



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:35 PM UTC

PDB ID : 6KCT / pdb_00006ket
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

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

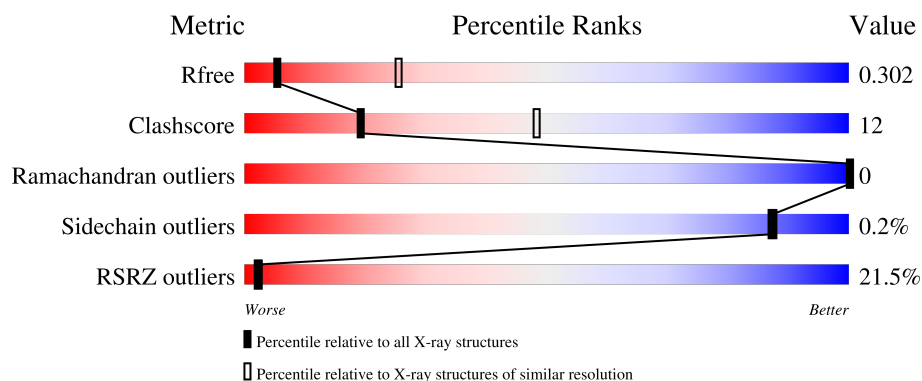
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (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 ≥ 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	20% 77% 21%
1	B	516	17% 78% 20%
1	C	516	26% 74% 23%
1	D	516	21% 76% 21%

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	LYS	C	602	-	-	X	-

2 Entry composition

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
1	A	506	Total	C	N	O	S	0	0	0
			3925	2522	655	731	17			
1	B	504	Total	C	N	O	S	0	0	0
			3910	2515	650	728	17			
1	C	498	Total	C	N	O	S	0	0	0
			3872	2491	644	721	16			
1	D	501	Total	C	N	O	S	0	0	0
			3921	2528	651	726	16			

There are 36 discrepancies between the modelled and reference sequences:

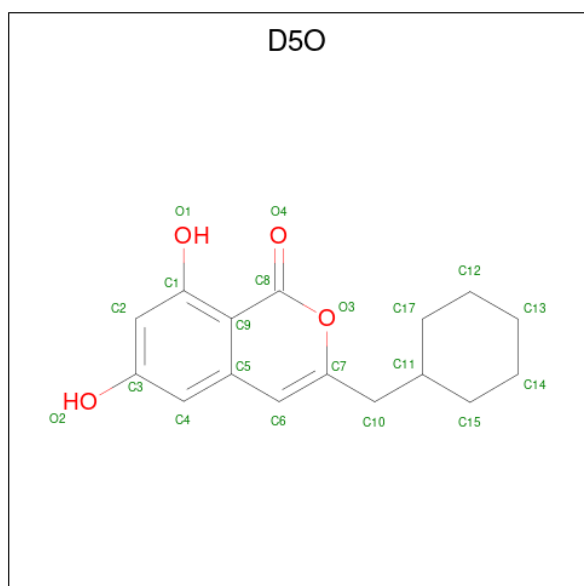
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	initiating methionine	UNP W7JP72
A	584	GLY	-	expression tag	UNP W7JP72
A	585	GLY	-	expression tag	UNP W7JP72
A	586	HIS	-	expression tag	UNP W7JP72
A	587	HIS	-	expression tag	UNP W7JP72
A	588	HIS	-	expression tag	UNP W7JP72
A	589	HIS	-	expression 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-(cyclohexylmethyl)-6,8-bis(oxidanyl)isochromen-1-one (CCD ID: D5O) (formula: C₁₆H₁₈O₄) (labeled as "Ligand of Interest" by depositor).



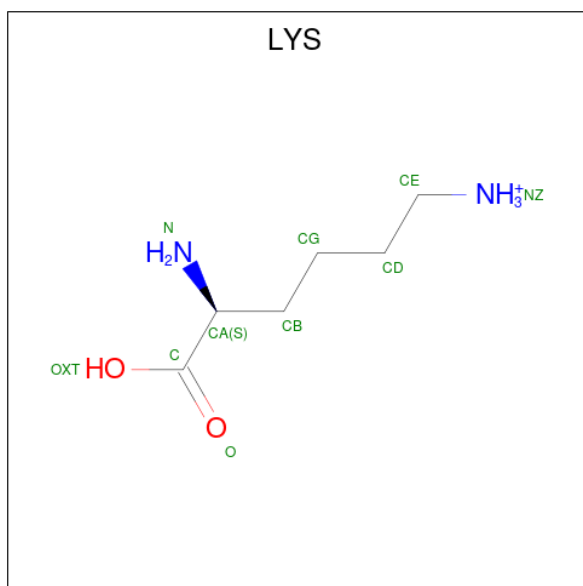
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	16	4		
2	B	1	Total	C	O	0	0
			20	16	4		
2	C	1	Total	C	O	0	0
			20	16	4		

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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 (CCD ID: 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		

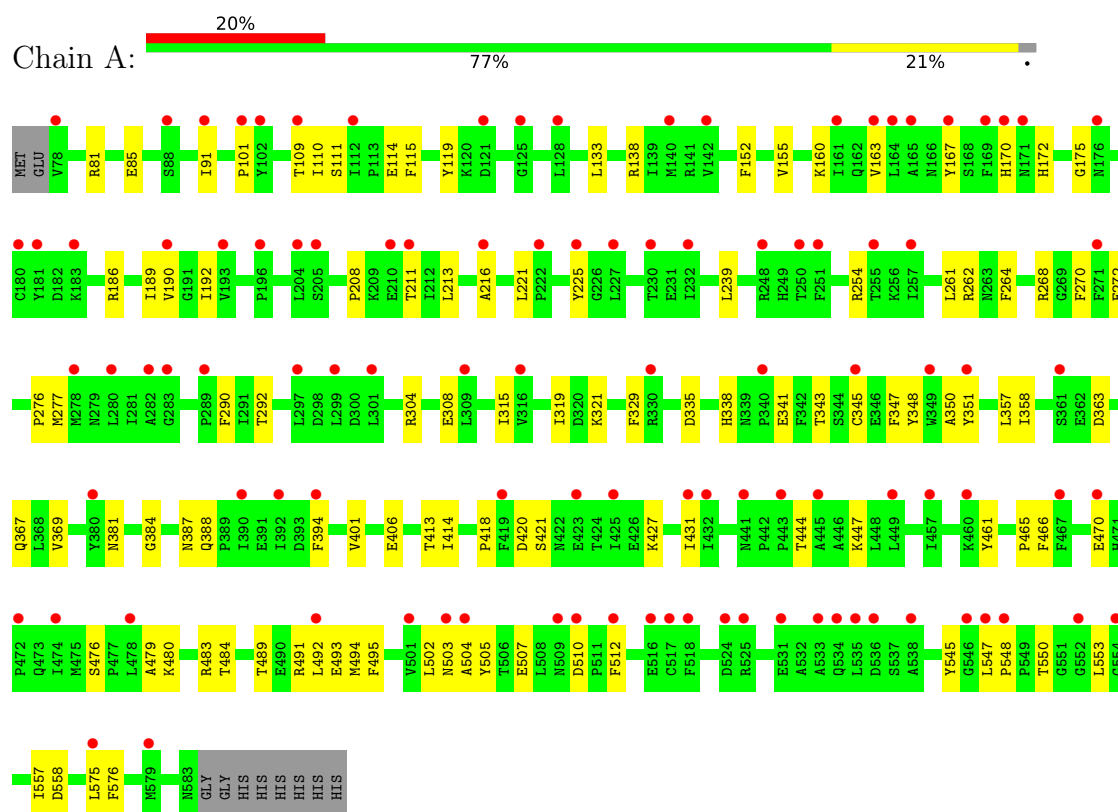
- Molecule 4 is water.

