



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:46 AM UTC

PDB ID : 2D41 / pdb\_00002d41  
Title : X-ray crystal structure of hepatitis C virus RNA-dependent RNA polymerase in complex with non-nucleoside inhibitor  
Authors : Biswal, B.K.; Wang, M.; Cherney, M.M.; Chan, L.; Yannopoulos, C.G.; Bilimoria, D.; Bedard, J.; James, M.N.G.  
Deposited on : 2005-10-05  
Resolution : 2.10 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](mailto: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>.

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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)  
Xtrriage (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

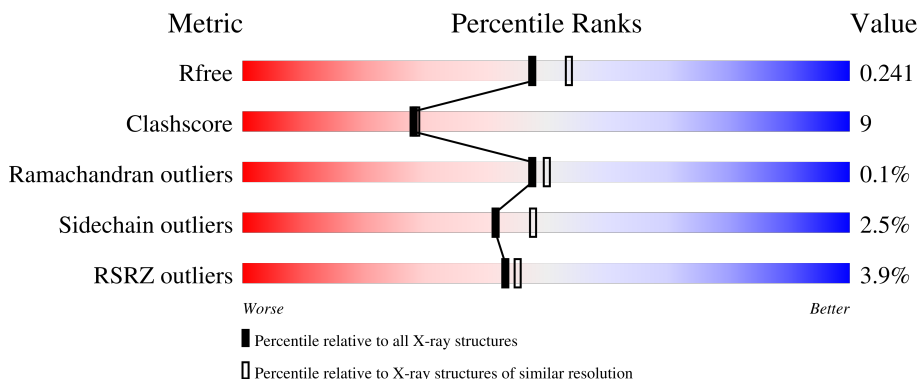
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

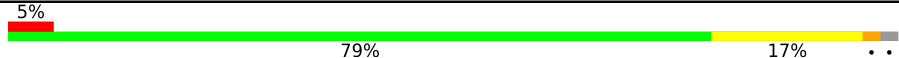
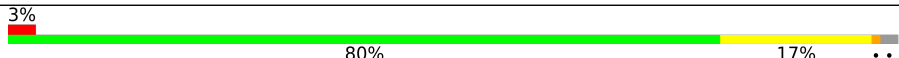
The reported resolution of this entry is 2.10 Å.

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  $\geq 3$ , 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	570	 5% 79% 17% ..
1	B	570	 3% 80% 17% ..

## 2 Entry composition [i](#)

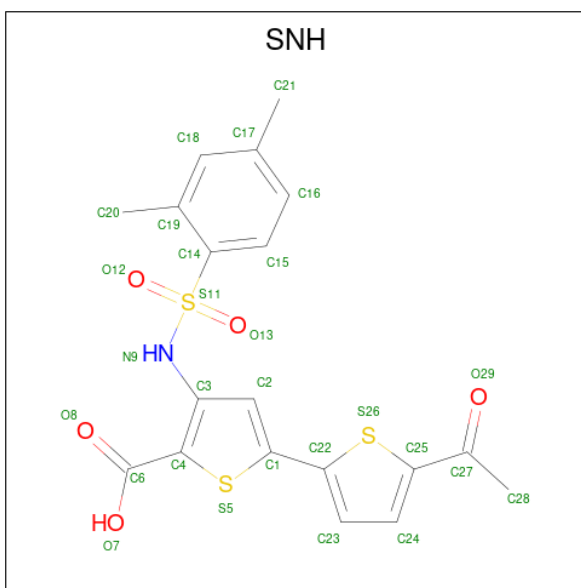
There are 3 unique types of molecules in this entry. The entry contains 9487 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	558	Total 4340	C 2738	N 765	O 806	S 31	0	0	0
1	B	558	Total 4340	C 2738	N 765	O 806	S 31	0	0	0

- Molecule 2 is 5'-ACETYL-4-[(2,4-DIMETHYLPHENYL)SULFONYL]AMINO}-2,2'-BITHIOPHENE-5-CARBOXYLIC ACID (CCD ID: SNH) (formula: C<sub>19</sub>H<sub>17</sub>NO<sub>5</sub>S<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total 28	C 19	N 1	O 5	S 3	0	0
2	A	1	Total 28	C 19	N 1	O 5	S 3	0	0
2	B	1	Total 28	C 19	N 1	O 5	S 3	0	0
2	B	1	Total 28	C 19	N 1	O 5	S 3	0	0

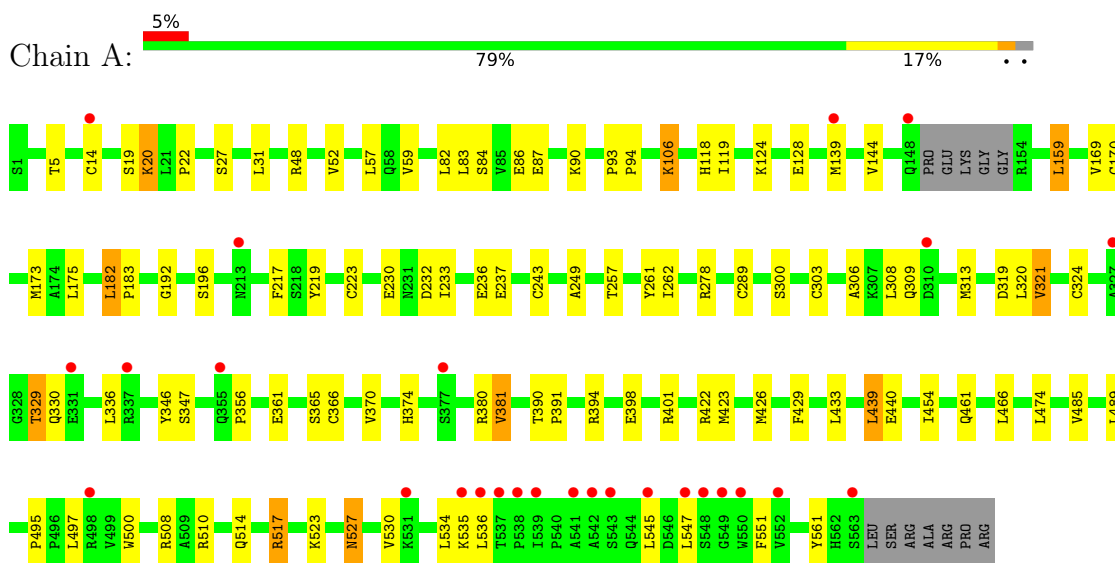
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	319	Total 319	O 319	0	0
3	B	376	Total 376	O 376	0	0

