



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2024 – 05:50 am BST

PDB ID : 4B2G  
Title : Crystal Structure of an Indole-3-Acetic Acid Amido Synthase from *Vitis vinifera* Involved in Auxin Homeostasis  
Authors : Peat, T.S.; Bottcher, C.; Newman, J.; Lucent, D.; Cowieson, N.; Davies, C.  
Deposited on : 2012-07-16  
Resolution : 2.40 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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

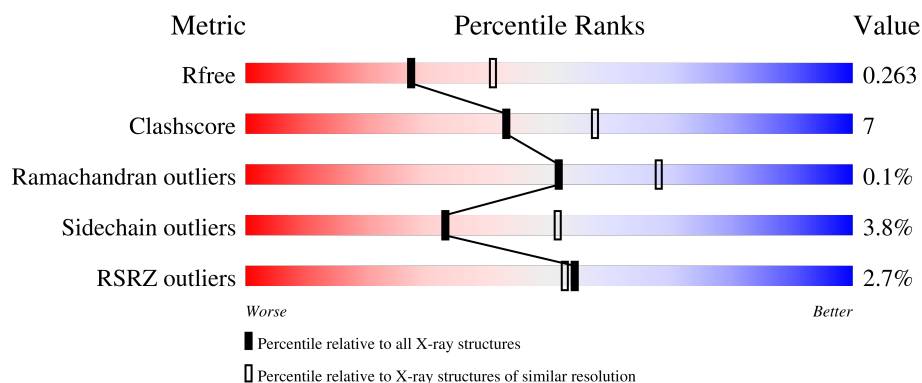
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	609	 3% 79% 12% • 7%
1	B	609	 2% 79% 12% • 6%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9364 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 GH3-1 AUXIN CONJUGATING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	34	8	0
			4524	2873	769	858	24			
1	B	572	Total	C	N	O	S	18	7	0
			4596	2922	782	868	24			

There are 22 discrepancies between the modelled and reference sequences:

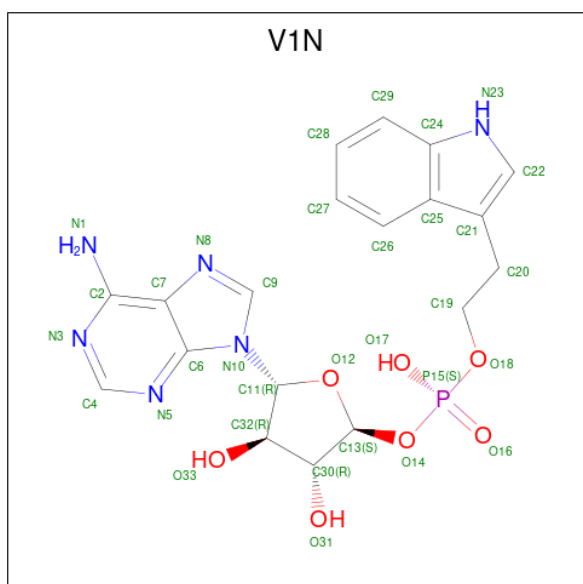
Chain	Residue	Modelled	Actual	Comment	Reference
A	599	ALA	-	expression tag	UNP F6H697
A	600	ALA	-	expression tag	UNP F6H697
A	601	ALA	-	expression tag	UNP F6H697
A	602	LEU	-	expression tag	UNP F6H697
A	603	GLU	-	expression tag	UNP F6H697
A	604	HIS	-	expression tag	UNP F6H697
A	605	HIS	-	expression tag	UNP F6H697
A	606	HIS	-	expression tag	UNP F6H697
A	607	HIS	-	expression tag	UNP F6H697
A	608	HIS	-	expression tag	UNP F6H697
A	609	HIS	-	expression tag	UNP F6H697
B	599	ALA	-	expression tag	UNP F6H697
B	600	ALA	-	expression tag	UNP F6H697
B	601	ALA	-	expression tag	UNP F6H697
B	602	LEU	-	expression tag	UNP F6H697
B	603	GLU	-	expression tag	UNP F6H697
B	604	HIS	-	expression tag	UNP F6H697
B	605	HIS	-	expression tag	UNP F6H697
B	606	HIS	-	expression tag	UNP F6H697
B	607	HIS	-	expression tag	UNP F6H697
B	608	HIS	-	expression tag	UNP F6H697
B	609	HIS	-	expression tag	UNP F6H697

- Molecule 2 is MALONATE ION (three-letter code: MLI) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		
2	A	1	Total	C	O	0	0
			7	3	4		
2	B	1	Total	C	O	0	0
			7	3	4		
2	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 3 is [(2S,3R,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl] 2-(1H-indol-3-yl)ethyl hydrogen phosphate (three-letter code: V1N) (formula: C<sub>19</sub>H<sub>21</sub>N<sub>6</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			33	19	6	7	1		
3	B	1	Total	C	N	O	P	0	0
			33	19	6	7	1		

