



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 10:46 PM UTC

PDB ID : 7WZV / pdb_00007wzv
Title : The structure of a Twitch Radical SAM Dehydrogenase SpeY
Authors : Zhou, J.H.; Hou, X.L.
Deposited on : 2022-02-19
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

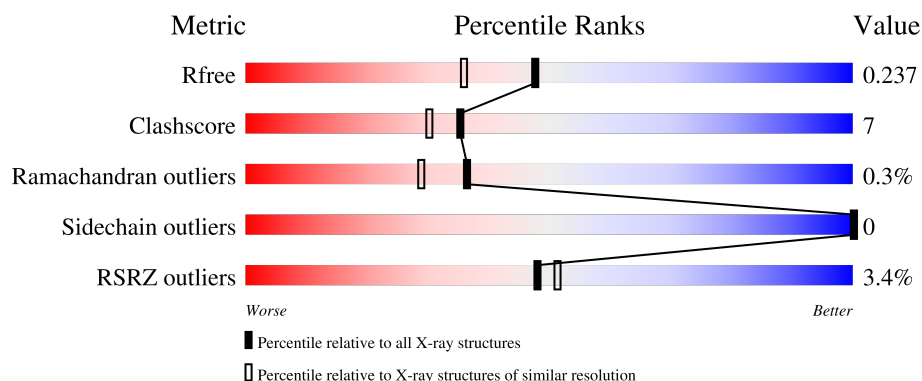
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	322	
1	B	322	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	B	408	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5311 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 4Fe-4S cluster-binding domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2362	1481	429	439	13			
1	B	297	Total	C	N	O	S	0	0	0
			2349	1474	426	436	13			

There are 44 discrepancies between the modelled and reference sequences:

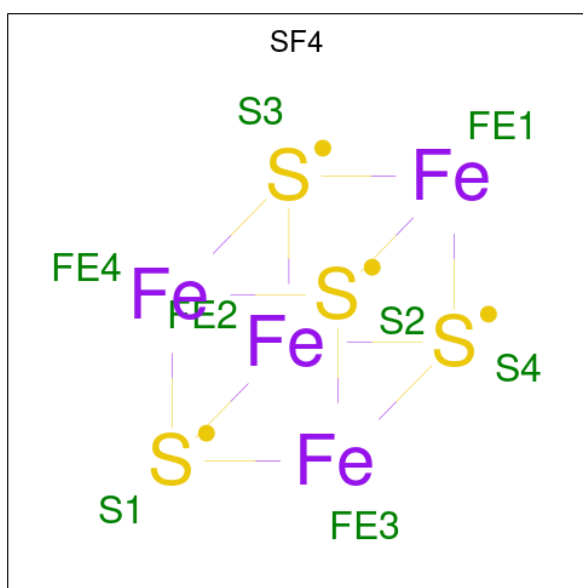
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A8WEZ7
A	-18	GLY	-	expression tag	UNP A8WEZ7
A	-17	SER	-	expression tag	UNP A8WEZ7
A	-16	SER	-	expression tag	UNP A8WEZ7
A	-15	HIS	-	expression tag	UNP A8WEZ7
A	-14	HIS	-	expression tag	UNP A8WEZ7
A	-13	HIS	-	expression tag	UNP A8WEZ7
A	-12	HIS	-	expression tag	UNP A8WEZ7
A	-11	HIS	-	expression tag	UNP A8WEZ7
A	-10	HIS	-	expression tag	UNP A8WEZ7
A	-9	SER	-	expression tag	UNP A8WEZ7
A	-8	SER	-	expression tag	UNP A8WEZ7
A	-7	GLY	-	expression tag	UNP A8WEZ7
A	-6	LEU	-	expression tag	UNP A8WEZ7
A	-5	VAL	-	expression tag	UNP A8WEZ7
A	-4	PRO	-	expression tag	UNP A8WEZ7
A	-3	ARG	-	expression tag	UNP A8WEZ7
A	-2	GLY	-	expression tag	UNP A8WEZ7
A	-1	SER	-	expression tag	UNP A8WEZ7
A	0	HIS	-	expression tag	UNP A8WEZ7
A	269	ALA	GLU	conflict	UNP A8WEZ7
A	270	ALA	GLU	conflict	UNP A8WEZ7
B	-19	MET	-	initiating methionine	UNP A8WEZ7
B	-18	GLY	-	expression tag	UNP A8WEZ7
B	-17	SER	-	expression tag	UNP A8WEZ7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP A8WEZ7
B	-15	HIS	-	expression tag	UNP A8WEZ7
B	-14	HIS	-	expression tag	UNP A8WEZ7
B	-13	HIS	-	expression tag	UNP A8WEZ7
B	-12	HIS	-	expression tag	UNP A8WEZ7
B	-11	HIS	-	expression tag	UNP A8WEZ7
B	-10	HIS	-	expression tag	UNP A8WEZ7
B	-9	SER	-	expression tag	UNP A8WEZ7
B	-8	SER	-	expression tag	UNP A8WEZ7
B	-7	GLY	-	expression tag	UNP A8WEZ7
B	-6	LEU	-	expression tag	UNP A8WEZ7
B	-5	VAL	-	expression tag	UNP A8WEZ7
B	-4	PRO	-	expression tag	UNP A8WEZ7
B	-3	ARG	-	expression tag	UNP A8WEZ7
B	-2	GLY	-	expression tag	UNP A8WEZ7
B	-1	SER	-	expression tag	UNP A8WEZ7
B	0	HIS	-	expression tag	UNP A8WEZ7
B	269	ALA	GLU	conflict	UNP A8WEZ7
B	270	ALA	GLU	conflict	UNP A8WEZ7

