



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:34 PM UTC

PDB ID : 3LP1 / pdb_00003lp1
Title : HIV-1 reverse transcriptase with inhibitor
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Deposited on : 2010-02-04
Resolution : 2.23 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

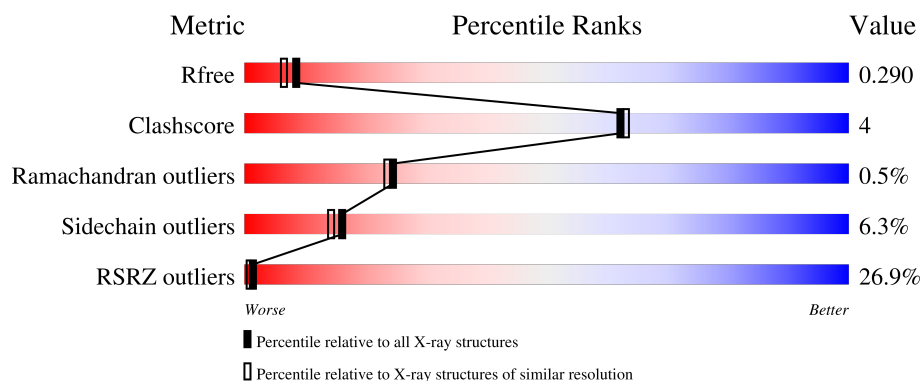
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	23% 83% 14% ..
2	B	443	29% 77% 12% • 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8029 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	554	Total	C	N	O	S	0	0	0
			4503	2911	751	833	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

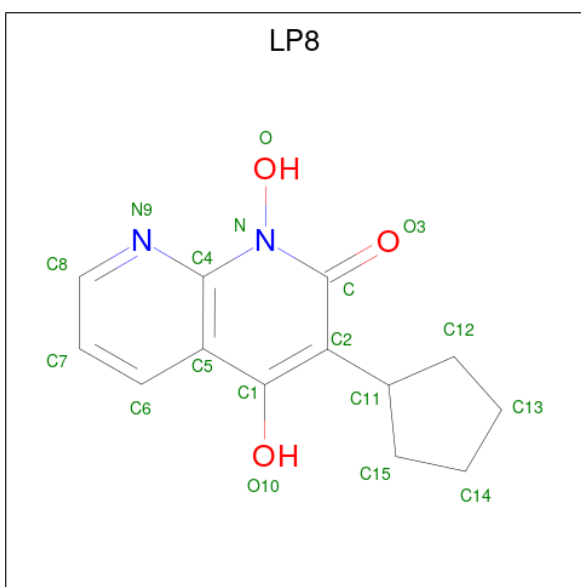
- Molecule 2 is a protein called p51 RT.

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 3-cyclopentyl-1,4-dihydroxy-1,8-naphthyridin-2(1H)-one (CCD ID: LP8) (formula: C₁₃H₁₄N₂O₃).

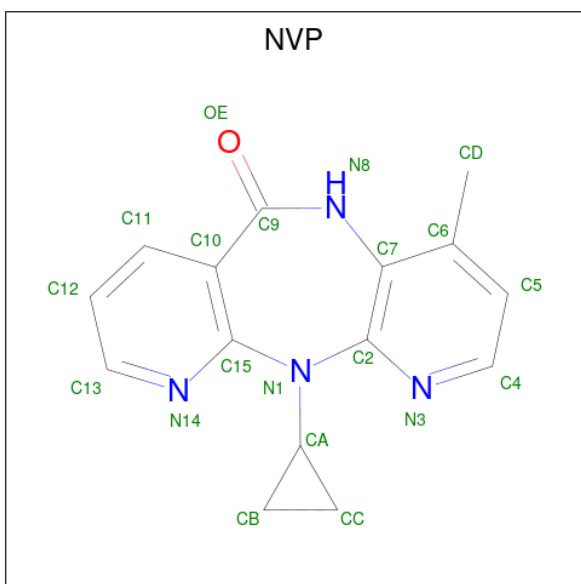


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	13	2	3		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- 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: C₁₅H₁₄N₄O).



