



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:24 AM UTC

PDB ID : 7QY9 / pdb_00007qy9
Title : The structure of T.forsythia NanH with oseltamivir
Authors : Rafferty, J.; Stafford, G.; Satur, M.
Deposited on : 2022-01-27
Resolution : 1.92 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

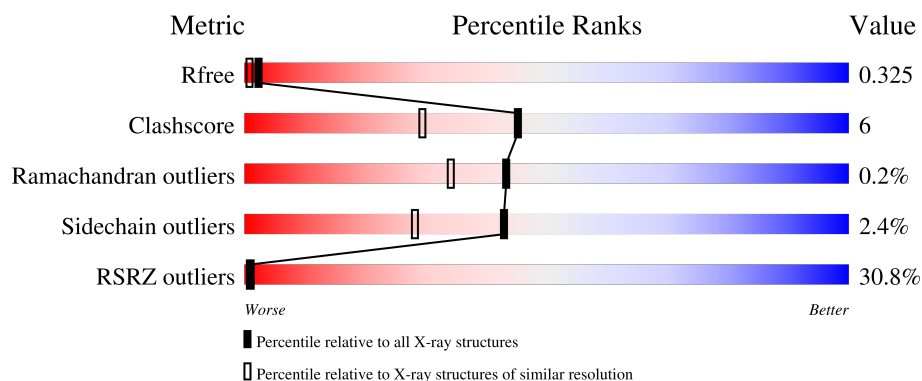
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	519	23% 86% 13%
1	B	519	39% 90% 9%

2 Entry composition [i](#)

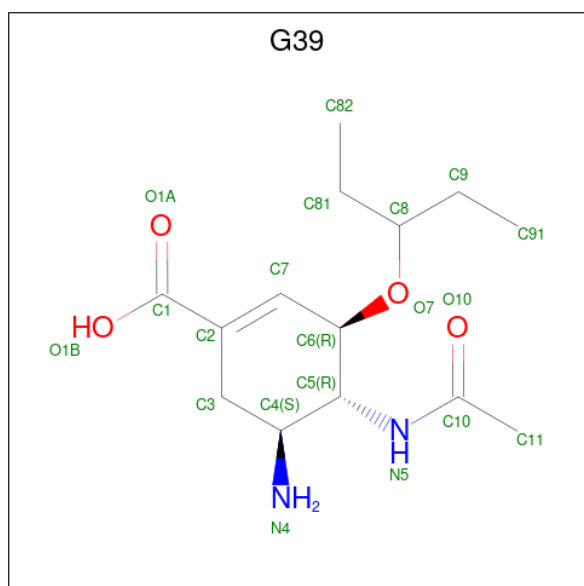
There are 3 unique types of molecules in this entry. The entry contains 16438 atoms, of which 8052 are hydrogens and 0 are deuteriums.

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 BNR/Asp-box repeat protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	519	Total	C	H	N	O	S	126	0	0
			8029	2505	4004	724	776	20			
1	B	519	Total	C	H	N	O	S	126	0	0
			8023	2503	4002	724	774	20			

- Molecule 2 is (3R,4R,5S)-4-(acetylamino)-5-amino-3-(pentan-3-yloxy)cyclohex-1-ene-1-carboxylic acid (CCD ID: G39) (formula: C₁₄H₂₄N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O		0	0
			43	14	23	2	4			
2	B	1	Total	C	H	N	O		0	0
			43	14	23	2	4			

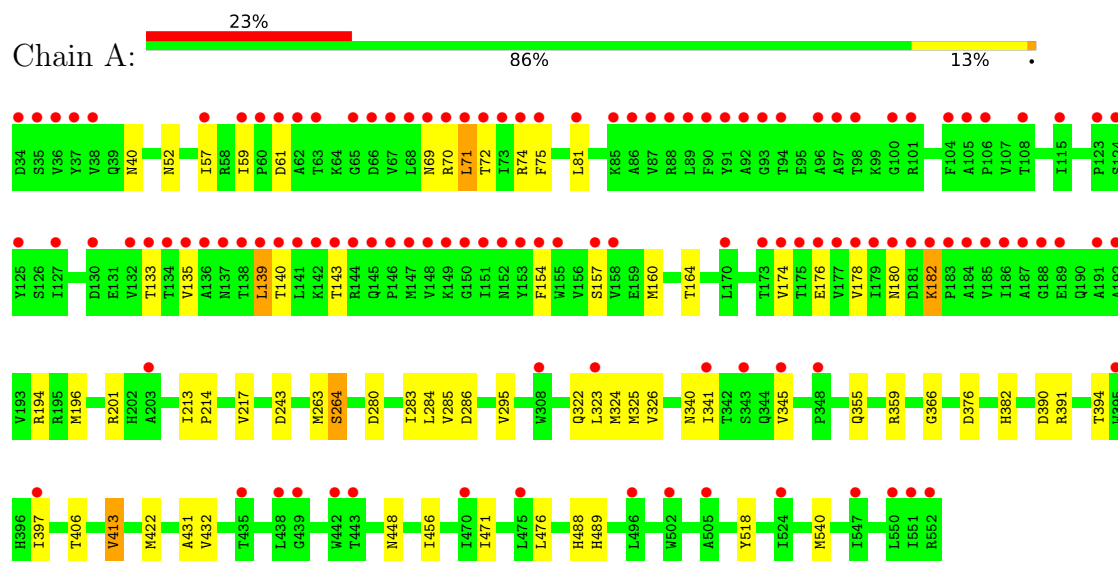
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total 161	O 161	0	0
3	B	139	Total 139	O 139	0	0

