



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:20 PM UTC

PDB ID : 3LP0 / pdb_00003lp0
Title : HIV-1 reverse transcriptase with inhibitor
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Deposited on : 2010-02-04
Resolution : 2.79 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

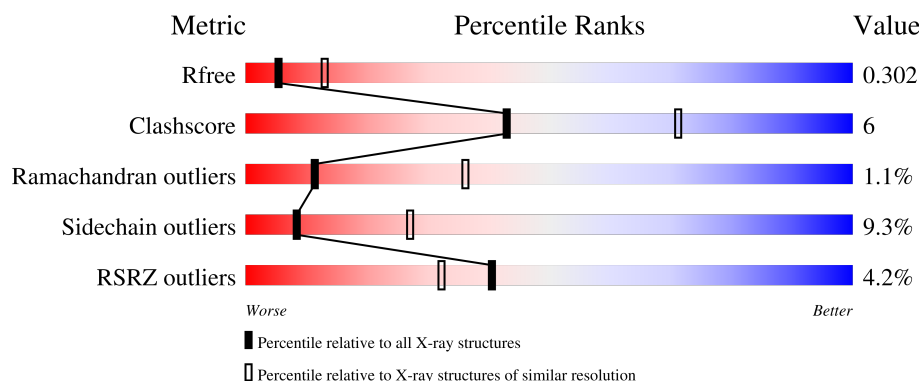
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	563	3% 75% 21% ..
2	B	443	6% 70% 17% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	LP7	A	601	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7913 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4510	2915	752	835	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP P04585
A	-1	ASN	-	expression tag	UNP P04585
A	0	SER	-	expression tag	UNP P04585

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total	C	N	O	S	0	0	0
			3311	2155	548	602	6			

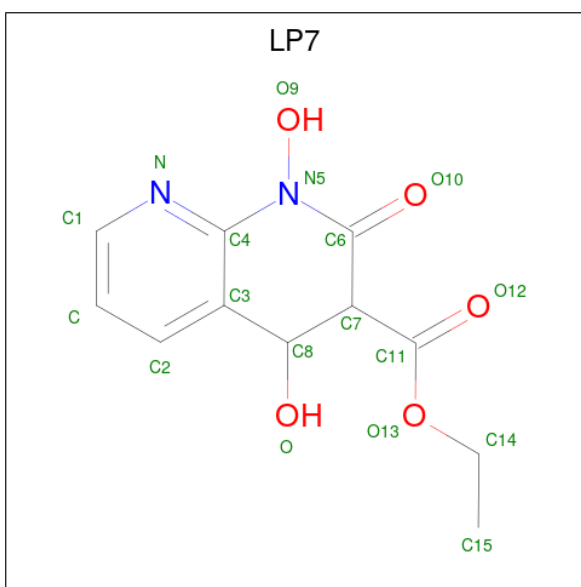
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP P04585
B	-1	ASN	-	expression tag	UNP P04585
B	0	SER	-	expression tag	UNP P04585

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

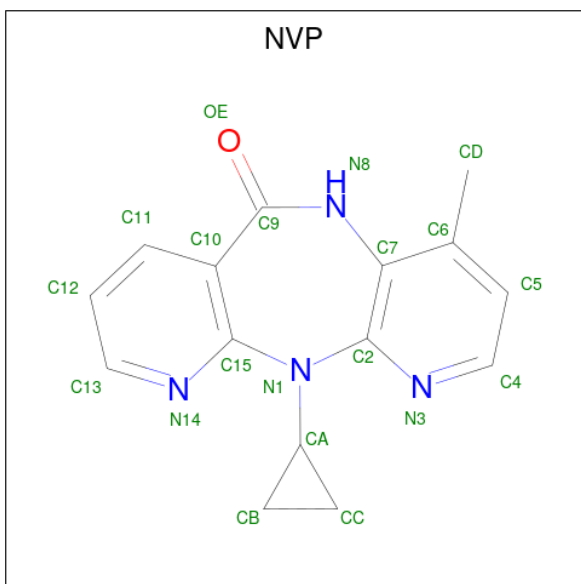
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is ethyl 1,4-dihydroxy-2-oxo-1,2-dihydro-1,8-naphthyridine-3-carboxylate (CCD ID: LP7) (formula: C₁₁H₁₂N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	11	2	5		

- Molecule 5 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (CCD ID: NVP) (formula: $C_{15}H_{14}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	15	4	1		

