Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2024 – 05:27 PM EST

PDB ID	:	3HCD
Title	:	Crystal Structure of hPNMT in Complex With Noradrenaline and AdoHcy
Authors	:	Drinkwater, N.; Martin, J.L.
Deposited on	:	2009-05-06
Resolution	:	2.39 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

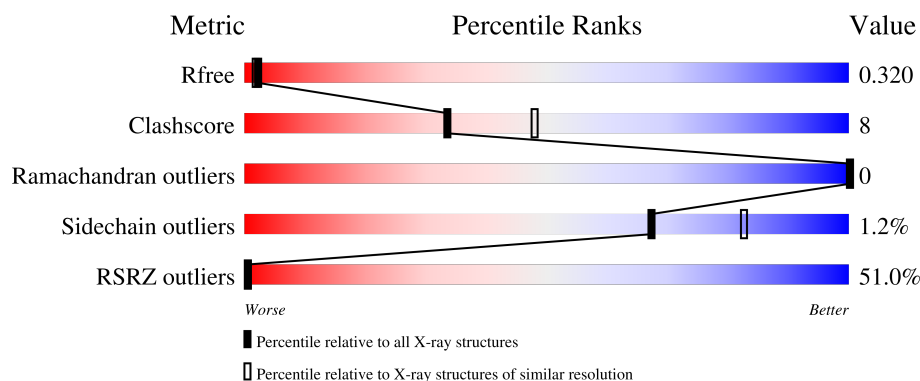|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.39 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	Percentile Ranks	Value
Rfree		0.320
Clashscore		8
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		51.0%

Worse　　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	289	33% / 73% / 15% · 11%
1	B	289	60% / 77% / 16% 7%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4421 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 Phenylethanolamine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total 2016	C 1280	N 358	O 369	S 9	1	0	0
1	B	268	Total 2089	C 1324	N 371	O 385	S 9	0	1	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	GLU	-	expression tag	UNP P11086
A	284	HIS	-	expression tag	UNP P11086
A	285	HIS	-	expression tag	UNP P11086
A	286	HIS	-	expression tag	UNP P11086
A	287	HIS	-	expression tag	UNP P11086
A	288	HIS	-	expression tag	UNP P11086
A	289	HIS	-	expression tag	UNP P11086
B	283	GLU	-	expression tag	UNP P11086
B	284	HIS	-	expression tag	UNP P11086
B	285	HIS	-	expression tag	UNP P11086
B	286	HIS	-	expression tag	UNP P11086
B	287	HIS	-	expression tag	UNP P11086
B	288	HIS	-	expression tag	UNP P11086
B	289	HIS	-	expression tag	UNP P11086

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).

SAH

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is L-NOREPINEPHRINE (three-letter code: LNR) (formula: $C_8H_{11}NO_3$).

