



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:00 PM UTC

PDB ID : 3QIP / pdb_00003qip
Title : Structure of HIV-1 reverse transcriptase in complex with an RNase H inhibitor and nevirapine
Authors : Lansdon, E.B.; Kirschberg, T.A.
Deposited on : 2011-01-27
Resolution : 2.09 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

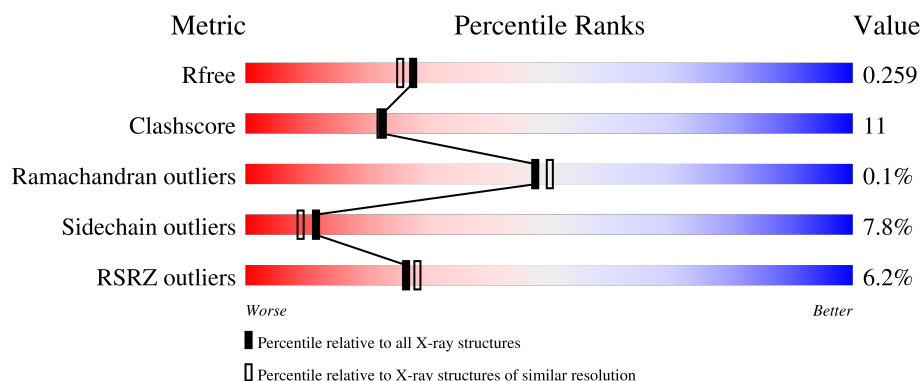
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	560	6% 74% 22% • •
2	B	440	5% 69% 18% • 9%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8317 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.

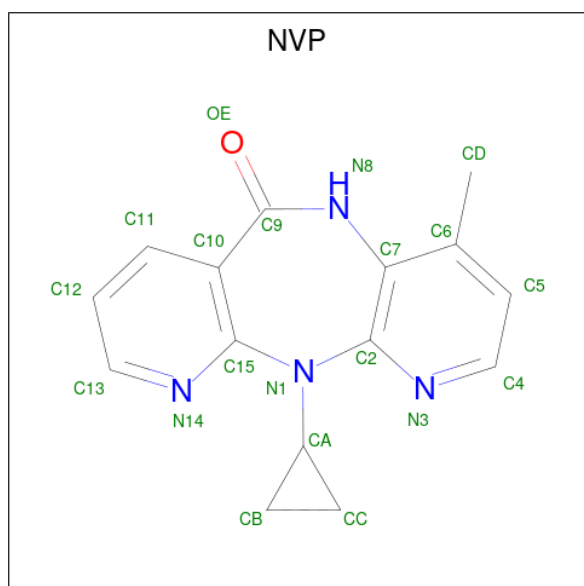
- Molecule 1 is a protein called Reverse HIV-1 reverse transcriptase p66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4508	2915	752	833	8			

- Molecule 2 is a protein called p51.

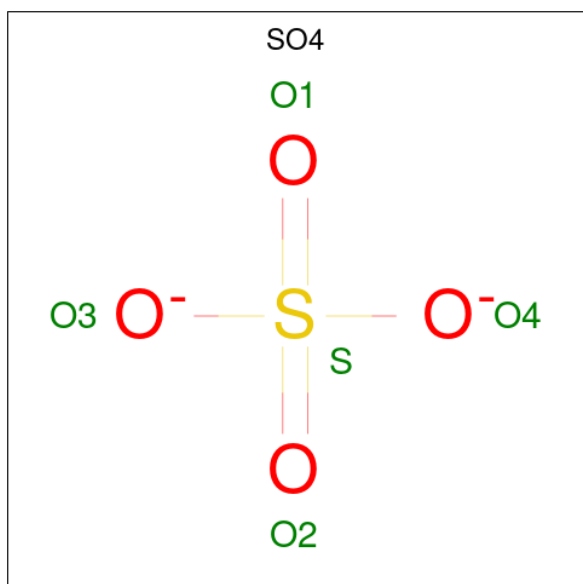
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3330	2169	549	606	6			

- Molecule 3 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
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

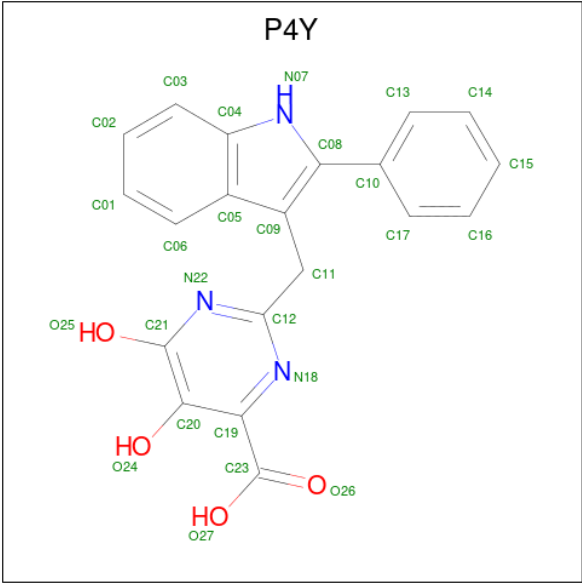


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 5,6-dihydroxy-2-[(2-phenyl-1H-indol-3-yl)methyl]pyrimidine-4-carboxylic acid (CCD ID: P4Y) (formula: C₂₀H₁₅N₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			27	20	3	4		

