



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:08 PM UTC

PDB ID : 3KQP / pdb_00003kqp
Title : Crystal Structure of hPNMT in Complex AdoHcy and 6-Aminoquinoline
Authors : Drinkwater, N.; Martin, J.L.
Deposited on : 2009-11-17
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

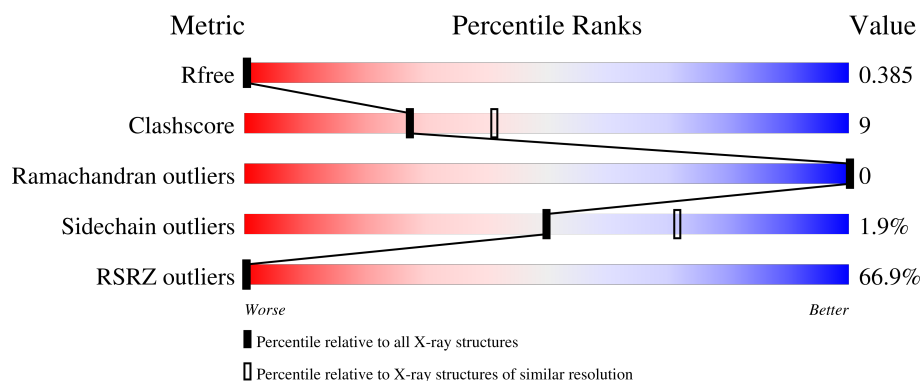
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	289	45% 71% 18% • 11%
1	B	289	77% 75% 17% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4337 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.

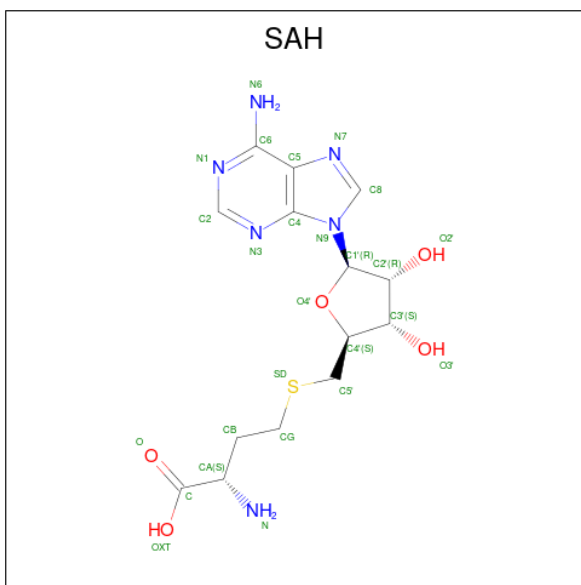
- Molecule 1 is a protein called Phenylethanolamine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2016	1280	358	369	9			
1	B	268	Total	C	N	O	S	0	0	0
			2083	1320	370	384	9			

There are 14 discrepancies between the modelled and reference sequences:

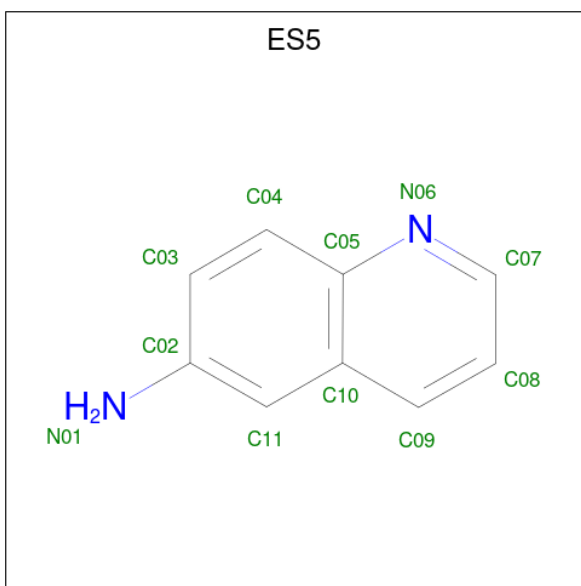
Chain	Residue	Modelled	Actual	Comment	Reference
A	283	GLU	-	expression tag	UNP P11086
A	284	HIS	-	expression tag	UNP P11086
A	285	HIS	-	expression tag	UNP P11086
A	286	HIS	-	expression tag	UNP P11086
A	287	HIS	-	expression tag	UNP P11086
A	288	HIS	-	expression tag	UNP P11086
A	289	HIS	-	expression tag	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 (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



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 quinolin-6-amine (CCD ID: ES5) (formula: $C_9H_8N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			11	9	2		
3	B	1	Total	C	N	0	0
			11	9	2		

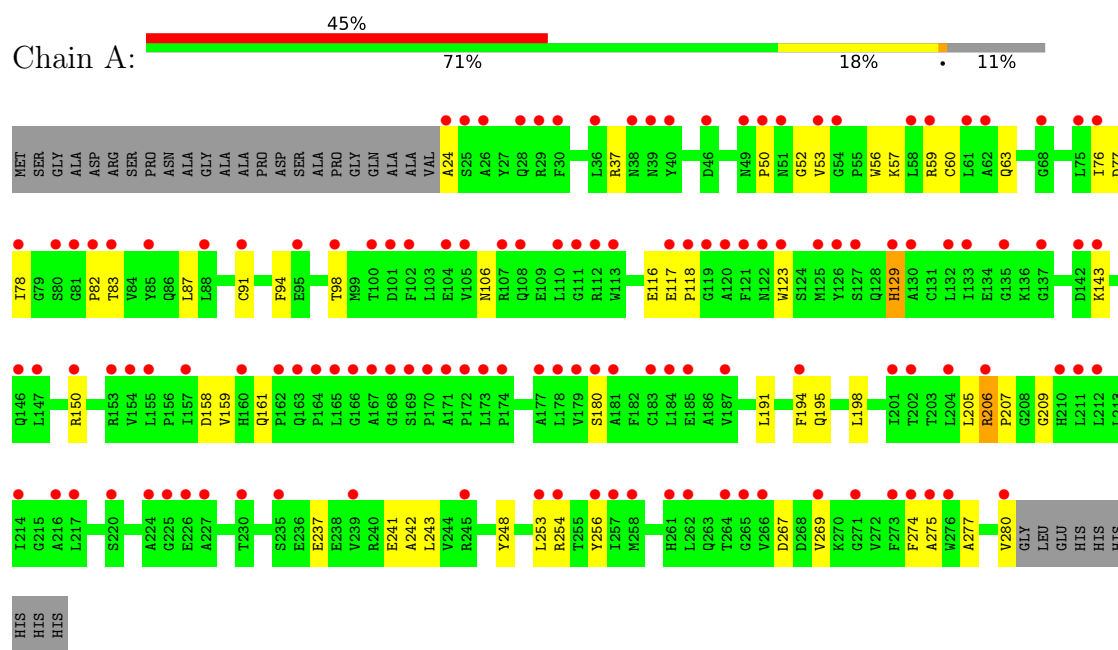
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total 71	O 71	0	0
4	B	93	Total 93	O 93	0	0