LNR
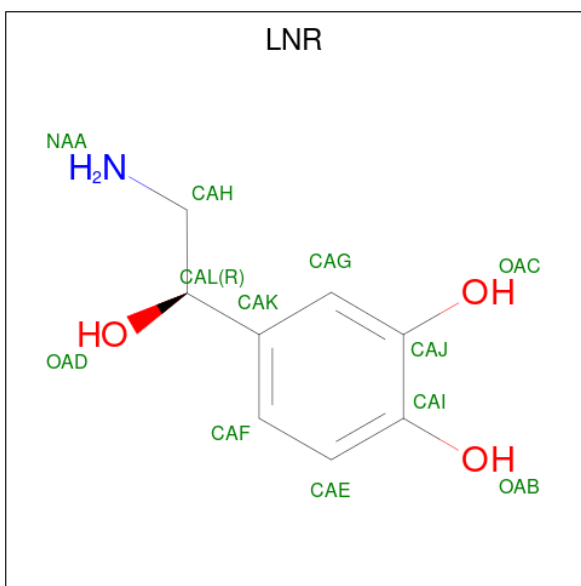
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	8	1	3		
3	B	1	Total	C	N	O	0	0
			12	8	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total O 114 114		0	0
4	B	126	Total O 126 126		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. 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. 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: Phenylethanolamine N-methyltransferase
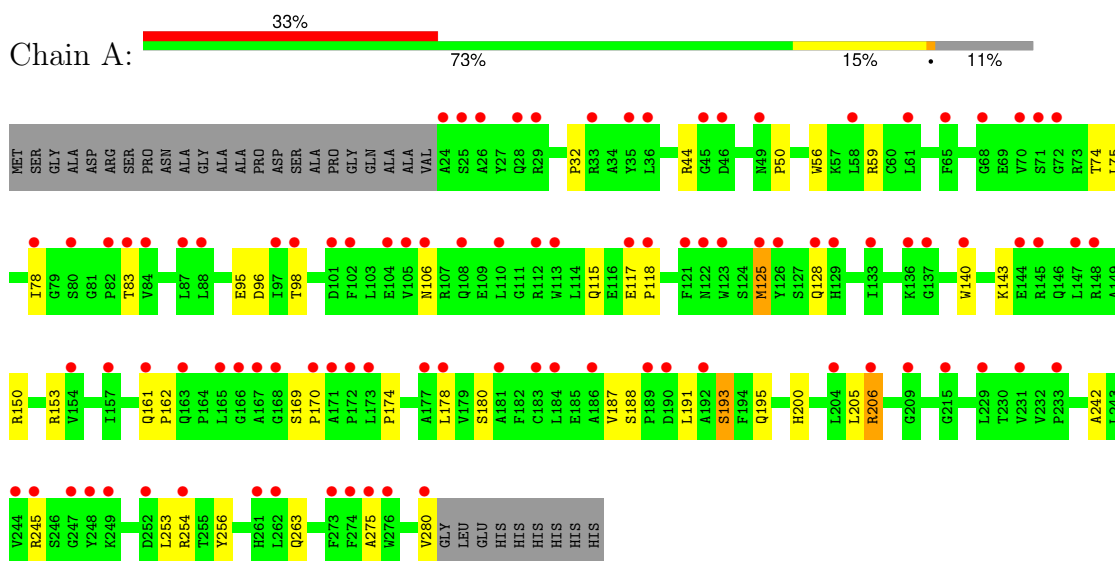
- Molecule 1: Phenylethanolamine N-methyltransferase
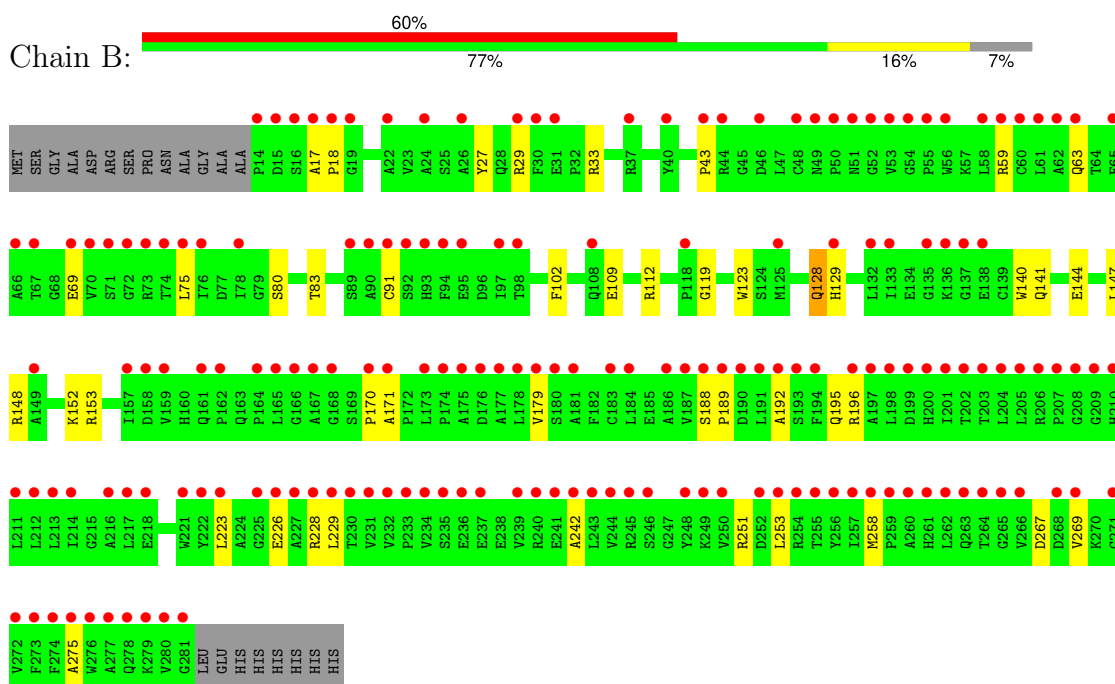
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	93.65Å 93.65Å 187.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.78 – 2.39 34.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.2 (34.78-2.39) 99.9 (34.78-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 2.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.181 , 0.230 0.321 , 0.320	Depositor DCC
R_{free} test set	3381 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.3	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4421	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LNR, SAH

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	0.46	0/2067	0.59	0/2813
1	B	0.53	0/2145	0.62	0/2920
All	All	0.50	0/4212	0.60	0/5733

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2016	0	1983	34	0
1	B	2089	0	2053	32	0
2	A	26	0	19	2	0
2	B	26	0	20	2	0
3	A	12	0	11	1	0
3	B	12	0	11	1	0
4	A	114	0	0	6	0
4	B	126	0	0	3	0
All	All	4421	0	4097	63	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 8.