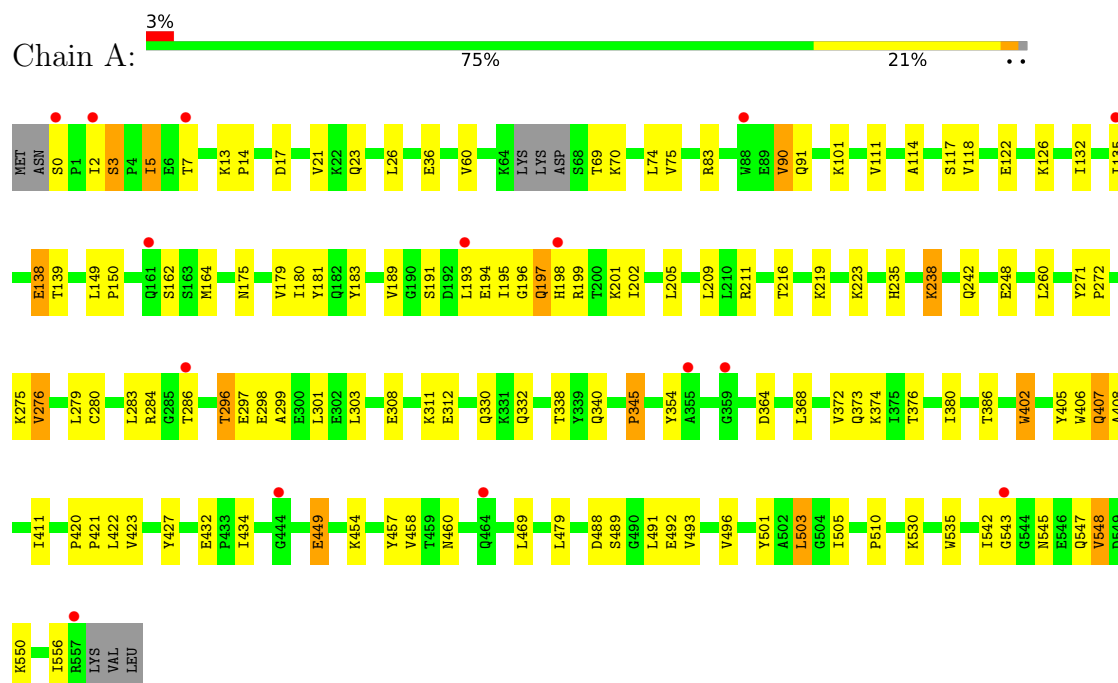
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total 31	O 31	0	0
6	B	21	Total 21	O 21	0	0

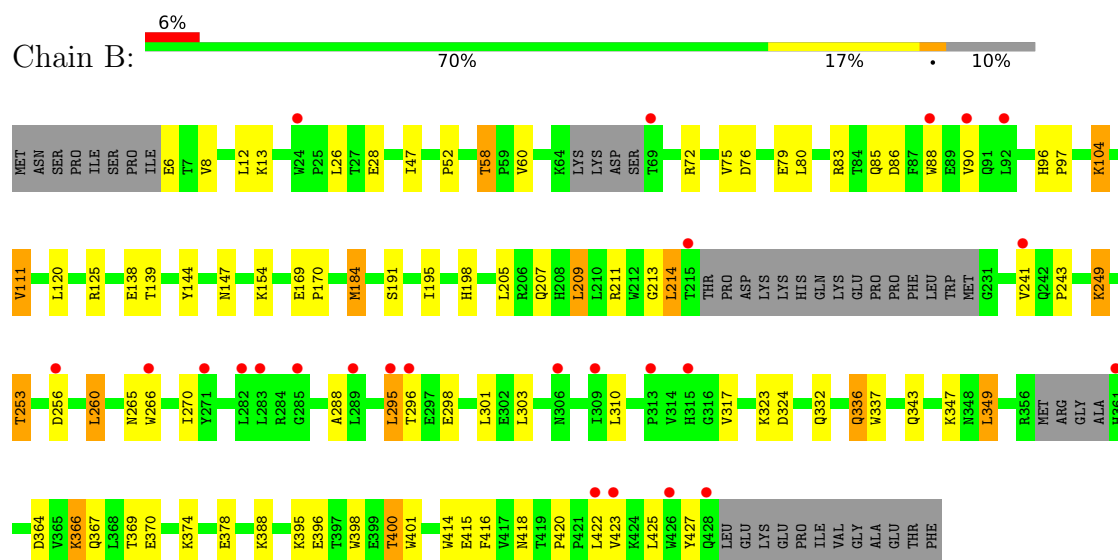
3 Residue-property plots

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: Reverse transcriptase/ribonuclease H



• Molecule 2: p51 RT



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.30Å 154.18Å 153.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.79 50.00 – 2.79	Depositor EDS
% Data completeness (in resolution range)	91.7 (50.00-2.79) 91.7 (50.00-2.79)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.248 , 0.310 0.244 , 0.302	Depositor DCC
R_{free} test set	1618 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7913	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: LP7, MN, NVP

