



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:20 PM UTC

PDB ID : 3KPY / pdb_00003kpy
Title : Crystal Structure of hPNMT in Complex AdoHcy and 6-Chlorooxindole
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.

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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

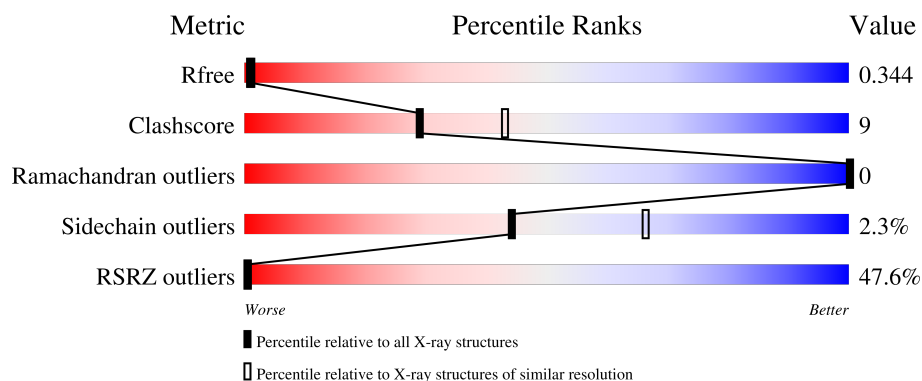
1 Overall quality at a glance

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	37% 70% 19% 11%
1	B	289	49% 78% 15% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4441 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.

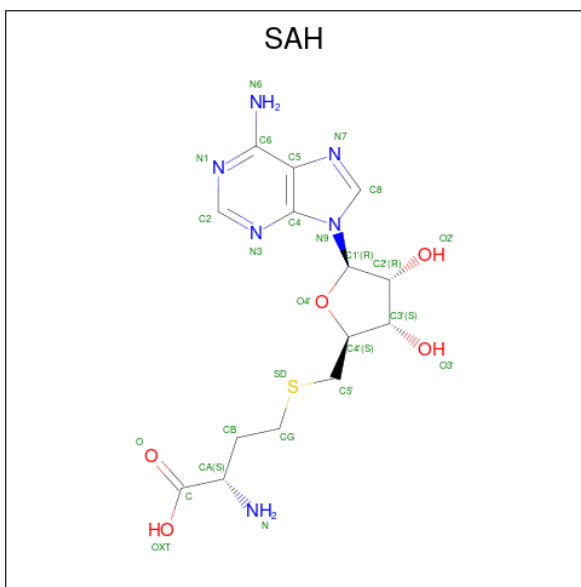
- Molecule 1 is a protein called Phenylethanolamine N-methyltransferase.

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:

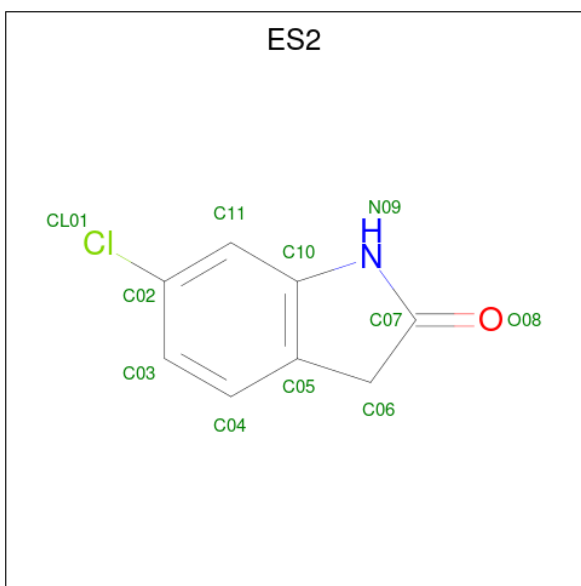
Chain	Residue	Modelled	Actual	Comment	Reference
A	283	GLU	-	expression tag	UNP P11086
A	284	HIS	-	expression tag	UNP P11086
A	285	HIS	-	expression tag	UNP P11086
A	286	HIS	-	expression tag	UNP P11086
A	287	HIS	-	expression tag	UNP P11086
A	288	HIS	-	expression tag	UNP P11086
A	289	HIS	-	expression tag	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: $C_{14}H_{20}N_6O_5S$).