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

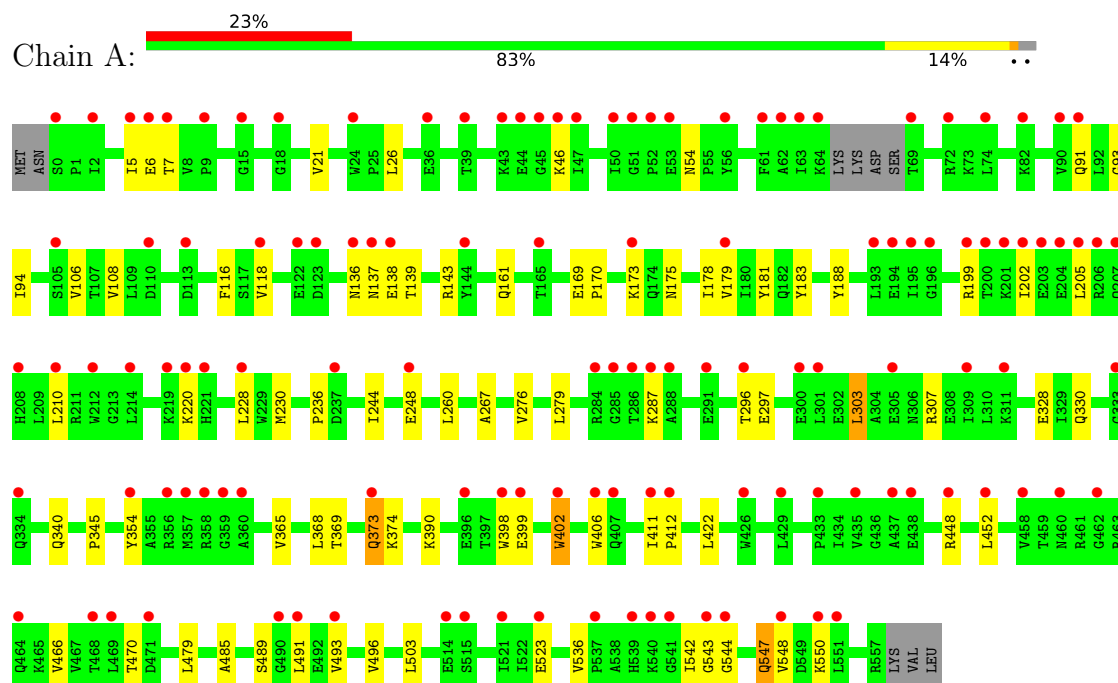
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	108	Total	O	0	0
			108	108		
6	B	67	Total	O	0	0
			67	67		

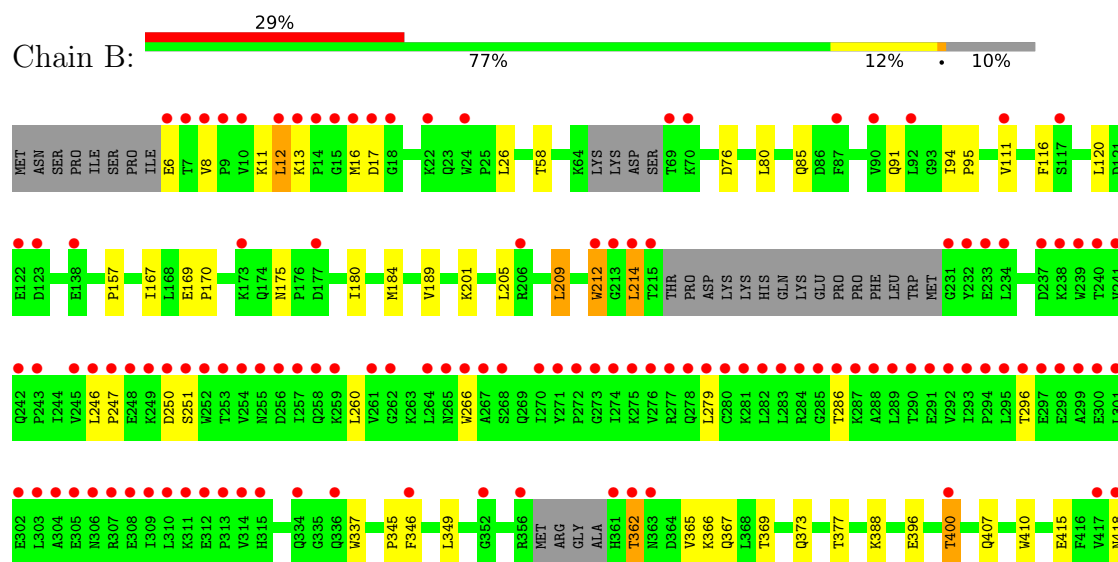
3 Residue-property plots

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



T419	T420	T421	L422	V423	K424	L425	K426	Y427	Q428	LEU	GLU	LYS	GLU	PRO	ILE	VAL	GLY	ALA	GLU	THR	PHE
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.78Å 155.26Å 155.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.23 50.00 – 2.23	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.23) 96.4 (50.00-2.23)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.22Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.268 , 0.292 0.265 , 0.290	Depositor DCC
R_{free} test set	3410 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8029	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: MN, NVP, LP8