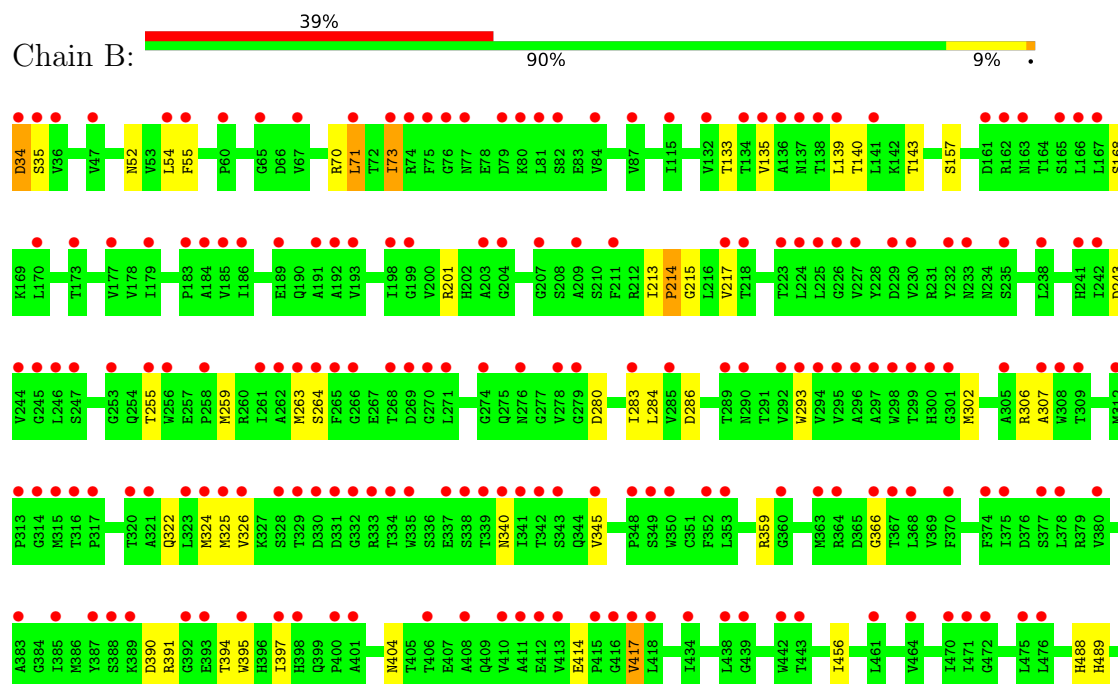
3 Residue-property plots

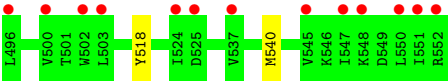
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: BNR/Asp-box repeat protein



- Molecule 1: BNR/Asp-box repeat protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	79.50Å 79.50Å 348.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.63 – 1.92 77.63 – 1.92	Depositor EDS
% Data completeness (in resolution range)	95.1 (77.63-1.92) 93.0 (77.63-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.313 , 0.346 0.295 , 0.325	Depositor DCC
R_{free} test set	4324 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 27.5	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	0.89	EDS
Total number of atoms	16438	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 3.51% 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: G39

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	1.00	0/4103	1.23	0/5572
1	B	1.01	0/4099	1.23	3/5567 (0.1%)
All	All	1.00	0/8202	1.23	3/11139 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	PRO	CA-C-N	5.21	125.62	121.61
1	B	214	PRO	C-N-CA	5.21	125.62	121.61
1	B	215	GLY	CA-C-O	-5.07	117.16	121.57