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	0.48	0/4626	0.83	6/6288 (0.1%)
2	B	0.45	0/3404	0.80	2/4627 (0.0%)
All	All	0.47	0/8030	0.81	8/10915 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	LYS	CA-C-N	6.64	128.13	119.84
1	A	13	LYS	C-N-CA	6.64	128.13	119.84
1	A	0	SER	CA-C-N	5.60	125.60	119.89
1	A	0	SER	C-N-CA	5.60	125.60	119.89
1	A	242	GLN	CA-C-N	5.19	126.33	119.84
1	A	242	GLN	C-N-CA	5.19	126.33	119.84
2	B	195	ILE	N-CA-C	5.19	115.40	110.42
2	B	414	TRP	N-CA-C	5.14	117.19	109.23

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	4510	0	4547	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3311	0	3326	46	0
3	A	2	0	0	0	0
4	A	18	0	8	0	0
5	A	20	0	14	1	0
6	A	31	0	0	1	0
6	B	21	0	0	0	0
All	All	7913	0	7895	98	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 (98) 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)
2:B:209:LEU:HG	2:B:214:LEU:HD12	1.58	0.84
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.19	0.78
1:A:296:THR:HG22	1:A:299:ALA:H	1.53	0.74
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.38	0.72
1:A:283:LEU:O	1:A:286:THR:HB	1.91	0.69
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.28	0.69
2:B:396:GLU:O	2:B:400:THR:HG22	1.97	0.63
2:B:154:LYS:HG2	2:B:184:MET:CE	2.29	0.62
1:A:162:SER:HB2	2:B:52:PRO:HG3	1.81	0.62
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.48	0.61
2:B:213:GLY:C	2:B:214:LEU:HD23	2.26	0.60
2:B:154:LYS:HG2	2:B:184:MET:HE2	1.84	0.59
2:B:396:GLU:O	2:B:400:THR:CG2	2.50	0.59
1:A:308:GLU:HA	1:A:311:LYS:HE2	1.85	0.59
1:A:308:GLU:O	1:A:311:LYS:HB2	2.03	0.58
2:B:298:GLU:HA	2:B:301:LEU:HD12	1.85	0.58
1:A:492:GLU:HG3	1:A:530:LYS:HB2	1.86	0.57
1:A:235:HIS:HB2	1:A:238:LYS:HG2	1.87	0.57
2:B:111:VAL:HG22	2:B:214:LEU:HD13	1.86	0.57
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.86	0.56
1:A:3:SER:OG	1:A:5:ILE:HD11	2.06	0.55
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.21	0.55
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.42	0.54
1:A:2:ILE:HG22	1:A:2:ILE:O	2.09	0.53
2:B:60:VAL:HG23	2:B:75:VAL:HG22	1.91	0.52
2:B:266:TRP:HZ2	2:B:427:TYR:CZ	2.28	0.52
2:B:138:GLU:HG3	2:B:139:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:PRO:HA	1:A:421:PRO:C	2.35	0.51
2:B:295:LEU:H	2:B:295:LEU:HD23	1.76	0.50
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.47	0.50
1:A:191:SER:OG	1:A:198:HIS:HD2	1.94	0.49
1:A:175:ASN:HD21	1:A:201:LYS:NZ	2.09	0.49
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.95	0.49
1:A:503:LEU:HD12	1:A:535:TRP:HB2	1.94	0.49
2:B:241:VAL:O	2:B:243:PRO:HD3	2.13	0.49
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.94	0.49
2:B:366:LYS:O	2:B:370:GLU:HG3	2.13	0.48
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.48	0.48
2:B:317:VAL:HG12	2:B:349:LEU:HD13	1.96	0.48
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.76	0.48
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.95	0.47
1:A:194:GLU:C	1:A:196:GLY:H	2.22	0.47
2:B:104:LYS:O	2:B:104:LYS:HD2	2.15	0.47
1:A:179:VAL:HG13	5:A:701:NVP:HCC1	1.96	0.47
1:A:275:LYS:HE3	1:A:332:GLN:NE2	2.30	0.47
1:A:454:LYS:HG3	1:A:556:ILE:HG13	1.96	0.47
2:B:58:THR:HG23	2:B:76:ASP:O	2.14	0.47
1:A:376:THR:HG23	1:A:386:THR:HG22	1.96	0.47
2:B:79:GLU:O	2:B:83:ARG:HG3	2.15	0.47
1:A:199:ARG:HA	1:A:202:ILE:HD12	1.97	0.46
1:A:457:TYR:HA	1:A:548:VAL:HG11	1.98	0.46
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.49	0.46
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.98	0.46
1:A:17:ASP:O	1:A:83:ARG:NH1	2.48	0.45
2:B:388:LYS:HE2	2:B:415:GLU:HG3	1.98	0.45
1:A:298:GLU:HA	1:A:301:LEU:HD12	1.99	0.45
2:B:374:LYS:O	2:B:378:GLU:HG3	2.15	0.45
1:A:427:TYR:OH	1:A:510:PRO:HD2	2.17	0.45
2:B:332:GLN:HB2	2:B:336:GLN:HB3	1.98	0.45
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.99	0.44
1:A:175:ASN:HD21	1:A:201:LYS:HZ1	1.65	0.44
1:A:180:ILE:HG23	1:A:189:VAL:HG22	2.00	0.44
1:A:380:ILE:HD11	1:A:386:THR:HG23	1.99	0.44
1:A:458:VAL:HG13	1:A:548:VAL:HG13	2.00	0.43
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.52	0.43
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.53	0.43
1:A:542:ILE:HB	1:A:545:ASN:HB3	2.01	0.43
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.90	0.43
2:B:400:THR:HG1	2:B:401:TRP:CD1	2.37	0.43
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.84	0.43
2:B:96:HIS:HA	2:B:97:PRO:HD3	1.87	0.43
1:A:449:GLU:H	1:A:449:GLU:HG2	1.65	0.42
2:B:260:LEU:HD11	2:B:303:LEU:HD21	2.00	0.42
2:B:191:SER:OG	2:B:198:HIS:ND1	2.46	0.42
1:A:135:ILE:H	1:A:135:ILE:HD12	1.85	0.42
1:A:211:ARG:HG3	6:A:574:HOH:O	2.20	0.41
1:A:489:SER:OG	1:A:493:VAL:HG21	2.19	0.41
2:B:337:TRP:HE1	2:B:367:GLN:NE2	2.11	0.41
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.02	0.41
1:A:489:SER:HB2	1:A:493:VAL:CG2	2.50	0.41
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.55	0.41
2:B:323:LYS:O	2:B:343:GLN:NE2	2.45	0.41
1:A:3:SER:HB2	1:A:117:SER:O	2.21	0.41
2:B:324:ASP:O	2:B:343:GLN:HG2	2.20	0.41
1:A:90:VAL:O	1:A:91:GLN:HG2	2.20	0.41
1:A:197:GLN:NE2	1:A:197:GLN:H	2.18	0.41
1:A:458:VAL:HG22	1:A:548:VAL:HG13	2.01	0.41
2:B:253:THR:HG22	2:B:256:ASP:CG	2.46	0.41
1:A:406:TRP:CH2	1:A:407:GLN:HG3	2.55	0.41
1:A:460:ASN:HD22	2:B:288:ALA:HB2	1.86	0.40
2:B:125:ARG:HD3	2:B:147:ASN:HA	2.03	0.40
2:B:207:GLN:O	2:B:211:ARG:HD3	2.20	0.40
1:A:402:TRP:CD1	1:A:402:TRP:C	2.98	0.40
2:B:13:LYS:HE3	2:B:86:ASP:HB2	2.03	0.40
1:A:23:GLN:HE22	1:A:60:VAL:H	1.69	0.40
1:A:209:LEU:HD13	1:A:216:THR:HG21	2.04	0.40
2:B:249:LYS:HE2	2:B:249:LYS:HB3	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/563 (98%)	507 (92%)	35 (6%)	9 (2%)	7	27
2	B	392/443 (88%)	366 (93%)	25 (6%)	1 (0%)	36	66
All	All	943/1006 (94%)	873 (93%)	60 (6%)	10 (1%)	11	36

