



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 10:02 PM EDT

PDB ID : 4JTW
Title : Crystal structure of HCV NS5B polymerase in complex with compound 1
Authors : Coulombe, R.
Deposited on : 2013-03-24
Resolution : 3.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

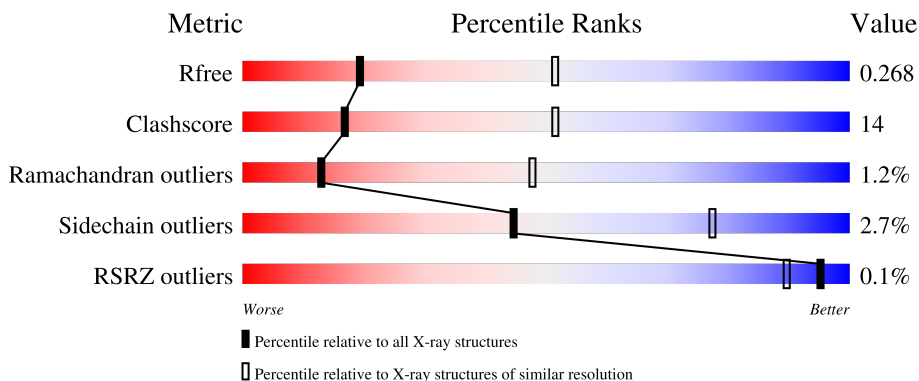
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	576	
1	B	576	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9122 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	560	4362	2747	771	812	32	0	0	0
1	B	560	4362	2747	771	812	32	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

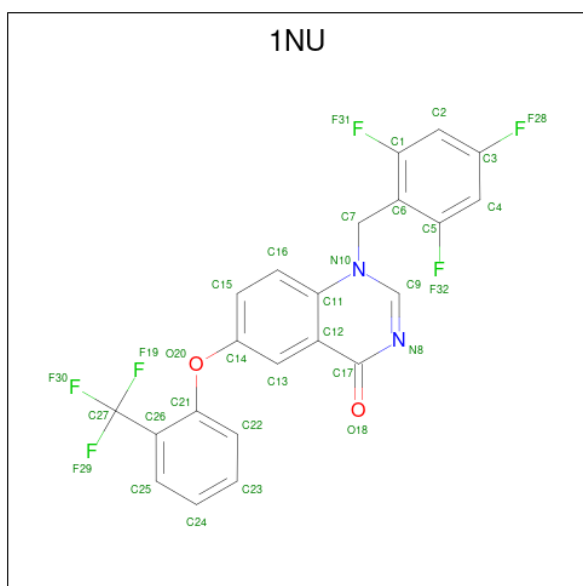
Chain	Residue	Modelled	Actual	Comment	Reference
A	571	HIS	-	expression tag	UNP O92972
A	572	HIS	-	expression tag	UNP O92972
A	573	HIS	-	expression tag	UNP O92972
A	574	HIS	-	expression tag	UNP O92972
A	575	HIS	-	expression tag	UNP O92972
A	576	HIS	-	expression tag	UNP O92972
B	571	HIS	-	expression tag	UNP O92972
B	572	HIS	-	expression tag	UNP O92972
B	573	HIS	-	expression tag	UNP O92972
B	574	HIS	-	expression tag	UNP O92972
B	575	HIS	-	expression tag	UNP O92972
B	576	HIS	-	expression tag	UNP O92972

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1-(2,4,6-trifluorobenzyl)-6-[2-(trifluoromethyl)phenoxy]quinazolin-4(1H)-one (three-letter code: 1NU) (formula: C₂₂H₁₂F₆N₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			32	22	6	2	2		

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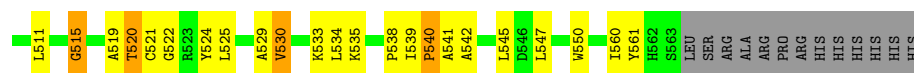
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			32	22	6	2	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	169	Total	O	0	0
			169	169		
5	B	149	Total	O	0	0
			149	149		



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.43Å 108.00Å 134.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 39.19 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 97.1 (39.19-2.99)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.01Å)	Xtrriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.200 , 0.274 0.197 , 0.268	Depositor DCC
R_{free} test set	3118 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtrriage
Anisotropy	0.343	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.008 for k,h,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9122	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: MG, GOL, 1NU

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	0.37	0/4457	0.63	1/6049 (0.0%)
1	B	0.34	0/4457	0.60	0/6049
All	All	0.35	0/8914	0.61	1/12098 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	GLY	N-CA-C	-5.18	100.15	113.10

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	4362	0	4374	104	0
1	B	4362	0	4374	145	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
3	A	32	0	12	1	0
3	B	32	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	169	0	0	7	0
5	B	149	0	0	12	0
All	All	9122	0	8788	247	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 14.