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 6-chloro-1,3-dihydro-2H-indol-2-one (CCD ID: ES2) (formula: C_8H_6ClNO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			11	8	1	1	1		
3	B	1	Total	C	Cl	N	O	0	0
			11	8	1	1	1		

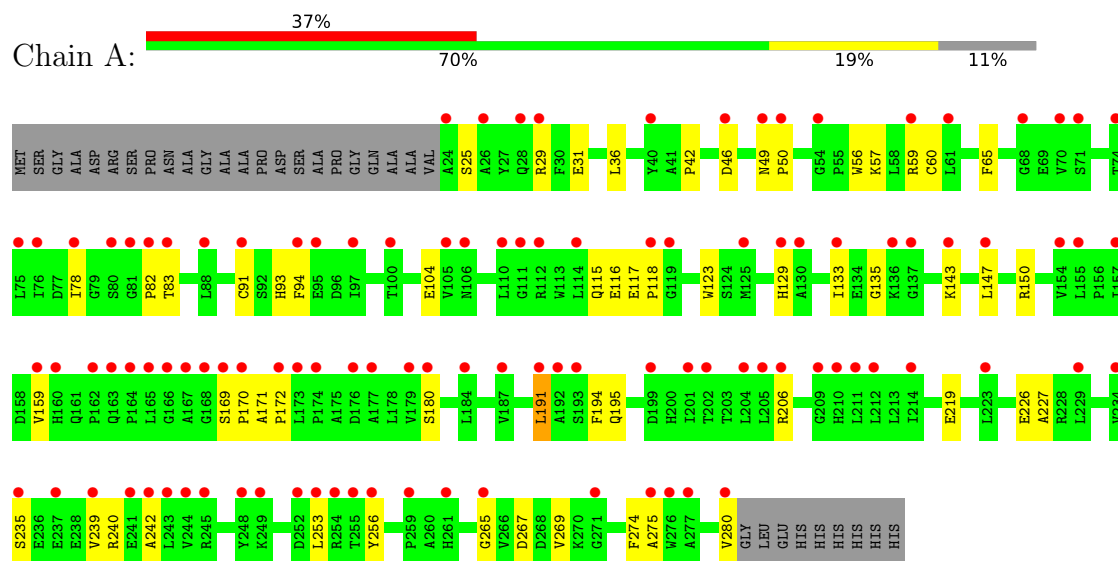
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	115	Total 115	O 115	0	0
4	B	153	Total 153	O 153	0	0

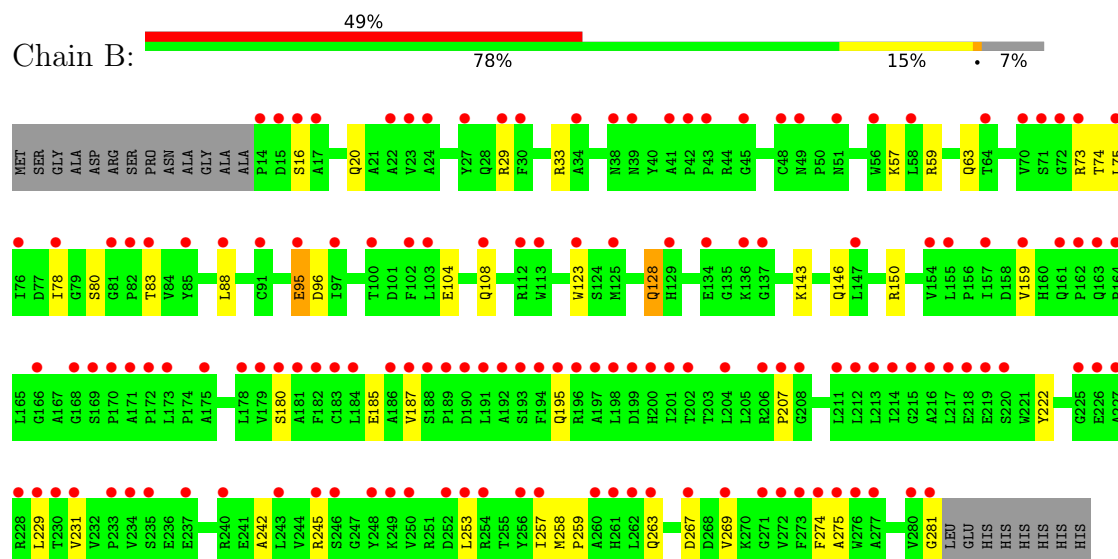
3 Residue-property plots [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.91Å 93.91Å 188.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.56 – 2.40 45.56 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (45.56-2.40) 90.1 (45.56-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.206 , 0.271 0.309 , 0.344	Depositor DCC
R_{free} test set	1583 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.2	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	0.88	EDS
Total number of atoms	4441	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ES2, 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	0.36	0/2067	0.75	0/2813
1	B	0.37	0/2136	0.75	0/2908
All	All	0.36	0/4203	0.75	0/5721