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	543	GLY
1	A	345	PRO
1	A	114	ALA
1	A	138	GLU
1	A	195	ILE
1	A	219	LYS
2	B	296	THR
1	A	14	PRO
1	A	276	VAL

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	493/503 (98%)	443 (90%)	50 (10%)	7	23
2	B	364/403 (90%)	334 (92%)	30 (8%)	10	33
All	All	857/906 (95%)	777 (91%)	80 (9%)	8	27

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	7	THR
1	A	21	VAL

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Mol	Chain	Res	Type
1	A	26	LEU
1	A	36	GLU
1	A	69	THR
1	A	70	LYS
1	A	74	LEU
1	A	90	VAL
1	A	101	LYS
1	A	118	VAL
1	A	122	GLU
1	A	126	LYS
1	A	132	ILE
1	A	138	GLU
1	A	139	THR
1	A	193	LEU
1	A	197	GLN
1	A	205	LEU
1	A	223	LYS
1	A	238	LYS
1	A	248	GLU
1	A	260	LEU
1	A	276	VAL
1	A	279	LEU
1	A	280	CYS
1	A	284	ARG
1	A	296	THR
1	A	297	GLU
1	A	303	LEU
1	A	312	GLU
1	A	338	THR
1	A	345	PRO
1	A	368	LEU
1	A	373	GLN
1	A	402	TRP
1	A	407	GLN
1	A	422	LEU
1	A	432	GLU
1	A	434	ILE
1	A	449	GLU
1	A	469	LEU
1	A	479	LEU
1	A	488	ASP
1	A	491	LEU

