



# Full wwPDB X-ray Structure Validation Report i

Sep 23, 2020 – 04:05 PM BST

PDB ID : 6SU7  
Title : Complex between a UDP-glucosyltransferase from Polygonum tinctorium capable of glucosylating indoxyl and 3,4-Dichloroaniline  
Authors : Fredslund, F.; Teze, D.; Svensson, B.; Adams, P.D.; Welner, D.H.  
Deposited on : 2019-09-13  
Resolution : 2.75 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 i symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

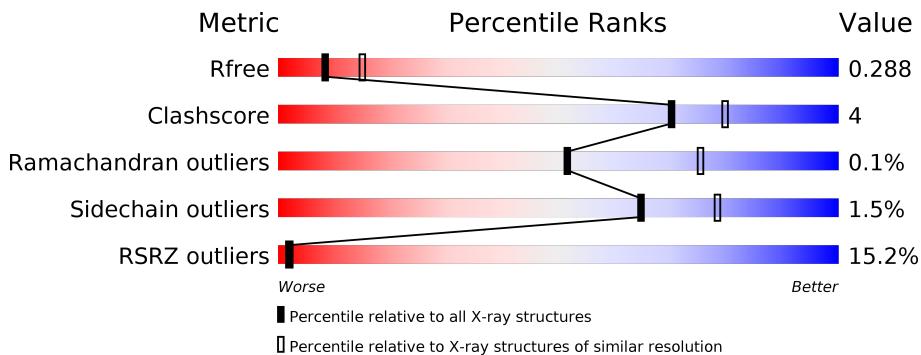
## 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.



## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 27755 atoms, of which 13943 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	H	N	O	S	0	1	0
			6981	2222	3508	597	640	14			
1	B	452	Total	C	H	N	O	S	0	0	0
			6980	2222	3507	597	640	14			
1	C	446	Total	C	H	N	O	S	0	0	0
			6910	2201	3473	590	633	13			
1	D	444	Total	C	H	N	O	S	0	0	0
			6875	2192	3455	585	630	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A0A2R2JFJ4
A	-20	GLY	-	expression tag	UNP A0A2R2JFJ4
A	-19	HIS	-	expression tag	UNP A0A2R2JFJ4
A	-18	HIS	-	expression tag	UNP A0A2R2JFJ4
A	-17	HIS	-	expression tag	UNP A0A2R2JFJ4
A	-16	HIS	-	expression tag	UNP A0A2R2JFJ4
A	-15	HIS	-	expression tag	UNP A0A2R2JFJ4
A	-14	HIS	-	expression tag	UNP A0A2R2JFJ4
A	-13	ASP	-	expression tag	UNP A0A2R2JFJ4
A	-12	TYR	-	expression tag	UNP A0A2R2JFJ4
A	-11	ASP	-	expression tag	UNP A0A2R2JFJ4
A	-10	ILE	-	expression tag	UNP A0A2R2JFJ4
A	-9	PRO	-	expression tag	UNP A0A2R2JFJ4
A	-8	THR	-	expression tag	UNP A0A2R2JFJ4
A	-7	THR	-	expression tag	UNP A0A2R2JFJ4
A	-6	GLU	-	expression tag	UNP A0A2R2JFJ4
A	-5	ASN	-	expression tag	UNP A0A2R2JFJ4
A	-4	LEU	-	expression tag	UNP A0A2R2JFJ4
A	-3	TYR	-	expression tag	UNP A0A2R2JFJ4
A	-2	PHE	-	expression tag	UNP A0A2R2JFJ4
A	-1	GLN	-	expression tag	UNP A0A2R2JFJ4