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



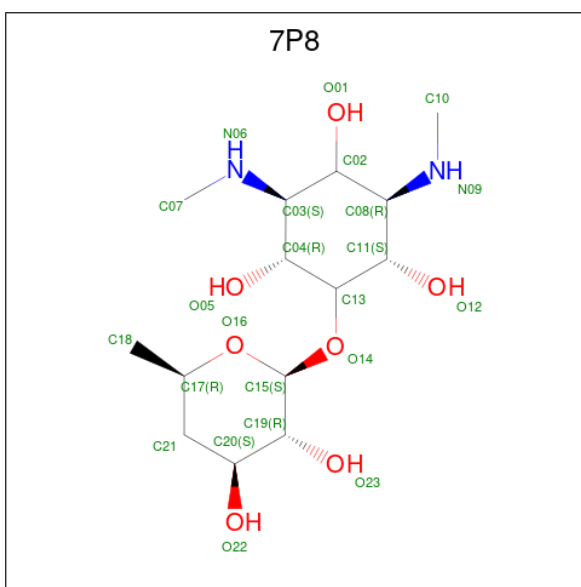
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0

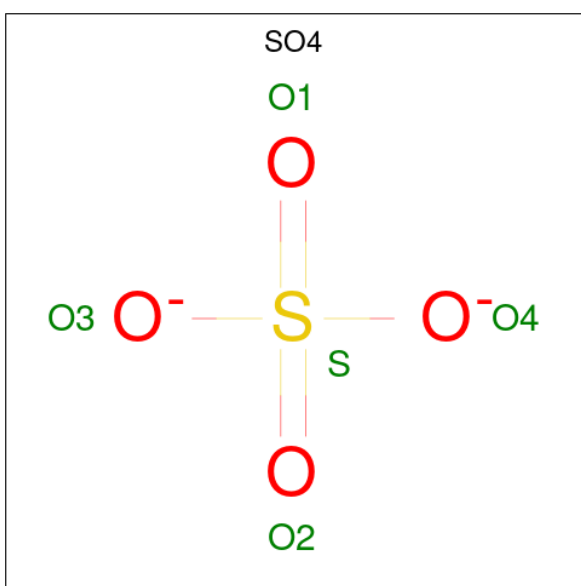
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- The chemical structure of SAM (S-adenosylmethionine) is shown. It consists of an adenosine ring (adenine base and ribose sugar) linked to a methionine side chain via a sulfur atom. The adenosine ring is labeled with atoms N1, N3, N6, N7, N9, C2, C4, C5, C6, C8, C9, C11(R), C12(R), C3(S), C4(S), and C5. The sulfur atom is labeled S1(S). The methionine side chain is labeled with atoms 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, C801, C802, C803, C804, C805, C806, C807, C808, C809, C810,

