



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:57 PM UTC

PDB ID : 6IX7 / pdb_00006ix7
Title : The structure of LepI C52A in complex with SAH and substrate analogue
Authors : Cai, Y.; Ohashi, M.; Hai, Y.; Tang, Y.; Zhou, J.
Deposited on : 2018-12-09
Resolution : 1.83 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

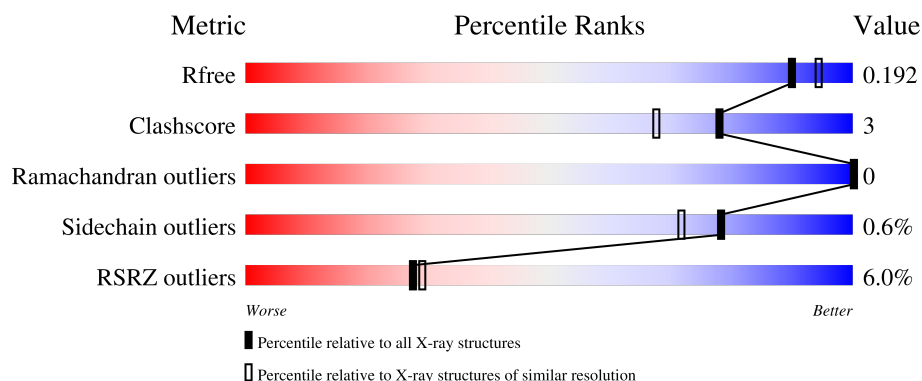
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	405	5% 90% 6% .
1	B	405	6% 90% 6% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7055 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 O-methyltransferase lepI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	7	0
			3117	1976	539	584	18			
1	B	389	Total	C	N	O	S	0	7	0
			3116	1977	538	583	18			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP B8NJH3
A	-16	GLY	-	expression tag	UNP B8NJH3
A	-15	SER	-	expression tag	UNP B8NJH3
A	-14	SER	-	expression tag	UNP B8NJH3
A	-13	HIS	-	expression tag	UNP B8NJH3
A	-12	HIS	-	expression tag	UNP B8NJH3
A	-11	HIS	-	expression tag	UNP B8NJH3
A	-10	HIS	-	expression tag	UNP B8NJH3
A	-9	HIS	-	expression tag	UNP B8NJH3
A	-8	HIS	-	expression tag	UNP B8NJH3
A	-7	GLU	-	expression tag	UNP B8NJH3
A	-6	ASN	-	expression tag	UNP B8NJH3
A	-5	LEU	-	expression tag	UNP B8NJH3
A	-4	TYR	-	expression tag	UNP B8NJH3
A	-3	PHE	-	expression tag	UNP B8NJH3
A	-2	GLN	-	expression tag	UNP B8NJH3
A	-1	SER	-	expression tag	UNP B8NJH3
A	0	ASN	-	expression tag	UNP B8NJH3
A	1	ALA	-	expression tag	UNP B8NJH3
A	52	ALA	CYS	engineered mutation	UNP B8NJH3
B	-17	MET	-	initiating methionine	UNP B8NJH3
B	-16	GLY	-	expression tag	UNP B8NJH3
B	-15	SER	-	expression tag	UNP B8NJH3
B	-14	SER	-	expression tag	UNP B8NJH3
B	-13	HIS	-	expression tag	UNP B8NJH3

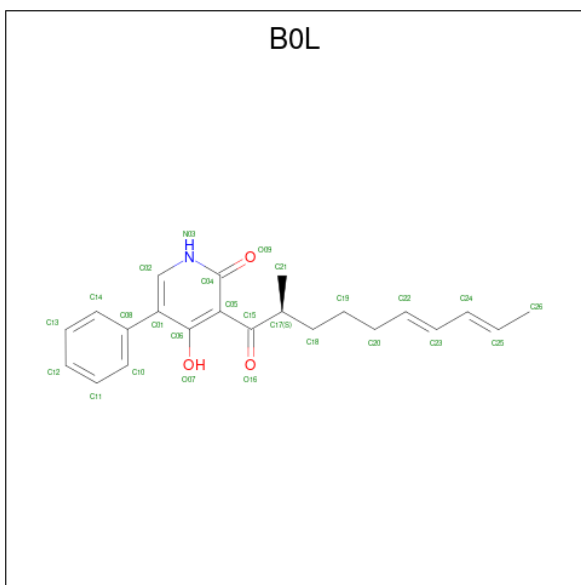
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP B8NJH3
B	-11	HIS	-	expression tag	UNP B8NJH3
B	-10	HIS	-	expression tag	UNP B8NJH3
B	-9	HIS	-	expression tag	UNP B8NJH3
B	-8	HIS	-	expression tag	UNP B8NJH3
B	-7	GLU	-	expression tag	UNP B8NJH3
B	-6	ASN	-	expression tag	UNP B8NJH3
B	-5	LEU	-	expression tag	UNP B8NJH3
B	-4	TYR	-	expression tag	UNP B8NJH3
B	-3	PHE	-	expression tag	UNP B8NJH3
B	-2	GLN	-	expression tag	UNP B8NJH3
B	-1	SER	-	expression tag	UNP B8NJH3
B	0	ASN	-	expression tag	UNP B8NJH3
B	1	ALA	-	expression tag	UNP B8NJH3
B	52	ALA	CYS	engineered mutation	UNP B8NJH3

-
- The chemical structure of S-adenosylmethionine (SAH) is shown. It consists of an adenosine moiety (adenine base and ribose sugar) linked to a methionine side chain. The adenosine part is highlighted in blue, and the methionine part is highlighted in red. The ribose sugar is shown in a chair conformation. The methionine side chain is attached to the 5' carbon of the ribose sugar via a sulfonium ylide linkage. The methionine side chain includes a methylene group (CH2) and a methyl group (CH3). The structure is labeled with atom names: N6, N7, N9, C6, C5, C8, C2, C4, C3, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C799, C800,