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	39	0
1	B	2083	0	2045	31	0
2	A	26	0	20	2	0
2	B	26	0	20	3	0
3	A	11	0	6	3	0
3	B	11	0	6	3	0
4	A	115	0	0	8	0
4	B	153	0	0	8	0
All	All	4441	0	4080	72	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 (72) 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	1.46	0.79
1:B:263:GLN:HB2	4:B:2039:HOH:O	1.86	0.75
1:A:46:ASP:HB2	4:A:2217:HOH:O	1.91	0.69
1:A:195:GLN:HE22	1:A:242:ALA:HA	1.59	0.67
1:B:263:GLN:HG3	4:B:2159:HOH:O	1.98	0.63
1:A:253:LEU:HD13	1:A:275:ALA:HB2	1.81	0.63
1:B:207:PRO:HB3	1:B:281:GLY:HA3	1.80	0.61
1:A:159:VAL:HG13	2:A:2001:SAH:H2	1.82	0.60
1:A:115:GLN:HB2	1:A:117:GLU:HG3	1.84	0.59
1:B:267:ASP:OD2	1:B:269:VAL:HG12	2.04	0.58
1:A:280:VAL:HA	4:A:2258:HOH:O	2.03	0.57
1:A:135:GLY:HA2	4:B:2110:HOH:O	2.04	0.57
1:A:78:ILE:HB	1:A:180:SER:HB2	1.86	0.56
1:A:267:ASP:OD1	1:A:269:VAL:HG12	2.07	0.55
1:B:222:TYR:CZ	1:B:229:LEU:HD13	2.40	0.55
1:B:57:LYS:HZ3	3:B:290:ES2:H06A	1.71	0.55
1:B:159:VAL:HG22	2:B:2002:SAH:N1	2.23	0.53
1:A:56:TRP:CE2	1:A:256:TYR:HB2	2.43	0.53
1:B:57:LYS:NZ	3:B:290:ES2:H06A	2.23	0.53
1:A:42:PRO:HG3	4:A:2217:HOH:O	2.08	0.53
1:A:57:LYS:HZ3	3:A:290:ES2:H06A	1.73	0.52
1:B:95:GLU:HG2	4:B:2273:HOH:O	2.09	0.52
1:A:94:PHE:O	1:A:150:ARG:HD3	2.10	0.52
1:B:59:ARG:HG2	1:B:63:GLN:NE2	2.25	0.51
1:B:73:ARG:HG3	1:B:95:GLU:HG3	1.91	0.51
1:B:83:THR:HA	1:B:123:TRP:CZ2	2.46	0.51
1:A:83:THR:HA	1:A:123:TRP:CZ2	2.46	0.51
1:A:129:HIS:HE1	4:B:2109:HOH:O	1.93	0.51
3:B:290:ES2:H03	4:B:2309:HOH:O	2.10	0.50
1:B:146:GLN:HG2	1:B:150:ARG:HD2	1.93	0.49
1:A:265:GLY:N	4:A:2296:HOH:O	2.40	0.49
1:B:74:THR:HG22	1:B:96:ASP:HB3	1.95	0.49
3:A:290:ES2:H03	4:A:2311:HOH:O	2.13	0.49
1:A:56:TRP:CD2	1:A:256:TYR:HB2	2.48	0.48
1:A:31:GLU:OE2	1:A:226:GLU:HG2	2.15	0.47
1:B:104:GLU:O	1:B:108:GLN:HG3	2.14	0.47
1:A:50:PRO:O	1:A:59:ARG:NH2	2.44	0.47
1:A:219:GLU:OE1	1:A:269:VAL:HB	2.14	0.47
1:B:281:GLY:HA2	4:B:2199:HOH:O	2.13	0.47
1:B:88:LEU:O	1:B:143:LYS:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LYS:NZ	3:A:290:ES2:H06A	2.30	0.46
1:B:95:GLU:HG2	1:B:95:GLU:H	1.61	0.46
1:B:159:VAL:HG13	2:B:2002:SAH:H2	1.95	0.46
1:A:116:GLU:HA	4:A:2269:HOH:O	2.15	0.45
1:B:75:LEU:C	1:B:75:LEU:HD23	2.41	0.45
1:A:143:LYS:HD3	4:A:2015:HOH:O	2.17	0.45
1:B:143:LYS:HD3	4:B:2009:HOH:O	2.15	0.45
1:A:117:GLU:HB3	1:A:118:PRO:CD	2.47	0.45
1:A:60:CYS:HB3	1:A:274:PHE:CD1	2.51	0.45
1:A:117:GLU:HB3	1:A:118:PRO:HD2	1.98	0.44
1:B:253:LEU:HD13	1:B:275:ALA:HB2	1.99	0.44
1:B:16:SER:HB2	1:B:20:GLN:NE2	2.32	0.44
1:B:258:MET:HA	1:B:259:PRO:HD3	1.89	0.43
1:A:36:LEU:HD11	1:A:82:PRO:HB2	2.01	0.43
1:A:169:SER:HA	1:A:170:PRO:HD3	1.85	0.43
1:A:82:PRO:HD2	1:A:83:THR:HG23	2.00	0.43
1:A:191:LEU:O	1:A:194:PHE:HB3	2.18	0.43
1:B:253:LEU:HA	1:B:274:PHE:O	2.19	0.43
1:B:78:ILE:HB	1:B:180:SER:HB2	2.01	0.42
1:A:240:ARG:NH2	4:A:2111:HOH:O	2.50	0.42
1:A:49:ASN:HA	1:A:50:PRO:HD3	1.87	0.41
1:A:171:ALA:HA	1:A:172:PRO:HD3	1.91	0.41
1:B:80:SER:O	2:B:2002:SAH:HA	2.20	0.41
1:A:159:VAL:HG22	2:A:2001:SAH:N1	2.36	0.41
1:A:91:CYS:HB3	1:A:147:LEU:HD13	2.03	0.41
1:B:33:ARG:HD3	1:B:33:ARG:HA	1.76	0.41
1:A:235:SER:O	1:A:239:VAL:HG23	2.21	0.41
1:B:185:GLU:O	1:B:231:VAL:HG13	2.21	0.40
1:A:29:ARG:C	1:A:227:ALA:HB2	2.46	0.40
1:A:65:PHE:HB3	1:A:93:HIS:CE1	2.56	0.40
1:B:128:GLN:HE21	1:B:128:GLN:HA	1.85	0.40
1:A:129:HIS:O	1:A:133:ILE:HG13	2.21	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	255/289 (88%)	250 (98%)	5 (2%)	0	100	100
1	B	266/289 (92%)	261 (98%)	5 (2%)	0	100	100
All	All	521/578 (90%)	511 (98%)	10 (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%)	50	71
1	B	218/233 (94%)	212 (97%)	6 (3%)	38	60
All	All	430/466 (92%)	420 (98%)	10 (2%)	44	66