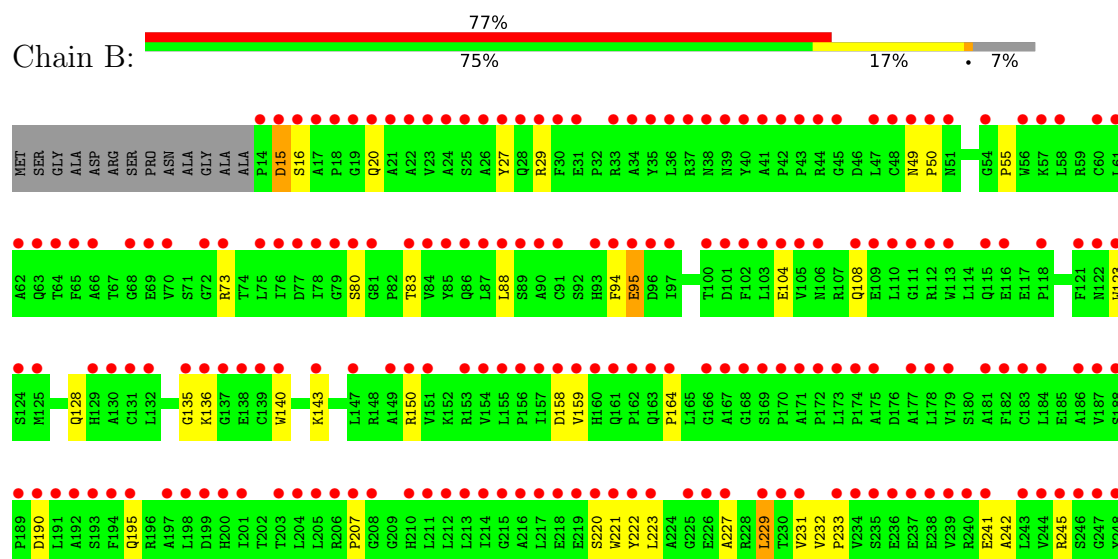
3 Residue-property plots [i](#)

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: Phenylethanolamine N-methyltransferase



• Molecule 1: Phenylethanolamine N-methyltransferase



K249	V250	R251	D252	L253	R254	T255	Y256	I257	M258	F259	A260	H261	L262	Q263	T264	G265	V266	D267	D268	V269	K270	G271	V272	F273	F274	A275	W276	K279	V280	G281	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.57Å 93.57Å 188.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.41 – 2.40 45.41 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (45.41-2.40) 90.2 (45.41-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.231 , 0.302 0.336 , 0.385	Depositor DCC
R_{free} test set	1557 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4337	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: ES5, 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	0.39	0/2067	0.76	2/2813 (0.1%)
1	B	0.42	0/2136	0.77	0/2908
All	All	0.40	0/4203	0.76	2/5721 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	GLN	CA-C-N	5.16	125.20	119.32
1	A	161	GLN	C-N-CA	5.16	125.20	119.32

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	2016	0	1983	37	0
1	B	2083	0	2045	38	1
2	A	26	0	20	1	0
2	B	26	0	20	4	0
3	A	11	0	8	1	0
3	B	11	0	8	2	0
4	A	71	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	93	0	0	9	0
All	All	4337	0	4084	75	1

