



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:47 PM UTC

PDB ID : 4B2G / pdb_00004b2g
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

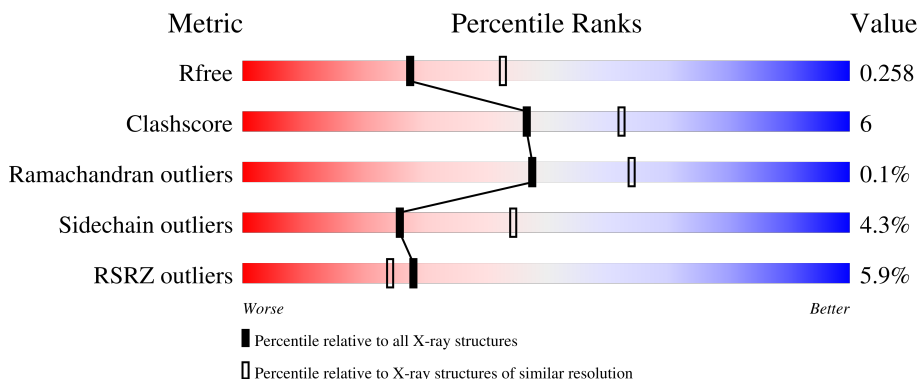
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 ≥ 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	 5% 79% 12% • 7%
1	B	609	 6% 80% 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.

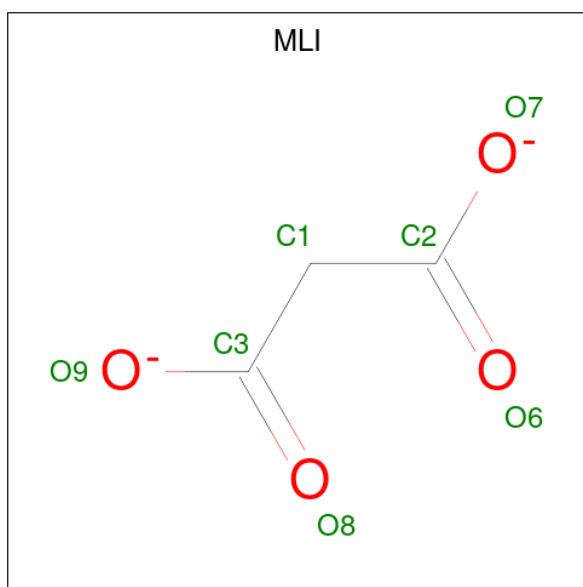
- Molecule 1 is a protein called GH3-1 AUXIN CONJUGATING ENZYME.

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:

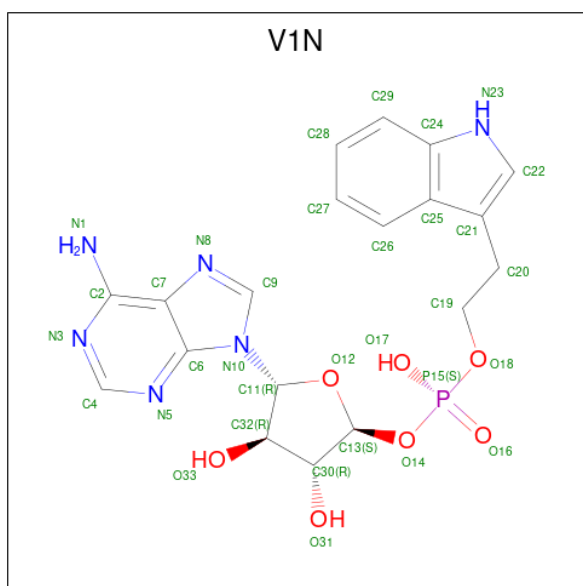
Chain	Residue	Modelled	Actual	Comment	Reference
A	599	ALA	-	expression tag	UNP F6H697
A	600	ALA	-	expression tag	UNP F6H697
A	601	ALA	-	expression tag	UNP F6H697
A	602	LEU	-	expression tag	UNP F6H697
A	603	GLU	-	expression tag	UNP F6H697
A	604	HIS	-	expression tag	UNP F6H697
A	605	HIS	-	expression tag	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 (CCD ID: MLI) (formula: C₃H₂O₄).



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 (CCD ID: V1N) (formula: $C_{19}H_{21}N_6O_7P$).



