



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:27 PM UTC

PDB ID : 9KGT / pdb\_00009kgt  
Title : Crystal structure of topoisomerase IV from *Klebsiella pneumoniae* in complex with DNA and BWC0977, a dual-targeting broad-spectrum novel bacterial topoisomerase inhibitor.  
Authors : Murakami, S.; Okada, U.; Yamashita, E.; Aoki, M.; Hameed, S.; Katagihallimath, N.; Balasubramanian, V.; Ramachandran, V.; Datta, S.  
Deposited on : 2024-11-09  
Resolution : 3.05 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](#) ①) 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

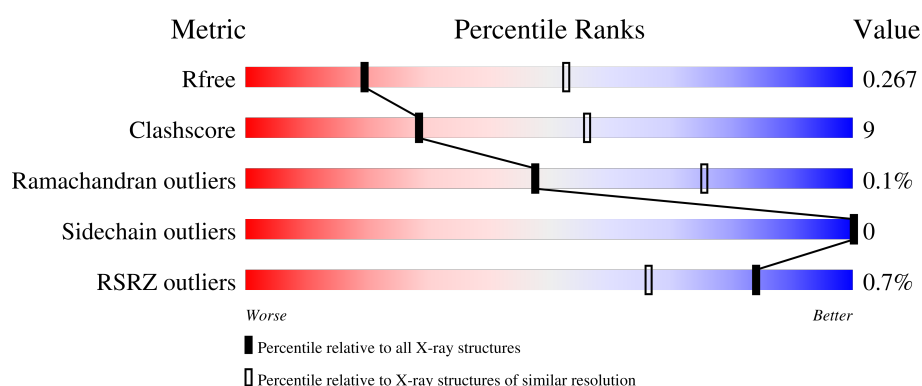
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	734	<div> <div>76%</div> <div>23%</div> <div>.</div> </div>
1	B	734	<div> <div>75%</div> <div>24%</div> <div>.</div> </div>
1	C	734	<div> <div>%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
1	D	734	<div> <div>%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
2	E	26	<div> <div>85%</div> <div>8%</div> <div>8%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	26	 62% 31% 8%
2	G	26	 54% 31% 15%
2	H	26	 62% 23% 15%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24940 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 DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5753	3607	1023	1094	29			
1	B	725	Total	C	N	O	S	0	0	0
			5757	3610	1025	1093	29			
1	C	722	Total	C	N	O	S	0	0	0
			5727	3592	1016	1090	29			
1	D	718	Total	C	N	O	S	0	0	0
			5697	3572	1011	1085	29			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	MET	-	initiating methionine	UNP A6TE19
A	397	GLY	-	expression tag	UNP A6TE19
A	398	SER	-	expression tag	UNP A6TE19
A	399	SER	-	expression tag	UNP A6TE19
A	999	GLU	-	linker	UNP A6TE19
A	1000	SER	-	linker	UNP A6TE19
A	1489	LEU	-	expression tag	UNP A6TE12
A	1490	GLU	-	expression tag	UNP A6TE12
A	1491	HIS	-	expression tag	UNP A6TE12
A	1492	HIS	-	expression tag	UNP A6TE12
A	1493	HIS	-	expression tag	UNP A6TE12
A	1494	HIS	-	expression tag	UNP A6TE12
A	1495	HIS	-	expression tag	UNP A6TE12
A	1496	HIS	-	expression tag	UNP A6TE12
B	396	MET	-	initiating methionine	UNP A6TE19
B	397	GLY	-	expression tag	UNP A6TE19
B	398	SER	-	expression tag	UNP A6TE19
B	399	SER	-	expression tag	UNP A6TE19
B	999	GLU	-	linker	UNP A6TE19
B	1000	SER	-	linker	UNP A6TE19

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	1489	LEU	-	expression tag	UNP A6TE12
B	1490	GLU	-	expression tag	UNP A6TE12
B	1491	HIS	-	expression tag	UNP A6TE12
B	1492	HIS	-	expression tag	UNP A6TE12
B	1493	HIS	-	expression tag	UNP A6TE12
B	1494	HIS	-	expression tag	UNP A6TE12
B	1495	HIS	-	expression tag	UNP A6TE12
B	1496	HIS	-	expression tag	UNP A6TE12
C	396	MET	-	initiating methionine	UNP A6TE19
C	397	GLY	-	expression tag	UNP A6TE19
C	398	SER	-	expression tag	UNP A6TE19
C	399	SER	-	expression tag	UNP A6TE19
C	999	GLU	-	linker	UNP A6TE19
C	1000	SER	-	linker	UNP A6TE19
C	1489	LEU	-	expression tag	UNP A6TE12
C	1490	GLU	-	expression tag	UNP A6TE12
C	1491	HIS	-	expression tag	UNP A6TE12
C	1492	HIS	-	expression tag	UNP A6TE12
C	1493	HIS	-	expression tag	UNP A6TE12
C	1494	HIS	-	expression tag	UNP A6TE12
C	1495	HIS	-	expression tag	UNP A6TE12
C	1496	HIS	-	expression tag	UNP A6TE12
D	396	MET	-	initiating methionine	UNP A6TE19
D	397	GLY	-	expression tag	UNP A6TE19
D	398	SER	-	expression tag	UNP A6TE19
D	399	SER	-	expression tag	UNP A6TE19
D	999	GLU	-	linker	UNP A6TE19
D	1000	SER	-	linker	UNP A6TE19
D	1489	LEU	-	expression tag	UNP A6TE12
D	1490	GLU	-	expression tag	UNP A6TE12
D	1491	HIS	-	expression tag	UNP A6TE12
D	1492	HIS	-	expression tag	UNP A6TE12
D	1493	HIS	-	expression tag	UNP A6TE12
D	1494	HIS	-	expression tag	UNP A6TE12
D	1495	HIS	-	expression tag	UNP A6TE12
D	1496	HIS	-	expression tag	UNP A6TE12

- Molecule 2 is a DNA chain called DNA (5'-D(P\*TP\*TP\*AP\*CP\*GP\*TP\*TP\*GP\*TP\*AP\*TP\*GP\*AP\*TP\*CP\*AP\*TP\*AP\*CP\*AP\*AP\*CP\*GP\*TP\*AP\*A)-3').

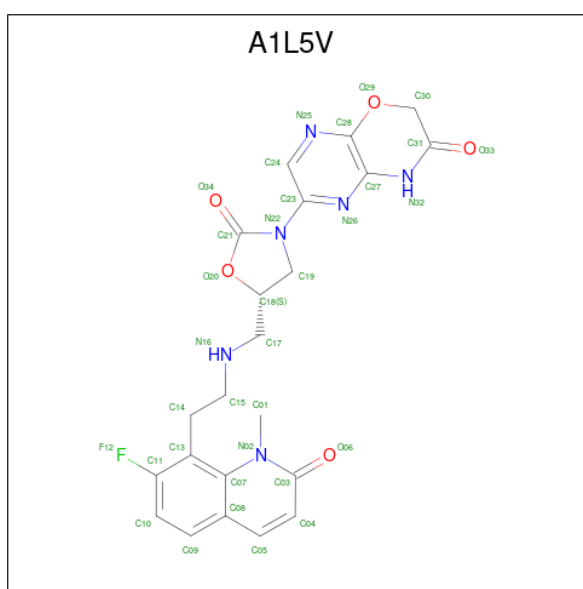
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	24	Total	C	N	O	P	0	0	0
			490	236	85	145	24			

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	24	Total	C	N	O	P	0	0	0
			493	236	91	142	24			
2	G	22	Total	C	N	O	P	0	0	0
			451	216	81	132	22			
2	H	22	Total	C	N	O	P	0	0	0
			451	216	81	132	22			

- Molecule 3 is 6-[(5S)-5-[[[2-(7-Fluoro-1,2-dihydro-1-methyl-2-oxo-8-quinolinyl)ethyl]amino]methyl]-2-oxo-3-oxazolidinyl]-2H-pyrazino[2,3-b]-1,4-oxazin-3(4H)-one (CCD ID: A1L5V) (formula: C<sub>22</sub>H<sub>21</sub>FN<sub>6</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	F	N	O	0	0
			34	22	1	6	5		
3	H	1	Total	C	F	N	O	0	0
			34	22	1	6	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	18	Total 18 O	0	0
4	B	19	Total 19 O	0	0
4	C	4	Total 4 O	0	0

Continued on next page...