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 (75) 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:195:GLN:HE22	1:B:242:ALA:HA	1.44	0.82
1:A:37:ARG:HD3	4:A:2175:HOH:O	1.84	0.77
1:A:253:LEU:HD13	1:A:275:ALA:HB2	1.71	0.71
1:B:159:VAL:HG13	2:B:2002:SAH:H2	1.76	0.67
1:A:143:LYS:HD3	4:A:2010:HOH:O	1.93	0.67
1:B:267:ASP:OD2	1:B:269:VAL:HG12	1.93	0.67
1:A:267:ASP:OD1	1:A:269:VAL:HG12	1.95	0.66
1:B:207:PRO:HB3	1:B:281:GLY:HA3	1.78	0.64
1:A:59:ARG:HG2	1:A:63:GLN:NE2	2.13	0.63
1:A:94:PHE:O	1:A:150:ARG:HD3	2.00	0.62
1:B:159:VAL:HG22	2:B:2002:SAH:N1	2.15	0.61
1:B:241:GLU:HG2	4:B:2183:HOH:O	1.99	0.61
1:B:135:GLY:O	1:B:136:LYS:HD3	2.04	0.58
1:A:159:VAL:HG13	2:A:2001:SAH:H2	1.85	0.57
1:B:104:GLU:O	1:B:108:GLN:HG3	2.05	0.57
1:A:195:GLN:HE22	1:A:242:ALA:HA	1.70	0.57
1:B:143:LYS:HD3	4:B:2017:HOH:O	2.04	0.56
1:A:116:GLU:HG2	4:A:2096:HOH:O	2.05	0.56
1:B:263:GLN:HB2	4:B:2031:HOH:O	2.06	0.55
1:A:52:GLY:HA3	4:A:2195:HOH:O	2.06	0.54
1:B:16:SER:HB2	1:B:20:GLN:NE2	2.23	0.53
1:B:280:VAL:HA	4:B:2073:HOH:O	2.08	0.53
1:A:83:THR:HA	1:A:123:TRP:CZ2	2.44	0.53
1:A:198:LEU:HD21	1:A:243:LEU:HD23	1.90	0.52
1:B:83:THR:HA	1:B:123:TRP:CZ2	2.46	0.51
1:B:222:TYR:CZ	1:B:229:LEU:HD13	2.46	0.50
1:A:254:ARG:NH2	4:A:2173:HOH:O	2.39	0.50
1:B:27:TYR:CZ	1:B:229:LEU:HD22	2.47	0.50
1:A:82:PRO:HD2	1:A:83:THR:HG23	1.94	0.49
1:A:56:TRP:CE2	1:A:256:TYR:HB2	2.47	0.49
1:B:253:LEU:HD13	1:B:275:ALA:HB2	1.94	0.49
1:B:73:ARG:HG3	1:B:95:GLU:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:VAL:HG11	3:B:290:ES5:H09	1.96	0.48
1:A:191:LEU:O	1:A:194:PHE:HB3	2.13	0.48
1:B:140:TRP:HD1	4:B:2180:HOH:O	1.95	0.48
1:A:253:LEU:HA	1:A:274:PHE:O	2.13	0.48
1:A:78:ILE:HB	1:A:180:SER:HB2	1.95	0.48
1:B:27:TYR:CE1	1:B:229:LEU:HD22	2.50	0.47
1:A:91:CYS:O	1:A:150:ARG:HD2	2.15	0.47
1:A:76:ILE:HG12	1:A:98:THR:HB	1.96	0.47
1:B:140:TRP:CD1	4:B:2180:HOH:O	2.67	0.47
1:B:159:VAL:HG13	2:B:2002:SAH:C2	2.44	0.46
1:B:258:MET:HE1	3:B:290:ES5:H08	1.97	0.46
1:B:220:SER:HA	1:B:231:VAL:O	2.15	0.46
1:A:24:ALA:HB3	4:A:2113:HOH:O	2.16	0.46
1:A:237:GLU:HG2	4:A:2027:HOH:O	2.15	0.46
1:A:77:ASP:HB2	1:A:87:LEU:HD21	1.97	0.45
1:B:135:GLY:C	1:B:136:LYS:HD3	2.40	0.45
1:A:117:GLU:HB3	1:A:118:PRO:CD	2.46	0.45
1:A:129:HIS:CE1	4:B:2047:HOH:O	2.69	0.45
1:B:94:PHE:O	1:B:150:ARG:HD3	2.17	0.44
1:B:88:LEU:O	1:B:143:LYS:HD2	2.17	0.44
1:A:50:PRO:O	1:A:59:ARG:NH2	2.44	0.43
1:B:158:ASP:O	1:B:164:PRO:HA	2.18	0.43
1:B:29:ARG:HB3	1:B:227:ALA:HB2	1.99	0.43
1:A:53:VAL:O	1:A:57:LYS:HG3	2.18	0.43
1:B:190:ASP:HB2	4:B:2087:HOH:O	2.18	0.43
1:B:29:ARG:C	1:B:227:ALA:HB2	2.44	0.43
1:B:221:TRP:HZ3	1:B:223:LEU:HG	1.84	0.43
1:A:56:TRP:CD2	1:A:256:TYR:HB2	2.54	0.42
1:B:261:HIS:CE1	1:B:262:LEU:HG	2.54	0.42
1:A:106:ASN:HD22	1:A:106:ASN:HA	1.58	0.42
1:B:49:ASN:O	1:B:55:PRO:HG2	2.19	0.42
1:A:158:ASP:OD1	1:A:158:ASP:C	2.63	0.42
1:B:261:HIS:HE1	4:B:2077:HOH:O	2.02	0.42
1:B:49:ASN:HA	1:B:50:PRO:HD3	1.91	0.42
1:A:60:CYS:HB3	1:A:274:PHE:CD1	2.55	0.41
1:B:232:VAL:HA	1:B:233:PRO:HD2	1.87	0.41
1:A:57:LYS:HE2	4:A:2192:HOH:O	2.19	0.41
1:A:237:GLU:O	1:A:241:GLU:HG3	2.21	0.41
1:B:80:SER:O	2:B:2002:SAH:HA	2.21	0.41
1:A:206:ARG:HG2	1:A:207:PRO:N	2.31	0.41
1:A:269:VAL:HG11	3:A:290:ES5:H09	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LEU:HD11	1:A:209:GLY:HA3	2.04	0.40
1:A:248:TYR:HB3	1:A:277:ALA:HB1	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ASP:OD2	1:B:29:ARG:NH1[8_664]	2.16	0.04

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	255/289 (88%)	245 (96%)	10 (4%)	0	100	100
1	B	266/289 (92%)	257 (97%)	9 (3%)	0	100	100
All	All	521/578 (90%)	502 (96%)	19 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	212/233 (91%)	209 (99%)	3 (1%)	59	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	218/233 (94%)	213 (98%)	5 (2%)	44 66
All	All	430/466 (92%)	422 (98%)	8 (2%)	50 71

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	206	ARG
1	A	280	VAL
1	B	15	ASP
1	B	95	GLU
1	B	128	GLN
1	B	229	LEU
1	B	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	93	HIS
1	A	106	ASN
1	A	129	HIS
1	A	160	HIS
1	A	195	GLN
1	A	261	HIS
1	B	20	GLN
1	B	106	ASN
1	B	128	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 [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$
3	ES5	A	290	-	12,12,12	1.63	4 (33%)	16,16,16	1.23	3 (18%)
3	ES5	B	290	-	12,12,12	1.60	3 (25%)	16,16,16	1.30	2 (12%)
2	SAH	B	2002	-	27,28,28	4.13	12 (44%)	36,40,40	2.21	13 (36%)
2	SAH	A	2001	-	27,28,28	4.13	12 (44%)	36,40,40	2.18	13 (36%)