All (247) 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:B:515:GLY:HA2	1:B:519:ALA:HB2	1.48	0.92
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.52	0.90
1:A:18:GLU:HG2	1:A:401:ARG:NH2	1.84	0.90
1:B:233:ILE:HD12	1:B:262:ILE:HA	1.59	0.84
1:A:394:ARG:O	1:A:398:GLU:HG3	1.77	0.84
1:A:503:ARG:O	1:A:507:VAL:HG23	1.81	0.80
1:B:9:ALA:HB3	1:B:274:CYS:HA	1.66	0.76
1:A:441:LYS:HE3	1:A:443:LEU:HD21	1.68	0.76
1:B:143:GLU:HG2	5:B:834:HOH:O	1.88	0.73
1:A:523:ARG:HG3	1:A:534:LEU:HD12	1.71	0.73
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.71	0.73
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.70	0.72
1:B:451:CYS:HB2	5:B:716:HOH:O	1.89	0.72
1:B:422:ARG:HH12	1:B:474:LEU:HB2	1.54	0.71
1:B:22:PRO:O	1:B:25:PRO:HD3	1.92	0.70
1:B:93:PRO:HG3	1:B:561:TYR:HB2	1.74	0.70
1:A:314:LEU:HB3	1:A:321:VAL:HG13	1.74	0.69
1:B:498:ARG:HB3	1:B:498:ARG:NH1	2.09	0.68
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.75	0.68
1:B:498:ARG:HB3	1:B:498:ARG:HH11	1.58	0.67
1:A:32:ARG:NH1	1:A:495:PRO:HG3	2.10	0.67
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.77	0.67
1:A:303:CYS:HB3	1:A:311:CYS:SG	2.35	0.66
1:A:423:MET:CE	1:A:497:LEU:HD13	2.26	0.66
1:A:377:SER:HB2	1:A:379:LYS:HD2	1.76	0.66
1:A:74:LYS:O	1:A:77:THR:HG23	1.94	0.66
1:A:24:ASN:HB2	1:A:25:PRO:HD2	1.81	0.63
1:A:57:LEU:HD23	1:A:57:LEU:O	2.00	0.62
1:A:22:PRO:HG2	1:A:400:ALA:HB1	1.81	0.61
1:A:79:LYS:HG3	1:A:244:ASP:HB3	1.81	0.61
1:B:31:LEU:HD12	1:B:31:LEU:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:GLY:CA	1:B:519:ALA:HB2	2.25	0.61
1:A:523:ARG:HD3	5:A:3168:HOH:O	2.00	0.61
1:B:439:LEU:HB3	1:B:457:LEU:HD21	1.82	0.61
1:A:175:LEU:HD21	1:A:253:ILE:HG12	1.82	0.61
1:B:508:ARG:HG3	1:B:522:GLY:O	2.01	0.60
1:A:211:LYS:HE3	1:A:323:ILE:HG22	1.82	0.60
1:B:118:HIS:O	1:B:122:VAL:HG23	2.02	0.60
1:A:14:CYS:O	1:A:15:ALA:HB2	2.00	0.59
1:A:217:PHE:HA	5:A:3267:HOH:O	2.02	0.59
1:B:533:LYS:H	1:B:533:LYS:HD2	1.68	0.58
1:B:481:GLU:O	1:B:485:VAL:HG23	2.03	0.58
1:B:233:ILE:CD1	1:B:262:ILE:HA	2.33	0.58
1:B:434:LEU:HD12	1:B:507:VAL:HG13	1.86	0.58
1:A:508:ARG:CZ	1:A:530:VAL:HG11	2.34	0.57
1:A:445:CYS:SG	1:A:454:ILE:HD13	2.44	0.57
1:B:11:ILE:HD12	1:B:11:ILE:N	2.18	0.57
1:B:422:ARG:NH1	1:B:474:LEU:HB2	2.20	0.57
1:B:530:VAL:CG2	1:B:533:LYS:HG3	2.35	0.57
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.85	0.57
1:B:204:LEU:HD21	1:B:314:LEU:HD22	1.87	0.57
1:B:303:CYS:HG	1:B:311:CYS:CB	2.18	0.56
1:B:31:LEU:HB3	1:B:494:VAL:HG22	1.87	0.56
1:B:143:GLU:OE1	1:B:158:ARG:NH1	2.38	0.56
1:B:303:CYS:SG	1:B:311:CYS:SG	3.04	0.56
1:B:327:ALA:O	1:B:331:GLU:HB2	2.04	0.56
1:B:39:ALA:HB2	1:B:397:TRP:CH2	2.41	0.56
1:B:199:GLN:O	1:B:202:GLU:HB3	2.06	0.56
1:B:303:CYS:HB3	1:B:311:CYS:HG	1.71	0.55
1:A:18:GLU:HG2	1:A:401:ARG:CZ	2.36	0.55
1:A:134:ILE:HG13	1:A:259:ARG:HB3	1.88	0.55
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.88	0.55
1:A:461:GLN:HG2	1:A:541:ALA:HB3	1.89	0.55
1:B:109:ARG:HH11	1:B:109:ARG:HG2	1.72	0.55
1:A:56:ARG:HD3	1:A:56:ARG:N	2.23	0.54
1:B:354:PRO:HA	5:B:800:HOH:O	2.06	0.54
1:B:263:GLY:HA2	1:B:277:ARG:NH1	2.22	0.54
1:A:303:CYS:CB	1:A:311:CYS:HG	2.20	0.54
1:B:390:THR:O	1:B:394:ARG:HG2	2.08	0.54
1:A:388:PRO:HG2	1:A:488:CYS:SG	2.48	0.54
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.90	0.54
1:B:470:SER:O	1:B:474:LEU:HG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLU:HG2	1:B:240:TYR:CE2	2.44	0.53
1:A:346:TYR:O	1:A:347:SER:HB3	2.08	0.53
1:B:303:CYS:HB3	1:B:311:CYS:SG	2.49	0.53
1:B:409:LEU:HD12	1:B:409:LEU:O	2.09	0.53
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.39	0.53
1:B:507:VAL:O	1:B:511:LEU:HG	2.09	0.53
1:A:124:GLU:O	1:A:128:GLU:HG3	2.08	0.52
1:A:115:ALA:O	1:A:119:ILE:HG13	2.08	0.52
1:B:12:THR:HG21	1:B:270:LYS:HE2	1.92	0.52