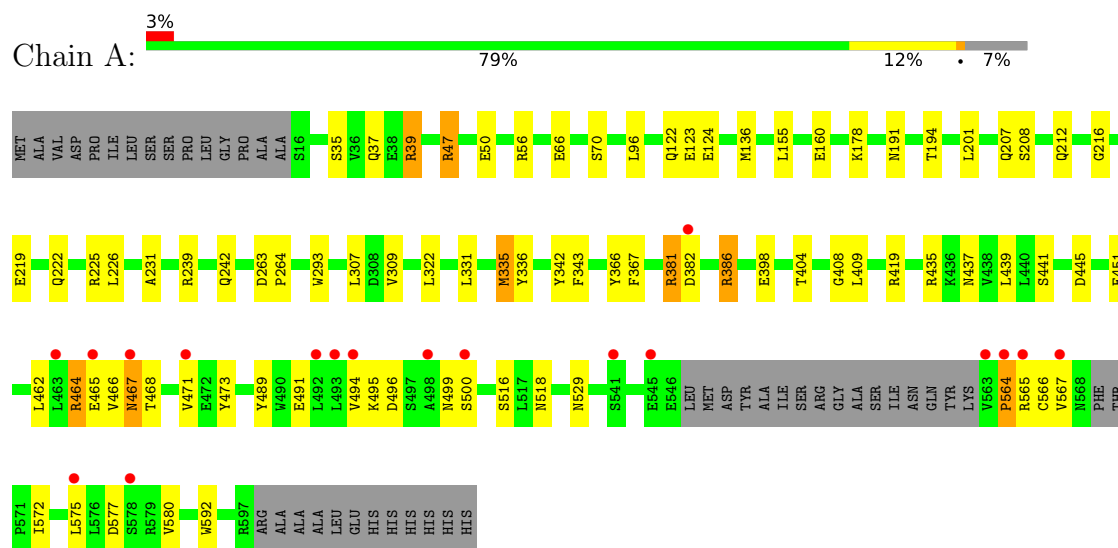
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	63	Total	O	0	0
			63	63		

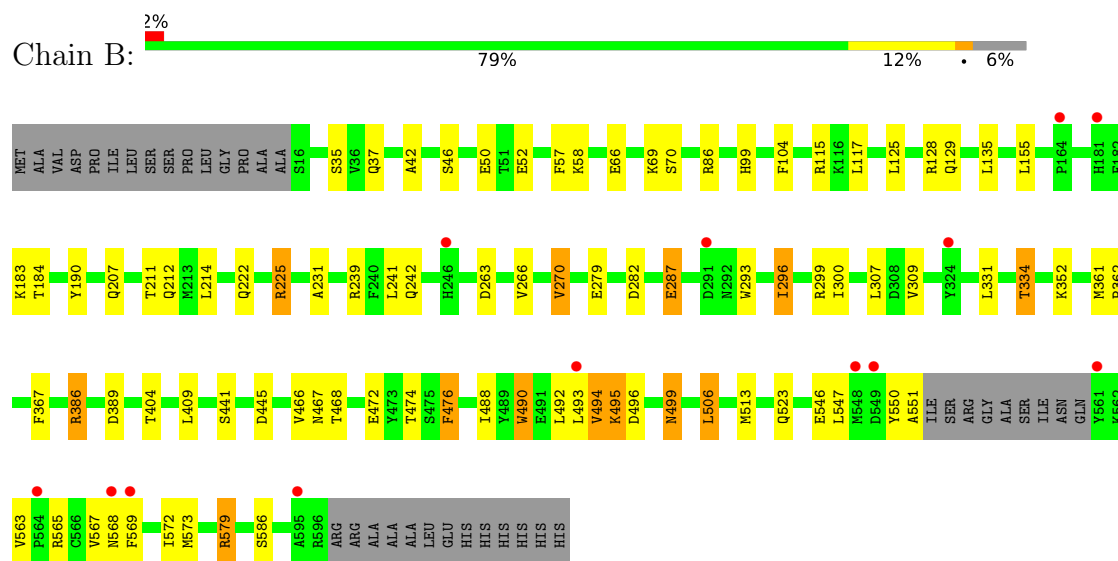
### 3 Residue-property plots

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: GH3-1 AUXIN CONJUGATING ENZYME



#### • Molecule 1: GH3-1 AUXIN CONJUGATING ENZYME



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.17Å 91.17Å 338.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.40) 100.0 (29.94-2.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.224 , 0.264 0.224 , 0.263	Depositor DCC
$R_{free}$ test set	2916 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 20.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9364	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: MLI, V1N

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	0.53	5/4630 (0.1%)	0.64	3/6282 (0.0%)
1	B	0.54	4/4705 (0.1%)	0.64	7/6385 (0.1%)
All	All	0.54	9/9335 (0.1%)	0.64	10/12667 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	ASP	CA-CB	-13.66	1.24	1.53
1	B	495	LYS	CB-CG	-9.30	1.27	1.52
1	A	496	ASP	CA-CB	-8.78	1.34	1.53
1	A	500	SER	CB-OG	-8.54	1.31	1.42
1	A	495	LYS	CA-CB	-8.01	1.36	1.53
1	A	465	GLU	CA-CB	-7.03	1.38	1.53
1	B	496	ASP	CA-CB	-7.02	1.38	1.53
1	B	490	TRP	CD2-CE2	5.28	1.47	1.41
1	A	592	TRP	CD2-CE2	5.12	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	506[A]	LEU	CB-CG-CD2	9.59	127.30	111.00
1	B	506[B]	LEU	CB-CG-CD2	9.59	127.30	111.00
1	A	496	ASP	N-CA-CB	-9.15	94.12	110.60
1	B	495	LYS	CA-CB-CG	7.35	129.56	113.40
1	A	467	ASN	N-CA-CB	7.28	123.71	110.60
1	A	465	GLU	N-CA-CB	7.18	123.52	110.60
1	B	282	ASP	N-CA-CB	6.55	122.40	110.60
1	B	282	ASP	CB-CA-C	6.48	123.36	110.40
1	B	496	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	494	VAL	CA-CB-CG1	-5.03	103.36	110.90



There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	4524	0	4500	61	0
1	B	4596	0	4573	63	0
2	A	14	0	4	0	0
2	B	14	0	4	0	0
3	A	33	0	20	0	0
3	B	33	0	20	0	0
4	A	87	0	0	4	0
4	B	63	0	0	0	0
All	All	9364	0	9121	124	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 7.