*Continued from previous page...*

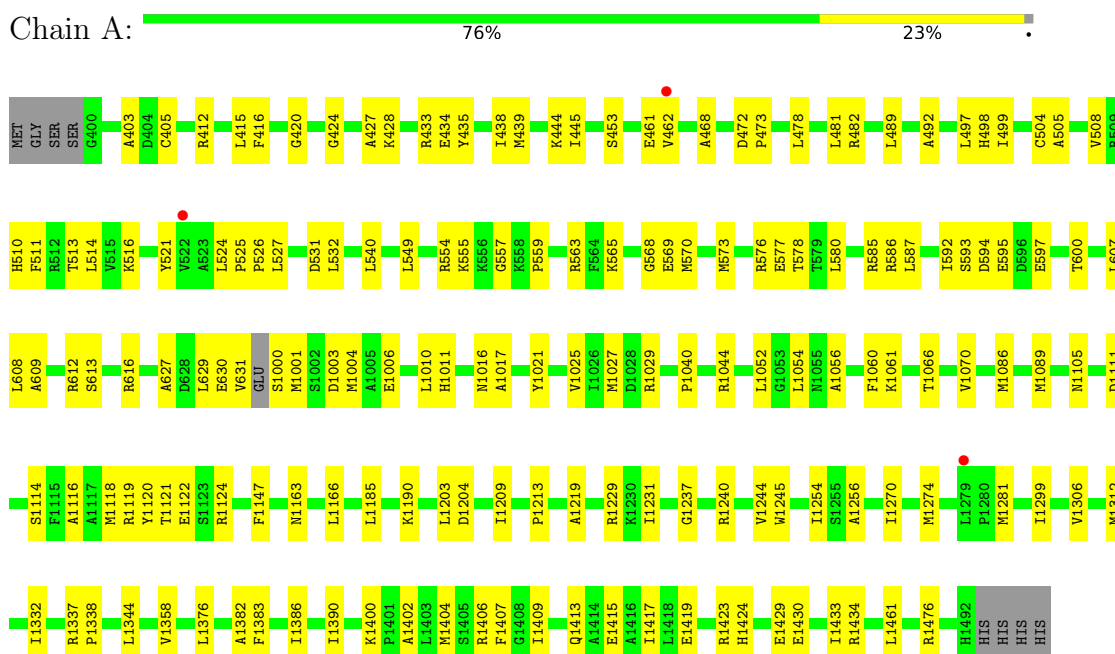
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	11	Total	O	0	0
			11	11		
4	H	1	Total	O	0	0
			1	1		



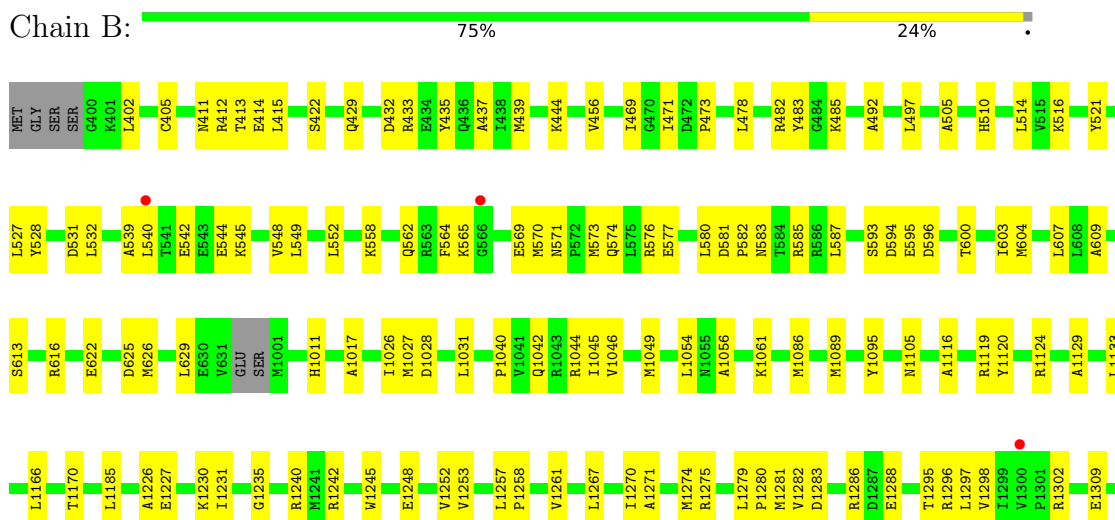
### 3 Residue-property plots

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: DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A




- Molecule 1: DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A





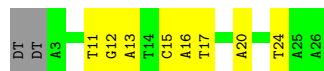
- Molecule 2: DNA (5'-D(P\*TP\*TP\*AP\*CP\*GP\*TP\*TP\*GP\*TP\*AP\*TP\*GP\*AP\*TP\*CP\*A P\*TP\*AP\*CP\*AP\*AP\*CP\*GP\*TP\*AP\*A)-3')

Chain E:  85% 8% 8%



- Molecule 2: DNA (5'-D(P\*TP\*TP\*AP\*CP\*GP\*TP\*TP\*GP\*TP\*AP\*TP\*GP\*AP\*TP\*CP\*A P\*TP\*AP\*CP\*AP\*AP\*CP\*GP\*TP\*AP\*A)-3')

Chain F:  62% 31% 8%



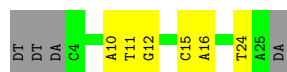
- Molecule 2: DNA (5'-D(P\*TP\*TP\*AP\*CP\*GP\*TP\*TP\*GP\*TP\*AP\*TP\*GP\*AP\*TP\*CP\*A P\*TP\*AP\*CP\*AP\*AP\*CP\*GP\*TP\*AP\*A)-3')

Chain G:  54% 31% 15%



- Molecule 2: DNA (5'-D(P\*TP\*TP\*AP\*CP\*GP\*TP\*TP\*GP\*TP\*AP\*TP\*GP\*AP\*TP\*CP\*A P\*TP\*AP\*CP\*AP\*AP\*CP\*GP\*TP\*AP\*A)-3')

Chain H:  62% 23% 15%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.44Å 163.26Å 145.84Å 90.00° 94.55° 90.00°	Depositor
Resolution (Å)	46.46 – 3.05 46.46 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.46-3.05) 99.9 (46.46-3.05)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.223 , 0.269 (Not available) , 0.267	Depositor DCC
$R_{free}$ test set	4289 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	109.7	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 98.1	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	0.95	EDS
Total number of atoms	24940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: A1L5V

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	0.10	0/5845	0.33	0/7888
1	B	0.09	0/5850	0.31	0/7895
1	C	0.09	0/5817	0.31	0/7850
1	D	0.09	0/5787	0.30	0/7810
2	E	0.18	0/548	0.36	0/843
2	F	0.19	0/553	0.37	0/851
2	G	0.17	0/505	0.34	0/777
2	H	0.19	0/505	0.35	0/777
All	All	0.10	0/25410	0.31	0/34691

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	5753	0	5816	110	0
1	B	5757	0	5818	119	0
1	C	5727	0	5797	100	0
1	D	5697	0	5762	107	0
2	E	490	0	274	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	493	0	272	8	0
2	G	451	0	250	6	0
2	H	451	0	250	6	0
3	F	34	0	0	0	0
3	H	34	0	0	1	0
4	A	18	0	0	1	0
4	B	19	0	0	0	0
4	C	4	0	0	0	0
4	D	11	0	0	0	0
4	H	1	0	0	0	0
All	All	24940	0	24239	426	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 9.

