



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:08 am BST

PDB ID : 6KAB
Title : Crystal structure of plasmodium lysyl-tRNA synthetase in complex with a cladosporin derivative 2
Authors : Zhou, J.; Fang, P.
Deposited on : 2019-06-21
Resolution : 2.89 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 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 : 2.11
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) : 2.11

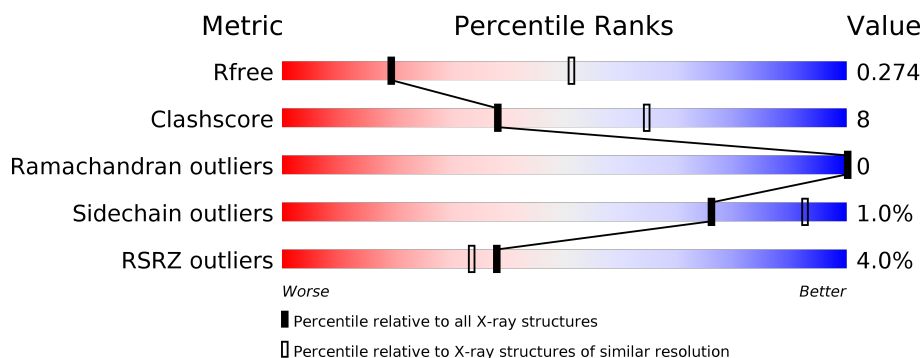
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	516	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div></div> </div> <div></div> </div>
1	B	516	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div></div> </div> <div></div> </div>
1	C	516	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div></div> </div> <div></div> </div>
1	D	516	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div></div> </div> <div></div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16261 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	506	Total	C	N	O	S	0	0	0
			3954	2544	659	734	17			
1	B	503	Total	C	N	O	S	0	0	0
			3944	2536	657	734	17			
1	C	498	Total	C	N	O	S	0	0	0
			3907	2516	652	722	17			
1	D	501	Total	C	N	O	S	0	0	0
			3924	2530	652	726	16			

There are 36 discrepancies between the modelled and reference sequences:

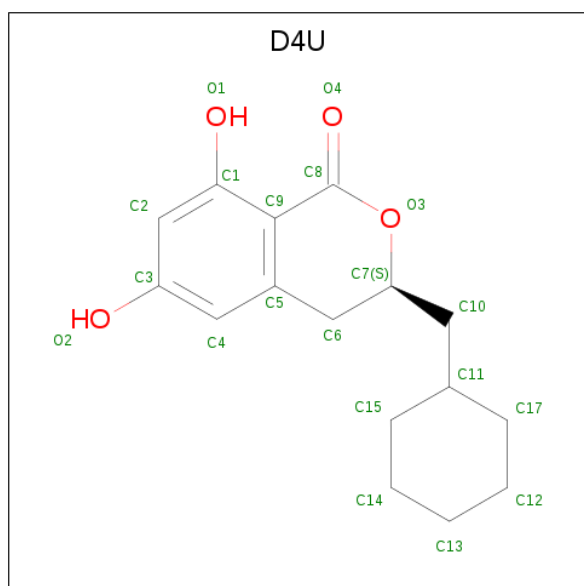
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	initiating methionine	UNP W7JP72
A	584	GLY	-	expression tag	UNP W7JP72
A	585	GLY	-	expression tag	UNP W7JP72
A	586	HIS	-	expression tag	UNP W7JP72
A	587	HIS	-	expression tag	UNP W7JP72
A	588	HIS	-	expression tag	UNP W7JP72
A	589	HIS	-	expression 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-(cyclohexylmethyl)-6,8-bis(oxidanyl)-3,4-dihydroisochromen-1-one (three-letter code: D4U) (formula: C₁₆H₂₀O₄) (labeled as "Ligand of Interest" by author).



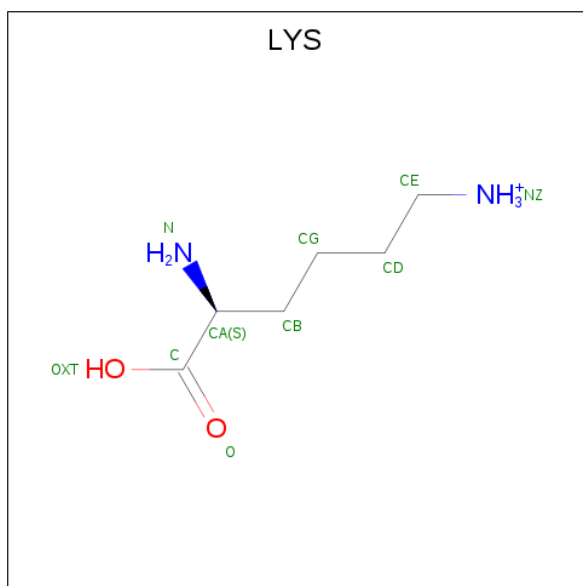
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	16	4		
2	B	1	Total	C	O	0	0
			20	16	4		
2	C	1	Total	C	O	0	0
			20	16	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			20	16	4		

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



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

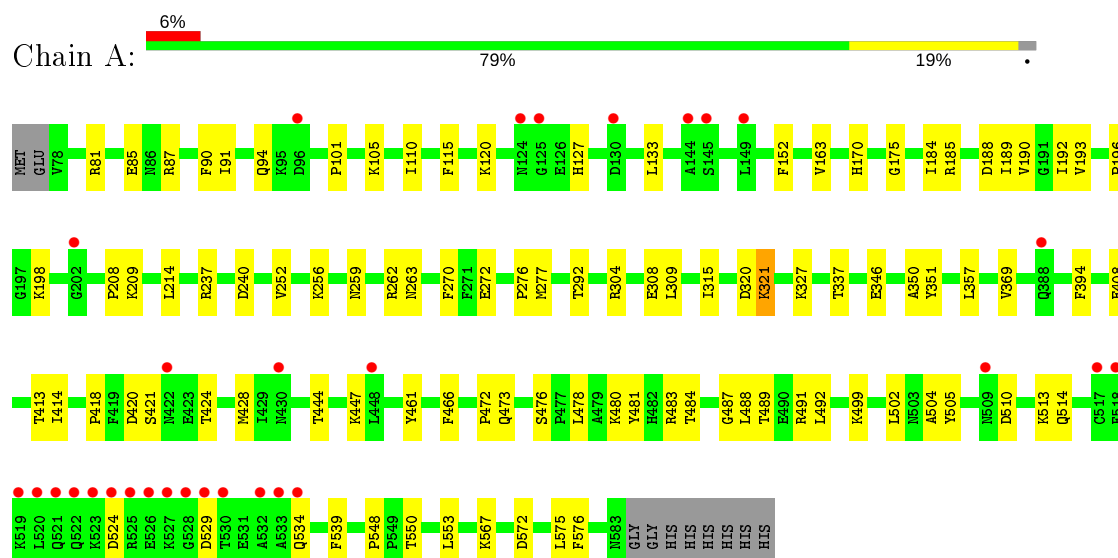
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	105	Total	O	0	0
			105	105		
4	C	108	Total	O	0	0
			108	108		
4	D	96	Total	O	0	0
			96	96		