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		

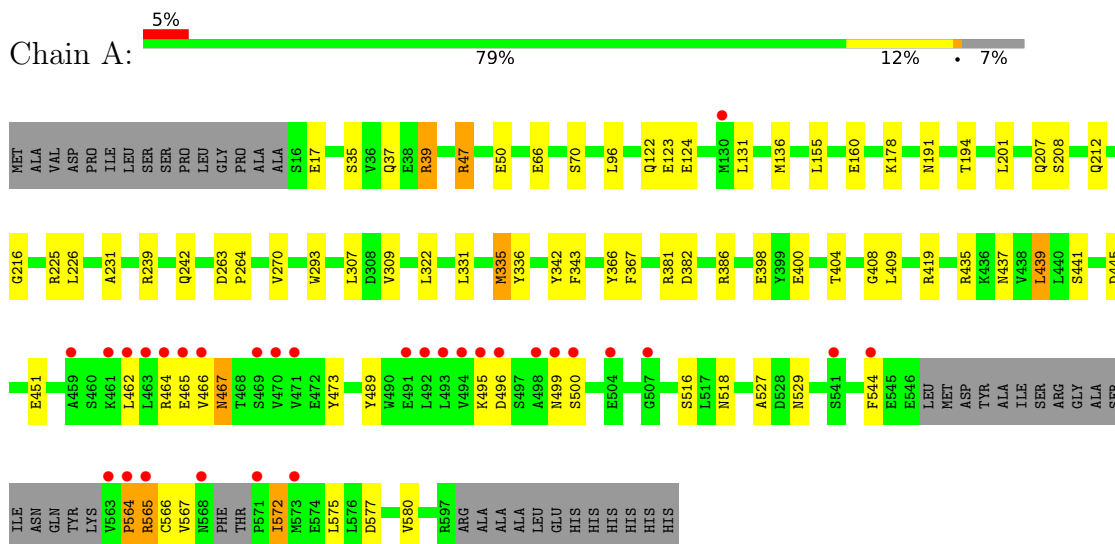
- Molecule 4 is water.