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	104	GLU
1	A	191	LEU
1	A	206	ARG
1	B	29	ARG
1	B	95	GLU
1	B	128	GLN
1	B	187	VAL
1	B	245	ARG
1	B	257	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	106	ASN
1	A	195	GLN
1	B	20	GLN
1	B	63	GLN
1	B	106	ASN
1	B	128	GLN
1	B	195	GLN
1	B	261	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	$\# Z > 2$
3	ES2	B	290	-	12,12,12	4.48	9 (75%)	17,17,17	4.06	3 (17%)
2	SAH	A	2001	-	27,28,28	4.11	12 (44%)	36,40,40	2.14	14 (38%)
2	SAH	B	2002	-	27,28,28	4.05	12 (44%)	36,40,40	2.24	15 (41%)
3	ES2	A	290	-	12,12,12	4.33	9 (75%)	17,17,17	4.17	3 (17%)

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	ES2	B	290	-	-	-	0/2/2/2
2	SAH	A	2001	-	-	6/15/31/31	0/3/3/3
2	SAH	B	2002	-	-	4/15/31/31	0/3/3/3
3	ES2	A	290	-	-	-	0/2/2/2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	290	ES2	C10-C05	10.35	1.49	1.39
3	A	290	ES2	C10-C05	9.75	1.48	1.39
2	B	2002	SAH	C2-N1	9.50	1.50	1.33
2	A	2001	SAH	C2-N1	9.48	1.50	1.33
2	A	2001	SAH	C2-N3	8.66	1.49	1.33
2	B	2002	SAH	C2-N3	8.37	1.48	1.33
2	A	2001	SAH	C8-N7	7.63	1.46	1.31
2	B	2002	SAH	C8-N7	7.49	1.46	1.31
2	A	2001	SAH	C4-N3	7.33	1.48	1.34
2	A	2001	SAH	C8-N9	7.12	1.49	1.37
2	B	2002	SAH	C4-N3	7.00	1.47	1.34
2	B	2002	SAH	C8-N9	6.91	1.49	1.37
3	B	290	ES2	C03-C02	5.70	1.48	1.38
3	A	290	ES2	C03-C02	5.69	1.48	1.38
2	B	2002	SAH	C5-C4	5.45	1.48	1.39
2	A	2001	SAH	C5-C4	5.40	1.48	1.39
3	B	290	ES2	C10-N09	5.24	1.48	1.38
3	A	290	ES2	C10-N09	4.95	1.47	1.38
2	A	2001	SAH	C6-N6	4.73	1.46	1.34
2	B	2002	SAH	C6-N6	4.71	1.46	1.34
3	B	290	ES2	C07-N09	4.62	1.46	1.36
2	A	2001	SAH	C5-N7	4.58	1.47	1.39
3	A	290	ES2	C07-N09	4.49	1.46	1.36
2	B	2002	SAH	C5-N7	4.38	1.47	1.39
3	A	290	ES2	C11-C02	4.27	1.45	1.38
3	B	290	ES2	C11-C02	4.22	1.45	1.38
2	A	2001	SAH	C6-N1	3.83	1.46	1.35
2	B	2002	SAH	C4-N9	3.75	1.45	1.37
2	B	2002	SAH	C6-N1	3.62	1.45	1.35
2	A	2001	SAH	C4-N9	3.59	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	SAH	C5-C6	3.51	1.50	1.41
2	A	2001	SAH	C5-C6	3.41	1.50	1.41
2	B	2002	SAH	OXT-C	3.17	1.40	1.30
3	B	290	ES2	C04-C05	3.08	1.44	1.39
3	A	290	ES2	C04-C03	3.01	1.43	1.38
2	A	2001	SAH	OXT-C	2.97	1.40	1.30
3	B	290	ES2	C04-C03	2.96	1.43	1.38
3	A	290	ES2	C04-C05	2.86	1.44	1.39
3	A	290	ES2	O08-C07	-2.51	1.18	1.23
3	B	290	ES2	O08-C07	-2.40	1.18	1.23
3	A	290	ES2	C11-C10	2.38	1.43	1.39
3	B	290	ES2	C11-C10	2.31	1.43	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	290	ES2	O08-C07-C06	-15.04	119.29	126.97
3	B	290	ES2	O08-C07-C06	-13.72	119.96	126.97
3	B	290	ES2	C10-N09-C07	-7.90	108.35	111.70
3	A	290	ES2	C10-N09-C07	-6.33	109.02	111.70
2	A	2001	SAH	N3-C2-N1	-5.81	119.79	128.58
2	B	2002	SAH	N3-C2-N1	-5.65	120.02	128.58
2	B	2002	SAH	C5-C4-N3	-4.88	120.00	126.72
2	B	2002	SAH	N9-C8-N7	-4.76	107.18	113.94
2	A	2001	SAH	C5-C4-N3	-4.37	120.70	126.72
2	A	2001	SAH	N9-C8-N7	-4.33	107.79	113.94
3	A	290	ES2	C05-C06-C07	4.05	105.08	103.13
3	B	290	ES2	C05-C06-C07	3.72	104.92	103.13
2	B	2002	SAH	O4'-C1'-C2'	-3.55	99.03	106.62
2	B	2002	SAH	C5-N7-C8	3.40	108.79	103.45
2	B	2002	SAH	C2-N3-C4	3.28	119.85	111.83
2	A	2001	SAH	C2-N3-C4	3.09	119.39	111.83
2	B	2002	SAH	N3-C4-N9	3.05	132.36	127.17
2	A	2001	SAH	O4'-C1'-C2'	-2.95	100.31	106.62
2	A	2001	SAH	C5-N7-C8	2.83	107.90	103.45
2	B	2002	SAH	C5'-SD-CG	2.78	110.50	102.26
2	B	2002	SAH	C4-N9-C8	2.78	108.65	105.74
2	A	2001	SAH	C5'-SD-CG	2.61	110.02	102.26
2	A	2001	SAH	N3-C4-N9	2.57	131.53	127.17
2	B	2002	SAH	C4-C5-N7	-2.49	107.73	110.58
2	A	2001	SAH	CB-CG-SD	-2.49	107.90	113.45
2	A	2001	SAH	C4-N9-C8	2.45	108.31	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2002	SAH	C6-C5-C4	2.39	120.44	117.18
2	B	2002	SAH	C2'-C1'-N9	-2.35	107.47	113.30
2	A	2001	SAH	OXT-C-O	-2.21	119.07	124.08
2	B	2002	SAH	C4'-O4'-C1'	-2.19	104.62	109.47
2	A	2001	SAH	C2'-C1'-N9	-2.09	108.11	113.30
2	A	2001	SAH	C6-C5-C4	2.08	120.02	117.18
2	A	2001	SAH	C4-C5-N7	-2.05	108.24	110.58
2	B	2002	SAH	CB-CG-SD	-2.04	108.90	113.45
2	B	2002	SAH	OXT-C-O	-2.02	119.49	124.08

There are no chirality outliers.

All (10) 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	A	2001	SAH	C4'-C5'-SD-CG
2	B	2002	SAH	C2'-C1'-N9-C8
2	A	2001	SAH	C2'-C1'-N9-C8
2	A	2001	SAH	C2'-C1'-N9-C4
2	B	2002	SAH	C2'-C1'-N9-C4
2	B	2002	SAH	O-C-CA-CB
2	A	2001	SAH	O4'-C1'-N9-C8
2	B	2002	SAH	O4'-C1'-N9-C8