All (63) 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:125:MET:HE2	1:B:141:GLN:HE22	1.17	1.07
1:A:125:MET:CE	1:B:141:GLN:HE22	1.86	0.89
1:B:29:ARG:HH21	1:B:226:GLU:HB3	1.41	0.85
1:A:125:MET:HB2	4:A:400:HOH:O	1.76	0.84
1:B:75:LEU:HD11	1:B:179:VAL:HG23	1.66	0.77
1:B:195:GLN:HE22	1:B:242:ALA:HA	1.50	0.75
1:B:29:ARG:NH2	1:B:226:GLU:HB3	2.05	0.71
1:A:125:MET:HE2	1:B:141:GLN:NE2	2.00	0.69
1:A:254:ARG:NH2	4:A:504:HOH:O	2.36	0.58
1:A:115:GLN:HB2	1:A:117:GLU:HG3	1.86	0.57
1:A:98:THR:HG23	1:A:153:ARG:HG3	1.87	0.56
1:A:143:LYS:HD3	4:A:320:HOH:O	2.04	0.56
1:A:125:MET:CE	1:B:141:GLN:NE2	2.61	0.56
1:B:69:GLU:OE1	1:B:251:ARG:NH2	2.38	0.56
1:A:83:THR:OG1	2:A:3001:SAH:HA	2.08	0.54
1:B:112:ARG:HH21	1:B:119:GLY:HA3	1.72	0.54
1:A:263:GLN:HG2	4:A:337:HOH:O	2.08	0.53
1:A:50:PRO:O	1:A:59:ARG:NH2	2.41	0.52
1:A:195:GLN:HE22	1:A:242:ALA:HA	1.75	0.51
1:B:17:ALA:HB3	1:B:18:PRO:HD3	1.93	0.50
1:B:253:LEU:HD13	1:B:275:ALA:HB2	1.94	0.50
1:A:253:LEU:HD13	1:A:275:ALA:HB2	1.94	0.50
1:B:128[A]:GLN:HE21	1:B:128[A]:GLN:HA	1.76	0.49
1:B:128[B]:GLN:HG2	1:B:140:TRP:CD1	2.47	0.48
1:B:148:ARG:HD2	4:B:414:HOH:O	2.12	0.48
1:A:161:GLN:HA	1:A:161:GLN:OE1	2.12	0.48
1:A:32:PRO:HG3	1:A:106:ASN:ND2	2.29	0.47
1:B:91:CYS:HB3	1:B:147:LEU:HD13	1.96	0.47
1:A:188:SER:HB3	1:A:193:SER:HB2	1.96	0.46
1:A:280:VAL:O	1:A:280:VAL:HG13	2.15	0.46
1:B:83:THR:HA	1:B:123:TRP:CZ2	2.51	0.46
1:B:129:HIS:ND1	4:B:445:HOH:O	2.35	0.46
1:B:170:PRO:O	1:B:171:ALA:C	2.54	0.46
1:B:43:PRO:HD2	4:B:426:HOH:O	2.14	0.46
1:A:187:VAL:HG11	2:A:3001:SAH:C5	2.45	0.45
1:B:102:PHE:HB2	2:B:3002:SAH:C4	2.45	0.45
1:A:74:THR:HG22	1:A:96:ASP:HB3	1.98	0.45
1:B:27:TYR:CE2	1:B:229:LEU:HD22	2.52	0.45
1:B:258:MET:HE3	3:B:2002:LNR:HAE	2.00	0.44
1:A:174:PRO:HG2	1:A:206:ARG:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:HE	1:A:245:ARG:HB2	1.62	0.43
1:A:195:GLN:NE2	1:A:245:ARG:HD2	2.34	0.43
1:B:59:ARG:HG2	1:B:63:GLN:NE2	2.33	0.43
1:B:188:SER:HA	1:B:189:PRO:HD3	1.90	0.43
1:B:192:ALA:O	1:B:196:ARG:HG3	2.18	0.43
1:A:56:TRP:CE2	1:A:256:TYR:HB2	2.54	0.43
1:A:128:GLN:HG2	1:A:140:TRP:CD1	2.54	0.43
1:A:44:ARG:HG3	4:A:294:HOH:O	2.18	0.43
1:A:178:LEU:HG	1:A:205:LEU:HD13	2.00	0.43
1:B:33:ARG:NH2	1:B:109:GLU:OE2	2.51	0.43
1:A:117:GLU:HB3	1:A:118:PRO:CD	2.50	0.42
1:A:75:LEU:C	1:A:75:LEU:HD23	2.39	0.42
1:A:162:PRO:HA	1:A:200:HIS:CD2	2.54	0.41
1:A:78:ILE:HB	1:A:180:SER:HB2	2.03	0.41
3:A:2001:LNR:HAHA	3:A:2001:LNR:HAG	1.81	0.41
1:A:169:SER:HA	1:A:170:PRO:HD3	1.94	0.41
1:B:267:ASP:OD2	1:B:269:VAL:HG12	2.21	0.41
1:A:95:GLU:HA	1:A:150:ARG:HD3	2.03	0.41
1:B:223:LEU:HD21	1:B:228:ARG:HD2	2.01	0.41
1:B:152:LYS:O	1:B:153:ARG:HB3	2.19	0.41
1:B:80:SER:O	2:B:3002:SAH:HA	2.20	0.41
1:A:125:MET:HG3	4:A:441:HOH:O	2.21	0.40
1:B:144:GLU:O	1:B:148:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	255/289 (88%)	247 (97%)	8 (3%)	0	100	100
1	B	267/289 (92%)	262 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	522/578 (90%)	509 (98%)	13 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	212/233 (91%)	208 (98%)	4 (2%)	52 72
1	B	219/233 (94%)	217 (99%)	2 (1%)	75 88
All	All	431/466 (92%)	425 (99%)	6 (1%)	67 79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	MET
1	A	191	LEU
1	A	193	SER
1	A	206	ARG
1	B	128[A]	GLN
1	B	128[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	195	GLN
1	B	106	ASN
1	B	141	GLN
1	B	195	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
3	LNR	A	2001	-	12,12,12	1.07	1 (8%)	16,16,16	1.04	0
2	SAH	A	3001	-	23,28,28	2.32	7 (30%)	22,40,40	2.71	4 (18%)
3	LNR	B	2002	-	12,12,12	1.02	0	16,16,16	0.89	0
2	SAH	B	3002	-	23,28,28	1.90	6 (26%)	22,40,40	2.21	7 (31%)