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	4025	4004	3989	51	0
1	B	4021	4002	3985	44	0
2	A	20	23	23	1	0
2	B	20	23	23	0	0
3	A	161	0	0	0	0
3	B	139	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8386	8052	8020	95	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 (95) 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:160:MET:HG3	1:A:196:MET:HE1	1.39	1.00
1:B:302:MET:HE1	1:B:307:ALA:HA	1.43	0.98
1:B:322:GLN:HB3	1:B:324:MET:HE3	1.53	0.91
1:A:322:GLN:HB3	1:A:324:MET:HE3	1.60	0.83
1:B:201:ARG:HH11	1:B:259:MET:HE2	1.48	0.78
1:A:324:MET:HE1	1:A:340:ASN:CG	2.08	0.78
1:B:324:MET:HE1	1:B:340:ASN:CG	2.12	0.74
1:A:243:ASP:CG	1:A:264:SER:HG	2.01	0.69
1:B:322:GLN:CB	1:B:324:MET:HE3	2.22	0.68
1:B:213:ILE:HG21	1:B:280:ASP:HA	1.77	0.67
1:B:302:MET:HE1	1:B:307:ALA:CA	2.24	0.67
1:A:243:ASP:CG	1:A:264:SER:OG	2.39	0.66
1:A:213:ILE:HG21	1:A:280:ASP:HA	1.79	0.65
1:A:432:VAL:H	1:A:448:ASN:HD22	1.46	0.63
1:B:488:HIS:HD2	1:B:489:HIS:ND1	1.96	0.62
1:B:201:ARG:HH11	1:B:259:MET:CE	2.13	0.61
1:B:54:LEU:HD12	1:B:55:PHE:CD2	2.36	0.61
1:A:160:MET:HG3	1:A:196:MET:CE	2.23	0.61
1:A:263:MET:HE1	1:A:324:MET:HB3	1.84	0.58
1:B:286:ASP:HB2	1:B:293:TRP:HZ3	1.69	0.58
1:A:263:MET:HE3	1:A:326:VAL:HG13	1.85	0.57
1:A:322:GLN:CB	1:A:324:MET:HE3	2.31	0.57
1:B:139:LEU:HD23	1:B:140:THR:N	2.21	0.56
1:A:57:ILE:HD11	1:A:154:PHE:HB2	1.88	0.55
1:B:414:GLU:HB2	1:B:417:VAL:CG1	2.37	0.55
1:B:135:VAL:HG13	1:B:139:LEU:HD12	1.89	0.54
1:A:263:MET:CE	1:A:324:MET:HB3	2.39	0.52
1:A:488:HIS:HD2	1:A:489:HIS:CD2	2.27	0.52
1:B:325:MET:HE1	1:B:395:TRP:CZ2	2.45	0.52
1:B:70:ARG:HG2	1:B:140:THR:HG23	1.92	0.51
1:B:71:LEU:C	1:B:71:LEU:HD12	2.34	0.51
1:A:263:MET:HE1	1:A:324:MET:CB	2.41	0.51
1:B:201:ARG:HB2	1:B:540:MET:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ASP:CB	1:B:293:TRP:HZ3	2.24	0.50
1:A:164:THR:HG21	1:A:196:MET:HE2	1.93	0.50
1:A:70:ARG:HB2	1:A:178:VAL:CG2	2.41	0.50
1:A:488:HIS:HD2	1:A:489:HIS:HD2	1.59	0.50
1:A:217:VAL:HB	1:A:285:VAL:HG23	1.94	0.50
1:A:71:LEU:CD1	1:A:174:VAL:HG13	2.42	0.50
1:A:201:ARG:HB2	1:A:540:MET:HB2	1.94	0.49
1:A:295:VAL:HB	1:A:325:MET:HE2	1.95	0.49
1:B:71:LEU:CD1	1:B:73:ILE:CD1	2.91	0.49
1:B:54:LEU:HD12	1:B:55:PHE:CE2	2.48	0.48
1:B:286:ASP:HB2	1:B:293:TRP:CZ3	2.46	0.48
1:B:293:TRP:CD1	1:B:325:MET:HE2	2.48	0.48
1:A:366:GLY:O	1:A:391:ARG:NH2	2.47	0.48
1:A:180:ASN:O	1:A:182:LYS:HD3	2.13	0.48
1:A:283:ILE:O	1:A:359:ARG:HA	2.14	0.47
1:B:366:GLY:O	1:B:391:ARG:NH2	2.46	0.47
1:A:390:ASP:OD2	1:A:394:THR:OG1	2.32	0.47
1:A:69:ASN:HB2	1:A:178:VAL:HG23	1.95	0.47
1:B:217:VAL:HG13	1:B:283:ILE:HG23	1.97	0.47
1:A:70:ARG:HB2	1:A:178:VAL:HG22	1.97	0.47
1:B:71:LEU:CD1	1:B:73:ILE:HD12	2.45	0.46
1:B:302:MET:CE	1:B:307:ALA:HA	2.29	0.46
1:B:283:ILE:O	1:B:359:ARG:HA	2.16	0.46
1:A:323:LEU:O	1:A:324:MET:HE2	2.16	0.46
1:B:54:LEU:C	1:B:54:LEU:HD13	2.42	0.45
1:A:139:LEU:HD23	1:A:140:THR:N	2.32	0.45
1:A:286:ASP:OD1	1:A:391:ARG:NH1	2.49	0.45
1:A:57:ILE:CG1	1:A:154:PHE:HB2	2.46	0.45
1:A:217:VAL:HG13	1:A:283:ILE:HG23	1.98	0.45
1:B:286:ASP:OD1	1:B:391:ARG:NH1	2.49	0.45
1:A:52:ASN:O	1:A:157:SER:HA	2.17	0.45
1:B:284:LEU:HD12	1:B:284:LEU:C	2.42	0.44
1:A:345:VAL:HB	1:A:397:ILE:HD12	1.99	0.44
1:B:293:TRP:HD1	1:B:325:MET:HE2	1.83	0.44
1:A:243:ASP:OD1	1:A:264:SER:OG	2.24	0.44
1:B:390:ASP:OD2	1:B:394:THR:OG1	2.31	0.44
1:B:243:ASP:OD1	1:B:264:SER:OG	2.30	0.44
1:B:263:MET:HE2	1:B:326:VAL:HG13	1.99	0.44
1:A:214:PRO:HD2	1:A:518:TYR:HB3	1.99	0.44
1:B:54:LEU:CD1	1:B:55:PHE:CE2	3.00	0.44
1:A:75:PHE:CG	1:A:81:LEU:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ASN:O	1:B:157:SER:HA	2.17	0.43
1:B:293:TRP:CZ2	1:B:391:ARG:O	2.71	0.43
1:A:284:LEU:HD12	1:A:284:LEU:C	2.43	0.43
1:B:201:ARG:NH1	1:B:259:MET:HE2	2.25	0.43
1:A:376:ASP:OD2	1:A:382:HIS:HE1	2.02	0.43
1:B:293:TRP:CH2	1:B:391:ARG:O	2.71	0.43
1:A:71:LEU:HD12	1:A:174:VAL:HG13	2.01	0.42
1:A:422:MET:HB2	1:A:431:ALA:HB3	2.02	0.42
1:B:345:VAL:HB	1:B:397:ILE:HD12	2.02	0.41
1:A:341:ILE:O	1:A:341:ILE:HG22	2.21	0.41
1:A:280:ASP:O	1:A:355:GLN:NE2	2.49	0.41
1:A:57:ILE:HD11	1:A:154:PHE:CD1	2.55	0.41
1:A:135:VAL:HG13	1:A:139:LEU:HD12	2.03	0.41
1:A:413:VAL:HG12	1:A:476:LEU:HD11	2.03	0.41
1:B:214:PRO:HD2	1:B:518:TYR:HB3	2.02	0.41
1:A:488:HIS:CD2	1:A:489:HIS:HD2	2.39	0.41
1:B:34:ASP:OD1	1:B:34:ASP:N	2.54	0.41
1:A:406:THR:HG21	2:A:601:G39:H911	2.03	0.40
1:A:72:THR:OG1	1:A:176:GLU:HB3	2.20	0.40
1:B:306:ARG:HA	1:B:306:ARG:NE	2.37	0.40
1:A:40:ASN:OD1	1:A:194:ARG:HD3	2.22	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	517/519 (100%)	491 (95%)	25 (5%)	1 (0%)	43	34
1	B	517/519 (100%)	490 (95%)	26 (5%)	1 (0%)	43	34
All	All	1034/1038 (100%)	981 (95%)	51 (5%)	2 (0%)	43	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	ILE
1	B	456	ILE