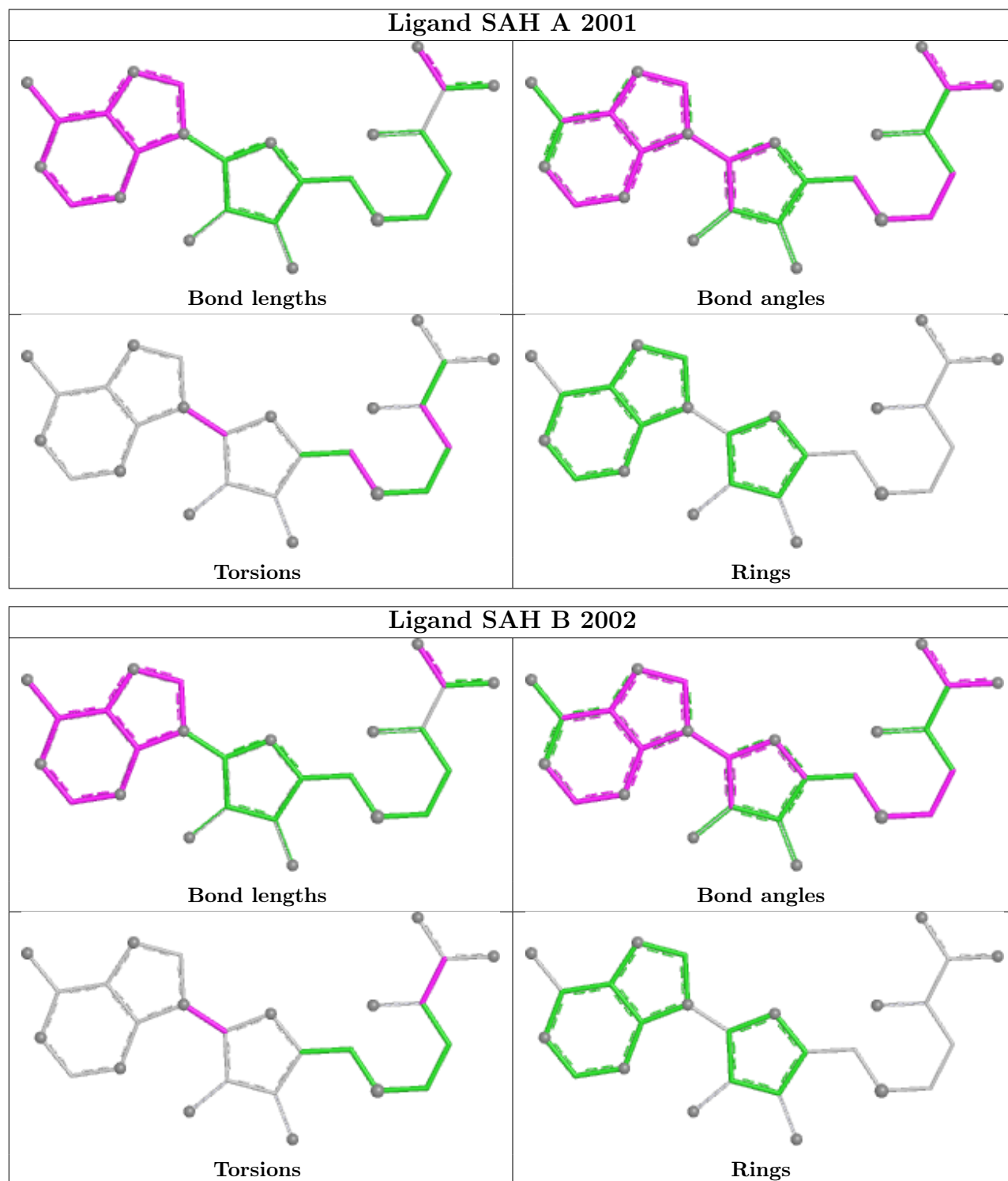
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	290	ES2	3	0
2	A	2001	SAH	2	0
2	B	2002	SAH	3	0
3	A	290	ES2	3	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%)	1.82	107 (41%) 0 0	25, 41, 68, 90	5 (1%)
1	B	268/289 (92%)	2.20	143 (53%) 0 0	25, 37, 63, 122	1 (0%)
All	All	525/578 (90%)	2.01	250 (47%) 0 0	25, 39, 66, 122	6 (1%)

