



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:48 pm BST

PDB ID : 3LP0
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

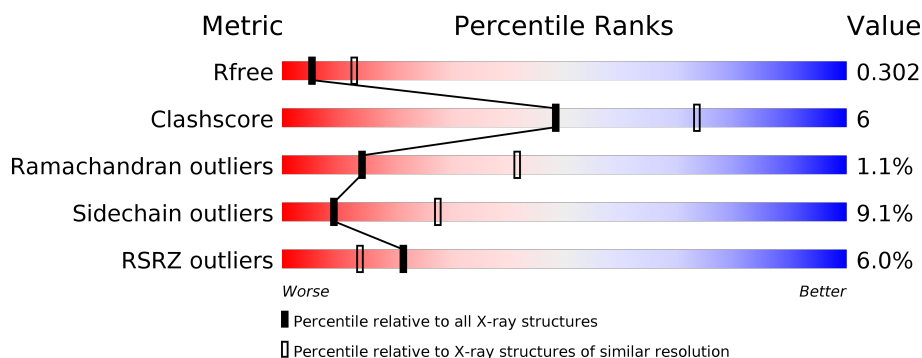
1 Overall quality at a glance ⓘ

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on 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	<div> <div>4%</div> <div>76%</div> <div>20%</div> <div>••</div> </div>
2	B	443	<div> <div>8%</div> <div>71%</div> <div>17%</div> <div>• 10%</div> </div>

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			

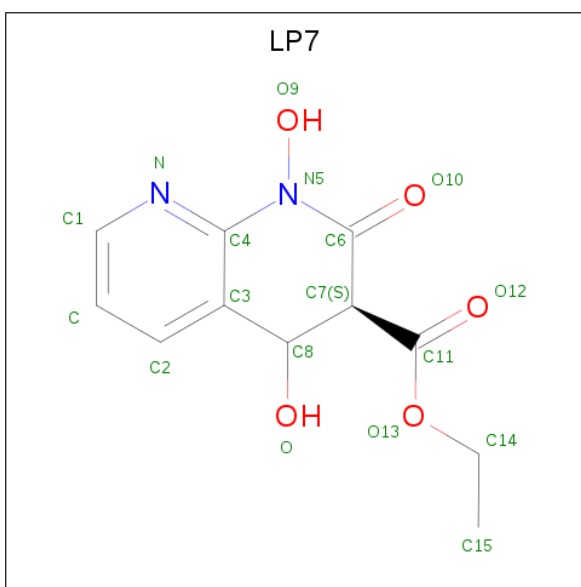
There are 3 discrepancies between the modelled and reference sequences:

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 (three-letter code: MN) (formula: Mn).

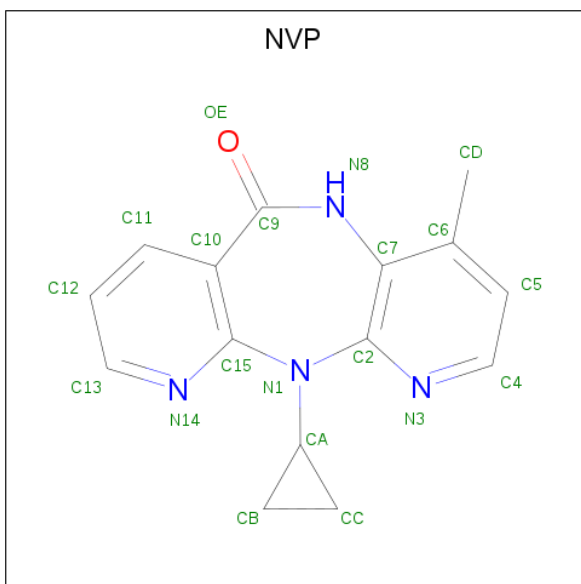
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is ethyl 1,4-dihydroxy-2-oxo-1,2-dihydro-1,8-naphthyridine-3-carboxylate (three-letter code: 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 (three-letter code: NVP) (formula: C₁₅H₁₄N₄O).