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Mol	Chain	Res	Type
1	A	496	VAL
1	A	503	LEU
1	A	547	GLN
1	A	548	VAL
1	A	550	LYS
2	B	6	GLU
2	B	8	VAL
2	B	12	LEU
2	B	26	LEU
2	B	28	GLU
2	B	58	THR
2	B	72	ARG
2	B	80	LEU
2	B	90	VAL
2	B	104	LYS
2	B	111	VAL
2	B	120	LEU
2	B	184	MET
2	B	205	LEU
2	B	209	LEU
2	B	214	LEU
2	B	249	LYS
2	B	253	THR
2	B	260	LEU
2	B	265	ASN
2	B	270	ILE
2	B	295	LEU
2	B	310	LEU
2	B	336	GLN
2	B	347	LYS
2	B	349	LEU
2	B	366	LYS
2	B	400	THR
2	B	422	LEU
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	136	ASN
1	A	147	ASN

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Mol	Chain	Res	Type
1	A	151	GLN
1	A	175	ASN
1	A	198	HIS
1	A	258	GLN
1	A	315	HIS
1	A	330	GLN
1	A	332	GLN
1	A	407	GLN
1	A	500	GLN
1	A	519	ASN
1	A	520	GLN
1	A	524	GLN
2	B	103	ASN
2	B	151	GLN
2	B	174	GLN
2	B	175	ASN
2	B	182	GLN
2	B	255	ASN
2	B	265	ASN
2	B	306	ASN
2	B	367	GLN
2	B	373	GLN
2	B	394	GLN
2	B	428	GLN

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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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
4	LP7	A	601	3	18,19,19	4.04	5 (27%)	18,27,27	2.36	4 (22%)
5	NVP	A	701	-	23,23,23	2.38	7 (30%)	34,34,34	2.11	8 (23%)

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
4	LP7	A	601	3	2/2/5/5	4/7/27/27	0/2/2/2
5	NVP	A	701	-	-	0/4/6/6	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	LP7	C7-C8	-11.83	1.40	1.54
4	A	601	LP7	C3-C8	-8.39	1.40	1.51
5	A	701	NVP	C10-C9	-6.50	1.41	1.49
4	A	601	LP7	O10-C6	6.33	1.33	1.22
4	A	601	LP7	O-C8	-4.81	1.33	1.42
5	A	701	NVP	C7-N8	-4.57	1.36	1.42
5	A	701	NVP	C2-N1	-4.40	1.37	1.42
5	A	701	NVP	C15-N1	-4.23	1.37	1.42
4	A	601	LP7	C7-C6	-3.47	1.40	1.51
5	A	701	NVP	CB-CA	2.26	1.53	1.48
5	A	701	NVP	C15-N14	2.21	1.38	1.34
5	A	701	NVP	CC-CA	2.07	1.53	1.48

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	LP7	C6-C7-C11	6.57	121.13	108.88
5	A	701	NVP	C7-N8-C9	6.40	133.57	128.29
5	A	701	NVP	C7-C2-N1	-5.46	118.05	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	NVP	N3-C2-N1	5.11	120.53	116.67
4	A	601	LP7	O-C8-C7	4.90	121.55	110.81
4	A	601	LP7	O-C8-C3	3.73	117.54	110.42
5	A	701	NVP	C15-N1-C2	3.49	119.13	115.29
5	A	701	NVP	CB-CA-N1	2.79	117.74	116.09
4	A	601	LP7	C4-N5-C6	2.66	126.42	121.57
5	A	701	NVP	OE-C9-N8	-2.57	117.87	120.38
5	A	701	NVP	C2-C7-N8	-2.42	119.18	121.46
5	A	701	NVP	C10-C9-N8	2.21	122.38	120.22

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	601	LP7	C7
4	A	601	LP7	C8

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	LP7	O12-C11-C7-C6
4	A	601	LP7	O13-C11-C7-C6
4	A	601	LP7	C7-C11-O13-C14
4	A	601	LP7	O12-C11-O13-C14