All (124) 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:A:471:VAL:CG1	1:A:491:GLU:HG2	1.52	1.38
1:A:466:VAL:HG11	1:A:499:ASN:O	1.40	1.21
1:B:579:ARG:HG2	1:B:579:ARG:HH11	0.99	1.12
1:A:464:ARG:HG2	1:A:464:ARG:HH11	1.15	1.07
1:A:466:VAL:CG1	1:A:499:ASN:O	2.02	1.06
1:B:579:ARG:HH11	1:B:579:ARG:CG	1.68	1.05
1:A:471:VAL:HG13	1:A:491:GLU:HG2	1.32	1.02
1:A:37:GLN:HE22	1:A:367:PHE:H	1.10	0.98
1:A:464:ARG:HH11	1:A:464:ARG:CG	1.77	0.97
1:B:37:GLN:HE22	1:B:367:PHE:H	1.10	0.95
1:A:564:PRO:HB2	1:A:565:ARG:HA	1.49	0.95
1:A:194[B]:THR:HG22	4:A:2044:HOH:O	1.67	0.93
1:B:579:ARG:HG2	1:B:579:ARG:NH1	1.80	0.89
1:A:471:VAL:CG1	1:A:491:GLU:CG	2.48	0.88
1:B:125:LEU:HD12	1:B:128:ARG:HH12	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:VAL:HG11	1:A:491:GLU:HG2	1.56	0.86
1:B:207:GLN:HE22	1:B:263:ASP:H	1.25	0.82
1:B:125:LEU:HD12	1:B:128:ARG:NH1	1.94	0.81
1:A:160:GLU:OE2	1:A:178:LYS:NZ	2.16	0.77
1:A:471:VAL:HG12	1:A:491:GLU:HG2	1.63	0.77
1:B:579:ARG:CG	1:B:579:ARG:NH1	2.39	0.75
1:A:437[B]:ASN:O	1:A:437[B]:ASN:OD1	2.04	0.75
1:B:466:VAL:CG1	1:B:499:ASN:O	2.34	0.75
1:A:564:PRO:CB	1:A:565:ARG:HA	2.18	0.73
1:A:219:GLU:OE1	1:A:222:GLN:OE1	2.06	0.73
1:A:239:ARG:HH11	1:A:242:GLN:HE21	1.34	0.73
1:A:464:ARG:HG2	1:A:464:ARG:NH1	1.96	0.71
1:A:464:ARG:CG	1:A:464:ARG:NH1	2.48	0.70
1:A:435:ARG:NH2	4:A:2017:HOH:O	2.25	0.70
1:A:207:GLN:HE22	1:A:263:ASP:H	1.40	0.67
1:A:35:SER:O	1:A:39:ARG:HG2	1.95	0.66
1:B:239:ARG:NH1	1:B:242:GLN:OE1	2.28	0.65
1:B:155:LEU:H	1:B:212:GLN:HE22	1.45	0.64
1:B:211:THR:HG21	1:B:266:VAL:HG12	1.78	0.64
1:B:466:VAL:HG13	1:B:499:ASN:O	1.99	0.62
1:A:194[B]:THR:HG21	1:A:216:GLY:HA2	1.82	0.62
1:B:547:LEU:HD11	1:B:572:ILE:HG23	1.82	0.62
1:A:466:VAL:HG12	1:A:467:ASN:H	1.65	0.61
1:A:466:VAL:HG13	1:A:499:ASN:O	1.97	0.61
1:A:441:SER:HB2	1:A:445:ASP:O	2.00	0.61
1:A:70:SER:HB3	1:A:386:ARG:HH21	1.66	0.61
1:A:335:MET:HE3	1:A:342:TYR:CD2	2.37	0.59
1:A:381:ARG:NH2	4:A:2010:HOH:O	2.35	0.59
1:A:47:ARG:NH2	1:A:123:GLU:OE2	2.30	0.59
1:A:437[B]:ASN:OD1	1:A:437[B]:ASN:C	2.41	0.58
1:B:441:SER:HB2	1:B:445:ASP:O	2.04	0.58
1:A:239:ARG:NH1	1:A:242:GLN:HE21	2.01	0.58
1:B:135:LEU:HD22	1:B:334[A]:THR:HG23	1.86	0.58
1:B:115:ARG:HH21	1:B:523:GLN:HE22	1.52	0.57
1:A:439:LEU:HD13	1:A:566:CYS:HB3	1.85	0.57
1:B:287:GLU:HG3	1:B:299:ARG:HH11	1.70	0.57
1:B:468:THR:CG2	1:B:492:LEU:HD23	2.34	0.57
1:B:466:VAL:HG12	1:B:467:ASN:H	1.70	0.56
1:A:398:GLU:OE2	1:A:419[A]:ARG:NH1	2.38	0.56
1:A:471:VAL:HG13	1:A:491:GLU:CG	2.21	0.56
1:B:488:ILE:HD13	1:B:513:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLN:NE2	1:B:367:PHE:H	1.91	0.54
1:A:37:GLN:NE2	1:A:367:PHE:H	1.93	0.52
1:B:550:TYR:O	1:B:551:ALA:CB	2.58	0.51
1:B:466:VAL:HG11	1:B:499:ASN:O	2.11	0.51
1:B:476:PHE:HB2	1:B:567:VAL:O	2.10	0.51
1:B:135:LEU:HD13	1:B:334[A]:THR:HG21	1.92	0.50
1:A:404:THR:HA	1:A:409:LEU:O	2.11	0.50