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		

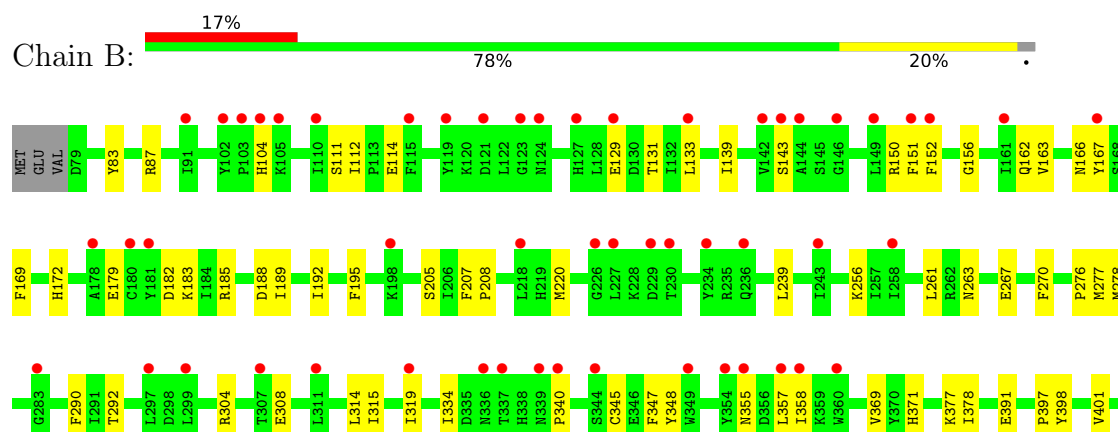
3 Residue-property plots [i](#)

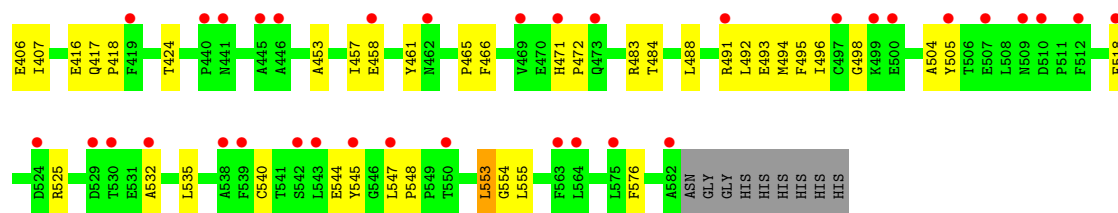
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

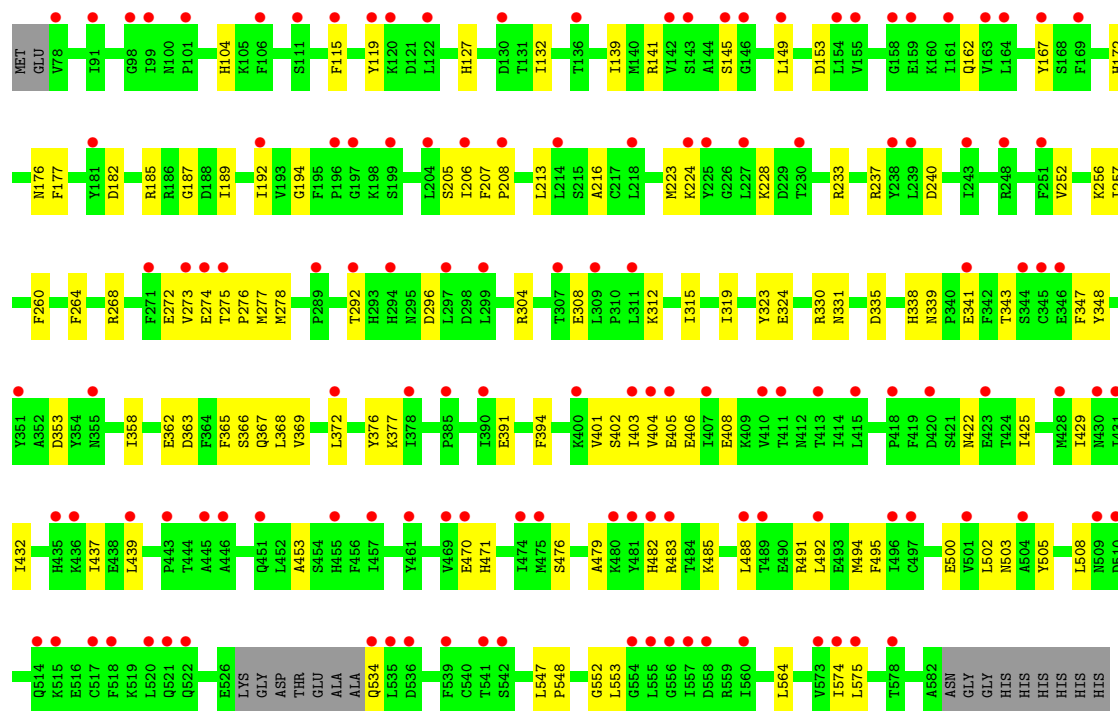
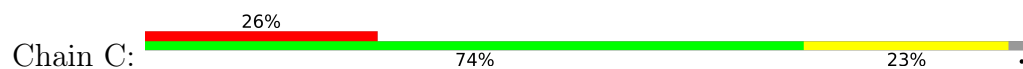


• Molecule 1: Lysine-tRNA ligase

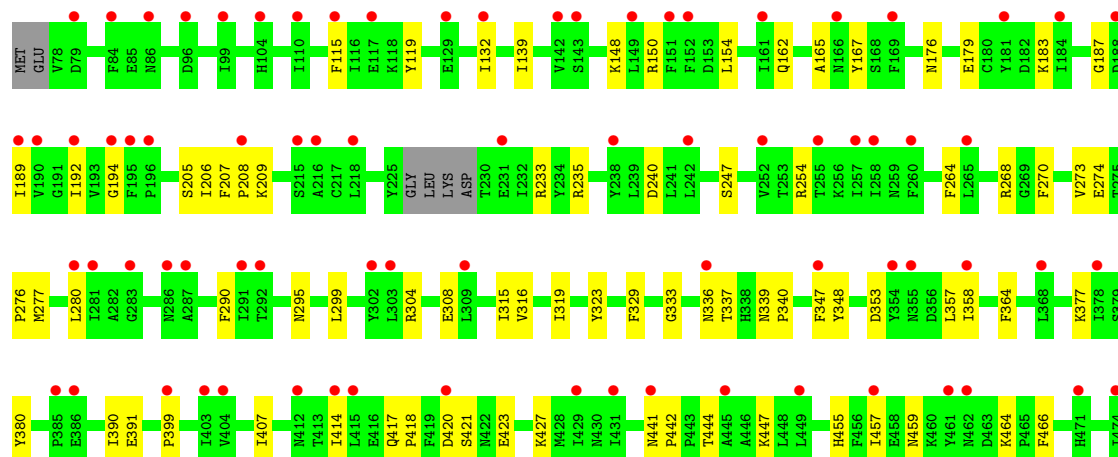
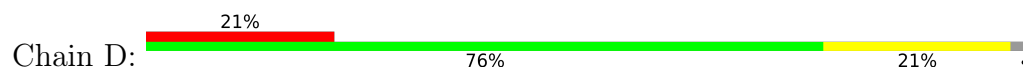