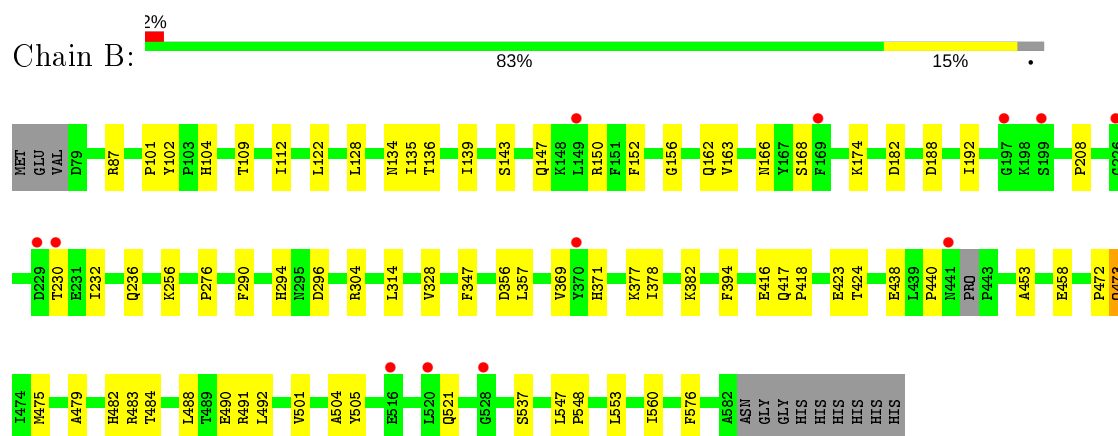
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

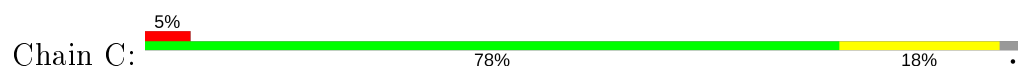
• Molecule 1: Lysine-tRNA ligase

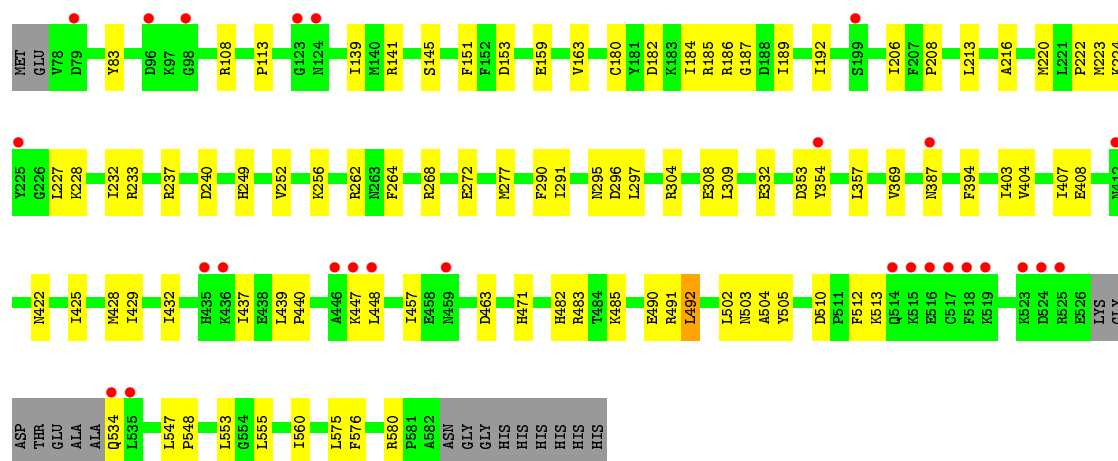


• Molecule 1: Lysine-tRNA ligase

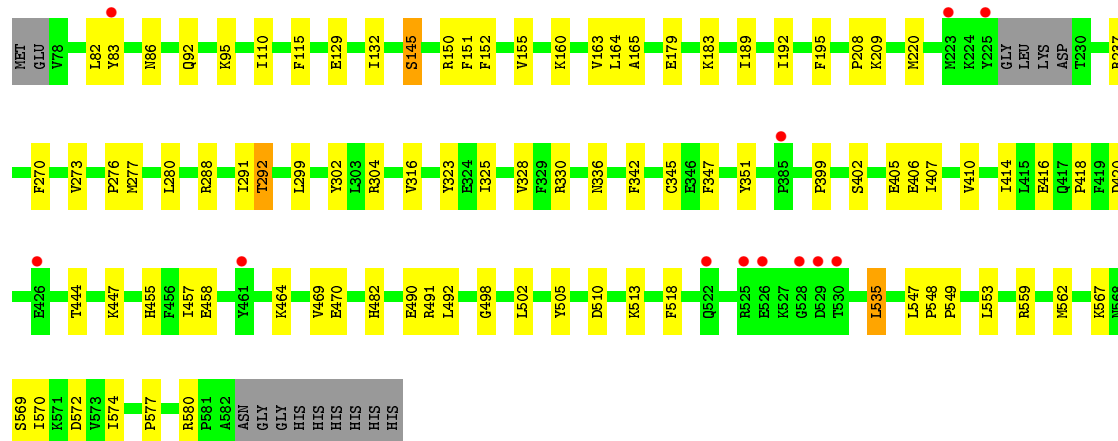
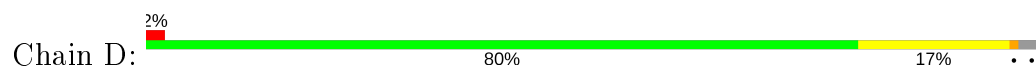


• Molecule 1: Lysine-tRNA ligase





• 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	71.05Å 90.01Å 100.62Å 76.43° 72.92° 79.76°	Depositor
Resolution (Å)	46.17 – 2.89 46.17 – 2.89	Depositor EDS
% Data completeness (in resolution range)	93.5 (46.17-2.89) 93.5 (46.17-2.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.224 , 0.273 0.224 , 0.274	Depositor DCC
R_{free} test set	2423 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.1	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	0.90	EDS
Total number of atoms	16261	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.49% 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: D4U

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	0.26	0/4052	0.45	0/5500
1	B	0.26	0/4040	0.45	0/5482
1	C	0.25	0/4003	0.44	0/5431
1	D	0.27	0/4022	0.45	0/5459
All	All	0.26	0/16117	0.45	0/21872

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	3954	0	3754	65	0
1	B	3944	0	3734	51	0
1	C	3907	0	3726	72	0
1	D	3924	0	3740	65	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	1	0
2	D	20	0	0	0	0
3	A	10	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	12	0	0
3	C	10	0	12	4	0
3	D	10	0	12	0	0
4	A	103	0	0	3	0
4	B	105	0	0	3	0
4	C	108	0	0	7	0
4	D	96	0	0	2	0
All	All	16261	0	15002	233	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 8.