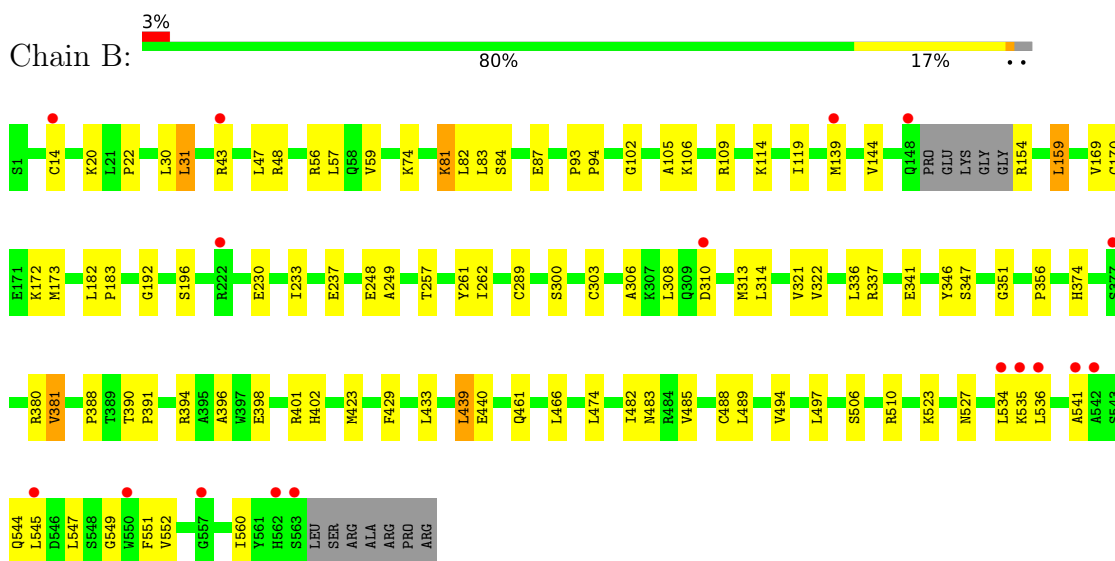
### 3 Residue-property plots [i](#)

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: polyprotein



- Molecule 1: polyprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.53Å 105.98Å 126.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.66 – 2.10 39.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.66-2.10) 94.8 (39.66-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.10Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.240 0.205 , 0.241	Depositor DCC
$R_{free}$ test set	3233 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtrriage
Anisotropy	0.468	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9487	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3336e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SNH

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	0.38	0/4434	0.87	6/6017 (0.1%)
1	B	0.38	0/4434	0.87	5/6017 (0.1%)
All	All	0.38	0/8868	0.87	11/12034 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	SER	N-CA-C	-9.08	99.69	110.13
1	B	196	SER	N-CA-C	-6.68	100.31	110.07
1	A	192	GLY	N-CA-C	6.13	121.58	113.37
1	B	494	VAL	CA-C-N	6.05	124.08	119.66
1	B	494	VAL	C-N-CA	6.05	124.08	119.66
1	B	351	GLY	N-CA-C	-5.72	99.63	113.18
1	B	192	GLY	N-CA-C	5.52	120.77	113.37
1	A	175	LEU	N-CA-C	5.46	121.71	114.12
1	A	454	ILE	N-CA-C	5.21	116.22	108.46
1	A	27	SER	N-CA-C	5.15	117.30	111.02
1	A	182	LEU	N-CA-C	5.02	119.58	112.75

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	4340	0	4357	81	0
1	B	4340	0	4357	77	0
2	A	56	0	32	1	0
2	B	56	0	32	2	0
3	A	319	0	0	5	0
3	B	376	0	0	8	0
All	All	9487	0	8778	157	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 9.