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

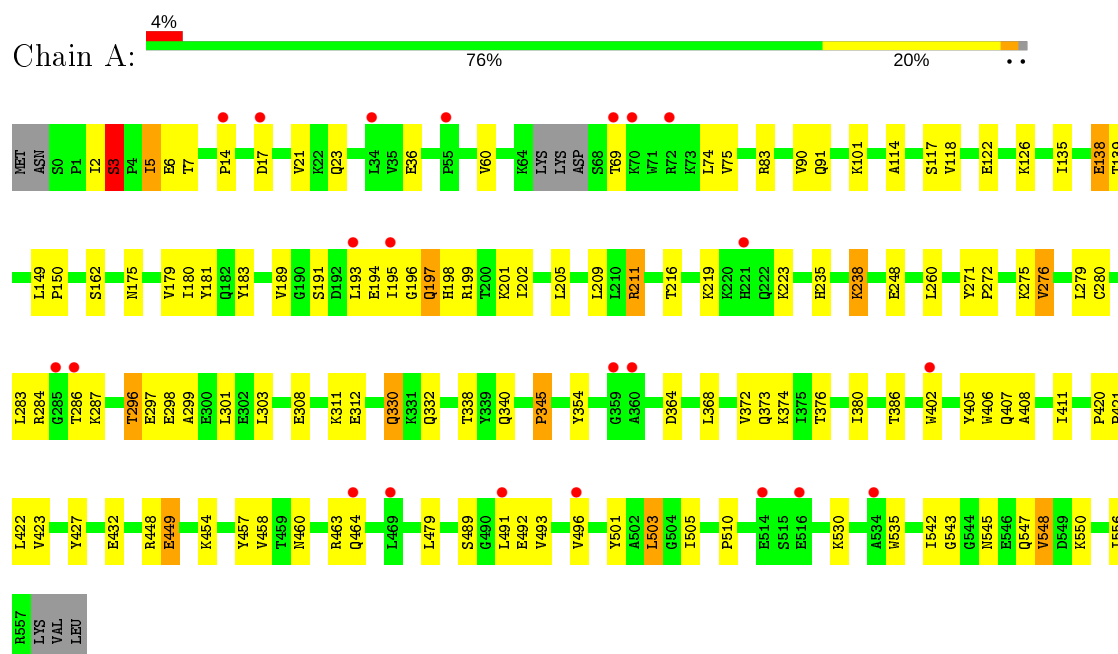
- Molecule 6 is water.

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

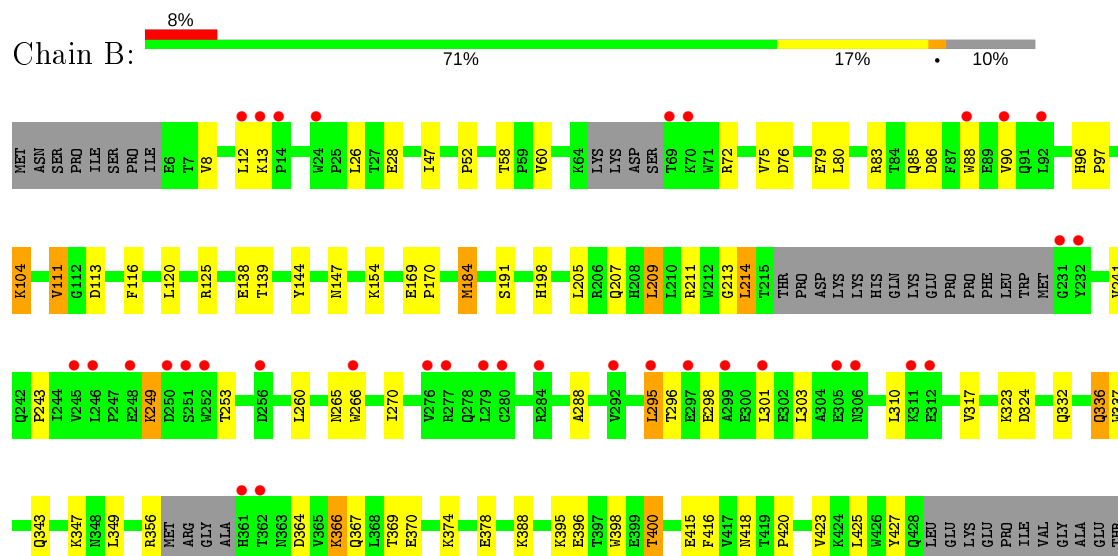
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