All (233) 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:D:291:ILE:HD12	1:D:302:TYR:CE2	2.12	0.85
1:B:230:THR:CB	4:B:767:HOH:O	2.26	0.83
1:B:382:LYS:CB	4:B:761:HOH:O	2.26	0.82
1:D:291:ILE:CD1	1:D:302:TYR:CD2	2.62	0.82
1:A:315:ILE:HG21	1:A:550:THR:HG21	1.63	0.81
1:D:447:LYS:CB	4:D:736:HOH:O	2.28	0.80
1:C:141:ARG:HB3	1:C:153:ASP:HB2	1.63	0.79
1:D:291:ILE:CD1	1:D:302:TYR:CE2	2.65	0.79
1:A:350:ALA:HA	1:A:550:THR:HG22	1.65	0.78
1:A:418:PRO:HG2	1:A:421:SER:HB3	1.65	0.78
1:D:407:ILE:HG13	1:D:457:ILE:HD11	1.69	0.74
1:D:444:THR:HG23	1:D:447:LYS:H	1.53	0.73
1:A:259:ASN:O	1:A:263:ASN:ND2	2.22	0.71
1:C:534:GLN:N	4:C:701:HOH:O	2.21	0.71
1:D:291:ILE:HD13	1:D:302:TYR:CD2	2.26	0.70
1:B:473:GLN:NE2	1:B:479:ALA:O	2.28	0.67
1:D:192:ILE:HG23	1:D:208:PRO:HB3	1.76	0.66
1:B:256:LYS:HE3	1:B:371:HIS:NE2	2.09	0.66
1:C:233:ARG:CG	4:C:706:HOH:O	2.43	0.65
1:B:147:GLN:HA	1:B:150:ARG:HH21	1.62	0.65
1:B:192:ILE:HG23	1:B:208:PRO:HB3	1.78	0.65
1:D:150:ARG:HB2	1:D:165:ALA:HB3	1.79	0.64
1:C:505:TYR:CZ	3:C:602:LYS:HE3	2.33	0.63
1:A:337:THR:HG21	1:A:499:LYS:HD2	1.80	0.63
1:B:521:GLN:NE2	4:B:702:HOH:O	2.32	0.63
1:B:369:VAL:HG13	1:B:378:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:ARG:NH2	4:C:704:HOH:O	2.32	0.63
1:D:547:LEU:HD12	1:D:548:PRO:HD2	1.81	0.62
1:A:120:LYS:O	1:A:198:LYS:NZ	2.33	0.61
1:C:228:LYS:O	1:C:233:ARG:NH1	2.31	0.61
1:A:170:HIS:NE2	1:A:175:GLY:O	2.32	0.61
1:C:512:PHE:CB	4:C:746:HOH:O	2.50	0.59
1:B:483:ARG:HG3	1:B:484:THR:HG23	1.85	0.59
1:D:444:THR:HG22	4:D:736:HOH:O	2.03	0.59
1:A:308:GLU:HG2	1:A:309:LEU:HD23	1.84	0.59
1:A:351:TYR:CZ	1:B:136:THR:HG21	2.38	0.58
1:A:262:ARG:NH1	1:A:272:GLU:OE1	2.37	0.58
1:B:232:ILE:HG13	1:B:236:GLN:HE21	1.69	0.58
1:C:429:ILE:HG12	1:C:439:LEU:HD11	1.85	0.58
1:C:290:PHE:HB3	1:D:292:THR:HG21	1.86	0.57
1:A:502:LEU:HD11	1:A:553:LEU:HD11	1.86	0.57
1:C:113:PRO:HG3	1:C:159:GLU:HG3	1.85	0.57
1:C:233:ARG:HG3	4:C:706:HOH:O	2.04	0.57
1:A:476:SER:HB2	1:A:489:THR:HG21	1.85	0.57
1:C:184:ILE:O	1:C:185:ARG:NH1	2.38	0.57
1:C:192:ILE:HG23	1:C:208:PRO:HB3	1.87	0.57
1:B:109:THR:HG23	1:B:134:ASN:HB2	1.87	0.56
1:C:407:ILE:HG13	1:C:457:ILE:HD11	1.85	0.56
1:C:510:ASP:HB3	1:C:513:LYS:HB2	1.88	0.56
1:D:502:LEU:HD11	1:D:553:LEU:HD11	1.88	0.56
1:C:237:ARG:NH1	1:C:240:ASP:OD2	2.38	0.56
1:D:277:MET:HA	1:D:304:ARG:HD3	1.86	0.56
1:B:491:ARG:HA	1:B:505:TYR:HB3	1.86	0.55
1:D:92:GLN:HA	1:D:95:LYS:HB2	1.88	0.55
1:A:87:ARG:NH2	1:A:188:ASP:OD1	2.40	0.54
1:A:270:PHE:HA	1:A:321:LYS:HB3	1.89	0.54
1:B:166:ASN:ND2	1:B:168:SER:H	2.06	0.54
1:B:547:LEU:HD12	1:B:548:PRO:HD2	1.90	0.54
1:A:548:PRO:O	1:A:550:THR:HG23	2.08	0.54
1:C:403:ILE:HD12	1:C:457:ILE:HD13	1.90	0.54
1:C:404:VAL:O	1:C:408:GLU:HG3	2.08	0.53
1:C:439:LEU:HD11	1:C:448:LEU:HD21	1.89	0.53
1:D:336:ASN:O	1:D:570:ILE:N	2.37	0.53
1:D:155:VAL:HG12	1:D:160:LYS:HB2	1.90	0.53
1:A:81:ARG:O	1:A:85:GLU:HG3	2.08	0.53
1:D:510:ASP:OD2	1:D:513:LYS:NZ	2.42	0.53
1:C:163:VAL:HG13	1:C:206:ILE:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:MET:HA	1:C:304:ARG:HD3	1.91	0.53
1:D:330:ARG:HG3	1:D:342:PHE:HE1	1.74	0.53
1:C:548:PRO:HB3	1:D:189:ILE:HG21	1.91	0.52
1:A:192:ILE:HG23	1:A:208:PRO:HB3	1.91	0.52
1:D:402:SER:HB3	1:D:405:GLU:HB2	1.90	0.52
1:A:444:THR:HG23	1:A:447:LYS:H	1.75	0.52
1:A:480:LYS:HD3	1:B:104:HIS:CD2	2.45	0.52
1:B:87:ARG:NH2	1:B:188:ASP:OD1	2.42	0.52
1:C:403:ILE:HG21	1:C:471:HIS:HA	1.92	0.52
1:B:423:GLU:OE1	1:B:423:GLU:N	2.43	0.52
1:C:252:VAL:O	1:C:256:LYS:HG3	2.09	0.52
1:C:504:ALA:HA	3:C:602:LYS:HE2	1.92	0.52
1:D:152:PHE:HB2	1:D:163:VAL:HB	1.92	0.52
1:B:501:VAL:HG22	1:B:560:ILE:HG13	1.92	0.51
1:D:237:ARG:HH21	1:D:577:PRO:HD3	1.75	0.51
1:A:491:ARG:HA	1:A:505:TYR:HB3	1.92	0.51
1:C:432:ILE:HD12	1:C:439:LEU:HD12	1.91	0.51
1:A:357:LEU:HD13	1:A:504:ALA:HB1	1.91	0.51
1:C:555:LEU:HD22	1:C:560:ILE:HD11	1.93	0.51
1:C:291:ILE:O	1:D:292:THR:HG22	2.11	0.51
1:C:491:ARG:HA	1:C:505:TYR:HB3	1.93	0.51
1:A:575:LEU:HD13	1:B:314:LEU:HD11	1.92	0.50
1:C:432:ILE:HG23	1:C:437:ILE:HB	1.93	0.50
1:A:491:ARG:HG3	1:A:505:TYR:HD2	1.76	0.50
1:C:463:ASP:OD1	1:C:463:ASP:N	2.44	0.50
1:C:502:LEU:HD11	1:C:553:LEU:HD11	1.93	0.50
1:D:491:ARG:HA	1:D:505:TYR:HB3	1.93	0.50
1:C:189:ILE:HG21	1:D:548:PRO:HB3	1.92	0.50
1:A:190:VAL:HG12	1:A:192:ILE:HG13	1.93	0.50
1:C:353:ASP:CG	1:C:483:ARG:HH22	2.14	0.50
1:D:455:HIS:O	1:D:455:HIS:ND1	2.36	0.50
1:D:316:VAL:HG12	1:D:547:LEU:HA	1.94	0.50
1:A:184:ILE:O	1:A:185:ARG:NH1	2.45	0.49
1:B:453:ALA:O	1:B:458:GLU:HG3	2.12	0.49
1:C:262:ARG:NH1	1:C:272:GLU:OE1	2.45	0.49
1:D:83:TYR:CD1	1:D:220:MET:HG3	2.47	0.49
1:D:518:PHE:CB	1:D:535:LEU:HD12	2.42	0.49
1:D:458:GLU:O	1:D:498:GLY:HA2	2.13	0.49
1:B:357:LEU:HD13	1:B:504:ALA:HB1	1.95	0.49
1:A:277:MET:HA	1:A:304:ARG:HD3	1.95	0.49
1:B:304:ARG:HG3	1:B:328:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PHE:HB2	1:A:163:VAL:HB	1.94	0.48
1:D:145:SER:HB3	1:D:151:PHE:HE2	1.77	0.48
1:B:139:ILE:HG23	1:B:152:PHE:HB3	1.96	0.48
1:A:481:TYR:CZ	1:B:104:HIS:HE1	2.32	0.48
1:C:369:VAL:HG21	1:C:394:PHE:CD2	2.48	0.48
1:C:428:MET:O	1:C:432:ILE:HG13	2.14	0.47
1:A:510:ASP:OD2	1:A:513:LYS:HG3	2.14	0.47
1:D:418:PRO:HB2	1:D:420:ASP:OD1	2.15	0.47
1:D:237:ARG:NH2	1:D:574:ILE:O	2.47	0.47
1:B:416:GLU:O	1:B:424:THR:HG21	2.15	0.47
1:A:351:TYR:CE2	1:B:136:THR:HG21	2.48	0.47
1:A:237:ARG:NH1	1:A:240:ASP:OD2	2.47	0.47
1:B:482:HIS:HA	1:B:490:GLU:HG2	1.96	0.47
1:C:308:GLU:OE1	1:C:505:TYR:OH	2.28	0.46