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	446/446 (100%)	435 (98%)	11 (2%)	42	26
1	B	445/446 (100%)	435 (98%)	10 (2%)	45	32
All	All	891/892 (100%)	870 (98%)	21 (2%)	43	28

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	61	ASP
1	A	71	LEU
1	A	74	ARG
1	A	133	THR
1	A	139	LEU
1	A	143	THR
1	A	182	LYS
1	A	264	SER
1	A	413	VAL
1	A	471	ILE
1	B	34	ASP
1	B	35	SER
1	B	71	LEU
1	B	73	ILE
1	B	133	THR
1	B	143	THR
1	B	168	SER
1	B	255	THR
1	B	404	ASN
1	B	417	VAL

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	163	ASN
1	A	382	HIS
1	A	448	ASN
1	A	488	HIS
1	B	163	ASN
1	B	304	ASN
1	B	488	HIS

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](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	G39	A	601	-	19,20,20	0.76	1 (5%)	20,27,27	1.18	1 (5%)
2	G39	B	601	-	19,20,20	0.85	1 (5%)	20,27,27	1.03	1 (5%)

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
2	G39	A	601	-	-	0/16/32/32	0/1/1/1
2	G39	B	601	-	-	1/16/32/32	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	G39	O1B-C1	-2.86	1.22	1.30
2	B	601	G39	O1B-C1	-2.71	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	G39	C4-C3-C2	3.34	113.50	109.72
2	B	601	G39	C4-C3-C2	3.22	113.36	109.72

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	G39	C9-C8-C81-C82

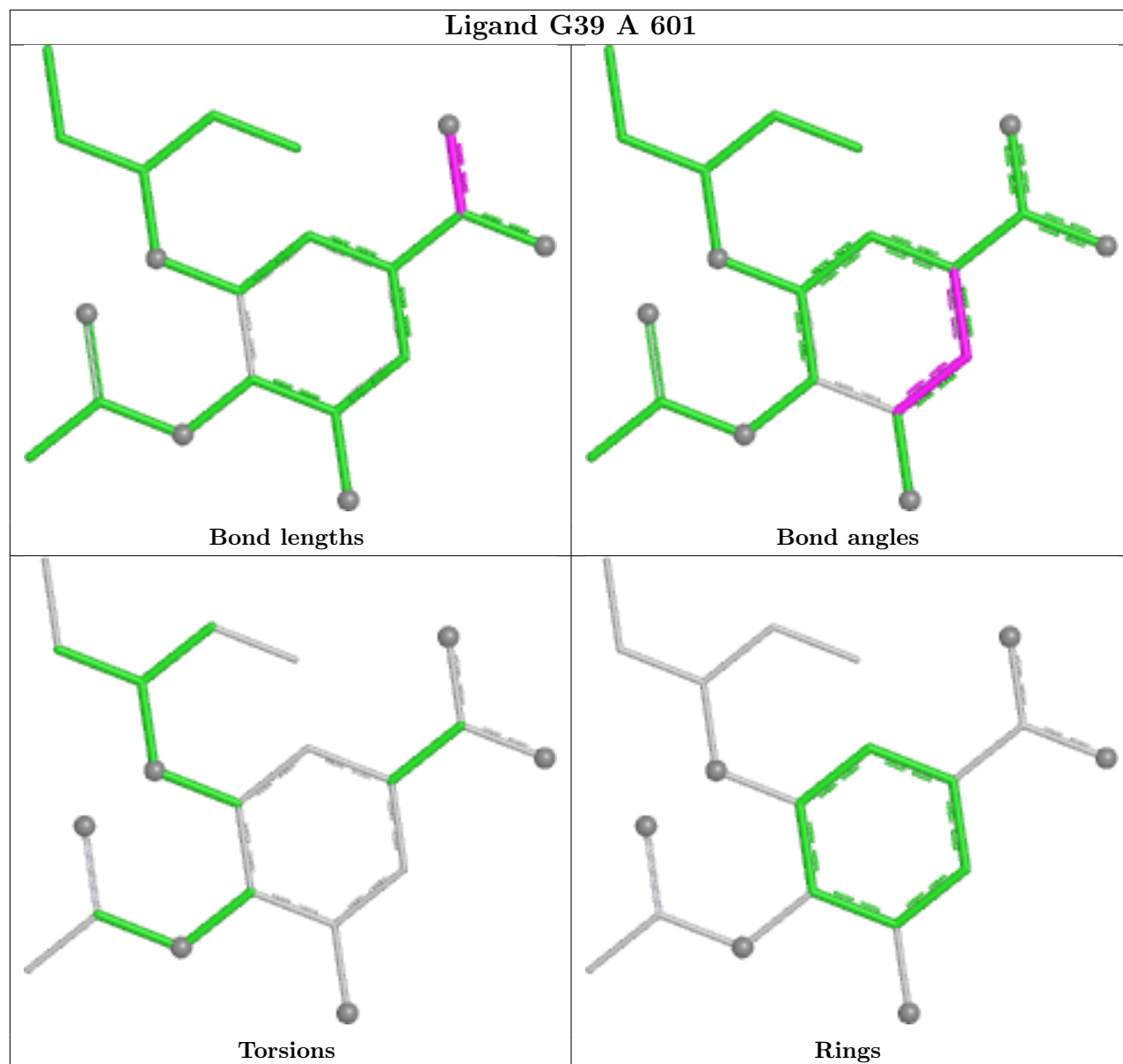
There are no ring outliers.