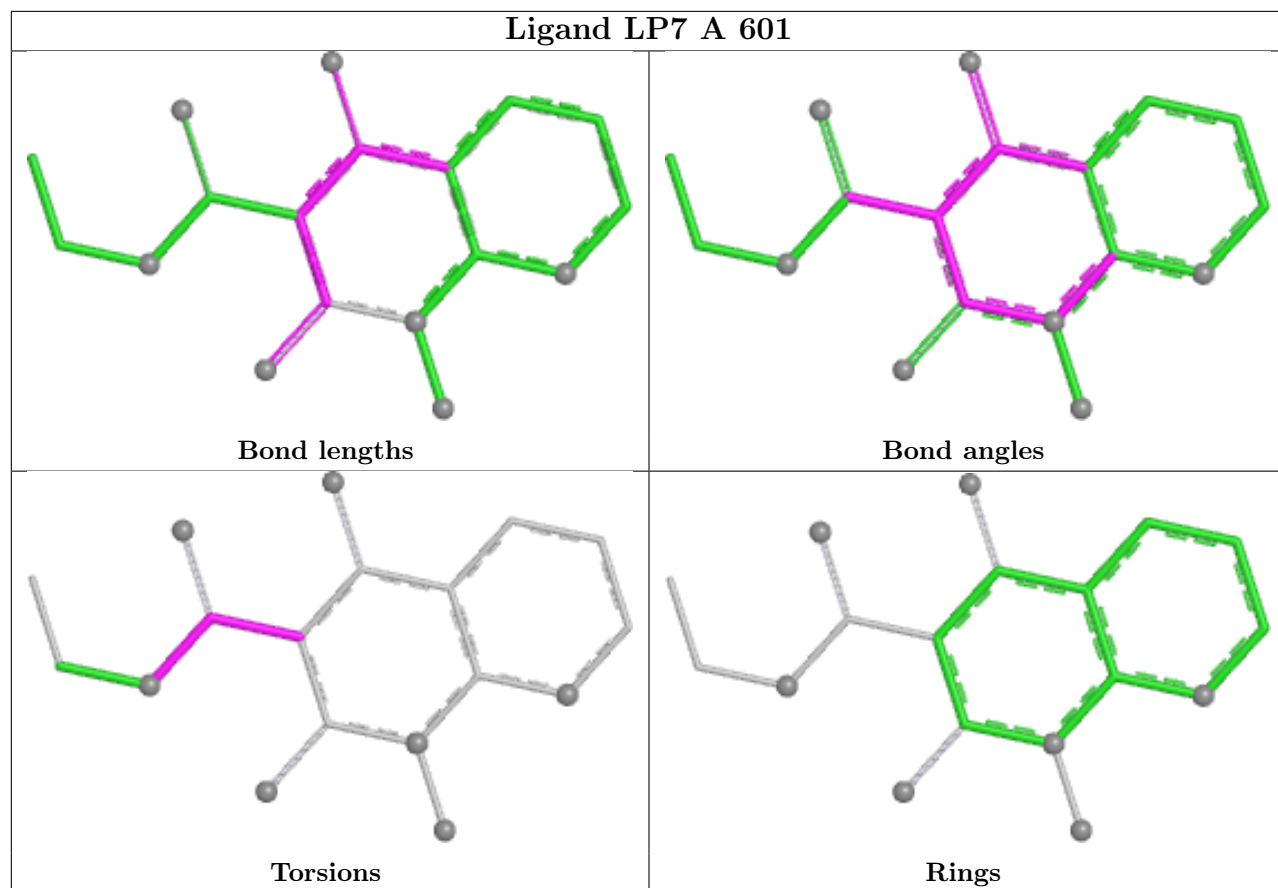
There are no ring outliers.

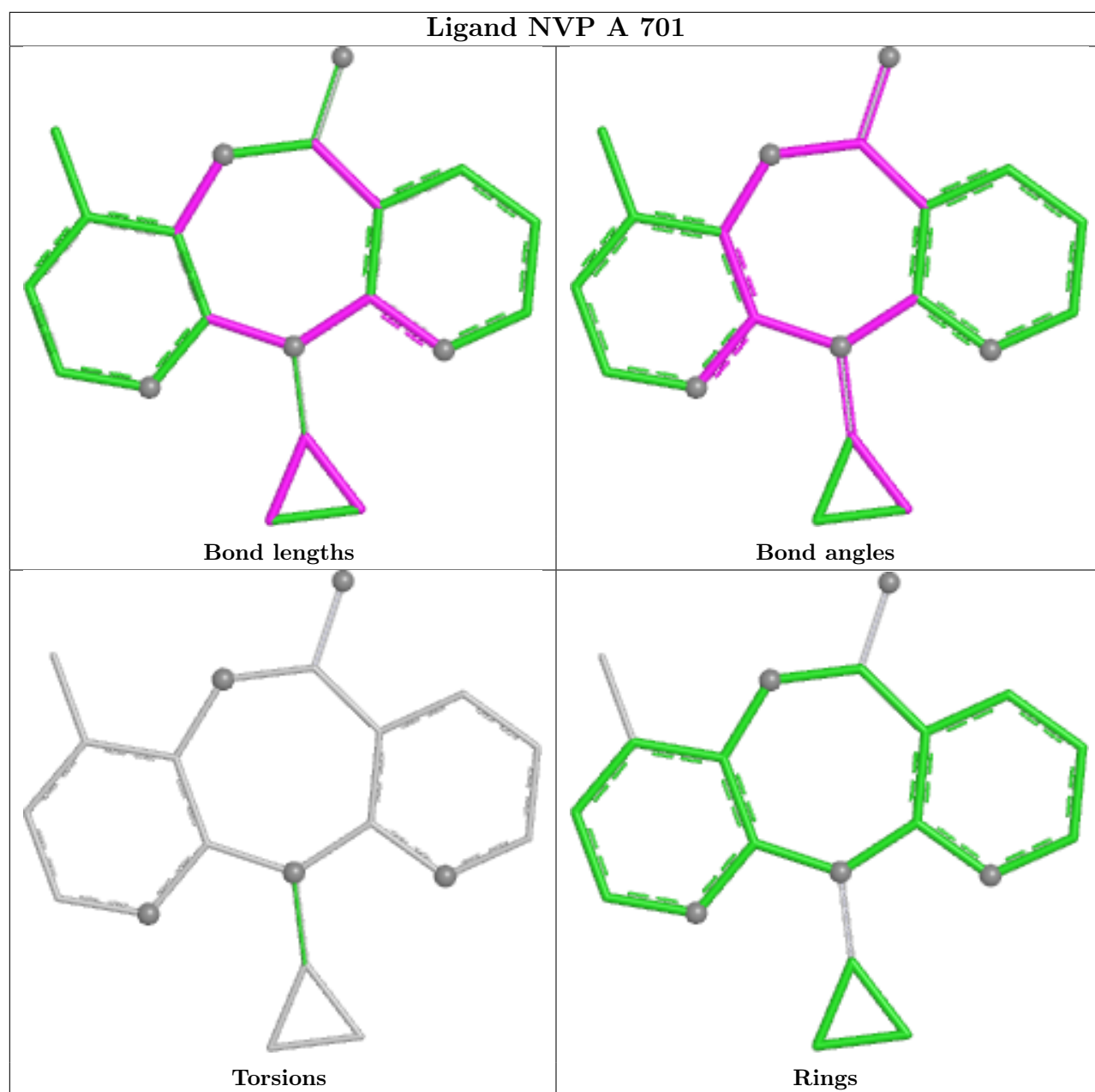
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	NVP	1	0