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	0.44	0/4619	0.78	0/6279
2	B	0.43	0/3404	0.77	0/4627
All	All	0.44	0/8023	0.78	0/10906

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	4503	0	4540	38	0
2	B	3311	0	3326	29	0
3	A	18	0	12	0	0
4	A	2	0	0	0	0
5	A	20	0	14	1	0
6	A	108	0	0	2	0
6	B	67	0	0	0	0
All	All	8029	0	7892	65	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 4.

All (65) 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:330:GLN:HE22	1:A:340:GLN:HE22	1.28	0.80
2:B:396:GLU:O	2:B:400:THR:HG22	1.84	0.78
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.32	0.75
2:B:12:LEU:HD23	2:B:17:ASP:HA	1.78	0.65
1:A:91:GLN:HG3	1:A:93:GLY:O	1.97	0.65
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.78	0.64
2:B:373:GLN:O	2:B:377:THR:HG23	1.98	0.64
2:B:266:TRP:HH2	2:B:427:TYR:CZ	2.16	0.62
1:A:369:THR:CG2	1:A:398:TRP:HZ3	2.12	0.62
2:B:214:LEU:HD23	2:B:214:LEU:H	1.67	0.60
1:A:199:ARG:HA	1:A:202:ILE:HD12	1.84	0.58
1:A:373:GLN:HG3	6:A:562:HOH:O	2.04	0.57
2:B:388:LYS:HE2	2:B:415:GLU:HG3	1.86	0.57
1:A:91:GLN:HG3	1:A:93:GLY:H	1.69	0.56
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.40	0.56
1:A:46:LYS:HE3	1:A:116:PHE:HB3	1.87	0.56
1:A:365:VAL:O	1:A:369:THR:HG23	2.06	0.55
1:A:94:ILE:HD13	1:A:230:MET:HG2	1.90	0.54
1:A:369:THR:HG22	1:A:398:TRP:HZ3	1.72	0.54
2:B:209:LEU:HG	2:B:214:LEU:HD12	1.89	0.53
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.43	0.53
1:A:91:GLN:CG	1:A:93:GLY:O	2.57	0.53
1:A:369:THR:HG22	1:A:398:TRP:CZ3	2.44	0.53
1:A:106:VAL:HG12	1:A:236:PRO:HB3	1.91	0.53
2:B:13:LYS:HE3	2:B:85:GLN:HB3	1.91	0.52
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.91	0.52
2:B:373:GLN:HE22	2:B:407:GLN:H	1.58	0.51
2:B:377:THR:HG22	2:B:410:TRP:HZ2	1.76	0.51
2:B:373:GLN:NE2	2:B:407:GLN:H	2.09	0.50
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.92	0.50
1:A:179:VAL:HG23	5:A:701:NVP:HCC1	1.93	0.50
2:B:345:PRO:O	2:B:346:PHE:HB2	2.10	0.49
2:B:362:THR:HG22	2:B:367:GLN:HG3	1.93	0.49
2:B:362:THR:HG23	2:B:366:LYS:HE3	1.95	0.49
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.95	0.49
1:A:303:LEU:O	1:A:307:ARG:HG3	2.14	0.48
1:A:183:TYR:OH	1:A:230:MET:CE	2.62	0.48
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.78	0.47
1:A:402:TRP:CD1	1:A:402:TRP:C	2.92	0.47
1:A:91:GLN:HG2	6:A:573:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.49	0.46
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.98	0.46
2:B:13:LYS:O	2:B:16:MET:HG2	2.16	0.45
2:B:250:ASP:O	2:B:251:SER:HB3	2.17	0.45
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.97	0.45
1:A:136:ASN:HB3	1:A:137:ASN:H	1.63	0.45
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.99	0.45
2:B:58:THR:HG23	2:B:76:ASP:O	2.17	0.44
1:A:230:MET:HA	1:A:230:MET:HE2	2.00	0.44
1:A:183:TYR:OH	1:A:230:MET:HE1	2.18	0.44
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.54	0.43
1:A:108:VAL:HG22	1:A:188:TYR:CE2	2.54	0.43
1:A:452:LEU:HD23	1:A:470:THR:HA	2.01	0.42
1:A:547:GLN:HA	1:A:550:LYS:HE2	2.00	0.42
2:B:157:PRO:HG3	2:B:184:MET:HA	2.01	0.42
1:A:536:VAL:HB	1:A:542:ILE:HD13	2.01	0.41
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.86	0.41
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.18	0.41
1:A:485:ALA:O	1:A:489:SER:HB3	2.21	0.41
2:B:365:VAL:O	2:B:369:THR:HG23	2.21	0.41
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.07	0.41
1:A:411:ILE:HG22	1:A:412:PRO:O	2.20	0.41
2:B:94:ILE:HA	2:B:95:PRO:HD3	1.91	0.41
2:B:116:PHE:CD1	2:B:116:PHE:C	2.99	0.40
2:B:246:LEU:HA	2:B:247:PRO:HD3	1.92	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	550/563 (98%)	532 (97%)	14 (2%)	4 (1%)	18 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	392/443 (88%)	377 (96%)	14 (4%)	1 (0%)	36	38
All	All	942/1006 (94%)	909 (96%)	28 (3%)	5 (0%)	24	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	GLU
1	A	543	GLY
2	B	296	THR
1	A	345	PRO
1	A	287	LYS