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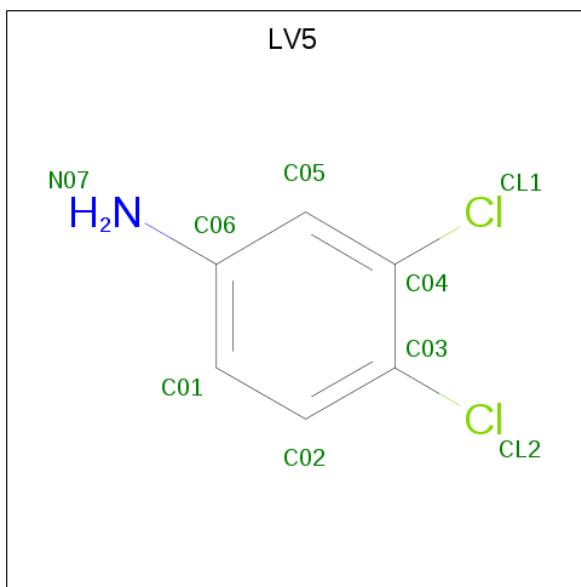
Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	initiating methionine	UNP A0A2R2JFJ4
B	-20	GLY	-	expression tag	UNP A0A2R2JFJ4
B	-19	HIS	-	expression tag	UNP A0A2R2JFJ4
B	-18	HIS	-	expression tag	UNP A0A2R2JFJ4
B	-17	HIS	-	expression tag	UNP A0A2R2JFJ4
B	-16	HIS	-	expression tag	UNP A0A2R2JFJ4
B	-15	HIS	-	expression tag	UNP A0A2R2JFJ4
B	-14	HIS	-	expression tag	UNP A0A2R2JFJ4
B	-13	ASP	-	expression tag	UNP A0A2R2JFJ4
B	-12	TYR	-	expression tag	UNP A0A2R2JFJ4
B	-11	ASP	-	expression tag	UNP A0A2R2JFJ4
B	-10	ILE	-	expression tag	UNP A0A2R2JFJ4
B	-9	PRO	-	expression tag	UNP A0A2R2JFJ4
B	-8	THR	-	expression tag	UNP A0A2R2JFJ4
B	-7	THR	-	expression tag	UNP A0A2R2JFJ4
B	-6	GLU	-	expression tag	UNP A0A2R2JFJ4
B	-5	ASN	-	expression tag	UNP A0A2R2JFJ4
B	-4	LEU	-	expression tag	UNP A0A2R2JFJ4
B	-3	TYR	-	expression tag	UNP A0A2R2JFJ4
B	-2	PHE	-	expression tag	UNP A0A2R2JFJ4
B	-1	GLN	-	expression tag	UNP A0A2R2JFJ4
C	-21	MET	-	initiating methionine	UNP A0A2R2JFJ4
C	-20	GLY	-	expression tag	UNP A0A2R2JFJ4
C	-19	HIS	-	expression tag	UNP A0A2R2JFJ4
C	-18	HIS	-	expression tag	UNP A0A2R2JFJ4
C	-17	HIS	-	expression tag	UNP A0A2R2JFJ4
C	-16	HIS	-	expression tag	UNP A0A2R2JFJ4
C	-15	HIS	-	expression tag	UNP A0A2R2JFJ4
C	-14	HIS	-	expression tag	UNP A0A2R2JFJ4
C	-13	ASP	-	expression tag	UNP A0A2R2JFJ4
C	-12	TYR	-	expression tag	UNP A0A2R2JFJ4
C	-11	ASP	-	expression tag	UNP A0A2R2JFJ4
C	-10	ILE	-	expression tag	UNP A0A2R2JFJ4
C	-9	PRO	-	expression tag	UNP A0A2R2JFJ4
C	-8	THR	-	expression tag	UNP A0A2R2JFJ4
C	-7	THR	-	expression tag	UNP A0A2R2JFJ4
C	-6	GLU	-	expression tag	UNP A0A2R2JFJ4
C	-5	ASN	-	expression tag	UNP A0A2R2JFJ4
C	-4	LEU	-	expression tag	UNP A0A2R2JFJ4
C	-3	TYR	-	expression tag	UNP A0A2R2JFJ4
C	-2	PHE	-	expression tag	UNP A0A2R2JFJ4
C	-1	GLN	-	expression tag	UNP A0A2R2JFJ4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	MET	-	initiating methionine	UNP A0A2R2JFJ4
D	-20	GLY	-	expression tag	UNP A0A2R2JFJ4
D	-19	HIS	-	expression tag	UNP A0A2R2JFJ4
D	-18	HIS	-	expression tag	UNP A0A2R2JFJ4
D	-17	HIS	-	expression tag	UNP A0A2R2JFJ4
D	-16	HIS	-	expression tag	UNP A0A2R2JFJ4
D	-15	HIS	-	expression tag	UNP A0A2R2JFJ4
D	-14	HIS	-	expression tag	UNP A0A2R2JFJ4
D	-13	ASP	-	expression tag	UNP A0A2R2JFJ4
D	-12	TYR	-	expression tag	UNP A0A2R2JFJ4
D	-11	ASP	-	expression tag	UNP A0A2R2JFJ4
D	-10	ILE	-	expression tag	UNP A0A2R2JFJ4
D	-9	PRO	-	expression tag	UNP A0A2R2JFJ4
D	-8	THR	-	expression tag	UNP A0A2R2JFJ4
D	-7	THR	-	expression tag	UNP A0A2R2JFJ4
D	-6	GLU	-	expression tag	UNP A0A2R2JFJ4
D	-5	ASN	-	expression tag	UNP A0A2R2JFJ4
D	-4	LEU	-	expression tag	UNP A0A2R2JFJ4
D	-3	TYR	-	expression tag	UNP A0A2R2JFJ4
D	-2	PHE	-	expression tag	UNP A0A2R2JFJ4
D	-1	GLN	-	expression tag	UNP A0A2R2JFJ4

- Molecule 2 is 3,4-Dichloroaniline (three-letter code: LV5) (formula: C<sub>6</sub>H<sub>5</sub>Cl<sub>2</sub>N) (labeled as "Ligand of Interest" by author).

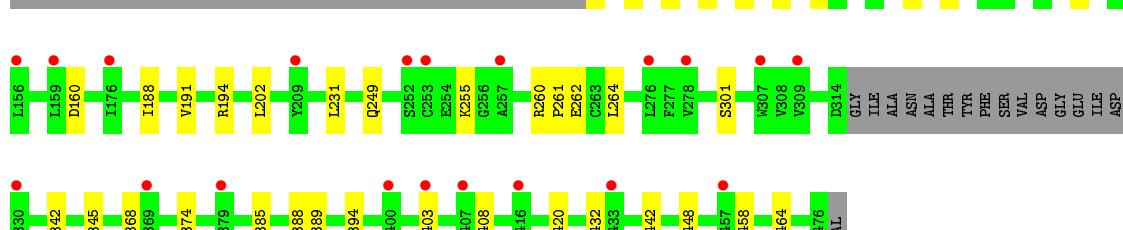
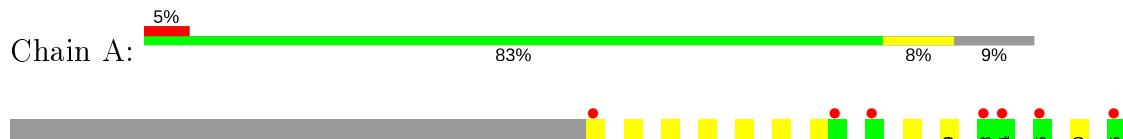