1:B:182:LEU:N	1:B:183:PRO:HD2	2.25	0.52
1:B:346:TYR:O	1:B:347:SER:HB3	2.10	0.52
1:B:464:GLU:OE2	1:B:538:PRO:HA	2.10	0.52
1:B:196:SER:H	1:B:199:GLN:HB2	1.75	0.51
1:A:5:THR:O	1:A:275:GLY:HA3	2.10	0.51
1:B:108:VAL:O	1:B:111:LEU:HD23	2.10	0.51
1:B:141:LYS:NZ	1:B:158:ARG:HH22	2.08	0.51
1:B:94:PRO:HB3	1:B:106:LYS:HE2	1.93	0.51
1:A:123:TRP:CH2	1:A:174:ALA:HB2	2.46	0.51
1:A:108:VAL:HG21	1:A:165:LEU:HD21	1.93	0.51
1:A:215:MET:HG3	1:A:332:ASP:OD2	2.10	0.51
1:B:196:SER:OG	1:B:199:GLN:HG3	2.10	0.51
1:A:42:SER:HA	1:A:140:ALA:CB	2.40	0.50
1:B:160:ILE:HA	1:B:282:SER:OG	2.11	0.50
1:B:138:ILE:O	1:B:139:MET:HG2	2.11	0.50
1:B:303:CYS:CB	1:B:311:CYS:HG	2.24	0.50
1:A:13:PRO:HB3	1:A:17:GLU:OE2	2.12	0.50
1:A:68:LEU:HG	5:A:3249:HOH:O	2.11	0.50
1:A:436:GLN:O	1:A:437:GLU:HB2	2.12	0.50
1:B:268:ASN:HB2	5:B:707:HOH:O	2.12	0.50
1:A:374:HIS:O	1:A:474:LEU:HA	2.12	0.50
1:B:82:LEU:HD12	1:B:173:MET:O	2.12	0.50
1:B:459:LEU:O	1:B:463:ILE:HG13	2.12	0.50
1:A:21:LEU:HD23	1:A:34:HIS:HB2	1.94	0.49
1:A:303:CYS:CB	1:A:311:CYS:SG	3.00	0.49
1:B:204:LEU:HD21	1:B:314:LEU:CD2	2.42	0.49
1:B:246:ALA:O	1:B:247:PRO:C	2.51	0.49
1:B:141:LYS:HZ3	1:B:158:ARG:HH22	1.59	0.49
1:A:423:MET:HE2	1:A:497:LEU:HD13	1.93	0.49
1:B:221:THR:N	5:B:724:HOH:O	2.44	0.49
1:B:296:TYR:HB2	1:B:315:VAL:HG21	1.95	0.49
1:B:313:MET:SD	1:B:322:VAL:HG22	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:HIS:O	1:B:474:LEU:HA	2.13	0.49
1:A:57:LEU:HD23	1:A:57:LEU:C	2.33	0.48
1:B:231:SER:O	1:B:235:VAL:HG23	2.14	0.48
1:A:21:LEU:HD23	1:A:34:HIS:CB	2.43	0.48
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.94	0.48
1:A:454:ILE:N	1:A:454:ILE:HD12	2.28	0.48
1:B:215:MET:SD	1:B:215:MET:C	2.92	0.48
1:B:303:CYS:HG	1:B:311:CYS:HG	1.55	0.48
1:B:311:CYS:HA	1:B:324:CYS:HB3	1.96	0.48
1:A:461:GLN:HB3	1:A:545:LEU:HD11	1.95	0.48
1:B:408:TRP:O	1:B:412:ILE:HG13	2.13	0.48
1:B:497:LEU:HD21	1:B:501:ARG:HH21	1.79	0.48
1:A:187:MET:SD	1:A:292:THR:HG22	2.54	0.48
1:B:241:GLN:OE1	1:B:250:ARG:HG3	2.14	0.48
1:B:257:THR:O	1:B:262:ILE:HG23	2.14	0.48
1:B:540:PRO:C	1:B:542:ALA:H	2.18	0.47
1:A:254:ARG:HG2	1:B:251:GLN:NE2	2.30	0.47
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.96	0.47
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.54	0.47
1:A:26:LEU:O	1:A:29:SER:HB3	2.14	0.47
1:B:182:LEU:O	1:B:186:VAL:HG23	2.15	0.47
1:A:508:ARG:HH11	1:A:508:ARG:HG2	1.80	0.47
1:A:545:LEU:HB3	1:A:547:LEU:HD13	1.96	0.47
1:B:422:ARG:HG2	1:B:426:MET:HE3	1.95	0.47
1:A:14:CYS:O	1:A:15:ALA:CB	2.63	0.47
1:B:134:ILE:HG13	1:B:259:ARG:HB3	1.96	0.47
1:B:464:GLU:OE1	1:B:539:ILE:HB	2.14	0.47
1:B:359:ASP:HB3	1:B:362:LEU:HG	1.96	0.47
1:A:334:ALA:HA	5:A:3149:HOH:O	2.15	0.47
1:A:434:LEU:HD13	1:A:434:LEU:C	2.34	0.47
1:B:375:ASP:OD1	1:B:379:LYS:HB3	2.14	0.47
1:B:23:ILE:O	1:B:24:ASN:HB2	2.15	0.46
1:A:120:ARG:O	1:A:124:GLU:HG2	2.15	0.46
1:A:48:ARG:HD3	1:A:157:ALA:O	2.16	0.46
1:A:175:LEU:HD21	1:A:253:ILE:CD1	2.45	0.46
1:B:143:GLU:CD	1:B:158:ARG:HH12	2.18	0.46
1:B:505:ARG:HG3	1:B:529:ALA:HB1	1.98	0.46
1:B:191:TYR:CZ	1:B:193:PHE:HB2	2.51	0.46
1:A:21:LEU:HD12	1:A:22:PRO:HD2	1.97	0.46
1:A:24:ASN:ND2	1:A:400:ALA:HA	2.30	0.46
1:A:438:GLN:HE21	1:A:438:GLN:HB2	1.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:VAL:HB	5:B:790:HOH:O	2.15	0.46
1:B:177:ASP:O	1:B:181:THR:HG23	2.16	0.46
1:B:201:VAL:O	1:B:205:VAL:HG23	2.15	0.46
1:A:175:LEU:HD21	1:A:253:ILE:CG1	2.46	0.46
1:B:419:LEU:HB2	1:B:477:TYR:CE1	2.51	0.46
1:A:444:ASP:HA	1:A:452:TYR:O	2.16	0.45
1:B:67:VAL:O	1:B:71:MET:HG3	2.17	0.45
1:B:306:ALA:HB2	1:B:339:PHE:N	2.32	0.45
1:A:434:LEU:HD13	1:A:434:LEU:O	2.16	0.45
1:B:6:TRP:CZ2	1:B:49:GLN:HG2	2.52	0.45
1:B:535:LYS:N	1:B:535:LYS:HD2	2.32	0.45
1:B:32:ARG:O	1:B:34:HIS:N	2.46	0.45
1:A:24:ASN:CB	1:A:25:PRO:HD2	2.46	0.45