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	LNR	A	2001	-	-	5/6/6/6	0/1/1/1
2	SAH	A	3001	-	-	2/11/31/31	0/3/3/3
3	LNR	B	2002	-	-	4/6/6/6	0/1/1/1
2	SAH	B	3002	-	-	2/11/31/31	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	SAH	O-C	5.94	1.39	1.22
2	A	3001	SAH	C2'-C3'	-5.38	1.38	1.53
2	B	3002	SAH	C2'-C3'	-4.86	1.40	1.53
2	A	3001	SAH	OXT-C	-4.27	1.17	1.30
2	B	3002	SAH	C6-N6	4.10	1.48	1.34
2	B	3002	SAH	C2-N3	3.03	1.36	1.32
2	A	3001	SAH	O4'-C4'	-2.91	1.38	1.45
2	A	3001	SAH	C6-N6	2.70	1.43	1.34
2	B	3002	SAH	OXT-C	2.44	1.38	1.30
2	A	3001	SAH	C2-N3	2.43	1.35	1.32
3	A	2001	LNR	OAC-CAJ	2.34	1.41	1.36
2	B	3002	SAH	O4'-C4'	-2.34	1.39	1.45
2	B	3002	SAH	C2-N1	2.26	1.38	1.33
2	A	3001	SAH	C8-N7	2.22	1.38	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	SAH	C4'-O4'-C1'	-8.68	101.97	109.92
2	A	3001	SAH	N3-C2-N1	-7.52	118.47	128.67
2	B	3002	SAH	N3-C2-N1	-6.04	120.47	128.67
2	B	3002	SAH	C4'-O4'-C1'	-3.92	106.34	109.92
2	B	3002	SAH	CB-CA-N	3.16	118.36	110.12
2	A	3001	SAH	O4'-C4'-C5'	-3.07	100.92	108.83
2	B	3002	SAH	C4-C5-N7	-2.93	106.24	109.34
2	B	3002	SAH	C4'-C5'-SD	2.38	122.27	113.78
2	B	3002	SAH	O3'-C3'-C4'	-2.16	104.88	111.08
2	B	3002	SAH	C5-C6-N6	2.14	123.57	120.31
2	A	3001	SAH	O2'-C2'-C3'	2.07	118.44	111.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	LNR	CAG-CAK-CAL-CAH
3	A	2001	LNR	CAF-CAK-CAL-CAH
3	B	2002	LNR	CAG-CAK-CAL-CAH
3	A	2001	LNR	NAA-CAH-CAL-OAD
3	B	2002	LNR	CAF-CAK-CAL-CAH
2	A	3001	SAH	O-C-CA-CB
2	B	3002	SAH	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	B	3002	SAH	CB-CG-SD-C5'
3	A	2001	LNR	CAF-CAK-CAL-OAD
3	B	2002	LNR	CAG-CAK-CAL-OAD
3	B	2002	LNR	CAF-CAK-CAL-OAD
3	A	2001	LNR	CAG-CAK-CAL-OAD
2	A	3001	SAH	CB-CG-SD-C5'

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	LNR	1	0
2	A	3001	SAH	2	0
3	B	2002	LNR	1	0
2	B	3002	SAH	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 then 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 SAH A 3001