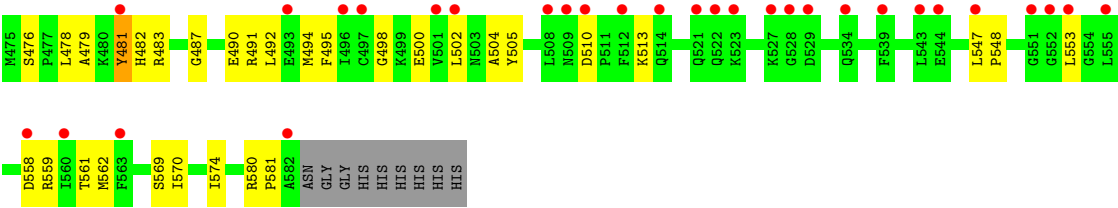


• Molecule 1: Lysine-tRNA ligase



• Molecule 1: Lysine-tRNA ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 94.2 (48.95-3.25)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.292 , 0.312 (Not available) , 0.302	Depositor DCC
R_{free} test set	1655 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.828	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	15828	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage'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.*

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: 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	0.22	0/4023	0.62	0/5467
1	B	0.26	0/4008	0.64	0/5453
1	C	0.26	0/3968	0.64	0/5392
1	D	0.24	0/4019	0.61	0/5456
All	All	0.24	0/16018	0.63	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	91	0
1	B	3910	0	3656	89	0
1	C	3872	0	3640	101	0
1	D	3921	0	3731	103	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	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	12	1	0
3	C	10	0	12	8	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	358	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 12.

All (358) 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:B:553:LEU:C	1:B:553:LEU:HD23	2.11	0.76
1:A:350:ALA:HA	1:A:550:THR:HG22	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:PHE:CE2	1:B:347:PHE:HD2	2.07	0.73
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: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:A:277:MET:HE1	1:B:277:MET:HE1	1.76	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:TYR:CD1	3:C:602:LYS:HE2	2.37	0.60
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:D:337:THR:HG22	1:D:562:MET:HE1	1.86	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:C:552:GLY:C	3:C:602:LYS:HZ3	2.13	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:C:278:MET:HE1	1:D:340:PRO:HB2	1.86	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:315:ILE:HD13	1:B:319:ILE:O	2.09	0.52
1:C:353:ASP:CG	1:C:483:ARG:HH22	2.15	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: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:A:465:PRO:HB2	1:A:494:MET:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:240:ASP:OD1	1:D:247:SER:OG	2.27	0.49
1:D:559:ARG:HA	1:D:562:MET:HE2	1.93	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:C:347:PHE:C	1:C:348:TYR:HD1	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:494:MET:C	1:B:495:PHE:HD1	2.21	0.47
1:C:277:MET:HA	1:C:304:ARG:HD3	1.95	0.47
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:C:365:PHE:CD2	1:C:494:MET:HE1	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:559:ARG:HG2	1:D:562:MET:HE2	1.99	0.45
1:A:109:THR:HG22	1:A:110:ILE:HG23	1.99	0.45
1:B:83:TYR:HD2	1:B:220:MET:HE2	1.81	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:D:494:MET:C	1:D:495:PHE:HD1	2.25	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:505:TYR:CE1	3:A:602:LYS:NZ	2.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:552:GLY:C	3:C:602:LYS:NZ	2.76	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
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:479:ALA:C	1:C:508:LEU:HB2	2.44	0.43
1:C:358:ILE:HD13	1:C:492:LEU:HD13	2.00	0.43
1:D:478:LEU:C	1:D:505:TYR:HE2	2.25	0.43
1:B:348:TYR:CD1	1:B:348:TYR:N	2.87	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:B:417:GLN:HA	1:B:418:PRO:C	2.45	0.42
1:C:402:SER:HB3	1:C:405:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ASP:OD1	1:A:335:ASP:N	2.51	0.42
1:A:189:ILE:HD13	1:B:548:PRO:HB3	2.02	0.42
1:A:465:PRO:CB	1:A:494:MET:HE3	2.49	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:B:553:LEU:C	1:B:553:LEU:CD2	2.84	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
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:329:PHE:HD2	1:B:278:MET:HE2	1.85	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:D:115:PHE:CD1	1:D:115:PHE:C	2.98	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: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:C:365:PHE:CE2	1:C:494:MET:HE1	2.56	0.40
1:D:329:PHE:CD1	1:D:329:PHE:N	2.89	0.40
1:A:115:PHE:CD1	1:A:115:PHE:C	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:PRO:HB2	1:A:420:ASP:OD1	2.21	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%)	401 (100%)	0	100	100
1	B	398/464 (86%)	396 (100%)	2 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	397/464 (86%)	397 (100%)	0	100	100
1	D	407/464 (88%)	406 (100%)	1 (0%)	87	87
All	All	1603/1856 (86%)	1600 (100%)	3 (0%)	87	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	397	PRO
1	B	553	LEU
1	D	481	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	473	GLN
1	A	514	GLN
1	B	92	GLN
1	B	104	HIS
1	B	162	GLN
1	B	170	HIS
1	B	172	HIS
1	C	92	GLN
1	C	172	HIS
1	C	279	ASN
1	C	451	GLN
1	D	92	GLN
1	D	355	ASN
1	D	417	GLN
1	D	471	HIS

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 [i](#)

There are no oligosaccharides 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
3	LYS	D	602	-	8,9,9	0.85	1 (12%)	7,10,10	1.09	1 (14%)
2	D5O	B	601	-	22,22,22	1.97	3 (13%)	29,31,31	1.56	5 (17%)
2	D5O	A	601	-	22,22,22	1.98	3 (13%)	29,31,31	1.49	4 (13%)
3	LYS	C	602	-	8,9,9	1.05	1 (12%)	7,10,10	1.12	1 (14%)
3	LYS	A	602	-	8,9,9	0.86	1 (12%)	7,10,10	1.12	1 (14%)
2	D5O	D	601	-	22,22,22	1.92	3 (13%)	29,31,31	1.59	5 (17%)
3	LYS	B	602	-	8,9,9	0.85	1 (12%)	7,10,10	1.02	1 (14%)
2	D5O	C	601	-	22,22,22	1.97	3 (13%)	29,31,31	1.56	5 (17%)