1:B:468:THR:HG21	1:B:492:LEU:HD23	1.94	0.49
1:A:155:LEU:H	1:A:212:GLN:HE22	1.61	0.48
1:B:231:ALA:HA	1:B:309:VAL:CG2	2.44	0.48
1:B:231:ALA:HA	1:B:309:VAL:HG21	1.96	0.48
1:A:124:GLU:HG2	4:A:2023:HOH:O	2.13	0.48
1:A:178:LYS:HG3	1:A:201:LEU:HD22	1.96	0.48
1:A:466:VAL:HG12	1:A:467:ASN:N	2.29	0.47
1:B:293:TRP:CE3	1:B:296:ILE:HG21	2.50	0.47
1:A:208:SER:O	1:A:212:GLN:HG3	2.15	0.47
1:B:293:TRP:CD2	1:B:296:ILE:HD13	2.50	0.47
1:B:70:SER:HB3	1:B:386[B]:ARG:NH2	2.29	0.47
1:A:191:ASN:HA	1:A:225:ARG:HH22	1.79	0.47
1:B:66:GLU:HA	1:B:386[B]:ARG:HH12	1.80	0.46
1:B:490:TRP:HB3	1:B:492:LEU:CD1	2.45	0.46
1:B:494:VAL:O	1:B:495:LYS:C	2.54	0.46
1:B:546:GLU:OE1	1:B:579:ARG:CZ	2.63	0.46
1:B:42:ALA:O	1:B:46:SER:HB2	2.15	0.46
1:A:572:ILE:HA	1:A:575:LEU:HD12	1.98	0.46
1:A:307:LEU:HB2	1:A:331:LEU:HD23	1.97	0.46
1:B:568:ASN:HA	1:B:573:MET:HE1	1.99	0.45
1:A:239:ARG:HH11	1:A:242:GLN:NE2	2.07	0.45
1:B:211:THR:HG21	1:B:266:VAL:CG1	2.46	0.45
1:B:404:THR:HA	1:B:409:LEU:O	2.17	0.45
1:A:194[B]:THR:HG21	1:A:216:GLY:CA	2.47	0.44
1:B:104:PHE:CD1	1:B:117:LEU:HB3	2.52	0.44
1:B:468:THR:HG22	1:B:492:LEU:HD23	1.98	0.44
1:B:490:TRP:HB3	1:B:492:LEU:HD11	1.99	0.44
1:A:336:TYR:O	1:A:343:PHE:HB2	2.17	0.44
1:B:547:LEU:CD1	1:B:572:ILE:HG23	2.46	0.44
1:A:464:ARG:HD3	1:A:464:ARG:N	2.33	0.44
1:A:242:GLN:HA	1:A:293:TRP:CH2	2.53	0.44
1:B:287:GLU:HG3	1:B:299:ARG:NH1	2.31	0.44
1:B:57:PHE:C	1:B:58:LYS:HG2	2.37	0.44
1:B:474:THR:OG1	1:B:567:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LYS:NZ	1:B:389:ASP:OD1	2.46	0.43
1:A:464:ARG:N	1:A:464:ARG:CD	2.81	0.43
1:B:115:ARG:HH21	1:B:523:GLN:NE2	2.15	0.43
1:A:263:ASP:HA	1:A:264:PRO:HD3	1.93	0.43
1:B:466:VAL:HG12	1:B:467:ASN:N	2.33	0.43
1:A:231:ALA:HB1	1:A:322:LEU:HD11	2.01	0.43
1:A:37:GLN:HE22	1:A:367:PHE:N	1.93	0.42
1:B:468:THR:HA	1:B:493:LEU:O	2.19	0.42
1:A:468:THR:HG23	1:A:494:VAL:HG22	2.00	0.42
1:A:471:VAL:HG11	1:A:491:GLU:CG	2.38	0.42
1:A:577:ASP:HA	1:A:580:VAL:HG23	2.01	0.42
1:B:361:MET:HA	1:B:362:PRO:HD3	1.71	0.42
1:A:96:LEU:HB3	1:A:408:GLY:HA3	2.02	0.42
1:B:190:TYR:O	1:B:225:ARG:NH2	2.52	0.42
1:B:52:GLU:OE2	1:B:86:ARG:NH1	2.42	0.41
1:B:293:TRP:CE3	1:B:296:ILE:HD13	2.56	0.41
1:B:472:GLU:HG2	1:B:563:VAL:HG21	2.02	0.41
1:B:569:PHE:HD2	1:B:572:ILE:HG13	1.85	0.41
1:B:307:LEU:HB2	1:B:331:LEU:HD23	2.02	0.41
1:A:451:GLU:OE2	1:A:518:ASN:HB3	2.20	0.41
1:A:473:TYR:HA	1:A:489:TYR:O	2.21	0.41
1:B:241:LEU:HD21	1:B:300:ILE:HD13	2.03	0.41
1:B:441:SER:CB	1:B:445:ASP:O	2.68	0.41
1:B:506[A]:LEU:H	1:B:506[A]:LEU:HG	1.72	0.41
1:A:366:TYR:HB3	1:A:404:THR:HB	2.03	0.41
1:B:242:GLN:HG2	1:B:293:TRP:CZ2	2.56	0.40
1:B:214:LEU:HD23	1:B:270:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	566/609 (93%)	550 (97%)	15 (3%)	1 (0%)	47	62
1	B	575/609 (94%)	556 (97%)	19 (3%)	0	100	100
All	All	1141/1218 (94%)	1106 (97%)	34 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	564	PRO