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	492/503 (98%)	458 (93%)	34 (7%)	14	11
2	B	364/403 (90%)	344 (94%)	20 (6%)	19	18
All	All	856/906 (94%)	802 (94%)	54 (6%)	16	14

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	21	VAL
1	A	26	LEU
1	A	118	VAL
1	A	139	THR
1	A	161	GLN
1	A	173	LYS
1	A	205	LEU
1	A	210	LEU

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Mol	Chain	Res	Type
1	A	220	LYS
1	A	228	LEU
1	A	248	GLU
1	A	260	LEU
1	A	276	VAL
1	A	279	LEU
1	A	296	THR
1	A	297	GLU
1	A	303	LEU
1	A	368	LEU
1	A	373	GLN
1	A	402	TRP
1	A	422	LEU
1	A	448	ARG
1	A	466	VAL
1	A	479	LEU
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	503	LEU
1	A	523	GLU
1	A	547	GLN
1	A	548	VAL
2	B	6	GLU
2	B	8	VAL
2	B	11	LYS
2	B	12	LEU
2	B	26	LEU
2	B	80	LEU
2	B	91	GLN
2	B	111	VAL
2	B	120	LEU
2	B	205	LEU
2	B	209	LEU
2	B	212	TRP
2	B	214	LEU
2	B	260	LEU
2	B	279	LEU
2	B	349	LEU
2	B	362	THR
2	B	400	THR
2	B	422	LEU

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Mol	Chain	Res	Type
2	B	425	LEU

Sometimes 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	103	ASN
1	A	137	ASN
1	A	175	ASN
1	A	198	HIS
1	A	235	HIS
1	A	258	GLN
1	A	278	GLN
1	A	330	GLN
1	A	407	GLN
1	A	500	GLN
1	A	507	GLN
1	A	509	GLN
1	A	520	GLN
1	A	524	GLN
2	B	147	ASN
2	B	175	ASN
2	B	208	HIS
2	B	255	ASN
2	B	258	GLN
2	B	269	GLN
2	B	306	ASN
2	B	367	GLN
2	B	373	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	$\# Z > 2$
5	NVP	A	701	-	23,23,23	2.40	6 (26%)	34,34,34	2.23	7 (20%)
3	LP8	A	601	4	20,20,20	1.72	4 (20%)	22,29,29	1.13	2 (9%)

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	-	-	0/4/6/6	0/4/4/4
3	LP8	A	601	4	-	0/0/11/11	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	NVP	C10-C9	-7.13	1.40	1.49
3	A	601	LP8	O3-C	5.22	1.33	1.23
5	A	701	NVP	C2-N1	-4.72	1.37	1.42
5	A	701	NVP	C7-N8	-4.50	1.36	1.42
5	A	701	NVP	C15-N1	-4.43	1.37	1.42
3	A	601	LP8	C5-C1	-3.59	1.40	1.45
3	A	601	LP8	C1-C2	2.47	1.40	1.36
3	A	601	LP8	C4-N	-2.45	1.35	1.38
5	A	701	NVP	CB-CA	2.27	1.53	1.48
5	A	701	NVP	CC-CA	2.23	1.53	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	NVP	C7-N8-C9	7.65	134.60	128.29
5	A	701	NVP	CB-CA-N1	5.06	119.08	116.09
5	A	701	NVP	N3-C2-N1	4.62	120.15	116.67
5	A	701	NVP	C7-C2-N1	-4.39	118.46	120.14
3	A	601	LP8	C5-C4-N	-3.38	116.62	119.51
5	A	701	NVP	C15-N1-C2	2.89	118.47	115.29
3	A	601	LP8	N9-C4-N	2.33	119.97	117.35
5	A	701	NVP	C10-C9-N8	2.25	122.41	120.22
5	A	701	NVP	C5-C4-N3	-2.13	121.36	123.97

There are no chirality outliers.

