



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:35 PM UTC

PDB ID : 6KA6 / pdb_00006ka6
Title : Crystal structure of plasmodium lysyl-tRNA synthetase in complex with a cladosporin derivative 1
Authors : Zhou, J.; Fang, P.
Deposited on : 2019-06-21
Resolution : 1.89 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

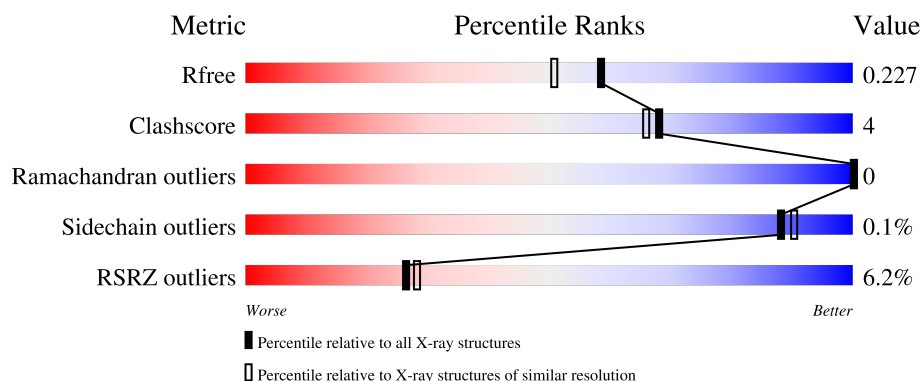
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	516	5% 89% 6% 6%
1	B	516	7% 89% 9% .
1	C	516	8% 84% 10% 6%
1	D	516	5% 88% 9% .

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
3	GOL	B	603	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17294 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	487	Total	C	N	O	S	0	1	0
			3872	2500	643	712	17			
1	B	504	Total	C	N	O	S	0	0	0
			3972	2558	662	735	17			
1	C	486	Total	C	N	O	S	0	0	0
			3847	2482	638	710	17			
1	D	501	Total	C	N	O	S	0	0	0
			3954	2547	657	734	16			

There are 36 discrepancies between the modelled and reference sequences:

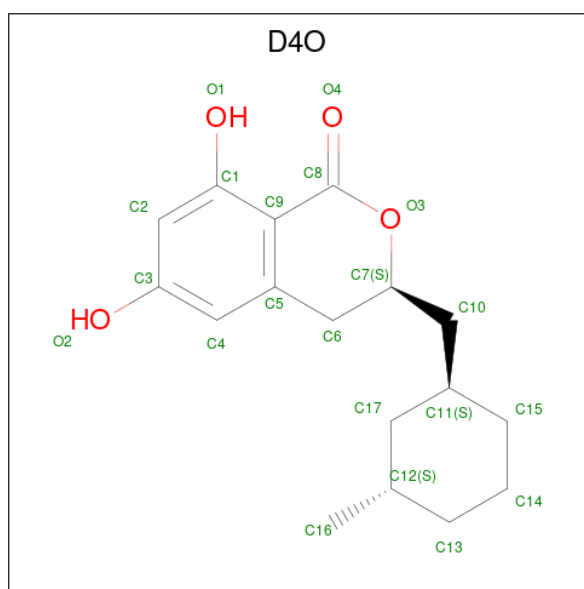
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	initiating methionine	UNP W7JP72
A	584	GLY	-	expression tag	UNP W7JP72
A	585	GLY	-	expression tag	UNP W7JP72
A	586	HIS	-	expression tag	UNP W7JP72
A	587	HIS	-	expression tag	UNP W7JP72
A	588	HIS	-	expression tag	UNP W7JP72
A	589	HIS	-	expression tag	UNP W7JP72
A	590	HIS	-	expression tag	UNP W7JP72
A	591	HIS	-	expression tag	UNP W7JP72
B	76	MET	-	initiating methionine	UNP W7JP72
B	584	GLY	-	expression tag	UNP W7JP72
B	585	GLY	-	expression tag	UNP W7JP72
B	586	HIS	-	expression tag	UNP W7JP72
B	587	HIS	-	expression tag	UNP W7JP72
B	588	HIS	-	expression tag	UNP W7JP72
B	589	HIS	-	expression tag	UNP W7JP72
B	590	HIS	-	expression tag	UNP W7JP72
B	591	HIS	-	expression tag	UNP W7JP72
C	76	MET	-	initiating methionine	UNP W7JP72
C	584	GLY	-	expression tag	UNP W7JP72
C	585	GLY	-	expression tag	UNP W7JP72

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Chain	Residue	Modelled	Actual	Comment	Reference
C	586	HIS	-	expression tag	UNP W7JP72
C	587	HIS	-	expression tag	UNP W7JP72
C	588	HIS	-	expression tag	UNP W7JP72
C	589	HIS	-	expression tag	UNP W7JP72
C	590	HIS	-	expression tag	UNP W7JP72
C	591	HIS	-	expression tag	UNP W7JP72
D	76	MET	-	initiating methionine	UNP W7JP72
D	584	GLY	-	expression tag	UNP W7JP72
D	585	GLY	-	expression tag	UNP W7JP72
D	586	HIS	-	expression tag	UNP W7JP72
D	587	HIS	-	expression tag	UNP W7JP72
D	588	HIS	-	expression tag	UNP W7JP72
D	589	HIS	-	expression tag	UNP W7JP72
D	590	HIS	-	expression tag	UNP W7JP72
D	591	HIS	-	expression tag	UNP W7JP72

- Molecule 2 is (3 {S})-3-[[[(1 {S}),3 {S})-3-methylcyclohexyl]methyl]-6,8-bis(oxidanyl)-3,4-dihydroisochromen-1-one (CCD ID: D4O) (formula: C₁₇H₂₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	17	4		
2	B	1	Total	C	O	0	0
			21	17	4		
2	C	1	Total	C	O	0	0
			21	17	4		

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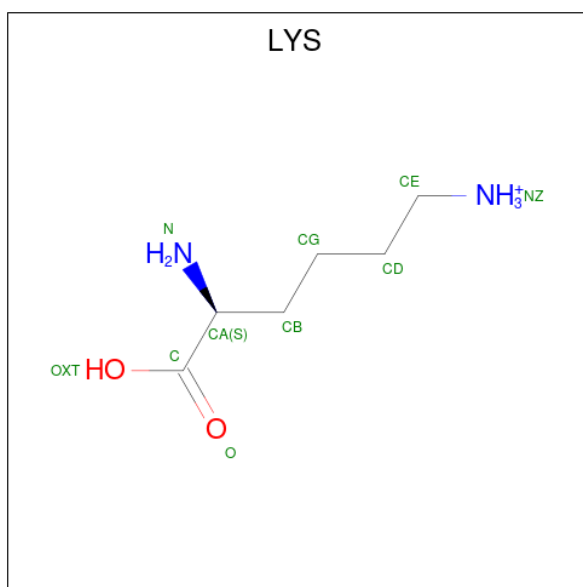
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			21	17	4		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