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
3	LYS	D	602	-	-	0/9/9/9	-
2	D5O	B	601	-	-	0/4/12/12	0/3/3/3
2	D5O	A	601	-	-	0/4/12/12	0/3/3/3
3	LYS	C	602	-	-	0/9/9/9	-
3	LYS	A	602	-	-	0/9/9/9	-
2	D5O	D	601	-	-	0/4/12/12	0/3/3/3
3	LYS	B	602	-	-	0/9/9/9	-
2	D5O	C	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	8.18	1.39	1.33
2	B	601	D5O	C6-C7	8.12	1.39	1.33
2	C	601	D5O	C6-C7	8.08	1.39	1.33
2	D	601	D5O	C6-C7	7.83	1.39	1.33
2	D	601	D5O	C5-C6	-2.46	1.38	1.43
2	C	601	D5O	C5-C6	-2.35	1.39	1.43
2	B	601	D5O	C5-C6	-2.35	1.39	1.43
2	A	601	D5O	C5-C6	-2.31	1.39	1.43
3	C	602	LYS	OXT-C	-2.26	1.23	1.30
3	B	602	LYS	OXT-C	-2.26	1.23	1.30
3	A	602	LYS	OXT-C	-2.25	1.23	1.30
3	D	602	LYS	OXT-C	-2.24	1.23	1.30
2	C	601	D5O	C9-C5	-2.23	1.38	1.42
2	A	601	D5O	C9-C5	-2.20	1.38	1.42
2	B	601	D5O	C9-C5	-2.19	1.39	1.42
2	D	601	D5O	C9-C5	-2.19	1.39	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	D5O	C10-C7-C6	-5.01	118.68	127.19
2	A	601	D5O	C10-C7-C6	-4.81	119.01	127.19
2	C	601	D5O	C10-C7-C6	-4.79	119.05	127.19
2	B	601	D5O	C10-C7-C6	-4.67	119.25	127.19
2	C	601	D5O	O3-C8-O4	3.62	120.77	116.45
2	B	601	D5O	O3-C8-O4	3.59	120.73	116.45
2	D	601	D5O	O3-C8-O4	3.46	120.58	116.45
2	A	601	D5O	O3-C8-O4	3.43	120.55	116.45
2	D	601	D5O	C15-C11-C10	-2.88	107.73	111.48
2	B	601	D5O	C8-O3-C7	-2.79	120.30	122.18
2	D	601	D5O	C8-O3-C7	-2.74	120.33	122.18
3	D	602	LYS	OXT-C-O	-2.72	117.90	124.08
2	C	601	D5O	C8-O3-C7	-2.72	120.34	122.18
2	B	601	D5O	C15-C11-C10	-2.67	107.99	111.48
3	A	602	LYS	OXT-C-O	-2.67	118.03	124.08
2	A	601	D5O	C8-O3-C7	-2.61	120.42	122.18
3	B	602	LYS	OXT-C-O	-2.56	118.27	124.08
2	B	601	D5O	C17-C11-C10	-2.50	108.22	111.48
2	C	601	D5O	C15-C11-C10	-2.46	108.28	111.48
2	C	601	D5O	C17-C11-C10	-2.42	108.32	111.48
3	C	602	LYS	OXT-C-O	-2.33	118.80	124.08
2	A	601	D5O	C15-C11-C10	-2.20	108.61	111.48
2	D	601	D5O	C17-C11-C10	-2.16	108.67	111.48

There are no chirality outliers.

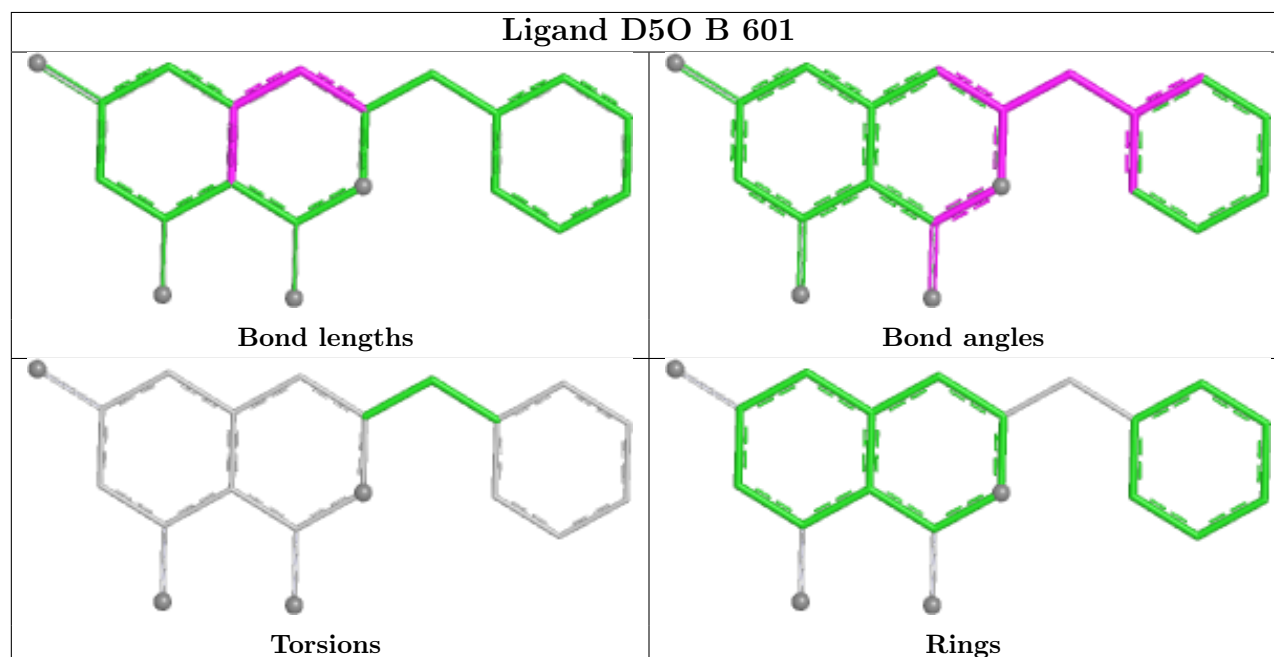
There are no torsion outliers.

There are no ring outliers.

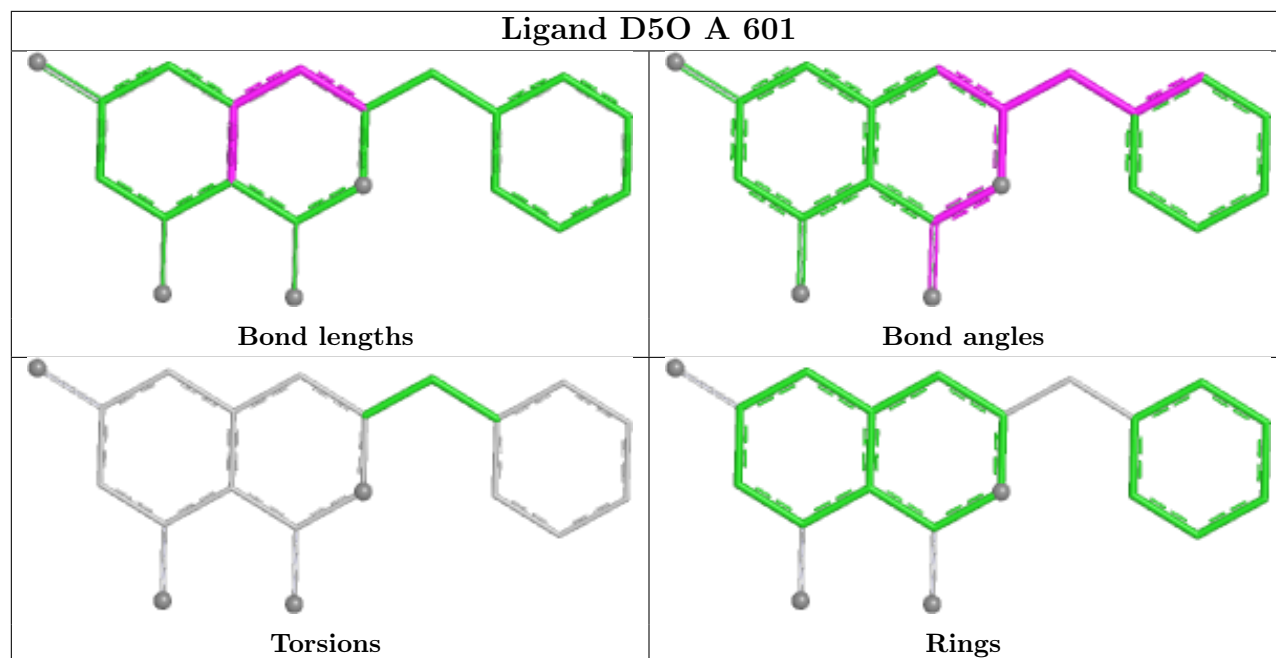
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	LYS	8	0
3	A	602	LYS	4	0
3	B	602	LYS	1	0