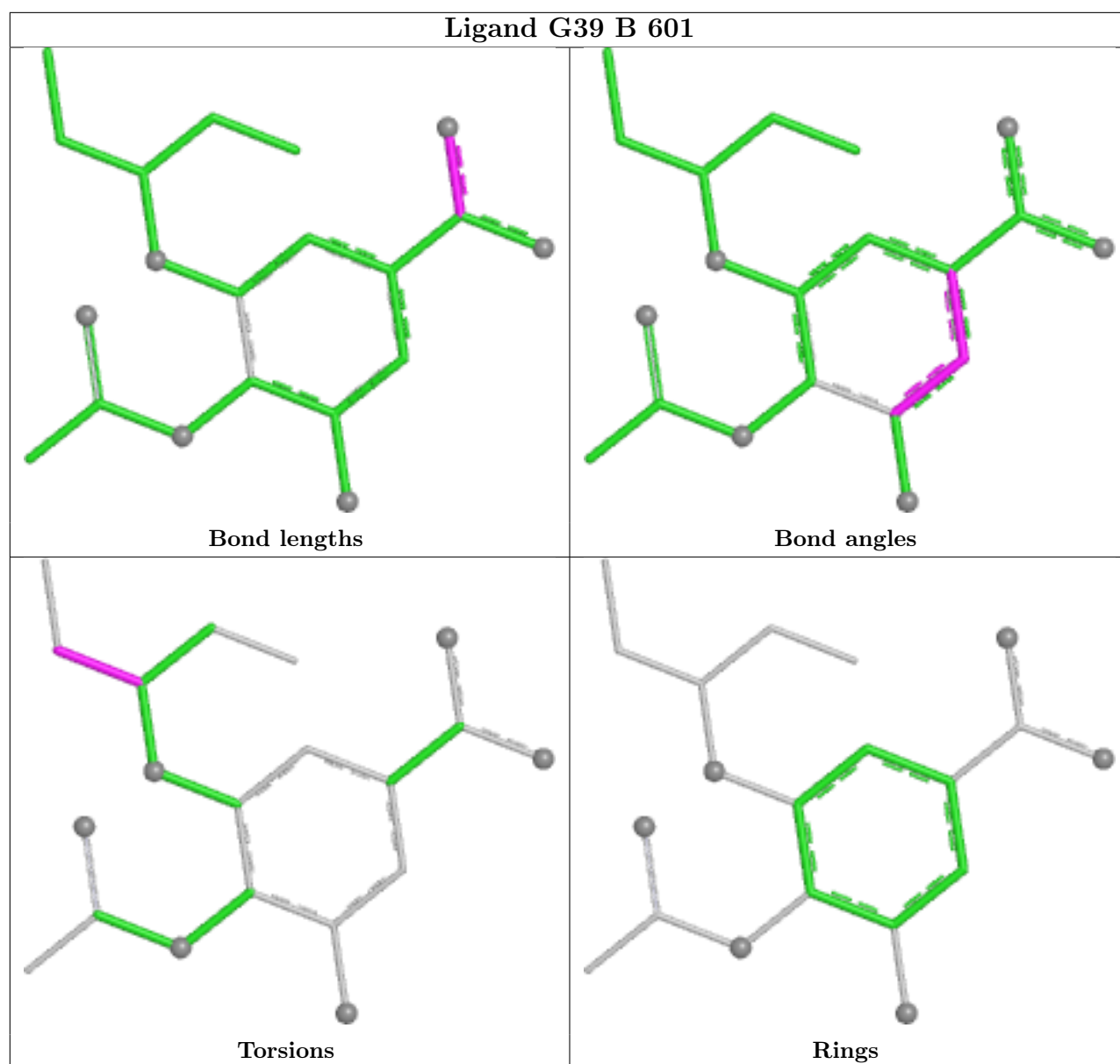
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	G39	1	0