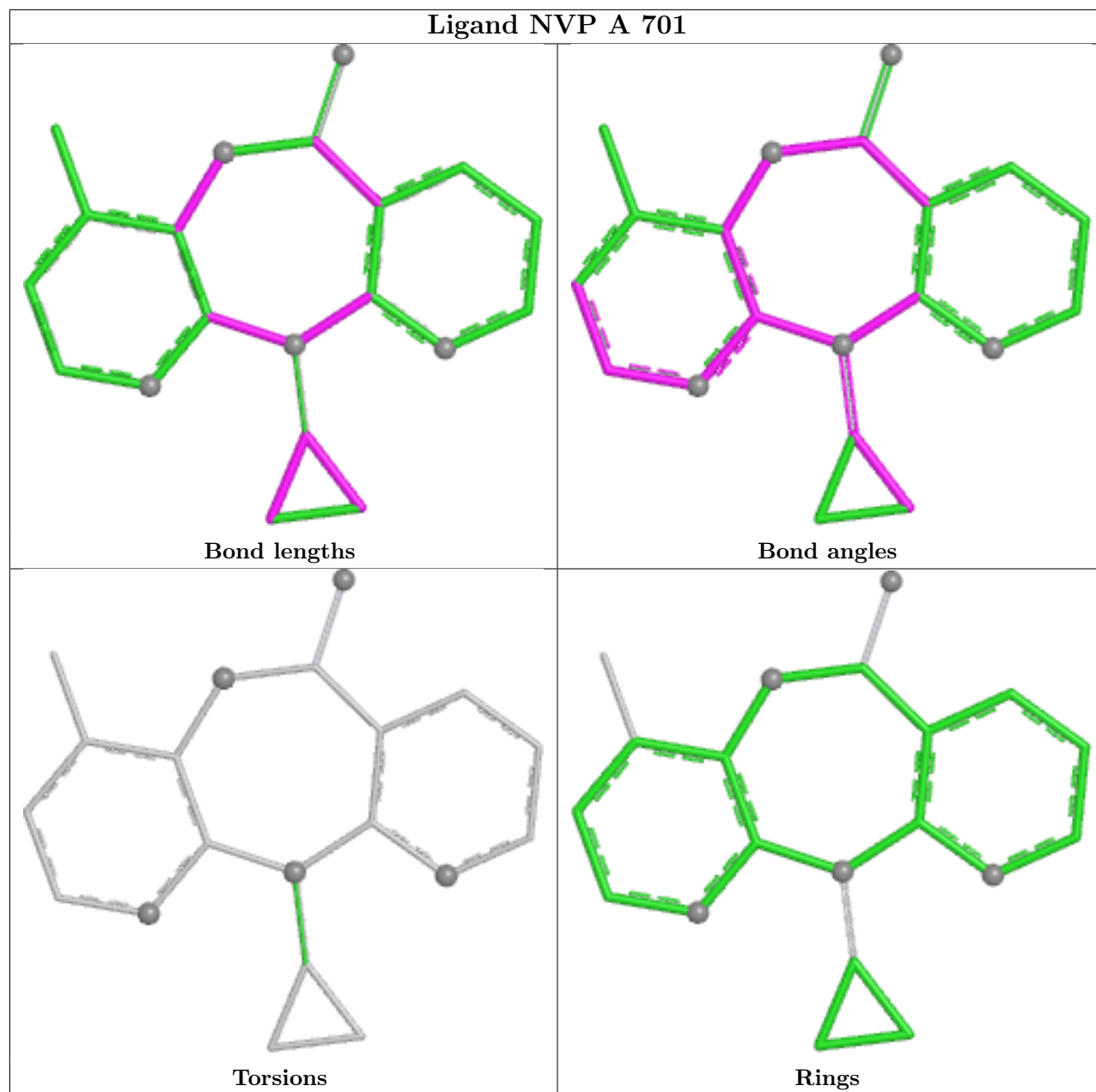
There are no torsion outliers.