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

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	22	1	3		
3	B	1	Total	C	N	O	0	0
			26	22	1	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

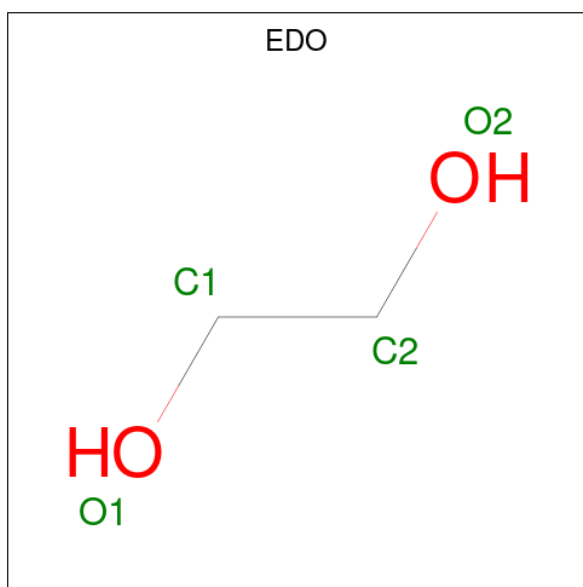
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	2	Total	Cl	0	0
			2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

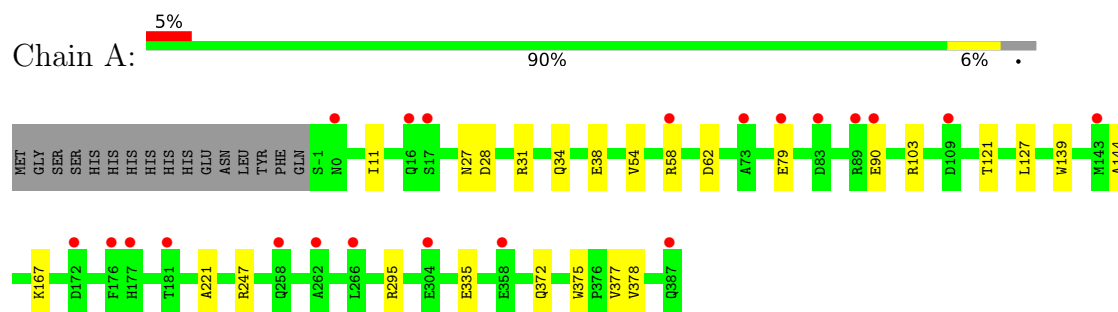
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	347	Total	O	0	1
			348	348		
7	B	331	Total	O	0	1
			332	332		

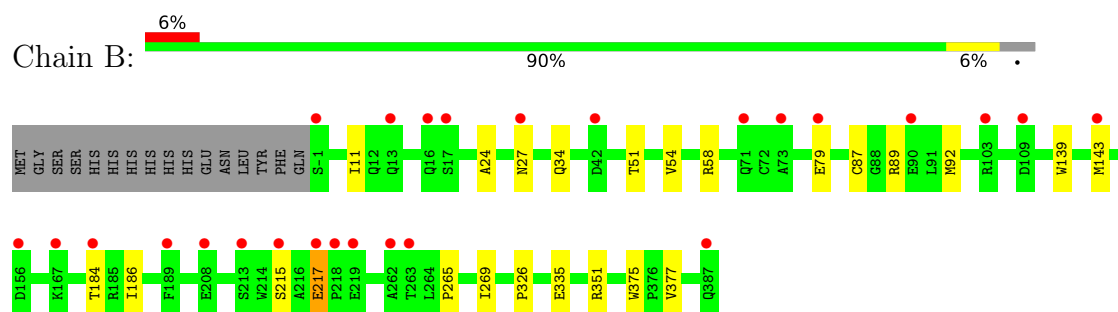
3 Residue-property plots [i](#)

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: O-methyltransferase lepI



- Molecule 1: O-methyltransferase lepI



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.28Å 62.13Å 113.59Å 90.00° 113.66° 90.00°	Depositor
Resolution (Å)	32.96 – 1.83 32.96 – 1.83	Depositor EDS
% Data completeness (in resolution range)	98.6 (32.96-1.83) 97.5 (32.96-1.83)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 1.83Å)	Xtriage
Refinement program	PHENIX v1.12_2829	Depositor
R, R_{free}	0.181 , 0.191 0.181 , 0.192	Depositor DCC
R_{free} test set	2000 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7055	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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: GOL, CL, B0L, SAH, EDO

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	0.31	0/3192	0.49	0/4335
1	B	0.30	0/3191	0.48	0/4334
All	All	0.30	0/6383	0.48	0/8669

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 [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	3117	0	3088	24	0
1	B	3116	0	3092	18	0
2	A	26	0	19	1	0
2	B	26	0	19	0	0
3	A	26	0	0	0	0
3	B	26	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	12	0	16	2	0
5	B	6	0	8	0	0
6	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	12	0	18	2	0
7	A	348	0	0	3	0
7	B	332	0	0	1	0
All	All	7055	0	6266	36	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 3.