All (157) 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:170:CYS:HA	1:B:173:MET:HE3	1.44	1.00
1:B:14:CYS:HB2	1:B:139:MET:HE1	1.44	0.96
1:A:422:ARG:HA	1:A:426:MET:HE2	1.46	0.95
1:A:423:MET:HE2	1:A:497:LEU:HD13	1.56	0.88
1:A:232:ASP:O	1:A:236:GLU:HG3	1.78	0.83
1:B:423:MET:HE1	2:B:3001:SNH:S26	2.19	0.83
1:A:170:CYS:HA	1:A:173:MET:HE3	1.59	0.82
1:B:423:MET:HE2	1:B:497:LEU:HD13	1.61	0.82
1:A:422:ARG:CA	1:A:426:MET:HE2	2.10	0.81
1:A:423:MET:HE1	2:A:1001:SNH:S26	2.20	0.81
1:B:483:ASN:HB3	3:B:4303:HOH:O	1.80	0.81
1:B:94:PRO:HB3	1:B:106:LYS:NZ	2.01	0.76
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.17	0.75
1:B:48:ARG:HG2	1:B:159:LEU:HD13	1.69	0.73
1:B:337:ARG:O	1:B:341:GLU:HG3	1.89	0.72
1:B:14:CYS:CB	1:B:139:MET:HE1	2.18	0.71
1:B:541:ALA:O	1:B:544:GLN:HG2	1.92	0.69
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.74	0.68
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.76	0.68
1:B:336:LEU:HD12	1:B:356:PRO:HD3	1.75	0.67
1:B:94:PRO:HB3	1:B:106:LYS:HZ3	1.58	0.67
1:A:48:ARG:HG2	1:A:159:LEU:HD13	1.77	0.67
1:A:321:VAL:HG23	1:A:365:SER:HB3	1.75	0.67
1:B:523:LYS:HE2	1:B:534:LEU:HD23	1.78	0.66
1:A:508:ARG:NE	3:A:2107:HOH:O	2.29	0.65
1:A:14:CYS:HB2	1:A:139:MET:HE1	1.80	0.64
1:A:5:THR:HG23	1:A:278:ARG:HH22	1.62	0.63
1:A:321:VAL:CG2	1:A:365:SER:HB3	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LYS:HE2	1:A:536:LEU:HD12	1.80	0.62
1:B:423:MET:CE	1:B:497:LEU:HD13	2.31	0.61
1:A:124:LYS:HE2	1:A:128:GLU:OE2	2.01	0.60
1:A:423:MET:CE	1:A:497:LEU:HD13	2.30	0.60
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.84	0.60
1:A:230:GLU:HG3	1:A:262:ILE:HG23	1.83	0.60
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.83	0.59
1:A:14:CYS:CB	1:A:139:MET:HE1	2.34	0.57
1:A:508:ARG:HE	1:A:530:VAL:HG11	1.69	0.57
1:A:182:LEU:HD23	1:A:182:LEU:C	2.29	0.57
1:B:535:LYS:HG3	1:B:536:LEU:H	1.70	0.56
1:B:182:LEU:C	1:B:182:LEU:HD23	2.30	0.56
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.71	0.56
1:A:86:GLU:O	1:A:90:LYS:HG3	2.05	0.55
1:A:527:ASN:HD21	1:A:534:LEU:H	1.55	0.55
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.90	0.54
1:B:248:GLU:HB2	3:B:4355:HOH:O	2.08	0.54
1:A:22:PRO:HG2	1:A:401:ARG:HG3	1.90	0.54
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.72	0.54
1:B:461:GLN:NE2	1:B:541:ALA:HB3	2.23	0.53
1:B:510:ARG:HG2	1:B:510:ARG:HH11	1.73	0.53
1:B:381:VAL:HG11	1:B:474:LEU:CD2	2.39	0.53
1:A:19:SER:H	1:A:20:LYS:NZ	2.07	0.53
1:A:508:ARG:CZ	3:A:2107:HOH:O	2.56	0.53
1:A:510:ARG:HH11	1:A:510:ARG:HG2	1.73	0.53
1:B:74:LYS:HE2	3:B:4108:HOH:O	2.08	0.52
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.91	0.52
1:B:390:THR:HB	1:B:391:PRO:HD3	1.92	0.52
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.91	0.52
1:A:461:GLN:HB2	1:A:545:LEU:HD11	1.90	0.52
1:B:84:SER:OG	1:B:87:GLU:HG3	2.10	0.52
1:B:506:SER:O	1:B:510:ARG:HD3	2.10	0.52
1:A:535:LYS:HG3	1:A:536:LEU:H	1.74	0.52
1:B:313:MET:HG2	1:B:322:VAL:HG22	1.92	0.52
1:A:230:GLU:HG3	1:A:262:ILE:CG2	2.40	0.52
1:A:20:LYS:HD2	1:A:20:LYS:H	1.75	0.51
1:B:81:LYS:HD2	3:B:4371:HOH:O	2.11	0.51
1:B:549:GLY:HA2	1:B:552:VAL:CG2	2.41	0.51
1:A:20:LYS:H	1:A:20:LYS:CD	2.23	0.51
1:A:535:LYS:CG	1:A:536:LEU:H	2.23	0.51
1:A:361:GLU:HG2	1:A:370:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ALA:HB3	1:A:308:LEU:HD13	1.93	0.50
1:B:230:GLU:HG3	1:B:262:ILE:HG23	1.94	0.50
1:A:390:THR:HB	1:A:391:PRO:HD3	1.94	0.50
1:B:527:ASN:HD21	1:B:534:LEU:H	1.58	0.50
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.93	0.50
1:B:14:CYS:HB2	1:B:139:MET:CE	2.30	0.50
1:A:84:SER:OG	1:A:87:GLU:HG3	2.12	0.49
1:A:508:ARG:NH1	1:A:523:LYS:HA	2.26	0.49
1:A:237:GLU:HG3	1:A:257:THR:OG1	2.12	0.49
1:A:124:LYS:O	1:A:128:GLU:HG3	2.13	0.49
1:B:300:SER:OG	1:B:313:MET:HE1	2.13	0.49
1:B:94:PRO:HB3	1:B:106:LYS:HZ1	1.75	0.48
1:B:433:LEU:HB3	1:B:439:LEU:HD12	1.96	0.48
1:A:93:PRO:HG3	1:A:561:TYR:HB2	1.96	0.48
1:B:394:ARG:O	1:B:398:GLU:HG3	2.13	0.48
1:B:402:HIS:HE1	3:B:4199:HOH:O	1.97	0.48
1:B:102:GLY:O	1:B:114:LYS:HE3	2.14	0.47
1:B:466:LEU:HD22	1:B:551:PHE:HE2	1.79	0.47
1:A:182:LEU:HD12	1:A:243:CYS:SG	2.55	0.47
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.94	0.47
1:A:485:VAL:O	1:A:489:LEU:HG	2.15	0.47
1:A:52:VAL:HG12	1:A:223:CYS:SG	2.55	0.47
1:B:374:HIS:HE1	1:B:380:ARG:HG3	1.80	0.47
1:B:510:ARG:HG2	1:B:510:ARG:NH1	2.31	0.46
1:A:319:ASP:CG	1:A:366:CYS:H	2.23	0.46
1:B:535:LYS:HG3	1:B:536:LEU:N	2.30	0.46
1:A:31:LEU:C	1:A:31:LEU:HD23	2.41	0.46
1:B:22:PRO:HG2	1:B:401:ARG:HG3	1.98	0.46
1:A:433:LEU:HB3	1:A:439:LEU:HD12	1.98	0.46
1:A:510:ARG:HG2	1:A:510:ARG:NH1	2.30	0.46
1:A:523:LYS:HG3	1:A:534:LEU:HD22	1.98	0.45
1:B:230:GLU:HG3	1:B:262:ILE:CG2	2.45	0.45
1:B:346:TYR:O	1:B:347:SER:HB3	2.17	0.45
1:A:20:LYS:HD2	1:A:20:LYS:N	2.31	0.45
1:A:381:VAL:HG11	1:A:474:LEU:CD2	2.47	0.45
1:A:517:ARG:HG2	1:A:517:ARG:NH1	2.32	0.45
1:A:59:VAL:CG1	1:B:59:VAL:HG13	2.46	0.45
1:B:545:LEU:HB3	1:B:547:LEU:CD1	2.47	0.45
1:A:313:MET:HE2	3:A:2233:HOH:O	2.16	0.44
1:B:233:ILE:HD13	1:B:261:TYR:O	2.17	0.44
1:B:388:PRO:HG2	1:B:488:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:GLY:HA2	1:B:552:VAL:HG21	1.99	0.44
1:A:217:PHE:CD2	1:A:336:LEU:HD21	2.51	0.44
1:A:545:LEU:HB3	1:A:547:LEU:CD1	2.48	0.44
1:B:43:ARG:HH11	1:B:43:ARG:HG3	1.81	0.44
1:B:56:ARG:O	1:B:57:LEU:HD12	2.18	0.44
1:A:535:LYS:HG3	1:A:536:LEU:N	2.33	0.43
1:B:237:GLU:HG3	1:B:257:THR:OG1	2.18	0.43
1:B:535:LYS:CG	1:B:536:LEU:H	2.32	0.43
1:B:374:HIS:CE1	1:B:380:ARG:HG3	2.54	0.43
1:A:508:ARG:HH12	1:A:523:LYS:HA	1.84	0.43
1:B:154:ARG:N	3:B:4154:HOH:O	2.51	0.43
1:B:336:LEU:CD1	1:B:356:PRO:HD3	2.48	0.43
1:B:105:ALA:O	1:B:109:ARG:HG3	2.19	0.43
1:B:527:ASN:ND2	3:B:4117:HOH:O	2.52	0.43
1:B:429:PHE:O	1:B:433:LEU:HG	2.18	0.42
1:A:309:GLN:O	1:A:324:CYS:HB2	2.20	0.42
1:A:329:THR:HG23	1:A:330:GLN:H	1.83	0.42
1:A:535:LYS:CG	1:A:536:LEU:N	2.82	0.42
1:A:106:LYS:NZ	3:A:2266:HOH:O	2.52	0.42
1:A:300:SER:OG	1:A:313:MET:HE1	2.19	0.42
1:B:482:ILE:HG23	2:B:3001:SNH:H23	2.02	0.42
1:B:527:ASN:HD21	1:B:534:LEU:N	2.17	0.42
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.91	0.42
1:A:394:ARG:O	1:A:398:GLU:HG3	2.20	0.42
1:B:313:MET:HE2	3:B:4234:HOH:O	2.19	0.42
1:A:144:VAL:HB	1:A:394:ARG:HG2	2.00	0.42
1:A:495:PRO:HG2	1:A:500:TRP:NE1	2.35	0.41
1:B:485:VAL:O	1:B:489:LEU:HG	2.19	0.41
1:A:19:SER:H	1:A:20:LYS:HZ2	1.66	0.41
1:A:118:HIS:HE1	3:A:2132:HOH:O	2.01	0.41
1:B:523:LYS:HG3	1:B:534:LEU:HD22	2.02	0.41
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.97	0.41
1:B:31:LEU:C	1:B:31:LEU:HD23	2.45	0.41
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.60	0.41
1:A:374:HIS:HE1	1:A:380:ARG:HG3	1.86	0.41
1:A:429:PHE:O	1:A:433:LEU:HG	2.21	0.41
1:B:30:LEU:HD23	1:B:396:ALA:HA	2.03	0.41
1:A:374:HIS:CE1	1:A:380:ARG:HG3	2.56	0.41
1:A:169:VAL:HG12	1:A:173:MET:HE2	2.02	0.41
1:A:346:TYR:O	1:A:347:SER:HB3	2.21	0.41
1:B:381:VAL:HG11	1:B:474:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LEU:CD2	1:A:551:PHE:HE2	2.34	0.41
1:A:233:ILE:HD13	1:A:261:TYR:O	2.20	0.40
1:B:183:PRO:HG3	1:B:289:CYS:SG	2.61	0.40
1:B:306:ALA:HB3	1:B:308:LEU:HD13	2.02	0.40
1:B:106:LYS:HA	1:B:106:LYS:HD3	1.90	0.40
1:B:527:ASN:HD22	1:B:527:ASN:HA	1.74	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	554/570 (97%)	539 (97%)	15 (3%)	0	100	100
1	B	554/570 (97%)	541 (98%)	12 (2%)	1 (0%)	43	44
All	All	1108/1140 (97%)	1080 (98%)	27 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	310	ASP