All (426) 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:1388:GLU:OE2	1:C:1406:ARG:NH1	1.66	1.26
1:B:1283:ASP:HB2	1:B:1302:ARG:HG2	1.61	0.82
1:A:607:LEU:O	1:A:616:ARG:NH2	2.13	0.80
1:A:526:PRO:HA	1:A:540:LEU:HB3	1.61	0.80
1:B:600:THR:HG22	1:B:1011:HIS:HB3	1.65	0.78
1:C:576:ARG:HA	1:C:580:LEU:HB2	1.65	0.76
1:B:571:ASN:HB2	1:B:574:GLN:HG3	1.69	0.74
1:A:1060:PHE:HB3	1:A:1122:GLU:HB3	1.70	0.73
1:D:1404:MET:HA	1:D:1409:ILE:HG22	1.71	0.72
1:D:1214:ASP:HB2	1:D:1476:ARG:HH21	1.54	0.72
1:B:576:ARG:HA	1:B:580:LEU:HB2	1.71	0.72
1:A:492:ALA:HB3	1:A:527:LEU:HG	1.72	0.71
1:D:576:ARG:HA	1:D:580:LEU:HB2	1.73	0.70
1:A:1056:ALA:O	1:A:1124:ARG:NH1	2.24	0.70
1:A:1400:LYS:HD3	1:A:1415:GLU:HG2	1.72	0.69
1:C:1388:GLU:CD	1:C:1406:ARG:HH12	2.00	0.69
1:D:1039:LYS:HG3	1:D:1042:GLN:HG3	1.75	0.69
1:A:563:ARG:HD3	1:A:1147:PHE:HB2	1.75	0.68
1:A:1105:ASN:HB3	1:A:1116:ALA:HB2	1.76	0.68
1:B:1376:LEU:HD22	1:B:1433:ILE:HG23	1.77	0.67
1:D:542:GLU:HA	1:D:545:LYS:HB2	1.77	0.67
1:A:557:GLY:HA2	1:B:1406:ARG:HH12	1.58	0.67
1:B:1054:LEU:HD21	1:B:1061:LYS:HE3	1.76	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ARG:HD3	1:A:587:LEU:HB2	1.78	0.66
1:D:456:VAL:HG22	1:D:462:VAL:HG11	1.78	0.66
1:D:1424:HIS:HA	1:D:1429:GLU:HG3	1.78	0.66
1:C:406:THR:H	1:C:434:GLU:HA	1.61	0.65
1:B:1166:LEU:HD22	1:B:1185:LEU:HD12	1.79	0.65
1:C:1431:MET:HE3	1:D:1436:GLU:HA	1.78	0.65
1:B:444:LYS:HG3	2:G:11:DT:H1'	1.80	0.64
1:A:1244:VAL:HB	1:A:1256:ALA:HB3	1.79	0.64
1:D:1060:PHE:HB3	1:D:1122:GLU:HB3	1.80	0.63
1:B:1056:ALA:O	1:B:1124:ARG:NH1	2.31	0.63
1:C:1025:VAL:HA	1:C:1029:ARG:HB3	1.80	0.63
1:D:1240:ARG:NH1	1:D:1322:GLU:OE2	2.31	0.63
1:C:403:ALA:HB2	1:C:428:LYS:HD3	1.80	0.63
1:D:592:ILE:HG23	1:D:1010:LEU:HD23	1.80	0.62
1:D:609:ALA:O	1:D:616:ARG:NH2	2.26	0.62
1:C:1279:LEU:HD13	1:C:1311:VAL:HG13	1.81	0.62
1:D:406:THR:HB	1:D:434:GLU:HG3	1.82	0.62
1:A:1001:MET:HG3	1:A:1003:ASP:H	1.64	0.62
1:C:432:ASP:HB2	1:C:576:ARG:HH22	1.64	0.62
1:B:1258:PRO:HG2	1:B:1261:VAL:HG21	1.81	0.62
1:D:512:ARG:NH1	1:D:597:GLU:OE2	2.33	0.62
1:C:1376:LEU:HD22	1:C:1433:ILE:HG23	1.82	0.61
1:A:613:SER:OG	1:A:616:ARG:NH2	2.27	0.61
1:A:1120:TYR:OH	2:F:12:DG:OP2	2.18	0.61
1:D:1355:ARG:NH2	1:D:1458:ASN:OD1	2.34	0.61
1:B:1253:VAL:HG22	1:B:1298:VAL:HG12	1.81	0.61
1:D:1179:ASP:OD2	1:D:1326:ARG:NH1	2.34	0.61
1:A:568:GLY:HA3	1:C:1120:TYR:HB3	1.82	0.60
1:D:1409:ILE:HG12	1:D:1413:GLN:HB2	1.83	0.60
1:D:444:LYS:HG3	2:H:11:DT:H1'	1.82	0.60
1:D:485:LYS:HB3	1:D:521:TYR:HE2	1.65	0.60
1:A:1213:PRO:O	1:A:1476:ARG:NH2	2.34	0.60
1:D:1383:PHE:HA	1:D:1386:ILE:HG23	1.83	0.60
1:C:1281:MET:HE1	1:C:1311:VAL:HG21	1.82	0.60
1:A:516:LYS:NZ	1:A:592:ILE:O	2.32	0.60
1:C:420:GLY:HA3	2:F:12:DG:H4'	1.83	0.60
1:C:1404:MET:HA	1:C:1409:ILE:HG22	1.84	0.60
1:A:1054:LEU:HD21	1:A:1061:LYS:HB2	1.84	0.59
1:C:448:THR:HG21	1:C:506:LEU:HD12	1.84	0.59
1:D:427:ALA:HB1	1:D:438:ILE:HG12	1.85	0.59
1:A:1402:ALA:O	1:A:1406:ARG:HG2	2.03	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1424:HIS:HA	1:C:1429:GLU:HG3	1.85	0.59
1:B:549:LEU:HD22	1:B:552:LEU:HD11	1.84	0.59
1:A:1424:HIS:HA	1:A:1429:GLU:HG3	1.85	0.59
1:D:1242:ARG:NH2	1:D:1484:GLU:O	2.35	0.59
1:A:427:ALA:HB1	1:A:438:ILE:HG12	1.84	0.58
1:C:1054:LEU:HD21	1:C:1061:LYS:HB2	1.85	0.58
1:D:495:ASP:OD1	1:D:1029:ARG:NH2	2.37	0.58
1:D:1198:GLN:O	1:D:1201:THR:OG1	2.21	0.58
1:D:1231:ILE:HG12	1:D:1237:GLY:HA3	1.85	0.58
1:B:1424:HIS:HA	1:B:1429:GLU:HG3	1.85	0.58
1:C:1432:LYS:HD3	1:D:1428:LEU:HD23	1.86	0.58
1:D:449:TRP:HA	1:D:509:ARG:HD2	1.83	0.58
1:A:1166:LEU:HD22	1:A:1185:LEU:HA	1.85	0.58
1:A:565:LYS:HD2	1:C:1062:LYS:HE2	1.86	0.58
1:B:1235:GLY:HA2	1:B:1329:LEU:HD12	1.85	0.58
1:C:1219:ALA:HB3	1:C:1241:MET:HE2	1.86	0.58
1:C:1166:LEU:HD22	1:C:1185:LEU:HA	1.84	0.58
1:C:1110:ASP:OD1	1:C:1110:ASP:N	2.36	0.57
1:B:531:ASP:OD1	1:B:531:ASP:N	2.35	0.57
1:D:462:VAL:HA	1:D:465:ILE:HD12	1.86	0.57
1:C:427:ALA:HB1	1:C:438:ILE:HG12	1.87	0.57
1:D:1308:MET:HA	1:D:1311:VAL:HG22	1.87	0.56
1:A:461:GLU:HG2	1:A:462:VAL:H	1.70	0.56
1:C:488:ILE:HG23	1:C:503:LEU:HD23	1.85	0.56
1:B:1248:GLU:OE1	1:B:1296:ARG:NH2	2.38	0.56
1:B:1446:GLN:O	1:B:1450:ILE:HG12	2.04	0.56
1:D:529:ARG:NH2	1:D:531:ASP:OD2	2.39	0.56
1:A:1240:ARG:NH2	2:F:24:DT:OP2	2.38	0.56
1:B:435:TYR:OH	1:B:585:ARG:NH2	2.38	0.56
1:C:432:ASP:O	1:C:435:TYR:HB3	2.06	0.56
1:B:1242:ARG:HD3	1:B:1316:PHE:CE2	2.42	0.55
1:C:491:ASP:HB3	1:C:566:GLY:HA2	1.89	0.55
1:A:1358:VAL:HG21	1:A:1461:LEU:HD21	1.87	0.55
1:B:432:ASP:O	1:B:435:TYR:HB3	2.05	0.55
1:C:1289:SER:HB2	1:C:1296:ARG:H	1.72	0.55
1:C:1040:PRO:O	1:C:1044:ARG:HG3	2.07	0.55
1:A:1040:PRO:O	1:A:1044:ARG:HG3	2.07	0.54
1:D:1211:GLN:HB2	1:D:1476:ARG:NH1	2.21	0.54
1:B:469:ILE:HG22	1:B:471:ILE:HG22	1.89	0.54
1:D:1242:ARG:HG2	1:D:1322:GLU:HG3	1.89	0.54
1:A:1119:ARG:NH1	1:A:1120:TYR:OH	2.41	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:PHE:CD1	1:B:570:MET:HG2	2.43	0.53
1:C:614:GLU:O	1:C:618:ASN:ND2	2.42	0.53
1:D:546:THR:HA	1:D:549:LEU:HB2	1.88	0.53
1:D:1267:LEU:HD21	1:D:1297:LEU:HD21	1.91	0.53
1:A:405:CYS:HB2	1:A:434:GLU:HA	1.90	0.53
1:A:1016:ASN:ND2	4:A:1502:HOH:O	2.42	0.53
1:B:1378:GLY:HA3	1:B:1413:GLN:HG2	1.89	0.53
1:C:619:TRP:HE1	1:C:623:LYS:HE3	1.74	0.53
1:D:621:GLN:NE2	1:D:625:ASP:OD1	2.40	0.53
1:D:1376:LEU:HD22	1:D:1433:ILE:HG23	1.90	0.52
1:A:497:LEU:HB3	1:A:1017:ALA:HB1	1.90	0.52
1:A:511:PHE:HB3	1:A:514:LEU:HD12	1.91	0.52
1:A:1086:MET:HA	1:A:1089:MET:HE2	1.92	0.52
1:B:1404:MET:HA	1:B:1409:ILE:HG22	1.91	0.52
1:A:505:ALA:HB2	1:A:608:LEU:HD13	1.91	0.52
1:A:1376:LEU:HD22	1:A:1433:ILE:HG23	1.92	0.52
1:D:448:THR:HG21	1:D:506:LEU:HD13	1.90	0.52
1:D:1040:PRO:O	1:D:1044:ARG:HG3	2.09	0.52
1:D:1382:ALA:HB2	1:D:1417:ILE:HG12	1.92	0.52
1:A:600:THR:HG22	1:A:1011:HIS:HB2	1.90	0.52
1:C:1195:LEU:HD13	1:C:1206:LEU:HD21	1.91	0.52
1:D:508:VAL:HG21	1:D:604:MET:HE3	1.92	0.52
1:B:1166:LEU:HD22	1:B:1185:LEU:HA	1.92	0.52
1:C:431:ARG:HH21	1:C:437:ALA:HA	1.75	0.52
1:C:1242:ARG:HG3	1:C:1322:GLU:HG3	1.91	0.52
1:D:492:ALA:HB3	1:D:527:LEU:HB2	1.92	0.52
1:B:573:MET:O	1:B:577:GLU:HG3	2.10	0.51
1:D:507:PHE:HA	1:D:511:PHE:HB2	1.92	0.51
1:A:1281:MET:HB2	1:A:1306:VAL:HG11	1.93	0.51
1:B:1120:TYR:OH	2:H:12:DG:OP2	2.27	0.51
1:B:594:ASP:OD1	1:B:594:ASP:N	2.42	0.51
1:B:607:LEU:O	1:B:616:ARG:NH1	2.40	0.51
1:D:1211:GLN:HB2	1:D:1476:ARG:HH12	1.76	0.51
1:B:1382:ALA:HB2	1:B:1417:ILE:HD13	1.92	0.51
1:B:625:ASP:O	1:B:629:LEU:HG	2.11	0.51
1:B:1383:PHE:HE2	1:B:1433:ILE:HD12	1.76	0.51
1:D:403:ALA:HB2	1:D:428:LYS:HE3	1.93	0.51
2:H:15:DC:H2'	2:H:16:DA:C8	2.46	0.51