All (36) 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:34[A]:GLN:OE1	1:B:34[A]:GLN:NE2	1.86	1.09
1:A:139[B]:TRP:HE3	1:B:143[B]:MET:HG2	1.57	0.70
1:A:38[B]:GLU:HG3	1:B:27:ASN:ND2	2.07	0.68
1:B:215:SER:HB3	1:B:217:GLU:OE1	1.94	0.67
1:A:31:ARG:HD3	7:A:518:HOH:O	1.98	0.64
1:A:372[B]:GLN:NE2	1:A:378:VAL:HG22	2.12	0.64
1:A:38[B]:GLU:HG3	1:B:27:ASN:HD22	1.63	0.61
1:A:139[B]:TRP:CE3	1:B:143[B]:MET:HG2	2.37	0.60
1:A:58[A]:ARG:NH2	1:A:62:ASP:OD2	2.38	0.56
1:A:54:VAL:HB	1:A:139[B]:TRP:CZ2	2.40	0.56
1:B:54:VAL:HB	1:B:139[A]:TRP:CZ2	2.43	0.54
1:A:79:GLU:OE1	1:A:79:GLU:N	2.30	0.53
1:B:24:ALA:HB1	6:B:407:EDO:H12	1.92	0.52
1:A:335:GLU:HG2	1:A:377:VAL:HG13	1.91	0.51
1:A:372[B]:GLN:HE22	1:A:378:VAL:HG22	1.74	0.50
1:A:11:ILE:HD11	1:B:11[A]:ILE:HD11	1.94	0.49
1:A:103:ARG:NH2	7:A:508:HOH:O	2.45	0.49
1:A:28:ASP:OD1	5:A:405:GOL:O3	2.31	0.48
1:A:144:ALA:HB1	1:A:167:LYS:HD3	1.96	0.47
1:A:372[B]:GLN:NE2	1:A:375:TRP:CD1	2.82	0.47
1:B:87:CYS:HB3	1:B:92:MET:HE2	1.97	0.47
2:A:401:SAH:HG1	2:A:401:SAH:H4'	1.81	0.44
1:A:295:ARG:HD3	7:A:600:HOH:O	2.17	0.44
1:B:375:TRP:O	6:B:406:EDO:H21	2.18	0.44
1:B:326:PRO:HD2	1:B:351:ARG:O	2.18	0.44
1:A:139[B]:TRP:CD1	1:B:51:THR:HG21	2.53	0.43
1:B:184:THR:HG22	7:B:531:HOH:O	2.19	0.43
1:A:372[B]:GLN:CD	1:A:378:VAL:HG13	2.43	0.43
1:A:377:VAL:HG11	5:A:406:GOL:H31	2.02	0.41
1:B:79:GLU:HG3	1:B:89:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:PRO:HD2	1:B:269:ILE:HD12	2.03	0.41
1:B:186:ILE:HD13	1:B:186:ILE:HA	1.85	0.40
1:A:121:THR:HG23	1:A:127:LEU:HD13	2.03	0.40
1:A:221:ALA:HA	1:A:247:ARG:HB2	2.02	0.40
1:B:335:GLU:HG2	1:B:377:VAL:HG13	2.02	0.40
1:A:372[B]:GLN:HG3	1:A:378:VAL:HG13	2.04	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	394/405 (97%)	387 (98%)	7 (2%)	0	100	100
1	B	394/405 (97%)	386 (98%)	8 (2%)	0	100	100
All	All	788/810 (97%)	773 (98%)	15 (2%)	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	334/342 (98%)	332 (99%)	2 (1%)	78	72
1	B	334/342 (98%)	331 (99%)	3 (1%)	70	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	668/684 (98%)	663 (99%)	5 (1%)	78	68

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	90	GLU
1	B	58[A]	ARG
1	B	58[B]	ARG
1	B	217	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	173	GLN
1	A	300	HIS
1	A	301	GLN
1	A	379	ASN
1	B	244	GLN
1	B	301	GLN
1	B	379	ASN

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 ⓘ

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

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$
6	EDO	A	407	-	3,3,3	0.54	0	2,2,2	0.84	0
2	SAH	B	401	-	27,28,28	1.11	4 (14%)	36,40,40	1.95	9 (25%)
5	GOL	A	406	-	5,5,5	0.33	0	5,5,5	0.30	0
3	B0L	B	402	-	26,27,27	1.45	6 (23%)	30,35,35	1.88	3 (10%)
3	B0L	A	402	-	26,27,27	1.37	6 (23%)	30,35,35	1.79	5 (16%)
5	GOL	B	405	-	5,5,5	0.39	0	5,5,5	0.63	0
2	SAH	A	401	-	27,28,28	1.00	3 (11%)	36,40,40	1.87	8 (22%)
5	GOL	A	405	-	5,5,5	0.38	0	5,5,5	0.26	0
6	EDO	B	407	-	3,3,3	0.54	0	2,2,2	0.12	0
6	EDO	B	408	-	3,3,3	0.48	0	2,2,2	0.66	0
6	EDO	B	406	-	3,3,3	0.40	0	2,2,2	0.31	0