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH B 3002

Bond lengths

Bond angles

Torsions

Rings
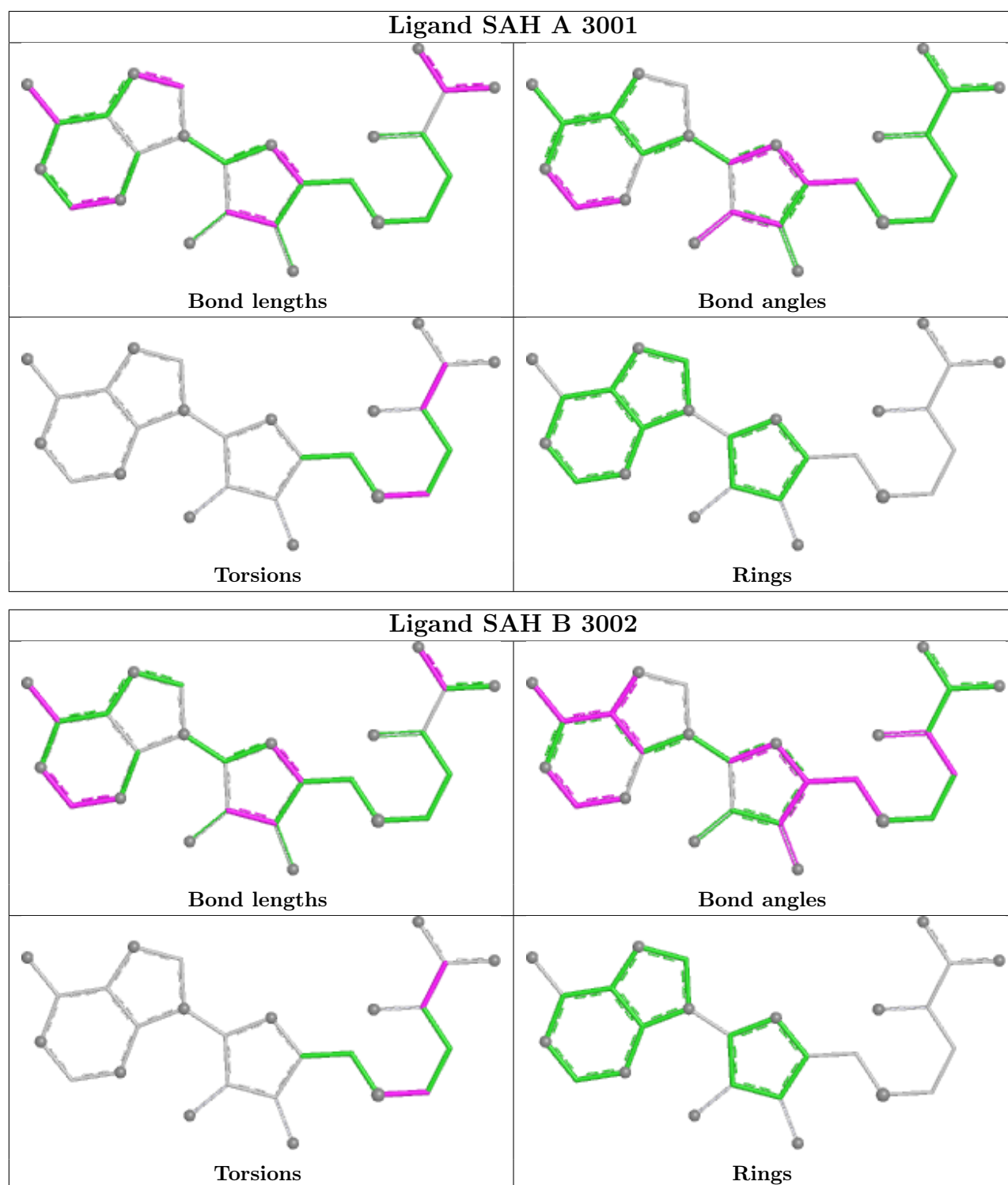
5.7 Other polymers ⓘ

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 ⓘ

Warning: The R factor obtained from EDS is 0.3156, which does not match the depositor's R factor of 0.181. Please interpret the results in this section carefully.

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(Å²)	Q<0.9
1	A	257/289 (88%)	1.79	95 (36%)	1	1	33, 51, 82, 113	4 (1%)
1	B	268/289 (92%)	2.59	173 (64%)	0	0	22, 46, 71, 112	6 (2%)
All	All	525/578 (90%)	2.20	268 (51%)	0	0	22, 48, 78, 113	10 (1%)