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	554/563 (98%)	1.34	127 (22%) 2 1	27, 44, 56, 62	0
2	B	400/443 (90%)	1.59	130 (32%) 1 0	29, 40, 80, 83	0
All	All	954/1006 (94%)	1.45	257 (26%) 1 1	27, 43, 71, 83	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	362	THR	6.5
2	B	293	ILE	6.2
2	B	310	LEU	6.2
1	A	286	THR	6.1
2	B	301	LEU	6.1
2	B	288	ALA	6.0
2	B	309	ILE	5.9
1	A	543	GLY	5.6
2	B	90	VAL	5.5
2	B	299	ALA	5.4
2	B	313	PRO	5.4
2	B	257	ILE	5.3
2	B	346	PHE	5.3
2	B	24	TRP	5.2
2	B	274	ILE	5.2
2	B	361	HIS	5.2
1	A	24	TRP	5.2
2	B	295	LEU	5.0
2	B	266	TRP	4.9
2	B	247	PRO	4.9
2	B	273	GLY	4.9
1	A	90	VAL	4.9
2	B	278	GLN	4.8
2	B	426	TRP	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	357	MET	4.8
2	B	283	LEU	4.6
2	B	422	LEU	4.6
1	A	550	LYS	4.5
2	B	285	GLY	4.4
2	B	306	ASN	4.4
2	B	282	LEU	4.4
1	A	360	ALA	4.4
2	B	290	THR	4.4
2	B	298	GLU	4.4
2	B	241	VAL	4.4
2	B	262	GLY	4.4
2	B	8	VAL	4.3
1	A	287	LYS	4.3
2	B	240	THR	4.3
2	B	248	GLU	4.3
2	B	303	LEU	4.3
1	A	402	TRP	4.2
2	B	6	GLU	4.2
2	B	420	PRO	4.2
1	A	356	ARG	4.2
2	B	253	THR	4.2
2	B	286	THR	4.1
2	B	231	GLY	4.1
2	B	304	ALA	4.0
1	A	359	GLY	4.0
2	B	232	TYR	4.0
2	B	242	GLN	4.0
1	A	203	GLU	3.9
1	A	47	ILE	3.9
1	A	91	GLN	3.9
1	A	2	ILE	3.9
2	B	212	TRP	3.9
1	A	69	THR	3.8
1	A	207	GLN	3.8
1	A	237	ASP	3.7
2	B	314	VAL	3.7
2	B	294	PRO	3.7
2	B	246	LEU	3.7
1	A	0	SER	3.7
2	B	213	GLY	3.7
2	B	308	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	234	LEU	3.6
2	B	267	ALA	3.6
2	B	17	ASP	3.6
2	B	255	ASN	3.6
2	B	423	VAL	3.6
2	B	243	PRO	3.6
2	B	252	TRP	3.6
2	B	268	SER	3.6
1	A	43	LYS	3.6
2	B	22	LYS	3.5
2	B	334	GLN	3.5
2	B	261	VAL	3.5
1	A	136	ASN	3.5
1	A	137	ASN	3.5
2	B	16	MET	3.4
1	A	52	PRO	3.4
1	A	44	GLU	3.4
2	B	418	ASN	3.4
2	B	70	LYS	3.3
1	A	311	LYS	3.3
2	B	425	LEU	3.3
2	B	271	TYR	3.2
1	A	541	GLY	3.2
1	A	63	ILE	3.2
2	B	276	VAL	3.2
2	B	281	LYS	3.2
1	A	74	LEU	3.2
1	A	462	GLY	3.1
2	B	214	LEU	3.1
2	B	311	LYS	3.1
2	B	292	VAL	3.1
2	B	279	LEU	3.1
2	B	249	LYS	3.1
1	A	514	GLU	3.1
2	B	289	LEU	3.1
2	B	259	LYS	3.1
2	B	428	GLN	3.1
1	A	202	ILE	3.0
1	A	358	ARG	3.0
2	B	9	PRO	3.0
1	A	228	LEU	3.0
1	A	36	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	305	GLU	3.0
2	B	312	GLU	3.0
2	B	302	GLU	3.0
1	A	118	VAL	3.0
2	B	14	PRO	3.0
1	A	437	ALA	2.9
2	B	277	ARG	2.9
1	A	334	GLN	2.9
2	B	254	VAL	2.9
2	B	270	ILE	2.9
1	A	200	THR	2.8
2	B	250	ASP	2.8
1	A	464	GLN	2.8
1	A	7	THR	2.8