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	ES5	A	290	-	-	-	0/2/2/2
3	ES5	B	290	-	-	-	0/2/2/2
2	SAH	B	2002	-	-	3/15/31/31	0/3/3/3
2	SAH	A	2001	-	-	6/15/31/31	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	SAH	C2-N1	9.76	1.51	1.33
2	A	2001	SAH	C2-N1	9.66	1.51	1.33
2	A	2001	SAH	C2-N3	8.76	1.49	1.33
2	B	2002	SAH	C2-N3	8.42	1.48	1.33
2	A	2001	SAH	C8-N7	7.45	1.46	1.31
2	A	2001	SAH	C4-N3	7.35	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	SAH	C4-N3	7.34	1.48	1.34
2	B	2002	SAH	C8-N7	7.18	1.45	1.31
2	B	2002	SAH	C8-N9	7.11	1.49	1.37
2	A	2001	SAH	C8-N9	7.07	1.49	1.37
2	B	2002	SAH	C5-C4	5.50	1.48	1.39
2	A	2001	SAH	C5-C4	5.46	1.48	1.39
2	B	2002	SAH	C6-N6	4.92	1.46	1.34
2	A	2001	SAH	C6-N6	4.77	1.46	1.34
2	A	2001	SAH	C5-N7	4.53	1.47	1.39
2	B	2002	SAH	C5-N7	4.48	1.47	1.39
2	B	2002	SAH	C6-N1	3.89	1.46	1.35
2	A	2001	SAH	C6-N1	3.86	1.46	1.35
2	B	2002	SAH	C4-N9	3.76	1.45	1.37
2	A	2001	SAH	C4-N9	3.72	1.45	1.37
2	B	2002	SAH	C5-C6	3.68	1.51	1.41
2	B	2002	SAH	OXT-C	3.40	1.41	1.30
2	A	2001	SAH	C5-C6	3.34	1.50	1.41
3	B	290	ES5	C07-N06	3.28	1.38	1.32
3	A	290	ES5	C07-N06	3.23	1.38	1.32
2	A	2001	SAH	OXT-C	2.99	1.40	1.30
3	A	290	ES5	C04-C03	2.36	1.41	1.36
3	A	290	ES5	C02-N01	2.35	1.46	1.38
3	B	290	ES5	C04-C03	2.33	1.41	1.36
3	B	290	ES5	C02-N01	2.24	1.46	1.38
3	A	290	ES5	C11-C02	2.03	1.42	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	SAH	N3-C2-N1	-5.83	119.75	128.58
2	B	2002	SAH	N3-C2-N1	-5.80	119.80	128.58
2	B	2002	SAH	N9-C8-N7	-4.77	107.17	113.94
2	A	2001	SAH	N9-C8-N7	-4.55	107.48	113.94
2	B	2002	SAH	C5-C4-N3	-4.48	120.55	126.72
2	A	2001	SAH	C5-C4-N3	-4.33	120.76	126.72
2	B	2002	SAH	O4'-C1'-C2'	-3.52	99.08	106.62
2	B	2002	SAH	C5-N7-C8	3.41	108.81	103.45
2	B	2002	SAH	C2-N3-C4	3.22	119.70	111.83
2	A	2001	SAH	CB-CG-SD	-3.15	106.42	113.45
2	A	2001	SAH	C2-N3-C4	3.06	119.30	111.83
2	A	2001	SAH	C5-N7-C8	2.97	108.12	103.45
2	A	2001	SAH	C4-N9-C8	2.93	108.82	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2002	SAH	N3-C4-N9	2.91	132.12	127.17
2	A	2001	SAH	N3-C4-N9	2.91	132.11	127.17
2	B	2002	SAH	C4-N9-C8	2.91	108.79	105.74
2	A	2001	SAH	O4'-C1'-C2'	-2.81	100.61	106.62
3	B	290	ES5	C08-C07-N06	-2.63	120.10	123.97
3	A	290	ES5	C08-C07-N06	-2.51	120.28	123.97
2	A	2001	SAH	C5'-SD-CG	2.44	109.50	102.26
2	A	2001	SAH	OXT-C-O	-2.40	118.63	124.08
2	B	2002	SAH	C5'-SD-CG	2.38	109.32	102.26
2	B	2002	SAH	C4-C5-N7	-2.34	107.91	110.58
3	B	290	ES5	C02-C11-C10	-2.23	119.63	121.11
2	B	2002	SAH	C2'-C1'-N9	-2.16	107.94	113.30
2	A	2001	SAH	C4'-O4'-C1'	-2.16	104.70	109.47
2	A	2001	SAH	C6-C5-C4	2.15	120.11	117.18
2	B	2002	SAH	C6-C5-C4	2.11	120.06	117.18
2	B	2002	SAH	CB-CG-SD	-2.09	108.80	113.45
3	A	290	ES5	C02-C11-C10	-2.07	119.74	121.11
3	A	290	ES5	C07-N06-C05	2.02	119.98	116.93

There are no chirality outliers.

All (9) torsion outliers are listed below:

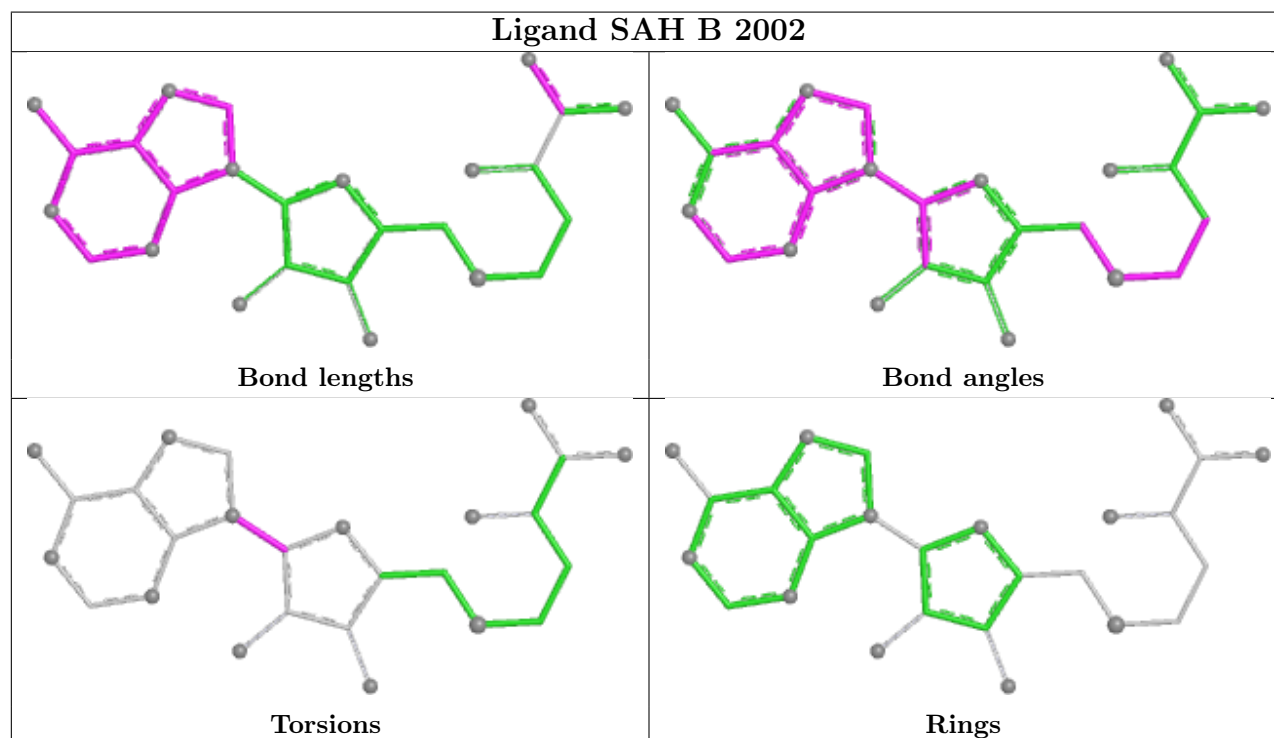
Mol	Chain	Res	Type	Atoms
2	A	2001	SAH	N-CA-CB-CG
2	A	2001	SAH	C-CA-CB-CG
2	B	2002	SAH	C2'-C1'-N9-C4
2	A	2001	SAH	C2'-C1'-N9-C8
2	B	2002	SAH	C2'-C1'-N9-C8
2	A	2001	SAH	C4'-C5'-SD-CG
2	A	2001	SAH	C2'-C1'-N9-C4
2	A	2001	SAH	O4'-C1'-N9-C8
2	B	2002	SAH	O4'-C1'-N9-C8

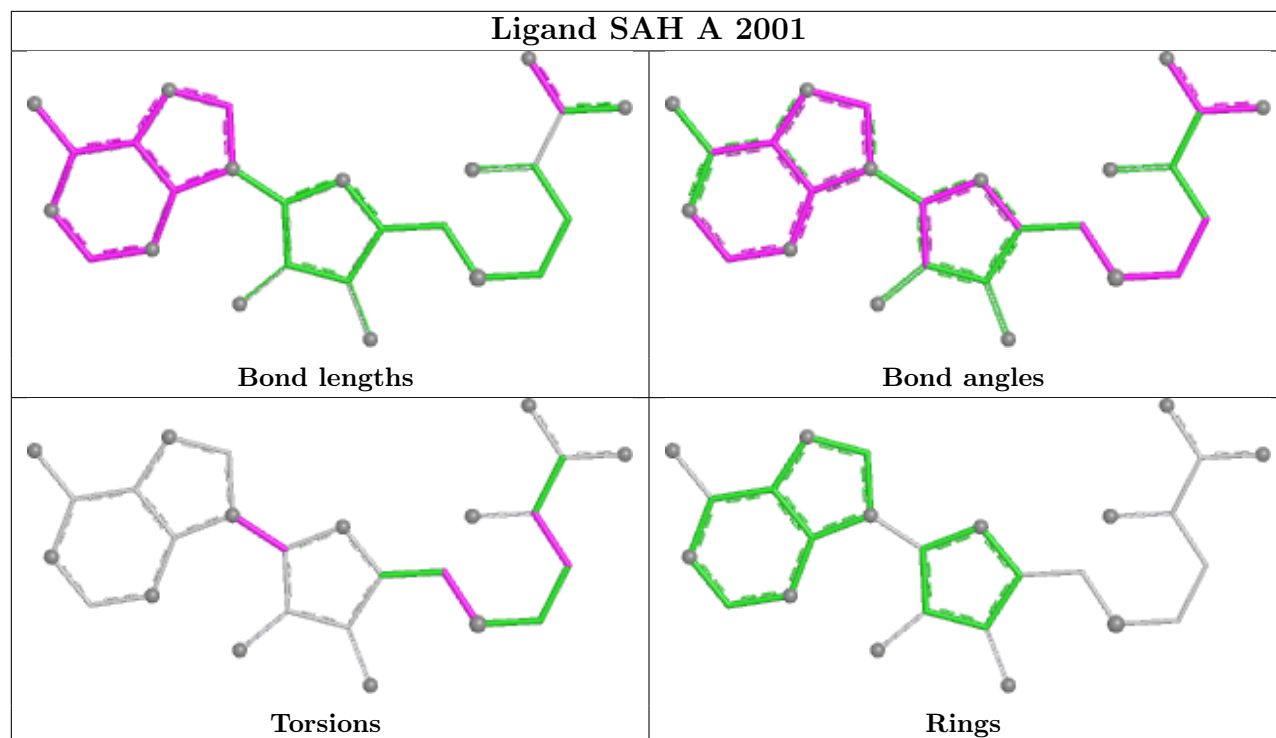
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	290	ES5	1	0
3	B	290	ES5	2	0
2	B	2002	SAH	4	0
2	A	2001	SAH	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	257/289 (88%)	2.14	129 (50%) 0 0	26, 46, 70, 86	5 (1%)
1	B	268/289 (92%)	2.98	222 (82%) 0 0	30, 42, 67, 117	1 (0%)
All	All	525/578 (90%)	2.57	351 (66%) 0 0	26, 44, 68, 117	6 (1%)