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

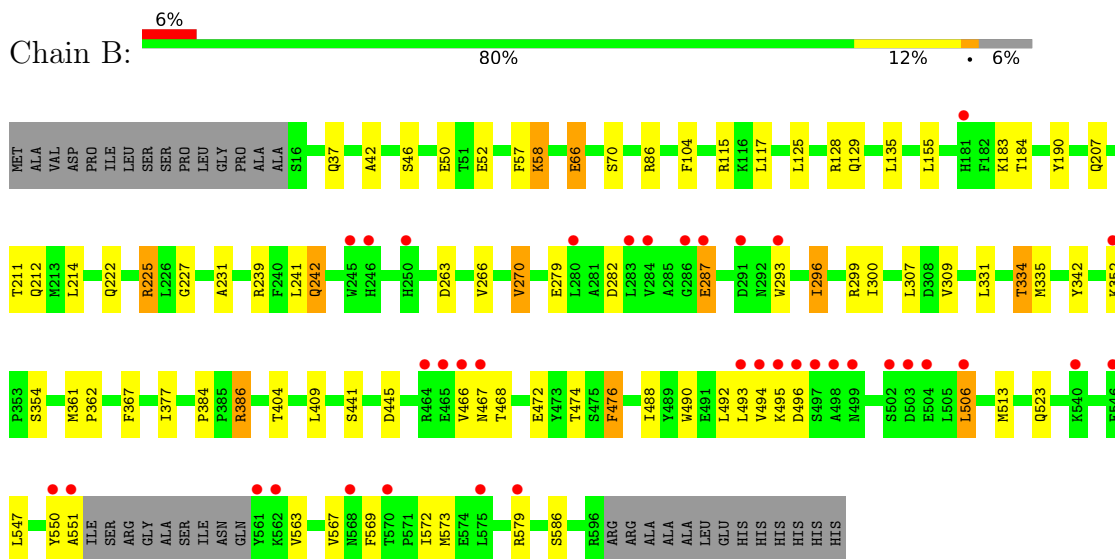
3 Residue-property plots

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, α , β , γ	91.17Å 91.17Å 338.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.40) 99.9 (30.00-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.224 , 0.264 (Not available) , 0.258	Depositor DCC
R_{free} test set	2916 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9364	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.69	4/4630 (0.1%)	0.91	9/6282 (0.1%)
1	B	0.69	4/4705 (0.1%)	0.86	6/6385 (0.1%)
All	All	0.69	8/9335 (0.1%)	0.88	15/12667 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	ASP	CA-CB	-17.49	1.24	1.53
1	A	495	LYS	CA-CB	-10.87	1.36	1.53
1	A	496	ASP	CA-CB	-10.83	1.34	1.53
1	B	496	ASP	CA-CB	-9.58	1.38	1.53
1	B	495	LYS	CB-CG	-8.34	1.27	1.52
1	A	465	GLU	CA-CB	-7.99	1.38	1.53
1	B	494	VAL	CA-CB	7.43	1.62	1.53
1	A	500	SER	CB-OG	-5.50	1.31	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	ASN	CA-CB-CG	10.77	123.36	112.60
1	A	496	ASP	N-CA-CB	-10.28	94.12	110.87
1	A	467	ASN	N-CA-CB	9.06	123.71	110.57
1	A	499	ASN	CA-CB-CG	-8.21	104.39	112.60
1	B	495	LYS	CA-CB-CG	7.73	129.56	114.10
1	A	465	GLU	N-CA-CB	7.25	123.52	110.32
1	B	282	ASP	N-CA-CB	7.05	122.40	110.49
1	B	282	ASP	CB-CA-C	6.50	123.36	110.42
1	A	500	SER	CA-CB-OG	6.14	123.38	111.10
1	A	527	ALA	N-CA-C	5.81	117.42	111.14
1	A	495	LYS	N-CA-CB	5.75	118.58	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	GLY	N-CA-C	5.72	118.94	110.42
1	B	384	PRO	O-C-N	5.51	123.74	121.15
1	A	544	PHE	N-CA-C	5.34	117.18	111.36
1	B	494	VAL	N-CA-CB	-5.27	105.27	111.60

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	48	0
1	B	4596	0	4573	55	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	103	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 6.

All (103) 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:37:GLN:HE22	1:A:367:PHE:H	1.10	0.98
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:125:LEU:HD12	1:B:128:ARG:HH12	1.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437[B]:ASN:O	1:A:437[B]:ASN:OD1	2.04	0.75
1:A:564:PRO:CB	1:A:565:ARG:HA	2.18	0.73
1:A:239:ARG:HH11	1:A:242:GLN:HE21	1.34	0.73
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:A:437[B]:ASN:OD1	1:A:437[B]:ASN:C	2.41	0.63
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: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: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:B:488:ILE:HD13	1:B:513:MET:HE1	1.84	0.59
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:A:335:MET:HE1	1:A:342:TYR:CE2	2.38	0.57
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:A:335:MET:HE1	1:A:342:TYR:CD2	2.41	0.56
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:B:488:ILE:HD13	1:B:513:MET:CE	2.36	0.55
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: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:57:PHE:C	1:B:58:LYS:HG2	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:131:LEU:HD23	1:A:335:MET:HE3	1.97	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:567:VAL:HG12	1:B:573:MET:HE1	1.96	0.46
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: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:474:THR:OG1	1:B:567:VAL:HG23	2.18	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:B:335:MET:HE2	1:B:342:TYR:CD2	2.54	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:335:MET:CE	1:A:342:TYR:CD2	3.04	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:A:160:GLU:CD	1:A:178:LYS:HZ3	2.21	0.40
1:B:242:GLN:HG2	1:B:293:TRP:CZ2	2.56	0.40
1:A:437[B]:ASN:O	1:A:437[B]:ASN:CG	2.64	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%)	43	58
1	B	575/609 (94%)	556 (97%)	19 (3%)	0	100	100
All	All	1141/1218 (94%)	1106 (97%)	34 (3%)	1 (0%)	48	64

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%)	485 (96%)	21 (4%)	26	45
1	B	512/535 (96%)	486 (95%)	26 (5%)	21	37
All	All	1018/1070 (95%)	971 (95%)	47 (5%)	26	41

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	39	ARG
1	A	47	ARG
1	A	50	GLU
1	A	66	GLU
1	A	122	GLN
1	A	136	MET
1	A	226	LEU
1	A	270	VAL
1	A	309	VAL
1	A	335	MET
1	A	382	ASP
1	A	400	GLU
1	A	439	LEU
1	A	462	LEU
1	A	464	ARG
1	A	516	SER
1	A	529	ASN
1	A	565	ARG
1	A	567	VAL
1	A	572	ILE
1	B	50	GLU
1	B	58	LYS
1	B	66	GLU
1	B	129	GLN
1	B	183	LYS
1	B	184	THR

