



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 01:21 AM JST

PDB ID : 6KCT  
Title : Crystal structure of plasmodium lysyl-tRNA synthetase in complex with a cladosporin derivative 5  
Authors : Zhou, J.; Fang, P.  
Deposited on : 2019-06-29  
Resolution : 3.25 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](mailto: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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

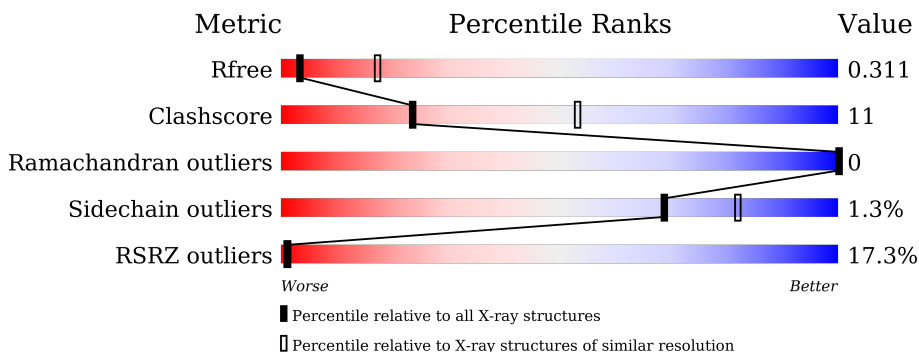
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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  $\geq 3$ , 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	 17% 77% 20% ..
1	B	516	 12% 78% 19% ..
1	C	516	 22% 74% 22% .
1	D	516	 17% 76% 20% ..

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LYS	B	602	-	-	-	X
3	LYS	C	602	-	-	X	X
3	LYS	D	602	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15828 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
			Total	C	N	O	S			
1	A	506	Total 3925	C 2522	N 655	O 731	S 17	0	0	0
1	B	504	Total 3910	C 2515	N 650	O 728	S 17	0	0	0
1	C	498	Total 3872	C 2491	N 644	O 721	S 16	0	0	0
1	D	501	Total 3921	C 2528	N 651	O 726	S 16	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

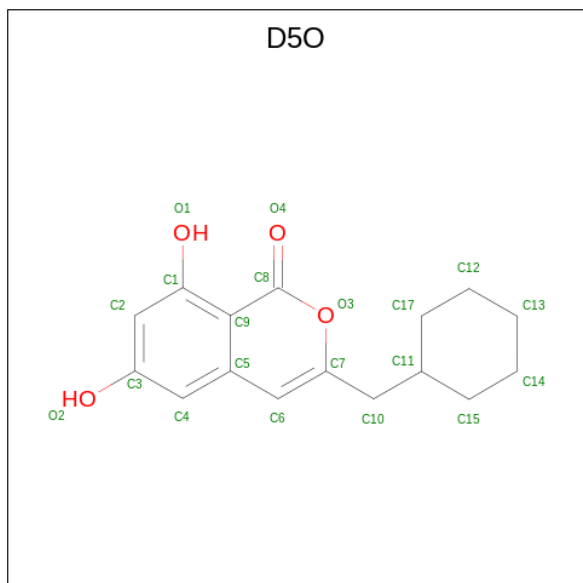
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	initiating methionine	UNP W7JP72
A	584	GLY	-	expression tag	UNP W7JP72
A	585	GLY	-	expression tag	UNP W7JP72
A	586	HIS	-	expression tag	UNP W7JP72
A	587	HIS	-	expression tag	UNP W7JP72
A	588	HIS	-	expression tag	UNP W7JP72
A	589	HIS	-	expression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

*Continued on next page...*

Continued from previous page...

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-(cyclohexylmethyl)-6,8-bis(oxidanyl)isochromen-1-one (three-letter code: D5O) (formula: C<sub>16</sub>H<sub>18</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



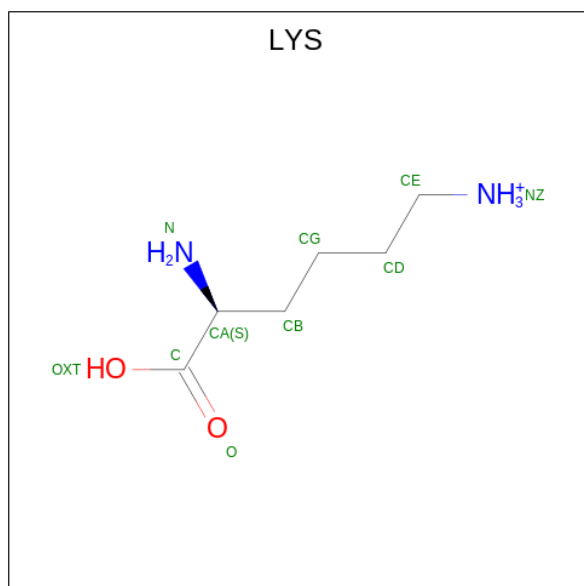
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	A	1	Total	C	O	0	0
			20	16	4		
2	B	1	Total	C	O	0	0
			20	16	4		
2	C	1	Total	C	O	0	0
			20	16	4		

Continued on next page...

Continued from previous page...

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		

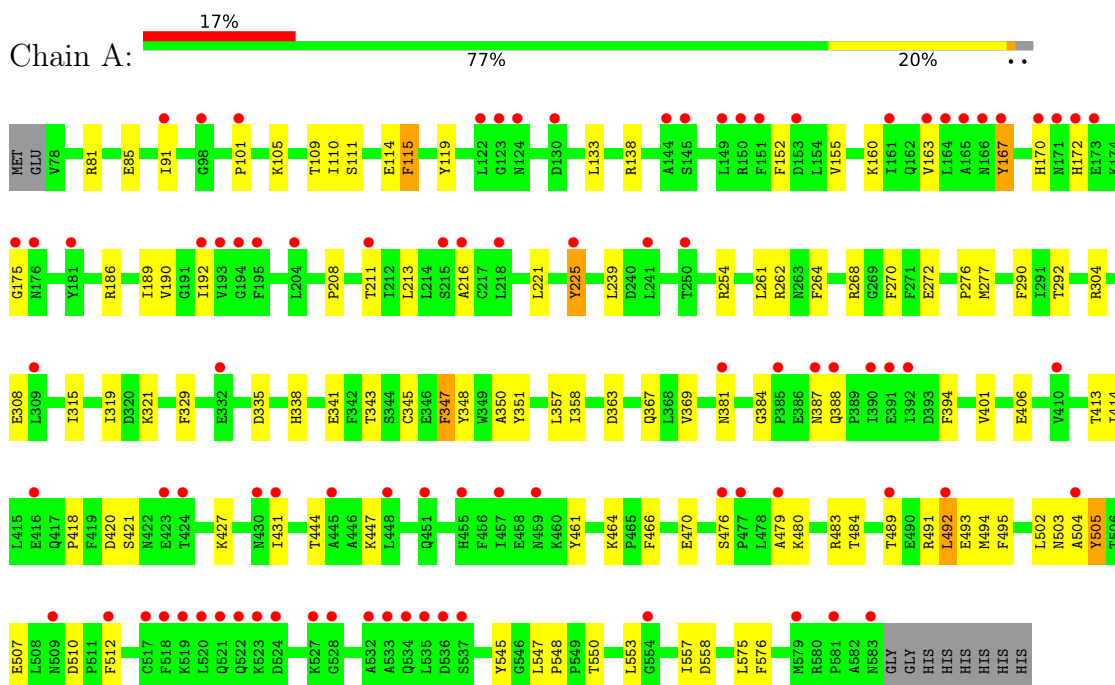
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	20	Total	O	0	0
			20	20		
4	C	20	Total	O	0	0
			20	20		
4	D	19	Total	O	0	0
			19	19		

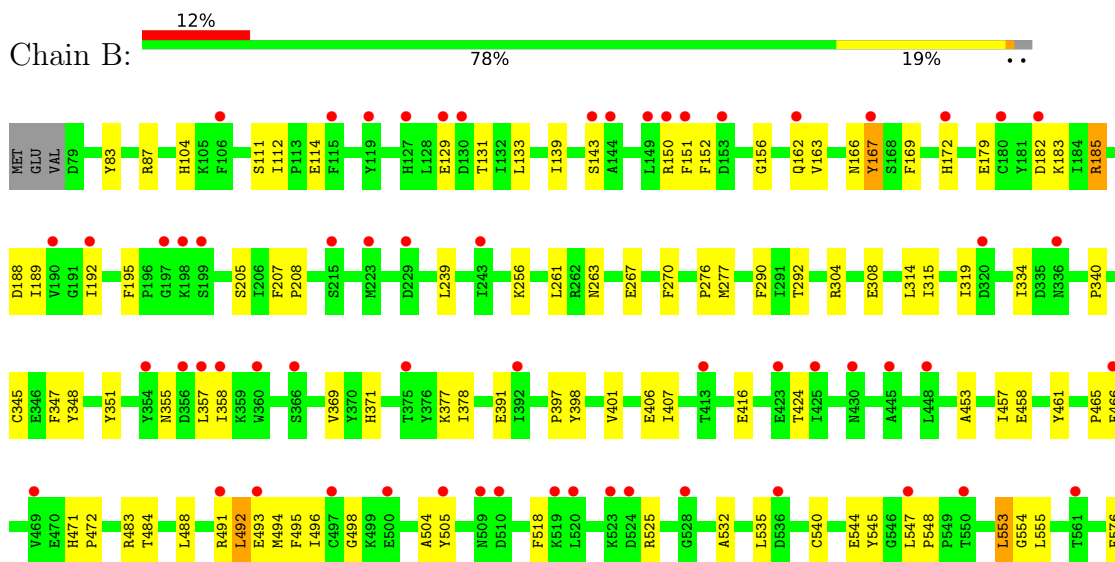
### 3 Residue-property plots [i](#)

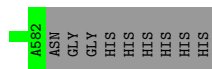
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