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

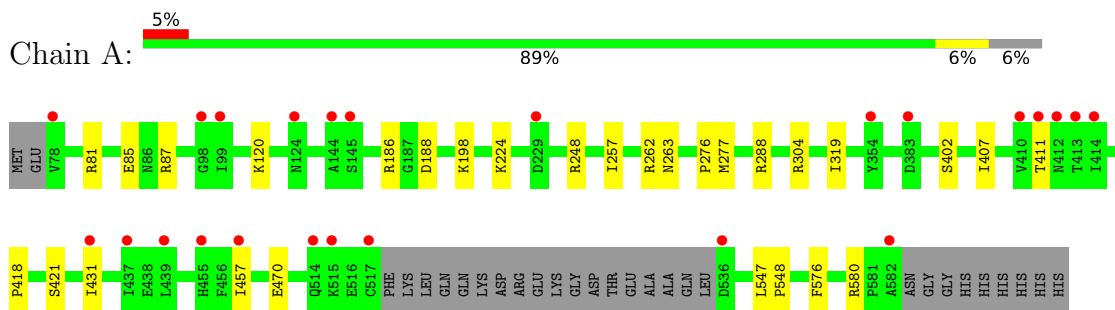
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	391	Total	O	0	0
			391	391		
5	B	391	Total	O	0	0
			391	391		
5	C	332	Total	O	0	0
			332	332		
5	D	387	Total	O	0	0
			387	387		

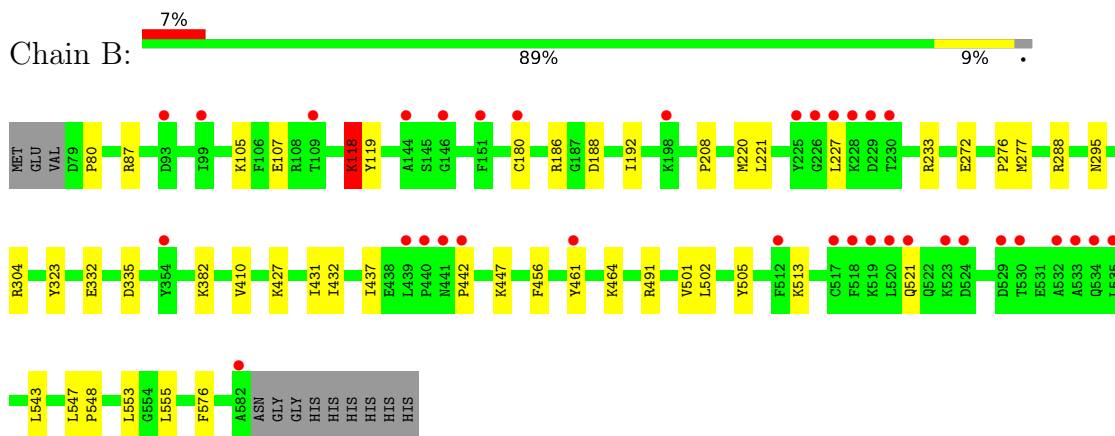
3 Residue-property plots [i](#)

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.

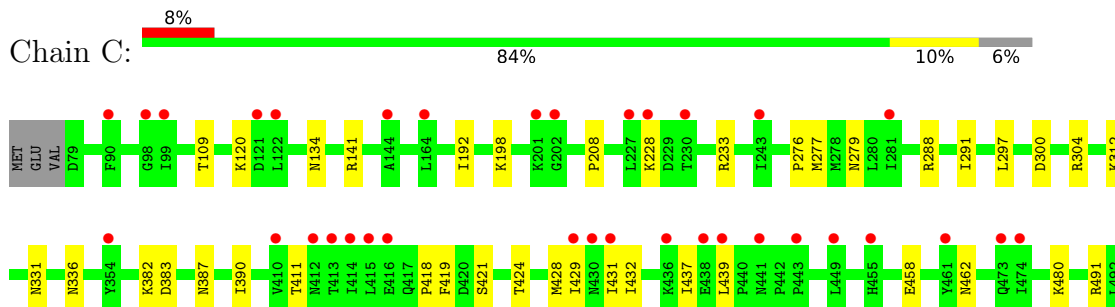
• Molecule 1: Lysine-tRNA ligase

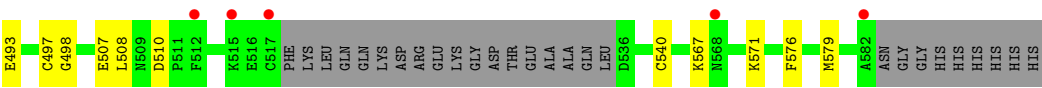


• Molecule 1: Lysine-tRNA ligase

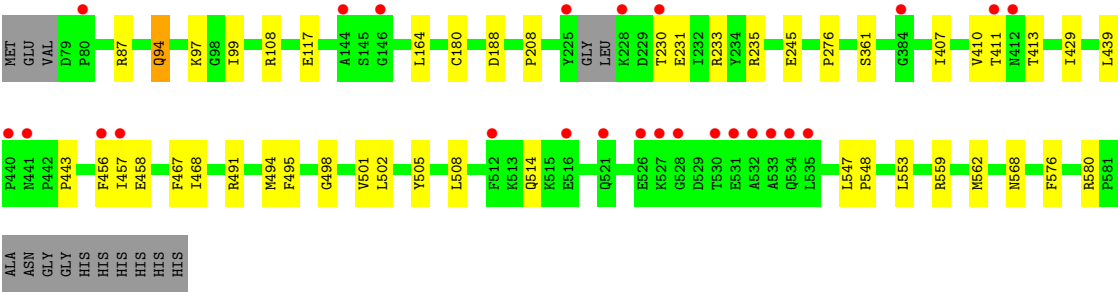
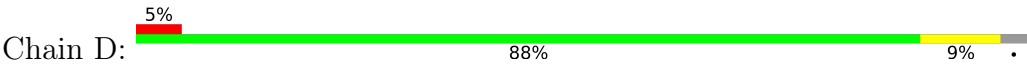


• Molecule 1: Lysine-tRNA ligase





● 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	71.48Å 90.20Å 100.72Å 76.70° 72.91° 80.03°	Depositor
Resolution (Å)	32.60 – 1.89 32.60 – 1.89	Depositor EDS
% Data completeness (in resolution range)	88.5 (32.60-1.89) 88.6 (32.60-1.89)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.191 , 0.227 0.192 , 0.227	Depositor DCC
R_{free} test set	8289 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17294	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: GOL, D4O