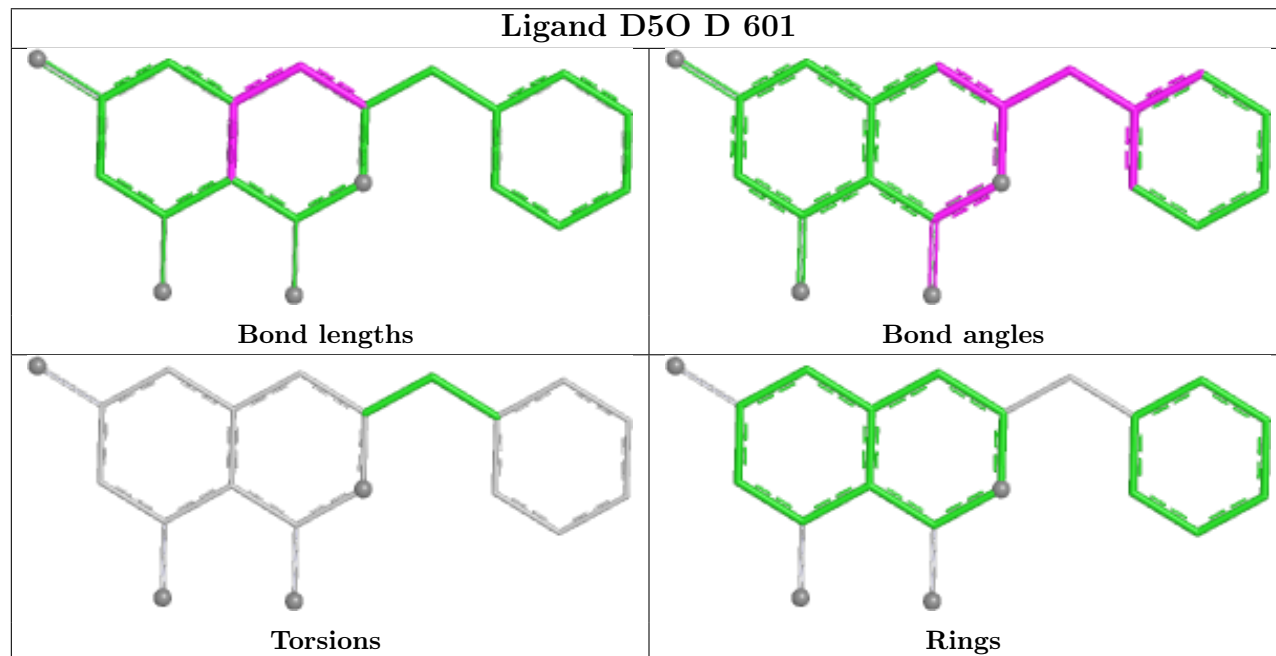
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

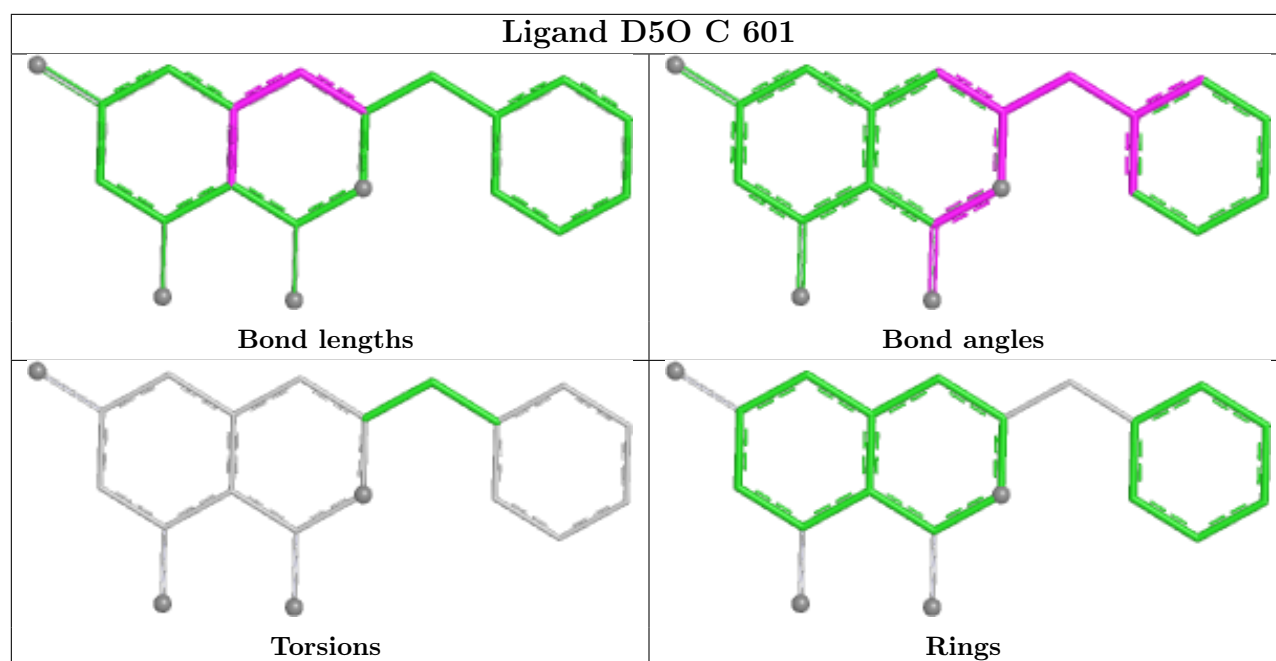


Ligand D5O A 601



Ligand D5O D 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	506/516 (98%)	1.39	104 (20%) 2 2	34, 60, 83, 95	0
1	B	504/516 (97%)	1.30	88 (17%) 4 4	35, 58, 80, 90	0
1	C	498/516 (96%)	1.54	133 (26%) 1 1	42, 64, 83, 107	0
1	D	501/516 (97%)	1.43	107 (21%) 2 2	39, 61, 78, 95	0
All	All	2009/2064 (97%)	1.41	432 (21%) 2 2	34, 61, 82, 107	0