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			9	6	2	1		

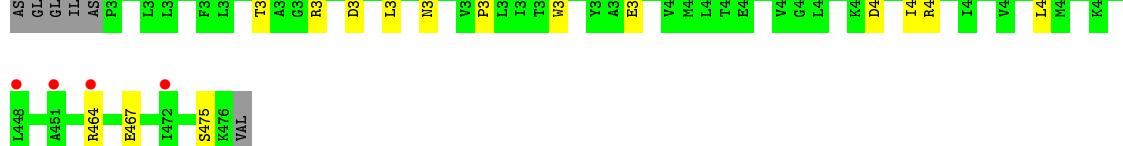
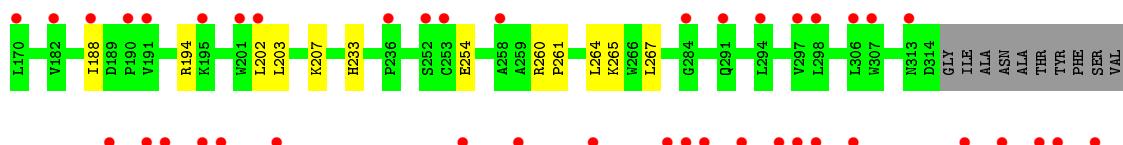
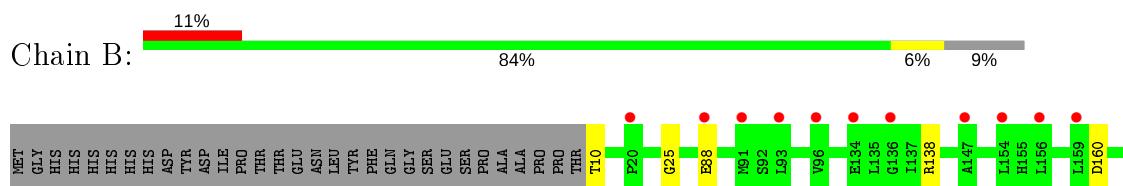
### 3 Residue-property plots [\(i\)](#)

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.

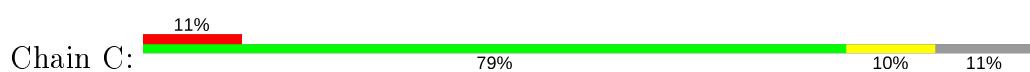
- Molecule 1: Glycosyltransferase

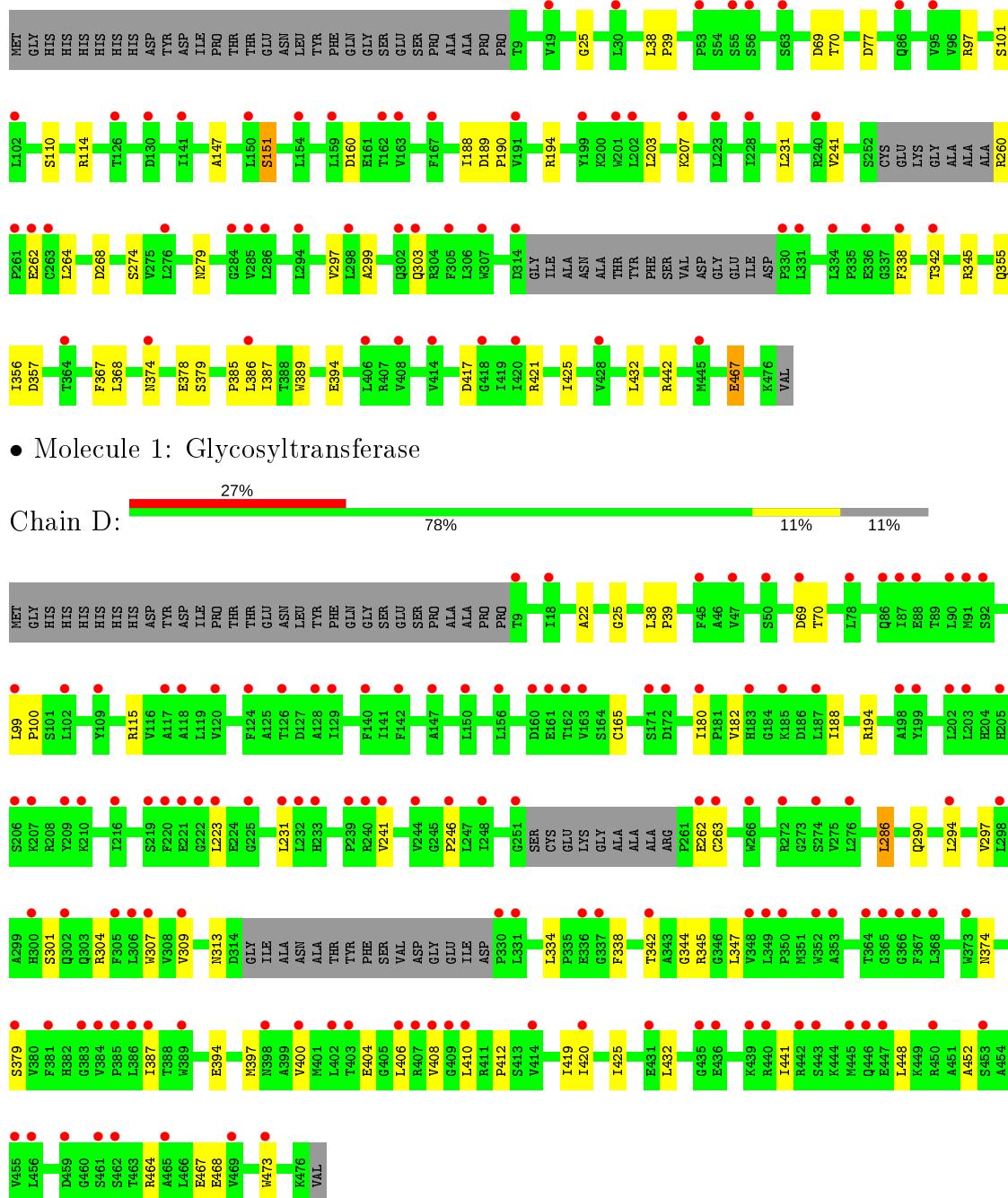


- Molecule 1: Glycosyltransferase



- Molecule 1: Glycosyltransferase





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.35 Å    119.36 Å    170.63 Å 90.00°    90.00°    90.00°	Depositor
Resolution (Å)	50.28 – 2.75 51.34 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.28-2.75) 99.5 (51.34-2.75)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.70 (at 2.73 Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
$R$ , $R_{free}$	0.256 , 0.287 0.259 , 0.288	Depositor DCC
$R_{free}$ test set	2475 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.1	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	27755	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6138e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: LV5