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	0.35	3/3972 (0.1%)	0.46	0/5385
1	B	0.38	5/4071 (0.1%)	0.51	4/5523 (0.1%)
1	C	0.30	0/3944	0.45	0/5349
1	D	0.33	2/4052 (0.0%)	0.48	1/5495 (0.0%)
All	All	0.34	10/16039 (0.1%)	0.48	5/21752 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	CYS	CA-C	7.62	1.62	1.52
1	B	382	LYS	C-O	-6.80	1.16	1.24
1	B	335	ASP	C-O	6.55	1.28	1.24
1	A	319[A]	ILE	CA-C	6.53	1.61	1.52
1	A	319[B]	ILE	CA-C	6.53	1.61	1.52
1	B	543	LEU	C-O	-5.82	1.16	1.24
1	B	501	VAL	C-O	-5.33	1.17	1.24
1	D	501	VAL	C-O	-5.25	1.18	1.24
1	D	117	GLU	C-O	-5.23	1.18	1.24
1	A	257	ILE	C-O	-5.14	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	CYS	CA-C-O	8.47	129.53	120.55
1	B	180	CYS	N-CA-C	7.52	119.47	111.28
1	D	501	VAL	CB-CA-C	-6.34	103.77	110.62
1	B	118	LYS	N-CA-C	5.95	117.84	111.36
1	B	501	VAL	CB-CA-C	-5.52	104.66	110.62

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	3872	0	3744	19	0
1	B	3972	0	3806	29	0
1	C	3847	0	3688	34	0
1	D	3954	0	3789	36	0
2	A	21	0	0	0	0
2	B	21	0	0	1	0
2	C	21	0	0	0	0
2	D	21	0	0	0	0
3	A	6	0	8	0	0
3	B	12	0	16	1	0
3	D	6	0	8	0	0
4	A	10	0	12	0	0
4	B	10	0	12	0	0
4	C	10	0	12	0	0
4	D	10	0	12	0	0
5	A	391	0	0	6	0
5	B	391	0	0	6	0
5	C	332	0	0	7	0
5	D	387	0	0	4	0
All	All	17294	0	15107	112	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 (112) 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:521:GLN:HG3	5:B:1007:HOH:O	1.61	1.00
1:C:540:CYS:SG	5:C:938:HOH:O	2.28	0.92
1:D:559:ARG:HA	1:D:562:MET:HE3	1.52	0.88
1:D:233:ARG:HH11	1:D:233:ARG:CB	1.99	0.76
1:D:411:THR:HG23	1:D:413:THR:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:THR:HG21	1:C:431:ILE:HD11	1.71	0.71
1:B:432:ILE:HG23	1:B:437:ILE:HB	1.73	0.70
1:D:429:ILE:HD13	1:D:439:LEU:HD11	1.74	0.69
1:C:336:ASN:ND2	5:C:702:HOH:O	2.25	0.69
1:D:233:ARG:HH11	1:D:233:ARG:HB2	1.56	0.69
1:D:233:ARG:HB2	1:D:233:ARG:NH1	2.10	0.66
1:A:262:ARG:HH12	3:B:602:GOL:H31	1.62	0.65
1:D:407:ILE:HG13	1:D:457:ILE:HD11	1.78	0.65
1:D:410:VAL:HG21	1:D:456:PHE:HB3	1.79	0.64
1:A:186:ARG:NH1	5:A:706:HOH:O	2.28	0.63
1:B:87:ARG:NH2	1:B:188:ASP:OD1	2.32	0.63
1:C:383:ASP:O	1:C:387:ASN:ND2	2.32	0.62
1:C:276:PRO:HG3	1:D:576:PHE:HB2	1.82	0.62
1:A:224:LYS:NZ	5:A:707:HOH:O	2.29	0.62
1:C:288:ARG:NH1	5:C:711:HOH:O	2.33	0.61
1:A:407:ILE:HG13	1:A:457:ILE:HD11	1.82	0.60
1:C:432:ILE:HG23	1:C:437:ILE:HB	1.84	0.60
1:D:230:THR:HG22	1:D:231:GLU:H	1.68	0.58
1:B:233:ARG:NH1	5:B:709:HOH:O	2.31	0.58
1:C:228:LYS:O	1:C:233:ARG:NH1	2.35	0.58
1:C:291:ILE:HD11	1:C:300:ASP:HB3	1.84	0.57
1:C:120:LYS:O	1:C:198:LYS:NZ	2.37	0.57
1:B:288:ARG:NH1	5:B:712:HOH:O	2.37	0.57
1:D:87:ARG:NH2	1:D:188:ASP:OD1	2.38	0.57
1:A:81:ARG:O	1:A:85:GLU:HG3	2.04	0.57
1:B:332:GLU:OE1	2:B:601:D4O:O2	2.23	0.57
1:D:233:ARG:HD2	5:D:774:HOH:O	2.05	0.57
1:C:141:ARG:NH1	5:C:715:HOH:O	2.36	0.57
1:D:235:ARG:NH1	1:D:580:ARG:O	2.26	0.56
1:A:87:ARG:NH2	1:A:188:ASP:OD1	2.40	0.54
1:A:418:PRO:HG2	1:A:421:SER:HB3	1.89	0.54
1:A:402:SER:OG	1:A:470:GLU:OE1	2.26	0.53
1:B:233:ARG:NH2	5:B:716:HOH:O	2.42	0.53
1:A:263:ASN:HB2	5:A:1022:HOH:O	2.09	0.53
1:B:192:ILE:HG23	1:B:208:PRO:HB3	1.90	0.53
1:A:576:PHE:HB2	1:B:276:PRO:HG3	1.91	0.52
1:B:513:LYS:NZ	5:B:718:HOH:O	2.43	0.52
1:D:502:LEU:HD11	1:D:553:LEU:HD11	1.92	0.51
1:B:491:ARG:HA	1:B:505:TYR:HB3	1.93	0.51
1:D:180:CYS:HB2	5:D:952:HOH:O	2.10	0.51
1:D:245:GLU:CD	1:D:245:GLU:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LYS:HD2	1:B:119:TYR:CZ	2.46	0.51
1:C:491:ARG:NH2	1:C:493:GLU:OE2	2.44	0.51
1:D:559:ARG:CA	1:D:562:MET:HE3	2.34	0.51
1:A:276:PRO:HG3	1:B:576:PHE:HB2	1.91	0.51
1:A:288:ARG:NH1	5:A:717:HOH:O	2.42	0.51
1:B:105:LYS:HE3	1:B:107:GLU:HG2	1.93	0.50
1:C:279:ASN:ND2	5:C:723:HOH:O	2.45	0.50
1:D:467:PHE:CZ	1:D:494:MET:HE2	2.47	0.50
1:C:390:ILE:HD11	1:C:497:CYS:SG	2.51	0.50
1:B:521:GLN:NE2	5:B:720:HOH:O	2.44	0.50
1:D:429:ILE:HD11	1:D:443:PRO:HB2	1.94	0.50
1:B:502:LEU:HD11	1:B:553:LEU:HD11	1.93	0.49
1:B:427:LYS:O	1:B:431:ILE:HG13	2.13	0.49
1:D:108:ARG:HD2	5:D:861:HOH:O	2.13	0.49
1:A:120:LYS:O	1:A:198:LYS:NZ	2.45	0.49
1:B:410:VAL:HG21	1:B:456:PHE:HB3	1.93	0.49
1:D:233:ARG:CB	1:D:233:ARG:NH1	2.71	0.48
1:C:109:THR:HG23	1:C:134:ASN:HB2	1.95	0.47
1:C:576:PHE:HB2	1:D:276:PRO:HG3	1.96	0.47
1:D:94:GLN:HG3	1:D:99:ILE:HB	1.96	0.47
1:B:502:LEU:HD12	1:B:555:LEU:HD21	1.96	0.47
1:C:428:MET:HA	1:C:431:ILE:HG22	1.96	0.47
1:D:97:LYS:HB3	1:D:97:LYS:HE2	1.76	0.47
1:A:288:ARG:HH11	1:B:295:ASN:HD21	1.60	0.47
1:D:411:THR:HG23	1:D:413:THR:HG23	1.97	0.47
1:D:547:LEU:HD12	1:D:548:PRO:HD2	1.96	0.47
1:A:580:ARG:NE	5:A:716:HOH:O	2.39	0.46
1:B:547:LEU:HD12	1:B:548:PRO:HD2	1.96	0.46
1:A:547:LEU:HD12	1:A:548:PRO:HD2	1.97	0.46
1:D:245:GLU:CD	1:D:245:GLU:N	2.73	0.46
1:D:361:SER:HB3	1:D:494:MET:HE3	1.97	0.46
1:C:480:LYS:HA	1:C:508:LEU:HD13	1.97	0.46
1:D:491:ARG:HA	1:D:505:TYR:HB3	1.98	0.45
1:B:461:TYR:CD1	1:B:464:LYS:HE2	2.51	0.45
1:A:248:ARG:NH2	5:A:701:HOH:O	2.23	0.45
1:D:468:ILE:HD12	1:D:495:PHE:CE1	2.52	0.45
1:D:568:ASN:ND2	5:D:714:HOH:O	2.46	0.45
1:B:227:LEU:HD22	1:B:233:ARG:HG2	1.99	0.45
1:C:419:PHE:HA	1:C:424:THR:HG21	1.99	0.45
1:D:233:ARG:HH11	1:D:233:ARG:HB3	1.78	0.44
1:A:411:THR:HB	1:A:431:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458:GLU:O	1:D:498:GLY:HA2	2.18	0.43
1:C:192:ILE:HG23	1:C:208:PRO:HB3	2.00	0.43
1:B:277:MET:HE2	1:B:304:ARG:NH2	2.33	0.43
1:C:297:LEU:HD22	1:D:580:ARG:HG3	2.00	0.43
1:D:508:LEU:HD22	1:D:514:GLN:HB2	2.01	0.43
1:C:571:LYS:HD3	1:C:579:MET:HE1	2.01	0.43
1:C:429:ILE:HG23	1:C:439:LEU:HD11	2.00	0.43
1:B:442:PRO:HD2	1:B:447:LYS:HE2	2.01	0.43
1:B:80:PRO:HA	1:B:220:MET:HE2	2.02	0.42
1:C:567:LYS:NZ	5:C:725:HOH:O	2.47	0.42
1:D:164:LEU:O	1:D:208:PRO:HD2	2.19	0.42
1:C:277:MET:HE2	1:C:304:ARG:NH2	2.35	0.42
1:C:288:ARG:NE	1:C:331:ASN:O	2.52	0.42
1:C:312:LYS:NZ	1:C:507:GLU:OE1	2.50	0.41
1:C:432:ILE:HG21	1:C:439:LEU:HD23	2.02	0.41
1:B:502:LEU:HD12	1:B:555:LEU:CD2	2.50	0.41
1:A:277:MET:HE2	1:A:304:ARG:NH2	2.35	0.41
1:B:272:GLU:HB2	1:B:323:TYR:CZ	2.56	0.41
1:C:510:ASP:OD2	5:C:701:HOH:O	2.22	0.41
1:C:418:PRO:HG2	1:C:421:SER:HB3	2.02	0.41
1:C:382:LYS:HE2	1:C:462:ASN:HD21	1.86	0.41
1:C:439:LEU:HD23	1:C:439:LEU:HA	1.88	0.41
1:B:186:ARG:NH1	1:B:221:LEU:O	2.54	0.41
1:C:571:LYS:CE	1:C:579:MET:HE1	2.51	0.41
1:C:458:GLU:O	1:C:498:GLY:HA2	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	484/516 (94%)	475 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	502/516 (97%)	493 (98%)	9 (2%)	0	100	100
1	C	482/516 (93%)	468 (97%)	14 (3%)	0	100	100
1	D	497/516 (96%)	485 (98%)	12 (2%)	0	100	100
All	All	1965/2064 (95%)	1921 (98%)	44 (2%)	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	410/464 (88%)	410 (100%)	0	100	100
1	B	416/464 (90%)	415 (100%)	1 (0%)	87	90
1	C	404/464 (87%)	404 (100%)	0	100	100
1	D	416/464 (90%)	415 (100%)	1 (0%)	87	90
All	All	1646/1856 (89%)	1644 (100%)	2 (0%)	88	90