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

Ligand G39 A 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	519/519 (100%)	1.40	118 (22%)	2 2	20, 37, 75, 98	0
1	B	519/519 (100%)	1.81	202 (38%)	1 0	26, 45, 63, 87	0
All	All	1038/1038 (100%)	1.60	320 (30%)	1 1	20, 42, 66, 98	0

All (320) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	VAL	6.1
1	B	308	TRP	5.5
1	A	71	LEU	5.5
1	B	395	TRP	5.4
1	A	186	ILE	5.3
1	A	183	PRO	5.3
1	A	67	VAL	5.3
1	A	185	VAL	5.2
1	A	36	VAL	5.2
1	A	148	VAL	5.2
1	A	134	THR	5.1
1	A	68	LEU	5.1
1	A	184	ALA	5.0
1	B	292	VAL	5.0
1	A	178	VAL	4.9
1	A	65	GLY	4.8
1	B	547	ILE	4.7
1	A	136	ALA	4.6
1	B	464	VAL	4.5
1	B	262	ALA	4.4
1	B	552	ARG	4.4
1	A	37	TYR	4.3
1	B	339	THR	4.2
1	A	86	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	551	ILE	4.2
1	B	345	VAL	4.1
1	B	246	LEU	4.1
1	B	335	TRP	4.1
1	A	177	VAL	4.1
1	B	410	VAL	4.1
1	B	413	VAL	4.1
1	A	73	ILE	4.1
1	A	35	SER	4.1
1	A	139	LEU	4.1
1	B	135	VAL	4.0
1	B	245	GLY	4.0
1	A	187	ALA	4.0
1	B	261	ILE	4.0
1	B	349	SER	4.0
1	A	135	VAL	4.0
1	B	470	ILE	4.0
1	A	69	ASN	3.9
1	B	270	GLY	3.9
1	A	59	ILE	3.9
1	B	258	PRO	3.8
1	A	308	TRP	3.8
1	B	442	TRP	3.8
1	B	294	VAL	3.8
1	A	146	PRO	3.8
1	B	471	ILE	3.8
1	A	34	ASP	3.7
1	B	183	PRO	3.7
1	B	550	LEU	3.7
1	B	293	TRP	3.7
1	B	285	VAL	3.7
1	B	340	ASN	3.7
1	A	141	LEU	3.7
1	A	179	ILE	3.7
1	B	334	THR	3.6
1	A	181	ASP	3.6
1	B	296	ALA	3.6
1	B	137	ASN	3.6
1	B	332	GLY	3.6
1	A	143	THR	3.6
1	B	75	PHE	3.6
1	B	438	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	475	LEU	3.6
1	B	298	TRP	3.5
1	B	387	TYR	3.5
1	B	47	VAL	3.5
1	B	315	MET	3.5
1	B	366	GLY	3.5
1	A	91	TYR	3.5
1	A	127	ILE	3.5
1	A	397	ILE	3.5
1	B	265	PHE	3.5
1	A	57	ILE	3.4
1	B	397	ILE	3.4
1	B	84	VAL	3.4
1	A	75	PHE	3.4
1	B	326	VAL	3.4
1	B	401	ALA	3.3
1	B	256	TRP	3.3
1	B	263	MET	3.3
1	B	374	PHE	3.3
1	A	62	ALA	3.3
1	B	209	ALA	3.3
1	A	133	THR	3.3
1	B	343	SER	3.3
1	B	217	VAL	3.2
1	B	417	VAL	3.2
1	B	268	THR	3.2
1	A	70	ARG	3.2
1	B	271	LEU	3.2
1	B	341	ILE	3.2
1	B	227	VAL	3.2
1	B	393	GLU	3.2
1	A	66	ASP	3.2
1	A	72	THR	3.2
1	A	153	TYR	3.2
1	B	321	ALA	3.2
1	B	500	VAL	3.2
1	B	199	GLY	3.2
1	A	151	ILE	3.1
1	B	411	ALA	3.1
1	A	550	LEU	3.1
1	A	144	ARG	3.1
1	A	182	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	324	MET	3.1
1	A	63	THR	3.1
1	B	138	THR	3.1
1	A	60	PRO	3.1
1	B	162	ARG	3.1
1	B	274	GLY	3.1
1	A	496	LEU	3.1
1	B	242	ILE	3.1
1	A	175	THR	3.1
1	B	134	THR	3.1
1	B	132	VAL	3.0
1	A	154	PHE	3.0
1	B	34	ASP	3.0
1	B	244	VAL	3.0
1	A	439	GLY	3.0
1	B	360	GLY	3.0
1	B	392	GLY	3.0
1	A	97	ALA	3.0
1	B	136	ALA	3.0
1	B	383	ALA	3.0
1	B	283	ILE	3.0
1	B	141	LEU	3.0
1	A	125	TYR	3.0
1	A	142	LYS	3.0
1	A	100	GLY	3.0
1	B	81	LEU	2.9
1	B	225	LEU	2.9
1	A	395	TRP	2.9
1	B	276	ASN	2.9
1	B	266	GLY	2.9
1	A	96	ALA	2.9
1	B	184	ALA	2.9
1	B	370	PHE	2.9
1	A	92	ALA	2.9
1	B	325	MET	2.9
1	A	552	ARG	2.8
1	B	211	PHE	2.8
1	B	352	PHE	2.8
1	B	167	LEU	2.8
1	B	170	LEU	2.8
1	B	224	LEU	2.8
1	B	253	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	295	VAL	2.8