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	0.24	0/3548	0.42	0/4820
1	B	0.24	0/3557	0.42	0/4833
1	C	0.24	0/3520	0.42	0/4783
1	D	0.24	0/3503	0.43	0/4760
All	All	0.24	0/14128	0.42	0/19196

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	3473	3508	3508	21	1
1	B	3473	3507	3508	21	0
1	C	3437	3473	3472	28	1
1	D	3420	3455	3455	32	0
2	A	9	0	0	0	0
All	All	13812	13943	13943	101	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:ASP:OD2	1:C:421:ARG:NH2	2.24	0.70
1:B:385:PRO:HB2	1:B:432:LEU:HD11	1.73	0.69
1:D:342:THR:HG22	1:D:345:ARG:HH11	1.57	0.68
1:A:385:PRO:HB2	1:A:432:LEU:HD11	1.77	0.66
1:C:342:THR:HG22	1:C:345:ARG:HH21	1.65	0.61
1:A:160:ASP:OD1	1:A:194:ARG:NH2	2.33	0.61
1:D:180:ILE:HD11	1:D:400:VAL:HG12	1.83	0.59
1:B:417:ASP:OD2	1:B:421:ARG:NH2	2.36	0.59
1:C:385:PRO:HB2	1:C:432:LEU:HD11	1.83	0.58
1:C:264:LEU:HD11	1:C:357:ASP:HB3	1.86	0.58
1:B:160:ASP:OD1	1:B:194:ARG:NH2	2.37	0.57
1:A:342:THR:HG22	1:A:345:ARG:NH2	2.20	0.56
1:D:304:ARG:NH1	1:D:344:GLY:O	2.38	0.56
1:B:25:GLY:O	1:B:374:ASN:ND2	2.36	0.56
1:C:25:GLY:O	1:C:374:ASN:ND2	2.35	0.55
1:C:297:VAL:HG21	1:C:425:ILE:HB	1.87	0.55
1:D:297:VAL:HG21	1:D:425:ILE:HB	1.89	0.54
1:C:203:LEU:HD22	1:C:207:LYS:HE3	1.89	0.54
1:C:299:ALA:HB2	1:C:338:PHE:CE1	2.44	0.53
1:D:286:LEU:HD12	1:D:286:LEU:H	1.73	0.53
1:C:160:ASP:OD1	1:C:194:ARG:NH2	2.41	0.52
1:B:264:LEU:HD23	1:B:267:LEU:HD12	1.92	0.52
1:C:274:SER:O	1:C:303:GLN:NE2	2.44	0.51
1:C:356:ILE:HD11	1:C:378:GLU:CD	2.32	0.50
1:D:394:GLU:OE1	1:D:394:GLU:N	2.39	0.50
1:A:150:LEU:HD23	1:A:231:LEU:HD13	1.93	0.50
1:D:387:ILE:CD1	1:D:432:LEU:HD22	2.42	0.50
1:B:368:LEU:HD21	1:B:389:TRP:CE3	2.46	0.50
1:B:394:GLU:N	1:B:394:GLU:OE1	2.38	0.50
1:C:260:ARG:NH1	1:C:268:ASP:OD2	2.44	0.50
1:D:223:LEU:O	1:D:406:LEU:HD11	2.13	0.49
1:A:261:PRO:HD2	1:A:264:LEU:HD12	1.94	0.48
1:B:464:ARG:O	1:B:467:GLU:N	2.47	0.48
1:A:28:ILE:HG23	1:A:249:GLN:HG3	1.95	0.48
1:D:165:CYS:O	1:D:194:ARG:NH1	2.46	0.48
1:D:301:SER:O	1:D:345:ARG:NH2	2.47	0.48
1:A:77:ASP:O	1:A:97:ARG:NH1	2.47	0.47
1:A:368:LEU:HD21	1:A:389:TRP:CE3	2.50	0.47
1:C:231:LEU:HB3	1:C:241:VAL:HG21	1.97	0.47
1:C:147:ALA:O	1:C:151:SER:OG	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:LEU:HD12	1:D:448:LEU:HD13	1.97	0.46
1:D:294:LEU:HD23	1:D:307:TRP:CZ2	2.50	0.46
1:C:367:PHE:HB3	1:C:386:LEU:HD23	1.97	0.46
1:C:387:ILE:HG13	1:C:432:LEU:HD22	1.96	0.46
1:D:188:ILE:HG22	1:D:394:GLU:HA	1.98	0.46
1:D:25:GLY:O	1:D:374:ASN:ND2	2.48	0.46
1:D:412:PRO:HG2	1:D:420:ILE:HD13	1.96	0.46
1:C:279:ASN:ND2	1:C:355:GLN:OE1	2.49	0.46
1:C:69:ASP:OD1	1:C:70:THR:N	2.47	0.45
1:A:188:ILE:HD11	1:A:202:LEU:HD21	1.98	0.45
1:C:188:ILE:HG22	1:C:394:GLU:HA	1.99	0.45
1:A:389:TRP:CE2	1:A:420:ILE:HD12	2.51	0.45
1:C:38:LEU:N	1:C:39:PRO:CD	2.79	0.45
1:D:286:LEU:N	1:D:286:LEU:HD12	2.31	0.45
1:D:182:VAL:HG11	1:D:397:MET:HG2	1.99	0.45
1:D:246:PRO:HG3	1:D:452:ALA:HB1	1.97	0.45
1:D:38:LEU:N	1:D:39:PRO:CD	2.79	0.45
1:C:394:GLU:OE1	1:C:394:GLU:N	2.41	0.45
1:A:394:GLU:N	1:A:394:GLU:OE1	2.41	0.44
1:D:400:VAL:HG13	1:D:404:GLU:OE1	2.18	0.44
1:D:223:LEU:CD1	1:D:448:LEU:HD13	2.48	0.44
1:B:188:ILE:HG22	1:B:394:GLU:HB2	2.00	0.44
1:D:307:TRP:CD2	1:D:309:VAL:HG22	2.52	0.44
1:D:313:ASN:O	1:D:313:ASN:ND2	2.51	0.43
1:A:301:SER:O	1:A:345:ARG:NH1	2.51	0.43
1:C:379:SER:OG	1:C:386:LEU:HD21	2.18	0.43
1:D:115:ARG:NH2	1:D:473:TRP:O	2.50	0.43
1:A:301:SER:O	1:A:345:ARG:CZ	2.66	0.43
1:A:17:ILE:HB	1:A:119:LEU:HD12	2.00	0.43
1:B:264:LEU:HD11	1:B:357:ASP:HB3	2.00	0.43
1:D:231:LEU:HB3	1:D:241:VAL:HG21	2.01	0.43
1:D:347:LEU:HD13	1:D:347:LEU:C	2.39	0.43
1:B:10:THR:O	1:B:10:THR:OG1	2.34	0.43
1:A:188:ILE:O	1:A:191:VAL:HG22	2.19	0.43
1:A:25:GLY:O	1:A:374:ASN:ND2	2.48	0.43
1:A:388:THR:HG21	1:A:403:THR:HG23	2.00	0.43
1:C:368:LEU:HD21	1:C:389:TRP:CE3	2.54	0.43
1:D:290:GLN:OE1	1:D:420:ILE:N	2.35	0.42
1:B:260:ARG:HG2	1:B:265:LYS:HG3	2.00	0.42
1:A:10:THR:OG1	1:A:10:THR:O	2.36	0.42
1:B:203:LEU:HD22	1:B:207:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ASP:OD1	1:D:70:THR:N	2.50	0.42
1:D:334:LEU:HD13	1:D:338:PHE:CD2	2.55	0.42
1:C:189:ASP:N	1:C:190:PRO:HD2	2.34	0.42
1:D:387:ILE:HD11	1:D:432:LEU:HD22	2.02	0.42
1:B:261:PRO:HD2	1:B:264:LEU:HD12	2.02	0.42
1:B:342:THR:HG22	1:B:345:ARG:NH2	2.36	0.41
1:B:188:ILE:HG22	1:B:394:GLU:CB	2.50	0.41
1:B:464:ARG:HH12	1:D:468:GLU:CG	2.34	0.41
1:D:99:LEU:N	1:D:100:PRO:HD2	2.35	0.41
1:B:138:ARG:NH2	1:B:475:SER:OG	2.53	0.41
1:C:356:ILE:HD11	1:C:378:GLU:CG	2.50	0.41
1:A:408:VAL:HG11	1:A:448:LEU:HD12	2.02	0.41
1:B:389:TRP:CE2	1:B:420:ILE:HD12	2.55	0.41
1:C:262:GLU:N	1:C:262:GLU:OE1	2.48	0.41
1:C:38:LEU:HD23	1:C:38:LEU:HA	1.95	0.41
1:A:49:THR:HG21	1:A:53:PRO:HG3	2.03	0.40
1:A:262:GLU:N	1:A:262:GLU:OE1	2.49	0.40
1:B:188:ILE:HD11	1:B:202:LEU:HD21	2.02	0.40
1:C:77:ASP:O	1:C:97:ARG:NH1	2.53	0.40
1:B:88:GLU:OE1	1:B:88:GLU:N	2.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ARG:NH2	1:C:467:GLU:OE1[1_455]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	448/499 (90%)	427 (95%)	21 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	448/499 (90%)	423 (94%)	25 (6%)	0	100	100
1	C	440/499 (88%)	414 (94%)	26 (6%)	0	100	100
1	D	438/499 (88%)	413 (94%)	24 (6%)	1 (0%)	47	69
All	All	1774/1996 (89%)	1677 (94%)	96 (5%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	22	ALA