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
6	EDO	A	407	-	-	0/1/1/1	-
2	SAH	B	401	-	-	5/15/31/31	0/3/3/3
5	GOL	A	406	-	-	3/4/4/4	-
3	B0L	B	402	-	-	4/20/20/20	0/2/2/2
3	B0L	A	402	-	-	7/20/20/20	0/2/2/2
5	GOL	B	405	-	-	3/4/4/4	-
2	SAH	A	401	-	-	5/15/31/31	0/3/3/3
5	GOL	A	405	-	-	2/4/4/4	-
6	EDO	B	407	-	-	0/1/1/1	-
6	EDO	B	408	-	-	1/1/1/1	-
6	EDO	B	406	-	-	1/1/1/1	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	B0L	C08-C01	3.39	1.53	1.48
3	A	402	B0L	C24-C23	3.00	1.53	1.44
3	B	402	B0L	C24-C23	2.96	1.53	1.44
3	A	402	B0L	C05-C15	2.74	1.55	1.47
3	A	402	B0L	C08-C01	2.63	1.52	1.48
3	B	402	B0L	C05-C15	2.51	1.54	1.47
3	B	402	B0L	O09-C04	-2.50	1.18	1.23
2	B	401	SAH	C2-N3	2.49	1.38	1.33
2	B	401	SAH	C2-N1	2.49	1.38	1.33
3	B	402	B0L	C04-N03	-2.43	1.34	1.39
2	B	401	SAH	OXT-C	-2.39	1.23	1.30
2	A	401	SAH	C8-N7	2.34	1.36	1.31
3	A	402	B0L	C04-N03	-2.27	1.34	1.39
2	B	401	SAH	C8-N7	2.25	1.36	1.31
3	A	402	B0L	O16-C15	-2.15	1.18	1.22
2	A	401	SAH	OXT-C	-2.14	1.23	1.30
3	B	402	B0L	C05-C04	-2.13	1.39	1.44
2	A	401	SAH	C2-N1	2.10	1.37	1.33
3	A	402	B0L	O09-C04	-2.08	1.19	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	B0L	C06-C05-C15	7.22	126.17	118.11
2	A	401	SAH	N3-C2-N1	-6.10	119.35	128.58
2	B	401	SAH	N3-C2-N1	-5.84	119.75	128.58
3	A	402	B0L	C06-C05-C15	5.57	124.33	118.11
2	B	401	SAH	N9-C8-N7	-4.78	107.16	113.94
2	A	401	SAH	N9-C8-N7	-4.22	107.95	113.94
3	A	402	B0L	C18-C19-C20	-3.75	106.33	114.47
2	B	401	SAH	C5-N7-C8	3.54	109.02	103.45
2	A	401	SAH	C5-C4-N3	-3.48	121.92	126.72
2	B	401	SAH	C5-C4-N3	-3.40	122.04	126.72
2	B	401	SAH	OXT-C-O	-3.40	116.37	124.08
3	B	402	B0L	C18-C19-C20	-3.30	107.31	114.47
2	A	401	SAH	C2-N3-C4	3.28	119.84	111.83
3	A	402	B0L	C05-C04-N03	3.13	120.49	114.65
3	B	402	B0L	C05-C04-N03	3.06	120.35	114.65
2	B	401	SAH	C2-N3-C4	2.98	119.10	111.83
2	A	401	SAH	C5-N7-C8	2.93	108.06	103.45
2	B	401	SAH	C4-N9-C8	2.92	108.80	105.74
2	A	401	SAH	C4-N9-C8	2.70	108.58	105.74
2	A	401	SAH	OXT-C-O	-2.61	118.15	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	SAH	C4-C5-N7	-2.31	107.94	110.58
2	A	401	SAH	N3-C4-N9	2.29	131.06	127.17
3	A	402	B0L	C02-N03-C04	-2.28	121.08	124.41
2	B	401	SAH	N3-C4-N9	2.19	130.90	127.17
3	A	402	B0L	C21-C17-C15	-2.10	105.28	110.42

There are no chirality outliers.

All (31) torsion outliers are listed below:

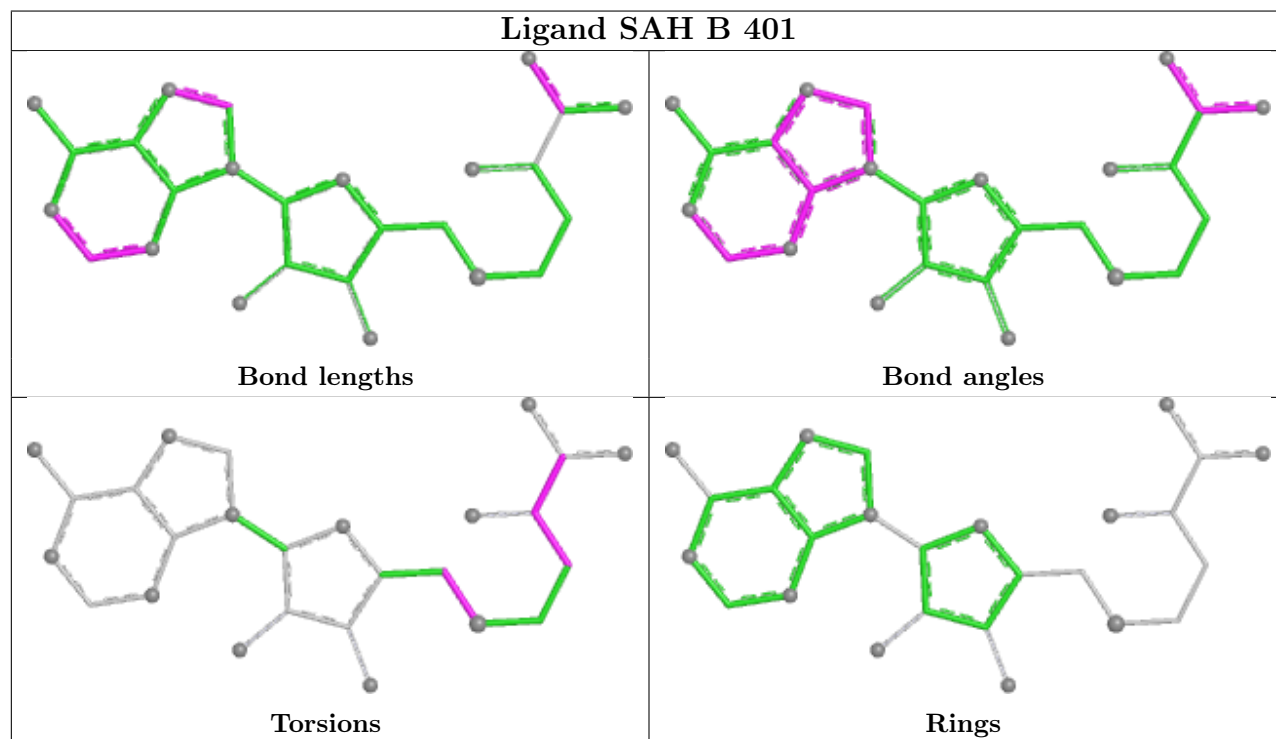
Mol	Chain	Res	Type	Atoms
2	A	401	SAH	N-CA-CB-CG
2	A	401	SAH	C-CA-CB-CG
2	B	401	SAH	N-CA-CB-CG
2	B	401	SAH	C-CA-CB-CG
5	A	405	GOL	C1-C2-C3-O3
2	B	401	SAH	OXT-C-CA-N
5	B	405	GOL	O1-C1-C2-C3
5	A	405	GOL	O2-C2-C3-O3
5	B	405	GOL	O1-C1-C2-O2
5	B	405	GOL	O2-C2-C3-O3
3	A	402	B0L	C04-C05-C15-C17
3	B	402	B0L	C04-C05-C15-C17
5	A	406	GOL	O2-C2-C3-O3
5	A	406	GOL	O1-C1-C2-O2
2	A	401	SAH	OXT-C-CA-N
2	A	401	SAH	C4'-C5'-SD-CG
2	B	401	SAH	C4'-C5'-SD-CG
3	A	402	B0L	C06-C05-C15-O16
3	B	402	B0L	C06-C05-C15-O16
3	A	402	B0L	C04-C05-C15-O16
3	B	402	B0L	C04-C05-C15-O16
3	A	402	B0L	C06-C05-C15-C17
3	B	402	B0L	C06-C05-C15-C17
6	B	406	EDO	O1-C1-C2-O2
2	A	401	SAH	O-C-CA-N
3	A	402	B0L	O16-C15-C17-C18
5	A	406	GOL	C1-C2-C3-O3
3	A	402	B0L	C22-C23-C24-C25
6	B	408	EDO	O1-C1-C2-O2
3	A	402	B0L	C19-C20-C22-C23
2	B	401	SAH	O-C-CA-N