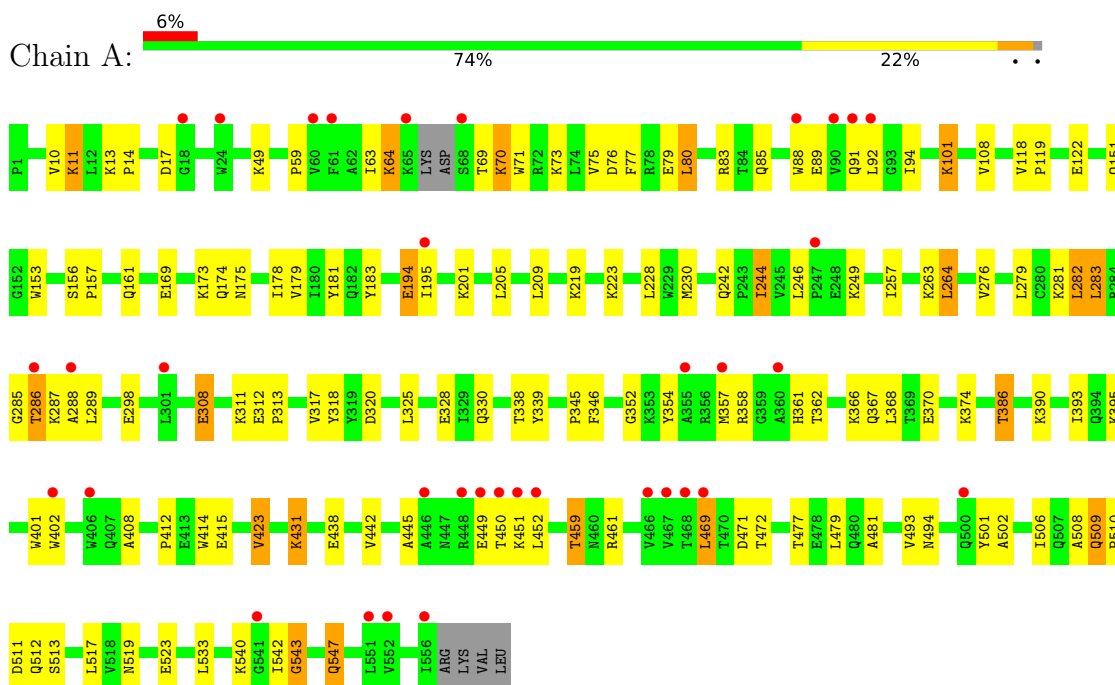
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	248	Total	O	0	0
			248	248		
8	B	170	Total	O	0	0
			170	170		

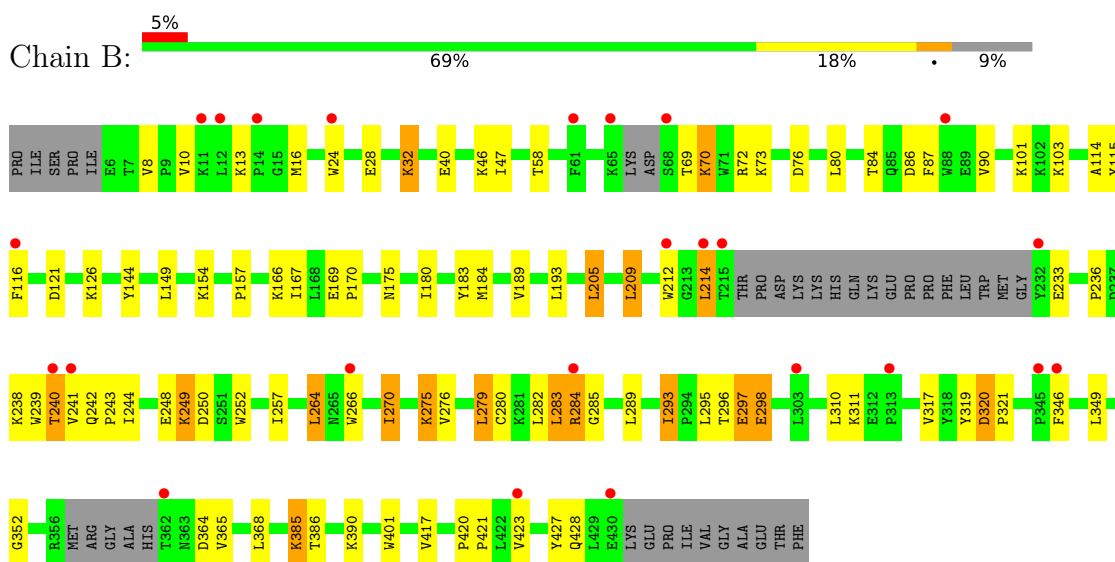
3 Residue-property plots [i](#)

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 HIV-1 reverse transcriptase p66



- Molecule 2: p51



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.90Å 154.88Å 153.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.35 – 2.09 47.35 – 2.09	Depositor EDS
% Data completeness (in resolution range)	91.7 (47.35-2.09) 91.0 (47.35-2.09)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.216 , 0.267 0.212 , 0.259	Depositor DCC
R_{free} test set	4099 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8317	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: SO4, CL, MN, P4Y, 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	0.49	0/4624	0.80	2/6282 (0.0%)
2	B	0.48	0/3422	0.81	6/4649 (0.1%)
All	All	0.49	0/8046	0.80	8/10931 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	320	ASP	CA-C-N	7.22	126.86	119.56
2	B	320	ASP	C-N-CA	7.22	126.86	119.56
2	B	175	ASN	CA-C-N	5.49	125.16	119.56
2	B	175	ASN	C-N-CA	5.49	125.16	119.56
2	B	270	ILE	CB-CA-C	-5.39	106.25	111.05
1	A	320	ASP	CA-C-N	5.25	124.92	119.56
1	A	320	ASP	C-N-CA	5.25	124.92	119.56
2	B	233	GLU	N-CA-C	5.12	116.86	108.52

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	4508	0	4559	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3330	0	3358	75	0
3	A	20	0	14	1	0
4	A	2	0	0	0	0
5	A	10	0	0	0	0
6	A	1	0	0	1	0
6	B	1	0	0	1	0
7	A	27	0	13	0	0
8	A	248	0	0	6	0
8	B	170	0	0	3	0
All	All	8317	0	7944	167	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 11.