- Molecule 4 is (1 {S},2 {R},4 {S},5 {R})-2,4-bis(methylamino)-6-[(2 {S},3 {R},4 {S},6 {R})-6-methyl-3,4-bis(oxidanyl)oxan-2-yl]oxy-cyclohexane-1,3,5-triol (CCD ID: 7P8) (formula: C₁₄H₂₈N₂O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			23	14	2	7		
4	B	1	Total	C	N	O	0	0
			23	14	2	7		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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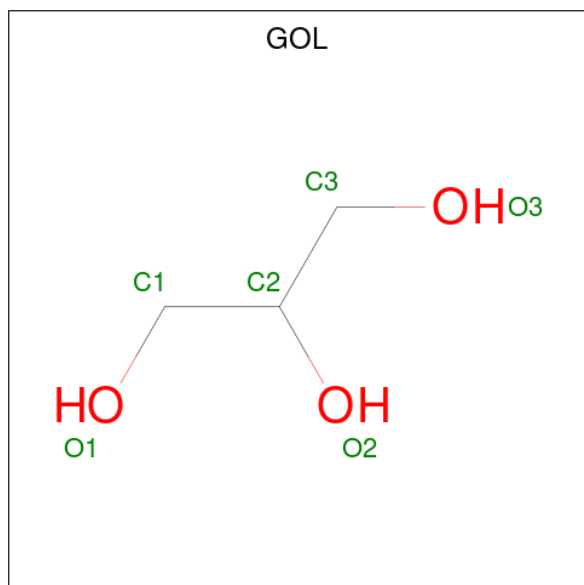
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	B	4	Total	Na	0	0
			4	4		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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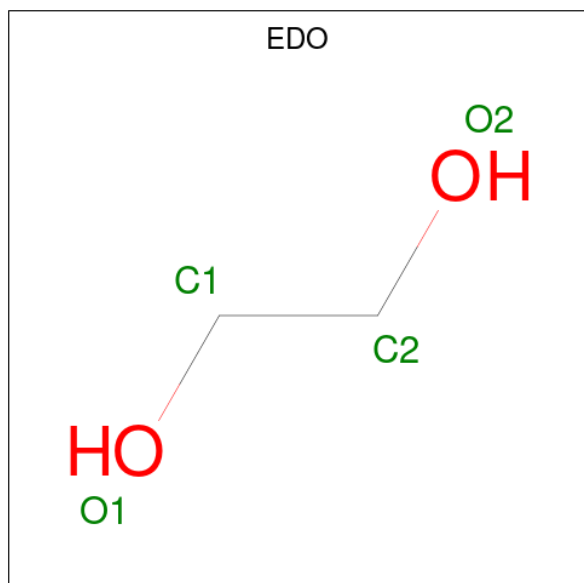
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

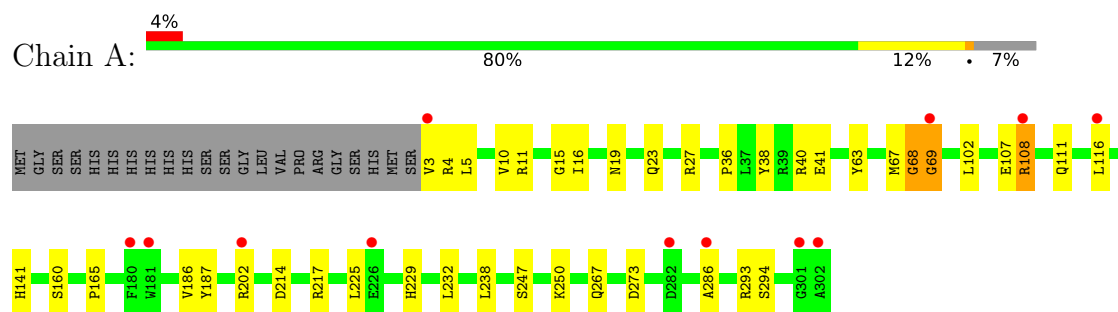
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	162	Total	O	0	0
			162	162		
10	B	195	Total	O	0	0
			195	195		