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	ALA	7.5
1	B	281	GLY	7.5
1	B	56	TRP	6.0
1	B	260	ALA	5.8
1	B	261	HIS	5.7
1	B	19	GLY	5.3
1	B	187	VAL	5.3
1	B	237	GLU	5.3
1	B	66	ALA	5.2
1	B	243	LEU	5.2
1	B	174	PRO	5.1
1	B	239	VAL	5.0
1	B	257	ILE	4.9
1	B	258	MET	4.9
1	B	221	TRP	4.8
1	B	263	GLN	4.7
1	B	279	LYS	4.7
1	B	244	VAL	4.7
1	B	70	VAL	4.7
1	B	184	LEU	4.6
1	B	255	THR	4.6
1	B	14	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	203	THR	4.5
1	B	216	ALA	4.5
1	B	241	GLU	4.5
1	B	167	ALA	4.4
1	B	269	VAL	4.4
1	B	232	VAL	4.4
1	B	280	VAL	4.4
1	B	159	VAL	4.4
1	B	256	TYR	4.3
1	B	46	ASP	4.2
1	B	204	LEU	4.1
1	A	167	ALA	4.1
1	B	59	ARG	4.1
1	B	202	THR	4.1
1	B	274	PHE	4.1
1	B	240	ARG	4.1
1	B	207	PRO	4.1
1	A	280	VAL	4.0
1	B	259	PRO	4.0
1	B	210	HIS	4.0
1	B	188	SER	3.9
1	B	177	ALA	3.9
1	B	133	ILE	3.9
1	B	52	GLY	3.9
1	B	209	GLY	3.9
1	B	37	ARG	3.9
1	B	95	GLU	3.9
1	B	137	GLY	3.9
1	B	71	SER	3.9
1	A	184	LEU	3.8
1	B	94	PHE	3.8
1	B	166	GLY	3.8
1	B	92	SER	3.8
1	B	277	ALA	3.8
1	A	189	PRO	3.8
1	B	253	LEU	3.7
1	B	170	PRO	3.7
1	B	272	VAL	3.7
1	B	22	ALA	3.7
1	B	262	LEU	3.7
1	B	201	ILE	3.7
1	B	73	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	264	THR	3.7
1	B	173	LEU	3.7
1	B	192	ALA	3.7
1	B	229	LEU	3.7
1	B	228	ARG	3.7
1	A	170	PRO	3.6
1	B	18	PRO	3.6
1	B	252	ASP	3.6
1	B	250	VAL	3.6
1	A	113	TRP	3.6
1	B	208	GLY	3.5
1	A	157	ILE	3.5
1	B	254	ARG	3.5
1	B	50	PRO	3.5
1	B	248	TYR	3.5
1	B	164	PRO	3.5
1	B	93	HIS	3.5
1	B	230	THR	3.5
1	B	43	PRO	3.5
1	B	191	LEU	3.5
1	A	45	GLY	3.5
1	A	261	HIS	3.5
1	B	223	LEU	3.4
1	B	29	ARG	3.4
1	B	226	GLU	3.4
1	B	234	VAL	3.4
1	B	49	ASN	3.4
1	B	178	LEU	3.3
1	B	217	LEU	3.3
1	B	51	ASN	3.3
1	A	108	GLN	3.3
1	A	105	VAL	3.3
1	B	249	LYS	3.3
1	A	154	VAL	3.3
1	A	140	TRP	3.3
1	B	222	TYR	3.3
1	B	242	ALA	3.3