1:A:115:PHE:CE1	1:A:196:PRO:HB3	2.51	0.46
1:C:222:PRO:HG2	1:C:227:LEU:HD11	1.98	0.46
1:A:277:MET:HE1	1:A:327:LYS:HB2	1.96	0.46
1:D:482:HIS:HA	1:D:490:GLU:HG3	1.98	0.46
1:D:469:VAL:HG23	1:D:470:GLU:HG2	1.96	0.46
1:D:518:PHE:HB2	1:D:535:LEU:HD12	1.98	0.46
1:A:576:PHE:HB2	1:B:276:PRO:CG	2.46	0.46
1:C:332:GLU:OE1	2:C:601:D4U:O2	2.34	0.46
1:A:369:VAL:HG21	1:A:394:PHE:CD2	2.50	0.46
1:C:83:TYR:CD1	1:C:220:MET:HG3	2.51	0.46
1:D:270:PHE:HB3	1:D:323:TYR:CD1	2.51	0.46
1:A:87:ARG:NH1	4:A:713:HOH:O	2.46	0.45
1:A:193:VAL:O	1:A:209:LYS:N	2.35	0.45
1:D:406:GLU:O	1:D:410:VAL:HG23	2.16	0.45
1:A:252:VAL:O	1:A:256:LYS:HG3	2.16	0.45
1:A:478:LEU:HD23	1:A:514:GLN:HE22	1.82	0.45
1:D:399:PRO:HG3	1:D:464:LYS:HE2	1.99	0.45
1:C:139:ILE:O	1:C:187:GLY:N	2.43	0.45
1:C:213:LEU:HD21	1:C:216:ALA:HB2	1.99	0.45
1:A:534:GLN:N	4:A:715:HOH:O	2.49	0.45
1:B:163:VAL:HG23	1:B:208:PRO:HD3	1.98	0.45
1:D:179:GLU:O	1:D:183:LYS:HG2	2.17	0.45
1:A:408:GLU:HG2	1:A:413:THR:O	2.17	0.44
1:D:559:ARG:HA	1:D:562:MET:HE2	1.99	0.44
1:D:82:LEU:O	1:D:86:ASN:HB2	2.17	0.44
1:C:422:ASN:O	1:C:425:ILE:HG22	2.17	0.44
1:C:227:LEU:HD23	1:C:232:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:LEU:HD11	1:D:273:VAL:HB	2.00	0.44
1:C:576:PHE:HB2	1:D:276:PRO:HG3	1.99	0.44
1:D:132:ILE:HD11	1:D:209:LYS:HD3	2.00	0.44
1:B:256:LYS:HA	1:B:256:LYS:HD2	1.69	0.44
1:C:492:LEU:HG	1:C:504:ALA:HB3	2.00	0.44
1:A:483:ARG:HG3	1:A:484:THR:HG23	1.99	0.44
1:C:357:LEU:HD22	1:C:553:LEU:HB2	2.00	0.44
1:C:439:LEU:HG	1:C:440:PRO:HD2	2.00	0.44
1:A:424:THR:O	1:A:428:MET:HG3	2.18	0.44
1:C:440:PRO:HB3	1:C:447:LYS:HE2	2.00	0.44
1:D:491:ARG:HG3	1:D:505:TYR:HD2	1.83	0.44
1:D:347:PHE:CE2	1:D:553:LEU:HD22	2.53	0.43
1:A:473:GLN:HG3	1:A:487:GLY:O	2.18	0.43
1:B:122:LEU:HD21	1:B:128:LEU:CD1	2.49	0.43
1:B:347:PHE:CE2	1:B:553:LEU:HB3	2.53	0.43
1:D:129:GLU:HA	1:D:195:PHE:CG	2.53	0.43
1:A:513:LYS:NZ	4:A:703:HOH:O	2.29	0.43
1:D:110:ILE:HD11	1:D:115:PHE:HA	1.99	0.43
1:A:91:ILE:HG23	1:A:101:PRO:HG3	2.00	0.43
1:A:189:ILE:HG22	1:A:214:LEU:HB2	2.01	0.43
1:C:503:ASN:HB3	3:C:602:LYS:HB3	1.99	0.43
1:D:183:LYS:HD3	1:D:183:LYS:HA	1.86	0.43
1:A:90:PHE:O	1:A:94:GLN:HG2	2.18	0.42
1:A:320:ASP:HB3	1:A:350:ALA:HB3	2.01	0.42
1:A:413:THR:HG22	1:A:414:ILE:H	1.85	0.42
1:B:472:PRO:HD2	1:B:475:MET:SD	2.59	0.42
1:C:447:LYS:HA	1:C:447:LYS:HD2	1.89	0.42
1:C:297:LEU:HD23	1:D:580:ARG:CZ	2.49	0.42
1:B:101:PRO:HG2	1:B:102:TYR:HD1	1.84	0.42
1:C:297:LEU:HD23	1:D:580:ARG:NH2	2.34	0.42
1:B:377:LYS:C	1:B:378:ILE:HD12	2.40	0.42
1:B:112:ILE:HD12	1:B:156:GLY:HA3	2.01	0.42
1:C:308:GLU:HG2	1:C:309:LEU:HD23	2.00	0.42
1:A:190:VAL:CG1	1:A:192:ILE:HG13	2.49	0.42
1:A:461:TYR:HB2	1:A:466:PHE:CD1	2.55	0.42
1:C:249:HIS:HD2	4:C:749:HOH:O	2.02	0.42
1:C:291:ILE:O	1:D:292:THR:CG2	2.67	0.42
1:A:292:THR:OG1	1:B:290:PHE:HB3	2.19	0.42
1:C:354:TYR:HA	1:C:357:LEU:HD12	2.02	0.42
1:C:482:HIS:HB3	1:C:485:LYS:O	2.20	0.42
1:C:547:LEU:HD12	1:C:548:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:PRO:HA	1:A:488:LEU:HA	2.02	0.42
1:B:150:ARG:NH1	1:B:182:ASP:OD1	2.48	0.42
1:D:336:ASN:HB3	1:D:569:SER:HA	2.02	0.42
1:C:482:HIS:HA	1:C:490:GLU:HG2	2.02	0.41
1:C:534:GLN:N	4:C:711:HOH:O	2.53	0.41
1:C:505:TYR:CE2	3:C:602:LYS:HE3	2.53	0.41
1:D:414:ILE:HG22	1:D:416:GLU:HG3	2.02	0.41
1:D:351:TYR:N	1:D:549:PRO:O	2.38	0.41
1:A:276:PRO:CG	1:B:576:PHE:HB2	2.50	0.41
1:B:294:HIS:CE1	1:B:296:ASP:HB2	2.56	0.41
1:A:110:ILE:HD13	1:A:133:LEU:HD13	2.01	0.41
1:A:351:TYR:CZ	1:B:136:THR:CG2	3.04	0.41
1:C:145:SER:HB3	1:C:151:PHE:HE2	1.86	0.41
1:A:444:THR:CG2	1:A:447:LYS:H	2.33	0.41
1:B:122:LEU:HD21	1:B:128:LEU:HD12	2.01	0.41
1:A:346:GLU:HA	1:A:553:LEU:O	2.20	0.41
1:A:567:LYS:HD2	1:A:572:ASP:HB3	2.01	0.41
1:D:280:LEU:HD21	1:D:299:LEU:HD21	2.03	0.41
1:A:418:PRO:HB2	1:A:420:ASP:OD1	2.21	0.41
1:A:105:LYS:NZ	1:B:356:ASP:OD2	2.52	0.41
1:C:407:ILE:HG13	1:C:457:ILE:CD1	2.51	0.41
1:D:164:LEU:O	1:D:208:PRO:HD2	2.21	0.41
1:D:491:ARG:HG3	1:D:505:TYR:HB3	2.03	0.41
1:B:417:GLN:HA	1:B:418:PRO:C	2.41	0.41
1:D:304:ARG:HE	1:D:328:VAL:HG12	1.85	0.41
1:B:162:GLN:HG3	1:B:163:VAL:N	2.36	0.41
1:B:369:VAL:HG21	1:B:394:PHE:CD1	2.56	0.41
1:B:135:ILE:HG23	1:B:135:ILE:HD12	1.90	0.41
1:B:438:GLU:O	1:B:440:PRO:HD3	2.21	0.41
1:D:325:ILE:HG12	1:D:345:CYS:HB2	2.03	0.41
1:A:478:LEU:HD23	1:A:514:GLN:NE2	2.36	0.40
1:B:472:PRO:HA	1:B:488:LEU:HA	2.03	0.40
1:C:295:ASN:HD22	1:D:288:ARG:NH1	2.19	0.40
1:A:524:ASP:O	1:A:529:ASP:HB3	2.21	0.40
1:B:152:PHE:HB2	1:B:163:VAL:CG1	2.52	0.40
1:C:182:ASP:O	1:C:185:ARG:NH1	2.53	0.40
1:C:223:MET:HG3	1:C:224:LYS:H	1.87	0.40
1:C:264:PHE:O	1:C:268:ARG:HD2	2.21	0.40
1:C:432:ILE:HD12	1:C:448:LEU:HD23	2.03	0.40
1:D:518:PHE:CD2	1:D:535:LEU:HA	2.56	0.40
1:A:514:GLN:HE21	1:A:539:PHE:HE2	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ARG:NH2	1:C:223:MET:SD	2.95	0.40
1:D:567:LYS:HD2	1:D:572:ASP:HB3	2.04	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	504/516 (98%)	489 (97%)	15 (3%)	0	100	100
1	B	499/516 (97%)	490 (98%)	9 (2%)	0	100	100
1	C	494/516 (96%)	484 (98%)	10 (2%)	0	100	100
1	D	497/516 (96%)	487 (98%)	10 (2%)	0	100	100
All	All	1994/2064 (97%)	1950 (98%)	44 (2%)	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	408/464 (88%)	405 (99%)	3 (1%)	84	95
1	B	407/464 (88%)	402 (99%)	5 (1%)	71	91
1	C	406/464 (88%)	401 (99%)	5 (1%)	71	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	408/464 (88%)	404 (99%)	4 (1%)	76	92
All	All	1629/1856 (88%)	1612 (99%)	17 (1%)	76	92