### 5.3.2 Protein sidechains ⓘ

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	506/535 (95%)	488 (96%)	18 (4%)	35	54
1	B	512/535 (96%)	489 (96%)	23 (4%)	27	44
All	All	1018/1070 (95%)	977 (96%)	41 (4%)	33	49

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	47	ARG
1	A	50	GLU
1	A	56	ARG
1	A	66	GLU
1	A	122	GLN
1	A	136	MET
1	A	226	LEU
1	A	309	VAL
1	A	335	MET
1	A	381	ARG
1	A	382	ASP
1	A	386	ARG
1	A	462	LEU
1	A	464	ARG

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Mol	Chain	Res	Type
1	A	516	SER
1	A	529	ASN
1	A	567	VAL
1	B	35	SER
1	B	50	GLU
1	B	99	HIS
1	B	129	GLN
1	B	183	LYS
1	B	184	THR
1	B	222[A]	GLN
1	B	222[B]	GLN
1	B	225	ARG
1	B	270	VAL
1	B	279	GLU
1	B	287	GLU
1	B	296	ILE
1	B	334[A]	THR
1	B	334[B]	THR
1	B	352	LYS
1	B	386[A]	ARG
1	B	386[B]	ARG
1	B	476	PHE
1	B	499	ASN
1	B	565	ARG
1	B	579	ARG
1	B	586	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	99	HIS
1	A	122	GLN
1	A	207	GLN
1	A	212	GLN
1	A	222	GLN
1	A	242	GLN
1	A	244	ASN
1	A	424	HIS
1	B	37	GLN
1	B	129	GLN
1	B	181	HIS

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Mol	Chain	Res	Type
1	B	207	GLN
1	B	212	GLN
1	B	244	ASN
1	B	372	HIS
1	B	374	HIS
1	B	499	ASN
1	B	523	GLN
1	B	584	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 ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	MLI	A	1599	-	6,6,6	1.14	0	7,7,7	1.27	1 (14%)
3	V1N	A	1600	-	32,37,37	1.56	6 (18%)	36,55,55	2.52	11 (30%)
3	V1N	B	1600	-	32,37,37	1.43	4 (12%)	36,55,55	2.39	11 (30%)
2	MLI	A	1598	-	6,6,6	1.12	0	7,7,7	0.99	0
2	MLI	B	1597	-	6,6,6	0.95	0	7,7,7	1.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MLI	B	1598	-	6,6,6	1.16	0	7,7,7	0.94	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	MLI	A	1599	-	-	0/4/4/4	-
3	V1N	A	1600	-	-	3/11/32/32	0/5/5/5
3	V1N	B	1600	-	-	3/11/32/32	0/5/5/5
2	MLI	A	1598	-	-	2/4/4/4	-
2	MLI	B	1597	-	-	0/4/4/4	-
2	MLI	B	1598	-	-	3/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1600	V1N	P15-O14	4.18	1.71	1.60
3	B	1600	V1N	P15-O14	3.94	1.70	1.60
3	A	1600	V1N	O12-C11	3.60	1.46	1.41
3	A	1600	V1N	C32-C11	-3.06	1.49	1.53
3	B	1600	V1N	O12-C11	2.98	1.45	1.41
3	B	1600	V1N	O12-C13	2.23	1.45	1.41
3	A	1600	V1N	O12-C13	2.23	1.45	1.41
3	A	1600	V1N	C29-C24	-2.22	1.38	1.41
3	A	1600	V1N	C13-C30	2.18	1.55	1.52
3	B	1600	V1N	C29-C24	-2.02	1.38	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1600	V1N	O14-C13-C30	5.99	116.85	106.72
3	A	1600	V1N	C13-O12-C11	5.80	115.47	106.28
3	B	1600	V1N	O12-C13-C30	-5.56	97.82	104.98
3	A	1600	V1N	O12-C13-C30	-5.41	98.01	104.98
3	B	1600	V1N	C13-O12-C11	5.06	114.30	106.28
3	B	1600	V1N	O14-C13-C30	4.93	115.07	106.72
3	B	1600	V1N	P15-O14-C13	4.59	137.49	119.74
3	A	1600	V1N	O31-C30-C32	-4.49	97.29	111.82
3	A	1600	V1N	P15-O14-C13	4.42	136.83	119.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1600	V1N	C13-C30-C32	4.22	107.64	102.30
3	B	1600	V1N	C13-C30-C32	4.06	107.44	102.30
3	B	1600	V1N	O31-C30-C32	-3.98	98.94	111.82
3	B	1600	V1N	C28-C29-C24	-3.81	114.60	120.08
3	A	1600	V1N	C28-C29-C24	-3.68	114.79	120.08
3	B	1600	V1N	C27-C26-C25	-3.22	116.42	120.89
3	A	1600	V1N	O31-C30-C13	3.04	120.33	111.83
3	A	1600	V1N	C27-C26-C25	-2.96	116.79	120.89
3	B	1600	V1N	C30-C32-C11	2.63	104.94	100.98
3	A	1600	V1N	C30-C32-C11	2.61	104.90	100.98
3	B	1600	V1N	O31-C30-C13	2.57	119.00	111.83
3	A	1600	V1N	C11-N10-C6	2.37	130.81	126.64
3	B	1600	V1N	C29-C24-C25	2.35	125.05	120.76
2	A	1599	MLI	O9-C3-C1	2.16	121.44	114.54

There are no chirality outliers.