PHE

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 34.63 – 2.79	Depositor EDS
% Data completeness (in resolution range)	91.7 (50.00-2.79) 91.7 (34.63-2.79)	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 (5.02%)	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 , 39.0	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

5.1 Standard geometry

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	0.36	0/4626	0.54	0/6288
2	B	0.35	0/3404	0.52	0/4627
All	All	0.36	0/8030	0.53	0/10915

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

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	55	0
2	B	3311	0	3326	44	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	94	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 (94) 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: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
2:B:213:GLY:C	2:B:214:LEU:HD23	2.26	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:266:TRP:HZ2	2:B:427:TYR:CZ	2.28	0.52
2:B:60:VAL:HG23	2:B:75:VAL:HG22	1.91	0.52
2:B:138:GLU:HG3	2:B:139:THR:HG23	1.92	0.52
2:B:154:LYS:HG2	2:B:184:MET:HE2	1.93	0.50
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:503:LEU:HD12	1:A:535:TRP:HB2	1.94	0.49
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:LYS:HD2	2:B:104:LYS:O	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
2:B:58:THR:HG23	2:B:76:ASP:O	2.14	0.47
1:A:454:LYS:HG3	1:A:556:ILE:HG13	1.96	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:420:PRO:HA	1:A:421:PRO:C	2.35	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: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
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.90	0.43
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.84	0.43
1:A:194:GLU:C	1:A:196:GLY:H	2.22	0.43
2:B:96:HIS:HA	2:B:97:PRO:HD3	1.87	0.43
1:A:449:GLU:HG2	1:A:449:GLU:H	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:HD12	1:A:135:ILE:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:197:GLN:H	1:A:197:GLN:NE2	2.18	0.41
1:A:458:VAL:HG22	1:A:548:VAL:HG13	2.01	0.41
1:A:90:VAL:O	1:A:91:GLN:HG2	2.20	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
2:B:13:LYS:HE3	2:B:86:ASP:HB2	2.03	0.40
1:A:209:LEU:HD13	1:A:216:THR:HG21	2.04	0.40
1:A:23:GLN:HE22	1:A:60:VAL:H	1.69	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 [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	551/563 (98%)	507 (92%)	35 (6%)	9 (2%)	9	31
2	B	392/443 (88%)	366 (93%)	25 (6%)	1 (0%)	41	72
All	All	943/1006 (94%)	873 (93%)	60 (6%)	10 (1%)	14	41

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

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Mol	Chain	Res	Type
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	22
2	B	364/403 (90%)	336 (92%)	28 (8%)	13	35
All	All	857/906 (95%)	779 (91%)	78 (9%)	9	27

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	21	VAL
1	A	36	GLU
1	A	69	THR
1	A	74	LEU
1	A	101	LYS
1	A	118	VAL
1	A	122	GLU
1	A	126	LYS
1	A	138	GLU
1	A	139	THR
1	A	193	LEU
1	A	197	GLN
1	A	205	LEU
1	A	211	ARG

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Mol	Chain	Res	Type
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	287	LYS
1	A	296	THR
1	A	297	GLU
1	A	303	LEU
1	A	312	GLU
1	A	330	GLN
1	A	338	THR
1	A	345	PRO
1	A	368	LEU
1	A	373	GLN
1	A	402	TRP
1	A	422	LEU
1	A	432	GLU
1	A	448	ARG
1	A	449	GLU
1	A	463	ARG
1	A	464	GLN
1	A	479	LEU
1	A	491	LEU
1	A	496	VAL
1	A	503	LEU
1	A	547	GLN
1	A	548	VAL
1	A	550	LYS
2	B	8	VAL
2	B	12	LEU
2	B	26	LEU
2	B	28	GLU
2	B	72	ARG
2	B	80	LEU
2	B	90	VAL
2	B	104	LYS
2	B	111	VAL
2	B	113	ASP