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Mol	Chain	Res	Type
1	B	222[A]	GLN
1	B	222[B]	GLN
1	B	225	ARG
1	B	242	GLN
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	354	SER
1	B	377	ILE
1	B	386[A]	ARG
1	B	386[B]	ARG
1	B	476	PHE
1	B	506[A]	LEU
1	B	506[B]	LEU
1	B	579	ARG
1	B	586	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	81	GLN
1	A	122	GLN
1	A	207	GLN
1	A	212	GLN
1	A	222	GLN
1	A	242	GLN
1	A	424	HIS
1	A	425	ASN
1	A	431	HIS
1	A	458	ASN
1	B	37	GLN
1	B	140	ASN
1	B	181	HIS
1	B	207	GLN
1	B	212	GLN
1	B	244	ASN
1	B	372	HIS

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Mol	Chain	Res	Type
1	B	374	HIS
1	B	431	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 oligosaccharides 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	$\# Z > 2$
3	V1N	A	1600	-	36,37,37	1.23	4 (11%)	54,55,55	2.06	9 (16%)
2	MLI	B	1598	-	6,6,6	1.19	0	7,7,7	0.98	0
2	MLI	A	1599	-	6,6,6	1.17	0	7,7,7	1.30	1 (14%)
3	V1N	B	1600	-	36,37,37	1.15	3 (8%)	54,55,55	1.97	11 (20%)
2	MLI	A	1598	-	6,6,6	1.15	0	7,7,7	1.02	0
2	MLI	B	1597	-	6,6,6	0.98	0	7,7,7	1.29	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
3	V1N	A	1600	-	-	2/15/32/32	0/5/5/5
2	MLI	B	1598	-	-	1/4/4/4	-
2	MLI	A	1599	-	-	0/4/4/4	-
3	V1N	B	1600	-	-	2/15/32/32	0/5/5/5
2	MLI	A	1598	-	-	2/4/4/4	-
2	MLI	B	1597	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1600	V1N	P15-O14	4.02	1.71	1.59
3	B	1600	V1N	P15-O14	3.81	1.70	1.59
3	B	1600	V1N	C2-N1	2.49	1.40	1.34
3	A	1600	V1N	C2-N1	2.38	1.40	1.34
3	B	1600	V1N	O12-C13	2.26	1.45	1.41
3	A	1600	V1N	O12-C13	2.26	1.45	1.41
3	A	1600	V1N	C13-C30	2.17	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1600	V1N	O14-C13-C30	6.29	116.85	106.65
3	B	1600	V1N	O12-C13-C30	-5.63	97.82	104.98
3	A	1600	V1N	O12-C13-C30	-5.48	98.01	104.98
3	A	1600	V1N	C13-O12-C11	5.28	115.47	106.05
3	B	1600	V1N	O14-C13-C30	5.19	115.07	106.65
3	B	1600	V1N	C13-O12-C11	4.62	114.30	106.05
3	A	1600	V1N	O31-C30-C32	-4.53	97.29	111.82
3	A	1600	V1N	C13-C30-C32	4.30	107.64	102.29
3	B	1600	V1N	C13-C30-C32	4.14	107.44	102.29
3	B	1600	V1N	O31-C30-C32	-4.02	98.94	111.82
3	B	1600	V1N	P15-O14-C13	4.00	137.49	121.21
3	A	1600	V1N	P15-O14-C13	3.83	136.83	121.21
3	A	1600	V1N	O31-C30-C13	3.02	120.33	111.82
3	B	1600	V1N	C29-C24-C25	2.96	125.05	122.19
3	A	1600	V1N	C21-C22-N23	-2.73	107.31	110.31
3	B	1600	V1N	O31-C30-C13	2.55	119.00	111.82
3	B	1600	V1N	C28-C27-C26	2.42	123.22	120.24
3	A	1600	V1N	C24-N23-C22	2.27	111.09	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1600	V1N	C32-C11-N10	-2.25	107.71	113.30
2	A	1599	MLI	O9-C3-C1	2.24	121.44	114.51
3	B	1600	V1N	C28-C29-C24	-2.01	114.60	118.69

There are no chirality outliers.