All (11) torsion outliers are listed below:

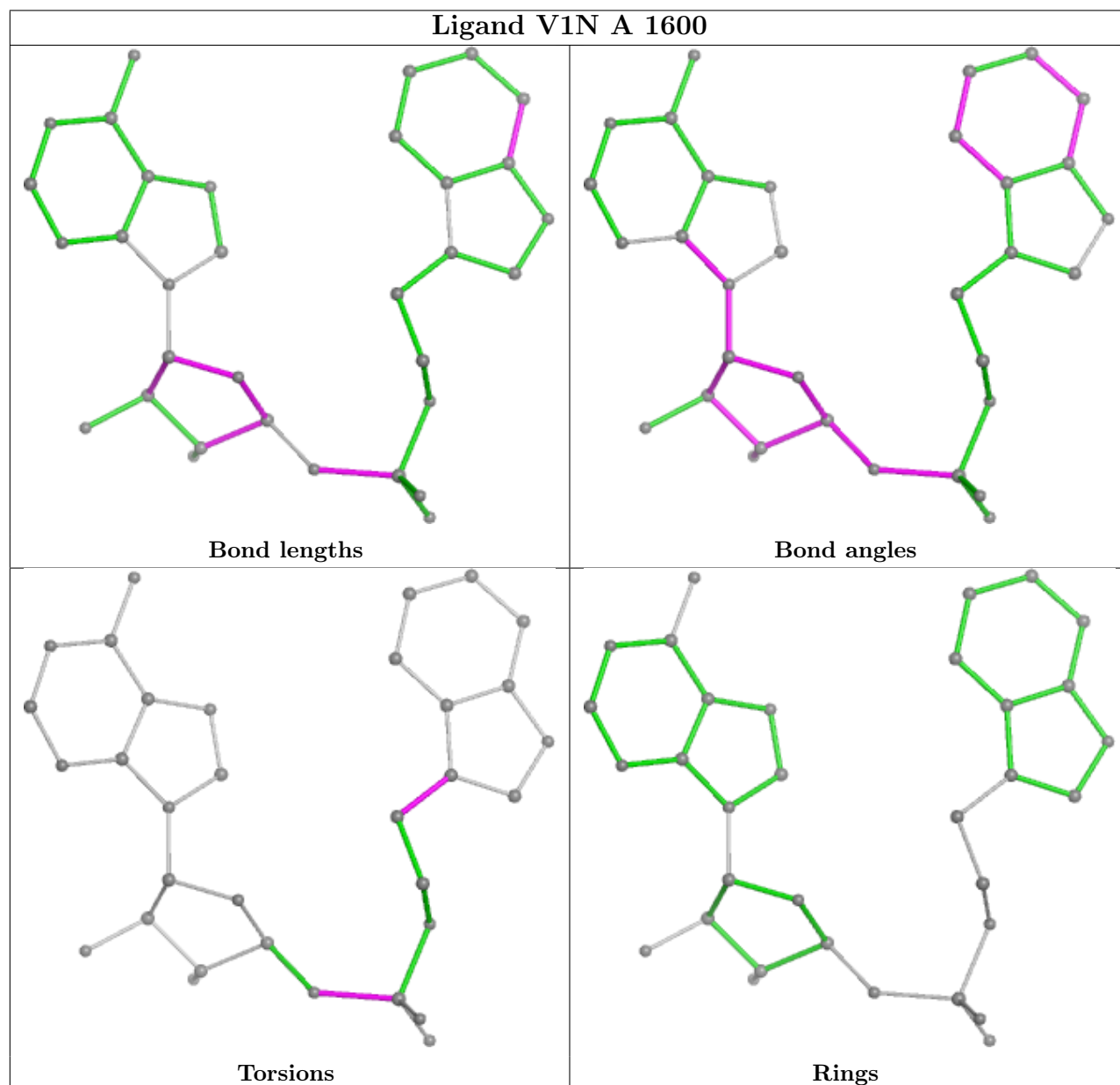
Mol	Chain	Res	Type	Atoms
3	A	1600	V1N	C13-O14-P15-O18
3	B	1600	V1N	C13-O14-P15-O18
3	A	1600	V1N	C19-C20-C21-C25
3	B	1600	V1N	C19-C20-C21-C25
3	B	1600	V1N	C13-O14-P15-O17
2	A	1598	MLI	C3-C1-C2-O6
2	A	1598	MLI	C3-C1-C2-O7
2	B	1598	MLI	C2-C1-C3-O8
2	B	1598	MLI	C2-C1-C3-O9
2	B	1598	MLI	C3-C1-C2-O7
3	A	1600	V1N	C13-O14-P15-O17