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	ALA	6.0
1	B	14	PRO	6.0
1	B	227	ALA	5.1
1	B	261	HIS	4.9
1	B	182	PHE	4.8
1	B	231	VAL	4.6
1	B	95	GLU	4.5
1	A	275	ALA	4.5
1	B	159	VAL	4.5
1	B	188	SER	4.4
1	B	281	GLY	4.4
1	B	212	LEU	4.1
1	B	234	VAL	4.0
1	B	263	GLN	4.0
1	B	27	TYR	4.0
1	B	248	TYR	4.0
1	B	170	PRO	4.0
1	A	82	PRO	3.9
1	B	23	VAL	3.9
1	B	30	PHE	3.8
1	B	233	PRO	3.8
1	B	169	SER	3.8
1	A	167	ALA	3.8
1	B	246	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	16	SER	3.7
1	B	200	HIS	3.7
1	B	181	ALA	3.7
1	B	235	SER	3.6
1	A	254	ARG	3.6
1	B	213	LEU	3.6
1	B	15	ASP	3.6
1	B	194	PHE	3.5
1	B	230	THR	3.5
1	A	157	ILE	3.5
1	A	81	GLY	3.5
1	A	245	ARG	3.4
1	A	177	ALA	3.4
1	B	22	ALA	3.4
1	A	170	PRO	3.3
1	A	280	VAL	3.3
1	B	272	VAL	3.3
1	A	75	LEU	3.3
1	A	172	PRO	3.3
1	A	80	SER	3.2
1	B	269	VAL	3.2
1	B	51	ASN	3.2
1	B	189	PRO	3.2
1	A	209	GLY	3.2
1	B	262	LEU	3.2
1	B	187	VAL	3.2
1	B	102	PHE	3.1
1	B	271	GLY	3.1
1	B	186	ALA	3.1
1	B	39	ASN	3.1
1	B	250	VAL	3.1
1	B	191	LEU	3.1
1	B	201	ILE	3.1
1	B	178	LEU	3.1
1	B	245	ARG	3.1
1	B	56	TRP	3.0
1	B	195	GLN	3.0
1	B	197	ALA	3.0
1	B	276	TRP	3.0
1	A	211	LEU	3.0
1	A	249	LYS	3.0
1	B	218	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	244	VAL	2.9
1	B	157	ILE	2.9
1	B	228	ARG	2.9
1	A	61	LEU	2.9
1	B	85	TYR	2.9
1	B	274	PHE	2.9
1	A	49	ASN	2.9
1	B	214	ILE	2.9
1	A	179	VAL	2.9
1	B	175	ALA	2.9
1	B	207	PRO	2.9
1	A	147	LEU	2.9
1	A	212	LEU	2.9
1	B	137	GLY	2.9
1	B	253	LEU	2.9
1	A	163	GLN	2.9
1	B	260	ALA	2.9
1	B	198	LEU	2.9
1	B	163	GLN	2.9
1	A	29	ARG	2.8
1	B	71	SER	2.8
1	A	159	VAL	2.8
1	A	229	LEU	2.8
1	B	41	ALA	2.8
1	A	94	PHE	2.8
1	A	168	GLY	2.8
1	B	215	GLY	2.8
1	B	49	ASN	2.8
1	A	26	ALA	2.8
1	A	155	LEU	2.8
1	B	192	ALA	2.8
1	B	199	ASP	2.8
1	A	201	ILE	2.7
1	A	71	SER	2.7
1	A	164	PRO	2.7
1	A	277	ALA	2.7
1	B	34	ALA	2.7
1	B	202	THR	2.7
1	B	273	PHE	2.7
1	B	75	LEU	2.7
1	B	275	ALA	2.7
1	B	237	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	164	PRO	2.7
1	A	184	LEU	2.7
1	B	256	TYR	2.7
1	B	254	ARG	2.7
1	A	78	ILE	2.7
1	A	110	LEU	2.7
1	A	187	VAL	2.7
1	B	196	ARG	2.7
1	B	108	GLN	2.7
1	A	271	GLY	2.6
1	B	173	LEU	2.6
1	A	180	SER	2.6
1	B	17	ALA	2.6
1	A	119	GLY	2.6
1	B	184	LEU	2.6
1	A	154	VAL	2.6
1	B	76	ILE	2.6
1	B	206	ARG	2.6