All (167) 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:154:LYS:HE2	2:B:184:MET:HE2	1.32	1.06
2:B:154:LYS:HE2	2:B:184:MET:CE	1.98	0.94
1:A:194:GLU:H	1:A:194:GLU:CD	1.71	0.94
1:A:547:GLN:HE21	1:A:547:GLN:H	1.18	0.91
6:B:441:CL:CL	8:B:557:HOH:O	2.25	0.89
1:A:70:LYS:HD3	1:A:71:TRP:H	1.39	0.87
2:B:13:LYS:HD3	2:B:86:ASP:H	1.44	0.80
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.83	0.78
1:A:70:LYS:HD3	1:A:71:TRP:N	1.97	0.78
1:A:509:GLN:HG2	8:A:805:HOH:O	1.83	0.78
1:A:543:GLY:O	1:A:547:GLN:NE2	2.16	0.76
2:B:297:GLU:CD	2:B:297:GLU:H	1.96	0.74
1:A:547:GLN:HE21	1:A:547:GLN:N	1.86	0.72
1:A:308:GLU:HA	1:A:311:LYS:HG3	1.73	0.71
1:A:244:ILE:HD11	1:A:246:LEU:HD21	1.73	0.71
1:A:386:THR:HG21	1:A:412:PRO:HB3	1.73	0.70
1:A:174:GLN:HG3	8:A:776:HOH:O	1.91	0.70
1:A:79:GLU:OE1	1:A:83:ARG:NH1	2.25	0.69
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.74	0.69
1:A:459:THR:CG2	1:A:461:ARG:H	2.05	0.69
1:A:195:ILE:HD12	1:A:195:ILE:H	1.57	0.68
1:A:64:LYS:HE3	1:A:69:THR:HA	1.76	0.68
1:A:451:LYS:HG2	1:A:471:ASP:HA	1.76	0.66
1:A:459:THR:HG22	1:A:461:ARG:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:HB3	1:A:178:ILE:HG12	1.79	0.65
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.33	0.63
1:A:298:GLU:CD	1:A:298:GLU:H	2.08	0.62
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.83	0.61
2:B:284:ARG:CZ	2:B:285:GLY:H	2.14	0.61
2:B:319:TYR:OH	2:B:385:LYS:HE3	2.01	0.60
2:B:244:ILE:HD13	2:B:266:TRP:HZ3	1.66	0.60
1:A:108:VAL:HG11	1:A:223:LYS:HE3	1.83	0.60
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.84	0.60
2:B:166:LYS:HE2	2:B:212:TRP:HH2	1.67	0.60
1:A:362:THR:HG22	1:A:366:LYS:HE2	1.83	0.60
2:B:183:TYR:CZ	2:B:184:MET:HE3	2.37	0.59
2:B:241:VAL:O	2:B:243:PRO:HD3	2.02	0.59
1:A:283:LEU:O	1:A:286:THR:HB	2.01	0.59
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.18	0.58
1:A:479:LEU:HD21	1:A:501:TYR:CE2	2.39	0.58
2:B:240:THR:HG22	2:B:241:VAL:O	2.03	0.58
1:A:89:GLU:HB3	1:A:92:LEU:HD21	1.86	0.57
1:A:194:GLU:CD	1:A:194:GLU:N	2.51	0.57
2:B:183:TYR:OH	2:B:184:MET:HE3	2.05	0.57
2:B:284:ARG:NE	2:B:284:ARG:HA	2.19	0.57
2:B:205:LEU:HD22	2:B:209:LEU:HD22	1.86	0.57
1:A:288:ALA:N	8:A:738:HOH:O	2.38	0.56
1:A:431:LYS:NZ	1:A:431:LYS:HB2	2.20	0.56
2:B:257:ILE:HG23	2:B:279:LEU:HD12	1.86	0.56
2:B:72:ARG:NH2	8:B:552:HOH:O	2.38	0.56
2:B:84:THR:HG22	2:B:84:THR:O	2.05	0.56
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.42	0.55
1:A:479:LEU:HD21	1:A:501:TYR:HE2	1.69	0.55
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.88	0.55
2:B:284:ARG:NH2	2:B:285:GLY:H	2.05	0.55
2:B:47:ILE:HD12	2:B:144:TYR:CG	2.43	0.54
2:B:114:ALA:CB	2:B:214:LEU:HD22	2.38	0.53
2:B:69:THR:C	2:B:70:LYS:HE3	2.34	0.53
1:A:390:LYS:HE2	1:A:415:GLU:OE1	2.09	0.53
1:A:219:LYS:C	1:A:219:LYS:HD3	2.34	0.53
1:A:450:THR:CG2	1:A:452:LEU:HB3	2.39	0.52
1:A:508:ALA:HB3	8:A:603:HOH:O	2.10	0.52
1:A:228:LEU:HD22	1:A:242:GLN:HG2	1.91	0.52
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.93	0.51
2:B:8:VAL:O	2:B:121:ASP:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LYS:HE2	8:A:744:HOH:O	2.09	0.51
1:A:179:VAL:HG12	3:A:561:NVP:HCB2	1.92	0.50
1:A:354:TYR:CD1	1:A:374:LYS:HD3	2.46	0.50
1:A:94:ILE:HD13	1:A:230:MET:HE2	1.94	0.50
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.94	0.49
2:B:101:LYS:O	2:B:236:PRO:HB2	2.12	0.49
2:B:28:GLU:O	2:B:32:LYS:HD2	2.12	0.49
1:A:17:ASP:O	1:A:83:ARG:HD3	2.13	0.49
1:A:361:HIS:CE1	1:A:513:SER:HG	2.30	0.49
2:B:69:THR:O	2:B:70:LYS:HE3	2.12	0.49
2:B:242:GLN:HB2	2:B:352:GLY:HA2	1.94	0.49
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.95	0.49
1:A:354:TYR:HD1	1:A:374:LYS:HD3	1.78	0.49
1:A:257:ILE:HG22	1:A:283:LEU:HD21	1.96	0.48
1:A:401:TRP:HD1	1:A:402:TRP:CD1	2.31	0.48
1:A:330:GLN:OE1	1:A:338:THR:HG23	2.13	0.48
1:A:509:GLN:N	1:A:510:PRO:CD	2.77	0.48
1:A:452:LEU:HD12	1:A:469:LEU:O	2.14	0.48
2:B:103:LYS:O	2:B:236:PRO:HG2	2.13	0.48
1:A:317:VAL:HG12	1:A:318:TYR:N	2.28	0.47
2:B:296:THR:HB	2:B:298:GLU:OE1	2.14	0.47
1:A:450:THR:HG22	1:A:452:LEU:HB3	1.95	0.47