1	A	147	LEU	3.2
1	A	245	ARG	3.2
1	A	249	LYS	3.2
1	B	194	PHE	3.2
1	B	198	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	121	PHE	3.1
1	B	63	GLN	3.1
1	A	83	THR	3.1
1	A	254	ARG	3.1
1	B	236	GLU	3.1
1	B	26	ALA	3.1
1	B	175	ALA	3.1
1	B	276	TRP	3.1
1	B	218	GLU	3.1
1	B	55	PRO	3.1
1	B	60	CYS	3.0
1	A	274	PHE	3.0
1	B	213	LEU	3.0
1	B	266	VAL	3.0
1	B	227	ALA	3.0
1	A	28	GLN	3.0
1	A	106	ASN	3.0
1	B	275	ALA	3.0
1	B	212	LEU	2.9
1	B	16	SER	2.9
1	A	177	ALA	2.9
1	B	189	PRO	2.9
1	A	88	LEU	2.9
1	A	97	ILE	2.9
1	B	72	GLY	2.9
1	B	125	MET	2.9
1	B	211	LEU	2.9
1	B	265	GLY	2.9
1	A	136	LYS	2.9
1	A	102	PHE	2.9
1	B	278	GLN	2.9
1	B	44	ARG	2.9
1	B	206	ARG	2.9
1	B	135	GLY	2.9
1	B	65	PHE	2.8
1	A	61	LEU	2.8
1	B	214	ILE	2.8
1	A	25	SER	2.8
1	B	31	GLU	2.8
1	A	125	MET	2.8
1	B	58	LEU	2.8
1	B	179	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	173	LEU	2.8
1	A	126	TYR	2.8
1	B	17	ALA	2.8
1	B	171	ALA	2.8
1	B	183	CYS	2.8
1	B	246	SER	2.7
1	B	225	GLY	2.7
1	B	205	LEU	2.7
1	A	71	SER	2.7
1	B	273	PHE	2.7
1	B	24	ALA	2.7
1	A	104	GLU	2.6
1	A	233	PRO	2.6
1	B	233	PRO	2.6
1	A	46	ASP	2.6
1	B	15	ASP	2.6
1	B	168	GLY	2.6
1	B	181	ALA	2.6
1	B	271	GLY	2.6
1	A	144	GLU	2.6
1	A	36	LEU	2.6
1	B	74	THR	2.6
1	B	231	VAL	2.6
1	A	248	TYR	2.6
1	A	172	PRO	2.5
1	A	29	ARG	2.5
1	A	190	ASP	2.5
1	A	231	VAL	2.5
1	B	235	SER	2.5
1	B	190	ASP	2.5
1	A	118	PRO	2.5
1	A	168	GLY	2.5
1	B	75	LEU	2.5
1	B	165	LEU	2.5
1	A	148	ARG	2.5
1	A	78	ILE	2.4
1	A	252	ASP	2.4
1	B	48	CYS	2.4
1	B	67	THR	2.4
1	B	89	SER	2.4
1	A	101	ASP	2.4
1	B	129	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	192	ALA	2.4
1	B	90	ALA	2.4
1	A	117	GLU	2.4
1	B	76	ILE	2.4
1	A	35	TYR	2.4
1	A	33	ARG	2.4
1	A	145	ARG	2.4
1	A	161	GLN	2.4
1	B	132	LEU	2.4
1	B	53	VAL	2.3
1	A	215	GLY	2.3
1	A	178	LEU	2.3
1	A	26	ALA	2.3