1	A	253	LEU	2.6
1	B	38	ASN	2.6
1	B	45	GLY	2.6
1	B	73	ARG	2.6
1	B	190	ASP	2.6
1	A	88	LEU	2.6
1	B	229	LEU	2.6
1	A	74	THR	2.6
1	A	68	GLY	2.5
1	B	72	GLY	2.5
1	B	280	VAL	2.5
1	A	242	ALA	2.5
1	A	40	TYR	2.5
1	B	24	ALA	2.5
1	B	226	GLU	2.5
1	B	252	ASP	2.5
1	A	204	LEU	2.5
1	A	243	LEU	2.5
1	B	217	LEU	2.5
1	A	261	HIS	2.5
1	B	216	ALA	2.5
1	A	54	GLY	2.5
1	A	166	GLY	2.5
1	A	237	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	103	LEU	2.5
1	A	100	THR	2.5
1	B	83	THR	2.5
1	A	162	PRO	2.4
1	A	241	GLU	2.4
1	B	267	ASP	2.4
1	A	129	HIS	2.4
1	A	210	HIS	2.4
1	A	83	THR	2.4
1	A	259	PRO	2.4
1	B	240	ARG	2.4
1	A	239	VAL	2.4
1	A	76	ILE	2.4
1	A	176	ASP	2.4
1	B	91	CYS	2.4
1	B	58	LEU	2.4
1	A	234	VAL	2.4
1	B	171	ALA	2.4
1	A	50	PRO	2.4
1	A	28	GLN	2.4
1	B	243	LEU	2.4
1	A	248	TYR	2.4
1	A	118	PRO	2.3
1	B	82	PRO	2.3
1	B	225	GLY	2.3
1	B	48	CYS	2.3
1	A	202	THR	2.3
1	A	137	GLY	2.3
1	A	265	GLY	2.3
1	A	160	HIS	2.3
1	A	214	ILE	2.3
1	A	223	LEU	2.3
1	A	59	ARG	2.3
1	B	220	SER	2.3
1	B	129	HIS	2.3
1	A	133	ILE	2.3
1	A	165	LEU	2.3
1	B	78	ILE	2.3
1	B	154	VAL	2.3
1	B	42	PRO	2.3
1	B	208	GLY	2.3
1	A	169	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	193	SER	2.3
1	B	204	LEU	2.3
1	B	219	GLU	2.3
1	A	91	CYS	2.3
1	B	43	PRO	2.3
1	B	161	GLN	2.2
1	A	46	ASP	2.2
1	A	105	VAL	2.2
1	B	162	PRO	2.2
1	B	134	GLU	2.2
1	B	29	ARG	2.2
1	B	112	ARG	2.2
1	B	166	GLY	2.2
1	B	168	GLY	2.2
1	A	199	ASP	2.2
1	A	252	ASP	2.2
1	A	112	ARG	2.2
1	B	172	PRO	2.2
1	B	70	VAL	2.2
1	B	147	LEU	2.2
1	B	193	SER	2.2
1	B	249	LYS	2.2
1	A	106	ASN	2.1
1	A	125	MET	2.1
1	A	111	GLY	2.1
1	A	114	LEU	2.1
1	B	100	THR	2.1
1	B	123	TRP	2.1
1	B	277	ALA	2.1
1	B	81	GLY	2.1
1	A	256	TYR	2.1
1	A	174	PRO	2.1
1	A	173	LEU	2.1
1	A	191	LEU	2.1
1	B	88	LEU	2.1
1	B	211	LEU	2.1
1	A	255	THR	2.1
1	B	64	THR	2.1
1	A	95	GLU	2.1
1	B	257	ILE	2.1
1	A	205	LEU	2.1
1	B	155	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	LYS	2.1
1	A	235	SER	2.1
1	B	183	CYS	2.1
1	B	125	MET	2.1
1	B	179	VAL	2.0
1	A	192	ALA	2.0
1	A	206	ARG	2.0
1	A	276	TRP	2.0
1	B	113	TRP	2.0
1	B	97	ILE	2.0
1	A	70	VAL	2.0
1	A	130	ALA	2.0
1	A	136	LYS	2.0
1	B	136	LYS	2.0
1	A	97	ILE	2.0
1	B	180	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 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.