1:A:630:GLU:OE2	1:A:631:VAL:HG22	2.10	0.51
1:B:1423:ARG:NH1	1:D:1419:GLU:OE2	2.44	0.51
1:B:405:CYS:HB2	1:B:437:ALA:HB2	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:LYS:HG3	2:F:11:DT:H1'	1.93	0.50
1:C:1010:LEU:O	1:C:1014:THR:OG1	2.29	0.50
1:C:1105:ASN:HB3	1:C:1116:ALA:HB2	1.93	0.50
1:C:1117:ALA:HB1	1:C:1119:ARG:HH21	1.76	0.50
1:C:607:LEU:O	1:C:616:ARG:NH1	2.37	0.50
1:C:1242:ARG:NH2	1:C:1484:GLU:O	2.44	0.50
1:A:576:ARG:HA	1:A:580:LEU:HB2	1.92	0.50
1:C:405:CYS:SG	1:C:437:ALA:HB2	2.52	0.50
1:D:563:ARG:HD3	1:D:1147:PHE:HB2	1.94	0.50
1:D:1270:ILE:O	1:D:1274:MET:HG2	2.12	0.50
1:D:532:LEU:HD12	1:D:559:PRO:HB3	1.93	0.50
1:D:1290:ASP:OD1	1:D:1291:HIS:N	2.44	0.50
1:D:1105:ASN:HB3	1:D:1116:ALA:HB2	1.93	0.50
1:B:613:SER:HA	1:B:616:ARG:HE	1.76	0.50
1:B:1240:ARG:NH2	2:H:24:DT:OP2	2.42	0.50
1:B:1245:TRP:HH2	1:B:1309:GLU:HG3	1.77	0.50
1:B:1315:LEU:O	1:B:1319:THR:OG1	2.30	0.50
1:D:515:VAL:HG12	1:D:592:ILE:HG12	1.93	0.50
1:B:1086:MET:HA	1:B:1089:MET:HE2	1.94	0.50
1:B:1227:GLU:O	1:B:1231:ILE:HG13	2.12	0.50
1:B:411:ASN:O	1:B:485:LYS:NZ	2.45	0.49
1:A:1027:MET:HA	1:A:1332:ILE:HD11	1.94	0.49
1:A:472:ASP:OD1	1:A:473:PRO:HD2	2.13	0.49
1:B:1428:LEU:HD12	1:B:1428:LEU:H	1.77	0.49
1:B:1314:HIS:HA	1:B:1488:ALA:HA	1.95	0.49
1:B:528:TYR:CG	1:B:545:LYS:HD3	2.48	0.49
1:B:1045:ILE:O	1:B:1049:MET:HG3	2.13	0.49
1:D:1166:LEU:HD22	1:D:1185:LEU:HA	1.93	0.49
1:B:521:TYR:HB3	1:B:587:LEU:HD22	1.95	0.49
1:C:422:SER:N	2:F:13:DA:OP1	2.46	0.49
1:C:1146:ASN:ND2	1:C:1148:ASP:OD1	2.46	0.49
1:A:1118:MET:HA	1:A:1121:THR:HG22	1.94	0.49
1:B:532:LEU:HA	1:B:532:LEU:HD23	1.67	0.48
1:C:1386:ILE:HD11	1:C:1425:LEU:HD13	1.94	0.48
1:D:616:ARG:NH1	2:G:20:DA:OP1	2.46	0.48
1:C:498:HIS:HB2	1:C:1021:TYR:CG	2.48	0.48
1:D:1054:LEU:HD21	1:D:1061:LYS:HB2	1.94	0.48
1:A:565:LYS:HE2	1:A:569:GLU:HB2	1.94	0.48
1:B:1042:GLN:NE2	1:B:1095:TYR:OH	2.45	0.48
1:D:430:ALA:HB1	1:D:576:ARG:HB2	1.94	0.48
1:A:1203:LEU:HD13	1:A:1344:LEU:HB2	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:VAL:HG13	1:D:455:GLU:HB3	1.96	0.48
1:B:1271:ALA:O	1:B:1275:ARG:HG3	2.13	0.48
1:A:531:ASP:OD1	1:A:531:ASP:N	2.46	0.48
1:D:1026:ILE:O	1:D:1031:LEU:HB2	2.14	0.48
1:B:1413:GLN:O	1:B:1417:ILE:HG13	2.14	0.48
1:D:1222:ILE:HD13	1:D:1242:ARG:HG3	1.95	0.48
1:B:415:LEU:HB2	1:B:483:TYR:CD2	2.49	0.48
1:B:1170:THR:HG23	2:G:8:DG:H5'	1.96	0.48
1:C:1281:MET:HB3	1:C:1302:ARG:HG2	1.95	0.48
1:D:606:MET:HE2	1:D:607:LEU:HD12	1.96	0.48
1:A:445:ILE:O	2:F:17:DT:H4'	2.14	0.47
1:B:1226:ALA:O	1:B:1230:LYS:HG3	2.14	0.47
1:D:609:ALA:HB3	1:D:612:ARG:HB2	1.95	0.47
1:D:1227:GLU:HA	1:D:1230:LYS:HE2	1.95	0.47
1:A:607:LEU:C	1:A:616:ARG:HH22	2.17	0.47
1:C:521:TYR:HB3	1:C:587:LEU:HD22	1.96	0.47
1:C:609:ALA:O	1:C:616:ARG:NH1	2.47	0.47
1:C:1320:ASP:HA	1:C:1323:LYS:HE2	1.96	0.47
1:D:1200:LYS:HD2	1:D:1200:LYS:O	2.15	0.47
1:D:1222:ILE:HG21	1:D:1242:ARG:HG3	1.95	0.47
1:A:478:LEU:HD21	1:A:513:THR:HB	1.96	0.47
1:B:1286:ARG:NH2	1:B:1288:GLU:OE2	2.31	0.47
1:A:1400:LYS:O	1:A:1404:MET:HG3	2.14	0.47
1:C:498:HIS:HB2	1:C:1021:TYR:CD1	2.50	0.47
1:D:1287:ASP:HA	1:D:1297:LEU:HD23	1.97	0.47
1:A:412:ARG:HB3	1:A:435:TYR:HE1	1.80	0.47
1:B:414:GLU:OE2	1:B:585:ARG:NH1	2.44	0.47
1:B:1458:ASN:O	1:B:1462:LYS:HG3	2.15	0.47
1:D:1309:GLU:HA	1:D:1312:MET:HE2	1.97	0.47
1:A:593:SER:HB3	1:A:595:GLU:OE1	2.15	0.47
1:A:1004:MET:HE2	1:A:1006:GLU:HG3	1.96	0.47
1:B:1388:GLU:OE2	1:B:1406:ARG:NE	2.43	0.47
1:C:495:ASP:O	1:C:499:ILE:HG13	2.15	0.47
1:C:1193:ILE:HG23	1:C:1462:LYS:HG2	1.95	0.47
1:D:1135:GLU:OE2	1:D:1361:ARG:NH2	2.43	0.47
1:C:1148:ASP:OD1	1:C:1148:ASP:N	2.42	0.47
1:A:403:ALA:HB2	1:A:428:LYS:HE3	1.96	0.46
1:C:625:ASP:OD1	1:C:1337:ARG:NH2	2.46	0.46
1:C:1413:GLN:O	1:C:1417:ILE:HG13	2.16	0.46
1:D:526:PRO:HA	1:D:540:LEU:HD23	1.96	0.46
1:A:439:MET:HE2	1:A:468:ALA:HB3	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ARG:HG2	1:B:435:TYR:CE1	2.50	0.46
1:B:582:PRO:HA	1:B:585:ARG:HG2	1.96	0.46
1:B:609:ALA:O	1:B:616:ARG:NH2	2.48	0.46
1:C:509:ARG:HG2	1:C:510:HIS:CE1	2.51	0.46
1:D:1008:LEU:HD21	1:D:1012:GLU:HB2	1.98	0.46
1:D:1067:VAL:HG11	1:D:1118:MET:HE1	1.98	0.46
1:D:549:LEU:HD23	1:D:549:LEU:HA	1.78	0.46
1:D:1274:MET:HE3	1:D:1282:VAL:HG23	1.97	0.46
1:B:596:ASP:O	1:B:600:THR:HG23	2.14	0.46
1:C:622:GLU:O	1:C:626:MET:HG2	2.15	0.46
2:G:15:DC:H2'	2:G:16:DA:C8	2.51	0.46
1:A:1404:MET:HA	1:A:1409:ILE:HG22	1.96	0.46
1:B:402:LEU:HG	1:B:439:MET:HG3	1.96	0.46
1:D:449:TRP:CZ3	1:D:509:ARG:HB2	2.50	0.46
1:D:487:CYS:HA	1:D:521:TYR:O	2.15	0.46
1:A:1430:GLU:OE2	1:A:1434:ARG:NH2	2.40	0.46
1:D:420:GLY:O	1:D:424:GLY:N	2.46	0.46
1:D:525:PRO:HB3	1:D:579:THR:HG21	1.98	0.46
2:E:15:DC:H2'	2:E:16:DA:C8	2.50	0.46
1:A:424:GLY:O	1:A:428:LYS:HD3	2.17	0.45
1:A:444:LYS:HG2	1:A:499:ILE:HD11	1.97	0.45
1:B:433:ARG:NH2	1:D:1287:ASP:OD2	2.49	0.45
1:C:590:LEU:HD13	1:C:1010:LEU:HD13	1.97	0.45
1:B:1129:ALA:O	1:B:1133:LEU:HD12	2.16	0.45
1:D:565:LYS:HD2	1:D:565:LYS:HA	1.83	0.45
1:A:594:ASP:HA	1:A:597:GLU:HG3	1.98	0.45
1:D:528:TYR:HE1	1:D:563:ARG:HD2	1.81	0.45
1:B:570:MET:HE2	1:B:570:MET:HB3	1.75	0.45
1:C:1083:TYR:O	1:C:1087:VAL:HG23	2.16	0.45
1:A:607:LEU:HA	1:A:616:ARG:HH12	1.81	0.45
1:C:447:ASN:HD21	1:C:608:LEU:HB3	1.81	0.45
1:C:523:ALA:HB1	1:C:579:THR:CG2	2.46	0.45
1:A:1386:ILE:O	1:A:1390:ILE:HG13	2.16	0.45
1:B:456:VAL:HG11	1:B:510:HIS:NE2	2.31	0.45
1:A:521:TYR:HB3	1:A:587:LEU:HD22	1.98	0.45
1:A:555:LYS:HD2	1:A:555:LYS:HA	1.65	0.45
1:A:627:ALA:C	1:A:629:LEU:H	2.25	0.45
1:B:1487:LYS:HD2	1:B:1487:LYS:HA	1.79	0.45
1:C:501:THR:HG21	1:C:1018:TYR:HD1	1.82	0.45
1:D:1307:ASP:O	1:D:1311:VAL:HG13	2.15	0.45
1:C:1270:ILE:O	1:C:1274:MET:HG2	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1271:ALA:HA	1:D:1274:MET:HG2	1.99	0.45
1:A:532:LEU:HD21	1:A:557:GLY:O	2.17	0.45
1:A:1413:GLN:O	1:A:1417:ILE:HG13	2.17	0.45
1:B:1105:ASN:HB3	1:B:1116:ALA:HB2	1.99	0.45
1:B:1321:LEU:HD23	1:B:1321:LEU:HA	1.87	0.45
1:C:600:THR:HG22	1:C:1011:HIS:N	2.32	0.45
1:C:623:LYS:HD3	1:C:1019:LEU:HD22	1.99	0.45
1:A:416:PHE:HB3	1:A:489:LEU:HD12	1.99	0.44
1:A:420:GLY:O	1:A:424:GLY:N	2.50	0.44
1:A:570:MET:HE1	1:A:578:THR:HG21	1.99	0.44
1:A:609:ALA:HB3	1:A:612:ARG:HB3	1.99	0.44
1:C:1427:LYS:O	1:C:1431:MET:HG2	2.16	0.44
1:A:573:MET:O	1:A:577:GLU:HG3	2.17	0.44
1:B:482:ARG:NH1	1:B:483:TYR:H	2.16	0.44
1:D:476:ASP:HB3	1:D:477:ASP:H	1.64	0.44
1:B:1026:ILE:O	1:B:1031:LEU:HB2	2.17	0.44
1:D:1254:ILE:HB	1:D:1297:LEU:HB2	2.00	0.44
1:A:504:CYS:O	1:A:508:VAL:HG22	2.17	0.44
1:B:497:LEU:HB3	1:B:1017:ALA:HB1	1.98	0.44
1:B:562:GLN:NE2	1:B:569:GLU:OE2	2.38	0.44