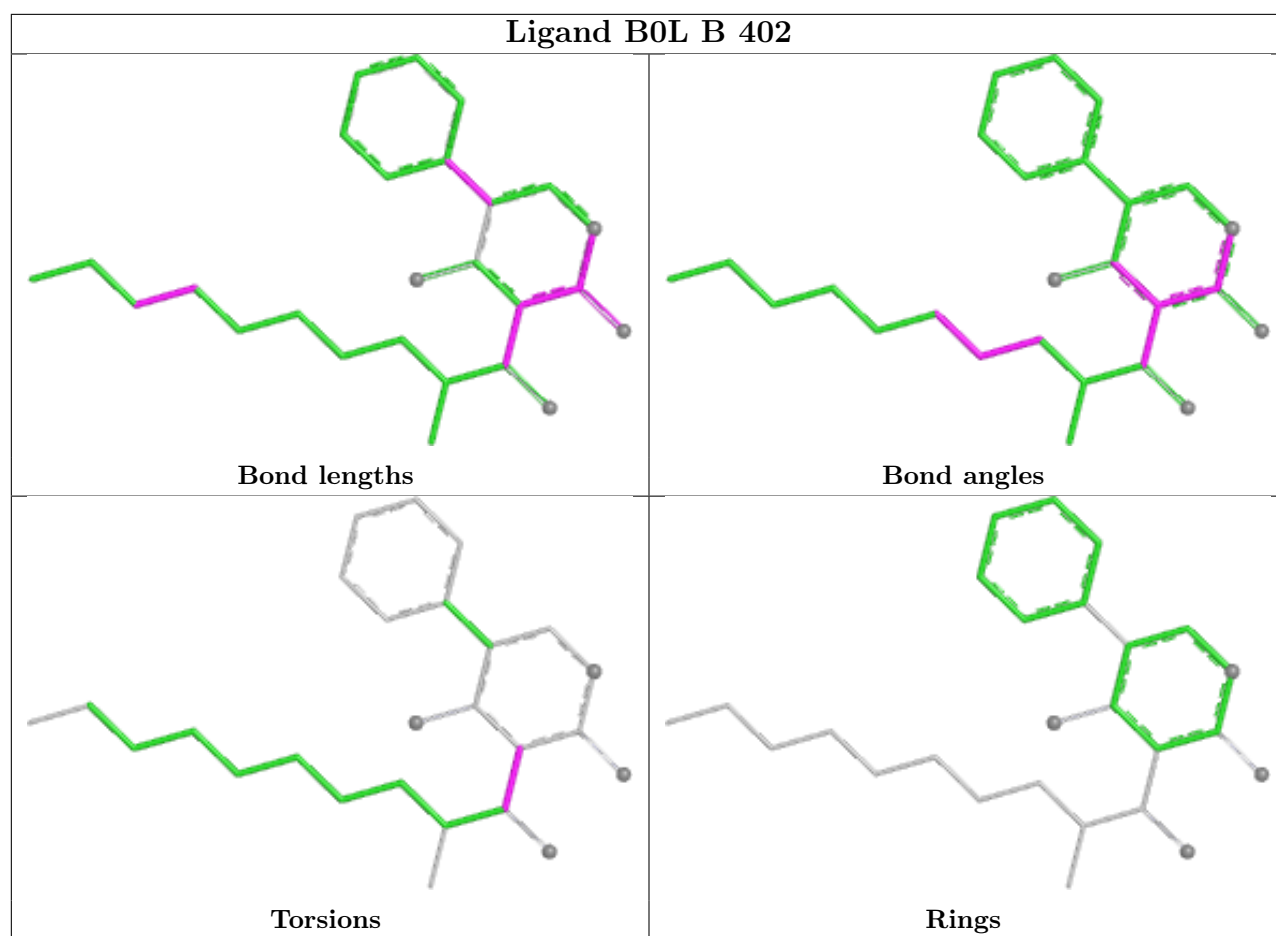
There are no ring outliers.