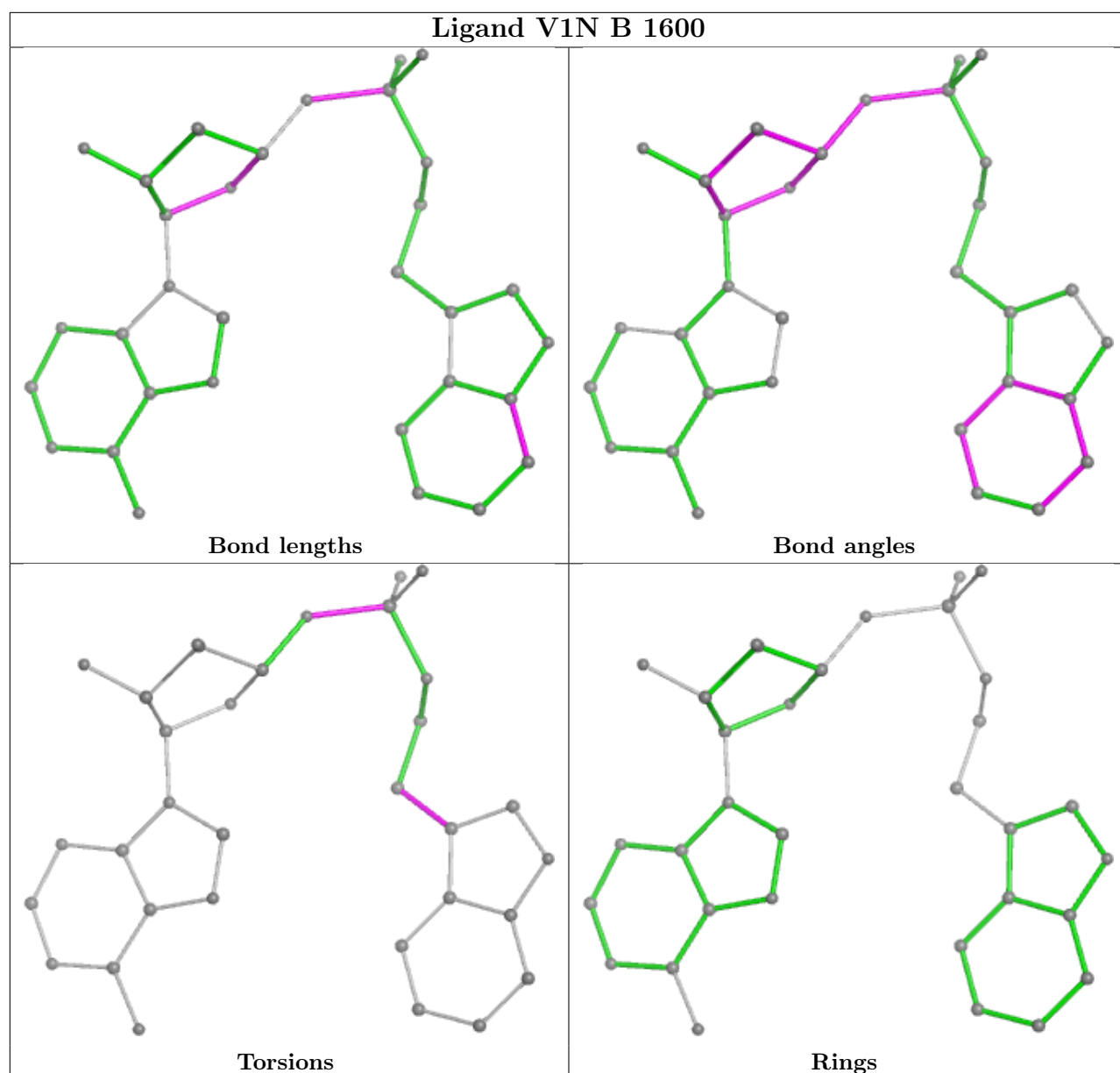
There are no ring outliers.

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

### 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	564/609 (92%)	-0.12	18 (3%)	47 46	15, 29, 63, 89	60 (10%)
1	B	572/609 (93%)	0.04	13 (2%)	60 58	18, 35, 60, 82	63 (11%)
All	All	1136/1218 (93%)	-0.04	31 (2%)	54 52	15, 32, 62, 89	123 (10%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	ALA	3.7
1	B	291	ASP	3.5
1	B	569	PHE	3.3
1	A	500	SER	3.0
1	A	563	VAL	2.9
1	A	467	ASN	2.8
1	B	246	HIS	2.8
1	A	575	LEU	2.7
1	A	565	ARG	2.7
1	A	463	LEU	2.6
1	A	541	SER	2.6
1	A	567	VAL	2.6
1	A	382	ASP	2.6
1	B	561	TYR	2.6
1	A	471	VAL	2.4
1	A	578	SER	2.4
1	B	568	ASN	2.3
1	B	548	MET	2.3
1	B	181	HIS	2.3
1	A	494	VAL	2.3
1	B	324	TYR	2.3
1	A	492	LEU	2.2
1	B	549	ASP	2.2
1	A	465	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	493	LEU	2.1
1	A	564	PRO	2.1
1	A	545	GLU	2.1
1	B	564	PRO	2.1
1	B	164	PRO	2.1
1	B	595	ALA	2.0
1	B	493	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](#)