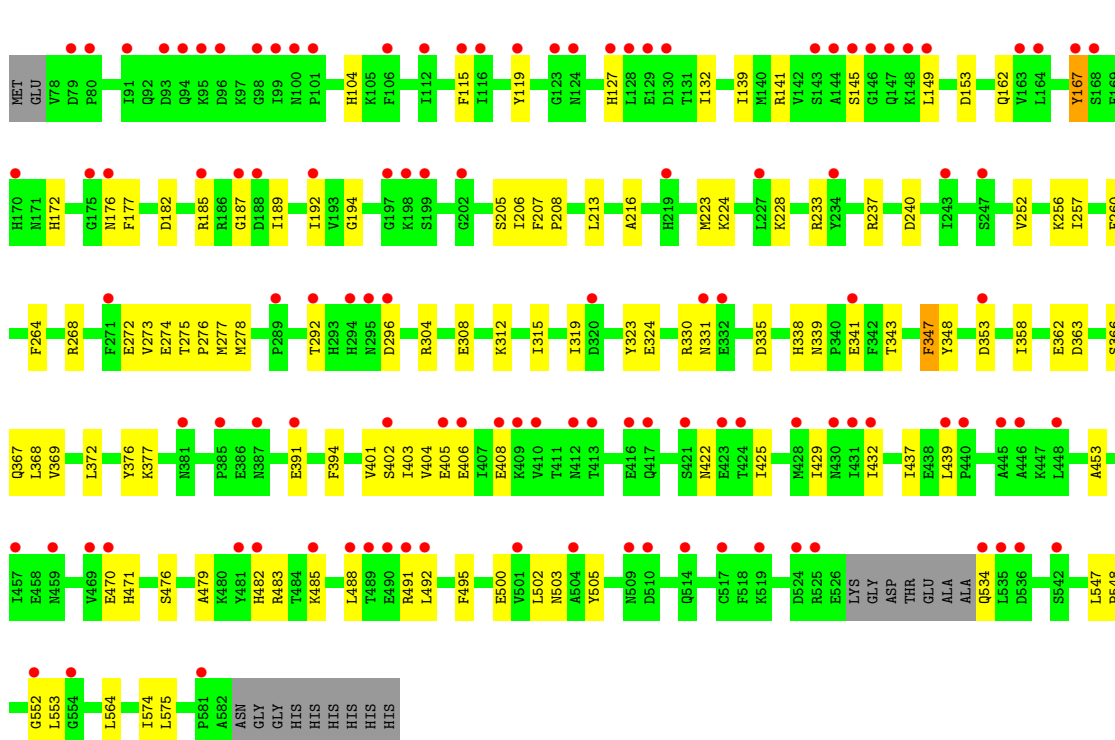
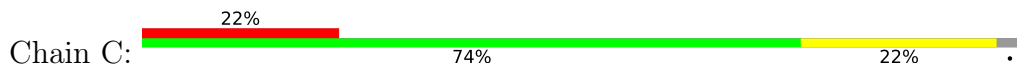


- Molecule 1: Lysine-tRNA ligase

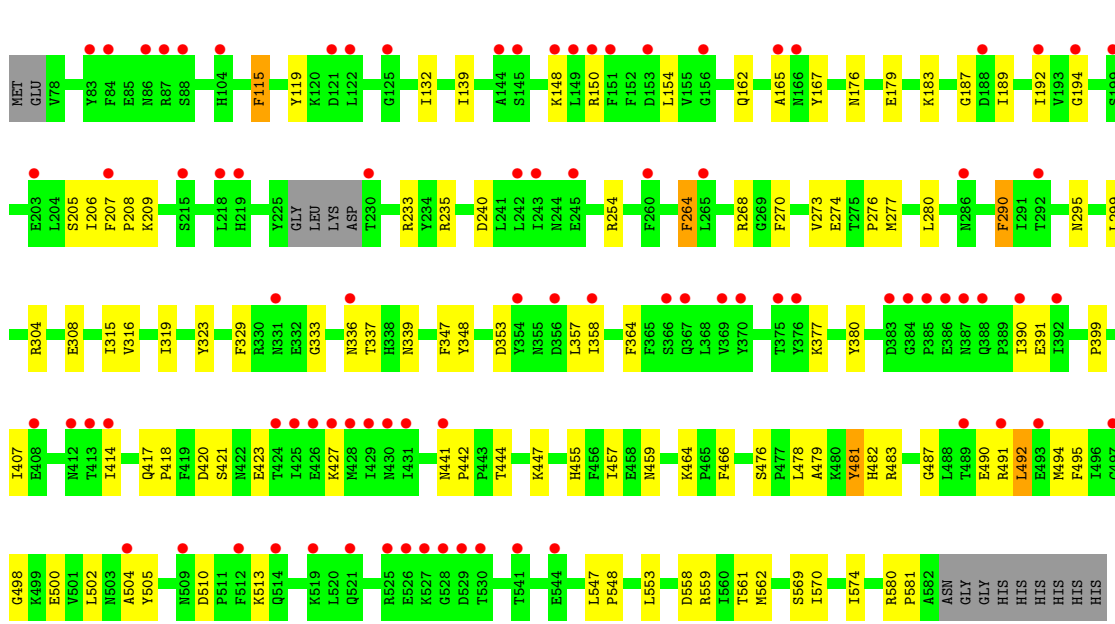
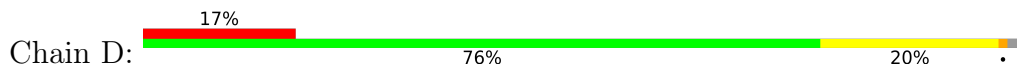




• Molecule 1: Lysine-tRNA ligase



• Molecule 1: Lysine-tRNA ligase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.11Å 89.70Å 100.05Å 76.76° 72.80° 80.03°	Depositor
Resolution (Å)	48.95 – 3.25 48.95 – 3.25	Depositor EDS
% Data completeness (in resolution range)	93.3 (48.95-3.25) 94.0 (48.95-3.25)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 3.25Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.292 , 0.312 0.292 , 0.311	Depositor DCC
$R_{free}$ test set	1655 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtrriage
Anisotropy	0.828	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 19.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.74	EDS
Total number of atoms	15828	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: D5O

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	0.34	0/4023	0.61	0/5467
1	B	0.37	0/4008	0.63	0/5453
1	C	0.37	0/3968	0.63	0/5392
1	D	0.34	0/4019	0.61	0/5456
All	All	0.35	0/16018	0.62	0/21768

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	3925	0	3687	86	0
1	B	3910	0	3656	86	0
1	C	3872	0	3640	96	0
1	D	3921	0	3731	97	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	0	0
3	A	10	0	12	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	12	1	0
3	C	10	0	12	7	0
3	D	10	0	12	0	0
4	A	21	0	0	0	0
4	B	20	0	0	1	0
4	C	20	0	0	1	0
4	D	19	0	0	0	0
All	All	15828	0	14762	341	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 11.