### 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	476/485 (98%)	462 (97%)	14 (3%)	37	42
1	B	476/485 (98%)	466 (98%)	10 (2%)	47	54
All	All	952/970 (98%)	928 (98%)	24 (2%)	42	48

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	57	LEU
1	A	83	LEU
1	A	106	LYS
1	A	159	LEU
1	A	303	CYS
1	A	321	VAL
1	A	329	THR
1	A	381	VAL
1	A	439	LEU
1	A	440	GLU
1	A	514	GLN
1	A	517	ARG
1	A	527	ASN
1	B	20	LYS
1	B	31	LEU
1	B	47	LEU
1	B	81	LYS
1	B	83	LEU
1	B	159	LEU
1	B	303	CYS
1	B	381	VAL
1	B	439	LEU
1	B	440	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	95	HIS
1	A	374	HIS
1	A	514	GLN
1	A	527	ASN
1	A	544	GLN

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Mol	Chain	Res	Type
1	A	562	HIS
1	B	49	GLN
1	B	95	HIS
1	B	374	HIS
1	B	402	HIS
1	B	406	ASN
1	B	446	GLN
1	B	461	GLN
1	B	483	ASN
1	B	527	ASN
1	B	544	GLN
1	B	562	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](#)

4 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	SNH	A	2001	-	30,30,30	2.10	11 (36%)	43,45,45	1.87	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SNH	B	4001	-	30,30,30	2.87	9 (30%)	43,45,45	1.84	11 (25%)
2	SNH	A	1001	-	30,30,30	1.62	9 (30%)	43,45,45	1.56	8 (18%)
2	SNH	B	3001	-	30,30,30	1.58	6 (20%)	43,45,45	1.53	8 (18%)

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	SNH	A	2001	-	-	2/23/23/23	0/3/3/3
2	SNH	B	4001	-	-	2/23/23/23	0/3/3/3
2	SNH	A	1001	-	-	1/23/23/23	0/3/3/3
2	SNH	B	3001	-	-	1/23/23/23	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4001	SNH	C19-C14	7.77	1.49	1.40
2	B	4001	SNH	O13-S11	6.65	1.51	1.43
2	B	4001	SNH	C14-S11	-6.61	1.68	1.77
2	B	4001	SNH	C15-C14	6.56	1.46	1.39
2	A	2001	SNH	C19-C14	5.09	1.46	1.40
2	A	2001	SNH	C15-C14	4.72	1.44	1.39
2	A	2001	SNH	C14-S11	4.10	1.83	1.77
2	B	4001	SNH	O12-S11	3.53	1.47	1.43
2	B	3001	SNH	C15-C14	3.25	1.43	1.39
2	A	2001	SNH	C27-C25	3.23	1.51	1.47
2	A	1001	SNH	C15-C14	3.21	1.42	1.39
2	B	3001	SNH	C19-C14	3.07	1.44	1.40
2	A	1001	SNH	C19-C14	3.04	1.44	1.40
2	B	3001	SNH	C18-C19	2.87	1.43	1.39
2	A	1001	SNH	C18-C19	2.80	1.43	1.39
2	A	2001	SNH	C16-C15	2.66	1.43	1.38
2	A	1001	SNH	C14-S11	2.62	1.81	1.77
2	B	4001	SNH	C18-C19	2.61	1.43	1.39
2	B	3001	SNH	C14-S11	2.56	1.81	1.77
2	A	1001	SNH	C18-C17	2.54	1.43	1.39
2	A	2001	SNH	O13-S11	2.47	1.46	1.43
2	B	4001	SNH	C27-C25	2.45	1.50	1.47
2	A	2001	SNH	S11-N9	2.33	1.69	1.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	SNH	O12-S11	2.31	1.46	1.43
2	A	2001	SNH	C18-C19	2.26	1.42	1.39
2	B	4001	SNH	C16-C15	2.21	1.42	1.38
2	B	3001	SNH	C18-C17	2.20	1.42	1.39
2	A	1001	SNH	C27-C25	2.20	1.50	1.47
2	A	2001	SNH	C18-C17	2.20	1.42	1.39
2	B	4001	SNH	C1-S5	-2.12	1.69	1.73
2	A	1001	SNH	O13-S11	2.12	1.46	1.43
2	A	2001	SNH	C3-C4	2.10	1.41	1.38
2	A	1001	SNH	O7-C6	-2.06	1.25	1.30
2	A	1001	SNH	C16-C15	2.03	1.42	1.38
2	B	3001	SNH	C27-C25	2.01	1.49	1.47

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	SNH	O13-S11-O12	-5.80	112.47	119.52
2	B	4001	SNH	C15-C14-C19	-5.30	116.37	121.17
2	B	4001	SNH	O13-S11-O12	-5.18	113.22	119.52
2	A	1001	SNH	O13-S11-O12	-5.11	113.32	119.52
2	B	3001	SNH	O13-S11-O12	-4.95	113.51	119.52
2	A	2001	SNH	C27-C25-S26	4.24	125.65	118.85
2	A	2001	SNH	C4-C3-N9	3.82	125.27	121.24
2	B	4001	SNH	C27-C25-S26	3.74	124.86	118.85
2	A	1001	SNH	C27-C25-S26	3.53	124.51	118.85
2	B	3001	SNH	C27-C25-S26	3.34	124.22	118.85
2	A	1001	SNH	C4-C3-N9	3.08	124.49	121.24
2	A	1001	SNH	C2-C3-C4	-2.93	110.66	113.80
2	B	4001	SNH	C18-C19-C14	2.85	118.94	116.99
2	A	2001	SNH	C19-C14-S11	2.85	124.54	122.02
2	A	2001	SNH	C2-C3-C4	-2.81	110.79	113.80
2	A	2001	SNH	C15-C14-C19	-2.78	118.65	121.17
2	A	2001	SNH	C14-S11-N9	2.73	109.35	105.96
2	B	3001	SNH	C14-S11-N9	2.72	109.34	105.96
2	B	3001	SNH	C4-C3-N9	2.70	124.09	121.24
2	B	3001	SNH	C2-C3-C4	-2.65	110.96	113.80
2	A	2001	SNH	C3-C2-C1	2.38	115.36	111.72
2	B	4001	SNH	O12-S11-C14	-2.34	103.82	107.68
2	B	4001	SNH	O13-S11-N9	2.29	113.32	106.77
2	B	4001	SNH	C20-C19-C18	-2.27	115.57	119.57
2	A	1001	SNH	C1-C22-S26	2.18	124.62	120.53
2	B	3001	SNH	C15-C14-C19	-2.17	119.20	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4001	SNH	C1-S5-C4	2.16	93.85	91.28
2	B	4001	SNH	C2-C3-C4	-2.16	111.48	113.80
2	B	4001	SNH	C6-C4-S5	2.15	123.74	115.13
2	A	1001	SNH	C14-S11-N9	2.13	108.60	105.96
2	B	3001	SNH	C1-C22-S26	2.11	124.49	120.53
2	B	3001	SNH	C6-C4-S5	2.05	123.33	115.13
2	A	1001	SNH	C15-C14-C19	-2.02	119.34	121.17
2	A	2001	SNH	C3-N9-S11	2.02	127.80	121.52
2	A	2001	SNH	C22-C1-S5	2.01	124.31	120.53
2	A	1001	SNH	C6-C4-S5	2.00	123.14	115.13
2	B	4001	SNH	C15-C14-S11	2.00	120.39	117.51

There are no chirality outliers.