1:B:128:GLU:HA	5:B:705:HOH:O	2.16	0.45
1:B:170:CYS:HA	1:B:173:MET:HE3	1.98	0.45
1:B:361:GLU:HG3	1:B:370:VAL:O	2.17	0.45
1:A:56:ARG:HD3	1:A:56:ARG:H	1.81	0.45
1:A:401:ARG:NH1	1:A:401:ARG:HG3	2.32	0.45
1:A:51:LYS:HD2	1:A:223:CYS:SG	2.57	0.45
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.86	0.45
1:A:215:MET:HB2	1:A:326:SER:HB2	1.99	0.44
1:B:207:THR:O	1:B:210:SER:OG	2.34	0.44
1:B:254:ARG:NH2	1:B:258:GLU:HG2	2.32	0.44
1:A:237:GLU:HA	1:A:240:TYR:CD2	2.52	0.44
1:B:61:ASP:HB2	5:B:796:HOH:O	2.17	0.44
1:B:489:LEU:HD22	1:B:494:VAL:HB	1.99	0.44
1:A:424:ILE:HG23	1:A:500:TRP:CZ2	2.52	0.44
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.80	0.44
1:B:56:ARG:N	1:B:56:ARG:HD3	2.33	0.44
1:B:201:VAL:CG2	1:B:384:LEU:HB2	2.47	0.44
1:B:224:PHE:O	1:B:227:THR:HG23	2.18	0.44
1:B:368:SER:HB2	1:B:385:THR:O	2.17	0.44
1:A:48:ARG:HD2	1:A:48:ARG:HA	1.76	0.44
1:B:109:ARG:HG2	1:B:109:ARG:NH1	2.33	0.44
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.58	0.43
1:A:422:ARG:HB2	3:A:3002:1NU:F28	2.08	0.43
1:A:207:THR:HG22	1:A:323:ILE:HG21	2.00	0.43
1:B:280:ARG:HG3	1:B:281:ALA:O	2.19	0.43
1:A:452:TYR:OH	1:A:562:HIS:HD2	2.01	0.43
1:B:19:SER:HA	1:B:39:ALA:HB3	2.00	0.43
1:A:508:ARG:HG2	1:A:508:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:O	1:A:69:LYS:HG3	2.18	0.43
1:A:336:LEU:HD23	1:A:336:LEU:HA	1.74	0.43
1:A:401:ARG:HG3	1:A:401:ARG:HH11	1.83	0.43
1:B:36:MET:O	1:B:146:CYS:HA	2.17	0.43
1:B:489:LEU:HD22	1:B:494:VAL:CG1	2.48	0.43
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.84	0.43
1:A:196:SER:H	1:A:199:GLN:HB2	1.84	0.43
1:B:545:LEU:HD23	5:B:840:HOH:O	2.19	0.43
1:B:184:GLN:HB2	5:B:741:HOH:O	2.19	0.43
1:B:451:CYS:HB3	1:B:561:TYR:HD1	1.83	0.42
1:B:455:GLU:HB2	1:B:458:ASP:OD2	2.18	0.42
1:A:485:VAL:O	1:A:489:LEU:HG	2.19	0.42
1:B:170:CYS:HA	1:B:173:MET:CE	2.49	0.42
1:B:403:THR:HA	1:B:404:PRO:HD3	1.81	0.42
1:B:14:CYS:HB3	1:B:269:SER:HB2	2.02	0.42
1:B:309:GLN:O	1:B:324:CYS:HB2	2.19	0.42
1:B:100:LYS:NZ	5:B:811:HOH:O	2.52	0.42
1:B:165:LEU:HD13	1:B:168:ARG:NH2	2.35	0.42
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.37	0.42
1:A:160:ILE:O	1:A:160:ILE:HG13	2.20	0.42
1:B:108:VAL:HG21	1:B:165:LEU:HD21	2.02	0.42
1:B:459:LEU:N	1:B:460:PRO:CD	2.83	0.41
1:A:404:PRO:HD2	5:A:3131:HOH:O	2.19	0.41
1:B:520:THR:HG22	1:B:524:TYR:HE1	1.84	0.41
1:A:416:ALA:N	1:A:417:PRO:HD2	2.35	0.41
1:B:39:ALA:O	1:B:41:THR:HG23	2.21	0.41
1:B:398:GLU:OE1	1:B:408:TRP:HD1	2.03	0.41
1:A:523:ARG:HB2	1:A:523:ARG:CZ	2.51	0.41
1:B:389:THR:HA	1:B:488:CYS:SG	2.61	0.41
1:B:465:ARG:HG2	1:B:545:LEU:HB3	2.03	0.41
1:B:141:LYS:NZ	1:B:158:ARG:NH2	2.69	0.41
1:B:144:VAL:HB	1:B:394:ARG:HB3	2.03	0.41
1:B:198:LYS:C	5:B:790:HOH:O	2.59	0.41
1:A:72:LYS:HB3	1:B:76:SER:HB2	2.03	0.41
1:A:93:PRO:O	1:A:105:ALA:HB1	2.21	0.41
1:B:419:LEU:HD11	1:B:423:MET:HE3	2.03	0.41
1:B:267:THR:HG23	1:B:272:GLN:O	2.20	0.40
1:A:390:THR:HB	1:A:391:PRO:HD3	2.03	0.40
1:A:445:CYS:HB2	5:A:3174:HOH:O	2.20	0.40
1:B:198:LYS:O	1:B:198:LYS:HG3	2.21	0.40
1:B:427:THR:O	1:B:431:SER:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:THR:HA	1:B:267:THR:O	2.21	0.40
1:B:497:LEU:HD21	1:B:501:ARG:NH2	2.35	0.40
1:A:292:THR:OG1	1:A:317:GLY:N	2.49	0.40
1:A:423:MET:HE2	1:A:497:LEU:CD1	2.51	0.40
1:A:539:ILE:O	1:A:542:ALA:HB3	2.22	0.40
1:B:22:PRO:HG2	1:B:400:ALA:HB1	2.04	0.40
1:B:217:PHE:CE1	1:B:322:VAL:HB	2.56	0.40
1:B:547:LEU:O	1:B:550:TRP:HB2	2.22	0.40
1:A:160:ILE:HA	1:A:282:SER:OG	2.22	0.40
1:A:441:LYS:HE3	1:A:443:LEU:CD2	2.44	0.40
1:A:505:ARG:NE	5:A:3265:HOH:O	2.53	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	556/576 (96%)	515 (93%)	38 (7%)	3 (0%)	29 68
1	B	556/576 (96%)	499 (90%)	47 (8%)	10 (2%)	8 37
All	All	1112/1152 (96%)	1014 (91%)	85 (8%)	13 (1%)	13 48