5 monomers are involved in 5 short contacts:

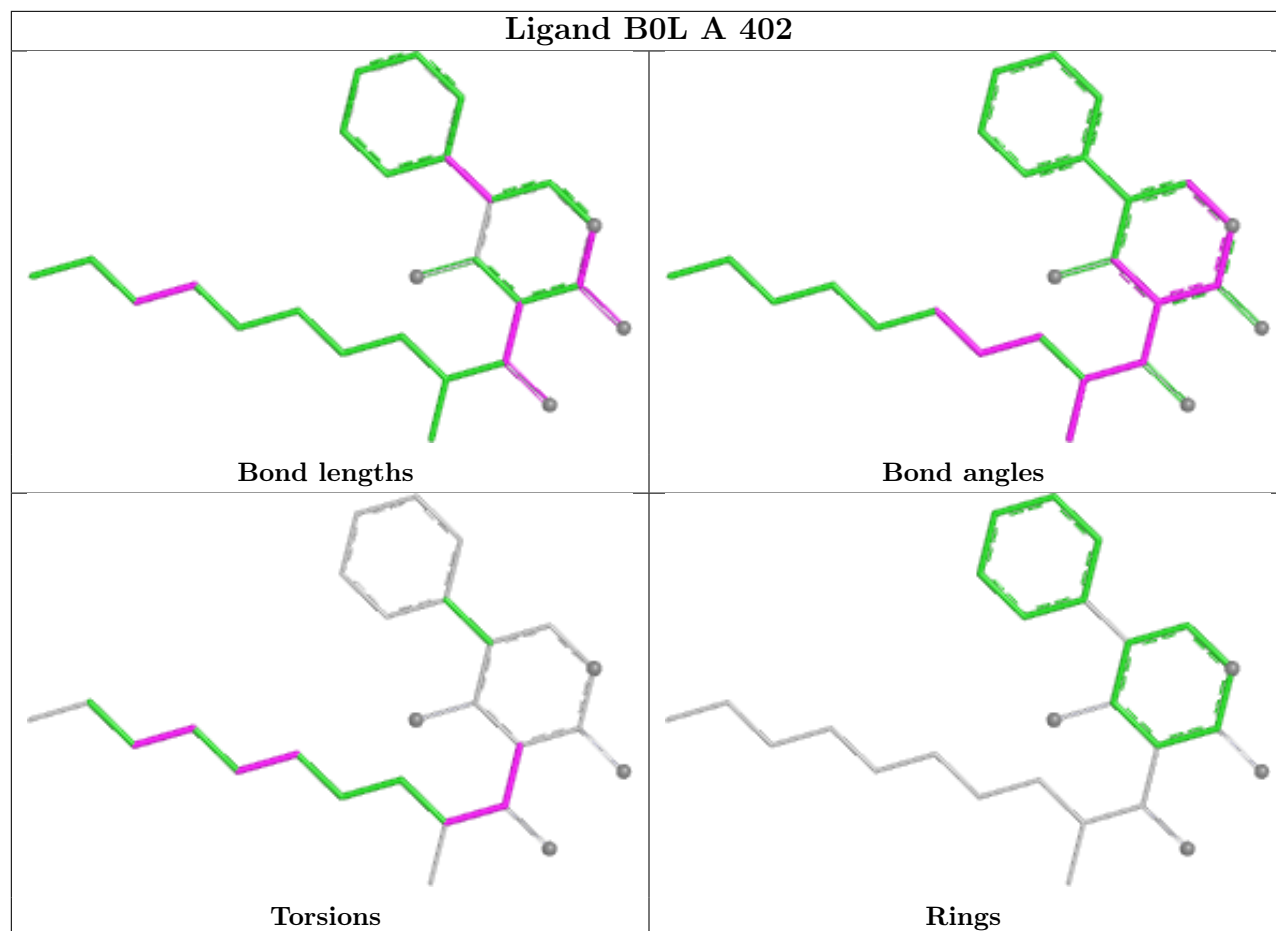
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	406	GOL	1	0
2	A	401	SAH	1	0
5	A	405	GOL	1	0
6	B	407	EDO	1	0
6	B	406	EDO	1	0