### 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	379/419 (90%)	375 (99%)	4 (1%)	73	84
1	B	380/419 (91%)	378 (100%)	2 (0%)	88	92
1	C	378/419 (90%)	372 (98%)	6 (2%)	62	77
1	D	376/419 (90%)	366 (97%)	10 (3%)	44	65
All	All	1513/1676 (90%)	1491 (98%)	22 (2%)	65	78

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	LYS
1	A	260	ARG
1	A	442	ARG
1	A	458	LYS
1	B	233	HIS
1	B	254	GLU
1	C	101	SER
1	C	110	SER
1	C	114	ARG
1	C	151	SER

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Mol	Chain	Res	Type
1	C	442	ARG
1	C	467	GLU
1	D	262	GLU
1	D	263	CYS
1	D	286	LEU
1	D	379	SER
1	D	408	VAL
1	D	410	LEU
1	D	419	ILE
1	D	441	ILE
1	D	464	ARG
1	D	467	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [\(i\)](#)

1 ligand is 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	LV5	A	1001	-	9,9,9	1.29	3 (33%)	12,12,12	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LV5	A	1001	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	LV5	C04-CL1	2.24	1.79	1.73
2	A	1001	LV5	C03-CL2	2.20	1.78	1.73
2	A	1001	LV5	C06-N07	2.11	1.45	1.38

There are no bond angle outliers.