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ALA
1	B	33	HIS
1	B	525	LEU
1	B	530	VAL
1	B	541	ALA
1	A	533	LYS
1	B	495	PRO

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Mol	Chain	Res	Type
1	B	515	GLY
1	B	22	PRO
1	A	33	HIS
1	B	247	PRO
1	B	400	ALA
1	B	540	PRO

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	477/491 (97%)	463 (97%)	14 (3%)	42	76
1	B	477/491 (97%)	465 (98%)	12 (2%)	47	79
All	All	954/982 (97%)	928 (97%)	26 (3%)	44	77

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	57	LEU
1	A	182	LEU
1	A	230	GLU
1	A	245	LEU
1	A	278	ARG
1	A	336	LEU
1	A	379	LYS
1	A	402	HIS
1	A	431	SER
1	A	438	GLN
1	A	505	ARG
1	A	544	GLN
1	A	547	LEU
1	B	34	HIS
1	B	50	LYS
1	B	139	MET

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Mol	Chain	Res	Type
1	B	182	LEU
1	B	303	CYS
1	B	311	CYS
1	B	315	VAL
1	B	352	ASP
1	B	383	TYR
1	B	520	THR
1	B	521	CYS
1	B	534	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	A	273	ASN
1	A	406	ASN
1	A	438	GLN
1	A	544	GLN
1	A	562	HIS
1	B	34	HIS
1	B	148	GLN
1	B	206	ASN
1	B	251	GLN
1	B	446	GLN
1	B	467	HIS
1	B	514	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 monosaccharides in this entry.