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

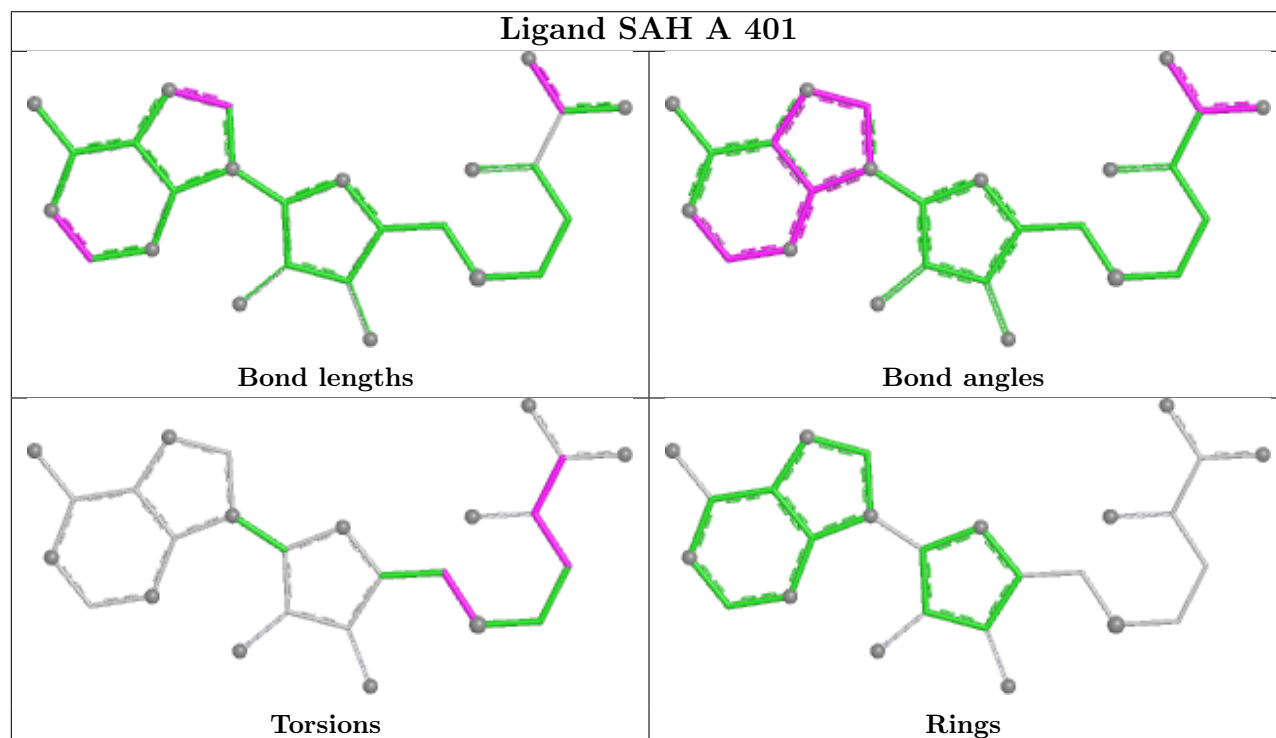




Ligand B0L A 402



Ligand SAH A 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	389/405 (96%)	0.28	21 (5%) 31 34	6, 18, 37, 61	9 (2%)
1	B	389/405 (96%)	0.31	26 (6%) 24 25	7, 18, 36, 99	10 (2%)
All	All	778/810 (96%)	0.30	47 (6%) 27 29	6, 18, 37, 99	19 (2%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	218	PRO	5.5
1	B	217	GLU	4.7
1	A	0	ASN	4.3
1	B	16	GLN	3.7
1	A	172	ASP	3.6
1	A	262	ALA	3.6
1	B	215	SER	3.4
1	B	73	ALA	3.1
1	A	16	GLN	3.1
1	B	-1	SER	3.1
1	B	219	GLU	3.0
1	B	262	ALA	2.9
1	A	387	GLN	2.8
1	A	258	GLN	2.7
1	B	17	SER	2.7
1	A	304	GLU	2.6
1	A	83	ASP	2.6
1	A	79	GLU	2.6
1	B	387	GLN	2.5
1	A	181	THR	2.5
1	A	109	ASP	2.5
1	A	17	SER	2.4
1	A	143[A]	MET	2.4
1	B	109	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	176	PHE	2.4
1	B	184	THR	2.4
1	B	79	GLU	2.4
1	B	263	THR	2.3
1	B	208	GLU	2.3
1	B	143[A]	MET	2.3
1	A	89	ARG	2.2
1	A	358	GLU	2.2
1	A	73	ALA	2.2
1	B	90	GLU	2.1
1	A	266	LEU	2.1
1	B	167	LYS	2.1
1	A	58[A]	ARG	2.1
1	A	90	GLU	2.1
1	B	13	GLN	2.1
1	B	71	GLN	2.1
1	B	42	ASP	2.1
1	B	213	SER	2.1
1	B	27	ASN	2.1
1	B	156	ASP	2.1
1	B	103	ARG	2.1
1	B	189	PHE	2.0
1	A	177	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 [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.

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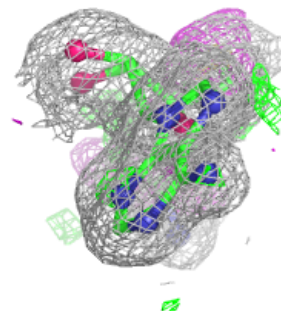
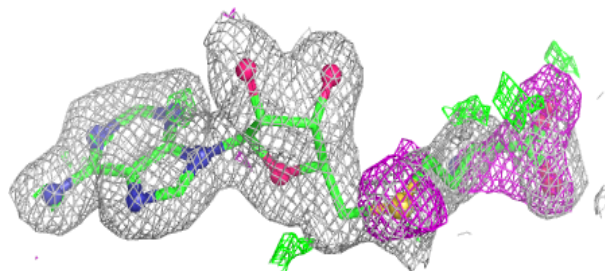
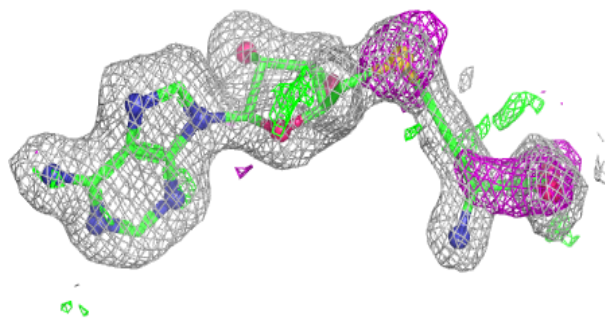
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	B	407	4/4	0.74	0.20	40,46,48,49	0
5	GOL	A	405	6/6	0.81	0.13	36,44,45,47	0
6	EDO	A	407	4/4	0.82	0.16	35,36,38,40	0
6	EDO	B	408	4/4	0.82	0.12	36,36,36,38	0
2	SAH	B	401	26/26	0.84	0.12	16,20,23,26	0
6	EDO	B	406	4/4	0.86	0.20	34,37,38,40	0
4	CL	B	403	1/1	0.87	0.17	70,70,70,70	0
2	SAH	A	401	26/26	0.88	0.10	20,23,26,26	0
5	GOL	A	406	6/6	0.88	0.15	28,32,34,38	0
5	GOL	B	405	6/6	0.89	0.12	23,27,31,31	0
3	B0L	B	402	26/26	0.92	0.09	16,19,25,28	0
4	CL	B	404	1/1	0.93	0.11	61,61,61,61	0
3	B0L	A	402	26/26	0.94	0.09	16,23,36,39	0
4	CL	A	404	1/1	0.99	0.10	19,19,19,19	0
4	CL	A	403	1/1	0.99	0.07	20,20,20,20	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.