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

Mol	Chain	Res	Type
1	B	118	LYS
1	D	94	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	459	ASN
1	B	162	GLN
1	B	286	ASN
1	C	127	HIS
1	C	355	ASN
1	C	459	ASN

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Mol	Chain	Res	Type
1	C	462	ASN
1	D	371	HIS
1	D	521	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](#)

12 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	$\# Z > 2$
4	LYS	B	604	-	8,9,9	0.94	1 (12%)	7,10,10	0.75	0
3	GOL	B	602	-	5,5,5	0.50	0	5,5,5	1.51	1 (20%)
3	GOL	A	602	-	5,5,5	0.92	0	5,5,5	1.13	0
4	LYS	D	603	-	8,9,9	0.80	1 (12%)	7,10,10	0.90	1 (14%)
2	D4O	A	601	-	23,23,23	1.68	1 (4%)	31,33,33	1.68	5 (16%)
2	D4O	B	601	-	23,23,23	1.69	1 (4%)	31,33,33	1.71	5 (16%)
3	GOL	B	603	-	5,5,5	0.93	0	5,5,5	1.64	2 (40%)
4	LYS	A	603	-	8,9,9	0.89	0	7,10,10	1.19	1 (14%)
4	LYS	C	602	-	8,9,9	1.00	1 (12%)	7,10,10	1.14	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	D4O	C	601	-	23,23,23	1.59	1 (4%)	31,33,33	1.56	4 (12%)
3	GOL	D	602	-	5,5,5	1.06	0	5,5,5	0.66	0
2	D4O	D	601	-	23,23,23	1.64	1 (4%)	31,33,33	1.41	5 (16%)