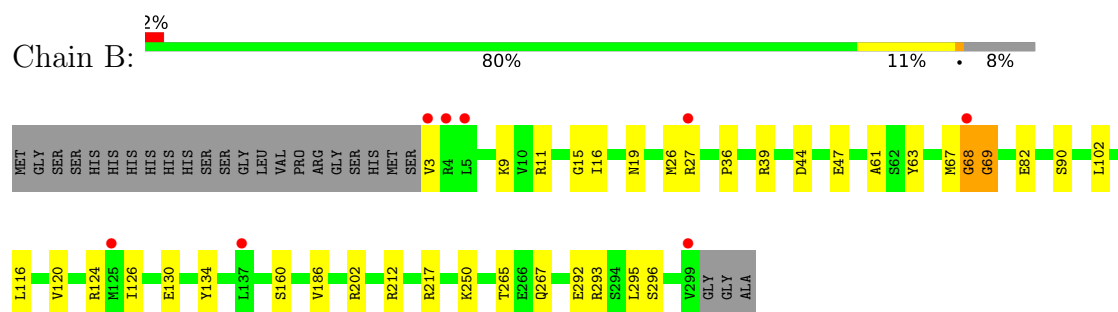
3 Residue-property plots [i](#)

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: 4Fe-4S cluster-binding domain-containing protein



- Molecule 1: 4Fe-4S cluster-binding domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.28Å 93.58Å 108.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.76 – 1.90 70.76 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.76-1.90) 99.9 (70.76-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.200 , 0.235 0.202 , 0.237	Depositor DCC
R_{free} test set	2623 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.1	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	5311	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0287e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NA, CL, SO4, GOL, SF4, SAM, 7P8, 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	0.28	0/2419	0.57	1/3292 (0.0%)
1	B	0.26	0/2406	0.53	0/3275
All	All	0.27	0/4825	0.55	1/6567 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ARG	CB-CG-CD	-9.59	89.25	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	68	GLY	Peptide
1	B	68	GLY	Peptide

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	2362	0	2290	36	0
1	B	2349	0	2279	31	0
2	A	16	0	0	1	0
2	B	16	0	0	1	0
3	A	27	0	22	2	0
3	B	27	0	22	1	0
4	A	23	0	0	1	0
4	B	23	0	0	0	0
5	A	10	0	0	1	0
5	B	25	0	0	2	0
6	A	1	0	0	0	0
6	B	4	0	0	0	0
7	A	48	0	64	7	0
7	B	18	0	24	4	0
8	A	1	0	0	0	0
9	B	4	0	6	1	0
10	A	162	0	0	8	1
10	B	195	0	0	8	1
All	All	5311	0	4707	71	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 7.

The worst 5 of 71 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:108:ARG:HH21	1:A:111:GLN:CD	1.58	1.11
1:A:108:ARG:HH21	1:A:111:GLN:NE2	1.58	0.99
1:B:27:ARG:NH1	10:B:501:HOH:O	1.99	0.94
1:A:108:ARG:NH2	1:A:111:GLN:NE2	2.17	0.91
1:A:3:VAL:N	10:A:504:HOH:O	2.15	0.80

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)
10:A:640:HOH:O	10:B:599:HOH:O[3_554]	2.17	0.03

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	298/322 (92%)	289 (97%)	8 (3%)	1 (0%)	36	29
1	B	295/322 (92%)	285 (97%)	9 (3%)	1 (0%)	36	29
All	All	593/644 (92%)	574 (97%)	17 (3%)	2 (0%)	36	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	GLY
1	B	69	GLY

