2.2
1	A	557	ILE	2.2
1	D	452	LEU	2.2
1	A	384	GLY	2.2
1	C	556	GLY	2.2
1	C	436	LYS	2.2
1	D	523	LYS	2.2
1	D	443	PRO	2.2
1	C	554	GLY	2.2
1	A	387	ASN	2.2
1	D	518	PHE	2.2
1	D	575	LEU	2.2
1	A	494	MET	2.2
1	B	212	ILE	2.2
1	B	412	ASN	2.2
1	C	342	PHE	2.2
1	C	99	ILE	2.1
1	C	495	PHE	2.1
1	A	130	ASP	2.1
1	B	383	ASP	2.1
1	D	125	GLY	2.1
1	A	311	LEU	2.1
1	A	212	ILE	2.1
1	B	391	GLU	2.1
1	A	344	SER	2.1
1	D	143	SER	2.1
1	B	80	PRO	2.1
1	C	137	GLY	2.1
1	A	99	ILE	2.1
1	C	390	ILE	2.1
1	A	530	THR	2.1
1	B	494	MET	2.1
1	A	316	VAL	2.1
1	D	502	LEU	2.1
1	C	546	GLY	2.1
1	D	519	LYS	2.1
1	A	190	VAL	2.0
1	A	553	LEU	2.0
1	C	325	ILE	2.0
1	D	99	ILE	2.0
1	C	310	PRO	2.0
1	B	439	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	117	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

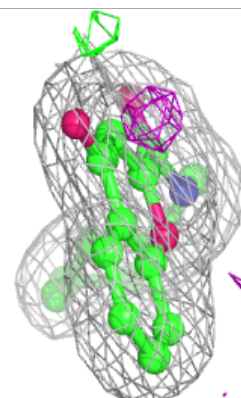
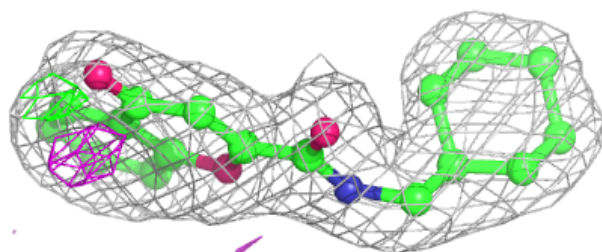
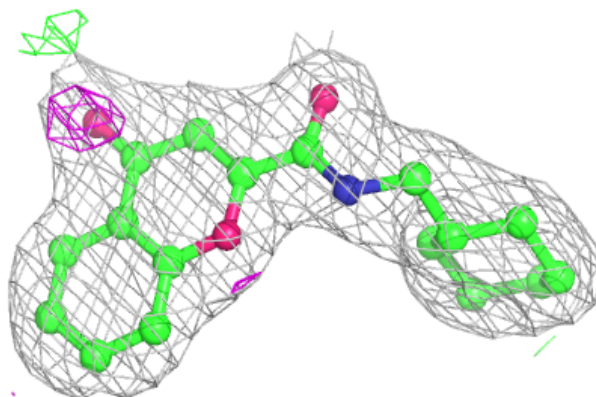
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CO	C	602	1/1	0.71	0.15	80,80,80,80	1
5	MLA	D	603	7/7	0.79	0.20	41,50,52,62	7
5	MLA	A	606	7/7	0.84	0.16	41,44,48,49	0
4	FMT	A	605	3/3	0.88	0.16	45,45,46,50	0
4	FMT	C	604	3/3	0.88	0.13	47,47,47,53	0
4	FMT	A	603	3/3	0.89	0.16	35,35,39,42	0
2	9X0	B	601	21/21	0.92	0.17	25,31,33,38	0
3	CO	D	602	1/1	0.92	0.13	67,67,67,67	1
6	LYS	D	604	10/10	0.92	0.19	28,33,42,43	0
4	FMT	C	605	3/3	0.93	0.30	32,32,34,39	3
4	FMT	A	604	3/3	0.93	0.15	40,40,49,58	0
2	9X0	D	601	21/21	0.95	0.18	30,33,37,38	0
2	9X0	C	601	21/21	0.95	0.19	27,30,35,36	0
6	LYS	A	607	10/10	0.95	0.23	23,27,31,35	0
6	LYS	C	606	10/10	0.95	0.28	25,28,34,35	0
2	9X0	A	601	21/21	0.95	0.20	26,31,35,42	0
6	LYS	B	603	10/10	0.96	0.15	24,28,35,36	0
3	CO	B	602	1/1	0.97	0.10	53,53,53,53	1
3	CO	C	603	1/1	0.98	0.09	66,66,66,66	0
3	CO	A	602	1/1	0.99	0.10	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.