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	HIS
1	A	321	LYS
1	A	492	LEU
1	B	143	SER
1	B	174	LYS
1	B	473	GLN
1	B	492	LEU
1	B	537	SER
1	C	108	ARG
1	C	180	CYS
1	C	296	ASP
1	C	387	ASN
1	C	492	LEU
1	D	145	SER
1	D	292	THR
1	D	492	LEU
1	D	535	LEU

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

Mol	Chain	Res	Type
1	A	451	GLN
1	B	104	HIS
1	B	236	GLN
1	B	336	ASN
1	C	249	HIS
1	C	279	ASN
1	C	355	ASN
1	C	387	ASN
1	D	417	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	D4U	C	601	-	22,22,22	1.62	1 (4%)	30,31,31	1.16	3 (10%)
2	D4U	D	601	-	22,22,22	1.62	1 (4%)	30,31,31	1.15	2 (6%)
2	D4U	A	601	-	22,22,22	1.58	1 (4%)	30,31,31	1.20	2 (6%)
2	D4U	B	601	-	22,22,22	1.62	1 (4%)	30,31,31	1.09	2 (6%)

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	D4U	C	601	-	-	0/4/24/24	0/3/3/3
2	D4U	D	601	-	-	0/4/24/24	0/3/3/3
2	D4U	A	601	-	-	0/4/24/24	0/3/3/3
2	D4U	B	601	-	-	0/4/24/24	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	D4U	O3-C8	6.99	1.46	1.35
2	B	601	D4U	O3-C8	6.97	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	D4U	O3-C8	6.94	1.45	1.35
2	A	601	D4U	O3-C8	6.74	1.45	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	D4U	C7-O3-C8	-4.09	112.39	118.69
2	D	601	D4U	C7-O3-C8	-3.90	112.67	118.69
2	C	601	D4U	C7-O3-C8	-3.77	112.88	118.69
2	B	601	D4U	C10-C7-C6	-3.06	107.68	113.44
2	B	601	D4U	C7-O3-C8	-2.44	114.94	118.69
2	A	601	D4U	C10-C7-C6	-2.37	108.99	113.44
2	C	601	D4U	C10-C7-C6	-2.20	109.30	113.44
2	D	601	D4U	C10-C7-C6	-2.13	109.44	113.44
2	C	601	D4U	O3-C7-C10	2.12	109.55	106.17

There are no chirality outliers.