1	B	232	TYR	2.8
1	B	186	ILE	2.8
1	A	38	VAL	2.8
1	A	158	VAL	2.8
1	A	61	ASP	2.8
1	A	192	ALA	2.8
1	B	299	THR	2.8
1	A	147	MET	2.8
1	B	278	VAL	2.8
1	B	333	ARG	2.7
1	A	90	PHE	2.7
1	B	389	LYS	2.7
1	B	418	LEU	2.7
1	B	115	ILE	2.7
1	B	338	SER	2.7
1	A	137	ASN	2.7
1	A	180	ASN	2.7
1	A	149	LYS	2.7
1	B	398	HIS	2.7
1	A	98	THR	2.7
1	A	140	THR	2.7
1	A	173	THR	2.7
1	B	323	LEU	2.7
1	B	368	LEU	2.7
1	B	378	LEU	2.7
1	B	337	GLU	2.7
1	A	442	TRP	2.7
1	A	443	THR	2.7
1	B	35	SER	2.7
1	A	547	ILE	2.7
1	B	380	VAL	2.7
1	B	76	GLY	2.6
1	B	297	ALA	2.6
1	B	307	ALA	2.6
1	A	155	TRP	2.6
1	A	74	ARG	2.6
1	A	152	ASN	2.6
1	A	341	ILE	2.6
1	A	345	VAL	2.6
1	B	36	VAL	2.6
1	B	77	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	317	PRO	2.6
1	A	115	ILE	2.6
1	B	524	ILE	2.6
1	A	145	GLN	2.6
1	A	502	TRP	2.6
1	B	385	ILE	2.6
1	B	204	GLY	2.6
1	A	87	VAL	2.6
1	A	174	VAL	2.6
1	A	348	PRO	2.5
1	B	177	VAL	2.5
1	B	348	PRO	2.5
1	B	388	SER	2.5
1	A	191	ALA	2.5
1	B	415	PRO	2.5
1	A	88	ARG	2.5
1	A	108	THR	2.5
1	B	230	VAL	2.5
1	A	150	GLY	2.4
1	B	226	GLY	2.4
1	B	241	HIS	2.4
1	B	496	LEU	2.4
1	B	363	MET	2.4
1	B	67	VAL	2.4
1	B	185	VAL	2.4
1	A	188	GLY	2.4
1	B	377	SER	2.4
1	B	139	LEU	2.4
1	B	55	PHE	2.4
1	B	375	ILE	2.4
1	B	165	SER	2.4
1	A	81	LEU	2.3
1	A	89	LEU	2.3
1	A	475	LEU	2.3
1	B	476	LEU	2.3
1	B	289	THR	2.3
1	A	85	LYS	2.3
1	B	290	ASN	2.3
1	A	93	GLY	2.3
1	B	235	SER	2.3
1	B	229	ASP	2.3
1	B	269	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	461	LEU	2.3
1	B	300	HIS	2.3
1	B	367	THR	2.3
1	B	207	GLY	2.3
1	B	472	GLY	2.3
1	B	79	ASP	2.3
1	B	54	LEU	2.3
1	B	166	LEU	2.3
1	B	179	ILE	2.2
1	B	80	LYS	2.2
1	A	101	ARG	2.2
1	B	223	THR	2.2
1	A	170	LEU	2.2
1	A	176	GLU	2.2
1	B	189	GLU	2.2
1	A	106	PRO	2.2
1	B	313	PRO	2.2
1	B	439	GLY	2.2
1	B	191	ALA	2.2
1	B	408	ALA	2.2
1	B	502	TRP	2.2
1	A	470	ILE	2.2
1	B	434	ILE	2.2
1	B	537	VAL	2.2
1	B	316	THR	2.2
1	B	247	SER	2.2
1	B	314	GLY	2.2
1	A	505	ALA	2.2
1	B	350	TRP	2.2
1	B	163	ASN	2.2
1	B	233	ASN	2.2
1	B	548	LYS	2.2
1	B	87	VAL	2.2
1	A	130	ASP	2.2
1	A	157	SER	2.2
1	B	416	GLY	2.2
1	B	74	ARG	2.2
1	A	435	THR	2.1
1	B	218	THR	2.1
1	B	443	THR	2.1
1	B	525	ASP	2.1
1	B	545	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	82	SER	2.1
1	B	301	GLY	2.1
1	A	438	LEU	2.1
1	B	71	LEU	2.1
1	B	238	LEU	2.1
1	B	503	LEU	2.1
1	B	312	MET	2.1
1	A	105	ALA	2.1
1	A	551	ILE	2.1
1	A	138	THR	2.1
1	B	412	GLU	2.1
1	A	323	LEU	2.1
1	B	60	PRO	2.1
1	B	353	LEU	2.1
1	B	192	ALA	2.1
1	B	193	VAL	2.1
1	A	123	PRO	2.1
1	B	400	PRO	2.1
1	A	203	ALA	2.1
1	B	330	ASP	2.1
1	A	189	GLU	2.0
1	B	73	ILE	2.0
1	B	198	ILE	2.0
1	B	328	SER	2.0
1	B	173	THR	2.0
1	B	320	THR	2.0
1	B	406	THR	2.0
1	B	203	ALA	2.0
1	B	305	ALA	2.0
1	B	161	ASP	2.0
1	B	331	ASP	2.0
1	A	124	SER	2.0
1	A	343	SER	2.0
1	B	264	SER	2.0
1	A	104	PHE	2.0
1	A	524	ILE	2.0
1	A	94	THR	2.0
1	B	65	GLY	2.0
1	B	255	THR	2.0
1	B	279	GLY	2.0
1	B	309	THR	2.0
1	B	329	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	342	THR	2.0
1	B	364	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