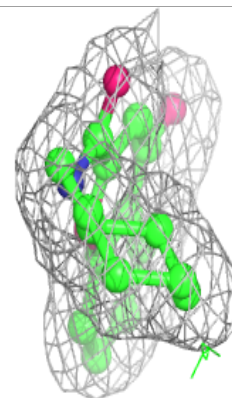
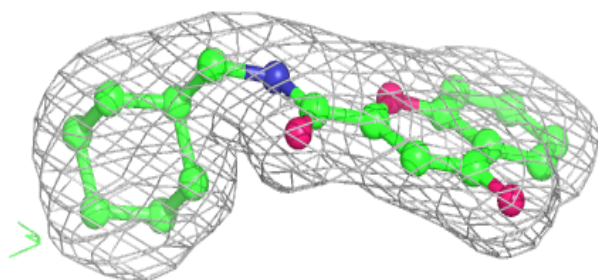
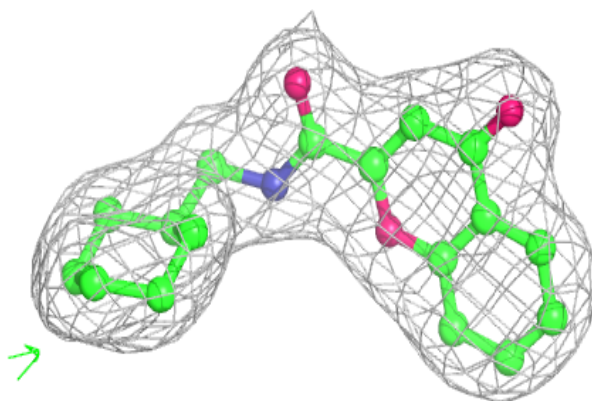
Electron density around 9X0 B 601:

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

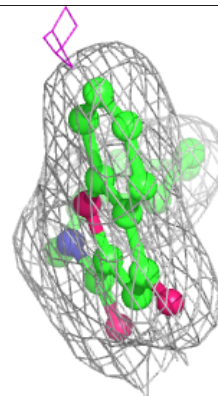
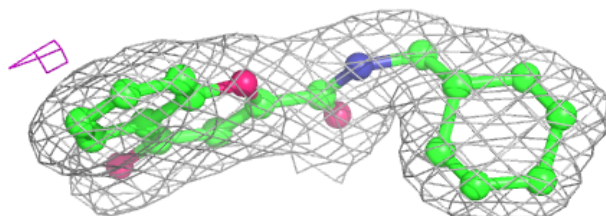
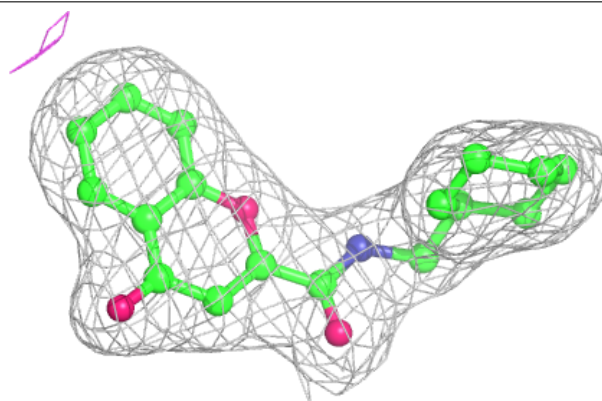


Electron density around 9X0 D 601:

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

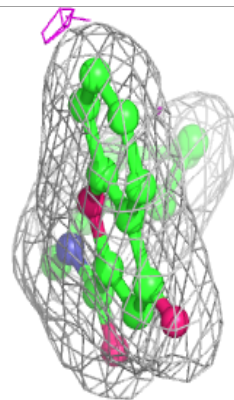
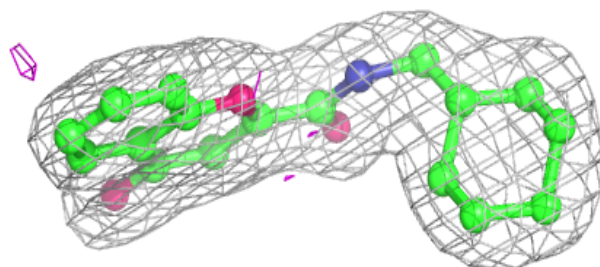
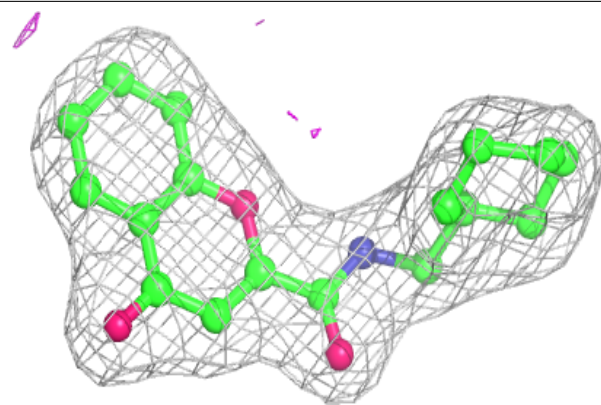
**Electron density around 9X0 C 601:**

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



Electron density around 9X0 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.