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	253/272 (93%)	253 (100%)	0	100	100
1	B	253/272 (93%)	253 (100%)	0	100	100
All	All	506/544 (93%)	506 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	243	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 33 ligands modelled in this entry, 6 are monoatomic - leaving 27 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	$\# Z > 2$
5	SO4	B	408	-	4,4,4	0.26	0	6,6,6	0.15	0
5	SO4	A	406	-	4,4,4	0.27	0	6,6,6	0.12	0
2	SF4	B	401	1	0,12,12	-	-	-		
2	SF4	A	401	3,1	0,12,12	-	-	-		
5	SO4	B	406	-	4,4,4	0.29	0	6,6,6	0.14	0
4	7P8	A	404	-	24,24,24	1.17	2 (8%)	33,35,35	1.33	5 (15%)
7	GOL	B	415	-	5,5,5	1.08	0	5,5,5	0.99	0
5	SO4	A	405	-	4,4,4	0.27	0	6,6,6	0.17	0
9	EDO	B	417	-	3,3,3	0.38	0	2,2,2	0.57	0
2	SF4	B	402	3,1	0,12,12	-	-	-		
4	7P8	B	404	-	24,24,24	1.06	2 (8%)	33,35,35	1.17	3 (9%)
5	SO4	B	407	-	4,4,4	0.29	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	405	-	4,4,4	0.28	0	6,6,6	0.12	0
5	SO4	B	409	-	4,4,4	0.25	0	6,6,6	0.13	0
7	GOL	A	415	-	5,5,5	0.99	0	5,5,5	1.07	0
7	GOL	A	411	-	5,5,5	0.84	0	5,5,5	0.93	0
3	SAM	A	403	2	27,29,29	1.12	4 (14%)	34,42,42	2.14	10 (29%)
7	GOL	B	414	-	5,5,5	0.90	0	5,5,5	1.00	0
2	SF4	A	402	1	0,12,12	-	-	-	-	-
7	GOL	A	409	-	5,5,5	0.97	0	5,5,5	1.15	1 (20%)
3	SAM	B	403	2	27,29,29	1.22	4 (14%)	34,42,42	2.09	10 (29%)
7	GOL	A	414	-	5,5,5	0.90	0	5,5,5	1.14	0
7	GOL	A	412	-	5,5,5	0.89	0	5,5,5	1.04	0
7	GOL	A	408	-	5,5,5	1.06	1 (20%)	5,5,5	1.09	0
7	GOL	A	410	-	5,5,5	0.85	0	5,5,5	1.06	1 (20%)
7	GOL	A	413	-	5,5,5	1.09	0	5,5,5	0.64	0
7	GOL	B	416	-	5,5,5	0.93	0	5,5,5	0.94	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
2	SF4	B	401	1	-	-	0/6/5/5
2	SF4	A	401	3,1	-	-	0/6/5/5
4	7P8	A	404	-	-	2/8/48/48	0/2/2/2
7	GOL	B	415	-	-	2/4/4/4	-
9	EDO	B	417	-	-	1/1/1/1	-
4	7P8	B	404	-	-	2/8/48/48	0/2/2/2
2	SF4	B	402	3,1	-	-	0/6/5/5
7	GOL	A	415	-	-	1/4/4/4	-
7	GOL	A	411	-	-	2/4/4/4	-
3	SAM	A	403	2	-	7/17/33/33	0/3/3/3
7	GOL	B	414	-	-	2/4/4/4	-
2	SF4	A	402	1	-	-	0/6/5/5
7	GOL	A	409	-	-	0/4/4/4	-
3	SAM	B	403	2	-	1/17/33/33	0/3/3/3
7	GOL	A	414	-	-	0/4/4/4	-
7	GOL	A	412	-	-	2/4/4/4	-
7	GOL	A	408	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	410	-	-	4/4/4/4	-
7	GOL	A	413	-	-	2/4/4/4	-
7	GOL	B	416	-	-	4/4/4/4	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	SAM	OXT-C	-3.17	1.20	1.30
4	A	404	7P8	O16-C15	2.90	1.49	1.41
3	B	403	SAM	C2-N1	2.88	1.39	1.33
3	B	403	SAM	C2-N3	2.74	1.38	1.33
3	A	403	SAM	OXT-C	-2.68	1.22	1.30