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.97	0.47
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.97	0.47
1:A:285:GLY:O	1:A:287:LYS:HE2	2.15	0.47
2:B:13:LYS:HD3	2:B:86:ASP:N	2.22	0.47
2:B:248:GLU:HA	2:B:248:GLU:OE1	2.14	0.47
2:B:284:ARG:NE	2:B:285:GLY:H	2.13	0.47
1:A:459:THR:HG22	1:A:461:ARG:N	2.27	0.47
2:B:266:TRP:CH2	2:B:427:TYR:CZ	3.03	0.46
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.50	0.46
2:B:257:ILE:HG22	2:B:283:LEU:HD21	1.98	0.46
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.41	0.46
1:A:279:LEU:O	1:A:282:LEU:HB2	2.15	0.46
1:A:519:ASN:O	1:A:523:GLU:HG2	2.15	0.46
2:B:266:TRP:CZ2	2:B:427:TYR:CZ	3.04	0.46
6:A:566:CL:CL	8:A:742:HOH:O	2.57	0.46
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.51	0.46
1:A:89:GLU:OE2	1:A:91:GLN:HG3	2.16	0.46
1:A:298:GLU:OE1	1:A:298:GLU:N	2.48	0.46
1:A:10:VAL:C	1:A:11:LYS:HG2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:TYR:CE2	2:B:184:MET:HE3	2.51	0.46
1:A:317:VAL:CG1	1:A:318:TYR:N	2.79	0.45
1:A:345:PRO:HA	1:A:346:PHE:HA	1.57	0.45
2:B:13:LYS:HE3	2:B:16:MET:HE1	1.98	0.45
1:A:101:LYS:N	1:A:101:LYS:HD3	2.31	0.45
2:B:266:TRP:HH2	2:B:427:TYR:CE1	2.35	0.45
2:B:10:VAL:HG13	2:B:87:PHE:CD1	2.52	0.45
2:B:282:LEU:HB3	2:B:293:ILE:HD11	1.97	0.45
2:B:24:TRP:N	2:B:24:TRP:CD1	2.85	0.45
2:B:183:TYR:OH	2:B:386:THR:HG23	2.17	0.45
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.99	0.44
2:B:244:ILE:CD1	2:B:266:TRP:CZ3	3.01	0.44
1:A:459:THR:HG23	1:A:461:ARG:H	1.81	0.44
2:B:317:VAL:HB	8:B:608:HOH:O	2.16	0.44
2:B:252:TRP:NE1	2:B:295:LEU:HD11	2.33	0.44
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.99	0.44
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.99	0.44
1:A:264:LEU:HD23	1:A:276:VAL:HG12	2.00	0.44
2:B:284:ARG:NE	2:B:284:ARG:CA	2.80	0.44
1:A:244:ILE:HD11	1:A:246:LEU:CD2	2.45	0.44
2:B:298:GLU:H	2:B:298:GLU:CD	2.25	0.43
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.83	0.43
2:B:236:PRO:C	2:B:238:LYS:H	2.27	0.43
1:A:368:LEU:HD22	1:A:423:VAL:HG11	2.01	0.43
2:B:46:LYS:HE2	2:B:116:PHE:HB3	1.99	0.43
2:B:390:LYS:HD2	2:B:417:VAL:HG11	2.01	0.43
2:B:115:TYR:HB3	2:B:149:LEU:HB2	2.00	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.19	0.42
2:B:214:LEU:HD23	2:B:214:LEU:N	2.34	0.42
2:B:297:GLU:CD	2:B:297:GLU:N	2.72	0.42
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.55	0.42
1:A:523:GLU:HG2	1:A:523:GLU:H	1.72	0.42
2:B:264:LEU:HB3	2:B:276:VAL:CG1	2.50	0.42
2:B:275:LYS:HE3	2:B:275:LYS:HB3	1.88	0.42
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.01	0.42
1:A:79:GLU:HG3	1:A:83:ARG:HH11	1.82	0.42
2:B:241:VAL:HG21	2:B:311:LYS:O	2.19	0.42
2:B:420:PRO:HA	2:B:421:PRO:HD2	1.92	0.42
1:A:511:ASP:OD1	1:A:511:ASP:C	2.63	0.42
1:A:219:LYS:HD3	1:A:219:LYS:O	2.20	0.41
1:A:118:VAL:HG13	1:A:119:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.55	0.41
1:A:173:LYS:HE3	1:A:173:LYS:HB2	1.82	0.41
1:A:393:ILE:HB	1:A:423:VAL:HG13	2.01	0.41
1:A:479:LEU:CD2	1:A:501:TYR:HE2	2.33	0.41
1:A:502:ALA:O	1:A:506:ILE:HG12	2.21	0.41
1:A:80:LEU:HD13	1:A:153:TRP:CD1	2.55	0.41
1:A:445:ALA:O	1:A:477:THR:HG21	2.21	0.41
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.94	0.41
1:A:494:ASN:HB3	2:B:289:LEU:HD12	2.03	0.41
1:A:175:ASN:OD1	1:A:201:LYS:HD2	2.20	0.41
1:A:75:VAL:HG11	1:A:77:PHE:CZ	2.56	0.41
2:B:420:PRO:HB2	2:B:423:VAL:HG23	2.03	0.41
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.56	0.40
2:B:157:PRO:HG3	2:B:184:MET:HA	2.03	0.40
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.56	0.40
1:A:11:LYS:O	1:A:85:GLN:HG2	2.22	0.40
1:A:367:GLN:NE2	1:A:512:GLN:NE2	2.69	0.40
2:B:320:ASP:C	2:B:320:ASP:OD1	2.64	0.40
2:B:320:ASP:HA	2:B:321:PRO:HD3	1.76	0.40
2:B:166:LYS:HE2	2:B:212:TRP:CH2	2.52	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	550/560 (98%)	532 (97%)	17 (3%)	1 (0%)	43	44
2	B	394/440 (90%)	378 (96%)	16 (4%)	0	100	100
All	All	944/1000 (94%)	910 (96%)	33 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	543	GLY