All (6) torsion outliers are listed below:

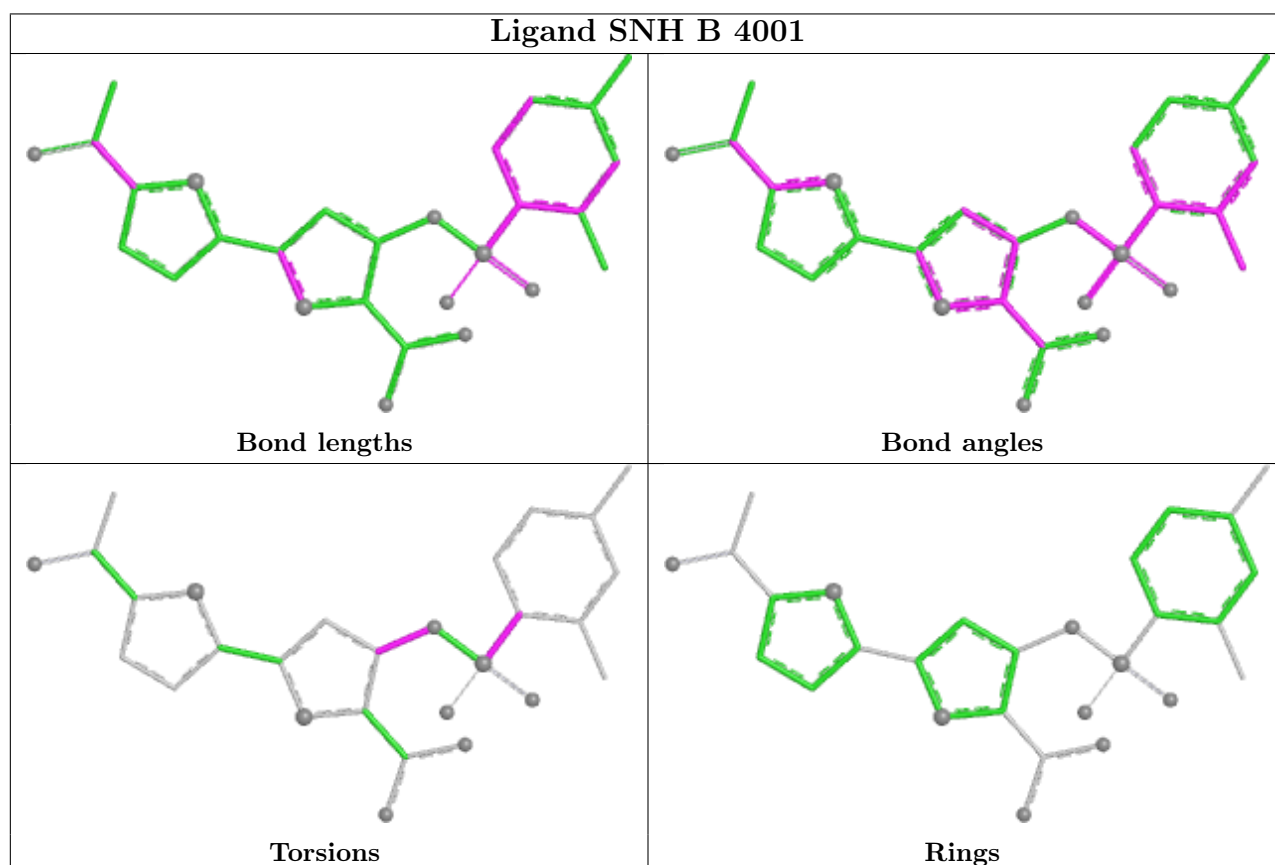
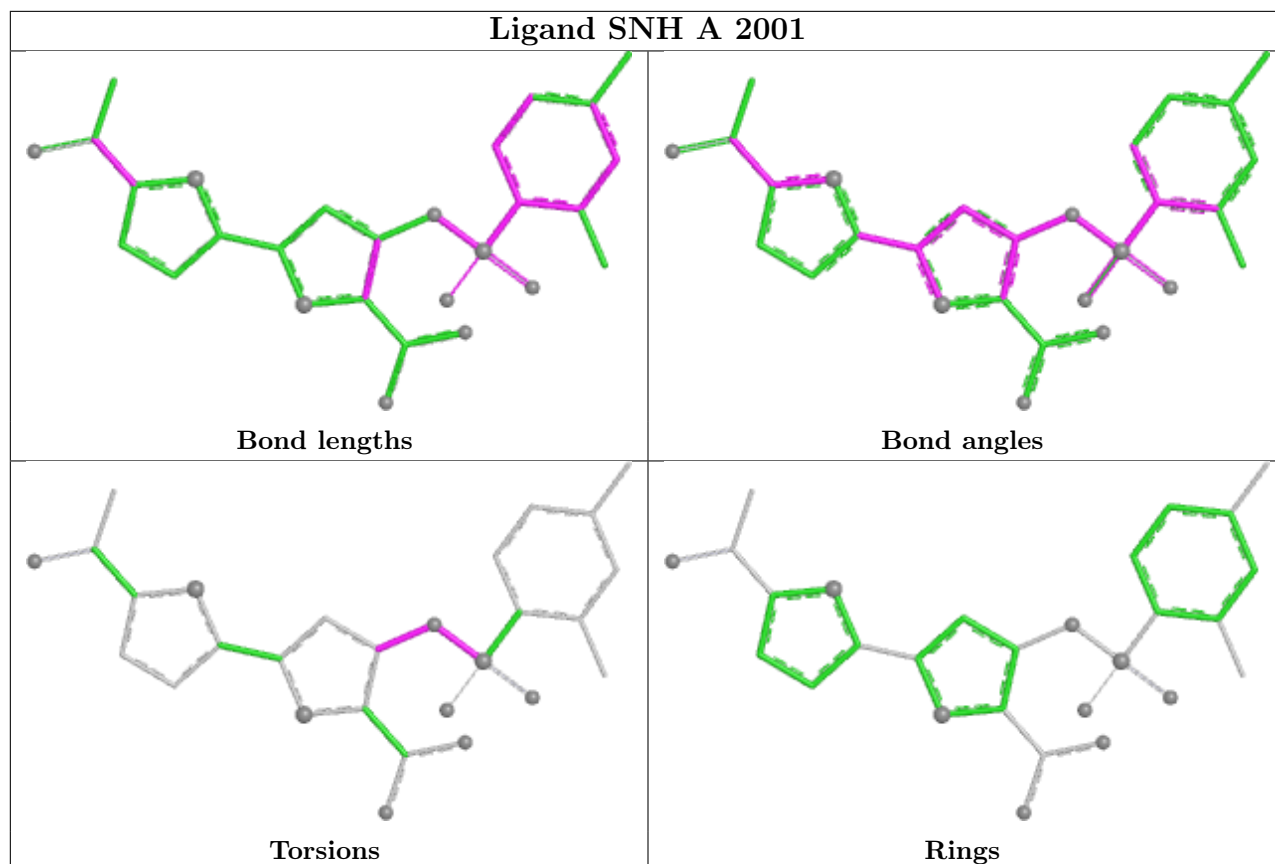
Mol	Chain	Res	Type	Atoms
2	B	4001	SNH	C4-C3-N9-S11
2	A	1001	SNH	C4-C3-N9-S11
2	B	3001	SNH	C4-C3-N9-S11
2	B	4001	SNH	C19-C14-S11-O12
2	A	2001	SNH	C4-C3-N9-S11
2	A	2001	SNH	C3-N9-S11-O13