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Mol	Chain	Res	Type
2	B	116	PHE
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	265	ASN
2	B	270	ILE
2	B	295	LEU
2	B	310	LEU
2	B	336	GLN
2	B	347	LYS
2	B	356	ARG
2	B	366	LYS
2	B	400	THR
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	136	ASN
1	A	147	ASN
1	A	175	ASN
1	A	198	HIS
1	A	258	GLN
1	A	330	GLN
1	A	336	GLN
1	A	407	GLN
1	A	519	ASN
1	A	520	GLN
1	A	524	GLN
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	175	ASN
2	B	182	GLN
2	B	208	HIS
2	B	258	GLN
2	B	265	ASN

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Mol	Chain	Res	Type
2	B	306	ASN
2	B	336	GLN
2	B	367	GLN
2	B	373	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	NVP	A	701	-	15,23,23	1.58	4 (26%)	13,34,34	1.15	1 (7%)
4	LP7	A	601	3	17,19,19	3.98	5 (29%)	16,27,27	2.01	2 (12%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	LP7	C7-C8	-11.34	1.40	1.54
4	A	601	LP7	C3-C8	-7.75	1.40	1.51
4	A	601	LP7	O10-C6	6.35	1.33	1.22
4	A	601	LP7	O-C8	-4.68	1.33	1.42
4	A	601	LP7	C7-C6	-3.28	1.40	1.50
5	A	701	NVP	C13-N14	2.61	1.37	1.32
5	A	701	NVP	C7-C2	2.60	1.41	1.38
5	A	701	NVP	C4-N3	2.42	1.37	1.32
5	A	701	NVP	C15-N14	2.11	1.38	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	LP7	C6-C7-C11	6.69	121.13	108.68
4	A	601	LP7	O-C8-C3	3.58	117.54	110.49
5	A	701	NVP	C10-C15-N14	-2.24	121.17	124.62

All (2) chirality outliers are listed below:

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

All (4) torsion outliers are listed below:

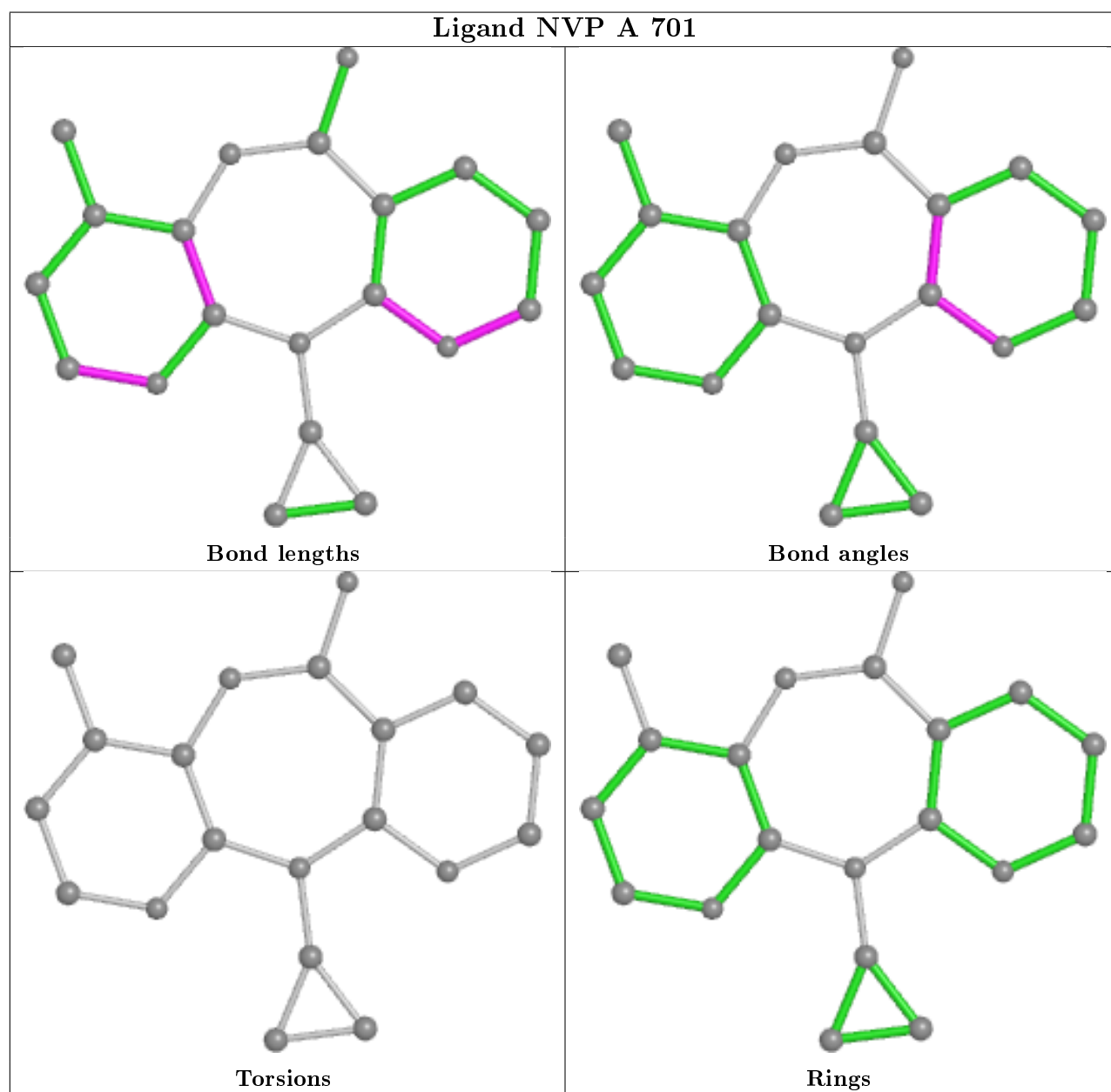
Mol	Chain	Res	Type	Atoms
4	A	601	LP7	O12-C11-C7-C6
4	A	601	LP7	O13-C11-C7-C6
4	A	601	LP7	C7-C11-O13-C14
4	A	601	LP7	O12-C11-O13-C14

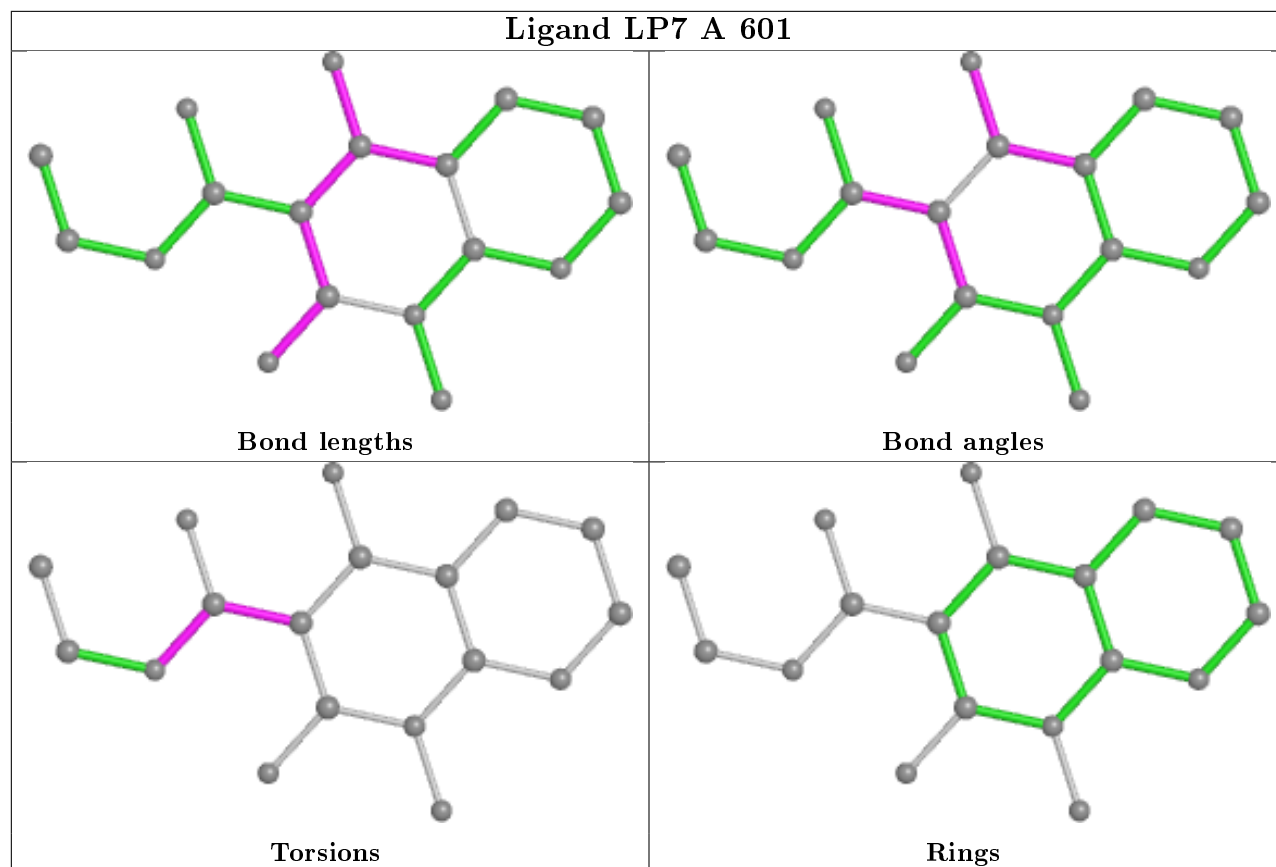
There are no ring outliers.