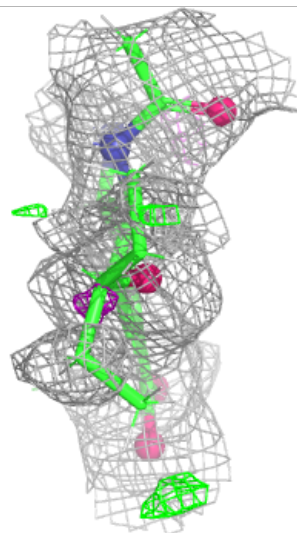
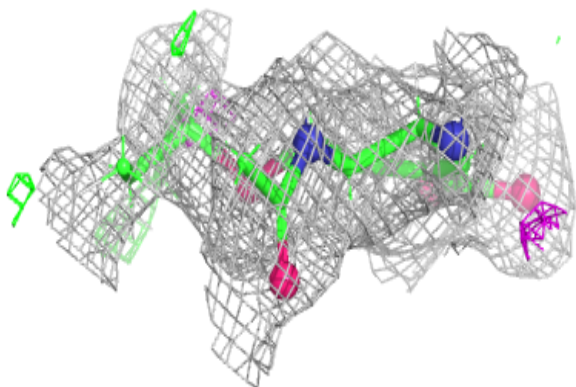
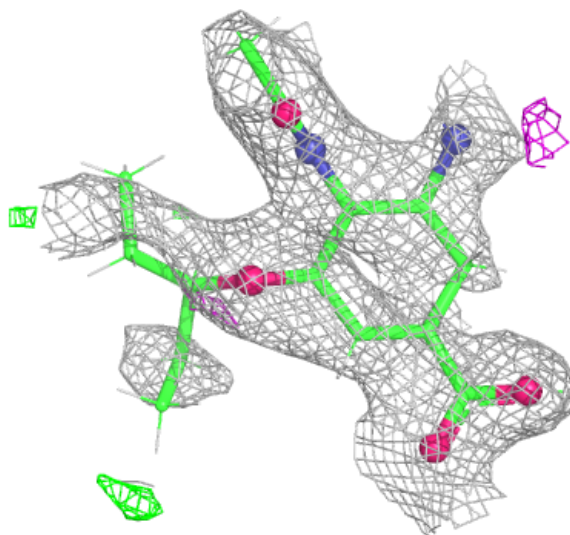
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	G39	B	601	20/20	0.75	0.17	47,53,60,61	0
2	G39	A	601	20/20	0.88	0.10	32,35,38,38	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.

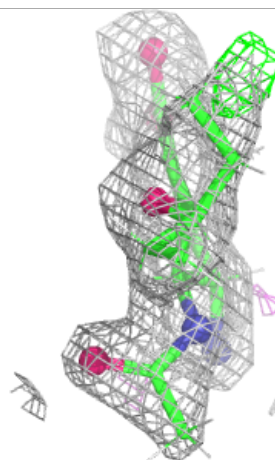
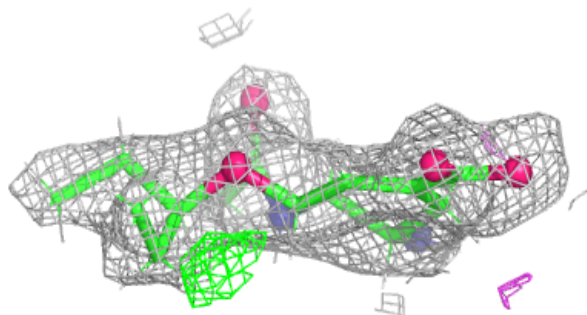
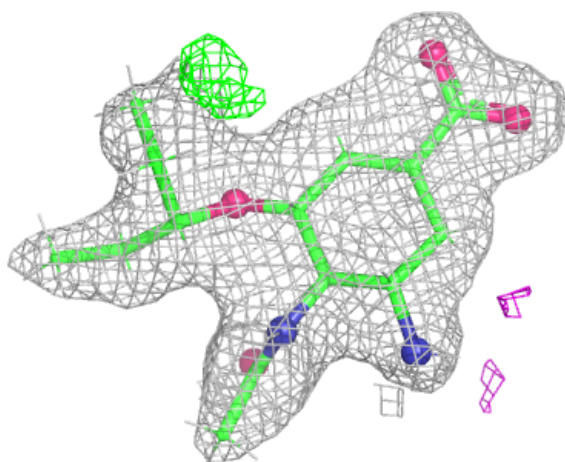
Electron density around G39 B 601:

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



Electron density around G39 A 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.