All (351) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	PRO	9.0
1	B	23	VAL	6.8
1	B	27	TYR	6.4
1	B	281	GLY	6.4
1	B	227	ALA	6.4
1	A	24	ALA	6.3
1	B	182	PHE	5.9
1	A	280	VAL	5.9
1	B	154	VAL	5.9
1	B	103	LEU	5.5
1	A	184	LEU	5.4
1	B	14	PRO	5.2
1	B	72	GLY	5.2
1	B	171	ALA	5.1
1	B	39	ASN	5.0
1	B	263	GLN	5.0
1	B	108	GLN	4.8
1	B	256	TYR	4.8
1	B	30	PHE	4.7
1	B	235	SER	4.7
1	B	231	VAL	4.7
1	B	189	PRO	4.6
1	B	261	HIS	4.6
1	B	203	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	95	GLU	4.6
1	A	167	ALA	4.6
1	B	22	ALA	4.6
1	B	85	TYR	4.5
1	B	207	PRO	4.5
1	A	155	LEU	4.5
1	A	201	ILE	4.5
1	A	147	LEU	4.5
1	B	216	ALA	4.5
1	B	206	ARG	4.5
1	B	158	ASP	4.5
1	A	85	TYR	4.4
1	B	45	GLY	4.4
1	B	137	GLY	4.4
1	B	222	TYR	4.4
1	B	187	VAL	4.3
1	A	261	HIS	4.3
1	B	233	PRO	4.3
1	B	248	TYR	4.3
1	B	16	SER	4.3
1	B	78	ILE	4.2
1	B	178	LEU	4.2
1	B	188	SER	4.2
1	B	91	CYS	4.2
1	B	225	GLY	4.2
1	B	280	VAL	4.1
1	A	275	ALA	4.1
1	A	83	THR	4.0
1	B	226	GLU	4.0
1	B	15	ASP	4.0
1	B	205	LEU	4.0
1	B	38	ASN	4.0
1	B	56	TRP	4.0
1	B	186	ALA	3.9
1	B	79	GLY	3.9
1	B	200	HIS	3.9
1	B	163	GLN	3.9
1	B	218	GLU	3.9
1	B	191	LEU	3.9
1	B	212	LEU	3.9
1	A	239	VAL	3.9
1	B	221	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	17	ALA	3.8
1	B	213	LEU	3.8
1	B	237	GLU	3.8
1	B	87	LEU	3.8
1	B	136	LYS	3.8
1	B	252	ASP	3.8
1	A	214	ILE	3.7
1	B	58	LEU	3.7
1	B	75	LEU	3.7
1	B	184	LEU	3.7
1	B	245	ARG	3.7
1	A	78	ILE	3.7
1	B	83	THR	3.7
1	B	234	VAL	3.7
1	B	253	LEU	3.7
1	B	204	LEU	3.6
1	B	220	SER	3.6
1	A	58	LEU	3.6
1	A	119	GLY	3.6
1	B	274	PHE	3.6
1	B	40	TYR	3.6
1	B	69	GLU	3.6
1	A	168	GLY	3.6
1	A	177	ALA	3.6
1	B	223	LEU	3.6
1	B	243	LEU	3.6
1	B	260	ALA	3.6
1	B	35	TYR	3.5
1	A	68	GLY	3.5
1	B	81	GLY	3.5
1	B	123	TRP	3.5
1	B	239	VAL	3.5
1	B	73	ARG	3.5
1	A	118	PRO	3.4
1	B	279	LYS	3.4
1	B	219	GLU	3.4
1	B	111	GLY	3.4
1	A	154	VAL	3.4
1	B	25	SER	3.4
1	A	40	TYR	3.4
1	B	159	VAL	3.4
1	B	173	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	199	ASP	3.3
1	A	204	LEU	3.3
1	B	198	LEU	3.3
1	A	29	ARG	3.3
1	A	157	ILE	3.3
1	B	26	ALA	3.3
1	B	97	ILE	3.3
1	B	201	ILE	3.3
1	B	102	PHE	3.3
1	B	121	PHE	3.3
1	A	54	GLY	3.3
1	A	25	SER	3.3
1	B	140	TRP	3.3
1	A	183	CYS	3.3
1	B	48	CYS	3.3
1	A	82	PRO	3.3
1	B	70	VAL	3.3
1	B	34	ALA	3.3
1	B	42	PRO	3.2
1	B	44	ARG	3.2
1	B	269	VAL	3.2
1	B	62	ALA	3.1
1	B	113	TRP	3.1
1	B	57	LYS	3.1
1	B	169	SER	3.1
1	A	166	GLY	3.1
1	A	80	SER	3.1
1	A	210	HIS	3.1
1	B	271	GLY	3.1
1	B	21	ALA	3.1
1	B	130	ALA	3.1
1	B	273	PHE	3.1
1	A	98	THR	3.1
1	B	76	ILE	3.1
1	A	75	LEU	3.1
1	B	129	HIS	3.0
1	A	216	ALA	3.0
1	A	170	PRO	3.0
1	B	262	LEU	3.0
1	A	265	GLY	3.0
1	A	126	TYR	3.0
1	A	110	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	132	LEU	3.0
1	B	122	ASN	3.0
1	B	155	LEU	3.0
1	A	102	PHE	3.0
1	B	246	SER	3.0
1	A	53	VAL	2.9
1	A	212	LEU	2.9
1	B	65	PHE	2.9
1	B	94	PHE	2.9
1	B	194	PHE	2.9
1	B	257	ILE	2.9
1	B	179	VAL	2.9
1	A	174	PRO	2.9
1	B	118	PRO	2.9
1	B	49	ASN	2.9
1	B	135	GLY	2.9
1	A	95	GLU	2.9
1	A	129	HIS	2.9
1	B	230	THR	2.9
1	B	177	ALA	2.9
1	A	178	LEU	2.9
1	B	276	TRP	2.9
1	A	169	SER	2.9
1	A	235	SER	2.9
1	B	161	GLN	2.9
1	B	166	GLY	2.9
1	B	29	ARG	2.8
1	B	214	ILE	2.8
1	B	229	LEU	2.8
1	B	265	GLY	2.8
1	A	211	LEU	2.8
1	B	28	GLN	2.8
1	B	172	PRO	2.8
1	A	133	ILE	2.8
1	A	49	ASN	2.8
1	A	125	MET	2.8
1	B	195	GLN	2.8
1	B	267	ASP	2.8
1	B	268	ASP	2.8
1	A	271	GLY	2.7
1	A	273	PHE	2.8
1	B	156	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	193	SER	2.7
1	B	131	CYS	2.7
1	A	135	GLY	2.7
1	B	106	ASN	2.7
1	A	62	ALA	2.7
1	B	190	ASP	2.7
1	B	215	GLY	2.7
1	A	113	TRP	2.7
1	A	256	TYR	2.7
1	B	217	LEU	2.7
1	B	175	ALA	2.7
1	B	241	GLU	2.7
1	A	50	PRO	2.7
1	B	240	ARG	2.7
1	A	185	GLU	2.7
1	A	164	PRO	2.6
1	B	88	LEU	2.6
1	A	104	GLU	2.6
1	B	138	GLU	2.6
1	A	224	ALA	2.6
1	B	24	ALA	2.6
1	B	64	THR	2.6
1	B	181	ALA	2.6
1	B	143	LYS	2.6
1	B	43	PRO	2.6
1	A	180	SER	2.6
1	A	257	ILE	2.6
1	A	173	LEU	2.6
1	B	20	GLN	2.6
1	B	264	THR	2.6
1	B	275	ALA	2.6
1	A	162	PRO	2.6
1	A	172	PRO	2.6
1	B	247	GLY	2.6
1	A	274	PHE	2.6
1	B	110	LEU	2.6
1	B	211	LEU	2.6
1	A	122	ASN	2.6
1	B	183	CYS	2.6
1	A	100	THR	2.6
1	A	194	PHE	2.5
1	B	47	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	272	VAL	2.5
1	B	157	ILE	2.5
1	A	88	LEU	2.5
1	B	41	ALA	2.5
1	B	197	ALA	2.5
1	B	68	GLY	2.5
1	A	121	PHE	2.5
1	B	250	VAL	2.5
1	A	26	ALA	2.5
1	B	80	SER	2.5
1	B	168	GLY	2.5
1	A	165	LEU	2.5
1	A	253	LEU	2.5
1	A	266	VAL	2.5
1	A	245	ARG	2.5
1	B	254	ARG	2.5
1	A	171	ALA	2.5
1	B	54	GLY	2.4
1	A	108	GLN	2.4
1	A	160	HIS	2.4
1	B	51	ASN	2.4
1	B	192	ALA	2.4
1	A	123	TRP	2.4
1	B	125	MET	2.4
1	B	236	GLU	2.4
1	B	238	GLU	2.4
1	A	111	GLY	2.4
1	B	61	LEU	2.4
1	B	18	PRO	2.4
1	A	46	ASP	2.4
1	A	142	ASP	2.4
1	A	150	ARG	2.4
1	A	163	GLN	2.4
1	A	105	VAL	2.4
1	A	130	ALA	2.4
1	B	90	ALA	2.4
1	A	202	THR	2.3
1	B	37	ARG	2.3
1	B	115	GLN	2.3
1	B	60	CYS	2.3
1	A	181	ALA	2.3
1	B	255	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	276	TRP	2.3
1	A	258	MET	2.3
1	A	30	PHE	2.3
1	B	244	VAL	2.3
1	B	104	GLU	2.3
1	B	50	PRO	2.3
1	B	162	PRO	2.3
1	A	61	LEU	2.3
1	A	76	ILE	2.3
1	B	147	LEU	2.3
1	B	84	VAL	2.3
1	A	112	ARG	2.3
1	A	254	ARG	2.3
1	A	28	GLN	2.3
1	B	86	GLN	2.3
1	B	160	HIS	2.3
1	B	210	HIS	2.3
1	A	143	LYS	2.3
1	B	31	GLU	2.3
1	A	51	ASN	2.2
1	A	81	GLY	2.2
1	A	217	LEU	2.2
1	A	101	ASP	2.2
1	B	101	ASP	2.2
1	A	153	ARG	2.2
1	B	139	CYS	2.2
1	B	19	GLY	2.2
1	B	164	PRO	2.2
1	A	91	CYS	2.2
1	A	264	THR	2.2
1	B	63	GLN	2.2
1	B	109	GLU	2.2
1	A	59	ARG	2.2
1	B	153	ARG	2.2
1	B	266	VAL	2.2
1	B	258	MET	2.2
1	B	124	SER	2.2
1	A	206	ARG	2.2
1	A	137	GLY	2.1
1	A	225	GLY	2.1
1	B	116	GLU	2.1
1	B	150	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	77	ASP	2.1
1	B	249	LYS	2.1
1	B	149	ALA	2.1
1	A	39	ASN	2.1
1	B	208	GLY	2.1
1	A	220	SER	2.1
1	A	187	VAL	2.1
1	B	66	ALA	2.1
1	A	36	LEU	2.1
1	A	132	LEU	2.1
1	A	230	THR	2.1
1	B	100	THR	2.1
1	A	107	ARG	2.1
1	B	33	ARG	2.1
1	A	117	GLU	2.1
1	A	146	GLN	2.1
1	A	269	VAL	2.1
1	A	38	ASN	2.1
1	B	36	LEU	2.1
1	B	96	ASP	2.1
1	B	89	SER	2.1
1	A	120	ALA	2.0
1	A	227	ALA	2.0
1	A	262	LEU	2.0
1	A	226	GLU	2.0
1	A	127	SER	2.0
1	A	179	VAL	2.0
1	B	105	VAL	2.0
1	B	112	ARG	2.0
1	B	151	VAL	2.0
1	B	167	ALA	2.0
1	B	174	PRO	2.0
1	B	93	HIS	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](#)