1:C:1231:ILE:HG12	1:C:1237:GLY:HA3	1.98	0.44
1:C:1342:ASN:ND2	1:C:1345:GLU:OE1	2.51	0.44
1:D:603:ILE:HD13	1:D:1011:HIS:ND1	2.32	0.44
1:A:1025:VAL:HA	1:A:1029:ARG:HB3	2.00	0.44
1:A:1111:ASP:CG	1:A:1114:SER:HB3	2.42	0.44
1:B:1252:VAL:HG11	1:B:1312:MET:SD	2.58	0.44
1:D:1025:VAL:HG22	1:D:1029:ARG:HH11	1.81	0.44
1:D:1207:LEU:HD13	1:D:1229:ARG:HG2	2.00	0.44
1:C:504:CYS:O	1:C:508:VAL:HG23	2.18	0.44
1:A:585:ARG:HG2	1:A:586:ARG:N	2.32	0.43
1:B:542:GLU:C	1:B:544:GLU:H	2.25	0.43
1:B:593:SER:OG	1:B:595:GLU:OE1	2.36	0.43
1:B:1450:ILE:HD13	1:B:1456:LYS:HG3	2.00	0.43
1:C:1388:GLU:O	1:C:1392:ILE:HG13	2.18	0.43
1:A:1299:ILE:HD12	1:A:1312:MET:HE1	1.99	0.43
1:C:1060:PHE:HB3	1:C:1122:GLU:HB3	1.99	0.43
1:D:493:ASP:OD1	1:D:494:SER:N	2.51	0.43
1:A:613:SER:HB3	2:F:20:DA:OP1	2.18	0.43
1:B:1257:LEU:HD11	1:B:1295:THR:HG21	2.00	0.43
1:A:525:PRO:O	1:A:540:LEU:HD13	2.19	0.43
1:A:1219:ALA:HA	1:A:1244:VAL:HG23	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:TRP:HA	1:A:1254:ILE:HA	2.00	0.43
1:B:478:LEU:HD21	1:B:514:LEU:HG	2.01	0.43
1:B:492:ALA:HB3	1:B:527:LEU:HD13	1.99	0.43
1:C:565:LYS:HA	1:C:565:LYS:HD2	1.86	0.43
1:A:1166:LEU:HD13	1:A:1185:LEU:HD12	2.00	0.43
1:B:1119:ARG:HG2	3:H:101:A1L5V:O34	2.18	0.43
1:C:412:ARG:HB2	1:C:435:TYR:HE1	1.83	0.43
1:B:473:PRO:HB3	1:B:510:HIS:HB3	2.00	0.43
1:B:505:ALA:HA	1:B:604:MET:HE1	2.00	0.43
1:B:1042:GLN:O	1:B:1046:VAL:HG23	2.19	0.43
1:B:1386:ILE:O	1:B:1390:ILE:HG13	2.18	0.43
1:C:470:GLY:HA3	1:C:480:GLN:O	2.18	0.43
1:A:453:SER:HA	1:A:510:HIS:CE1	2.53	0.43
1:A:554:ARG:C	1:B:1384:LEU:HD21	2.43	0.43
1:B:1281:MET:H	1:B:1281:MET:HG2	1.62	0.43
1:C:403:ALA:HB1	1:C:431:ARG:NH1	2.34	0.43
1:C:1400:LYS:HB2	1:C:1400:LYS:HE3	1.81	0.43
1:A:1382:ALA:HB2	1:A:1417:ILE:HD13	2.00	0.43
1:A:1390:ILE:HD13	1:C:1390:ILE:HD13	2.00	0.43
1:A:1419:GLU:OE2	1:C:1423:ARG:NH2	2.49	0.43
1:B:429:GLN:CD	1:D:1108:ALA:HB2	2.43	0.43
1:B:565:LYS:HG2	1:B:569:GLU:HB2	2.01	0.43
1:B:1242:ARG:O	1:B:1258:PRO:HD3	2.19	0.43
1:B:1270:ILE:O	1:B:1274:MET:HG3	2.18	0.43
1:B:1280:PRO:HD2	1:B:1281:MET:HE3	2.00	0.43
1:C:1254:ILE:HD11	1:C:1256:ALA:O	2.18	0.43
1:C:413:THR:HB	1:C:484:GLY:H	1.82	0.43
1:C:1116:ALA:HB3	1:C:1121:THR:HG23	1.99	0.43
1:C:1203:LEU:O	1:C:1207:LEU:HG	2.19	0.43
1:D:1026:ILE:HG23	1:D:1031:LEU:HD22	2.00	0.43
1:A:570:MET:HE2	1:A:570:MET:HB3	1.95	0.43
1:A:1066:THR:O	1:A:1070:VAL:HG23	2.19	0.43
1:A:1383:PHE:HE2	1:A:1433:ILE:HD12	1.83	0.43
1:C:1323:LYS:HA	1:C:1323:LYS:HD3	1.68	0.43
1:A:557:GLY:HA2	1:B:1406:ARG:NH1	2.30	0.42
1:C:1355:ARG:HE	1:C:1355:ARG:HB2	1.64	0.42
1:D:513:THR:O	1:D:514:LEU:HB2	2.18	0.42
1:B:422:SER:N	2:G:13:DA:OP1	2.42	0.42
1:B:1026:ILE:HG22	1:B:1027:MET:HG2	2.01	0.42
1:B:581:ASP:OD1	1:B:583:ASN:ND2	2.51	0.42
1:B:1279:LEU:HD21	1:B:1314:HIS:CD2	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1279:LEU:HD13	1:D:1311:VAL:HB	2.01	0.42
1:D:1297:LEU:HD23	1:D:1297:LEU:HA	1.88	0.42
1:A:580:LEU:HD23	1:A:580:LEU:HA	1.81	0.42
1:A:1000:SER:O	1:A:1001:MET:HG2	2.20	0.42
1:B:540:LEU:HD12	1:B:548:VAL:HG11	2.00	0.42
1:B:1379:LEU:HD22	1:B:1420:LEU:HD22	2.01	0.42
1:C:1042:GLN:O	1:C:1046:VAL:HG23	2.19	0.42
1:B:412:ARG:HG2	1:B:435:TYR:HE1	1.83	0.42
1:B:1040:PRO:O	1:B:1044:ARG:HG3	2.19	0.42
1:D:412:ARG:HB2	1:D:435:TYR:HE1	1.83	0.42
1:D:501:THR:HG21	1:D:1018:TYR:HD1	1.85	0.42
1:B:516:LYS:HD2	1:B:516:LYS:HA	1.81	0.42
1:C:1161:LEU:HB3	1:C:1166:LEU:HD11	2.01	0.42
1:D:1029:ARG:HH21	2:H:10:DA:H4'	1.82	0.42
2:F:15:DC:H2'	2:F:16:DA:C8	2.54	0.42
1:A:1163:ASN:HA	1:A:1166:LEU:HD12	2.02	0.42
1:C:414:GLU:HG2	1:C:485:LYS:HB2	2.01	0.42
1:B:1409:ILE:HG12	1:B:1413:GLN:HB3	2.02	0.42
1:C:548:VAL:C	1:C:550:GLU:H	2.28	0.42
1:D:514:LEU:HD23	1:D:514:LEU:HA	1.89	0.42
1:B:413:THR:HG23	1:B:483:TYR:O	2.21	0.41
1:B:1274:MET:HG2	1:B:1282:VAL:HG21	2.02	0.41
1:C:433:ARG:C	1:C:435:TYR:H	2.28	0.41
1:C:1045:ILE:HD13	1:C:1086:MET:HG3	2.01	0.41
1:C:1400:LYS:HB3	1:C:1401:PRO:HD3	2.01	0.41
1:C:494:SER:HB2	1:C:1021:TYR:HA	2.03	0.41
1:C:1036:ASP:OD1	1:C:1036:ASP:N	2.53	0.41
1:C:1206:LEU:O	1:C:1210:VAL:HG22	2.21	0.41
1:D:405:CYS:HB2	1:D:437:ALA:HB2	2.01	0.41
1:D:1066:THR:O	1:D:1070:VAL:HG23	2.20	0.41
1:A:1337:ARG:HG3	1:A:1338:PRO:HD2	2.03	0.41
1:B:432:ASP:HB3	1:B:435:TYR:HD2	1.86	0.41
1:B:1267:LEU:HD21	1:B:1297:LEU:HD22	2.02	0.41
1:B:1420:LEU:HD12	1:B:1420:LEU:HA	1.95	0.41
1:C:479:SER:O	1:C:480:GLN:C	2.63	0.41
1:D:498:HIS:HB2	1:D:1021:TYR:CD1	2.55	0.41
1:A:415:LEU:HD11	1:A:439:MET:HB2	2.03	0.41
1:B:528:TYR:CD1	1:B:545:LYS:HD3	2.55	0.41
1:C:431:ARG:NH2	1:C:437:ALA:HA	2.35	0.41
1:D:528:TYR:CE1	1:D:563:ARG:HD2	2.56	0.41
1:A:481:LEU:O	1:A:482:ARG:NH1	2.51	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:ILE:HG12	1:A:1237:GLY:HA3	2.02	0.41
1:B:1388:GLU:O	1:B:1392:ILE:HG13	2.21	0.41
1:B:1456:LYS:HA	1:B:1456:LYS:HD2	1.56	0.41
1:B:528:TYR:O	1:B:539:ALA:HB3	2.20	0.41
1:B:603:ILE:HD12	1:B:1011:HIS:HB2	2.03	0.41
1:B:622:GLU:O	1:B:626:MET:HG2	2.20	0.41
1:B:1460:LEU:O	1:B:1464:GLU:HG3	2.21	0.41
1:C:1052:LEU:HD23	1:C:1052:LEU:HA	1.94	0.41
1:A:433:ARG:HB3	1:A:434:GLU:H	1.59	0.41
1:A:524:LEU:HD23	1:A:524:LEU:HA	1.82	0.41
1:A:1270:ILE:O	1:A:1274:MET:HG3	2.20	0.41
1:D:1239:VAL:HG12	1:D:1325:TYR:HB2	2.02	0.41
1:D:1331:MET:HE2	1:D:1331:MET:HB3	1.97	0.41
2:G:2:DT:H2''	2:G:3:DA:H8	1.86	0.41
1:A:549:LEU:HD11	1:A:559:PRO:HG3	2.02	0.41
1:A:1105:ASN:HB2	1:C:426:SER:OG	2.21	0.41
1:B:1367:GLU:HG3	1:B:1371:LYS:HE2	2.02	0.41
1:A:1423:ARG:NH2	1:C:1415:GLU:OE2	2.50	0.40
1:B:1028:ASP:HA	1:B:1040:PRO:HG2	2.02	0.40
1:C:417:LEU:HD13	1:C:503:LEU:HD21	2.02	0.40
1:D:586:ARG:HD2	1:D:586:ARG:HA	1.79	0.40
1:D:1025:VAL:HA	1:D:1029:ARG:HB3	2.04	0.40
1:A:1052:LEU:HD23	1:A:1052:LEU:HA	1.89	0.40
1:A:1166:LEU:HD22	1:A:1185:LEU:HD12	2.04	0.40
1:A:1204:ASP:OD2	1:A:1229:ARG:NH1	2.54	0.40
1:D:1029:ARG:HE	2:H:10:DA:H4'	1.86	0.40
1:A:498:HIS:HB2	1:A:1021:TYR:CD1	2.57	0.40
1:A:1010:LEU:HD12	1:A:1010:LEU:HA	1.78	0.40
1:A:1407:PHE:O	1:B:558:LYS:HE3	2.22	0.40
1:D:1373:LEU:HD23	1:D:1373:LEU:HA	1.90	0.40
1:A:1190:LYS:HD3	1:A:1209:ILE:HD12	2.04	0.40
1:C:581:ASP:O	1:C:585:ARG:HB3	2.21	0.40
1:D:470:GLY:HA3	1:D:481:LEU:HB2	2.03	0.40
1:D:1241:MET:O	1:D:1322:GLU:HA	2.21	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	721/734 (98%)	660 (92%)	61 (8%)	0	100	100
1	B	721/734 (98%)	675 (94%)	46 (6%)	0	100	100
1	C	718/734 (98%)	665 (93%)	51 (7%)	2 (0%)	36	63
1	D	714/734 (97%)	670 (94%)	43 (6%)	1 (0%)	48	75
All	All	2874/2936 (98%)	2670 (93%)	201 (7%)	3 (0%)	48	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	401	LYS
1	C	1284	ASP
1	C	1487	LYS