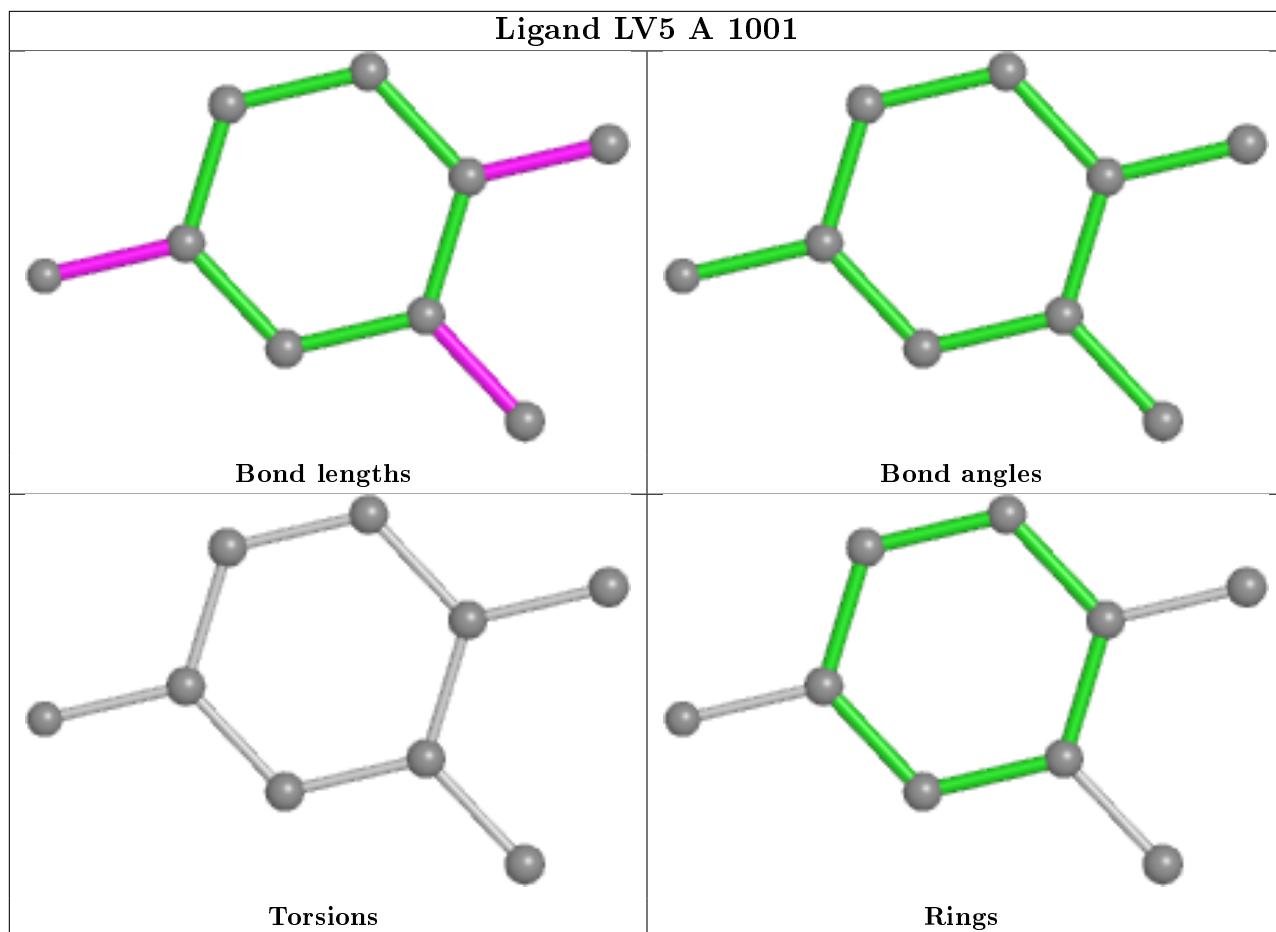
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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	452/499 (90%)	0.52	27 (5%) 21 26	27, 55, 104, 161	0
1	B	452/499 (90%)	0.88	57 (12%) 3 4	38, 75, 137, 211	0
1	C	446/499 (89%)	0.77	56 (12%) 3 4	42, 81, 136, 211	0
1	D	444/499 (88%)	1.60	133 (29%) 0 0	53, 136, 206, 269	0
All	All	1794/1996 (89%)	0.94	273 (15%) 2 2	27, 81, 174, 269	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	209	TYR	11.1
1	D	162	THR	9.9
1	D	436	GLU	9.5
1	D	223	LEU	9.2
1	D	336	GLU	8.9
1	D	406	LEU	8.8
1	D	348	VAL	8.2
1	D	202	LEU	8.0
1	D	445	MET	7.5
1	C	294	LEU	6.8
1	D	102	LEU	6.7
1	D	160	ASP	6.6
1	D	294	LEU	6.4
1	D	298	LEU	6.2
1	D	300	HIS	6.2
1	D	409	GLY	6.1
1	D	439	LYS	6.0
1	B	408	VAL	6.0
1	D	207	LYS	6.0
1	D	443	SER	5.9
1	D	140	PHE	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	298	LEU	5.8
1	D	435	GLY	5.7
1	D	383	GLY	5.6
1	D	86	GLN	5.6
1	B	330	PRO	5.6
1	D	91	MET	5.4
1	D	330	PRO	5.3
1	D	450	ARG	5.2
1	D	187	LEU	5.2
1	B	253	CYS	5.1
1	D	222	GLY	5.1
1	D	87	ILE	5.0
1	C	263	CYS	5.0
1	D	239	PRO	4.9
1	D	410	LEU	4.8
1	C	207	LYS	4.7
1	C	286	LEU	4.7
1	D	384	VAL	4.7
1	B	190	PRO	4.7
1	D	272	ARG	4.6
1	D	199	TYR	4.6
1	D	389	TRP	4.5
1	D	203	LEU	4.5
1	D	331	LEU	4.5
1	B	298	LEU	4.4
1	C	130	ASP	4.4
1	D	221	GLU	4.4
1	D	446	GLN	4.4
1	D	262	GLU	4.3
1	A	400	VAL	4.3
1	A	159	LEU	4.3
1	B	425	ILE	4.2
1	C	418	GLY	4.2
1	D	219	SER	4.2
1	D	307	TRP	4.1
1	D	305	PHE	4.1
1	C	285	VAL	4.0
1	B	297	VAL	4.0
1	B	188	ILE	3.9
1	C	305	PHE	3.9
1	C	159	LEU	3.9
1	D	198	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	409	GLY	3.8
1	D	78	LEU	3.8
1	B	182	VAL	3.7
1	D	124	PHE	3.7
1	D	408	VAL	3.7
1	C	163	VAL	3.6
1	A	276	LEU	3.6
1	D	205	HIS	3.6
1	D	225	GLY	3.6
1	B	410	LEU	3.6
1	C	191	VAL	3.5
1	D	385	PRO	3.5
1	D	246	PRO	3.5
1	D	447	GLU	3.5
1	C	330	PRO	3.5
1	C	408	VAL	3.5
1	B	339	LEU	3.5
1	B	159	LEU	3.4
1	D	302	GLN	3.4
1	D	241	VAL	3.4
1	C	420	ILE	3.4
1	D	180	ILE	3.4
1	D	373	TRP	3.3
1	A	369	THR	3.3
1	C	167	PHE	3.3
1	D	172	ASP	3.3
1	D	163	VAL	3.3
1	C	338	PHE	3.3
1	D	442	ARG	3.2
1	D	387	ILE	3.2
1	D	276	LEU	3.2
1	C	303	GLN	3.2
1	D	231	LEU	3.2
1	A	78	LEU	3.2
1	B	333	LEU	3.2
1	C	334	LEU	3.2
1	D	233	HIS	3.1
1	B	416	LYS	3.1
1	C	228	ILE	3.1
1	D	398	ASN	3.1
1	B	170	LEU	3.1
1	D	461	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	402	LEU	3.1
1	C	202	LEU	3.1
1	D	120	VAL	3.1
1	B	400	VAL	3.0
1	A	407	ARG	3.0
1	D	367	PHE	3.0
1	C	154	LEU	3.0
1	D	118	ALA	3.0
1	D	251	GLY	3.0
1	D	220	PHE	3.0
1	D	99	LEU	3.0
1	D	129	ILE	2.9
1	C	386	LEU	2.9
1	C	307	TRP	2.9
1	D	353	ALA	2.9
1	D	240	ARG	2.9
1	B	334	LEU	2.9
1	D	459	ASP	2.9