5.3.2 Protein sidechains [i](#)

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	494/500 (99%)	454 (92%)	40 (8%)	11	8
2	B	367/400 (92%)	340 (93%)	27 (7%)	13	10
All	All	861/900 (96%)	794 (92%)	67 (8%)	11	9

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	49	LYS
1	A	63	ILE
1	A	64	LYS
1	A	70	LYS
1	A	73	LYS
1	A	80	LEU
1	A	101	LYS
1	A	122	GLU
1	A	151	GLN
1	A	161	GLN
1	A	169	GLU
1	A	194	GLU
1	A	205	LEU
1	A	209	LEU
1	A	244	ILE
1	A	249	LYS
1	A	264	LEU
1	A	281	LYS
1	A	282	LEU
1	A	283	LEU
1	A	286	THR
1	A	289	LEU

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Mol	Chain	Res	Type
1	A	308	GLU
1	A	325	LEU
1	A	357	MET
1	A	386	THR
1	A	423	VAL
1	A	431	LYS
1	A	449	GLU
1	A	459	THR
1	A	469	LEU
1	A	472	THR
1	A	493	VAL
1	A	509	GLN
1	A	517	LEU
1	A	533	LEU
1	A	540	LYS
1	A	542	ILE
1	A	547	GLN
2	B	32	LYS
2	B	40	GLU
2	B	70	LYS
2	B	73	LYS
2	B	80	LEU
2	B	90	VAL
2	B	126	LYS
2	B	193	LEU
2	B	205	LEU
2	B	209	LEU
2	B	214	LEU
2	B	240	THR
2	B	249	LYS
2	B	250	ASP
2	B	264	LEU
2	B	275	LYS
2	B	279	LEU
2	B	280	CYS
2	B	283	LEU
2	B	284	ARG
2	B	293	ILE
2	B	297	GLU
2	B	298	GLU
2	B	310	LEU
2	B	368	LEU

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Mol	Chain	Res	Type
2	B	385	LYS
2	B	428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	GLN
1	A	474	ASN
1	A	500	GLN
1	A	509	GLN
1	A	547	GLN
2	B	147	ASN
2	B	265	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	SO4	A	565	-	4,4,4	0.21	0	6,6,6	0.36	0
3	NVP	A	561	-	23,23,23	1.04	2 (8%)	34,34,34	1.90	5 (14%)
7	P4Y	A	900	4	29,30,30	1.32	2 (6%)	34,43,43	1.56	5 (14%)
5	SO4	A	564	-	4,4,4	0.21	0	6,6,6	0.39	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	NVP	A	561	-	-	0/4/6/6	0/4/4/4
7	P4Y	A	900	4	-	0/12/12/12	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	900	P4Y	C08-C09	4.79	1.42	1.38
3	A	561	NVP	C15-N1	-2.46	1.39	1.42
7	A	900	P4Y	C19-C23	-2.40	1.47	1.51
3	A	561	NVP	C9-N8	2.32	1.37	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	561	NVP	CB-CA-N1	6.95	120.20	116.09
3	A	561	NVP	C15-N1-C2	5.18	121.00	115.29
7	A	900	P4Y	O26-C23-C19	3.86	128.71	120.80
7	A	900	P4Y	C11-C09-C08	3.85	132.71	128.33
3	A	561	NVP	CC-CA-N1	3.34	118.06	116.09
7	A	900	P4Y	C10-C08-C09	2.78	134.63	130.62
7	A	900	P4Y	C09-C08-N07	-2.56	107.76	109.61
3	A	561	NVP	N3-C2-N1	2.48	118.54	116.67
3	A	561	NVP	C15-N1-CA	-2.21	114.59	116.34
7	A	900	P4Y	C11-C12-N22	2.15	120.89	117.18