All (341) 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:264:PHE:HE1	1:D:268:ARG:CZ	1.63	1.12
1:C:347:PHE:HE1	1:C:553:LEU:HB3	1.33	0.90
1:A:347:PHE:HE1	1:A:553:LEU:HB3	1.35	0.90
1:B:347:PHE:CD1	1:B:553:LEU:HD22	2.06	0.90
1:D:264:PHE:CE1	1:D:268:ARG:CZ	2.54	0.89
1:B:347:PHE:CE1	1:B:553:LEU:HB3	2.06	0.89
1:C:505:TYR:CE1	3:C:602:LYS:HE2	2.08	0.88
1:D:254:ARG:HG3	1:D:561:THR:HG21	1.60	0.84
1:C:347:PHE:CE1	1:C:553:LEU:HB3	2.11	0.84
1:A:347:PHE:CE1	1:A:553:LEU:HB3	2.13	0.83
1:A:315:ILE:HG21	1:A:550:THR:HG21	1.61	0.81
1:B:192:ILE:HG23	1:B:208:PRO:HB3	1.64	0.80
1:B:525:ARG:HG2	1:B:532:ALA:HB3	1.63	0.80
1:B:347:PHE:HE1	1:B:553:LEU:HB3	1.46	0.79
1:D:192:ILE:HG23	1:D:208:PRO:HB3	1.63	0.79
1:D:270:PHE:CE2	1:D:347:PHE:HD2	2.02	0.78
1:A:418:PRO:HG2	1:A:421:SER:HB3	1.64	0.78
1:C:167:TYR:CE1	1:C:172:HIS:CE1	2.72	0.78
1:C:189:ILE:HG21	1:D:548:PRO:HB3	1.66	0.78
1:D:264:PHE:CE1	1:D:268:ARG:NH1	2.53	0.77
1:C:401:VAL:HG13	1:C:406:GLU:HG3	1.66	0.77
1:D:347:PHE:CE1	1:D:553:LEU:HB3	2.19	0.77
1:B:347:PHE:HD1	1:B:553:LEU:HD22	1.50	0.76
1:C:275:THR:HG23	1:C:276:PRO:HD2	1.67	0.76
1:A:350:ALA:HA	1:A:550:THR:HG22	1.68	0.73
1:B:270:PHE:CE2	1:B:347:PHE:HD2	2.07	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:PHE:CE1	1:B:553:LEU:HD13	2.23	0.72
1:C:331:ASN:ND2	1:D:295:ASN:OD1	2.22	0.72
1:B:553:LEU:C	1:B:553:LEU:HD23	2.11	0.71
1:D:444:THR:HG23	1:D:447:LYS:H	1.54	0.71
1:C:141:ARG:HB3	1:C:153:ASP:HB2	1.73	0.70
1:D:407:ILE:HG13	1:D:457:ILE:HD11	1.72	0.70
1:A:401:VAL:HG13	1:A:406:GLU:HG3	1.73	0.70
1:C:505:TYR:CE1	3:C:602:LYS:CE	2.74	0.69
1:D:510:ASP:OD2	1:D:513:LYS:NZ	2.23	0.69
1:B:347:PHE:HE1	1:B:553:LEU:HD13	1.56	0.69
1:D:264:PHE:HE1	1:D:268:ARG:NH1	1.91	0.69
1:D:399:PRO:HD3	1:D:464:LYS:HE2	1.73	0.68
1:C:192:ILE:HG23	1:C:208:PRO:HB3	1.74	0.68
1:A:167:TYR:CE1	1:A:172:HIS:NE2	2.62	0.68
1:D:481:TYR:HE2	1:D:513:LYS:HE2	1.60	0.67
1:D:254:ARG:NH1	1:D:558:ASP:OD1	2.25	0.67
1:D:347:PHE:HE1	1:D:553:LEU:HB3	1.58	0.65
1:B:182:ASP:O	1:B:185:ARG:NH1	2.29	0.65
1:A:507:GLU:OE2	3:A:602:LYS:NZ	2.30	0.65
1:D:417:GLN:NE2	1:D:487:GLY:HA3	2.12	0.64
1:A:167:TYR:HE1	1:A:172:HIS:NE2	1.96	0.64
1:D:479:ALA:HA	1:D:505:TYR:CE2	2.33	0.64
1:B:347:PHE:CE1	1:B:553:LEU:HD22	2.33	0.63
1:D:270:PHE:CE2	1:D:347:PHE:CD2	2.86	0.63
1:C:167:TYR:CE1	1:C:172:HIS:HE1	2.17	0.63
1:C:260:PHE:CE2	1:C:368:LEU:HA	2.34	0.63
1:B:518:PHE:CD2	1:B:535:LEU:HA	2.34	0.63
1:B:553:LEU:HD23	1:B:554:GLY:N	2.14	0.62
1:C:432:ILE:HG23	1:C:437:ILE:HB	1.80	0.62
1:D:353:ASP:OD2	1:D:483:ARG:NH2	2.27	0.62
1:C:491:ARG:HA	1:C:505:TYR:HB3	1.81	0.62
1:A:192:ILE:HG23	1:A:208:PRO:HB3	1.82	0.62
1:D:580:ARG:HG2	1:D:581:PRO:HD2	1.82	0.62
1:A:110:ILE:HD12	1:A:115:PHE:HB2	1.81	0.61
1:B:270:PHE:CE2	1:B:347:PHE:CD2	2.88	0.61
1:A:262:ARG:NH1	1:A:272:GLU:OE2	2.34	0.60
1:A:444:THR:HG23	1:A:447:LYS:H	1.66	0.60
1:B:369:VAL:HG13	1:B:378:ILE:HD11	1.84	0.60
1:C:548:PRO:HB3	1:D:189:ILE:HG21	1.82	0.60
1:A:152:PHE:HB2	1:A:163:VAL:HB	1.84	0.60
1:C:505:TYR:CD1	3:C:602:LYS:HE2	2.37	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HD21	1:A:216:ALA:HB2	1.84	0.59
1:B:358:ILE:HD13	1:B:492:LEU:HD13	1.83	0.59
1:A:155:VAL:HG12	1:A:160:LYS:HB2	1.85	0.59
1:C:223:MET:HG3	1:C:224:LYS:H	1.68	0.59
1:C:260:PHE:HE2	1:C:368:LEU:HA	1.67	0.58
1:C:470:GLU:HB3	1:C:488:LEU:HD23	1.84	0.58
1:B:347:PHE:HE1	1:B:553:LEU:CB	2.15	0.58
1:A:110:ILE:HD13	1:A:133:LEU:HD13	1.85	0.58
1:C:228:LYS:O	1:C:233:ARG:NH1	2.35	0.58
1:D:270:PHE:HE2	1:D:347:PHE:HD2	1.50	0.58
1:B:416:GLU:O	1:B:424:THR:HG21	2.03	0.58
1:D:115:PHE:HD1	1:D:119:TYR:HD2	1.52	0.58
1:A:358:ILE:HD13	1:A:492:LEU:HD13	1.85	0.58
1:C:401:VAL:CG1	1:C:406:GLU:HG3	2.33	0.57
1:A:239:LEU:HD21	1:B:545:TYR:CE2	2.39	0.57
1:A:502:LEU:HD11	1:A:553:LEU:HD11	1.86	0.57
1:B:483:ARG:HG3	1:B:484:THR:HG23	1.86	0.57
1:C:369:VAL:HG21	1:C:394:PHE:CD2	2.39	0.57
1:D:264:PHE:HD1	1:D:264:PHE:O	1.87	0.57
1:D:547:LEU:HD12	1:D:548:PRO:HD2	1.87	0.57
1:B:547:LEU:HD12	1:B:548:PRO:HD2	1.87	0.57
1:D:308:GLU:HG3	1:D:348:TYR:OH	2.04	0.56
1:B:398:TYR:N	1:B:398:TYR:CD1	2.72	0.56
1:D:179:GLU:O	1:D:183:LYS:HD3	2.06	0.56
1:C:308:GLU:OE2	1:C:505:TYR:OH	2.22	0.56
1:B:167:TYR:CE1	1:B:172:HIS:CE1	2.94	0.56
1:D:417:GLN:HE22	1:D:487:GLY:HA3	1.69	0.56
1:C:304:ARG:NH1	1:C:324:GLU:OE2	2.38	0.56
1:D:270:PHE:HE2	1:D:347:PHE:CD2	2.22	0.56
1:B:491:ARG:HA	1:B:505:TYR:HB3	1.87	0.56
1:B:166:ASN:HB3	1:B:169:PHE:HD2	1.71	0.55
1:C:503:ASN:O	3:C:602:LYS:HD2	2.07	0.55
1:C:312:LYS:HG3	1:C:348:TYR:CE2	2.41	0.55
1:D:139:ILE:O	1:D:187:GLY:N	2.31	0.55
1:D:264:PHE:HE2	1:D:364:PHE:HA	1.70	0.55
1:A:189:ILE:HG21	1:B:548:PRO:HB3	1.88	0.54
1:D:148:LYS:HG3	1:D:167:TYR:HB3	1.89	0.54
1:A:548:PRO:O	1:A:550:THR:HG23	2.07	0.54
1:C:252:VAL:HG12	1:C:256:LYS:HE2	1.88	0.54
1:A:308:GLU:HG3	1:A:348:TYR:OH	2.08	0.54
1:D:491:ARG:HA	1:D:505:TYR:HB3	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PHE:HD1	1:A:119:TYR:HD2	1.55	0.54
1:A:343:THR:HG22	1:A:557:ILE:HD12	1.90	0.54
1:B:179:GLU:O	1:B:183:LYS:HD3	2.07	0.54
1:B:167:TYR:HD1	1:B:167:TYR:O	1.91	0.53
1:A:81:ARG:O	1:A:85:GLU:HG3	2.08	0.53
1:C:115:PHE:HD1	1:C:119:TYR:HD2	1.56	0.53
1:D:483:ARG:HG3	1:D:490:GLU:OE2	2.09	0.53
1:B:308:GLU:HG3	1:B:348:TYR:OH	2.09	0.53
1:C:292:THR:OG1	1:D:290:PHE:HB3	2.09	0.53
1:D:377:LYS:HD3	1:D:391:GLU:OE2	2.09	0.53
1:A:292:THR:OG1	1:B:290:PHE:HB3	2.09	0.53
1:B:347:PHE:HE1	1:B:553:LEU:CD1	2.21	0.53
1:D:115:PHE:CD1	1:D:119:TYR:HD2	2.26	0.53
1:D:559:ARG:HA	1:D:562:MET:HE2	1.90	0.53
1:B:315:ILE:HD13	1:B:319:ILE:O	2.09	0.52
1:D:336:ASN:O	1:D:570:ILE:N	2.42	0.52
1:D:479:ALA:HA	1:D:505:TYR:HE2	1.74	0.52
1:C:273:VAL:HG22	1:C:274:GLU:H	1.72	0.52
1:D:233:ARG:HB3	1:D:240:ASP:OD2	2.09	0.52
1:A:461:TYR:HB2	1:A:466:PHE:CD1	2.45	0.52
1:A:483:ARG:HG3	1:A:484:THR:HG23	1.90	0.52
1:C:167:TYR:HD1	1:C:167:TYR:O	1.93	0.52
1:B:540:CYS:O	1:B:544:GLU:HG3	2.10	0.52
1:A:493:GLU:HB3	1:A:495:PHE:HE1	1.74	0.52
1:B:401:VAL:HG13	1:B:406:GLU:HG3	1.90	0.52
1:C:552:GLY:C	3:C:602:LYS:HZ3	2.13	0.51
1:D:339:ASN:HD22	1:D:574:ILE:HD13	1.75	0.51
1:A:510:ASP:OD1	1:A:512:PHE:HB2	2.10	0.51
1:A:341:GLU:OE2	1:B:276:PRO:HA	2.10	0.51
1:D:491:ARG:HA	1:D:505:TYR:CB	2.40	0.51
1:B:150:ARG:NH1	1:B:182:ASP:OD1	2.39	0.51
1:C:296:ASP:OD2	1:D:333:GLY:HA2	2.10	0.51
1:C:278:MET:HG3	1:D:329:PHE:HE2	1.75	0.51
1:C:404:VAL:O	1:C:408:GLU:HG3	2.10	0.51
1:A:167:TYR:HD1	1:A:167:TYR:O	1.93	0.51
1:D:455:HIS:O	1:D:455:HIS:ND1	2.44	0.51
1:B:263:ASN:O	1:B:267:GLU:HG3	2.11	0.51
1:C:104:HIS:CE1	1:D:481:TYR:HE1	2.29	0.50
1:C:505:TYR:HE1	3:C:602:LYS:CE	2.21	0.50
1:A:270:PHE:HA	1:A:321:LYS:HB3	1.93	0.50
1:A:357:LEU:HD13	1:A:504:ALA:HB1	1.92	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:LEU:HD11	1:D:553:LEU:HD11	1.92	0.50
1:D:358:ILE:HD13	1:D:492:LEU:HD13	1.93	0.50
1:A:480:LYS:HD3	1:B:104:HIS:CD2	2.47	0.50
1:B:205:SER:HB2	1:B:207:PHE:HE1	1.76	0.50
1:B:270:PHE:HE2	1:B:347:PHE:CD2	2.30	0.50
1:D:418:PRO:HB2	1:D:420:ASP:OD1	2.12	0.50
1:B:112:ILE:HD12	1:B:156:GLY:HA3	1.94	0.50
1:C:366:SER:HB2	1:C:376:TYR:HE2	1.77	0.50
1:C:495:PHE:CZ	1:C:500:GLU:HB2	2.47	0.49
1:D:316:VAL:HG12	1:D:547:LEU:HA	1.94	0.49
1:D:482:HIS:HA	1:D:490:GLU:HG3	1.92	0.49
1:A:491:ARG:NH2	1:A:493:GLU:OE2	2.45	0.49
1:D:132:ILE:HD11	1:D:209:LYS:HE2	1.94	0.49
1:A:167:TYR:HE1	1:A:172:HIS:CE1	2.31	0.49
1:D:176:ASN:HB3	1:D:179:GLU:HB3	1.94	0.49
1:C:237:ARG:NH1	1:C:240:ASP:OD2	2.45	0.49
1:A:190:VAL:HG12	1:A:192:ILE:HG13	1.95	0.49
1:C:182:ASP:O	1:C:185:ARG:NH1	2.46	0.49
1:D:399:PRO:HG2	1:D:466:PHE:HB2	1.93	0.49
1:A:369:VAL:HG21	1:A:394:PHE:CD2	2.48	0.49
1:A:504:ALA:O	1:A:505:TYR:HB3	2.12	0.49
1:B:334:ILE:HG12	1:B:340:PRO:HD3	1.95	0.49
1:D:414:ILE:O	1:D:427:LYS:NZ	2.38	0.49
1:A:270:PHE:CE1	1:A:321:LYS:HD2	2.48	0.48
1:B:401:VAL:CG1	1:B:406:GLU:HG3	2.43	0.48
1:A:545:TYR:CD2	1:B:239:LEU:HD21	2.48	0.48
1:C:575:LEU:HD11	1:D:273:VAL:HB	1.95	0.48
1:C:403:ILE:HD11	1:C:453:ALA:HB2	1.95	0.48
1:A:494:MET:HB3	1:A:502:LEU:HB3	1.96	0.48
1:A:505:TYR:HE1	3:A:602:LYS:CD	2.27	0.48
1:D:264:PHE:CD1	1:D:268:ARG:NH1	2.80	0.48
1:A:315:ILE:HD13	1:A:319:ILE:O	2.13	0.48
1:C:422:ASN:O	1:C:425:ILE:HG22	2.14	0.48
1:A:548:PRO:HB3	1:B:189:ILE:HG21	1.94	0.48
1:A:277:MET:HA	1:A:304:ARG:HD3	1.96	0.48
1:B:357:LEU:HD13	1:B:504:ALA:HB1	1.94	0.48
1:C:353:ASP:CG	1:C:483:ARG:HH22	2.15	0.48
1:C:115:PHE:HE2	1:C:206:ILE:HB	1.79	0.48
1:D:479:ALA:HA	1:D:505:TYR:CD2	2.48	0.47
1:A:290:PHE:HB3	1:B:292:THR:OG1	2.13	0.47
1:C:277:MET:HA	1:C:304:ARG:HD3	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:LYS:HD3	1:C:391:GLU:OE2	2.14	0.47
1:D:479:ALA:CA	1:D:505:TYR:CE2	2.97	0.47
1:C:341:GLU:OE2	1:D:276:PRO:HA	2.14	0.47
1:C:192:ILE:CG2	1:C:208:PRO:HB3	2.44	0.47
1:D:162:GLN:HB3	1:D:205:SER:OG	2.14	0.47
1:B:256:LYS:HE3	1:B:371:HIS:NE2	2.29	0.47
1:C:343:THR:OG1	1:D:274:GLU:OE1	2.29	0.47
1:A:261:LEU:HD21	1:A:345:CYS:SG	2.55	0.47
1:C:167:TYR:HE1	1:C:172:HIS:CE1	2.29	0.47
1:C:272:GLU:HB2	1:C:323:TYR:CZ	2.49	0.47
1:C:353:ASP:OD1	1:C:483:ARG:NH2	2.48	0.47
1:C:358:ILE:O	1:C:362:GLU:HG3	2.15	0.47
1:D:357:LEU:HD13	1:D:504:ALA:HB1	1.95	0.47
1:D:441:ASN:CB	1:D:442:PRO:HD3	2.45	0.47
1:D:491:ARG:HG3	1:D:505:TYR:HB3	1.96	0.47
1:D:194:GLY:HA3	1:D:207:PHE:O	2.15	0.47
1:A:547:LEU:HD12	1:A:548:PRO:HD2	1.96	0.47
1:A:111:SER:OG	1:A:114:GLU:HG2	2.13	0.47
1:A:479:ALA:HB2	1:A:505:TYR:HD2	1.80	0.47
1:B:369:VAL:CG1	1:B:378:ILE:HD11	2.44	0.47
1:C:403:ILE:HG21	1:C:471:HIS:HA	1.96	0.46
1:D:423:GLU:OE1	1:D:423:GLU:N	2.42	0.46
1:B:465:PRO:HB3	1:B:496:ILE:HG12	1.96	0.46
1:B:553:LEU:HD21	1:B:555:LEU:HG	1.97	0.46
1:A:239:LEU:HD21	1:B:545:TYR:CD2	2.50	0.46
1:B:518:PHE:HD2	1:B:535:LEU:HA	1.76	0.46
1:C:315:ILE:HD13	1:C:319:ILE:O	2.15	0.46
1:A:503:ASN:HB3	3:A:602:LYS:HB3	1.96	0.46
1:A:576:PHE:HB2	1:B:276:PRO:CG	2.46	0.46
1:D:347:PHE:CD1	1:D:553:LEU:HB3	2.51	0.46
1:B:471:HIS:CE1	1:B:493:GLU:HG3	2.51	0.46
1:C:502:LEU:HD11	1:C:553:LEU:HD11	1.97	0.46
1:A:276:PRO:CG	1:B:576:PHE:HB2	2.46	0.45
1:A:479:ALA:HB2	1:A:505:TYR:CD2	2.51	0.45
1:C:403:ILE:HG23	1:C:404:VAL:H	1.81	0.45
1:C:534:GLN:N	4:C:701:HOH:O	2.48	0.45
1:B:277:MET:HA	1:B:304:ARG:HD3	1.98	0.45
1:C:167:TYR:CD1	1:C:172:HIS:CE1	3.04	0.45
1:C:347:PHE:HE1	1:C:553:LEU:CB	2.17	0.45
1:D:150:ARG:HB2	1:D:165:ALA:HB3	1.98	0.45
1:C:264:PHE:O	1:C:268:ARG:HD3	2.16	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ARG:NH2	1:B:188:ASP:OD1	2.49	0.45
1:B:162:GLN:HG3	1:B:163:VAL:N	2.31	0.45
1:C:335:ASP:OD1	1:C:338:HIS:N	2.49	0.45
1:A:109:THR:HG22	1:A:110:ILE:HG23	1.99	0.45
1:C:162:GLN:HB3	1:C:205:SER:OG	2.17	0.45
1:B:143:SER:OG	1:B:151:PHE:HB2	2.17	0.45
1:D:418:PRO:HG2	1:D:421:SER:HB3	1.98	0.45
1:A:91:ILE:HG23	1:A:101:PRO:HG3	1.98	0.45
1:A:170:HIS:NE2	1:A:175:GLY:O	2.36	0.45
1:D:337:THR:O	1:D:559:ARG:NH2	2.47	0.45
1:D:504:ALA:O	1:D:505:TYR:HB3	2.16	0.45
1:B:472:PRO:HA	1:B:488:LEU:HA	1.99	0.45
1:D:380:TYR:O	1:D:390:ILE:HG22	2.16	0.45
1:A:138:ARG:NH2	1:A:189:ILE:HD11	2.32	0.45
1:A:254:ARG:NH2	1:A:558:ASP:OD1	2.39	0.45
1:B:131:THR:HG22	1:B:133:LEU:HG	1.98	0.45
1:D:481:TYR:HE2	1:D:513:LYS:CE	2.29	0.45
1:A:186:ARG:NH1	1:A:221:LEU:HB2	2.32	0.44
1:C:213:LEU:HD21	1:C:216:ALA:HB2	1.99	0.44
1:A:264:PHE:O	1:A:268:ARG:HD3	2.18	0.44
1:A:347:PHE:HE1	1:A:553:LEU:CB	2.18	0.44
1:B:183:LYS:HD2	1:B:183:LYS:N	2.33	0.44
1:B:256:LYS:HD2	1:B:256:LYS:HA	1.69	0.44
1:D:476:SER:HB3	1:D:479:ALA:CB	2.48	0.44
1:A:575:LEU:HD13	1:B:314:LEU:HD11	2.00	0.44
1:C:139:ILE:O	1:C:187:GLY:N	2.42	0.44
1:C:207:PHE:CD1	1:C:207:PHE:N	2.86	0.44
1:C:363:ASP:O	1:C:367:GLN:HG3	2.17	0.44
1:B:347:PHE:HE1	1:B:553:LEU:CG	2.31	0.44
1:A:363:ASP:O	1:A:367:GLN:HG3	2.18	0.44
1:A:413:THR:HG22	1:A:414:ILE:H	1.83	0.44
1:B:377:LYS:HD3	1:B:391:GLU:OE2	2.18	0.44
1:A:335:ASP:OD1	1:A:338:HIS:HB2	2.18	0.44
1:A:427:LYS:O	1:A:431:ILE:HD12	2.18	0.44
1:B:453:ALA:O	1:B:458:GLU:HG3	2.18	0.44
1:C:347:PHE:C	1:C:348:TYR:HD1	2.21	0.44
1:D:183:LYS:N	1:D:183:LYS:HD2	2.33	0.44
1:C:176:ASN:OD1	1:C:177:PHE:N	2.50	0.43
1:A:335:ASP:OD1	1:A:335:ASP:N	2.51	0.43
1:D:476:SER:HB3	1:D:479:ALA:HB2	1.99	0.43
1:D:495:PHE:CZ	1:D:500:GLU:HB2	2.53	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ARG:NH2	3:C:602:LYS:O	2.49	0.43
1:B:407:ILE:HG13	1:B:457:ILE:HD11	1.99	0.43
1:C:348:TYR:N	1:C:348:TYR:CD1	2.86	0.43
1:D:481:TYR:CE2	1:D:513:LYS:HE2	2.48	0.43
1:C:358:ILE:HD13	1:C:492:LEU:HD13	2.00	0.43
1:B:348:TYR:CD1	1:B:348:TYR:N	2.87	0.43
1:B:494:MET:C	1:B:495:PHE:HD1	2.21	0.43
1:C:491:ARG:HA	1:C:505:TYR:CB	2.47	0.43
1:A:401:VAL:HG13	1:A:406:GLU:CG	2.46	0.43
1:C:339:ASN:ND2	1:C:574:ILE:HD13	2.33	0.43
1:B:166:ASN:HB3	1:B:169:PHE:CD2	2.50	0.43
1:B:167:TYR:O	1:B:167:TYR:CD1	2.71	0.43
1:B:261:LEU:HD21	1:B:345:CYS:SG	2.59	0.43
1:D:115:PHE:CD1	1:D:119:TYR:CD2	3.06	0.43
1:B:355:ASN:ND2	4:B:701:HOH:O	2.32	0.42
1:C:547:LEU:HD12	1:C:548:PRO:HD2	2.00	0.42
1:B:111:SER:OG	1:B:114:GLU:HG3	2.19	0.42
1:D:270:PHE:HB3	1:D:323:TYR:HD1	1.83	0.42
1:C:223:MET:CG	1:C:224:LYS:H	2.32	0.42
1:C:275:THR:N	1:C:324:GLU:OE1	2.52	0.42
1:C:348:TYR:HD1	1:C:348:TYR:N	2.16	0.42
1:D:154:LEU:HD22	1:D:192:ILE:HD12	2.01	0.42
1:A:190:VAL:CG1	1:A:211:THR:HG23	2.50	0.42
1:D:280:LEU:HD21	1:D:299:LEU:HD21	2.01	0.42
1:B:129:GLU:HG2	1:B:195:PHE:CE2	2.54	0.42
1:B:461:TYR:HB2	1:B:466:PHE:CD1	2.54	0.42
1:A:167:TYR:O	1:A:167:TYR:CD1	2.72	0.42
1:C:402:SER:HB3	1:C:405:GLU:HB2	2.02	0.42
1:A:189:ILE:HD13	1:B:548:PRO:HB3	2.02	0.42
1:C:115:PHE:HD1	1:C:119:TYR:CD2	2.37	0.42
1:A:381:ASN:HB3	1:A:384:GLY:O	2.20	0.42
1:C:429:ILE:HG12	1:C:439:LEU:HD11	2.02	0.42
1:B:491:ARG:NH2	1:B:493:GLU:OE2	2.53	0.41
1:C:145:SER:O	1:C:149:LEU:HB2	2.19	0.41
1:C:205:SER:HB2	1:C:207:PHE:HE1	1.84	0.41
1:D:235:ARG:NH1	1:D:580:ARG:O	2.44	0.41
1:A:225:TYR:HD1	1:A:225:TYR:O	2.02	0.41
1:C:127:HIS:CE1	1:C:207:PHE:HE2	2.38	0.41
1:C:482:HIS:HB3	1:C:485:LYS:O	2.19	0.41
1:D:478:LEU:O	1:D:505:TYR:HE2	2.03	0.41
1:A:351:TYR:CE1	1:A:548:PRO:HB2	2.55	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:SER:HB2	1:A:489:THR:HG21	2.01	0.41
1:B:505:TYR:CZ	3:B:602:LYS:HD3	2.56	0.41
1:D:270:PHE:HB3	1:D:323:TYR:CD1	2.55	0.41
1:D:315:ILE:HD13	1:D:319:ILE:O	2.19	0.41
1:D:336:ASN:HB3	1:D:569:SER:HA	2.02	0.41
1:A:479:ALA:CB	1:A:505:TYR:HD2	2.33	0.41
1:A:387:ASN:OD1	1:A:388:GLN:N	2.52	0.41
1:B:139:ILE:HG23	1:B:152:PHE:HB3	2.03	0.41
1:B:553:LEU:C	1:B:553:LEU:CD2	2.84	0.41
1:D:459:ASN:OD1	1:D:498:GLY:HA3	2.20	0.41
1:B:458:GLU:O	1:B:498:GLY:HA2	2.21	0.41
1:C:275:THR:O	1:C:304:ARG:NH1	2.54	0.41
1:A:105:LYS:NZ	1:B:351:TYR:O	2.36	0.41
1:C:132:ILE:HA	1:C:194:GLY:O	2.21	0.41
1:C:372:LEU:HD12	1:C:564:LEU:HD13	2.03	0.41
1:C:476:SER:HB3	1:C:479:ALA:HB2	2.02	0.41
1:D:132:ILE:HD12	1:D:132:ILE:HA	1.97	0.41
1:D:277:MET:HA	1:D:304:ARG:HD3	2.02	0.41
1:C:505:TYR:CD1	1:C:505:TYR:N	2.89	0.41
1:C:167:TYR:O	1:C:167:TYR:CD1	2.73	0.40
1:A:470:GLU:HA	1:A:489:THR:O	2.22	0.40
1:C:167:TYR:CD1	1:C:172:HIS:HE1	2.37	0.40
1:D:329:PHE:CD1	1:D:329:PHE:N	2.89	0.40
1:A:418:PRO:HB2	1:A:420:ASP:OD1	2.21	0.40
1:D:494:MET:C	1:D:495:PHE:HD1	2.25	0.40
1:A:476:SER:HB3	1:A:479:ALA:HB2	2.03	0.40
1:C:257:ILE:HG12	1:C:372:LEU:HD11	2.04	0.40
1:D:115:PHE:HE2	1:D:206:ILE:HB	1.86	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%)	492 (98%)	12 (2%)	0	100	100
1	B	502/516 (97%)	488 (97%)	14 (3%)	0	100	100
1	C	494/516 (96%)	481 (97%)	13 (3%)	0	100	100
1	D	497/516 (96%)	485 (98%)	12 (2%)	0	100	100
All	All	1997/2064 (97%)	1946 (97%)	51 (3%)	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	401/464 (86%)	393 (98%)	8 (2%)	55	76
1	B	398/464 (86%)	392 (98%)	6 (2%)	65	80
1	C	397/464 (86%)	395 (100%)	2 (0%)	88	93
1	D	407/464 (88%)	402 (99%)	5 (1%)	71	83
All	All	1603/1856 (86%)	1582 (99%)	21 (1%)	69	82