5.6 Ligand geometry

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
3	1NU	B	602	-	35,35,35	2.21	15 (42%)	49,52,52	2.06	13 (26%)
2	GOL	A	3001	-	5,5,5	0.45	0	5,5,5	0.18	0
3	1NU	A	3002	-	35,35,35	1.93	11 (31%)	49,52,52	1.83	11 (22%)
2	GOL	B	601	-	5,5,5	0.43	0	5,5,5	0.18	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	1NU	B	602	-	-	0/14/14/14	0/4/4/4
2	GOL	A	3001	-	-	0/4/4/4	-
3	1NU	A	3002	-	-	0/14/14/14	0/4/4/4
2	GOL	B	601	-	-	0/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	1NU	C11-N10	4.91	1.46	1.40
3	B	602	1NU	C25-C26	4.14	1.44	1.39
3	A	3002	1NU	C11-N10	4.00	1.45	1.40
3	A	3002	1NU	C25-C26	3.82	1.44	1.39
3	B	602	1NU	C6-C5	3.81	1.44	1.38
3	B	602	1NU	C12-C11	3.24	1.46	1.41
3	B	602	1NU	C21-C26	3.21	1.45	1.39
3	B	602	1NU	C16-C15	3.01	1.44	1.38
3	A	3002	1NU	C4-C5	2.91	1.42	1.37
3	A	3002	1NU	C6-C1	2.90	1.43	1.38
3	A	3002	1NU	C7-N10	2.85	1.51	1.47
3	A	3002	1NU	C21-C26	2.81	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	1NU	C6-C1	2.77	1.42	1.38
3	B	602	1NU	C16-C11	2.76	1.44	1.39
3	A	3002	1NU	C12-C11	2.69	1.45	1.41
3	B	602	1NU	C2-C3	2.63	1.42	1.37
3	A	3002	1NU	C4-C3	2.56	1.42	1.37
3	B	602	1NU	C2-C1	2.51	1.41	1.37
3	B	602	1NU	C7-N10	2.48	1.50	1.47
3	B	602	1NU	C15-C14	2.38	1.43	1.38
3	B	602	1NU	C4-C5	2.31	1.41	1.37
3	B	602	1NU	C13-C12	2.25	1.43	1.39
3	A	3002	1NU	C9-N10	2.20	1.39	1.36
3	A	3002	1NU	C6-C5	2.20	1.41	1.38
3	B	602	1NU	C4-C3	2.10	1.41	1.37
3	A	3002	1NU	C2-C1	2.03	1.41	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	1NU	C16-C11-N10	8.71	126.68	121.16
3	A	3002	1NU	C16-C11-N10	7.24	125.75	121.16
3	A	3002	1NU	C4-C5-C6	-4.34	121.55	124.59
3	B	602	1NU	C4-C5-C6	-3.99	121.79	124.59
3	B	602	1NU	C2-C1-C6	-3.86	121.88	124.59
3	B	602	1NU	C13-C12-C11	3.48	122.79	118.73
3	A	3002	1NU	C13-C12-C11	3.18	122.44	118.73
3	A	3002	1NU	C2-C1-C6	-3.09	122.42	124.59
3	A	3002	1NU	N10-C9-N8	3.09	129.03	126.36
3	B	602	1NU	C11-C12-C17	-2.94	117.87	120.27
3	A	3002	1NU	C11-C12-C17	-2.73	118.04	120.27
3	B	602	1NU	N10-C9-N8	2.69	128.69	126.36
3	B	602	1NU	F32-C5-C6	2.55	120.67	117.63
3	B	602	1NU	C16-C11-C12	-2.45	115.27	119.10
3	B	602	1NU	C5-C4-C3	2.35	119.09	116.62
3	B	602	1NU	F31-C1-C6	2.34	120.43	117.63
3	B	602	1NU	O18-C17-C12	-2.33	117.98	121.54
3	A	3002	1NU	F31-C1-C6	2.31	120.38	117.63
3	A	3002	1NU	C16-C11-C12	-2.30	115.50	119.10
3	B	602	1NU	C1-C2-C3	2.27	119.01	116.62
3	A	3002	1NU	C1-C2-C3	2.26	119.00	116.62
3	A	3002	1NU	C5-C4-C3	2.23	118.96	116.62
3	B	602	1NU	C21-O20-C14	2.04	123.09	118.00
3	A	3002	1NU	O18-C17-C12	-2.00	118.49	121.54

There are no chirality outliers.

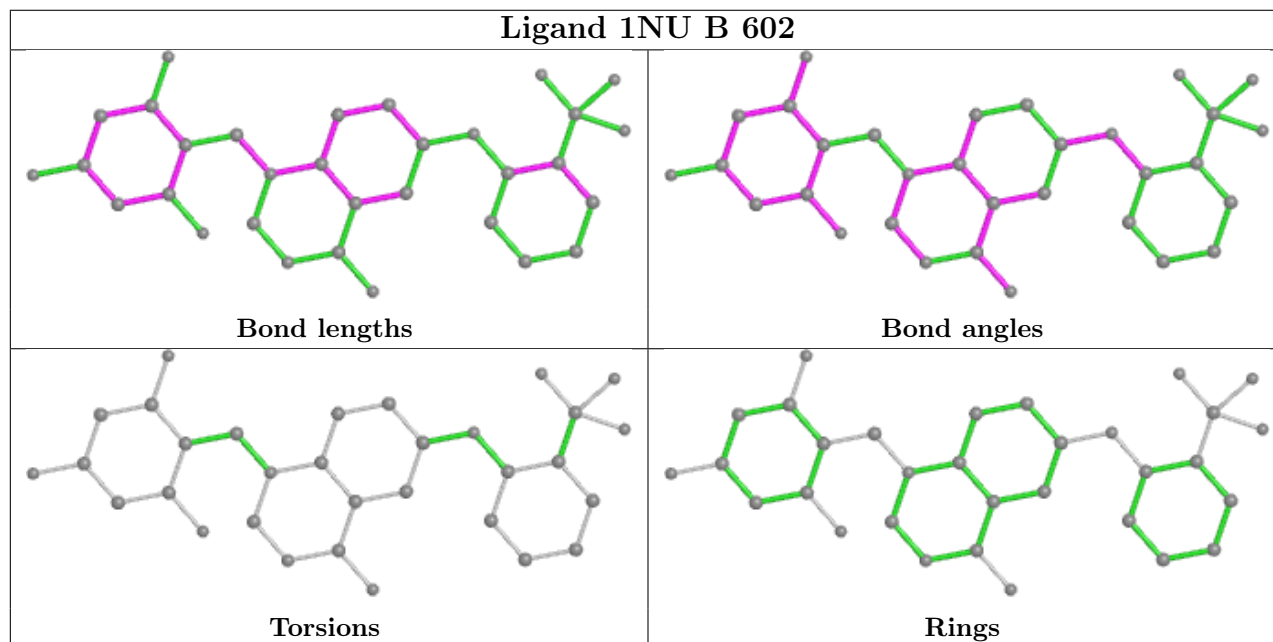
There are no torsion outliers.