All (432) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	227	LEU	6.0
1	C	470	GLU	5.7
1	C	534	GLN	5.0
1	D	292	THR	5.0
1	B	229	ASP	4.6
1	D	514	GLN	4.6
1	A	457	ILE	4.4
1	A	211	THR	4.4
1	C	115	PHE	4.4
1	C	514	GLN	4.3
1	C	119	TYR	4.3
1	C	192	ILE	4.2
1	D	512	PHE	4.1
1	A	503	ASN	4.0
1	D	218	LEU	4.0
1	C	271	PHE	3.9
1	C	489	THR	3.9
1	B	545	TYR	3.8
1	A	301	LEU	3.8
1	C	146	GLY	3.8
1	A	512	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	504	ALA	3.7
1	D	497	CYS	3.7
1	A	554	GLY	3.7
1	C	535	LEU	3.7
1	D	149	LEU	3.7
1	A	164	LEU	3.6
1	D	151	PHE	3.6
1	D	283	GLY	3.6
1	B	124	ASN	3.6
1	B	354	TYR	3.6
1	C	488	LEU	3.6
1	B	340	PRO	3.5
1	D	354	TYR	3.5
1	A	579	MET	3.5
1	A	181	TYR	3.5
1	B	307	THR	3.5
1	B	550	THR	3.5
1	C	501	VAL	3.5
1	D	129	GLU	3.4
1	C	208	PRO	3.4
1	B	230	THR	3.4
1	C	385	PRO	3.4
1	D	404	VAL	3.4
1	C	542	SER	3.4
1	C	439	LEU	3.4
1	D	104	HIS	3.4
1	A	190	VAL	3.4
1	C	481	TYR	3.4
1	B	152	PHE	3.3
1	C	556	GLY	3.3
1	B	512	PHE	3.3
1	C	457	ILE	3.3
1	C	299	LEU	3.3
1	C	145	SER	3.3
1	D	481	TYR	3.3
1	B	575	LEU	3.3
1	B	142	VAL	3.3
1	A	165	ALA	3.3
1	A	533	ALA	3.3
1	D	445	ALA	3.2
1	A	101	PRO	3.2
1	A	289	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	360	TRP	3.2
1	B	115	PHE	3.2
1	C	218	LEU	3.2
1	B	509	ASN	3.2
1	D	539	PHE	3.2
1	B	542	SER	3.2
1	A	443	PRO	3.1
1	C	443	PRO	3.1
1	C	341	GLU	3.1
1	C	294	HIS	3.1
1	A	467	PHE	3.1
1	B	336	ASN	3.1
1	B	499	LYS	3.1
1	B	146	GLY	3.1
1	B	226	GLY	3.1
1	C	517	CYS	3.1
1	A	91	ILE	3.1
1	A	349	TRP	3.1
1	C	492	LEU	3.0
1	C	404	VAL	3.0
1	C	243	ILE	3.0
1	C	510	ASP	3.0
1	C	469	VAL	3.0
1	D	493	GLU	3.0
1	A	525	ARG	3.0
1	B	144	ALA	3.0
1	A	470	GLU	2.9
1	B	446	ALA	2.9
1	A	297	LEU	2.9
1	A	251	PHE	2.9
1	C	122	LEU	2.9
1	B	497	CYS	2.9
1	A	271	PHE	2.9
1	A	361	SER	2.9
1	B	91	ILE	2.9
1	C	413	THR	2.9
1	D	462	ASN	2.9
1	A	518	PHE	2.9
1	B	129	GLU	2.9
1	A	248	ARG	2.9
1	C	297	LEU	2.9
1	D	449	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	471	HIS	2.8
1	A	216	ALA	2.8
1	B	357	LEU	2.8
1	D	195	PHE	2.8
1	B	441	ASN	2.8
1	A	392	ILE	2.8
1	A	394	PHE	2.8
1	D	169	PHE	2.8
1	A	205	SER	2.8
1	C	289	PRO	2.8
1	C	410	VAL	2.8
1	C	239	LEU	2.8
1	A	283	GLY	2.8
1	B	339	ASN	2.8
1	C	91	ILE	2.8
1	D	110	ILE	2.8
1	D	260	PHE	2.8
1	A	538	ALA	2.8
1	A	501	VAL	2.8
1	C	346	GLU	2.8
1	A	161	ILE	2.8
1	A	431	ILE	2.8
1	B	349	TRP	2.8
1	A	316	VAL	2.8
1	D	547	LEU	2.8
1	D	99	ILE	2.8
1	B	547	LEU	2.7
1	B	510	ASP	2.7
1	A	509	ASN	2.7
1	C	446	ALA	2.7
1	C	518	PHE	2.7
1	D	291	ILE	2.7
1	B	529	ASP	2.7
1	C	573	VAL	2.7
1	B	103	PRO	2.7
1	C	196	PRO	2.7
1	A	278	MET	2.7
1	C	169	PHE	2.7
1	D	543	LEU	2.7
1	B	445	ALA	2.7
1	C	461	TYR	2.7
1	D	303	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	536	ASP	2.7
1	B	524	ASP	2.7
1	A	340	PRO	2.6
1	D	522	GLN	2.6
1	A	535	LEU	2.6
1	D	190	VAL	2.6
1	C	435	HIS	2.6
1	C	206	ILE	2.6
1	D	188	ASP	2.6
1	D	358	ILE	2.6
1	C	101	PRO	2.6
1	D	84	PHE	2.6
1	D	528	GLY	2.6
1	A	575	LEU	2.6
1	C	164	LEU	2.6
1	D	302	TYR	2.6
1	D	385	PRO	2.6
1	A	552	GLY	2.6
1	C	292	THR	2.6
1	D	280	LEU	2.6
1	A	282	ALA	2.6
1	D	501	VAL	2.6
1	A	167	TYR	2.6
1	B	127	HIS	2.6
1	B	181	TYR	2.6
1	C	199	SER	2.6
1	B	419	PHE	2.6
1	C	420	ASP	2.6
1	B	462	ASN	2.6
1	C	309	LEU	2.6
1	C	415	LEU	2.6
1	A	230	THR	2.6
1	A	504	ALA	2.6
1	B	530	THR	2.6
1	C	230	THR	2.6
1	C	431	ILE	2.6
1	A	449	LEU	2.6
1	C	149	LEU	2.6
1	C	423	GLU	2.6
1	D	184	ILE	2.5
1	A	102	TYR	2.5
1	C	554	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	520	LEU	2.5
1	D	529	ASP	2.5
1	A	210	GLU	2.5
1	A	390	ILE	2.5
1	A	425	ILE	2.5
1	C	99	ILE	2.5
1	C	475	MET	2.5
1	A	492	LEU	2.5
1	C	555	LEU	2.5
1	A	78	VAL	2.5
1	A	176	ASN	2.5
1	D	558	ASP	2.5
1	B	110	ILE	2.5
1	C	411	THR	2.5
1	B	119	TYR	2.5
1	B	227	LEU	2.5
1	A	534	GLN	2.5
1	C	344	SER	2.5
1	C	445	ALA	2.5
1	C	536	ASP	2.5
1	C	428	MET	2.5
1	D	555	LEU	2.5
1	A	546	GLY	2.5
1	A	517	CYS	2.5
1	A	419	PHE	2.5
1	A	441	ASN	2.5
1	B	539	PHE	2.5
1	A	128	LEU	2.5
1	D	216	ALA	2.4
1	C	390	ILE	2.4
1	D	347	PHE	2.4
1	D	355	ASN	2.4
1	D	441	ASN	2.4
1	A	299	LEU	2.4
1	A	445	ALA	2.4
1	D	414	ILE	2.4
1	B	543	LEU	2.4
1	C	154	LEU	2.4
1	D	286	ASN	2.4
1	B	469	VAL	2.4
1	C	163	VAL	2.4
1	D	194	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	236	GLN	2.4
1	A	169	PHE	2.4
1	D	563	PHE	2.4
1	C	578	THR	2.4
1	B	167	TYR	2.4
1	B	319	ILE	2.4
1	B	358	ILE	2.4
1	D	534	GLN	2.4
1	B	151	PHE	2.4
1	A	478	LEU	2.4
1	B	133	LEU	2.4
1	B	149	LEU	2.4
1	B	297	LEU	2.4
1	D	265	LEU	2.4
1	C	345	CYS	2.4
1	A	193	VAL	2.4
1	C	155	VAL	2.4
1	B	121	ASP	2.4
1	D	258	ILE	2.4
1	D	281	ILE	2.4
1	D	386	GLU	2.4
1	B	143	SER	2.4
1	C	273	VAL	2.4
1	C	197	GLY	2.3
1	A	510	ASP	2.3
1	B	234	TYR	2.3
1	C	167	TYR	2.3
1	D	192	ILE	2.3
1	A	204	LEU	2.3
1	C	522	GLN	2.3
1	D	521	GLN	2.3
1	A	180	CYS	2.3
1	C	574	ILE	2.3
1	D	429	ILE	2.3
1	C	430	ASN	2.3
1	C	521	GLN	2.3
1	D	115	PHE	2.3
1	B	123	GLY	2.3
1	C	378	ILE	2.3
1	C	541	THR	2.3
1	D	215	SER	2.3
1	D	378	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	474	ILE	2.3
1	A	351	TYR	2.3
1	B	505	TYR	2.3
1	C	497	CYS	2.3
1	C	355	ASN	2.3
1	D	510	ASP	2.3
1	B	473	GLN	2.3
1	B	500	GLU	2.3
1	B	491	ARG	2.3
1	D	132	ILE	2.3
1	A	225	TYR	2.3
1	B	518	PHE	2.3
1	D	86	ASN	2.3
1	C	130	ASP	2.3
1	C	248	ARG	2.3
1	D	582	ALA	2.3
1	B	218	LEU	2.3
1	D	553	LEU	2.3
1	B	105	LYS	2.3
1	D	166	ASN	2.3
1	C	483	ARG	2.3
1	D	544	GLU	2.2
1	C	161	ILE	2.2
1	D	496	ILE	2.2
1	C	158	GLY	2.2
1	D	415	LEU	2.2
1	C	181	TYR	2.2
1	C	225	TYR	2.2
1	D	238	TYR	2.2
1	D	336	ASN	2.2
1	D	509	ASN	2.2
1	A	423	GLU	2.2
1	D	399	PRO	2.2
1	A	309	LEU	2.2
1	C	204	LEU	2.2
1	C	214	LEU	2.2
1	D	368	LEU	2.2
1	C	539	PHE	2.2
1	A	170	HIS	2.2
1	A	255	THR	2.2
1	C	275	THR	2.2
1	C	482	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	142	VAL	2.2
1	C	509	ASN	2.2
1	A	516	GLU	2.2
1	B	243	ILE	2.2
1	B	507	GLU	2.2
1	B	198	LYS	2.2
1	C	251	PHE	2.2
1	A	250	THR	2.2
1	D	255	THR	2.2
1	A	257	ILE	2.2
1	D	403	ILE	2.2
1	B	355	ASN	2.2
1	C	372	LEU	2.2
1	A	125	GLY	2.2
1	A	548	PRO	2.2
1	B	180	CYS	2.2
1	D	79	ASP	2.2
1	D	142	VAL	2.2
1	D	181	TYR	2.2
1	A	88	SER	2.2
1	A	432	ILE	2.2
1	C	451	GLN	2.2
1	A	227	LEU	2.2
1	B	564	LEU	2.2
1	C	274	GLU	2.2
1	C	418	PRO	2.2
1	D	196	PRO	2.2
1	D	152	PHE	2.2
1	C	311	LEU	2.1
1	D	508	LEU	2.1
1	C	515	LYS	2.1
1	D	527	LYS	2.1
1	D	231	GLU	2.1
1	C	98	GLY	2.1
1	D	412	ASN	2.1
1	B	563	PHE	2.1
1	D	471	HIS	2.1
1	C	136	THR	2.1
1	A	232	ILE	2.1
1	C	238	TYR	2.1
1	C	474	ILE	2.1
1	D	457	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	299	LEU	2.1
1	B	311	LEU	2.1
1	B	178	ALA	2.1
1	B	283	GLY	2.1
1	B	440	PRO	2.1
1	B	458	GLU	2.1
1	D	420	ASP	2.1
1	A	474	ILE	2.1
1	C	307	THR	2.1
1	D	189	ILE	2.1
1	C	351	TYR	2.1
1	A	140	MET	2.1
1	B	532	ALA	2.1
1	D	117	GLU	2.1
1	D	208	PRO	2.1
1	D	551	GLY	2.1
1	C	106	PHE	2.1
1	A	121	ASP	2.1
1	A	183	LYS	2.1
1	B	104	HIS	2.1
1	C	224	LYS	2.1
1	C	400	LYS	2.1
1	C	480	LYS	2.1
1	C	558	ASP	2.1
1	D	96	ASP	2.1
1	D	523	LYS	2.1
1	B	161	ILE	2.1
1	A	380	TYR	2.1
1	B	102	TYR	2.1
1	B	337	THR	2.1
1	D	461	TYR	2.1
1	D	287	ALA	2.1
1	D	552	GLY	2.1
1	A	222	PRO	2.1
1	A	531	GLU	2.1
1	C	159	GLU	2.1
1	D	143	SER	2.1
1	A	330	ARG	2.1
1	B	258	ILE	2.1
1	D	161	ILE	2.1
1	D	431	ILE	2.1
1	B	582	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	78	VAL	2.0
1	B	344	SER	2.0
1	C	143	SER	2.0
1	A	547	LEU	2.0
1	C	403	ILE	2.0
1	C	496	ILE	2.0
1	C	560	ILE	2.0
1	D	257	ILE	2.0
1	D	502	LEU	2.0
1	D	560	ILE	2.0
1	A	524	ASP	2.0
1	A	460	LYS	2.0
1	C	405	GLU	2.0
1	A	163	VAL	2.0
1	C	142	VAL	2.0
1	D	252	VAL	2.0
1	D	309	LEU	2.0
1	A	112	ILE	2.0
1	C	111	SER	2.0
1	C	557	ILE	2.0
1	A	171	ASN	2.0
1	C	455	HIS	2.0
1	A	109	THR	2.0
1	B	538	ALA	2.0
1	A	345	CYS	2.0
1	A	196	PRO	2.0
1	A	472	PRO	2.0
1	C	120	LYS	2.0
1	C	436	LYS	2.0
1	A	280	LEU	2.0
1	C	575	LEU	2.0
1	D	242	LEU	2.0
1	C	407	ILE	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](#)