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	PHE
1	A	167	TYR
1	A	225	TYR
1	A	329	PHE
1	A	347	PHE
1	A	464	LYS
1	A	492	LEU
1	A	505	TYR
1	B	83	TYR
1	B	167	TYR
1	B	185	ARG
1	B	397	PRO
1	B	492	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	553	LEU
1	C	167	TYR
1	C	347	PHE
1	D	115	PHE
1	D	264	PHE
1	D	290	PHE
1	D	481	TYR
1	D	492	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	473	GLN
1	B	104	HIS
1	B	170	HIS
1	B	172	HIS
1	C	162	GLN
1	C	172	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	D5O	C	601	-	22,22,22	1.89	3 (13%)	27,31,31	1.38	4 (14%)
3	LYS	D	602	-	8,9,9	0.82	1 (12%)	9,10,10	1.23	2 (22%)
3	LYS	B	602	-	8,9,9	0.82	1 (12%)	9,10,10	1.14	2 (22%)
3	LYS	C	602	-	8,9,9	1.00	1 (12%)	9,10,10	1.20	1 (11%)
3	LYS	A	602	-	8,9,9	0.82	1 (12%)	9,10,10	1.19	1 (11%)
2	D5O	B	601	-	22,22,22	1.89	3 (13%)	27,31,31	1.42	4 (14%)
2	D5O	D	601	-	22,22,22	1.84	3 (13%)	27,31,31	1.40	4 (14%)
2	D5O	A	601	-	22,22,22	1.90	3 (13%)	27,31,31	1.27	4 (14%)