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.





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%)	0.33	22 (3%)	38 28	53, 74, 89, 98	0
2	B	400/443 (90%)	0.61	35 (8%)	10 5	56, 72, 118, 122	0
All	All	955/1006 (94%)	0.45	57 (5%)	21 14	53, 74, 109, 122	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	90	VAL	6.7
2	B	361	HIS	5.9
1	A	193	LEU	4.2
1	A	69	THR	4.0
2	B	305	GLU	3.8
2	B	266	TRP	3.8
2	B	295	LEU	3.6
2	B	14	PRO	3.5
2	B	292	VAL	3.5
1	A	359	GLY	3.4
2	B	252	TRP	3.4
2	B	301	LEU	3.4
2	B	299	ALA	3.3
2	B	70	LYS	3.3
2	B	13	LYS	3.3
1	A	514	GLU	3.3
2	B	12	LEU	3.3
2	B	251	SER	3.2
2	B	276	VAL	3.1
2	B	362	THR	3.1
2	B	231	GLY	3.1
2	B	92	LEU	3.0
2	B	69	THR	3.0
1	A	469	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	311	LYS	2.9
2	B	277	ARG	2.9
1	A	221	HIS	2.9
2	B	250	ASP	2.8
2	B	245	VAL	2.8
2	B	232	TYR	2.7
2	B	312	GLU	2.7
1	A	34	LEU	2.7
1	A	402	TRP	2.6
1	A	285	GLY	2.5
1	A	516	GLU	2.5
1	A	286	THR	2.5
1	A	534	ALA	2.5
2	B	246	LEU	2.5
2	B	24	TRP	2.4
1	A	491	LEU	2.3
2	B	297	GLU	2.3
2	B	256	ASP	2.3
2	B	248	GLU	2.3
1	A	55	PRO	2.2
1	A	496	VAL	2.2
1	A	360	ALA	2.1
1	A	70	LYS	2.1
2	B	280	CYS	2.1
2	B	279	LEU	2.1
1	A	195	ILE	2.1
1	A	14	PRO	2.1
1	A	464	GLN	2.1
2	B	284	ARG	2.1
2	B	306	ASN	2.1
1	A	17	ASP	2.1
1	A	72	ARG	2.0
2	B	88	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