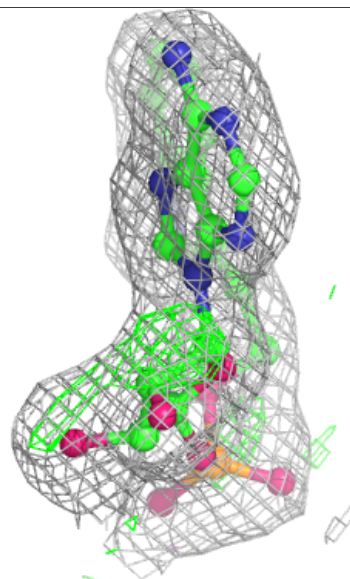
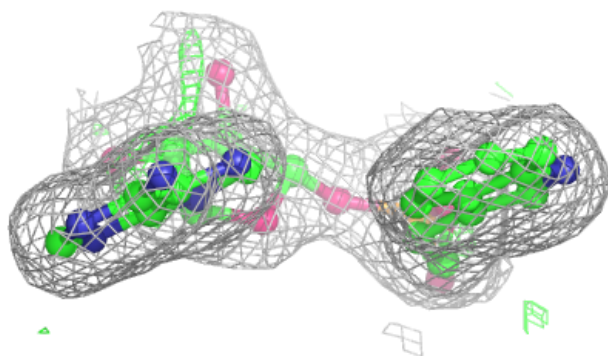
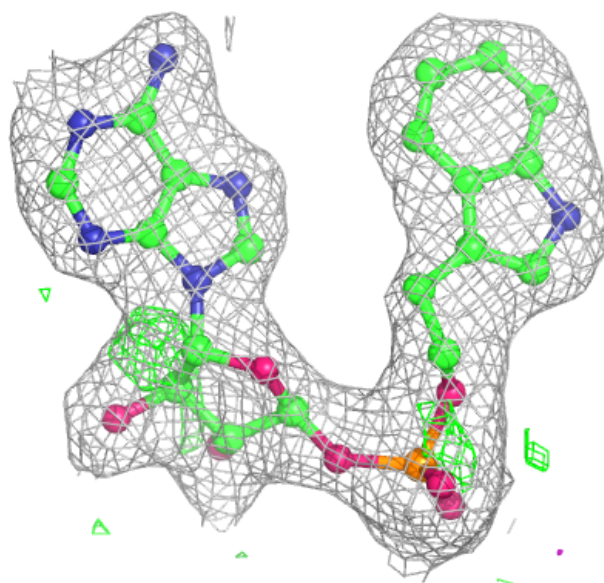
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MLI	B	1598	7/7	0.90	0.31	50,52,52,52	0
2	MLI	A	1598	7/7	0.93	0.19	39,41,43,45	0
2	MLI	B	1597	7/7	0.95	0.11	24,26,27,29	0
2	MLI	A	1599	7/7	0.96	0.12	26,27,30,32	0
3	V1N	A	1600	33/33	0.96	0.16	19,21,24,25	0
3	V1N	B	1600	33/33	0.96	0.15	19,21,23,23	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.

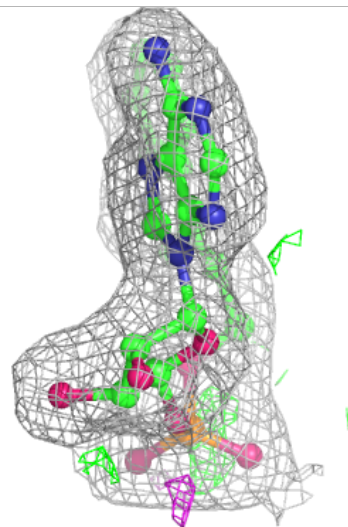
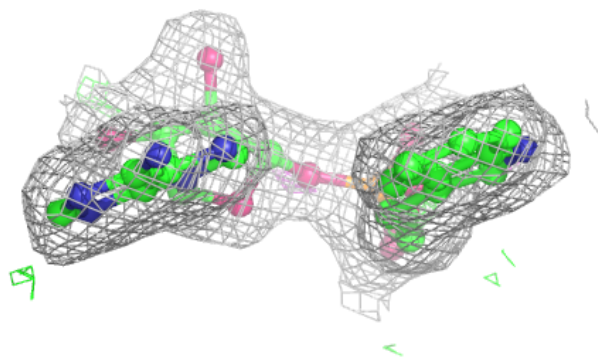
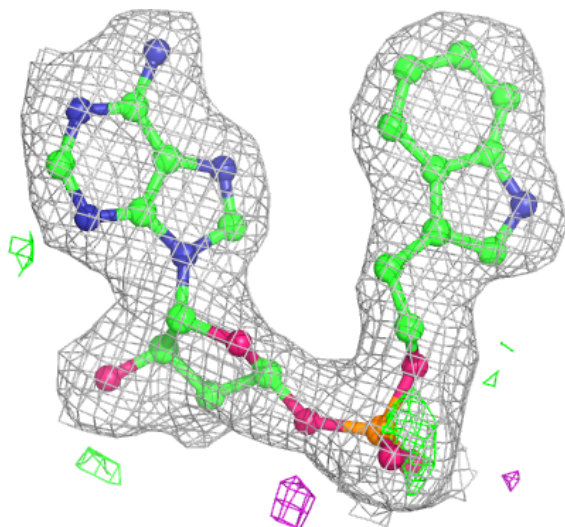
**Electron density around V1N A 1600:**

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



**Electron density around V1N B 1600:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.