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	D5O	C	601	-	-	0/4/12/12	0/3/3/3
3	LYS	D	602	-	-	0/9/9/9	-
3	LYS	B	602	-	-	0/9/9/9	-
3	LYS	C	602	-	-	0/9/9/9	-
3	LYS	A	602	-	-	0/9/9/9	-
2	D5O	B	601	-	-	0/4/12/12	0/3/3/3
2	D5O	D	601	-	-	0/4/12/12	0/3/3/3
2	D5O	A	601	-	-	0/4/12/12	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	D5O	C6-C7	7.82	1.39	1.33
2	B	601	D5O	C6-C7	7.76	1.39	1.33
2	C	601	D5O	C6-C7	7.73	1.39	1.33
2	D	601	D5O	C6-C7	7.49	1.39	1.33
2	D	601	D5O	C5-C6	-2.41	1.38	1.43
2	C	601	D5O	C5-C6	-2.31	1.39	1.43
2	B	601	D5O	C5-C6	-2.30	1.39	1.43
2	A	601	D5O	C5-C6	-2.27	1.39	1.43
2	C	601	D5O	C9-C5	-2.20	1.38	1.42
3	C	602	LYS	OXT-C	-2.17	1.23	1.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	D5O	C9-C5	-2.17	1.38	1.42
3	B	602	LYS	OXT-C	-2.17	1.23	1.30
2	B	601	D5O	C9-C5	-2.16	1.39	1.42
3	A	602	LYS	OXT-C	-2.16	1.23	1.30
2	D	601	D5O	C9-C5	-2.15	1.39	1.42
3	D	602	LYS	OXT-C	-2.15	1.23	1.30

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	D5O	O3-C8-O4	3.52	120.77	116.44
2	B	601	D5O	O3-C8-O4	3.48	120.73	116.44
2	D	601	D5O	O3-C8-O4	3.37	120.58	116.44
2	B	601	D5O	C8-O3-C7	-3.35	120.30	122.23
2	A	601	D5O	O3-C8-O4	3.34	120.55	116.44
2	D	601	D5O	C8-O3-C7	-3.29	120.33	122.23
2	C	601	D5O	C8-O3-C7	-3.27	120.34	122.23
2	D	601	D5O	C15-C11-C10	-3.26	107.73	111.52
2	A	601	D5O	C8-O3-C7	-3.14	120.42	122.23
2	B	601	D5O	C15-C11-C10	-3.03	107.99	111.52
2	B	601	D5O	C17-C11-C10	-2.84	108.22	111.52
2	C	601	D5O	C15-C11-C10	-2.79	108.28	111.52
2	C	601	D5O	C17-C11-C10	-2.75	108.32	111.52
3	D	602	LYS	OXT-C-O	-2.72	117.90	124.09
3	A	602	LYS	OXT-C-O	-2.67	118.03	124.09
3	B	602	LYS	OXT-C-O	-2.56	118.27	124.09
2	A	601	D5O	C15-C11-C10	-2.50	108.61	111.52
2	D	601	D5O	C17-C11-C10	-2.46	108.67	111.52
3	C	602	LYS	OXT-C-O	-2.33	118.80	124.09
3	D	602	LYS	OXT-C-CA	2.28	121.16	113.38
3	B	602	LYS	OXT-C-CA	2.06	120.41	113.38
2	A	601	D5O	C17-C11-C10	-2.04	109.15	111.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