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

Ligand LP7 A 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	555/563 (98%)	0.42	15 (2%) 56 46	53, 74, 89, 98	0
2	B	400/443 (90%)	0.46	25 (6%) 26 19	56, 72, 118, 122	0
All	All	955/1006 (94%)	0.44	40 (4%) 40 32	53, 74, 109, 122	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	SER	3.7
2	B	313	PRO	3.6
2	B	295	LEU	3.6
2	B	215	THR	3.5
2	B	266	TRP	3.2
1	A	7	THR	3.1
2	B	422	LEU	3.0
2	B	426	TRP	3.0
2	B	90	VAL	2.9
2	B	92	LEU	2.8
1	A	557	ARG	2.8
1	A	198	HIS	2.7
1	A	286	THR	2.7
2	B	69	THR	2.6
2	B	24	TRP	2.5
1	A	161	GLN	2.5
2	B	88	TRP	2.5
1	A	359	GLY	2.4
2	B	309	ILE	2.4
2	B	256	ASP	2.4
1	A	355	ALA	2.4
2	B	289	LEU	2.3
2	B	361	HIS	2.3
2	B	428	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	444	GLY	2.2
2	B	285	GLY	2.2
2	B	283	LEU	2.2
1	A	88	TRP	2.2
1	A	2	ILE	2.2
2	B	296	THR	2.2
1	A	543	GLY	2.2
2	B	282	LEU	2.2
2	B	241	VAL	2.1
2	B	315	HIS	2.1
1	A	464	GLN	2.1
1	A	135	ILE	2.1
2	B	423	VAL	2.1
2	B	306	ASN	2.0
1	A	193	LEU	2.0
2	B	271	TYR	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.

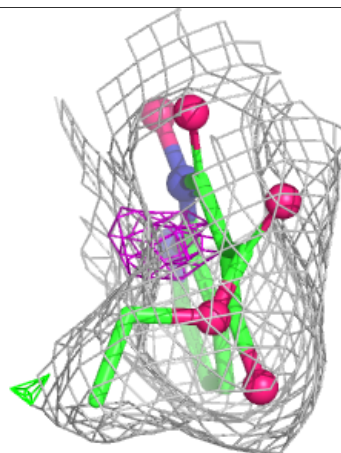
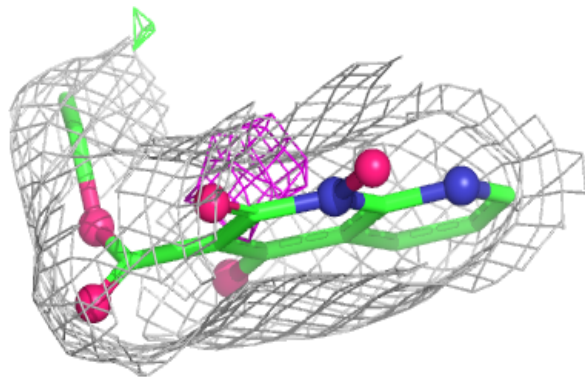
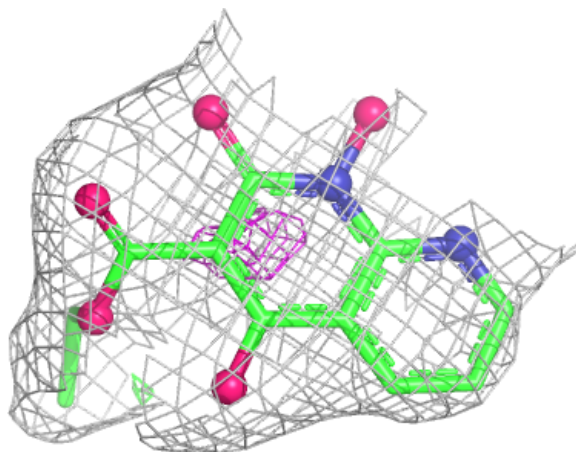
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	LP7	A	601	18/18	0.84	0.10	86,86,87,87	0
5	NVP	A	701	20/20	0.92	0.10	54,57,58,58	0
3	MN	A	602	1/1	0.99	0.07	77,77,77,77	0
3	MN	A	603	1/1	0.99	0.02	66,66,66,66	0