There are no chirality outliers.

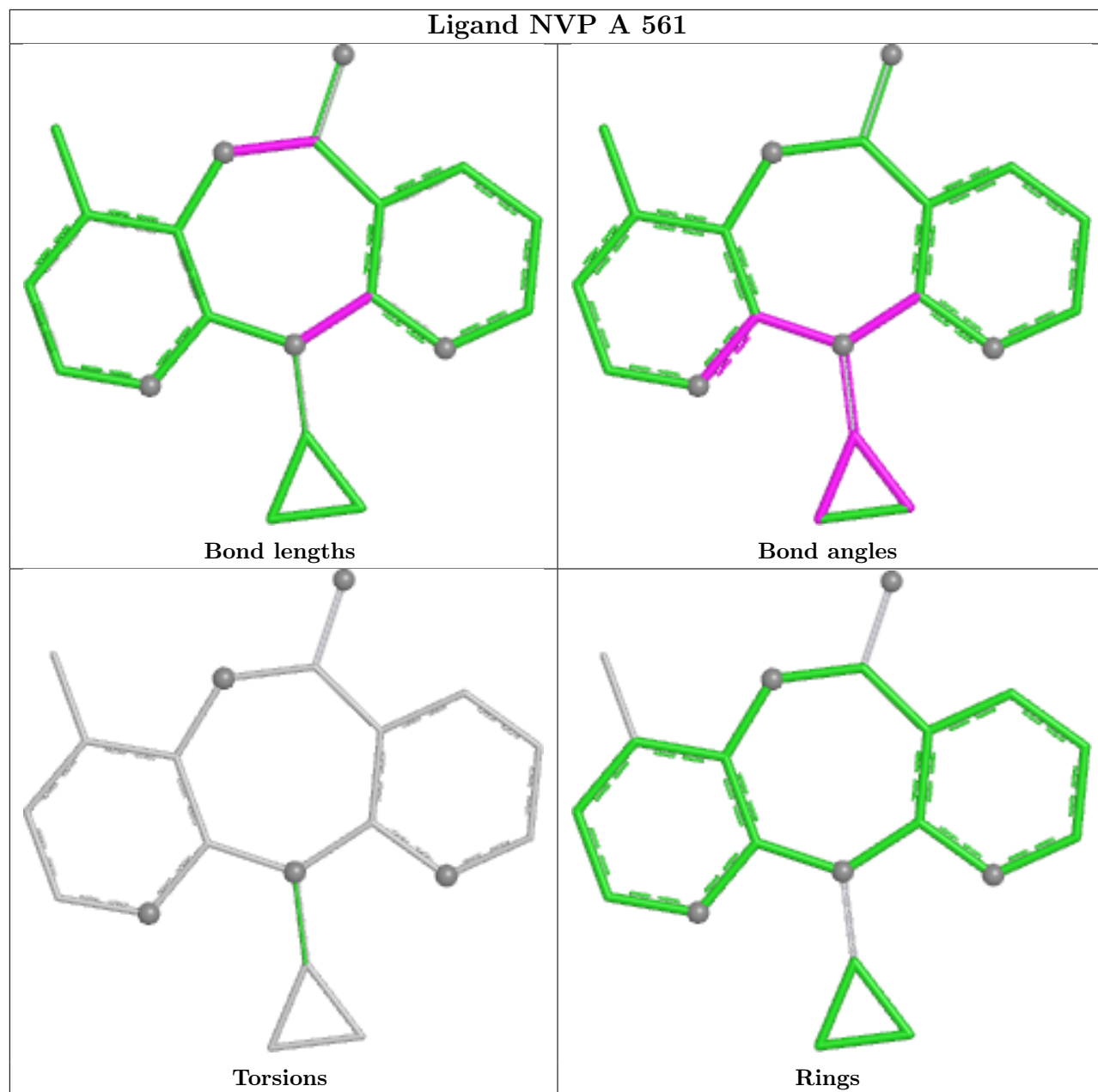
There are no torsion outliers.