1	A	195	ILE	2.8
2	B	419	THR	2.8
2	B	272	PRO	2.8
2	B	300	GLU	2.8
1	A	205	LEU	2.8
2	B	13	LYS	2.8
2	B	92	LEU	2.7
1	A	539	HIS	2.7
2	B	215	THR	2.7
1	A	45	GLY	2.7
1	A	196	GLY	2.7
1	A	193	LEU	2.7
1	A	199	ARG	2.7
1	A	406	TRP	2.7
1	A	301	LEU	2.7
2	B	123	ASP	2.7
1	A	333	GLY	2.7
2	B	280	CYS	2.7
1	A	399	GLU	2.6
2	B	245	VAL	2.6
1	A	284	ARG	2.6
1	A	61	PHE	2.6
2	B	256	ASP	2.6
2	B	427	TYR	2.6
2	B	400	THR	2.6
2	B	15	GLY	2.6
2	B	18	GLY	2.6
2	B	296	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	5	ILE	2.6
1	A	208	HIS	2.6
1	A	6	GLU	2.6
1	A	490	GLY	2.6
1	A	56	TYR	2.6
1	A	105	SER	2.6
2	B	69	THR	2.5
2	B	421	PRO	2.5
1	A	138	GLU	2.5
1	A	51	GLY	2.5
2	B	239	TRP	2.5
1	A	407	GLN	2.5
2	B	251	SER	2.5
1	A	521	ILE	2.5
1	A	448	ARG	2.5
1	A	551	LEU	2.5
1	A	113	ASP	2.5
1	A	411	ILE	2.4
1	A	540	LYS	2.4
2	B	275	LYS	2.4
1	A	373	GLN	2.4
1	A	248	GLU	2.4
2	B	284	ARG	2.4
2	B	307	ARG	2.4
1	A	515	SER	2.4
1	A	110	ASP	2.4
1	A	291	GLU	2.4
1	A	398	TRP	2.4
2	B	258	GLN	2.4
2	B	297	GLU	2.4
1	A	544	GLY	2.4
1	A	296	THR	2.4
2	B	7	THR	2.4
2	B	117	SER	2.4
1	A	354	TYR	2.3
1	A	460	ASN	2.3
1	A	173	LYS	2.3
1	A	548	VAL	2.3
2	B	315	HIS	2.3
1	A	144	TYR	2.3
1	A	201	LYS	2.3
1	A	219	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	39	THR	2.3
1	A	72	ARG	2.3
1	A	50	ILE	2.3
2	B	264	LEU	2.3
1	A	471	ASP	2.3
1	A	412	PRO	2.3
1	A	212	TRP	2.3
1	A	204	GLU	2.3
1	A	220	LYS	2.3
1	A	426	TRP	2.3
1	A	305	GLU	2.3
2	B	336	GLN	2.3
2	B	87	PHE	2.2
2	B	12	LEU	2.2
2	B	265	ASN	2.2
1	A	537	PRO	2.2
1	A	396	GLU	2.2
2	B	233	GLU	2.2
2	B	238	LYS	2.2
1	A	468	THR	2.2
1	A	210	LEU	2.2
1	A	206	ARG	2.2
2	B	356	ARG	2.2
1	A	53	GLU	2.2
1	A	194	GLU	2.2
2	B	291	GLU	2.2
2	B	363	ASN	2.2
1	A	300	GLU	2.2
2	B	138	GLU	2.2
1	A	165	THR	2.2
1	A	123	ASP	2.1
2	B	237	ASP	2.1
1	A	469	LEU	2.1
1	A	491	LEU	2.1
2	B	122	GLU	2.1
1	A	221	HIS	2.1
1	A	433	PRO	2.1
2	B	417	VAL	2.1
1	A	15	GLY	2.1
1	A	285	GLY	2.1
2	B	206	ARG	2.1
1	A	62	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	214	LEU	2.1
1	A	438	GLU	2.1
1	A	523	GLU	2.1
1	A	179	VAL	2.1
1	A	493	VAL	2.1
2	B	111	VAL	2.1
1	A	64	LYS	2.1
1	A	122	GLU	2.1
2	B	177	ASP	2.1
1	A	9	PRO	2.1
2	B	10	VAL	2.1
2	B	352	GLY	2.1
2	B	173	LYS	2.0
1	A	429	LEU	2.0
1	A	452	LEU	2.0
1	A	309	ILE	2.0
1	A	435	VAL	2.0
1	A	458	VAL	2.0
1	A	18	GLY	2.0
1	A	46	LYS	2.0
1	A	82	LYS	2.0
2	B	287	LYS	2.0
1	A	288	ALA	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](#)