1	D	185	LYS	2.9
1	C	201	TRP	2.9
1	D	50	SER	2.9
1	D	274	SER	2.9
1	D	379	SER	2.9
1	D	266	TRP	2.8
1	D	386	LEU	2.8
1	D	403	THR	2.8
1	C	414	VAL	2.8
1	C	336	GLU	2.8
1	C	223	LEU	2.8
1	D	210	LYS	2.8
1	C	261	PRO	2.8
1	B	258	ALA	2.8
1	C	406	LEU	2.8
1	B	252	SER	2.7
1	D	156	LEU	2.7
1	A	330	PRO	2.7
1	D	440	ARG	2.7
1	C	364	THR	2.7
1	C	428	VAL	2.7
1	B	134	GLU	2.7
1	B	294	LEU	2.7
1	B	432	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	307	TRP	2.7
1	B	464	ARG	2.7
1	B	284	GLY	2.7
1	B	433	MET	2.7
1	B	472	ILE	2.7
1	D	465	ALA	2.6
1	A	155	HIS	2.6
1	C	141	ILE	2.6
1	B	88	GLU	2.6
1	B	404	GLU	2.6
1	D	263	CYS	2.6
1	A	10	THR	2.6
1	D	216	ILE	2.6
1	D	407	ARG	2.6
1	D	366	GLY	2.6
1	D	462	SER	2.6
1	D	128	ALA	2.6
1	D	150	LEU	2.6
1	D	306	LEU	2.6
1	D	337	GLY	2.6
1	D	400	VAL	2.6
1	C	331	LEU	2.6
1	D	90	LEU	2.6
1	A	253	CYS	2.6
1	A	403	THR	2.5
1	A	433	MET	2.5
1	D	206	SER	2.5
1	D	161	GLU	2.5
1	A	135	LEU	2.5
1	B	402	LEU	2.5
1	D	453	SER	2.5
1	C	126	THR	2.5
1	A	209	TYR	2.5
1	B	154	LEU	2.5
1	D	473	TRP	2.5
1	B	91	MET	2.5
1	C	262	GLU	2.5
1	D	365	GLY	2.4
1	D	381	PHE	2.4
1	D	431	GLU	2.4
1	B	387	ILE	2.4
1	C	199	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	306	LEU	2.4
1	D	456	LEU	2.4
1	B	191	VAL	2.4
1	C	53	PRO	2.4
1	A	416	LYS	2.4
1	B	439	LYS	2.4
1	C	30	LEU	2.4
1	B	201	TRP	2.4
1	C	19	VAL	2.4
1	D	414	VAL	2.4
1	D	368	LEU	2.4
1	D	171	SER	2.4
1	D	309	VAL	2.4
1	A	252	SER	2.4
1	C	56	SER	2.4
1	A	309	VAL	2.4
1	B	202	LEU	2.3
1	D	45	PHE	2.3
1	D	147	ALA	2.3
1	D	232	LEU	2.3
1	C	162	THR	2.3
1	D	420	ILE	2.3
1	D	469	VAL	2.3
1	B	156	LEU	2.3
1	C	95	VAL	2.3
1	D	244	VAL	2.3
1	A	379	SER	2.2
1	C	302	GLN	2.2
1	A	91	MET	2.2
1	B	93	LEU	2.2
1	A	257	ALA	2.2
1	B	195	LYS	2.2
1	B	448	LEU	2.2
1	D	117	ALA	2.2
1	B	136	GLY	2.2
1	B	428	VAL	2.2
1	D	47	VAL	2.2
1	B	307	TRP	2.2
1	C	150	LEU	2.2
1	D	350	PRO	2.2
1	D	342	THR	2.2
1	B	338	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	55	SER	2.1
1	D	349	LEU	2.1
1	B	451	ALA	2.1
1	A	278	VAL	2.1
1	C	86	GLN	2.1
1	A	156	LEU	2.1
1	A	457	SER	2.1
1	C	284	GLY	2.1
1	C	445	MET	2.1
1	D	88	GLU	2.1
1	D	9	THR	2.1
1	D	126	THR	2.1
1	D	69	ASP	2.1
1	B	392	TYR	2.1
1	D	18	ILE	2.1
1	B	147	ALA	2.1
1	C	342	THR	2.1
1	D	352	TRP	2.1
1	D	92	SER	2.1
1	C	276	LEU	2.1
1	A	176	ILE	2.1
1	D	455	VAL	2.1
1	C	63	SER	2.1
1	C	240	ARG	2.1
1	D	183	HIS	2.1
1	B	236	PRO	2.1
1	D	109	TYR	2.1
1	B	96	VAL	2.0
1	B	401	MET	2.0
1	A	124	PHE	2.0
1	D	142	PHE	2.0
1	B	20	PRO	2.0
1	B	384	VAL	2.0
1	B	313	ASN	2.0
1	C	314	ASP	2.0
1	D	364	THR	2.0
1	B	291	GLN	2.0
1	A	123	LEU	2.0
1	D	248	ILE	2.0
1	B	343	ALA	2.0
1	C	374	ASN	2.0
1	C	102	LEU	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 [\(i\)](#)