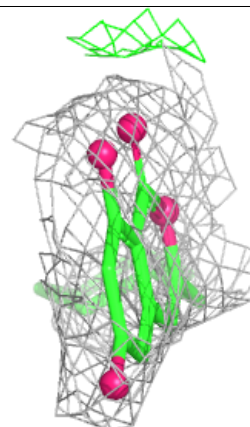
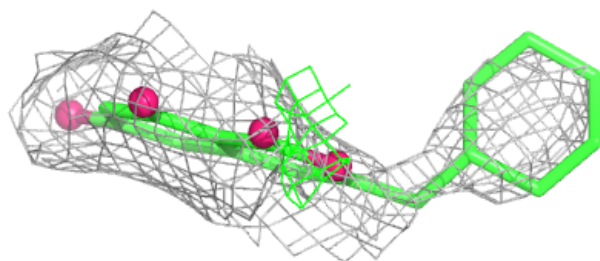
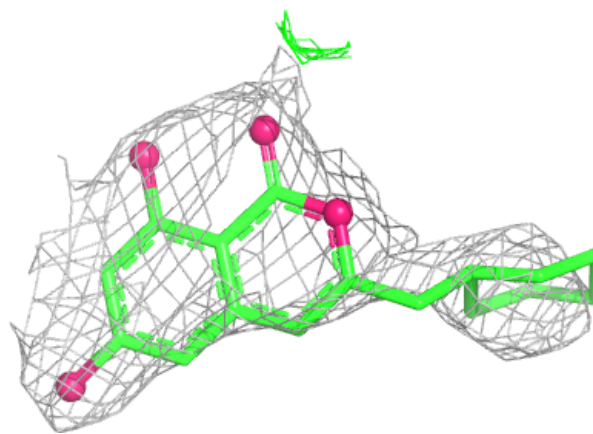
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LYS	B	602	10/10	0.60	0.21	44,45,48,48	0
3	LYS	C	602	10/10	0.73	0.26	54,56,56,57	0
2	D5O	C	601	20/20	0.74	0.19	54,55,57,57	0
3	LYS	A	602	10/10	0.79	0.23	48,49,50,51	0
2	D5O	D	601	20/20	0.82	0.16	39,40,43,43	0
2	D5O	B	601	20/20	0.82	0.16	44,45,46,46	0
3	LYS	D	602	10/10	0.82	0.19	42,45,51,51	0
2	D5O	A	601	20/20	0.84	0.15	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.