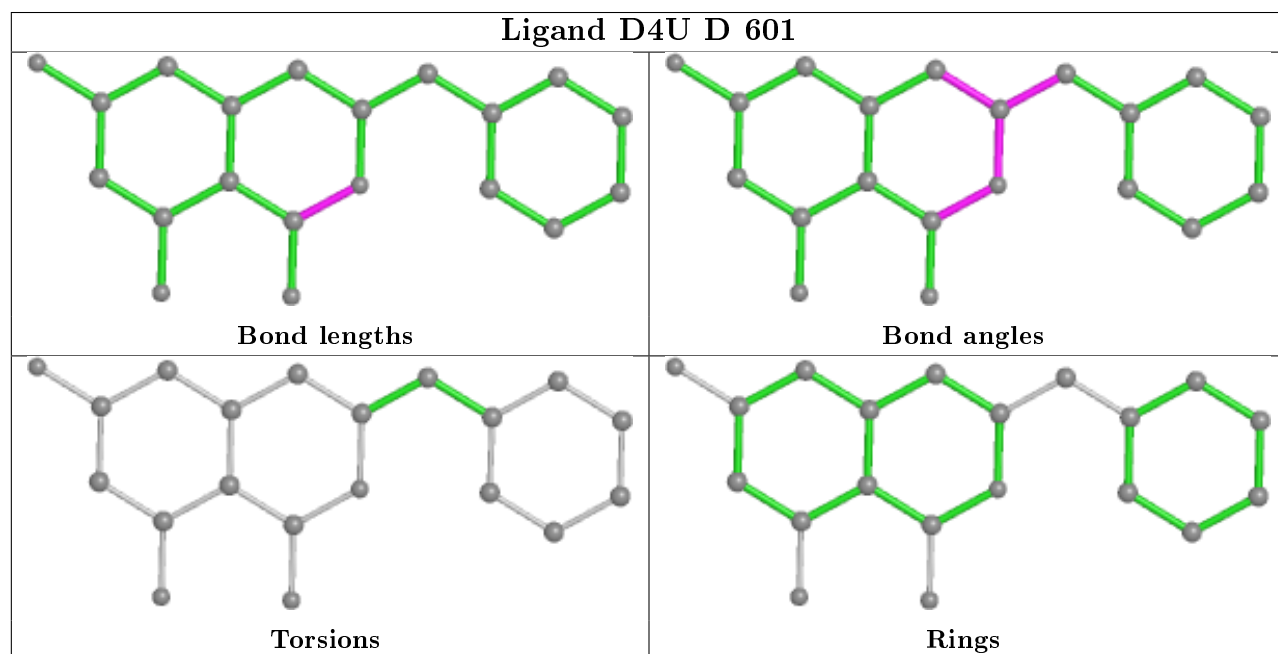
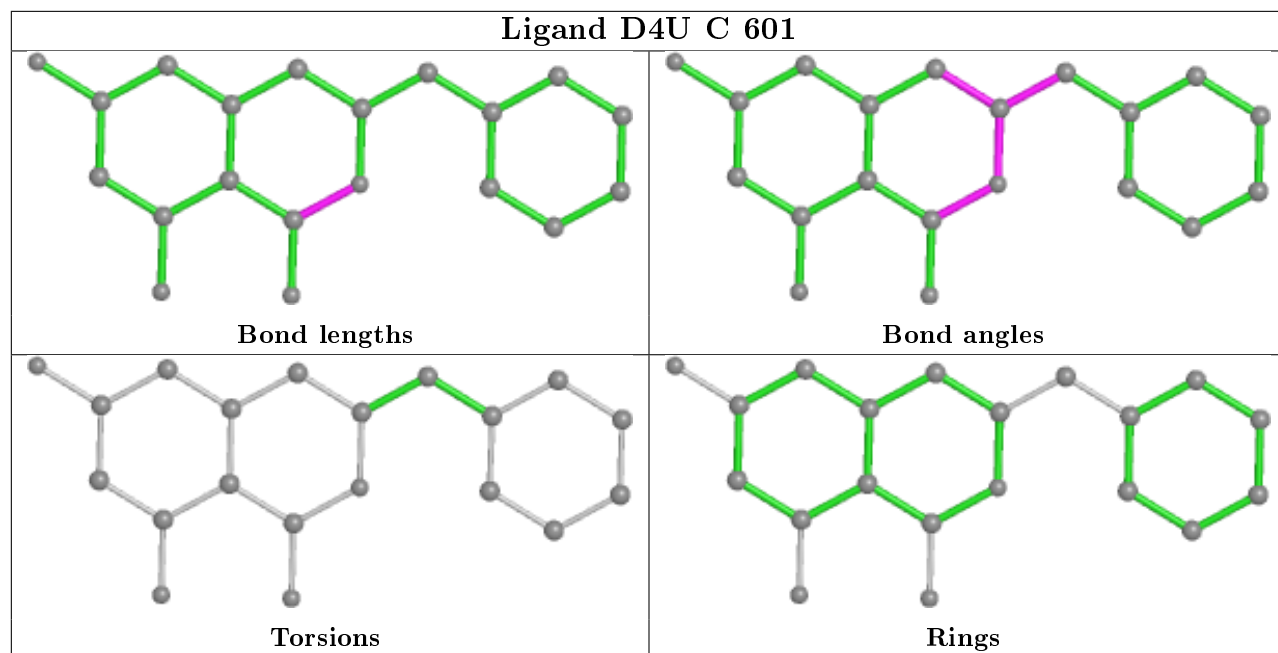
There are no torsion outliers.