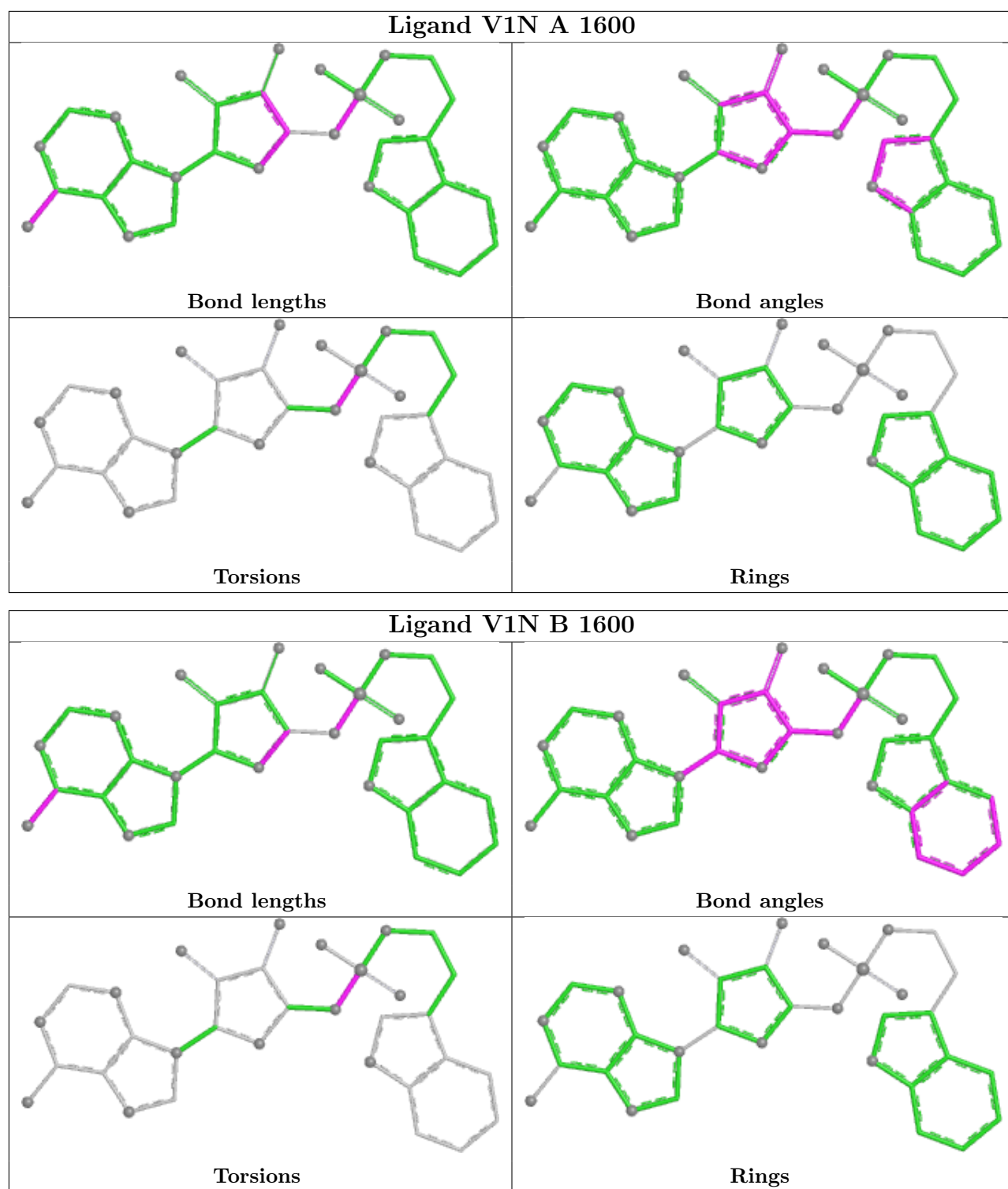
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1600	V1N	C13-O14-P15-O18
3	B	1600	V1N	C13-O14-P15-O18
2	A	1598	MLI	C3-C1-C2-O6
2	A	1598	MLI	C3-C1-C2-O7
3	A	1600	V1N	C13-O14-P15-O16
3	B	1600	V1N	C13-O14-P15-O16
2	B	1598	MLI	C3-C1-C2-O7