1	B	149	ALA	2.3
1	A	84	VAL	2.3
1	A	273	PHE	2.3
1	B	108	GLN	2.3
1	B	161	GLN	2.3
1	A	110	LEU	2.3
1	B	69	GLU	2.3
1	A	122	ASN	2.3
1	A	65	PHE	2.3
1	B	200	HIS	2.3
1	B	268	ASP	2.3
1	A	137	GLY	2.3
1	B	62	ALA	2.2
1	B	176	ASP	2.2
1	B	180	SER	2.2
1	A	68	GLY	2.2
1	A	87	LEU	2.2
1	B	61	LEU	2.2
1	A	186	ALA	2.2
1	B	118	PRO	2.2
1	A	183	CYS	2.2
1	B	157	ILE	2.2
1	B	196	ARG	2.2
1	A	171	ALA	2.2
1	B	162	PRO	2.2
1	B	186	ALA	2.2
1	B	197	ALA	2.2
1	A	128	GLN	2.2
1	A	133	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	78	ILE	2.2
1	B	97	ILE	2.2
1	A	49	ASN	2.2
1	A	82	PRO	2.2
1	A	129	HIS	2.2
1	A	244	VAL	2.2
1	B	54	GLY	2.1
1	A	206	ARG	2.1
1	A	229	LEU	2.1
1	A	262	LEU	2.1
1	A	275	ALA	2.1
1	A	98	THR	2.1
1	B	40	TYR	2.1
1	B	30	PHE	2.1
1	B	138	GLU	2.1
1	A	112	ARG	2.1
1	A	123	TRP	2.1
1	A	204	LEU	2.1
1	A	163	GLN	2.1
1	A	166	GLY	2.1
1	B	193	SER	2.1
1	B	245	ARG	2.1
1	A	58	LEU	2.1
1	A	276	TRP	2.1
1	A	181	ALA	2.1
1	A	70	VAL	2.0
1	A	72	GLY	2.0
1	A	247	GLY	2.0
1	B	158	ASP	2.0
1	B	199	ASP	2.0
1	B	136	LYS	2.0
1	A	165	LEU	2.0
1	B	91	CYS	2.0
1	B	98	THR	2.0
1	A	209	GLY	2.0
1	A	80	SER	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.
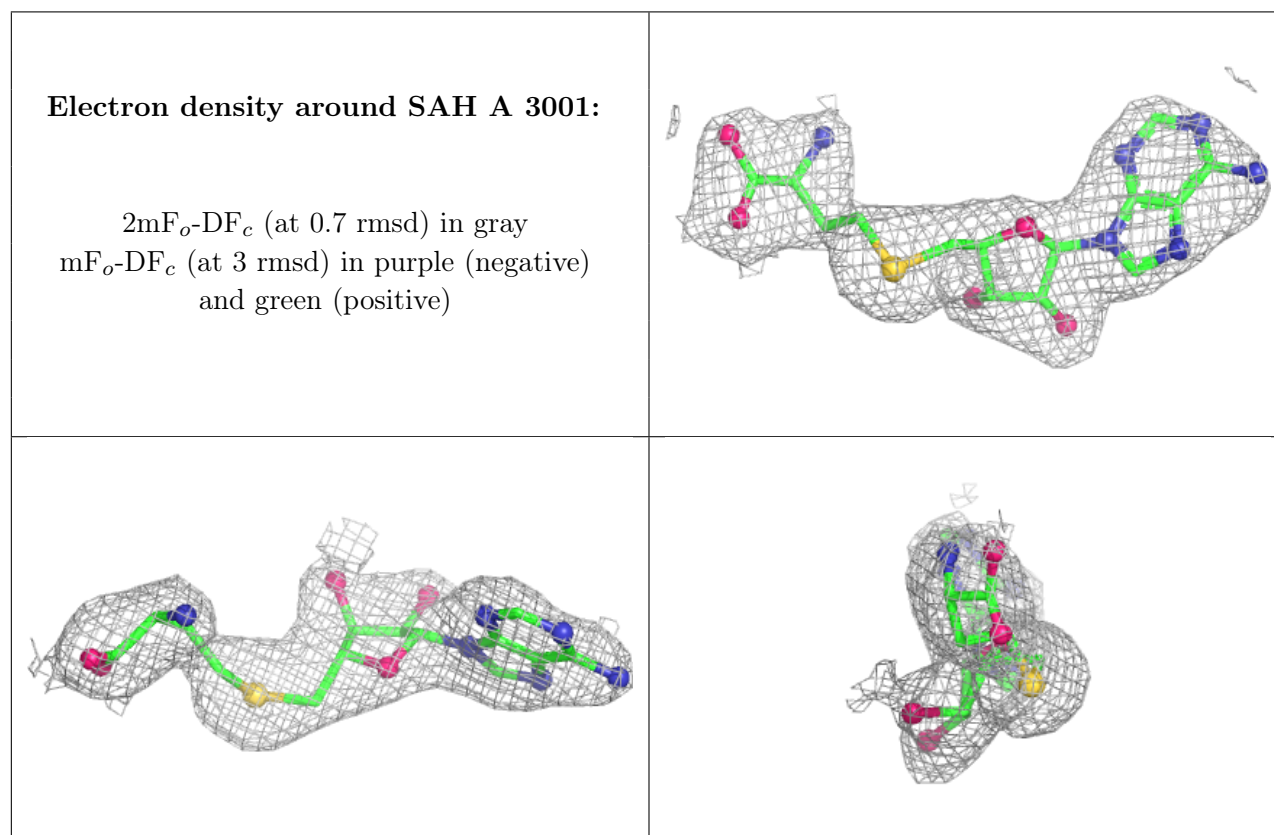
6.3 Carbohydrates (i)
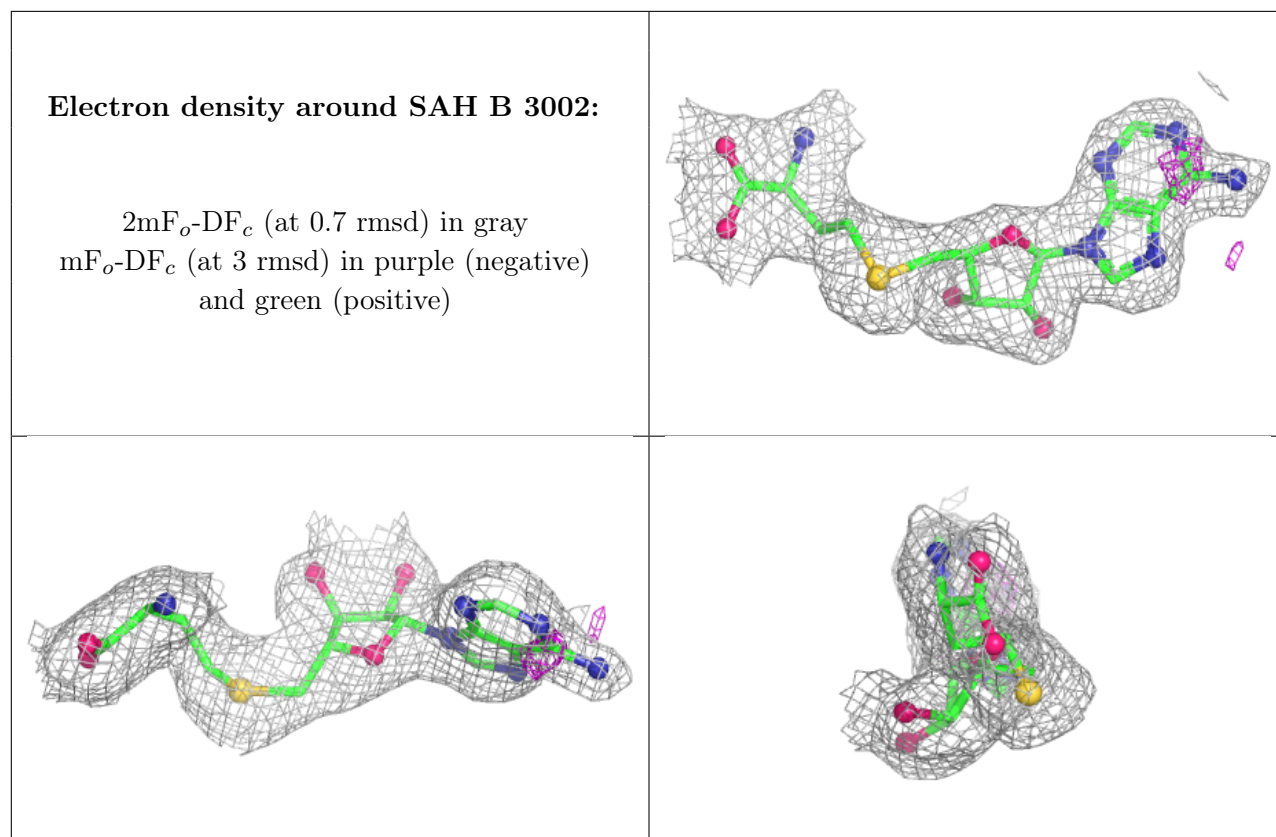
There are no monosaccharides in this entry.

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
3	LNR	B	2002	12/12	0.61	0.24	48,52,53,54	0
3	LNR	A	2001	12/12	0.69	0.21	46,49,53,54	0
2	SAH	A	3001	26/26	0.89	0.12	41,54,59,62	0
2	SAH	B	3002	26/26	0.89	0.13	30,40,47,47	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 SAH A 3001:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SAH B 3002:

$2mF_o$-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 ⓘ

There are no such residues in this entry.