### 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	624/632 (99%)	624 (100%)	0	100	100
1	B	624/632 (99%)	624 (100%)	0	100	100
1	C	621/632 (98%)	621 (100%)	0	100	100
1	D	619/632 (98%)	619 (100%)	0	100	100
All	All	2488/2528 (98%)	2488 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	460	GLN
1	A	1364	HIS
1	B	571	ASN
1	B	1233	GLN
1	B	1493	HIS
1	C	510	HIS
1	C	1459	ASN
1	D	1075	HIS
1	D	1152	GLN
1	D	1234	ASN
1	D	1260	GLN
1	D	1293	ASN
1	D	1310	GLN
1	D	1314	HIS
1	D	1385	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	A1L5V	H	101	-	36,38,38	3.36	15 (41%)	40,55,55	2.70	15 (37%)
3	A1L5V	F	101	-	36,38,38	3.35	16 (44%)	40,55,55	2.76	15 (37%)

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	A1L5V	H	101	-	-	2/11/32/32	0/5/5/5
3	A1L5V	F	101	-	-	4/11/32/32	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	101	A1L5V	C31-N32	8.81	1.45	1.35
3	H	101	A1L5V	C07-N02	8.55	1.55	1.40
3	F	101	A1L5V	C07-N02	8.49	1.55	1.40
3	F	101	A1L5V	C31-N32	8.22	1.44	1.35
3	F	101	A1L5V	C07-C13	8.02	1.54	1.41
3	H	101	A1L5V	C07-C13	7.86	1.53	1.41
3	F	101	A1L5V	C21-N22	5.39	1.42	1.36
3	H	101	A1L5V	C21-N22	4.99	1.42	1.36
3	F	101	A1L5V	C17-C18	4.99	1.58	1.51
3	H	101	A1L5V	C17-C18	4.55	1.57	1.51
3	H	101	A1L5V	C27-N32	4.47	1.43	1.38
3	H	101	A1L5V	C01-N02	4.46	1.53	1.46
3	F	101	A1L5V	C01-N02	4.42	1.53	1.46
3	F	101	A1L5V	C27-N32	3.99	1.43	1.38
3	F	101	A1L5V	C08-C05	3.93	1.52	1.44
3	H	101	A1L5V	C08-C05	3.80	1.52	1.44
3	F	101	A1L5V	C23-N22	3.67	1.48	1.41
3	F	101	A1L5V	C08-C07	3.40	1.45	1.41
3	H	101	A1L5V	C23-N22	3.40	1.47	1.41
3	H	101	A1L5V	C08-C07	3.29	1.45	1.41
3	F	101	A1L5V	C09-C08	3.23	1.46	1.41
3	H	101	A1L5V	C09-C08	3.22	1.46	1.41
3	H	101	A1L5V	C28-N25	3.04	1.38	1.32
3	F	101	A1L5V	C28-N25	2.98	1.38	1.32
3	H	101	A1L5V	C23-N26	2.89	1.38	1.34
3	F	101	A1L5V	C23-N26	2.61	1.38	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	101	A1L5V	C24-N25	2.25	1.39	1.34
3	H	101	A1L5V	C24-N25	2.25	1.39	1.34
3	F	101	A1L5V	C04-C05	2.22	1.38	1.34
3	H	101	A1L5V	C04-C05	2.19	1.38	1.34
3	F	101	A1L5V	C04-C03	2.01	1.48	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	101	A1L5V	C19-N22-C21	-7.48	105.64	111.17
3	H	101	A1L5V	C19-N22-C21	-7.46	105.66	111.17
3	F	101	A1L5V	C18-C19-N22	6.51	108.00	101.85
3	H	101	A1L5V	C18-C19-N22	6.31	107.81	101.85
3	F	101	A1L5V	O29-C28-N25	5.88	121.47	113.40
3	H	101	A1L5V	O29-C28-N25	5.71	121.24	113.40
3	F	101	A1L5V	O20-C18-C17	5.19	115.00	109.13
3	F	101	A1L5V	C23-N22-C21	4.66	132.41	125.40
3	H	101	A1L5V	N32-C27-N26	4.55	122.31	116.36
3	H	101	A1L5V	O34-C21-N22	-4.41	124.71	128.80
3	F	101	A1L5V	O34-C21-N22	-4.33	124.79	128.80
3	H	101	A1L5V	O20-C18-C17	4.32	114.02	109.13
3	F	101	A1L5V	N32-C27-N26	4.31	122.00	116.36
3	H	101	A1L5V	C23-N22-C21	4.20	131.72	125.40
3	F	101	A1L5V	O29-C30-C31	-2.92	107.36	114.81
3	F	101	A1L5V	C08-C07-N02	-2.90	115.37	118.43
3	H	101	A1L5V	O29-C30-C31	-2.87	107.49	114.81
3	H	101	A1L5V	C27-N32-C31	-2.84	120.00	124.50
3	H	101	A1L5V	C08-C07-N02	-2.82	115.45	118.43
3	F	101	A1L5V	C24-C23-N26	-2.80	117.69	121.22
3	F	101	A1L5V	C27-N32-C31	-2.67	120.27	124.50
3	H	101	A1L5V	C24-C23-N26	-2.56	117.98	121.22
3	F	101	A1L5V	O20-C18-C19	-2.56	102.02	104.50
3	H	101	A1L5V	C19-C18-C17	-2.54	110.50	113.38
3	H	101	A1L5V	O20-C18-C19	-2.53	102.04	104.50
3	F	101	A1L5V	C19-C18-C17	-2.52	110.52	113.38
3	H	101	A1L5V	N26-C23-N22	2.51	121.39	115.11
3	H	101	A1L5V	C18-O20-C21	2.29	111.93	110.10
3	F	101	A1L5V	N26-C23-N22	2.28	120.81	115.11
3	F	101	A1L5V	C18-O20-C21	2.09	111.77	110.10