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	564/609 (92%)	0.12	30 (5%)	32 28	9, 28, 56, 89	68 (12%)
1	B	572/609 (93%)	0.30	37 (6%)	25 21	11, 34, 60, 82	69 (12%)
All	All	1136/1218 (93%)	0.21	67 (5%)	28 24	9, 31, 59, 89	137 (12%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	SER	8.6
1	A	499	ASN	7.3
1	B	497	SER	6.6
1	A	496	ASP	6.5
1	B	496	ASP	6.4
1	B	494	VAL	6.2
1	A	494	VAL	5.8
1	A	495	LYS	5.7
1	B	551	ALA	5.7
1	B	499	ASN	5.5
1	B	498	ALA	5.4
1	A	563	VAL	5.1
1	B	495	LYS	5.0
1	B	561	TYR	4.6
1	A	498	ALA	4.3
1	A	565	ARG	4.2
1	A	573	MET	4.1
1	A	492	LEU	3.9
1	A	464	ARG	3.9
1	B	283	LEU	3.8
1	A	470	VAL	3.8
1	B	568	ASN	3.8
1	B	246	HIS	3.4
1	A	471	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	466	VAL	3.3
1	A	469	SER	3.3
1	B	575	LEU	3.3
1	B	291	ASP	3.2
1	A	462	LEU	3.2
1	B	540	LYS	3.0
1	B	506[A]	LEU	2.9
1	B	467	ASN	2.9
1	B	503	ASP	2.8
1	B	286	GLY	2.8
1	A	571	PRO	2.8
1	B	504	GLU	2.8
1	A	493	LEU	2.8
1	A	465	GLU	2.7
1	B	466	VAL	2.7
1	A	568	ASN	2.6
1	B	287	GLU	2.6
1	B	245	TRP	2.5
1	A	130[A]	MET	2.5
1	A	507	GLY	2.5
1	B	352	LYS	2.5
1	B	464	ARG	2.5
1	A	463	LEU	2.4
1	A	504	GLU	2.4
1	B	502	SER	2.4
1	B	570	THR	2.3
1	A	544	PHE	2.3
1	A	564	PRO	2.2
1	B	284	VAL	2.2
1	B	550	TYR	2.2
1	B	280	LEU	2.2
1	B	546	GLU	2.2
1	A	459	ALA	2.2
1	A	491	GLU	2.2
1	B	579	ARG	2.1
1	B	250	HIS	2.1
1	B	493	LEU	2.1
1	B	562	LYS	2.1
1	B	293	TRP	2.1
1	B	465	GLU	2.1
1	A	461	LYS	2.0
1	B	181	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	541	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

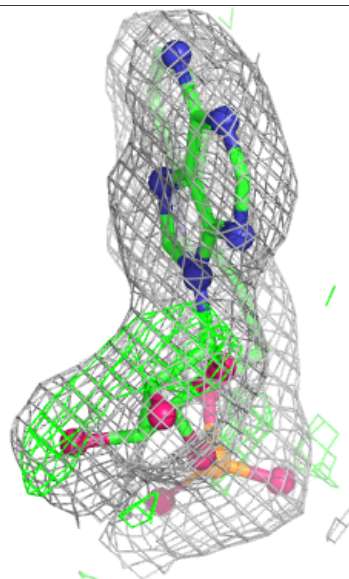
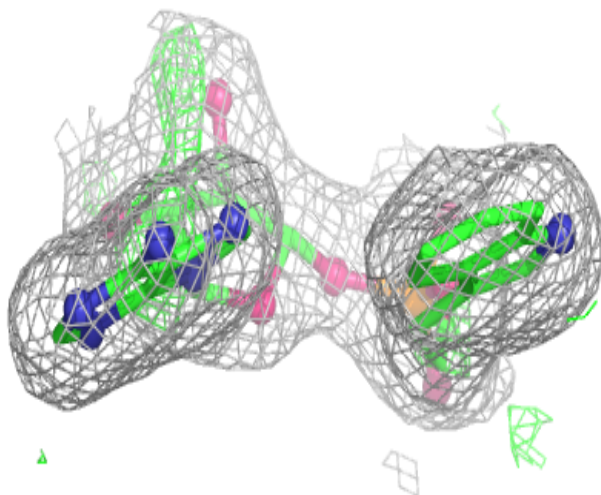
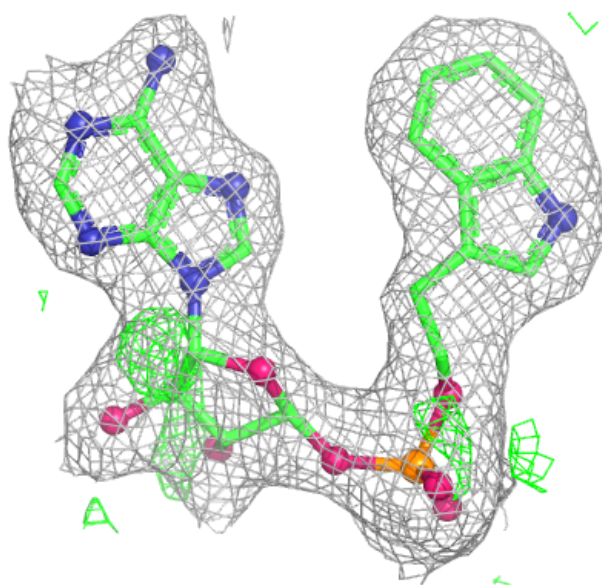
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MLI	B	1598	7/7	0.83	0.13	50,52,52,52	0
2	MLI	A	1598	7/7	0.93	0.08	39,41,43,45	0
2	MLI	B	1597	7/7	0.94	0.08	24,26,27,29	0
2	MLI	A	1599	7/7	0.94	0.07	26,27,30,32	0
3	V1N	A	1600	33/33	0.95	0.08	19,21,24,25	0
3	V1N	B	1600	33/33	0.96	0.07	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.