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	SAM	N3-C2-N1	-6.02	119.47	128.58
3	B	403	SAM	N3-C2-N1	-5.07	120.91	128.58
3	A	403	SAM	N9-C8-N7	-4.80	107.13	113.94
3	B	403	SAM	C5-C4-N3	-4.46	120.58	126.72
3	B	403	SAM	N9-C8-N7	-4.12	108.09	113.94

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	SAM	N-CA-CB-CG
3	A	403	SAM	C-CA-CB-CG
3	A	403	SAM	O4'-C4'-C5'-SD
3	A	403	SAM	C3'-C4'-C5'-SD
7	A	411	GOL	C1-C2-C3-O3

There are no ring outliers.

15 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	408	SO4	2	0
5	A	406	SO4	1	0
2	A	401	SF4	1	0
4	A	404	7P8	1	0

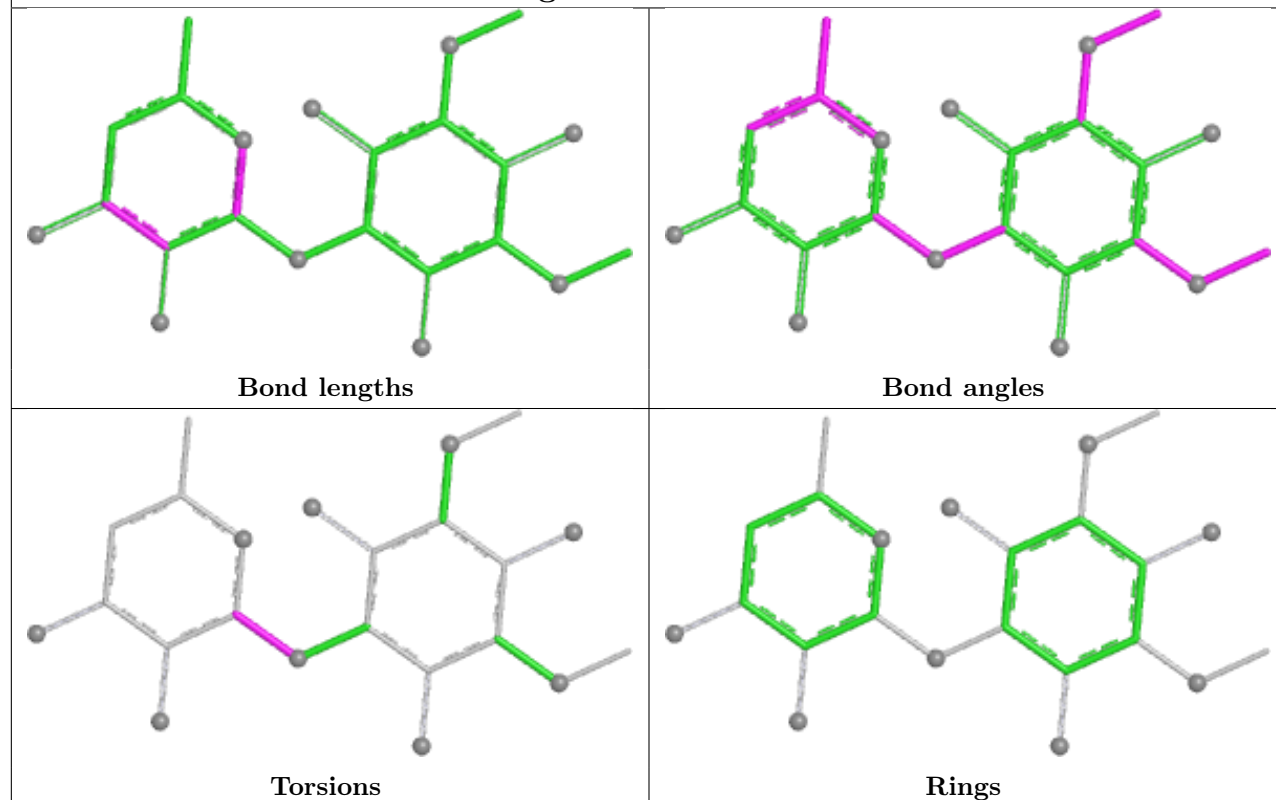
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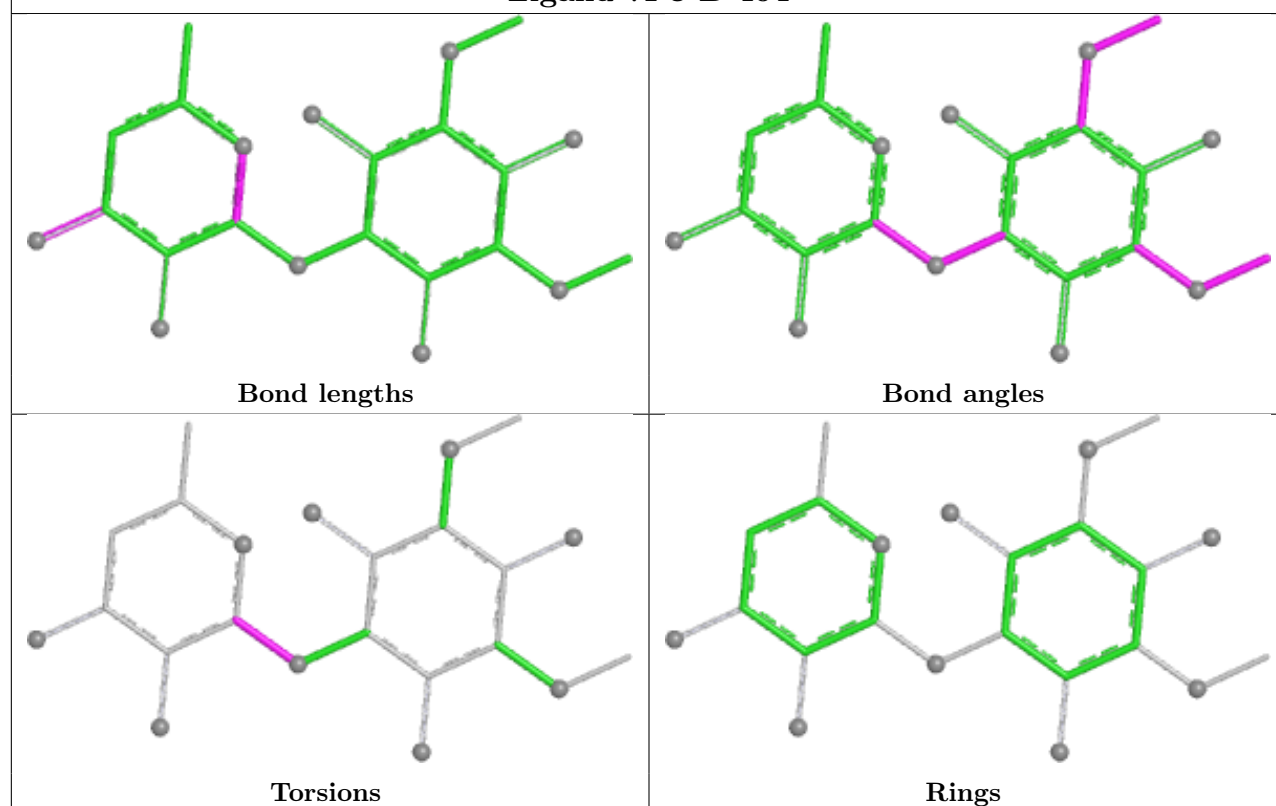
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	415	GOL	1	0
9	B	417	EDO	1	0
2	B	402	SF4	1	0
3	A	403	SAM	2	0
7	A	409	GOL	2	0
3	B	403	SAM	1	0
7	A	414	GOL	1	0
7	A	408	GOL	1	0
7	A	410	GOL	1	0
7	A	413	GOL	2	0
7	B	416	GOL	3	0