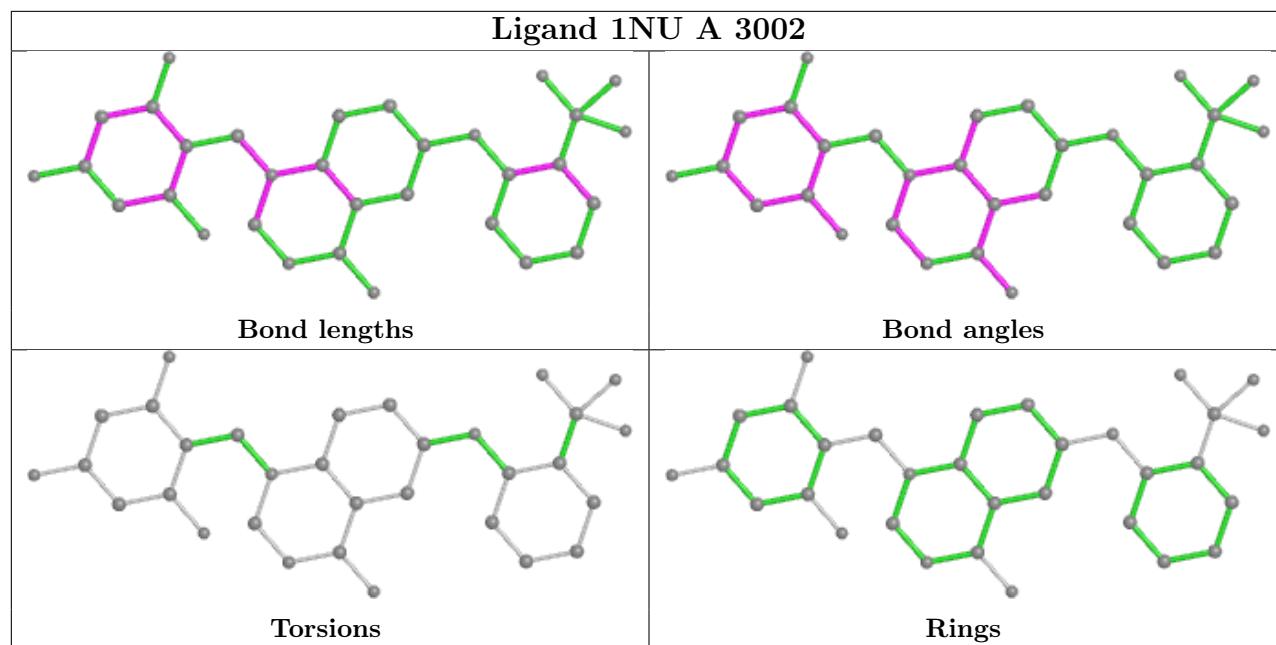
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3002	1NU	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	560/576 (97%)	-0.66	0 100 100	16, 36, 59, 79	0
1	B	560/576 (97%)	-0.40	1 (0%) 95 87	19, 50, 91, 103	0
All	All	1120/1152 (97%)	-0.53	1 (0%) 95 89	16, 42, 80, 103	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	ASN	2.3

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 monosaccharides 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.

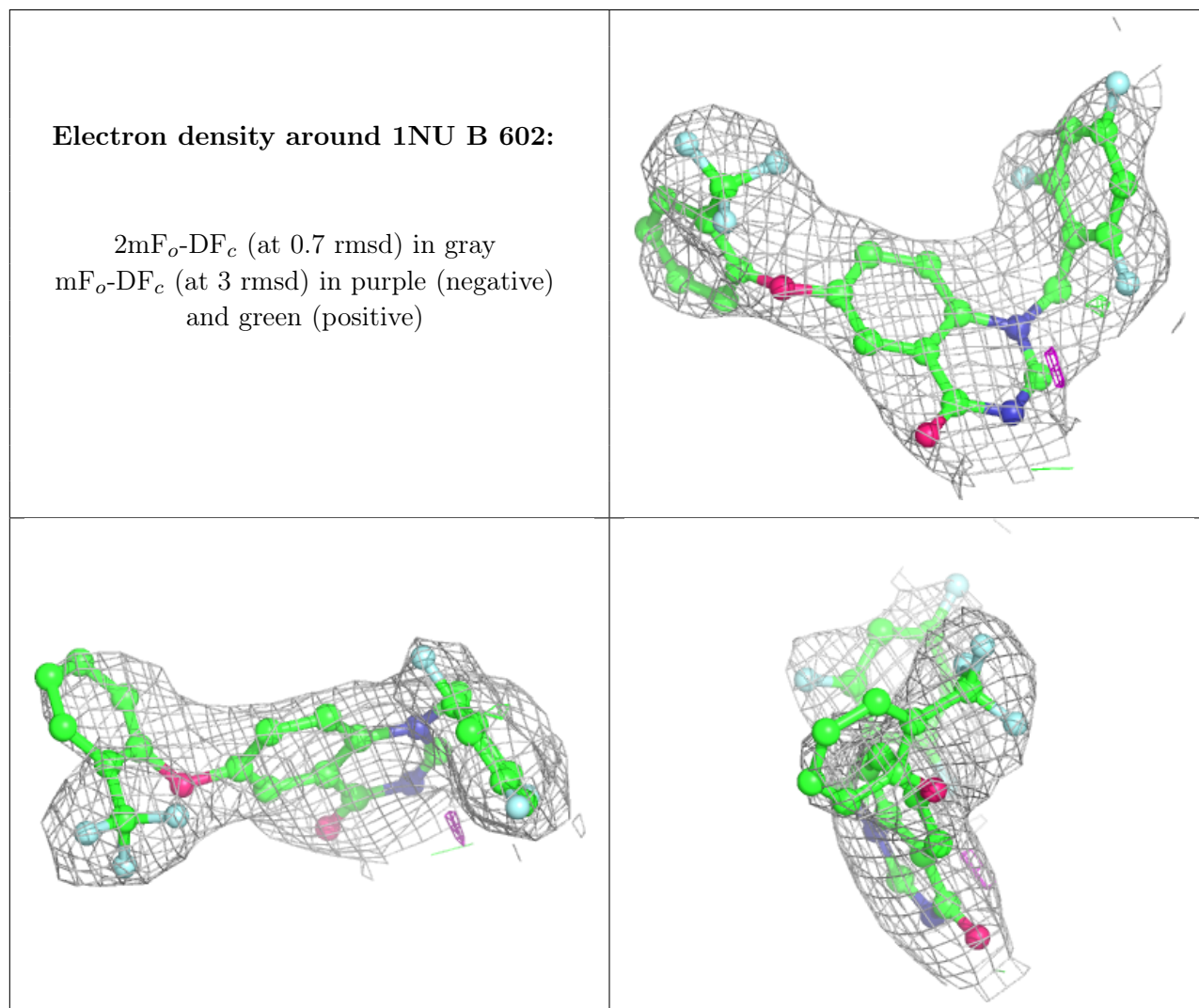
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	B	604	1/1	0.70	0.40	56,56,56,56	0
4	MG	A	3003	1/1	0.76	0.24	46,46,46,46	0
4	MG	A	3004	1/1	0.87	0.24	44,44,44,44	0
3	1NU	B	602	32/32	0.91	0.24	57,64,70,72	0