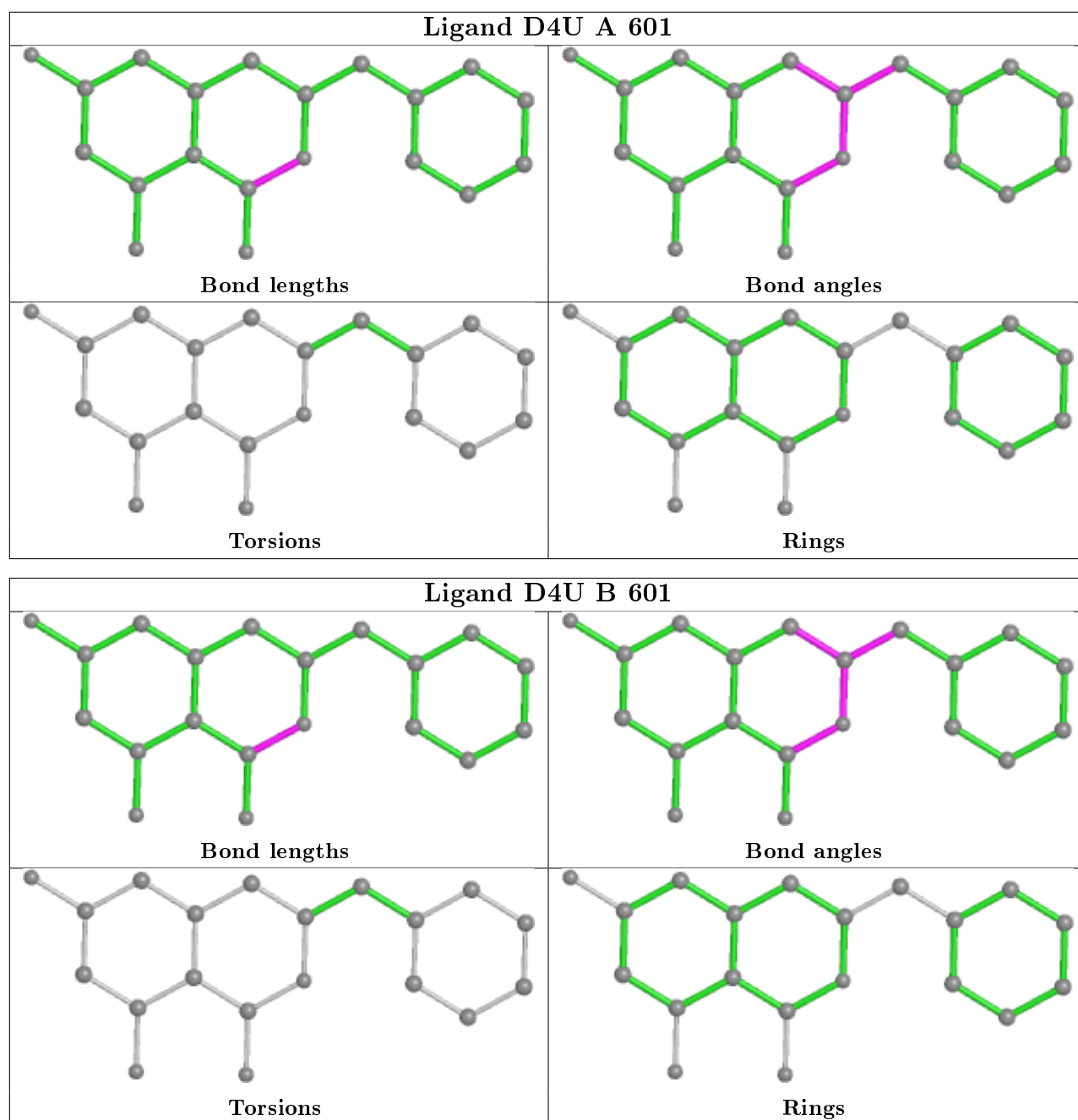
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	D4U	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	506/516 (98%)	0.16	30 (5%) 22 18	20, 36, 80, 111	0
1	B	503/516 (97%)	0.04	12 (2%) 59 56	21, 36, 75, 109	0
1	C	498/516 (96%)	0.19	27 (5%) 25 22	21, 38, 79, 106	0
1	D	501/516 (97%)	0.03	12 (2%) 59 56	20, 35, 65, 100	0
All	All	2008/2064 (97%)	0.11	81 (4%) 38 33	20, 36, 75, 111	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	533	ALA	5.5
1	C	517	CYS	4.7
1	D	526	GLU	4.5
1	C	518	PHE	4.4
1	C	519	LYS	4.3
1	A	524	ASP	4.2
1	A	530	THR	4.2
1	C	435	HIS	4.0
1	C	534	GLN	4.0
1	A	517	CYS	3.9
1	C	96	ASP	3.8
1	A	518	PHE	3.8
1	A	528	GLY	3.8
1	A	527	LYS	3.8
1	A	519	LYS	3.6
1	A	522	GLN	3.6
1	A	430	ASN	3.6
1	C	535	LEU	3.6
1	A	125	GLY	3.6
1	C	387	ASN	3.4
1	A	532	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	230	THR	3.3
1	C	523	LYS	3.3
1	A	422	ASN	3.3
1	D	529	ASP	3.2
1	D	530	THR	3.2
1	C	448	LEU	3.2
1	A	525	ARG	3.1
1	A	529	ASP	3.1
1	B	516	GLU	3.1
1	A	202	GLY	3.1
1	A	523	LYS	3.1
1	C	124	ASN	3.0
1	A	521	GLN	3.0
1	C	446	ALA	2.9
1	C	524	ASP	2.8
1	C	123	GLY	2.8
1	D	83	TYR	2.8
1	D	525	ARG	2.8
1	D	225	TYR	2.8
1	B	520	LEU	2.8
1	C	516	GLU	2.8
1	D	223	MET	2.7
1	C	98	GLY	2.7
1	B	149	LEU	2.7
1	D	528	GLY	2.7
1	A	534	GLN	2.7
1	D	522	GLN	2.7
1	D	426	GLU	2.6
1	B	528	GLY	2.6
1	A	526	GLU	2.5
1	A	520	LEU	2.5
1	C	515	LYS	2.4
1	C	514	GLN	2.4
1	D	461	TYR	2.4
1	B	441	ASN	2.4
1	C	459	ASN	2.4
1	B	370	TYR	2.4
1	C	199	SER	2.4
1	A	124	ASN	2.4
1	C	436	LYS	2.4
1	C	225	TYR	2.4
1	D	385	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	226	GLY	2.3
1	C	79	ASP	2.3
1	A	149	LEU	2.2
1	C	447	LYS	2.2
1	C	525	ARG	2.2
1	A	448	LEU	2.1
1	B	197	GLY	2.1
1	B	229	ASP	2.1
1	A	96	ASP	2.1
1	A	388	GLN	2.1
1	A	509	ASN	2.1
1	B	199	SER	2.1
1	C	354	TYR	2.1
1	A	145	SER	2.1
1	A	130	ASP	2.1
1	A	144	ALA	2.0
1	B	169	PHE	2.0
1	C	412	ASN	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 carbohydrates 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(\AA^2)	Q<0.9
3	LYS	D	602	10/10	0.92	0.19	20,21,21,21	0
3	LYS	C	602	10/10	0.92	0.20	23,25,26,26	0
2	D4U	C	601	20/20	0.93	0.18	28,29,30,30	0
2	D4U	B	601	20/20	0.94	0.19	22,23,25,25	0
2	D4U	D	601	20/20	0.94	0.17	27,27,28,28	0

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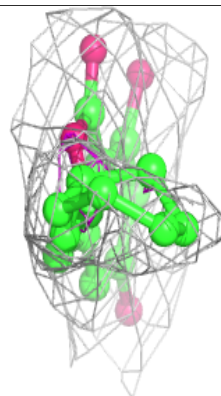
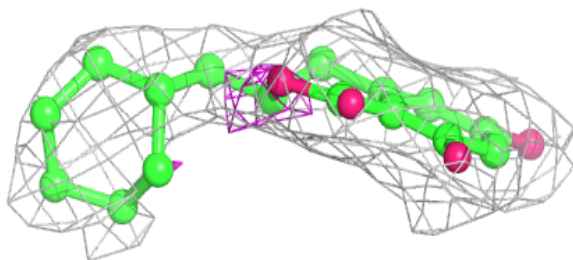
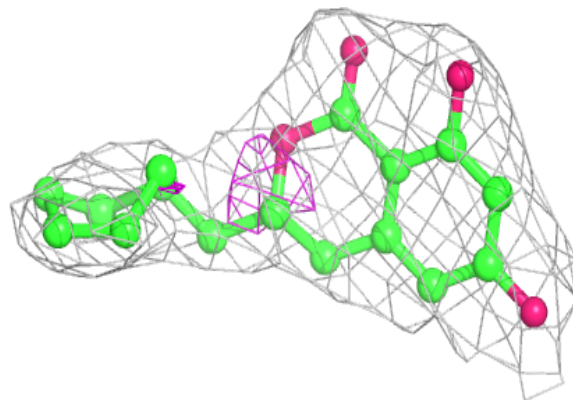
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	LYS	B	602	10/10	0.95	0.19	21,22,29,29	0
2	D4U	A	601	20/20	0.96	0.15	20,21,29,33	0
3	LYS	A	602	10/10	0.96	0.16	20,21,21,21	0

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.