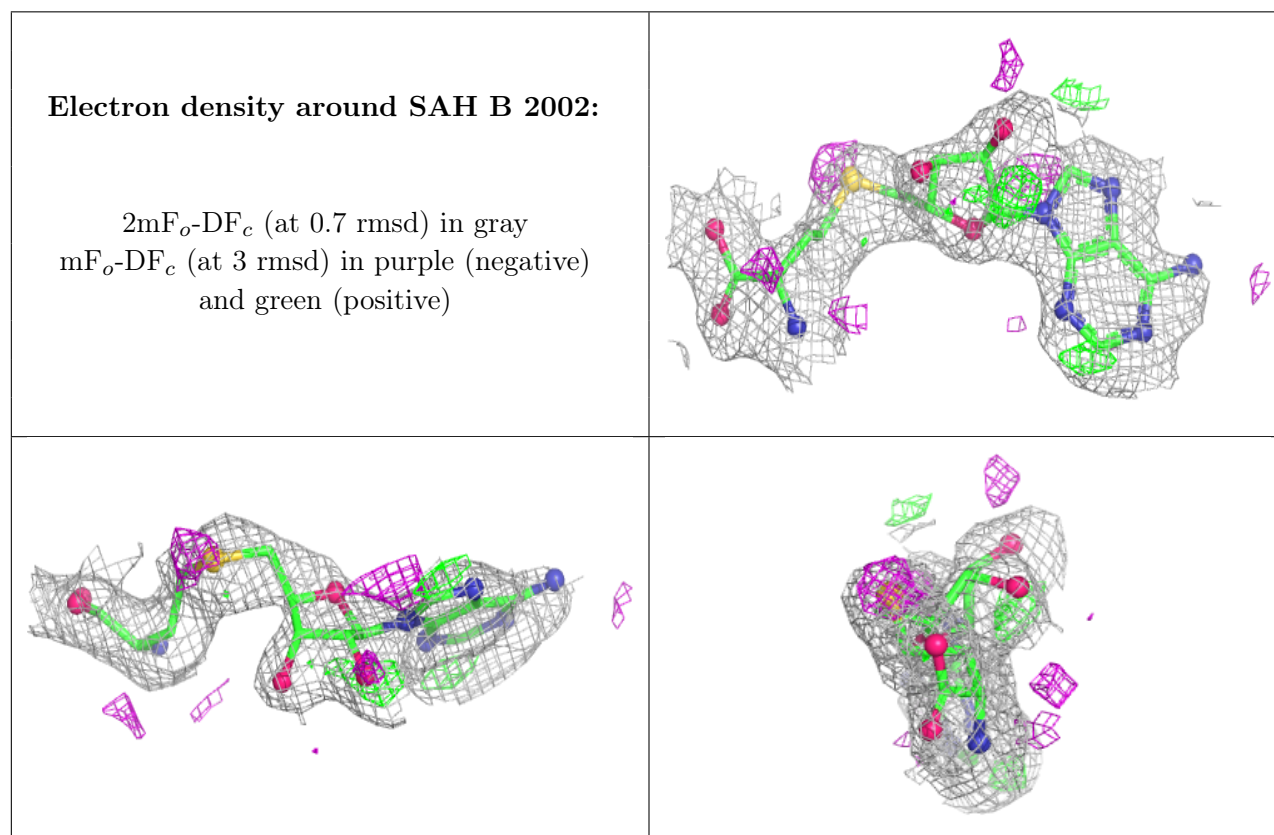
There are no oligosaccharides in this entry.