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
4	LYS	B	604	-	-	0/9/9/9	-
3	GOL	B	602	-	-	0/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-
4	LYS	D	603	-	-	1/9/9/9	-
2	D4O	A	601	-	-	0/4/26/26	0/3/3/3
2	D4O	B	601	-	-	0/4/26/26	0/3/3/3
3	GOL	B	603	-	-	4/4/4/4	-
4	LYS	A	603	-	-	0/9/9/9	-
4	LYS	C	602	-	-	0/9/9/9	-
2	D4O	C	601	-	-	0/4/26/26	0/3/3/3
3	GOL	D	602	-	-	0/4/4/4	-
2	D4O	D	601	-	-	0/4/26/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	D4O	O3-C8	7.35	1.46	1.34
2	B	601	D4O	O3-C8	7.32	1.46	1.34
2	D	601	D4O	O3-C8	7.17	1.45	1.34
2	C	601	D4O	O3-C8	6.83	1.45	1.34
4	C	602	LYS	OXT-C	-2.14	1.23	1.30
4	B	604	LYS	OXT-C	-2.11	1.23	1.30
4	D	603	LYS	OXT-C	-2.03	1.24	1.30

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	D4O	C10-C7-C6	-5.34	103.40	113.44
2	A	601	D4O	C10-C7-C6	-5.08	103.88	113.44
2	C	601	D4O	C10-C7-C6	-4.47	105.02	113.44
2	A	601	D4O	C7-O3-C8	-3.80	113.17	118.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	D4O	C7-O3-C8	-3.76	113.23	118.78
2	B	601	D4O	O3-C7-C10	3.70	111.94	106.10
2	D	601	D4O	C10-C7-C6	-3.58	106.71	113.44
2	C	601	D4O	O3-C7-C10	3.36	111.40	106.10
2	D	601	D4O	C7-O3-C8	-3.27	113.96	118.78
2	A	601	D4O	C10-C11-C15	-3.06	104.58	111.71
4	A	603	LYS	OXT-C-O	-3.05	117.15	124.08
2	C	601	D4O	C7-O3-C8	-3.00	114.36	118.78
2	C	601	D4O	C10-C11-C15	-2.95	104.84	111.71
2	B	601	D4O	C10-C11-C15	-2.95	104.85	111.71
4	C	602	LYS	OXT-C-O	-2.93	117.44	124.08
2	A	601	D4O	O3-C7-C10	2.89	110.65	106.10
3	B	602	GOL	C3-C2-C1	-2.61	102.23	111.80
2	A	601	D4O	O3-C8-O4	2.60	120.38	117.53
2	B	601	D4O	C3-C4-C5	-2.47	117.99	120.77
3	B	603	GOL	O1-C1-C2	2.44	121.36	110.38
4	D	603	LYS	OXT-C-O	-2.22	119.04	124.08
2	D	601	D4O	C17-C12-C13	2.09	112.61	109.42
2	D	601	D4O	O3-C7-C10	2.06	109.36	106.10
2	D	601	D4O	C1-C9-C5	2.06	120.76	118.61
3	B	603	GOL	C3-C2-C1	2.04	119.29	111.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

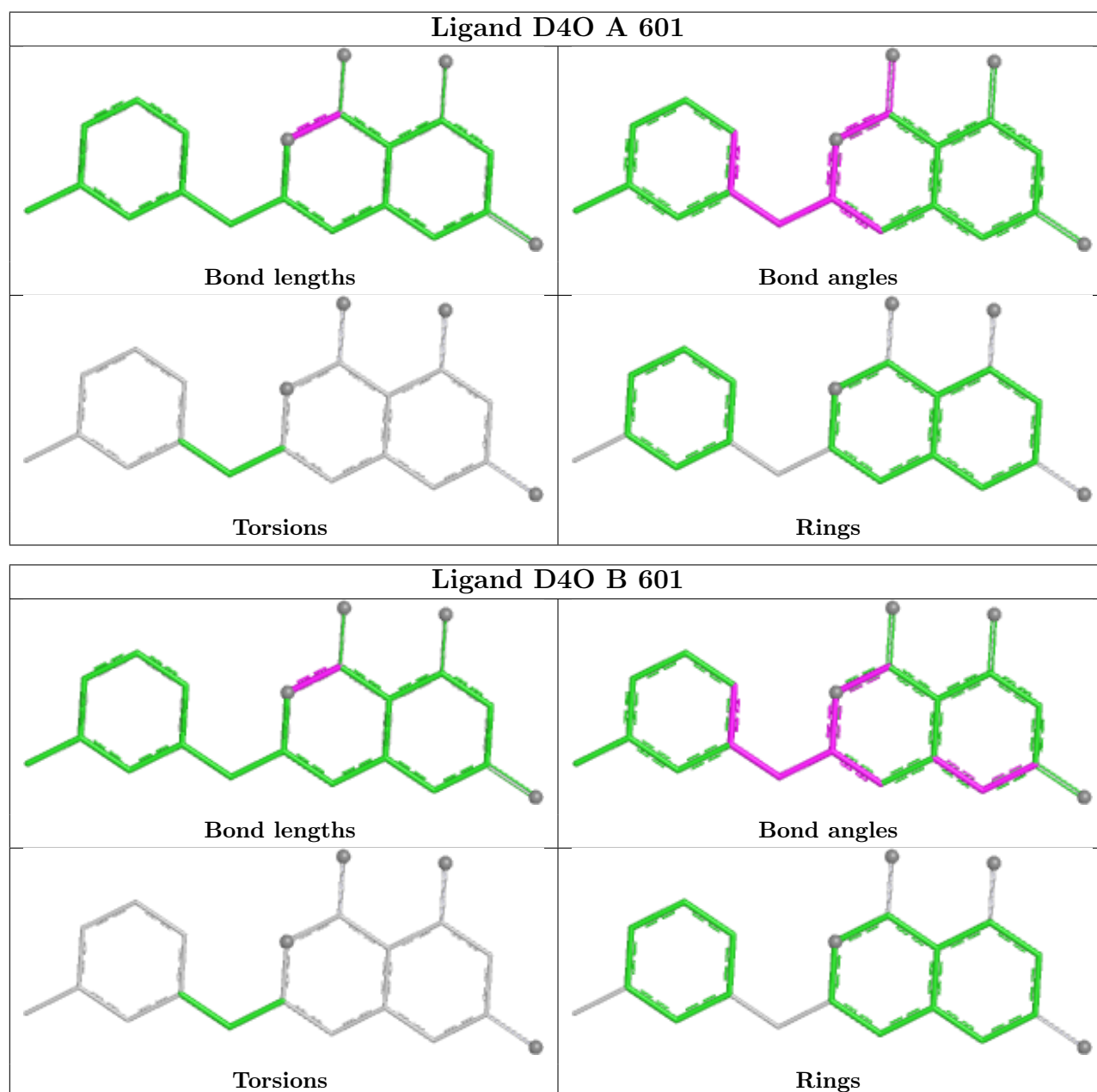
Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-C3
3	B	603	GOL	O1-C1-C2-O2
3	B	603	GOL	O1-C1-C2-C3
3	B	603	GOL	C1-C2-C3-O3
3	A	602	GOL	O1-C1-C2-O2
3	B	603	GOL	O2-C2-C3-O3
4	D	603	LYS	O-C-CA-N