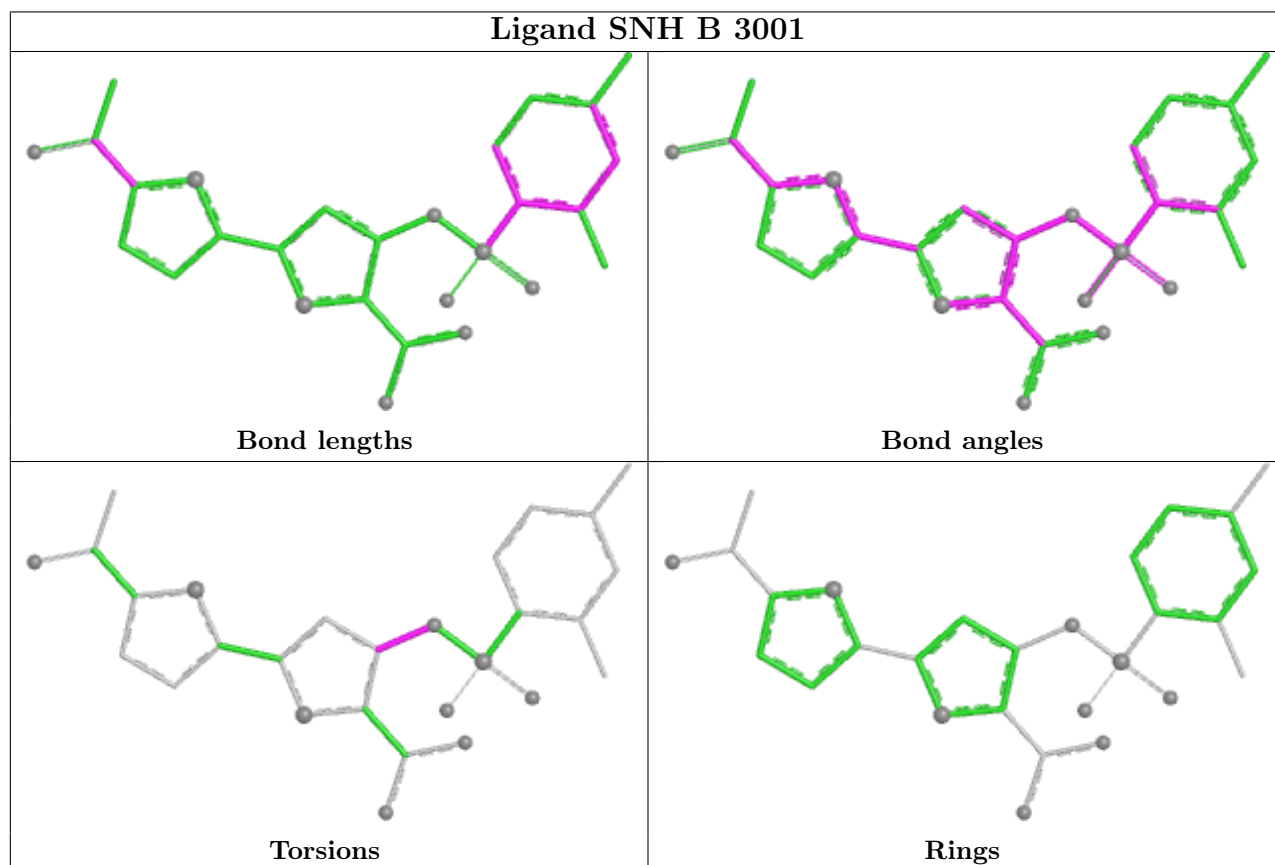
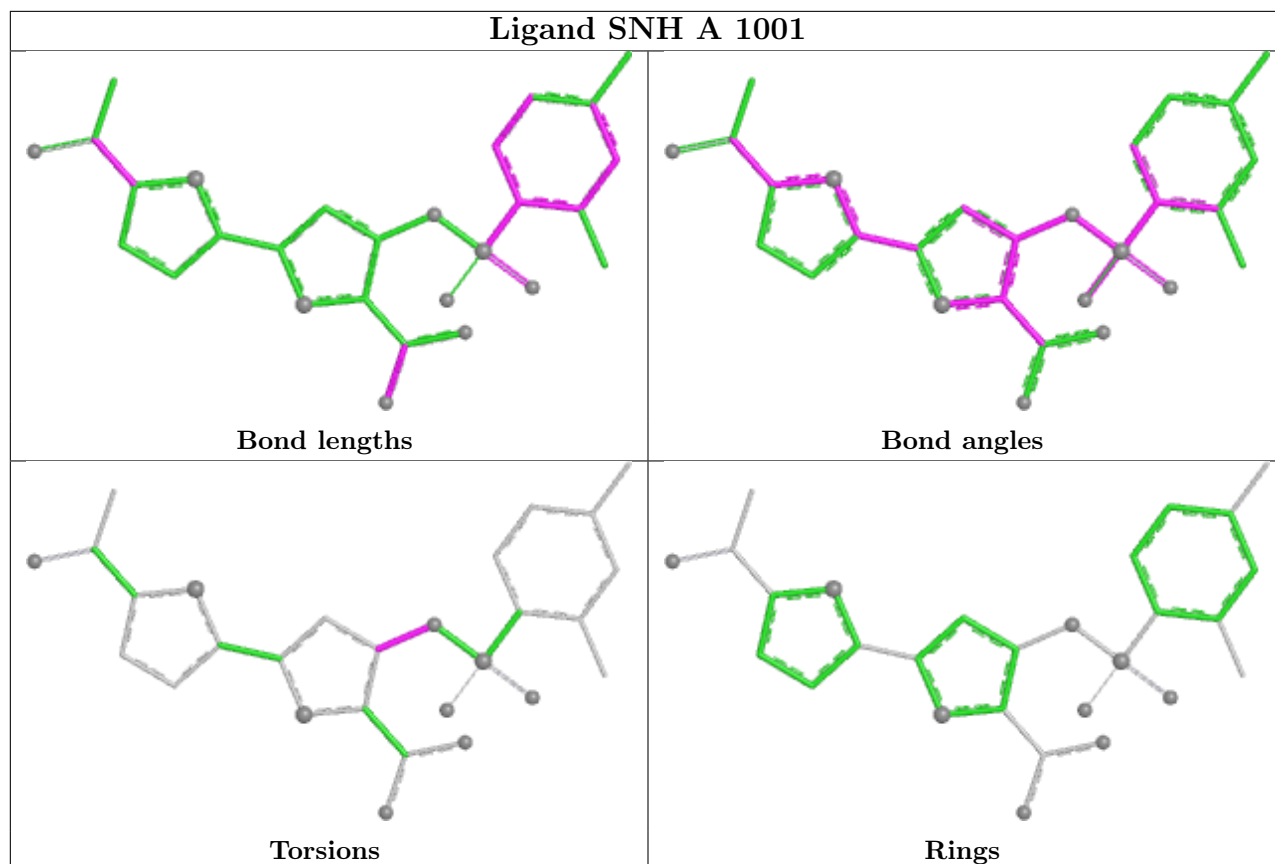
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SNH	1	0
2	B	3001	SNH	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	558/570 (97%)	0.21	27 (4%) 35 38	13, 26, 45, 72	0
1	B	558/570 (97%)	0.09	17 (3%) 52 55	14, 25, 44, 69	0
All	All	1116/1140 (97%)	0.15	44 (3%) 43 45	13, 25, 44, 72	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	LEU	4.6
1	B	536	LEU	3.4
1	B	148	GLN	3.4
1	A	535	LYS	3.4
1	A	14	CYS	3.2
1	B	377	SER	3.2
1	A	148	GLN	3.2
1	A	541	ALA	3.1
1	A	331	GLU	3.1
1	B	534	LEU	3.1
1	A	545	LEU	3.1
1	B	14	CYS	3.0
1	B	535	LYS	3.0
1	B	550	TRP	3.0
1	B	541	ALA	3.0
1	A	543	SER	2.9
1	A	563	SER	2.9
1	A	537	THR	2.9
1	A	538	PRO	2.8
1	B	139	MET	2.7
1	A	327	ALA	2.7
1	A	549	GLY	2.7
1	B	545	LEU	2.6
1	A	542	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	43	ARG	2.6
1	A	548	SER	2.6
1	B	562	HIS	2.5
1	A	531	LYS	2.5
1	A	539	ILE	2.5
1	B	310	ASP	2.4
1	A	213	ASN	2.4
1	B	563	SER	2.4
1	B	542	ALA	2.4
1	A	355	GLN	2.3
1	A	310	ASP	2.3
1	A	547	LEU	2.3
1	A	337	ARG	2.2
1	A	377	SER	2.2
1	A	498	ARG	2.2
1	A	550	TRP	2.1
1	A	552	VAL	2.1
1	B	222	ARG	2.1
1	A	139	MET	2.0
1	B	557	GLY	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, 95<sup>th</sup> 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.