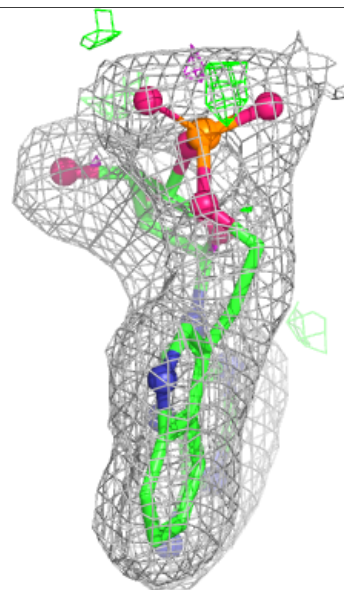
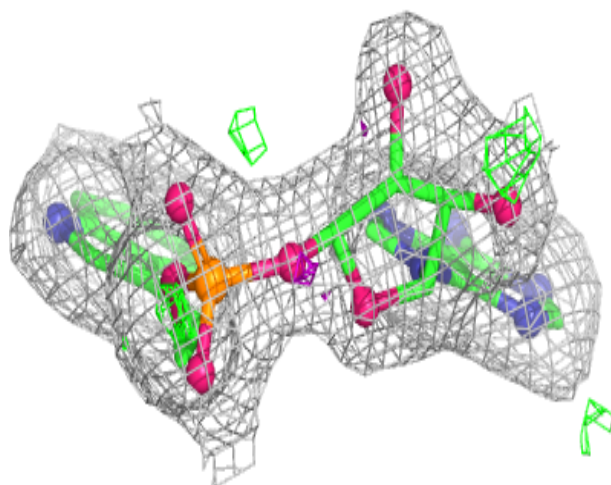
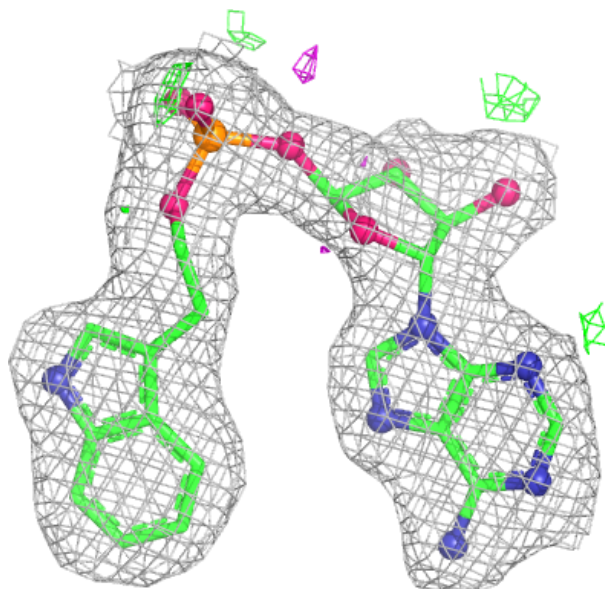
Electron density around V1N A 1600:

$2mF_o-DF_c$ (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:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.