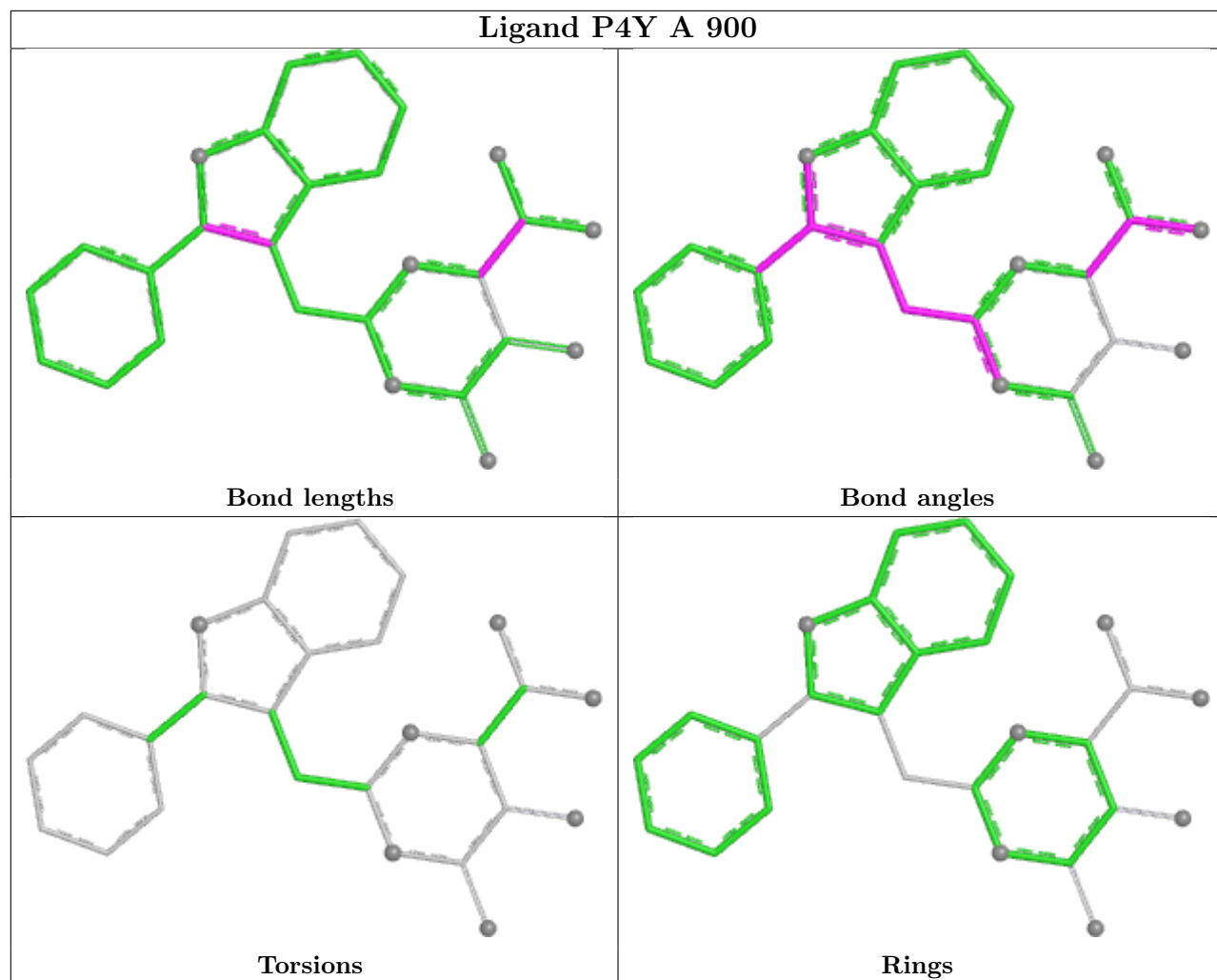
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	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	554/560 (98%)	0.60	35 (6%) 26 27	31, 48, 74, 98	0
2	B	402/440 (91%)	0.55	24 (5%) 27 29	31, 47, 75, 96	0
All	All	956/1000 (95%)	0.58	59 (6%) 26 28	31, 48, 75, 98	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	GLU	7.1
2	B	346	PHE	6.2
1	A	24	TRP	4.9
2	B	215	THR	4.8
1	A	61	PHE	4.7
2	B	214	LEU	4.3
1	A	556	ILE	4.2
1	A	90	VAL	4.1
1	A	18	GLY	4.1
1	A	88	TRP	4.0
1	A	91	GLN	4.0
2	B	68	SER	3.9
1	A	452	LEU	3.7
1	A	65	LYS	3.6
1	A	286	THR	3.6
2	B	116	PHE	3.6
1	A	92	LEU	3.3
1	A	406	TRP	3.3
2	B	24	TRP	3.2
1	A	466	VAL	3.2
2	B	232	TYR	3.1
2	B	241	VAL	3.1
1	A	500	GLN	3.1
1	A	467	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	448	ARG	2.9
2	B	284	ARG	2.9
1	A	469	LEU	2.9
2	B	345	PRO	2.8
1	A	301	LEU	2.8
2	B	65	LYS	2.8
2	B	14	PRO	2.7
2	B	362	THR	2.7
1	A	68	SER	2.7
2	B	212	TRP	2.7
1	A	451	LYS	2.6
1	A	446	ALA	2.6
2	B	88	TRP	2.6
1	A	450	THR	2.6
2	B	61	PHE	2.5
1	A	247	PRO	2.5
1	A	195	ILE	2.5
2	B	11	LYS	2.5
2	B	240	THR	2.5
2	B	266	TRP	2.5
1	A	355	ALA	2.4
1	A	357	MET	2.4
2	B	313	PRO	2.4
1	A	551	LEU	2.4
1	A	288	ALA	2.3
2	B	303	LEU	2.3
2	B	12	LEU	2.3
2	B	423	VAL	2.3
1	A	402	TRP	2.2
1	A	552	VAL	2.1
1	A	360	ALA	2.1
2	B	430	GLU	2.0
1	A	541	GLY	2.0
1	A	60	VAL	2.0
1	A	468	THR	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