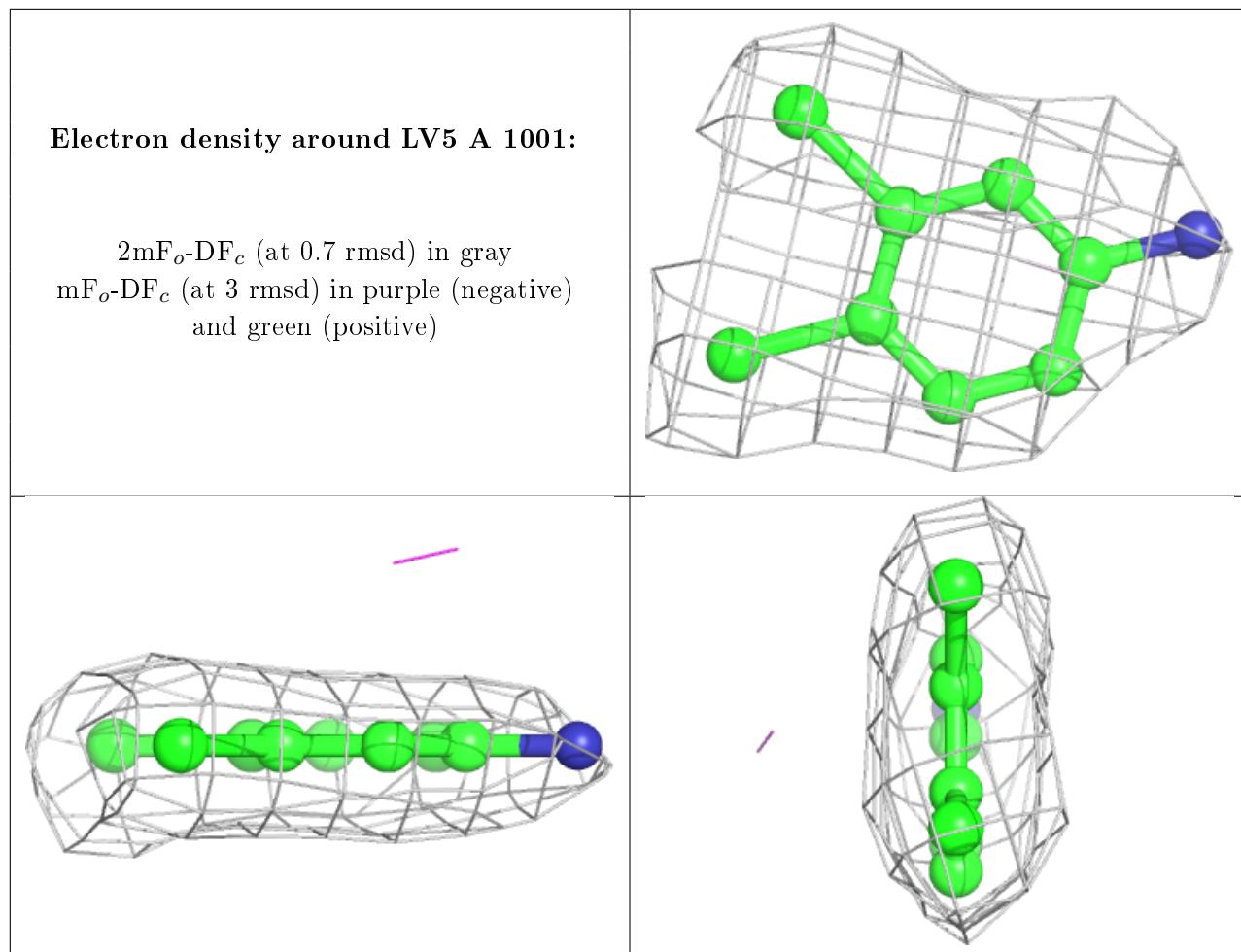
There are no monosaccharides in this entry.

## 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
2	LV5	A	1001	9/9	0.91	0.22	48,51,61,62	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.



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.