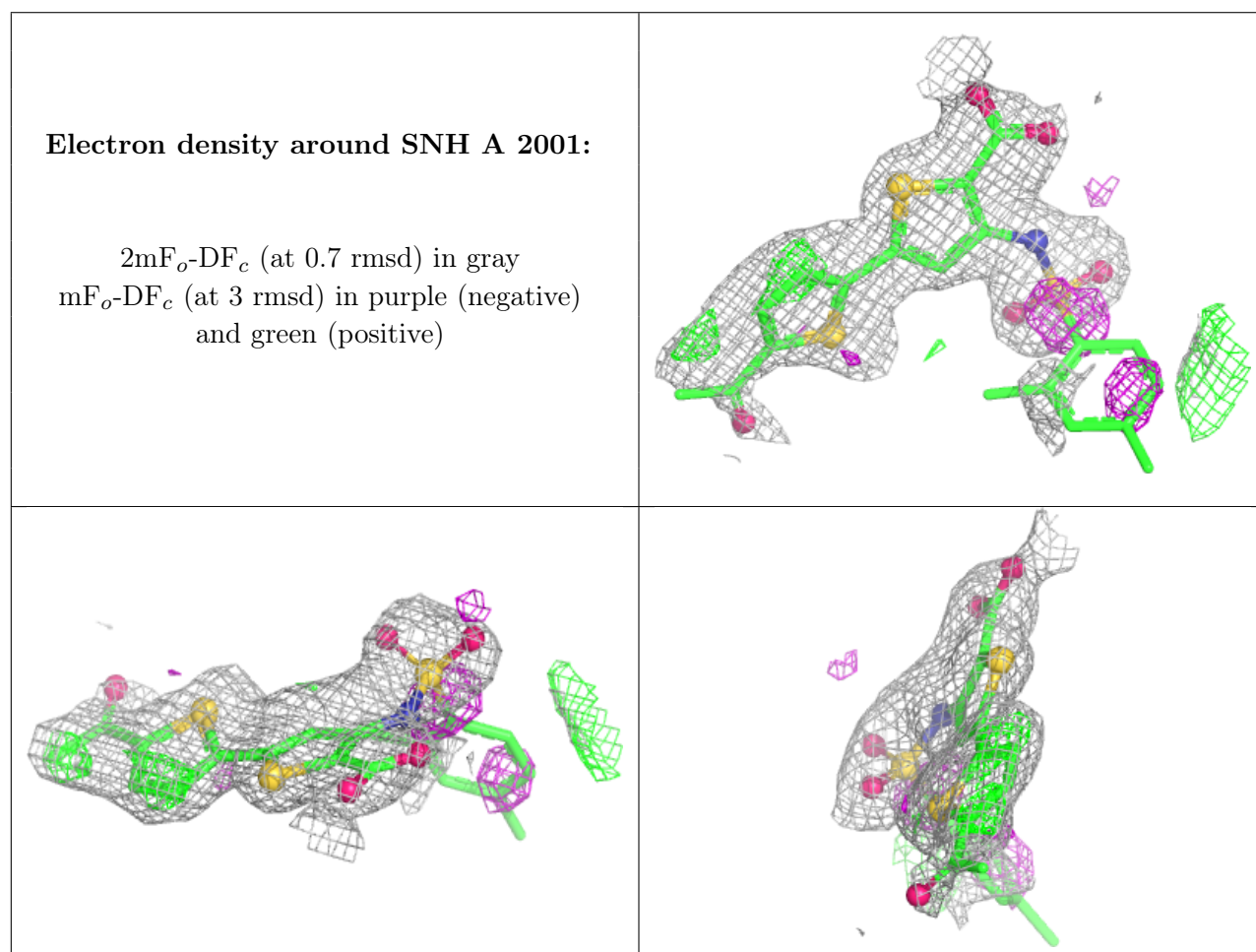
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SNH	A	2001	28/28	0.69	0.21	62,66,78,79	0
2	SNH	B	4001	28/28	0.89	0.14	40,45,47,49	0
2	SNH	B	3001	28/28	0.96	0.07	22,26,28,29	0

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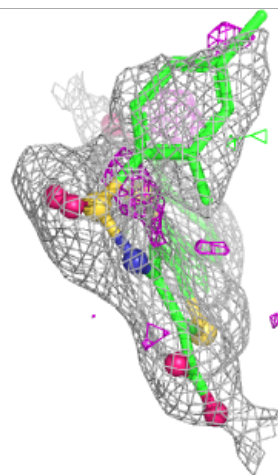
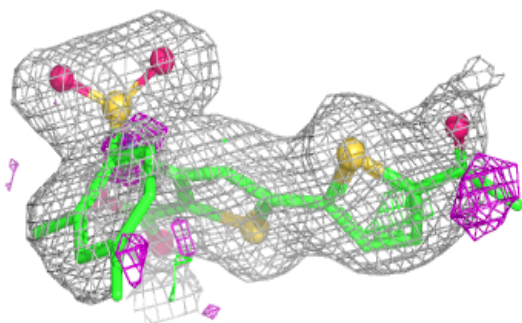
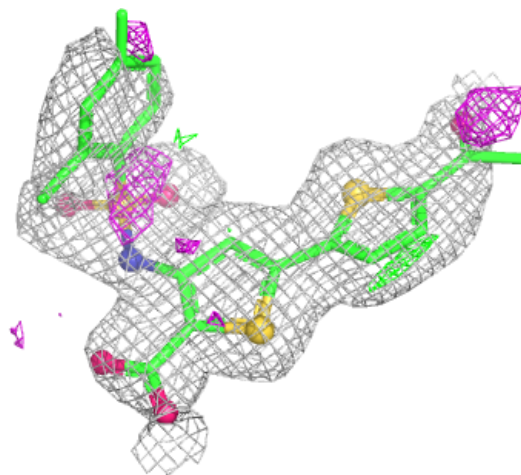
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SNH	A	1001	28/28	0.96	0.08	19,26,29,32	0