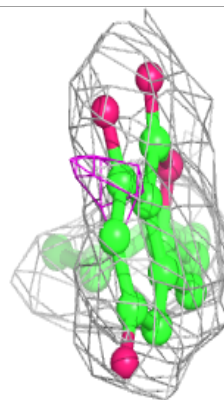
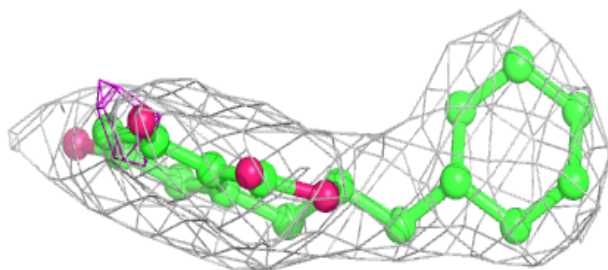
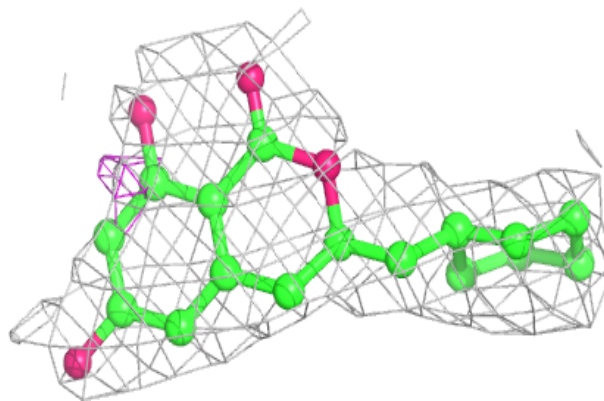
Electron density around D4U C 601:

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

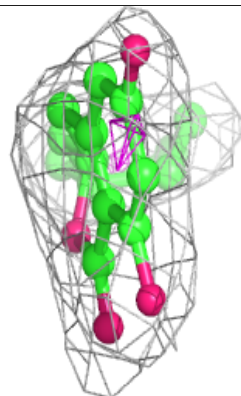
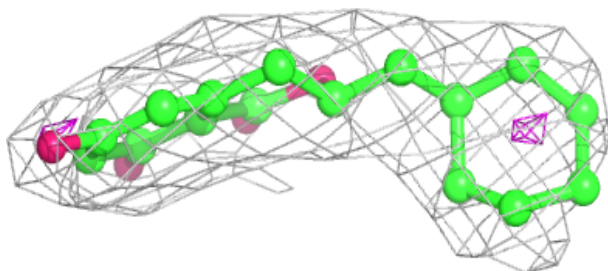
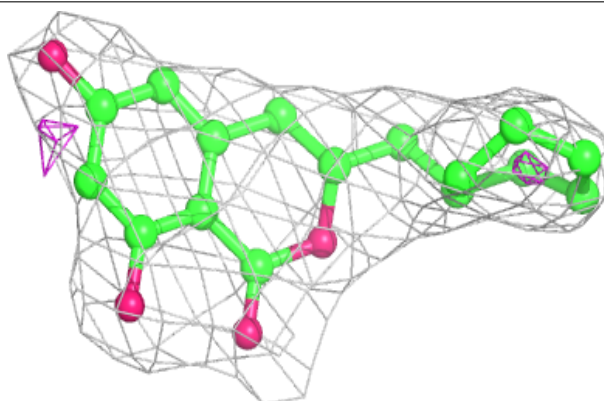


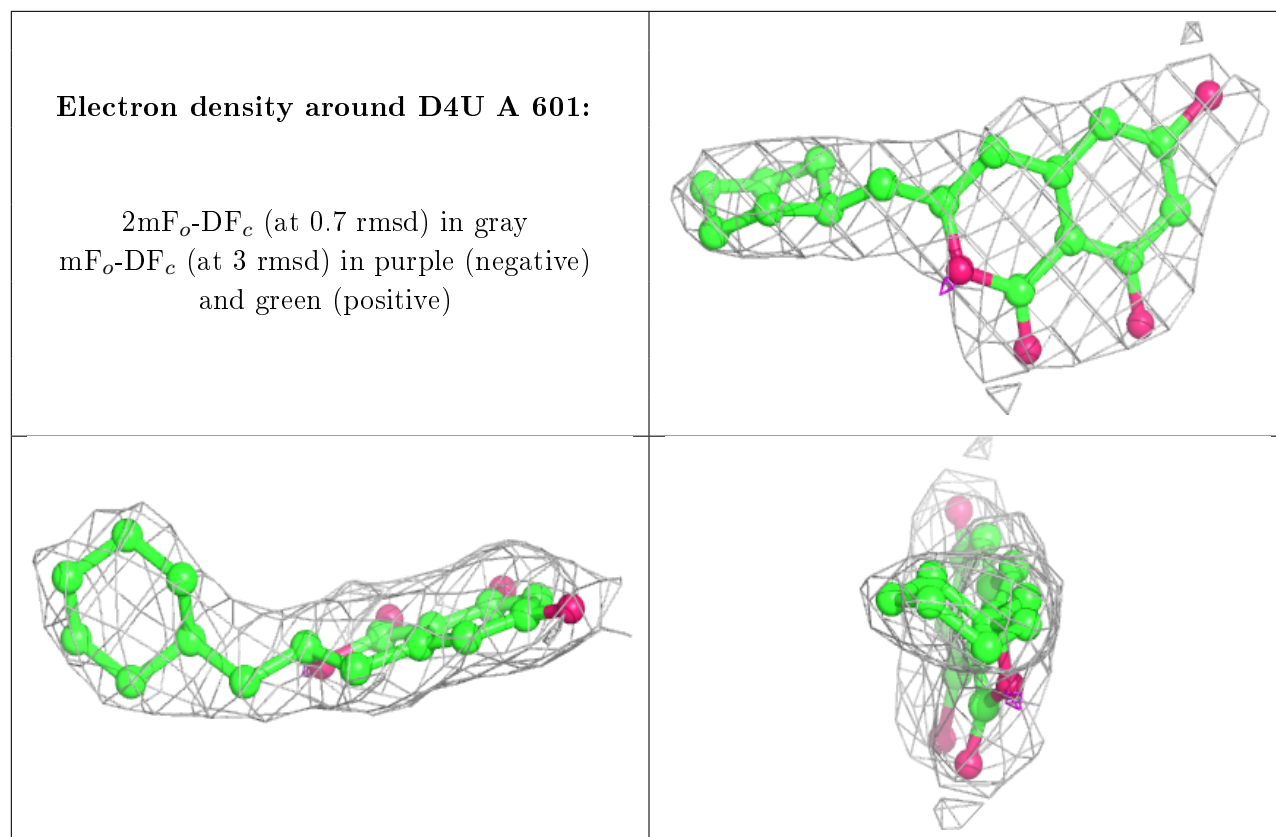
Electron density around D4U B 601:

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

**Electron density around D4U 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.