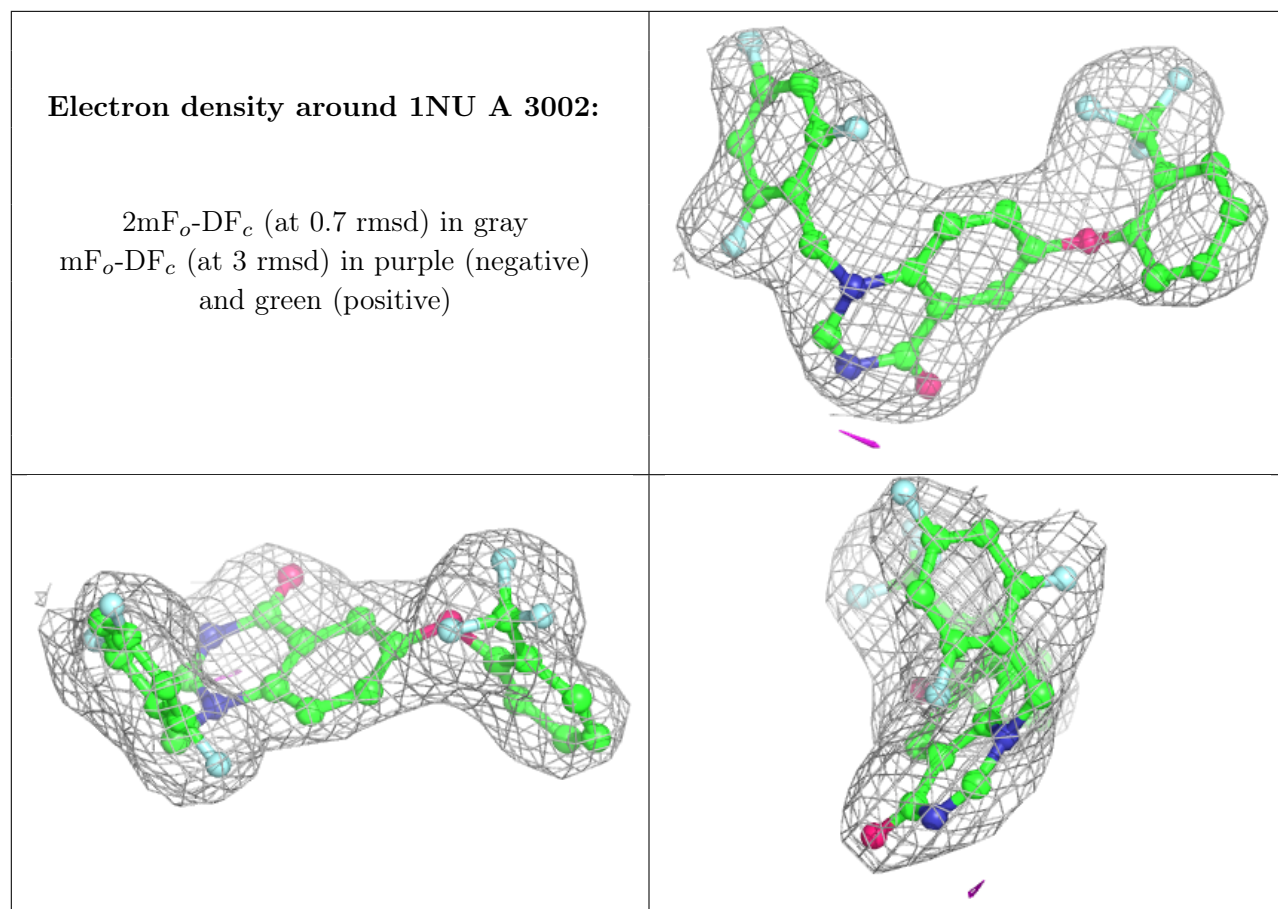
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	A	3001	6/6	0.92	0.22	50,52,53,53	0
2	GOL	B	601	6/6	0.92	0.26	44,46,47,48	0
4	MG	B	603	1/1	0.93	0.27	46,46,46,46	0
3	1NU	A	3002	32/32	0.96	0.18	37,43,52,54	0

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 [i](#)

There are no such residues in this entry.