There are no chirality outliers.

All (6) torsion outliers are listed below:

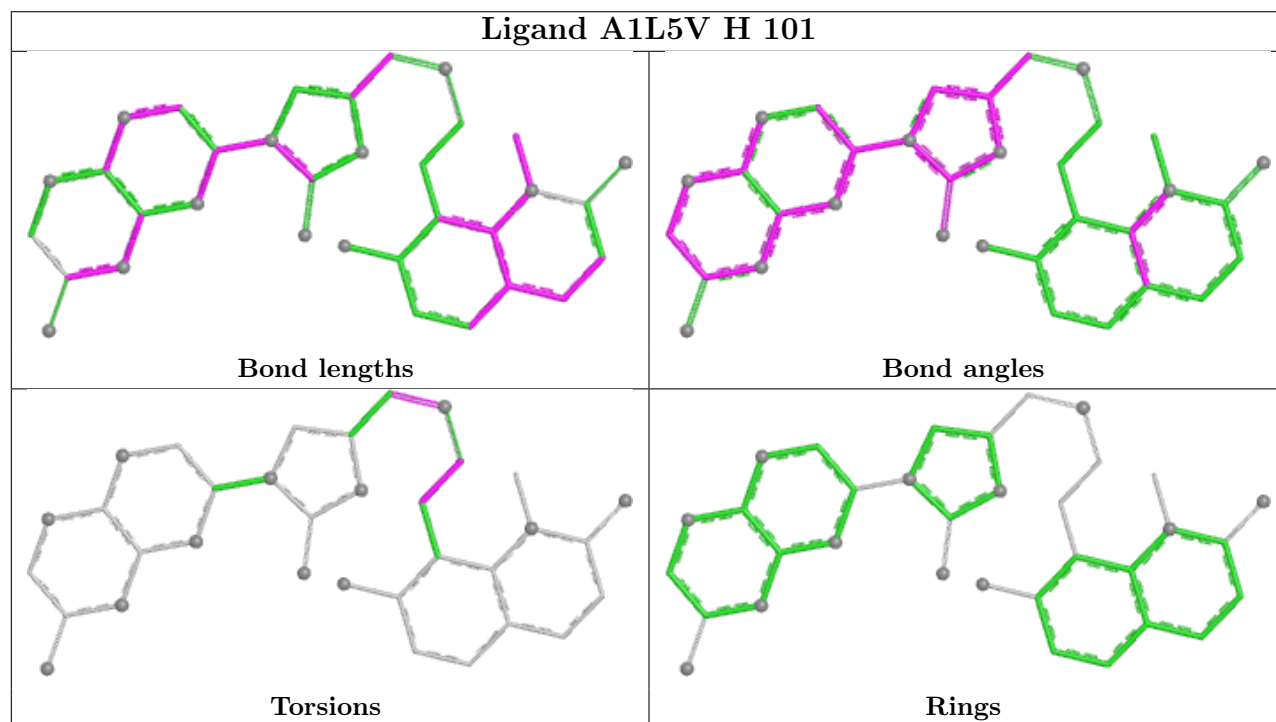
Mol	Chain	Res	Type	Atoms
3	F	101	A1L5V	C13-C14-C15-N16
3	F	101	A1L5V	N16-C17-C18-C19
3	F	101	A1L5V	N16-C17-C18-O20
3	F	101	A1L5V	C18-C17-N16-C15
3	H	101	A1L5V	C18-C17-N16-C15
3	H	101	A1L5V	C13-C14-C15-N16