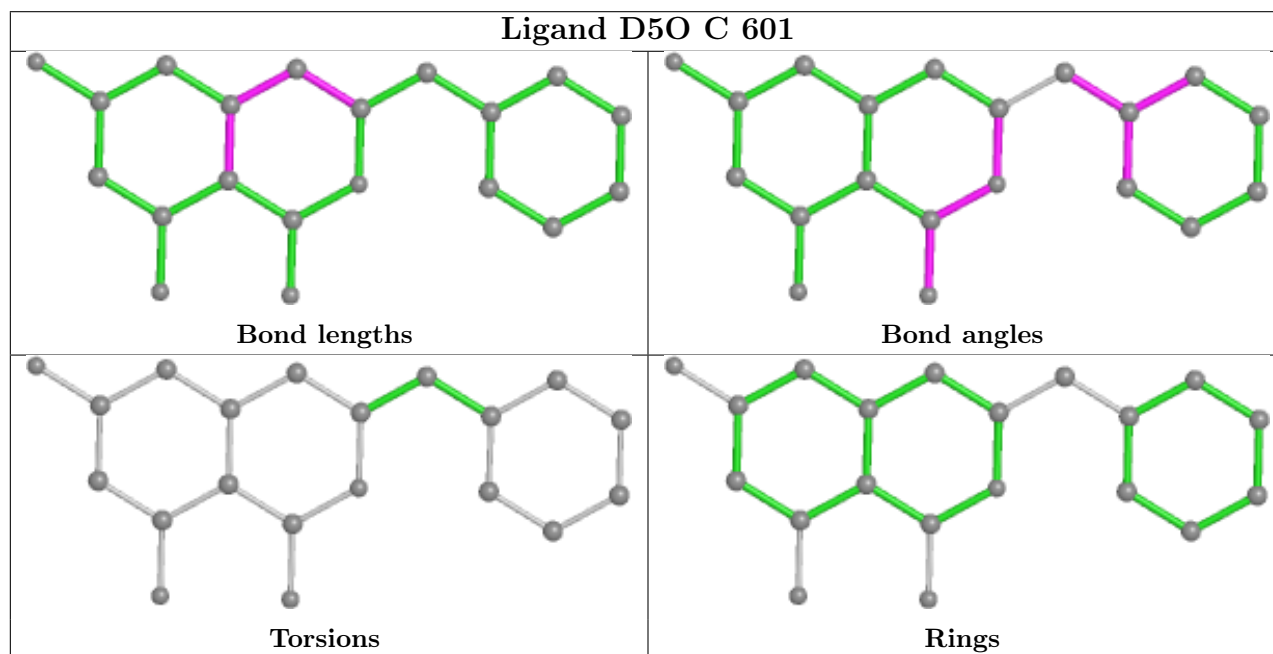
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	LYS	1	0
3	C	602	LYS	7	0

Continued on next page...

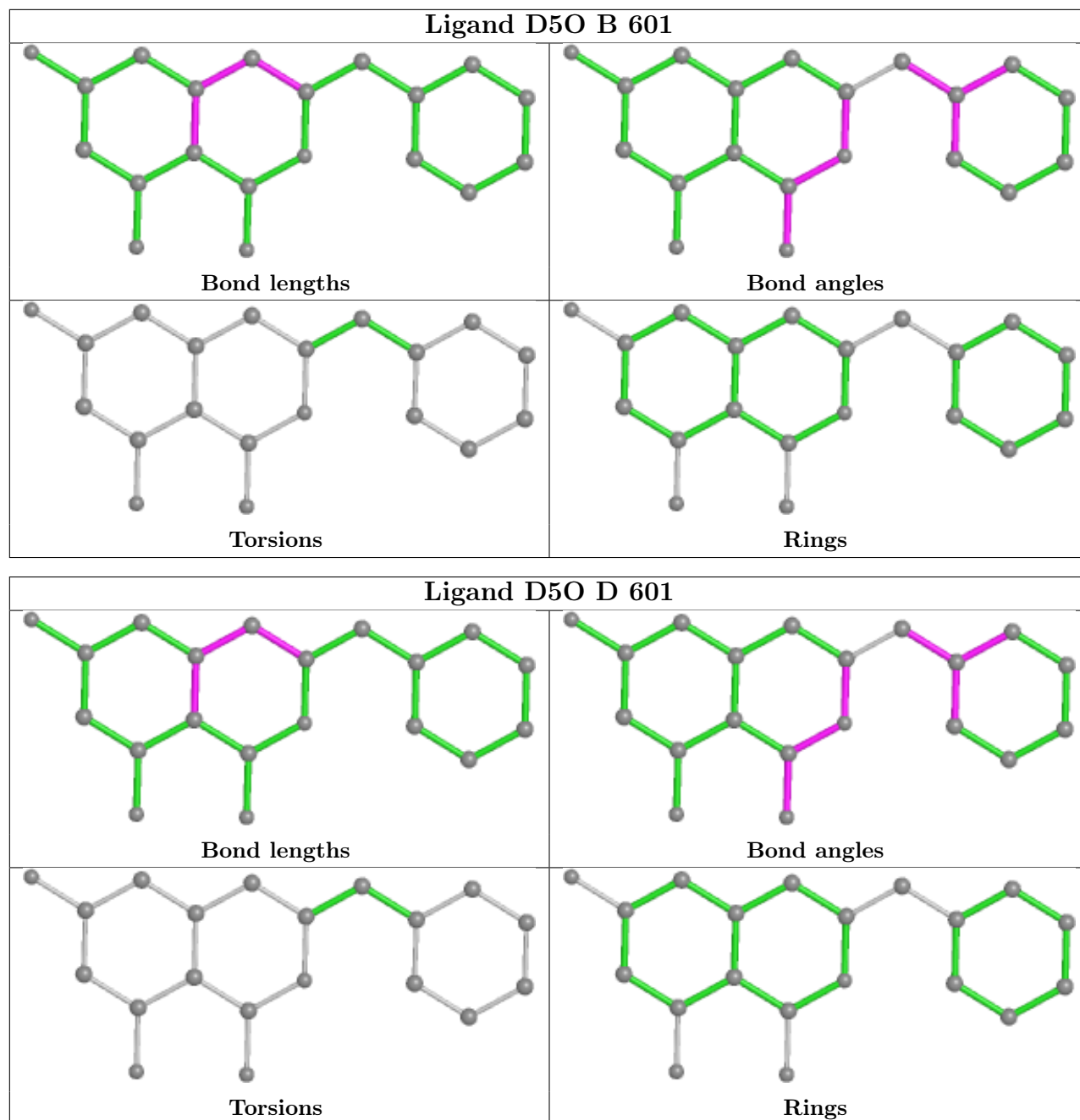
Continued from previous page...

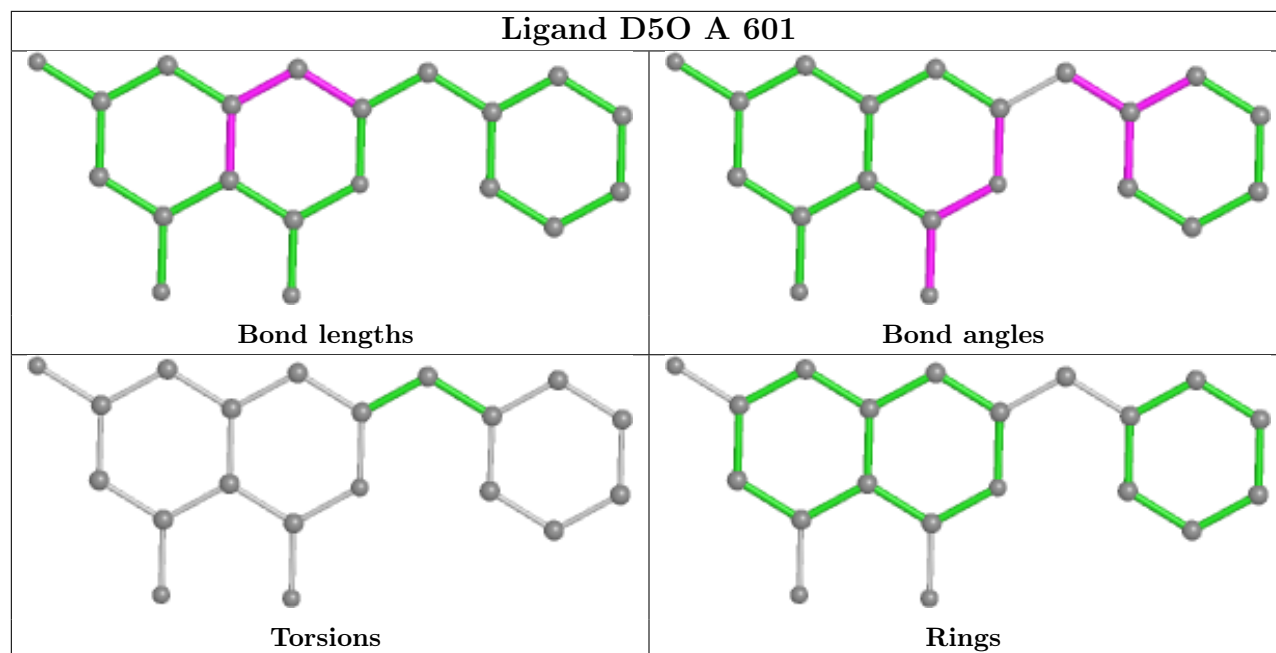
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	LYS	3	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	506/516 (98%)	1.04	87 (17%) <b>1</b> <b>1</b>	34, 60, 83, 95	0
1	B	504/516 (97%)	0.89	60 (11%) <b>4</b> <b>4</b>	35, 58, 80, 90	0
1	C	498/516 (96%)	1.28	114 (22%) <b>0</b> <b>1</b>	42, 64, 83, 107	0
1	D	501/516 (97%)	1.10	86 (17%) <b>1</b> <b>1</b>	39, 61, 78, 95	0
All	All	2009/2064 (97%)	1.08	347 (17%) <b>1</b> <b>1</b>	34, 61, 82, 107	0