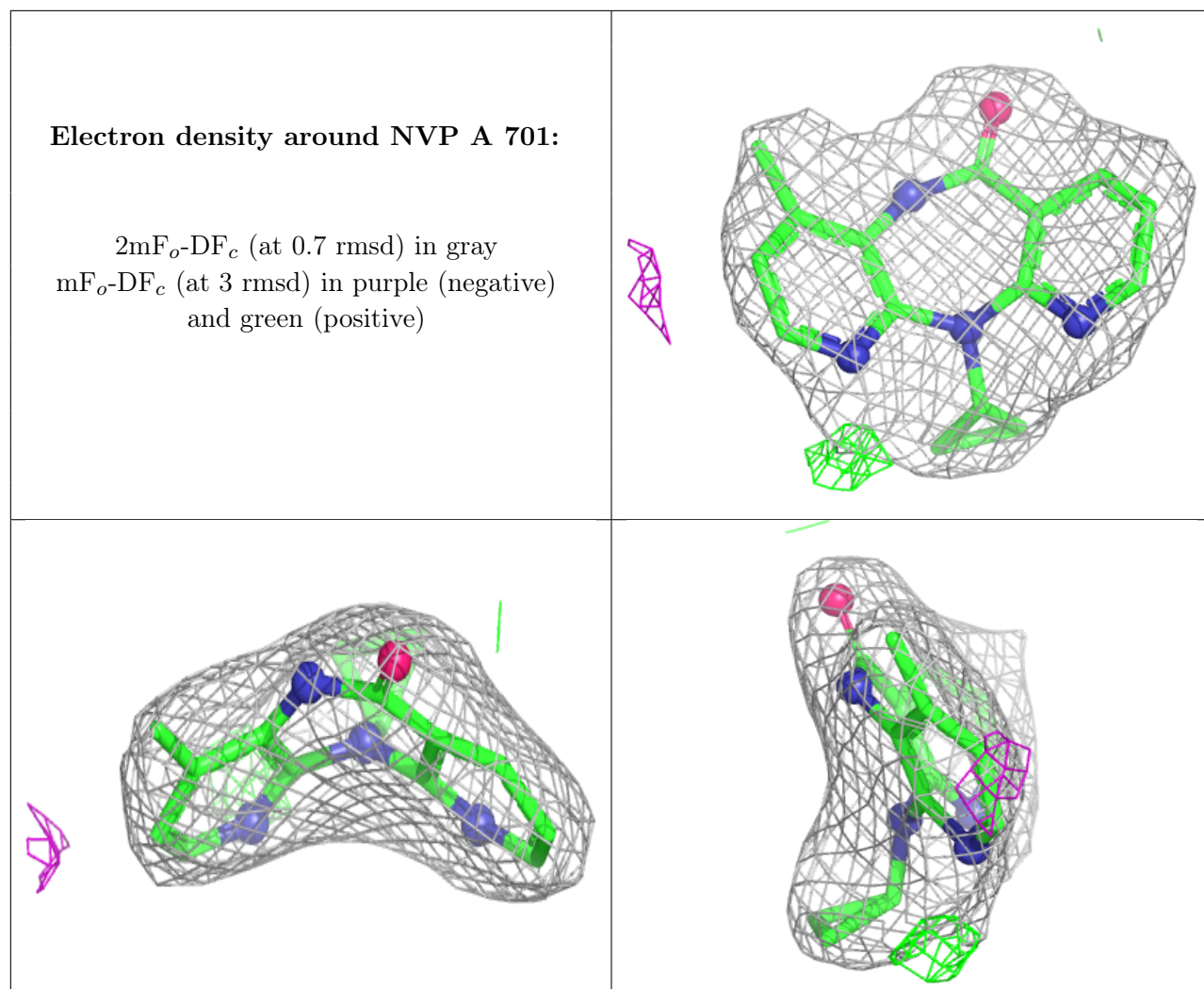
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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 LP7 A 601:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.