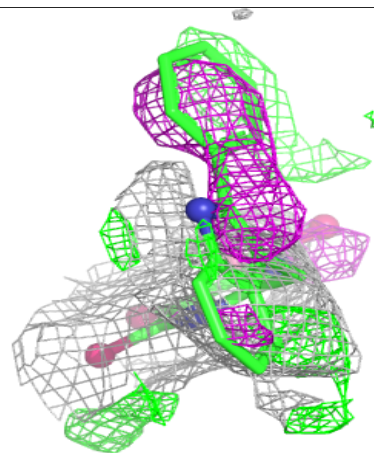
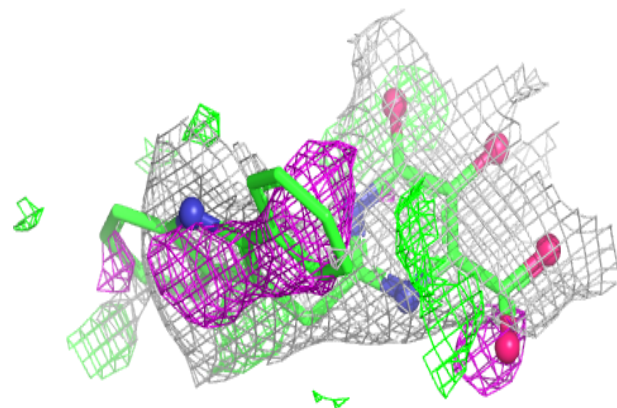
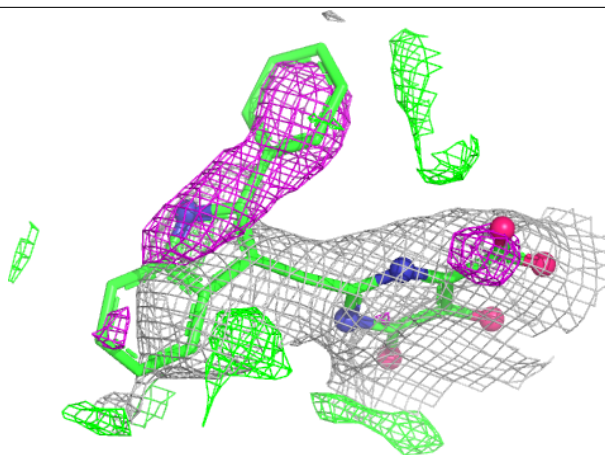
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	P4Y	A	900	27/27	0.67	0.22	56,80,90,92	0
5	SO4	A	565	5/5	0.89	0.09	59,59,65,75	0
5	SO4	A	564	5/5	0.90	0.11	48,51,57,58	0
6	CL	A	566	1/1	0.92	0.13	75,75,75,75	0
6	CL	B	441	1/1	0.94	0.09	67,67,67,67	0
3	NVP	A	561	20/20	0.96	0.08	25,33,36,41	0
4	MN	A	563	1/1	0.99	0.03	59,59,59,59	0
4	MN	A	562	1/1	0.99	0.03	51,51,51,51	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.

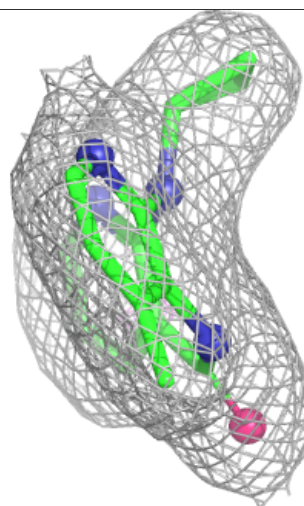
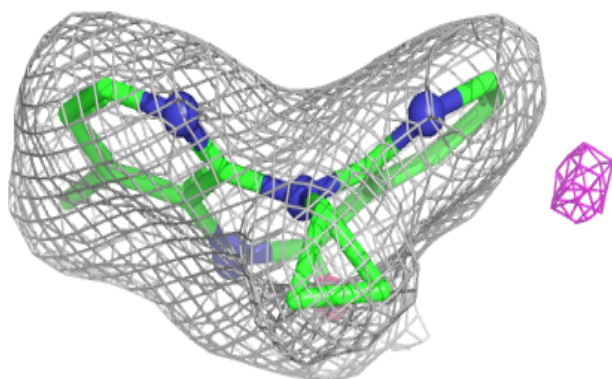
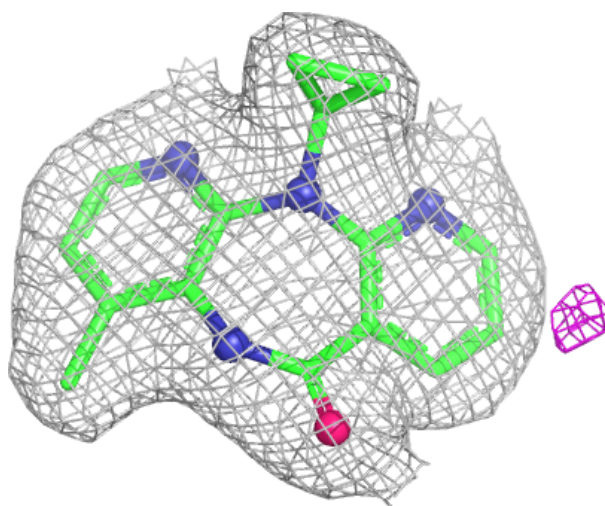
Electron density around P4Y A 900:

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



Electron density around NVP A 561:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.