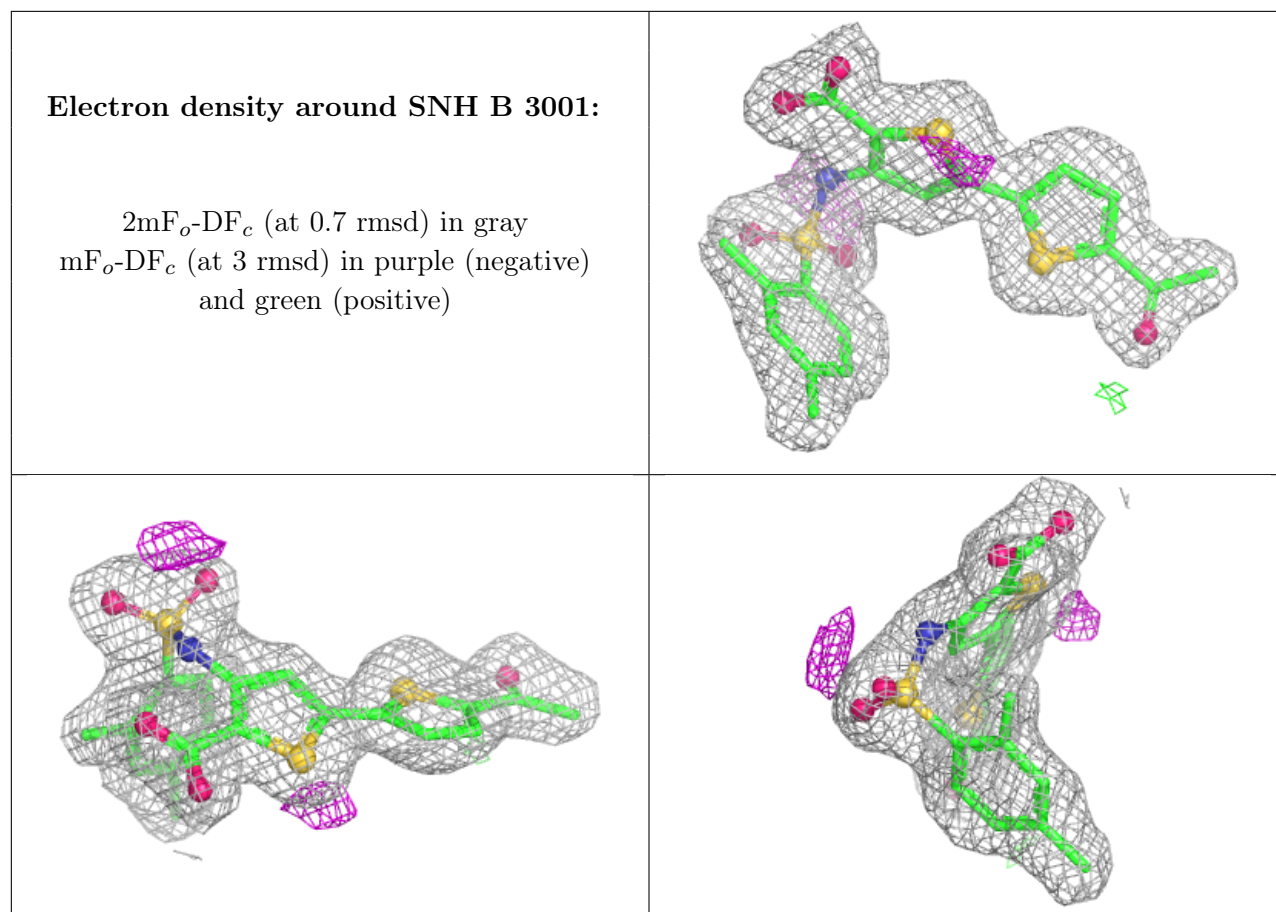
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

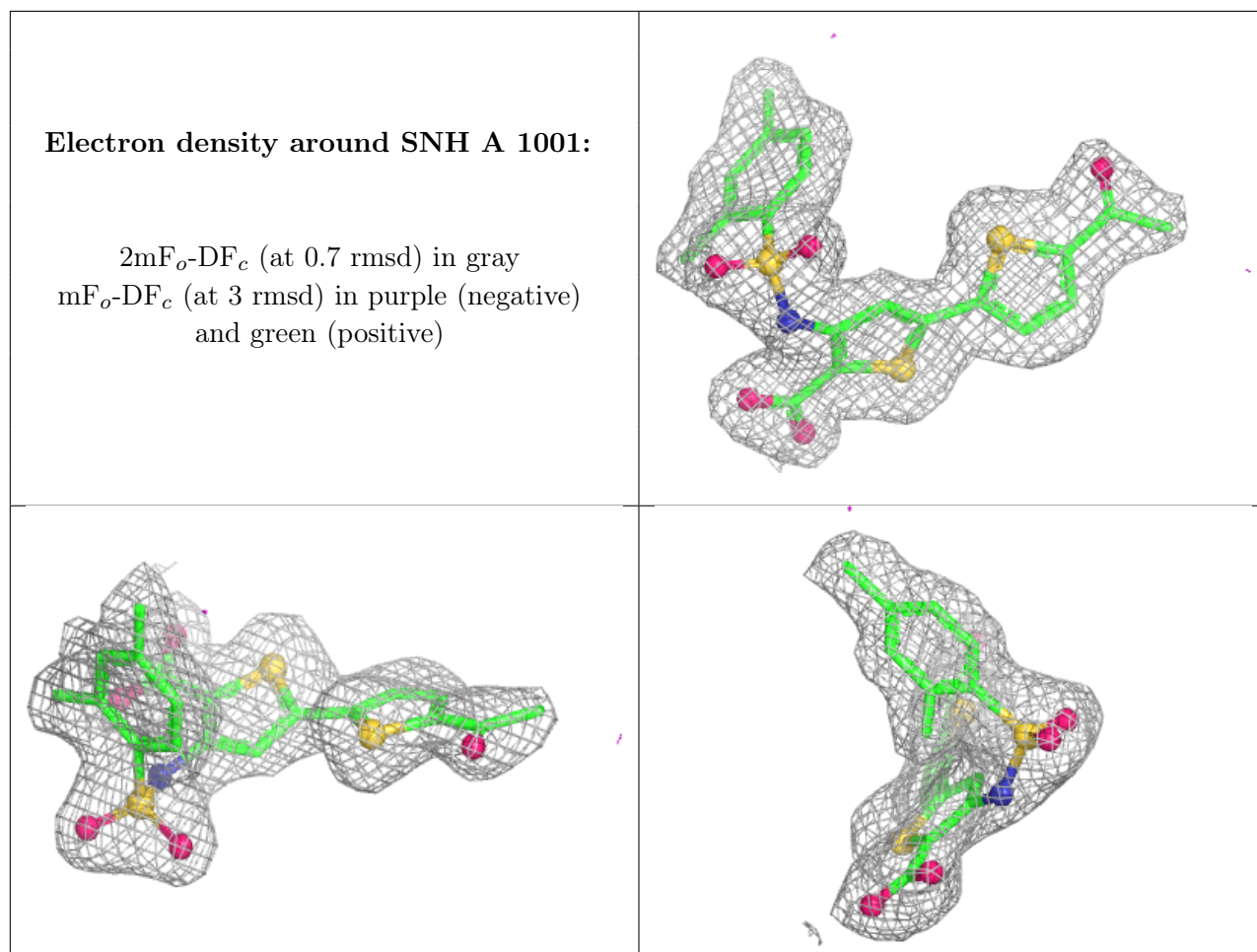


**Electron density around SNH B 4001:**

$2mF_o-DF_c$  (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.