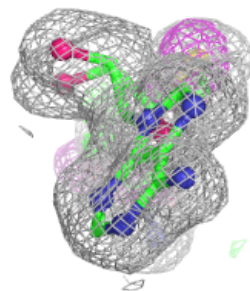
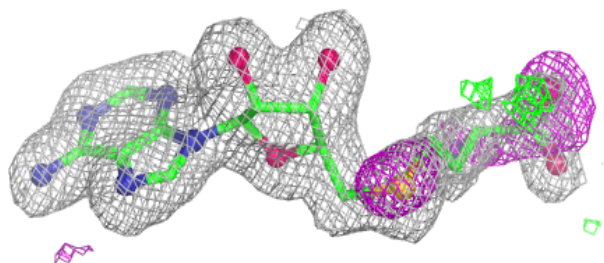
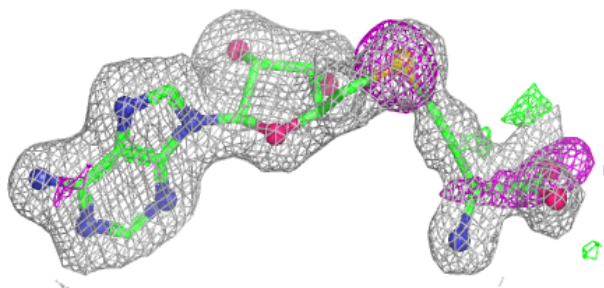
Electron density around SAH B 401:

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

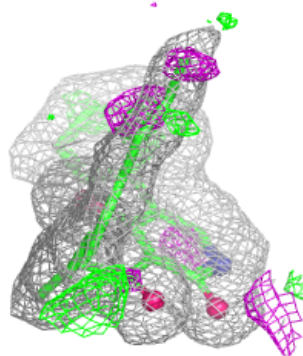
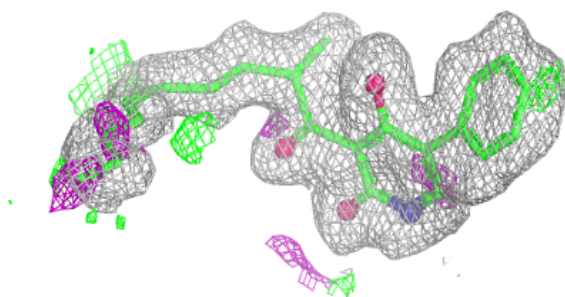
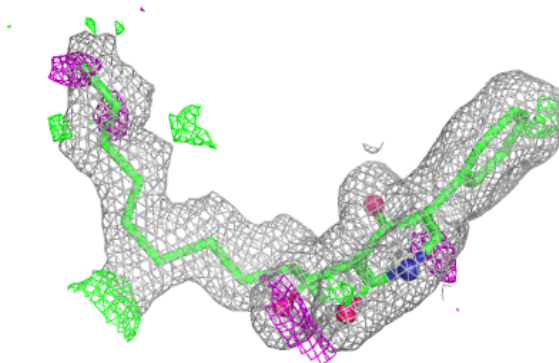


Electron density around SAH A 401:

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

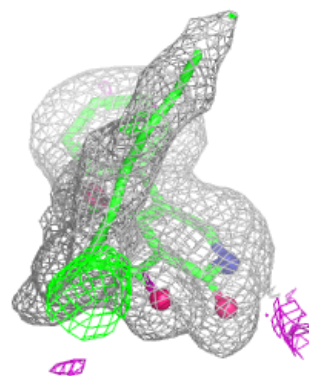
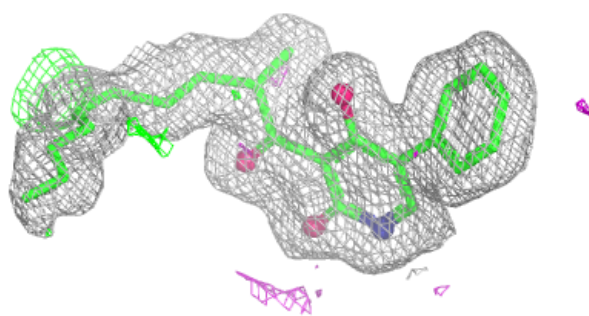
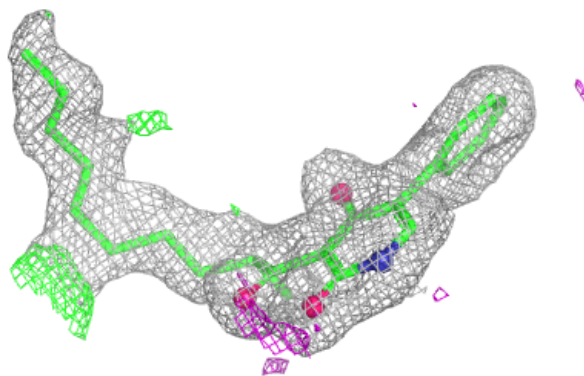
**Electron density around B0L B 402:**

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



Electron density around B0L A 402:

$2mF_o-DF_c$ (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.