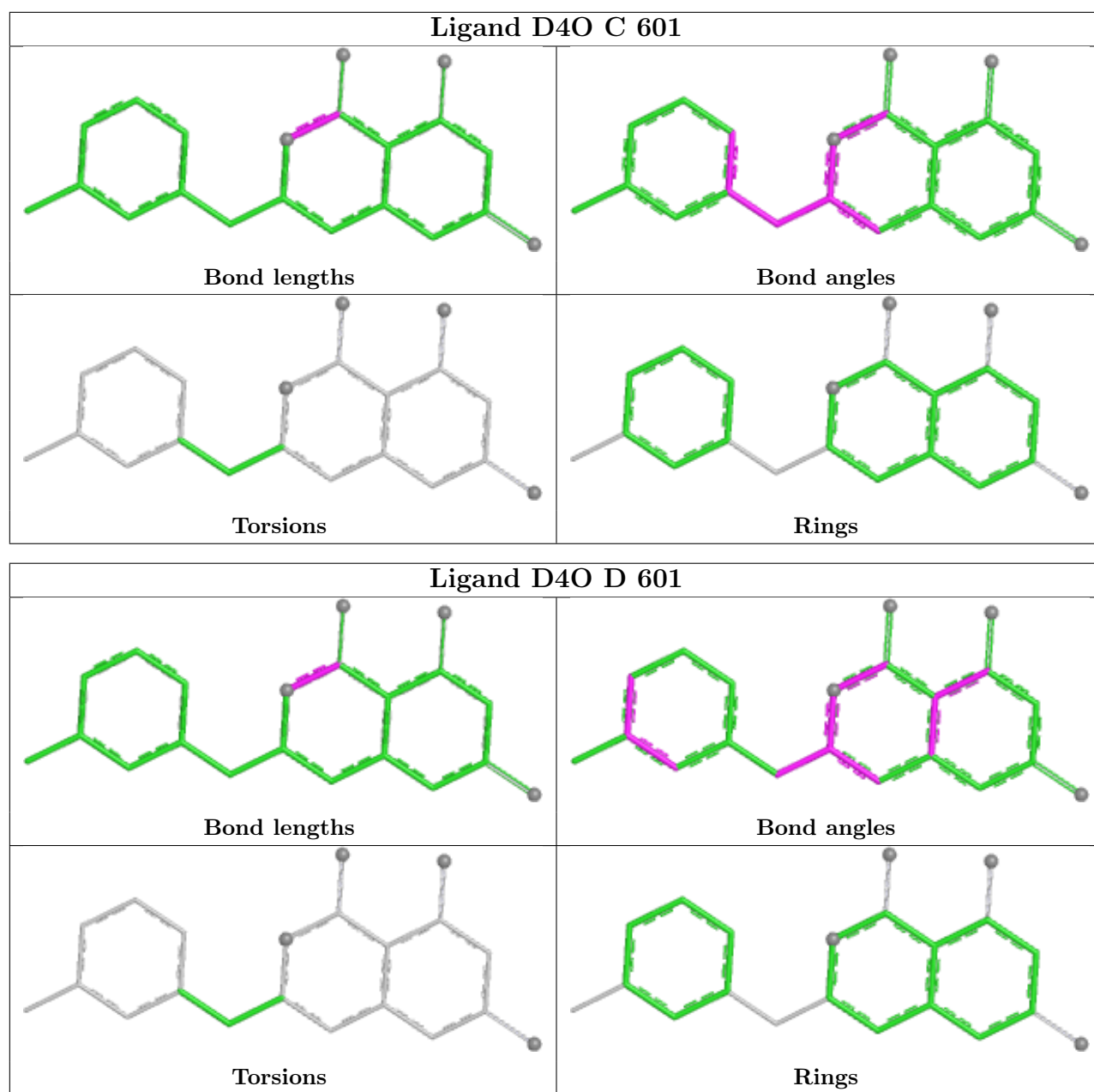
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	GOL	1	0
2	B	601	D4O	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	487/516 (94%)	0.34	24 (4%)	35	37	12, 29, 61, 77	1 (0%)
1	B	504/516 (97%)	0.40	35 (6%)	23	24	16, 30, 66, 111	0
1	C	486/516 (94%)	0.47	39 (8%)	18	19	17, 31, 66, 93	0
1	D	501/516 (97%)	0.38	25 (4%)	34	36	18, 30, 64, 91	0
All	All	1978/2064 (95%)	0.40	123 (6%)	26	28	12, 30, 65, 111	1 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	512	PHE	5.8
1	D	225	TYR	5.6
1	B	229	ASP	5.1
1	C	99	ILE	4.7
1	C	230	THR	4.6
1	B	441	ASN	4.5
1	B	518	PHE	4.4
1	A	99	ILE	4.2
1	A	457	ILE	4.2
1	D	230	THR	4.2
1	B	582	ALA	4.1
1	A	354	TYR	4.1
1	B	230	THR	4.1
1	C	415	LEU	4.0
1	C	461	TYR	3.9
1	B	533	ALA	3.9
1	A	437	ILE	3.7
1	D	533	ALA	3.7
1	B	535	LEU	3.7
1	C	515	LYS	3.7
1	D	526	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	439	LEU	3.6
1	B	534	GLN	3.5
1	D	384	GLY	3.5
1	C	121	ASP	3.5
1	A	515	LYS	3.4
1	A	145	SER	3.4
1	D	532	ALA	3.4
1	D	534	GLN	3.3
1	B	520	LEU	3.3
1	D	456	PHE	3.3
1	C	431	ILE	3.2
1	B	519	LYS	3.2
1	B	530	THR	3.1
1	C	413	THR	3.1
1	C	443	PRO	3.1
1	B	226	GLY	3.1
1	D	512	PHE	3.1
1	B	442	PRO	3.1
1	A	536	ASP	3.0
1	B	227	LEU	3.0
1	C	144	ALA	3.0
1	C	227	LEU	3.0
1	A	410	VAL	3.0
1	D	441	ASN	2.9
1	B	532	ALA	2.9
1	A	514	GLN	2.9
1	A	383	ASP	2.9
1	C	441	ASN	2.9
1	D	528	GLY	2.9
1	A	413	THR	2.8
1	A	582	ALA	2.8
1	C	436	LYS	2.8
1	B	354	TYR	2.7
1	C	517	CYS	2.7
1	C	228	LYS	2.7
1	C	412	ASN	2.7
1	B	461	TYR	2.7
1	D	531	GLU	2.6
1	C	201	LYS	2.6
1	B	225	TYR	2.6
1	A	431	ILE	2.6
1	D	530	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	440	PRO	2.5
1	B	529	ASP	2.5
1	B	99	ILE	2.5
1	A	144	ALA	2.5
1	C	98	GLY	2.5
1	A	414	ILE	2.5
1	A	411	THR	2.5
1	B	517	CYS	2.5
1	B	151	PHE	2.5
1	C	122	LEU	2.5
1	C	429	ILE	2.5
1	B	144	ALA	2.5
1	B	439	LEU	2.4
1	C	449	LEU	2.4
1	C	473	GLN	2.4
1	D	527	LYS	2.4
1	A	517	CYS	2.4
1	C	414	ILE	2.4
1	D	457	ILE	2.4
1	C	416	GLU	2.4
1	C	430	ASN	2.4
1	B	93	ASP	2.3
1	A	439	LEU	2.3
1	C	90	PHE	2.3
1	C	512	PHE	2.3
1	B	228	LYS	2.3
1	C	410	VAL	2.3
1	C	164	LEU	2.3
1	C	354	TYR	2.3
1	C	202	GLY	2.3
1	B	440	PRO	2.3
1	D	144	ALA	2.3
1	C	582	ALA	2.2
1	B	198	LYS	2.2
1	D	411	THR	2.2
1	D	535	LEU	2.2
1	A	229	ASP	2.2
1	A	412	ASN	2.2
1	C	455	HIS	2.2
1	D	228	LYS	2.2
1	A	78	VAL	2.2
1	B	521	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	146	GLY	2.2
1	D	516	GLU	2.2
1	D	521	GLN	2.2
1	B	146	GLY	2.2
1	B	180	CYS	2.1
1	A	455	HIS	2.1
1	C	568	ASN	2.1
1	C	438	GLU	2.1
1	D	412	ASN	2.1
1	C	243	ILE	2.0
1	B	109	THR	2.0
1	B	524	ASP	2.0
1	B	523	LYS	2.0
1	C	281	ILE	2.0
1	C	474	ILE	2.0
1	A	98	GLY	2.0
1	A	124	ASN	2.0
1	D	80	PRO	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(Å ²)	Q<0.9
3	GOL	B	602	6/6	0.86	0.14	40,43,44,45	0
3	GOL	B	603	6/6	0.86	0.13	39,41,42,43	0
3	GOL	A	602	6/6	0.88	0.11	44,49,49,50	0
2	D4O	B	601	21/21	0.93	0.07	19,21,26,26	0
3	GOL	D	602	6/6	0.93	0.08	31,31,33,34	0