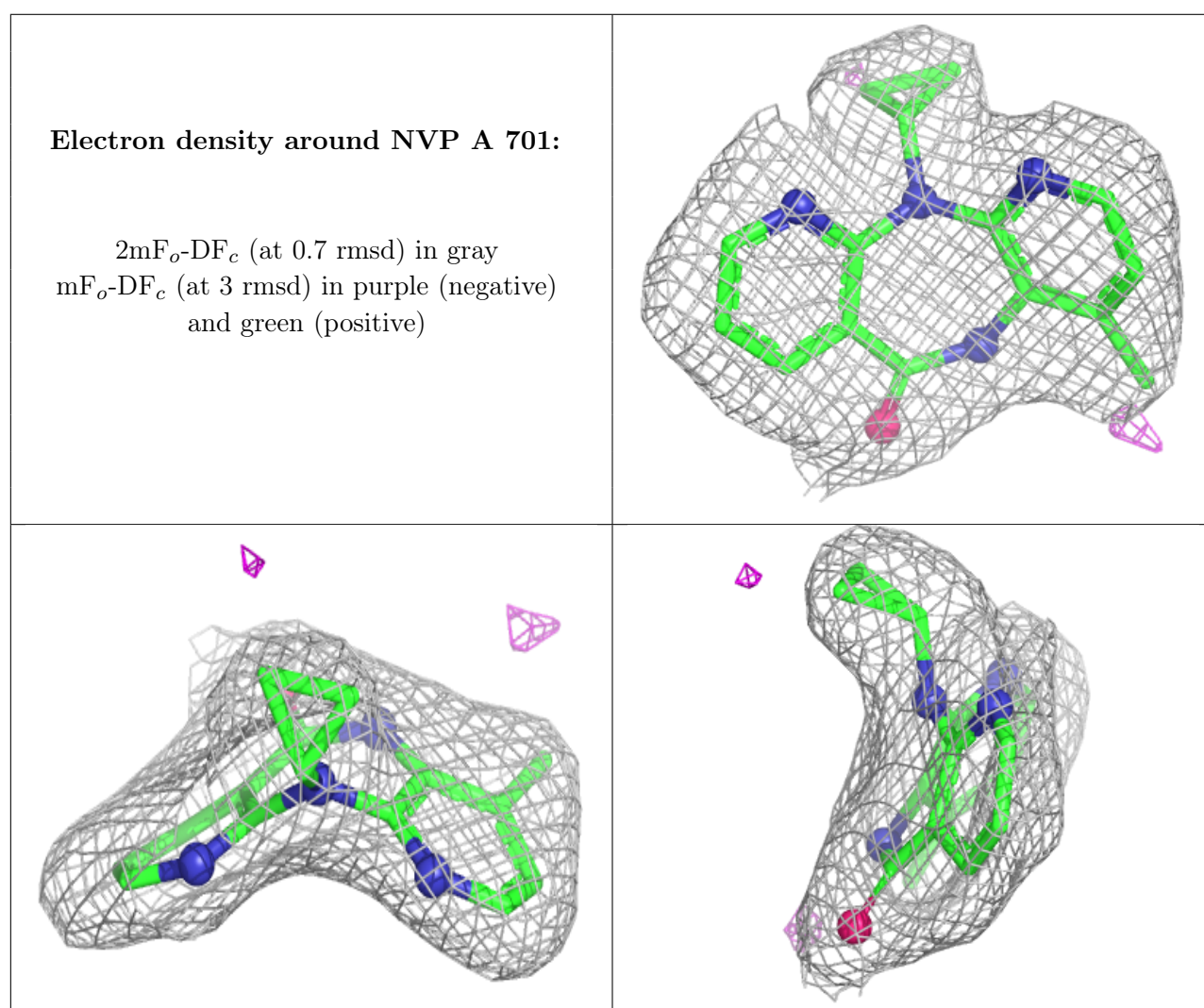
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LP8	A	601	18/18	0.84	0.13	44,44,45,45	0
5	NVP	A	701	20/20	0.92	0.09	35,35,36,36	0
4	MN	A	602	1/1	0.98	0.05	44,44,44,44	0
4	MN	A	603	1/1	0.99	0.04	37,37,37,37	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.