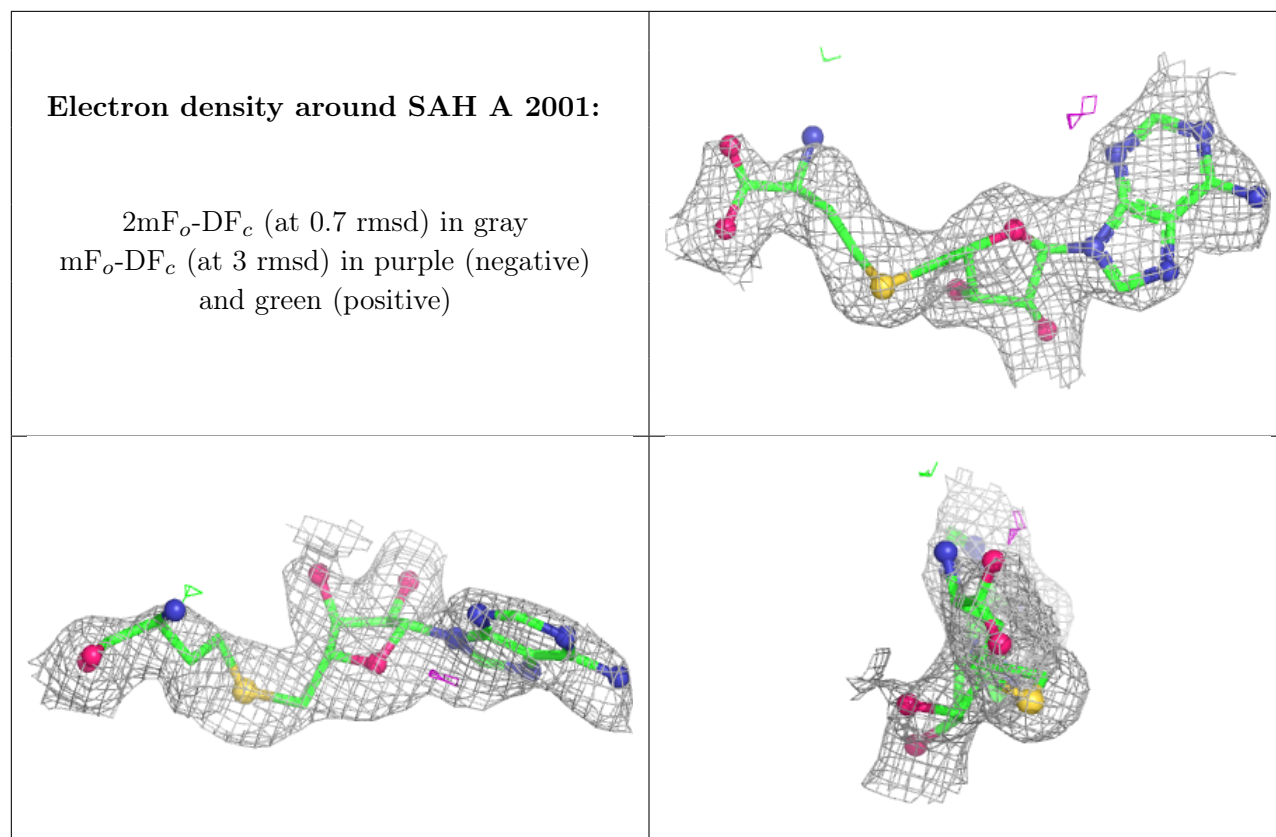
6.4 Ligands ⓘ

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
3	ES5	B	290	11/11	0.64	0.28	36,44,48,51	0
2	SAH	B	2002	26/26	0.72	0.20	29,35,44,44	0
2	SAH	A	2001	26/26	0.86	0.17	30,48,53,56	0
3	ES5	A	290	11/11	0.89	0.16	36,45,51,52	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.