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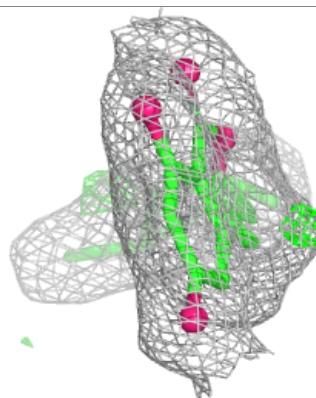
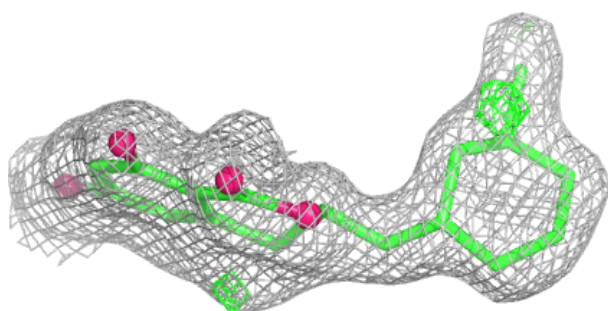
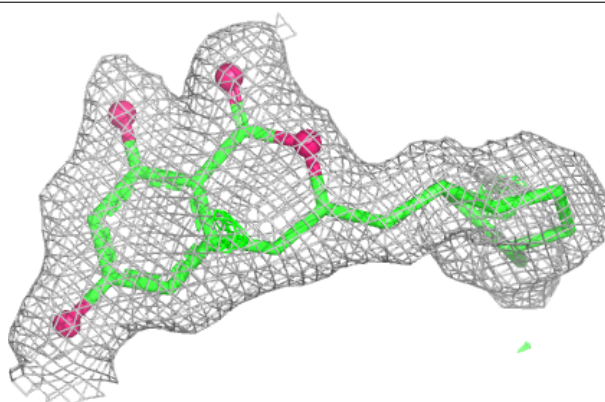
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	D4O	C	601	21/21	0.94	0.07	15,22,24,25	0
2	D4O	D	601	21/21	0.94	0.07	25,27,31,32	0
2	D4O	A	601	21/21	0.94	0.07	19,23,29,30	0
4	LYS	C	602	10/10	0.95	0.06	15,19,20,21	0
4	LYS	B	604	10/10	0.96	0.06	15,16,23,24	0
4	LYS	A	603	10/10	0.96	0.06	15,21,22,22	0
4	LYS	D	603	10/10	0.97	0.06	19,21,24,24	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.

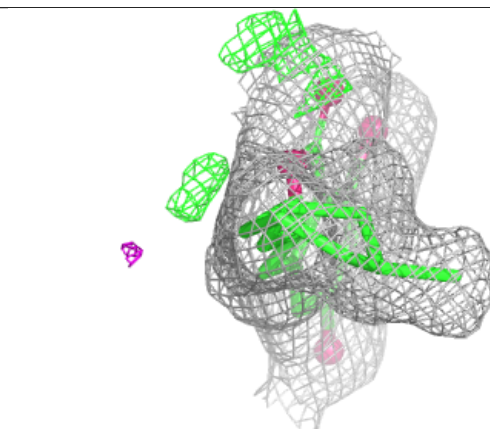
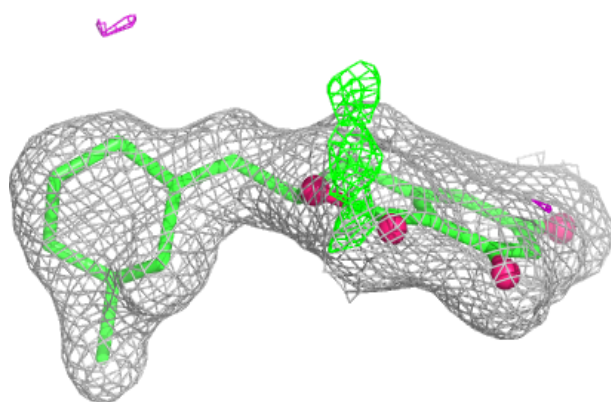
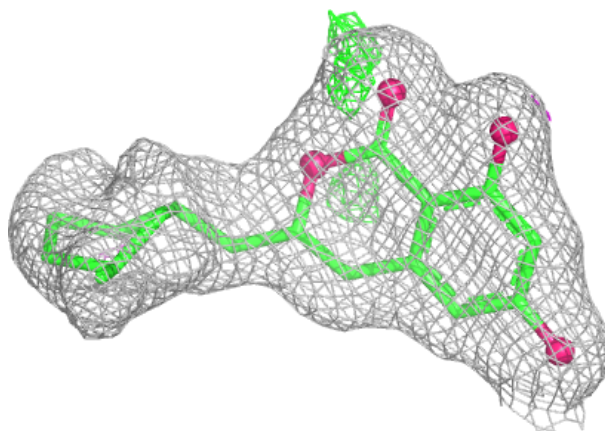
Electron density around D4O B 601:

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

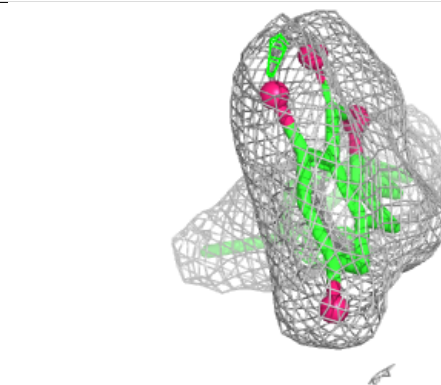
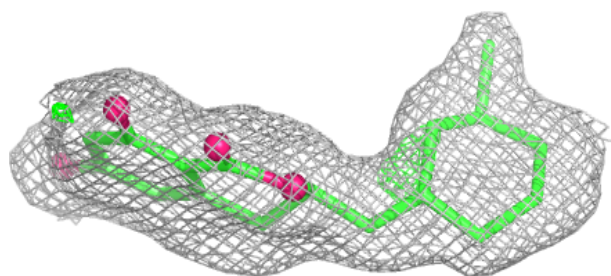
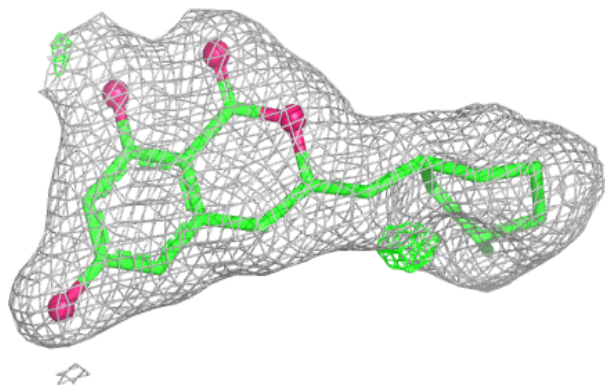


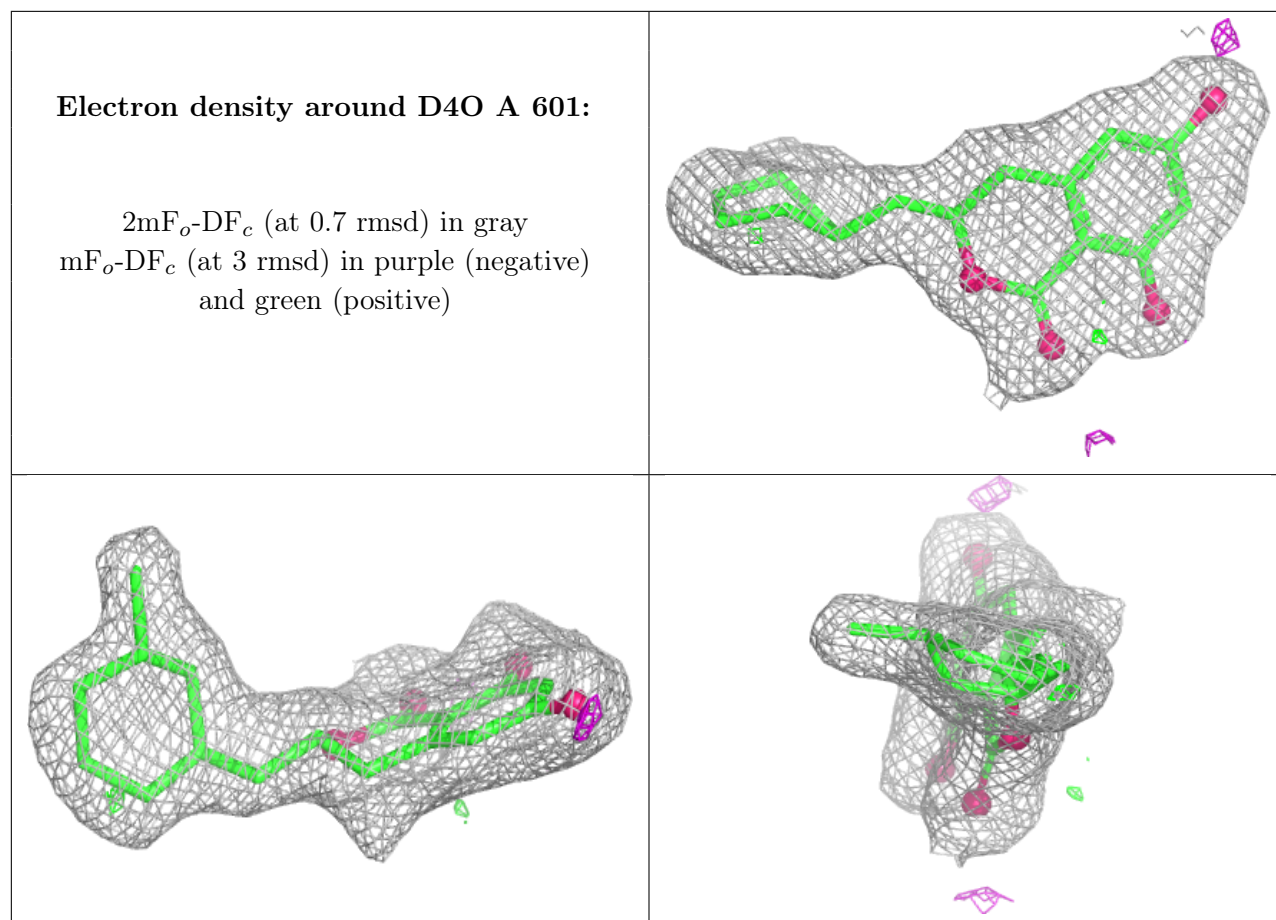
Electron density around D4O C 601:

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

**Electron density around D4O 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 ⓘ

There are no such residues in this entry.