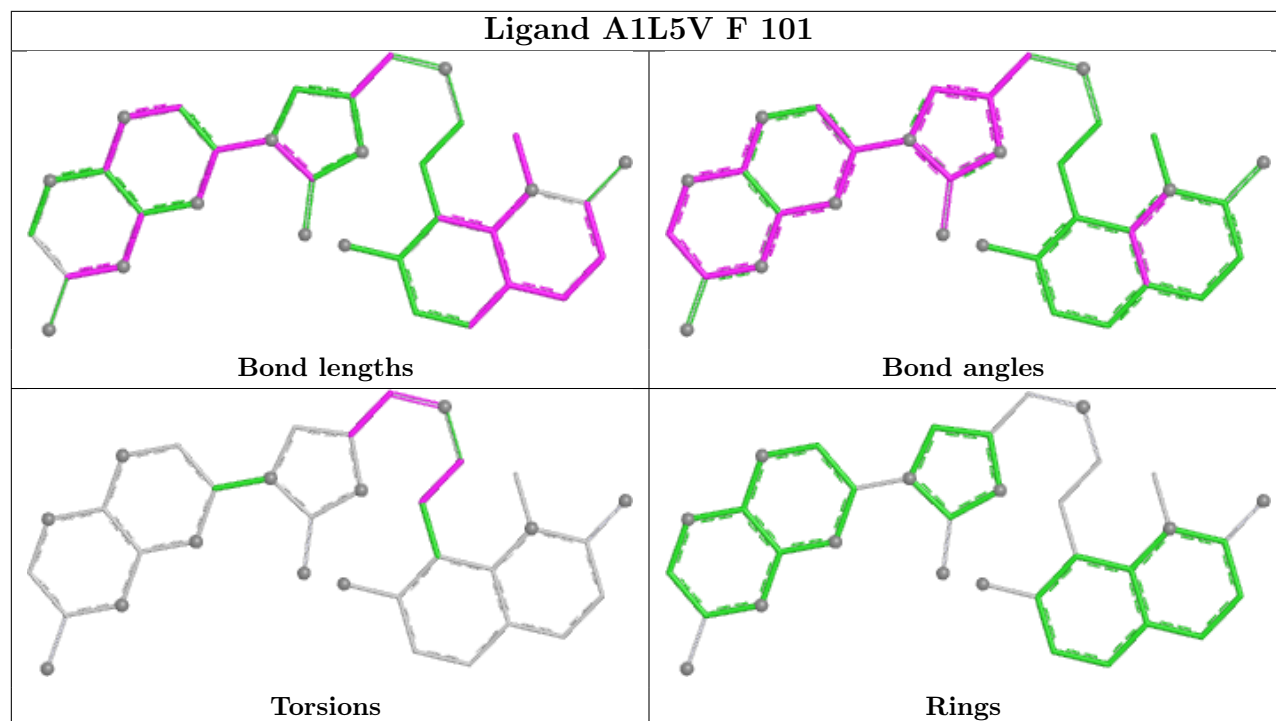
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	101	A1L5V	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	725/734 (98%)	-0.20	3 (0%) 88 75	68, 123, 240, 347	0
1	B	725/734 (98%)	-0.26	3 (0%) 88 75	68, 113, 207, 298	0
1	C	722/734 (98%)	-0.11	9 (1%) 76 55	81, 155, 276, 403	0
1	D	718/734 (97%)	-0.19	5 (0%) 84 66	75, 142, 260, 456	0
2	E	24/26 (92%)	-0.35	0 100 100	106, 214, 258, 276	0
2	F	24/26 (92%)	0.14	0 100 100	146, 221, 273, 310	0
2	G	22/26 (84%)	-0.04	0 100 100	94, 178, 226, 236	0
2	H	22/26 (84%)	-0.22	0 100 100	113, 174, 212, 273	0
All	All	2982/3040 (98%)	-0.19	20 (0%) 84 66	68, 133, 253, 456	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1299	ILE	3.4
1	D	1088	LEU	3.2
1	A	522	VAL	3.1
1	C	604	MET	3.0
1	D	465	ILE	2.9
1	B	1300	VAL	2.8
1	C	568	GLY	2.7
1	A	1279	LEU	2.7
1	D	1299	ILE	2.7
1	C	1026	ILE	2.6
1	C	600	THR	2.5
1	C	1297	LEU	2.5
1	D	505	ALA	2.4
1	D	1308	MET	2.3
1	A	462	VAL	2.3
1	B	540	LEU	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	505	ALA	2.2
1	B	566	GLY	2.2
1	C	504	CYS	2.2
1	C	507	PHE	2.2

## 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, 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.

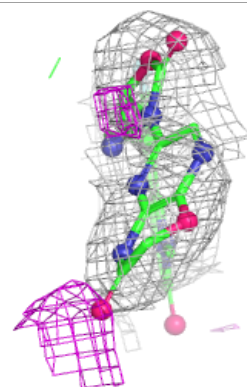
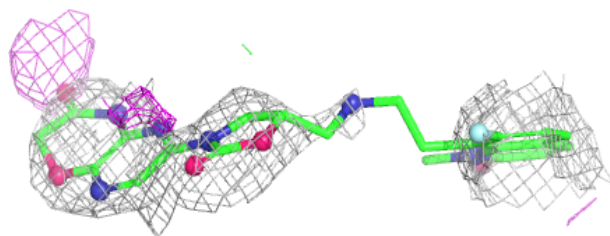
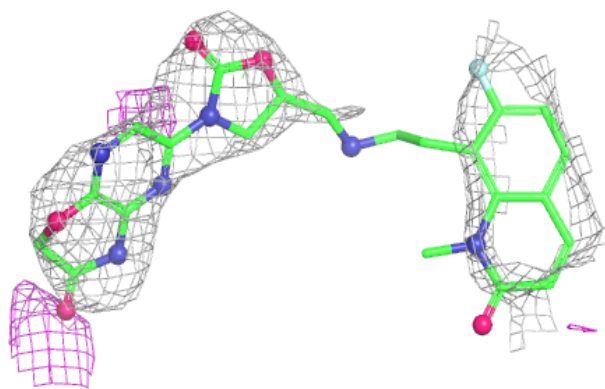
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A1L5V	H	101	34/34	0.85	0.13	87,147,216,217	0
3	A1L5V	F	101	34/34	0.88	0.13	102,149,255,259	0

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.

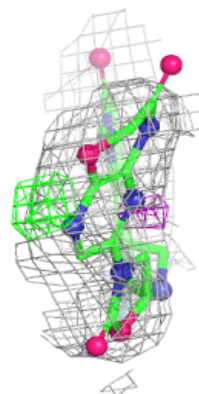
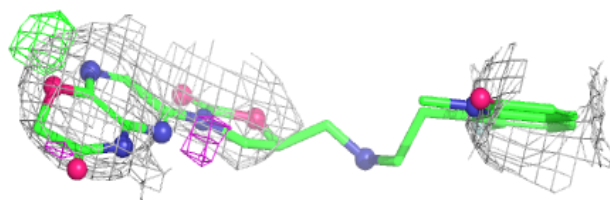
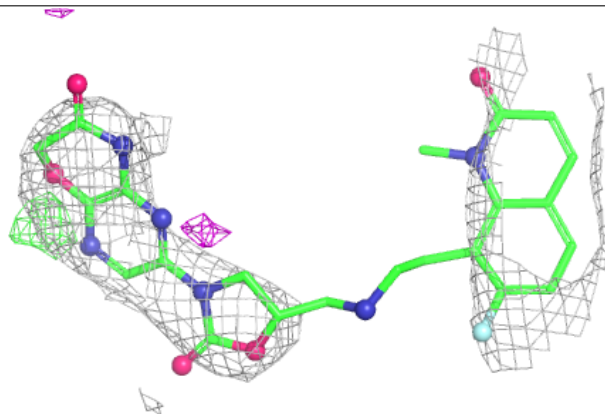


**Electron density around A1L5V H 101:**

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

**Electron density around A1L5V F 101:**

$2mF_o-DF_c$  (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.