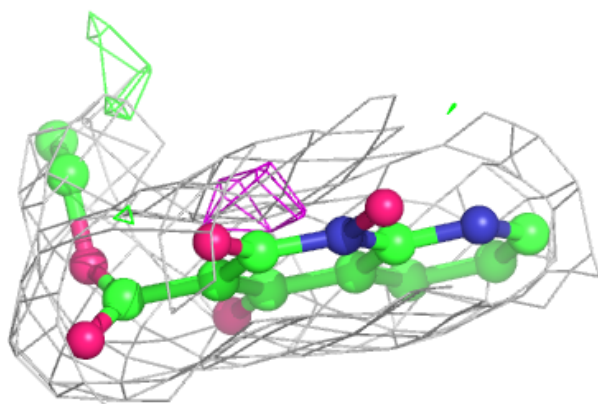
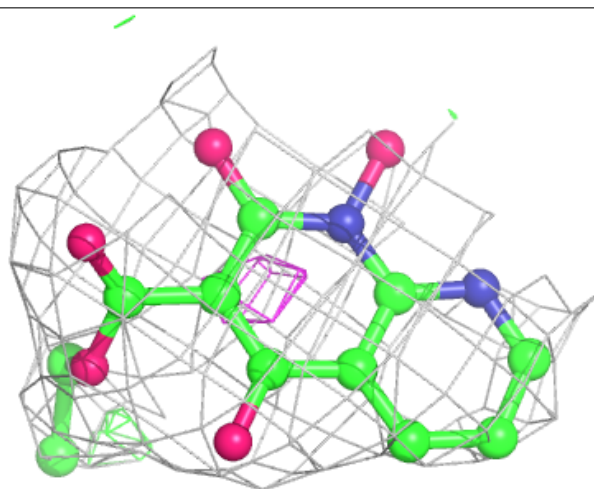
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LP7	A	601	18/18	0.91	0.16	86,86,87,87	0
5	NVP	A	701	20/20	0.95	0.18	54,57,58,58	0
3	MN	A	602	1/1	0.97	0.20	77,77,77,77	0
3	MN	A	603	1/1	0.98	0.16	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.

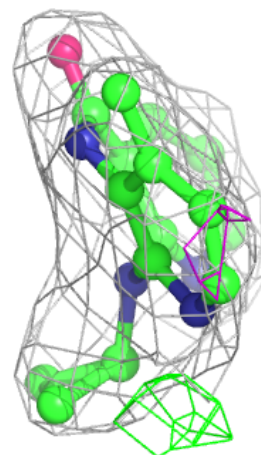
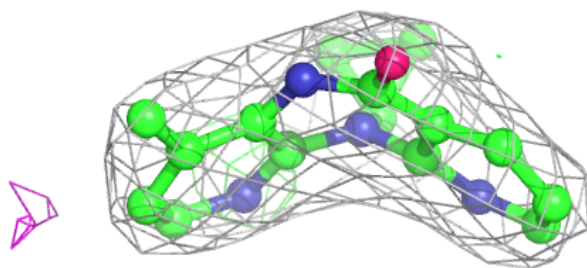
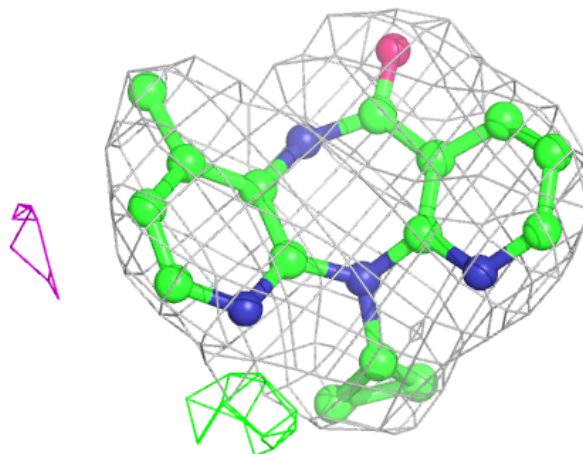
Electron density around LP7 A 601:

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



Electron density around NVP A 701:

$2mF_o-DF_c$ (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.