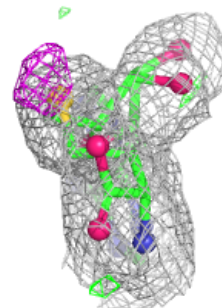
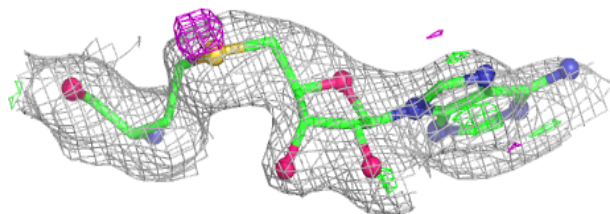
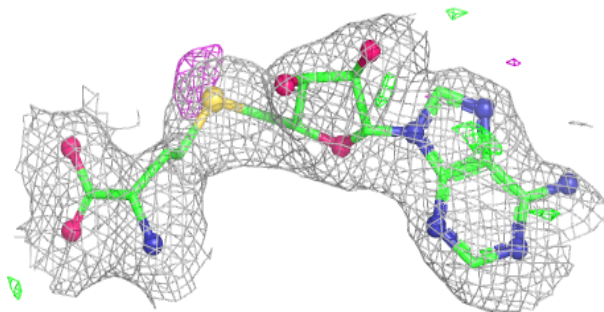
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ES2	A	290	11/11	0.71	0.31	54,63,75,81	0
3	ES2	B	290	11/11	0.72	0.30	58,71,88,89	0
2	SAH	B	2002	26/26	0.82	0.17	22,31,38,40	0
2	SAH	A	2001	26/26	0.87	0.15	30,39,44,58	0

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

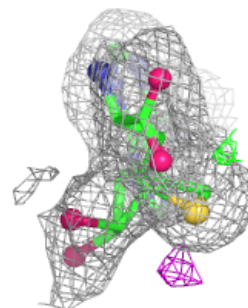
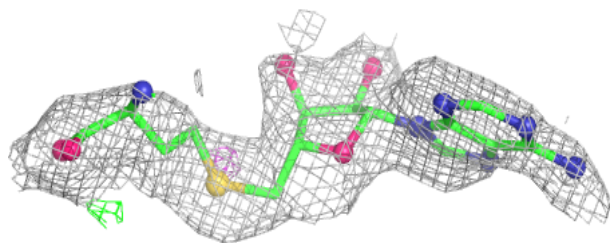
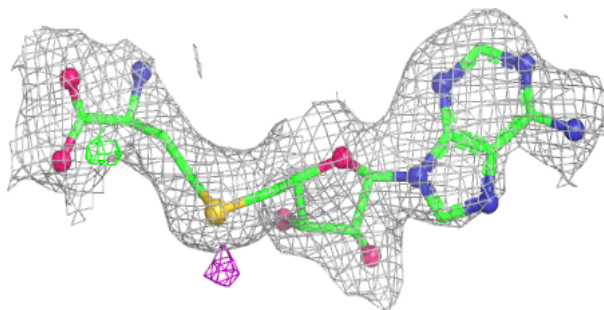
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAH B 2002:

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

**Electron density around SAH A 2001:**

$2mF_o-DF_c$ (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.