All (347) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	489	THR	10.1
1	D	149	LEU	8.7
1	D	528	GLY	7.6
1	C	517	CYS	7.2
1	C	535	LEU	7.0
1	A	517	CYS	7.0
1	C	534	GLN	6.3
1	A	165	ALA	6.3
1	A	522	GLN	6.3
1	C	430	ASN	6.1
1	A	535	LEU	5.8
1	C	130	ASP	5.8
1	C	536	ASP	5.7
1	A	524	ASP	5.6
1	C	488	LEU	5.5
1	A	164	LEU	5.4
1	C	514	GLN	5.4
1	A	527	LYS	5.4
1	A	533	ALA	5.2
1	C	149	LEU	5.2
1	D	430	ASN	5.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	218	LEU	5.0
1	C	143	SER	4.9
1	A	536	ASP	4.9
1	D	497	CYS	4.8
1	D	145	SER	4.8
1	A	176	ASN	4.8
1	C	115	PHE	4.7
1	D	366	SER	4.6
1	D	151	PHE	4.6
1	C	412	ASN	4.5
1	C	410	VAL	4.5
1	C	331	ASN	4.4
1	B	172	HIS	4.4
1	C	79	ASP	4.4
1	C	408	GLU	4.4
1	C	119	TYR	4.4
1	B	524	ASP	4.3
1	A	381	ASN	4.3
1	C	145	SER	4.3
1	D	384	GLY	4.3
1	B	127	HIS	4.2
1	C	470	GLU	4.2
1	A	430	ASN	4.2
1	C	188	ASP	4.2
1	D	144	ALA	4.2
1	C	144	ALA	4.1
1	A	175	GLY	4.1
1	C	542	SER	4.1
1	D	83	TYR	4.1
1	D	148	LYS	4.1
1	A	193	VAL	4.1
1	D	527	LYS	4.0
1	C	482	HIS	4.0
1	C	504	ALA	4.0
1	B	182	ASP	3.9
1	C	445	ALA	3.9
1	C	129	GLU	3.8
1	D	369	VAL	3.8
1	B	425	ILE	3.8
1	B	357	LEU	3.8
1	D	514	GLN	3.8
1	A	173	GLU	3.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	402	SER	3.8
1	A	520	LEU	3.7
1	C	492	LEU	3.7
1	C	432	ILE	3.7
1	A	523	LYS	3.7
1	B	561	THR	3.7
1	A	144	ALA	3.7
1	B	130	ASP	3.6
1	A	489	THR	3.6
1	A	534	GLN	3.6
1	D	521	GLN	3.6
1	A	455	HIS	3.6
1	D	414	ILE	3.6
1	D	385	PRO	3.5
1	C	295	ASN	3.5
1	C	100	ASN	3.5
1	D	265	LEU	3.5
1	C	123	GLY	3.5
1	B	143	SER	3.5
1	C	146	GLY	3.5
1	D	425	ILE	3.4
1	C	292	THR	3.4
1	B	223	MET	3.4
1	C	416	GLU	3.4
1	A	153	ASP	3.4
1	B	153	ASP	3.4
1	C	227	LEU	3.4
1	B	129	GLU	3.3
1	A	457	ILE	3.3
1	B	356	ASP	3.3
1	A	250	THR	3.3
1	D	199	SER	3.3
1	C	423	GLU	3.3
1	D	156	GLY	3.3
1	A	170	HIS	3.3
1	C	385	PRO	3.3
1	A	390	ILE	3.3
1	C	406	GLU	3.3
1	B	167	TYR	3.3
1	A	431	ILE	3.3
1	C	116	ILE	3.3
1	D	429	ILE	3.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	497	CYS	3.2
1	B	423	GLU	3.2
1	C	424	THR	3.2
1	C	552	GLY	3.2
1	B	354	TYR	3.2
1	B	198	LYS	3.2
1	D	412	ASN	3.2
1	D	493	GLU	3.2
1	A	476	SER	3.2
1	D	86	ASN	3.2
1	B	115	PHE	3.2
1	D	292	THR	3.2
1	C	127	HIS	3.2
1	C	106	PHE	3.1
1	A	581	PRO	3.1
1	D	375	THR	3.1
1	C	175	GLY	3.1
1	D	424	THR	3.1
1	D	122	LEU	3.1
1	B	448	LEU	3.1
1	D	413	THR	3.1
1	A	204	LEU	3.1
1	D	529	ASP	3.1
1	A	479	ALA	3.1
1	A	145	SER	3.0
1	D	383	ASP	3.0
1	B	550	THR	3.0
1	B	509	ASN	3.0
1	A	532	ALA	3.0
1	D	104	HIS	3.0
1	D	376	TYR	3.0
1	C	128	LEU	3.0
1	D	260	PHE	3.0
1	C	289	PRO	3.0
1	C	405	GLU	3.0
1	D	408	GLU	3.0
1	B	366	SER	3.0
1	A	150	ARG	2.9
1	C	491	ARG	2.9
1	C	387	ASN	2.9
1	C	457	ILE	2.9
1	A	424	THR	2.9

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	530	THR	2.9
1	A	579	MET	2.9
1	C	96	ASP	2.9
1	A	163	VAL	2.9
1	D	286	ASN	2.9
1	B	150	ARG	2.9
1	D	150	ARG	2.9
1	D	388	GLN	2.8
1	A	528	GLY	2.8
1	D	121	ASP	2.8
1	C	409	LYS	2.8
1	D	188	ASP	2.8
1	A	167	TYR	2.8
1	C	164	LEU	2.8
1	C	198	LYS	2.8
1	B	430	ASN	2.8
1	B	106	PHE	2.8
1	A	554	GLY	2.8
1	C	192	ILE	2.8
1	A	521	GLN	2.8
1	D	242	LEU	2.8
1	A	166	ASN	2.8
1	A	215	SER	2.8
1	A	172	HIS	2.7
1	B	360	TRP	2.7
1	C	243	ILE	2.7
1	C	439	LEU	2.7
1	B	144	ALA	2.7
1	A	192	ILE	2.7
1	D	215	SER	2.7
1	C	234	TYR	2.7
1	B	358	ILE	2.7
1	C	391	GLU	2.7
1	B	469	VAL	2.7
1	C	490	GLU	2.7
1	C	510	ASP	2.7
1	B	229	ASP	2.7
1	B	520	LEU	2.7
1	B	375	THR	2.7
1	A	123	GLY	2.7
1	C	112	ILE	2.6
1	A	194	GLY	2.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	528	GLY	2.6
1	B	523	LYS	2.6
1	B	215	SER	2.6
1	A	509	ASN	2.6
1	D	125	GLY	2.6
1	A	216	ALA	2.6
1	A	583	ASN	2.6
1	C	381	ASN	2.6
1	B	336	ASN	2.6
1	B	320	ASP	2.6
1	D	427	LYS	2.5
1	A	477	PRO	2.5
1	C	413	THR	2.5
1	D	219	HIS	2.5
1	A	388	GLN	2.5
1	C	341	GLU	2.5
1	D	370	TYR	2.5
1	C	554	GLY	2.5
1	D	207	PHE	2.5
1	B	180	CYS	2.5
1	B	197	GLY	2.5
1	A	416	GLU	2.5
1	A	445	ALA	2.5
1	C	219	HIS	2.5
1	D	367	GLN	2.5
1	D	153	ASP	2.5
1	A	98	GLY	2.5
1	C	176	ASN	2.5
1	C	296	ASP	2.5
1	A	218	LEU	2.5
1	A	124	ASN	2.5
1	A	512	PHE	2.5
1	B	445	ALA	2.5
1	C	485	LYS	2.5
1	D	192	ILE	2.5
1	D	243	ILE	2.5
1	A	181	TYR	2.5
1	C	80	PRO	2.5
1	C	353	ASP	2.5
1	A	122	LEU	2.5
1	A	241	LEU	2.5
1	A	519	LYS	2.5

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	481	TYR	2.5
1	D	489	THR	2.4
1	C	95	LYS	2.4
1	C	199	SER	2.4
1	D	525	ARG	2.4
1	C	428	MET	2.4
1	C	202	GLY	2.4
1	D	491	ARG	2.4
1	D	504	ALA	2.4
1	A	91	ILE	2.4
1	B	547	LEU	2.4
1	C	320	ASP	2.4
1	C	459	ASN	2.4
1	D	336	ASN	2.4
1	A	171	ASN	2.4
1	C	446	ALA	2.4
1	D	541	THR	2.4
1	C	247	SER	2.4
1	A	385	PRO	2.4
1	D	390	ILE	2.4
1	A	492	LEU	2.4
1	B	151	PHE	2.3
1	C	501	VAL	2.3
1	D	509	ASN	2.3
1	D	387	ASN	2.3
1	B	149	LEU	2.3
1	A	149	LEU	2.3
1	C	469	VAL	2.3
1	D	426	GLU	2.3
1	A	101	PRO	2.3
1	C	448	LEU	2.3
1	A	423	GLU	2.3
1	B	190	VAL	2.3
1	D	526	GLU	2.3
1	C	124	ASN	2.3
1	A	448	LEU	2.3
1	B	199	SER	2.3
1	B	119	TYR	2.3
1	C	187	GLY	2.3
1	A	392	ILE	2.3
1	C	431	ILE	2.3
1	B	162	GLN	2.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	294	HIS	2.2
1	A	161	ILE	2.2
1	C	101	PRO	2.2
1	D	165	ALA	2.2
1	B	466	PHE	2.2
1	C	509	ASN	2.2
1	C	524	ASP	2.2
1	B	505	TYR	2.2
1	C	99	ILE	2.2
1	C	98	GLY	2.2
1	C	519	LYS	2.2
1	C	525	ARG	2.2
1	A	225	TYR	2.2
1	D	356	ASP	2.2
1	A	309	LEU	2.2
1	B	192	ILE	2.2
1	B	519	LYS	2.2
1	C	91	ILE	2.2
1	D	230	THR	2.2
1	C	93	ASP	2.2
1	B	243	ILE	2.2
1	C	271	PHE	2.2
1	D	512	PHE	2.2
1	A	391	GLU	2.2
1	C	332	GLU	2.1
1	D	386	GLU	2.1
1	C	440	PRO	2.1
1	B	536	ASP	2.1
1	B	392	ILE	2.1
1	D	358	ILE	2.1
1	A	451	GLN	2.1
1	D	428	MET	2.1
1	C	148	LYS	2.1
1	C	185	ARG	2.1
1	D	544	GLU	2.1
1	D	194	GLY	2.1
1	D	84	PHE	2.1
1	A	504	ALA	2.1
1	C	147	GLN	2.1
1	C	581	PRO	2.1
1	B	491	ARG	2.1
1	C	197	GLY	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	211	THR	2.1
1	B	493	GLU	2.1
1	C	94	GLN	2.1
1	A	387	ASN	2.1
1	D	166	ASN	2.1
1	D	245	GLU	2.1
1	A	537	SER	2.1
1	A	130	ASP	2.1
1	A	151	PHE	2.0
1	D	441	ASN	2.0
1	D	431	ILE	2.0
1	B	510	ASP	2.0
1	C	170	HIS	2.0
1	C	421	SER	2.0
1	B	500	GLU	2.0
1	D	392	ILE	2.0
1	C	168	SER	2.0
1	C	167	TYR	2.0
1	D	354	TYR	2.0
1	A	518	PHE	2.0
1	B	413	THR	2.0
1	D	87	ARG	2.0
1	D	331	ASN	2.0
1	D	203	GLU	2.0
1	A	410	VAL	2.0
1	A	195	PHE	2.0
1	A	459	ASN	2.0
1	A	332	GLU	2.0
1	C	417	GLN	2.0
1	C	163	VAL	2.0
1	D	88	SER	2.0
1	D	519	LYS	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](#)