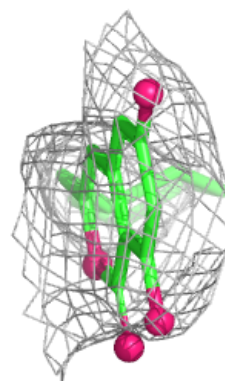
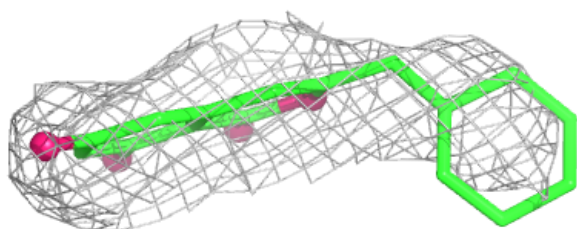
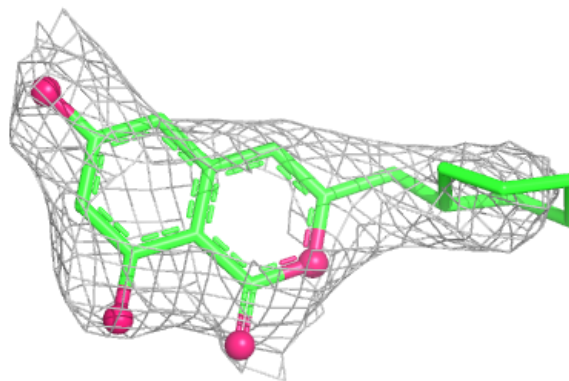
Electron density around D5O C 601:

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

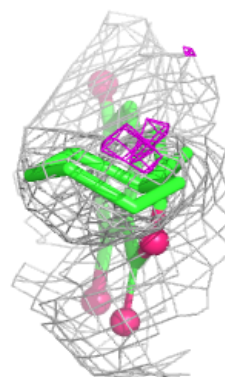
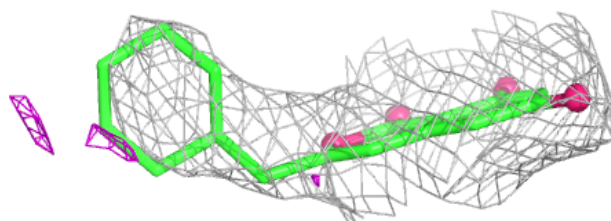
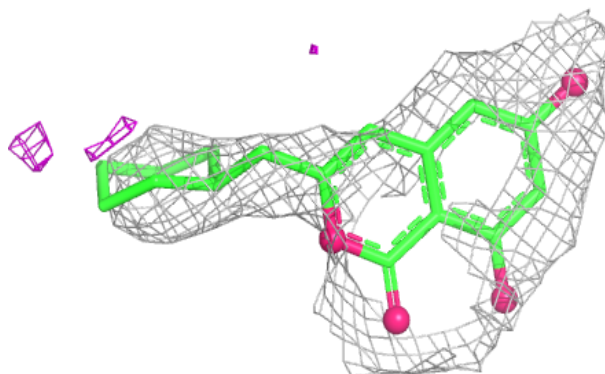


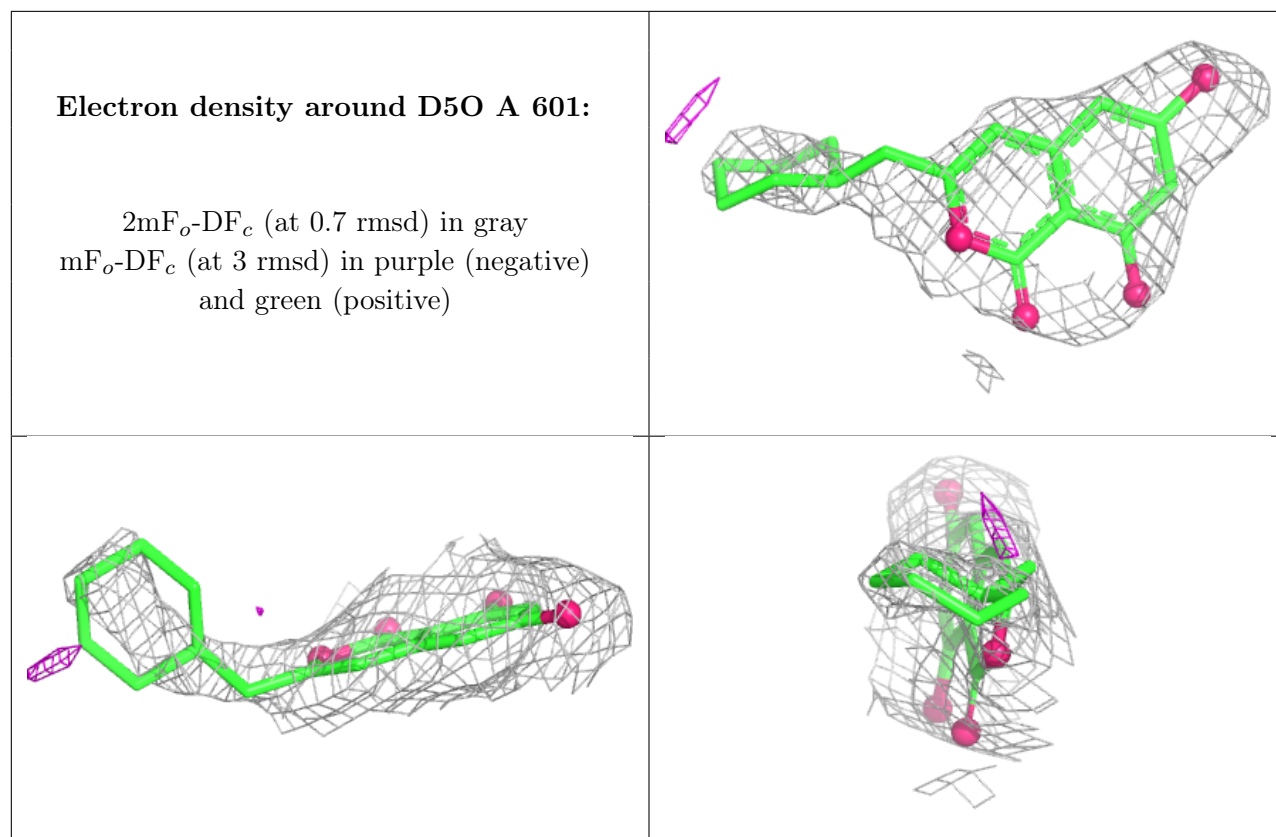
Electron density around D5O D 601:

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

**Electron density around D5O 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.