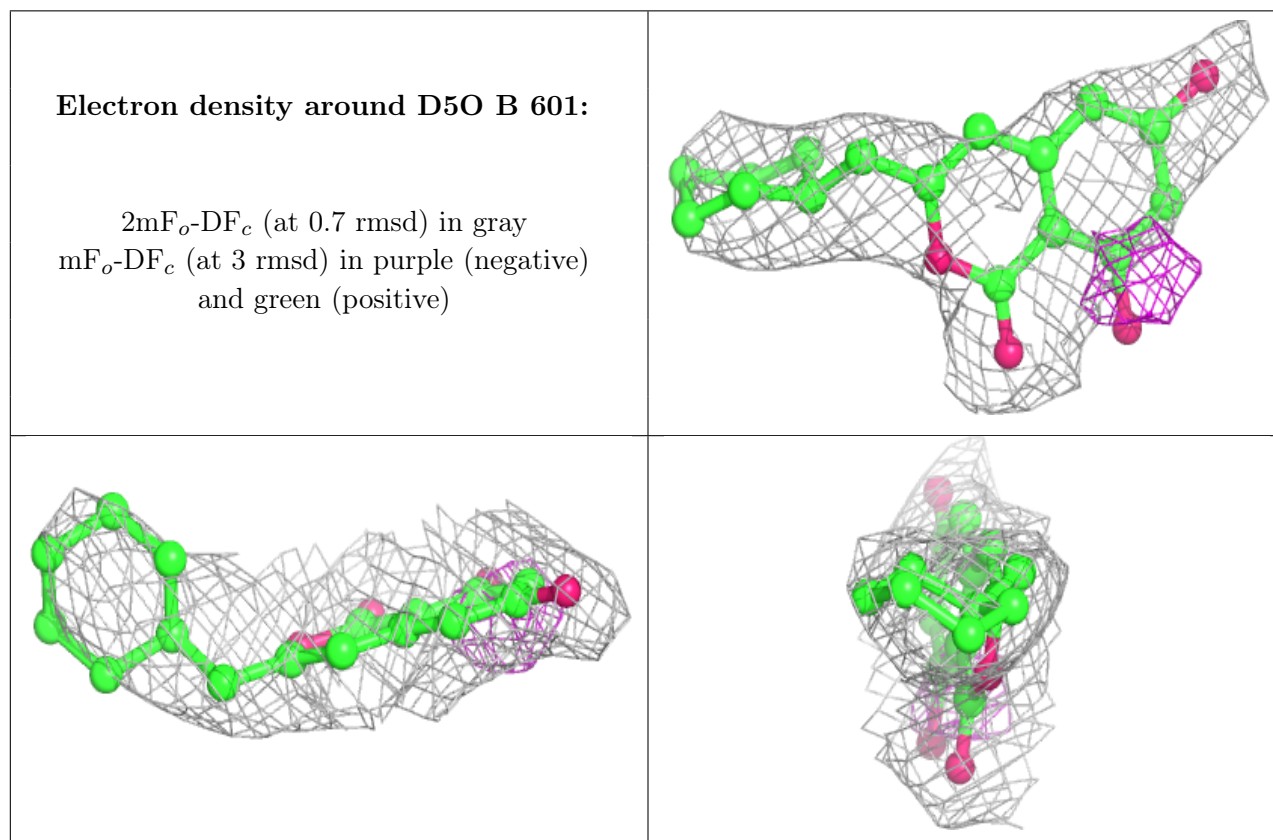
There are no monosaccharides in this entry.

## 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, 95<sup>th</sup> 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.

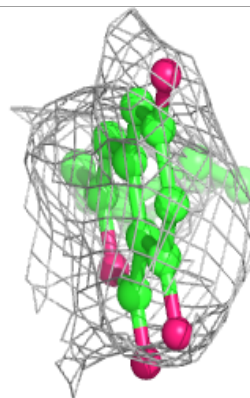
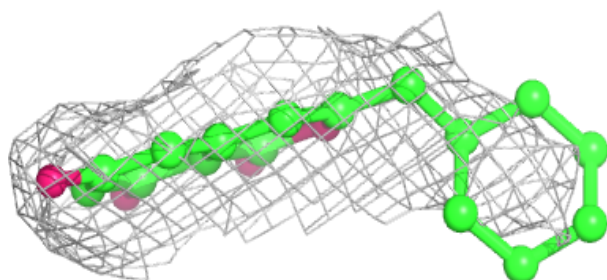
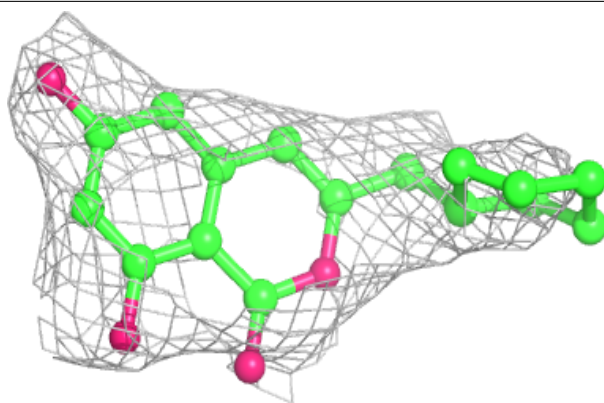
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	LYS	B	602	10/10	0.63	0.43	44,45,48,48	0
3	LYS	C	602	10/10	0.76	0.54	54,56,56,57	0
3	LYS	D	602	10/10	0.76	0.47	42,45,51,51	0
2	D5O	B	601	20/20	0.81	0.35	44,45,46,46	0
2	D5O	D	601	20/20	0.83	0.36	39,40,43,43	0
2	D5O	C	601	20/20	0.83	0.38	54,55,57,57	0
3	LYS	A	602	10/10	0.86	0.54	48,49,50,51	0
2	D5O	A	601	20/20	0.86	0.50	47,49,51,51	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.

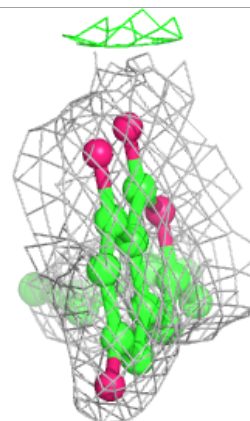
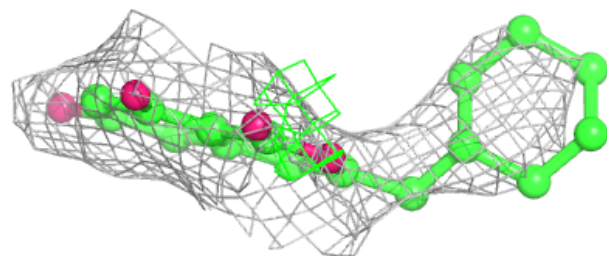
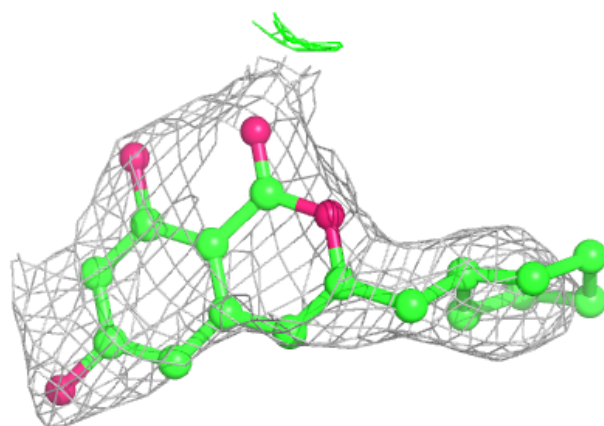


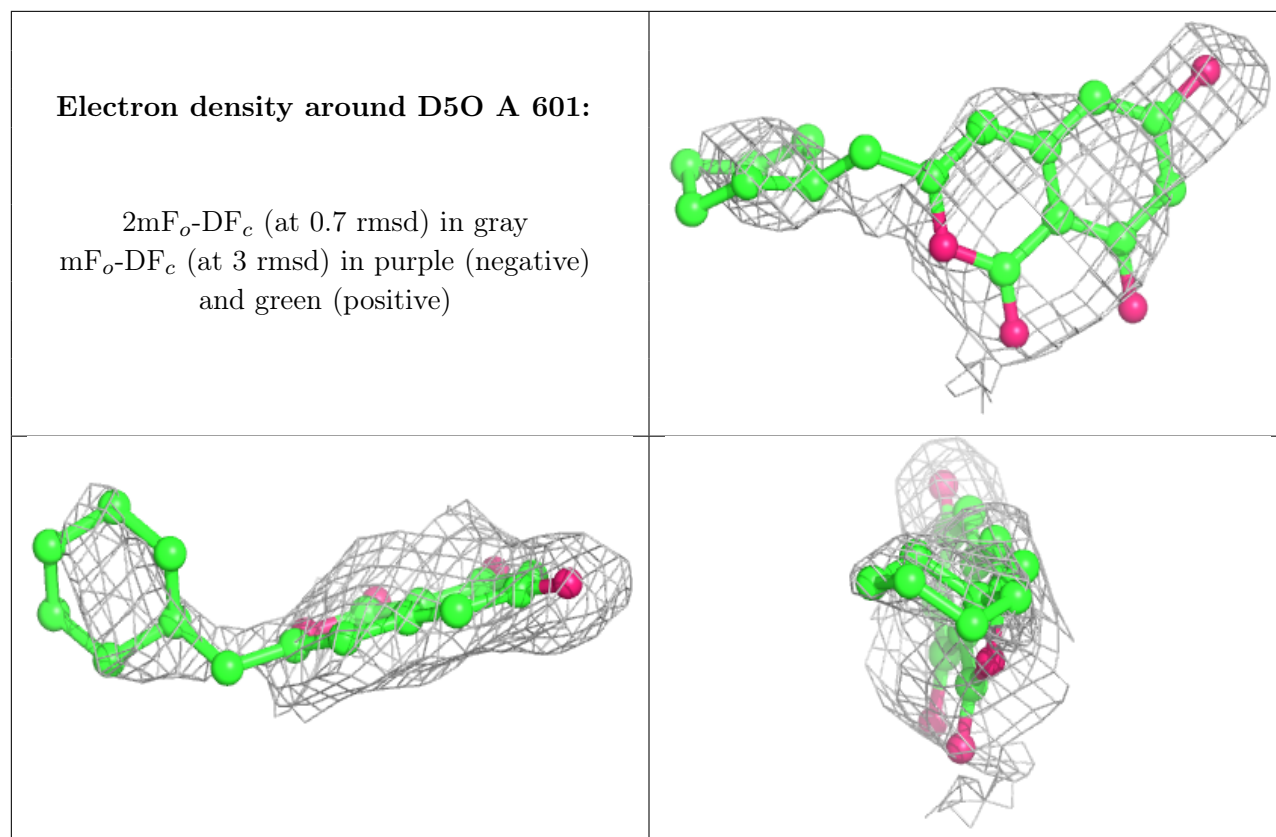
**Electron density around D5O D 601:**

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

**Electron density around D5O 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.