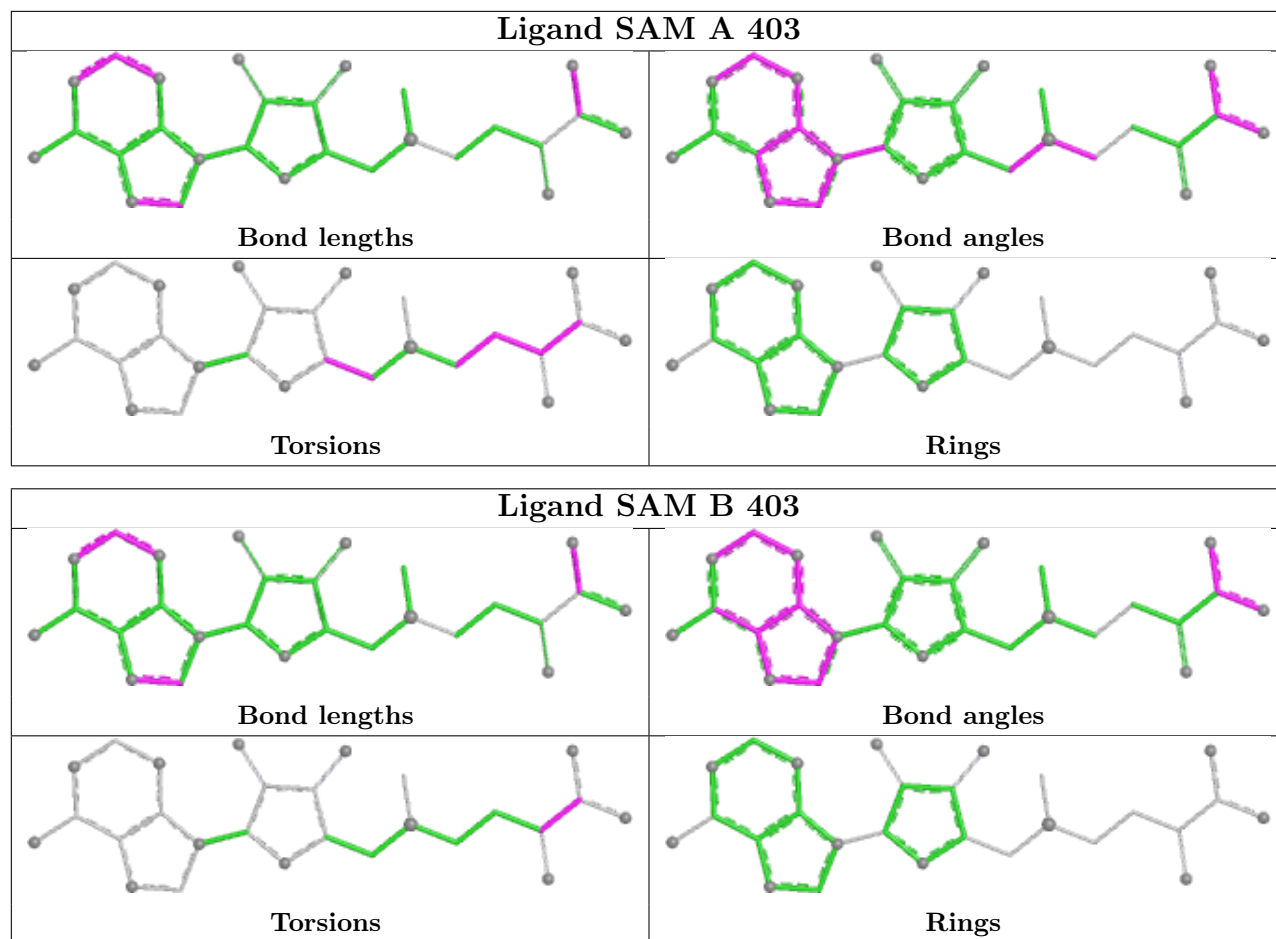
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 7P8 A 404



Ligand 7P8 B 404





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	300/322 (93%)	0.79	12 (4%) 42 45	25, 35, 50, 58	0
1	B	297/322 (92%)	0.69	8 (2%) 56 60	25, 33, 45, 54	0
All	All	597/644 (92%)	0.74	20 (3%) 48 51	25, 34, 49, 58	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	302	ALA	3.7
1	A	116	LEU	3.6
1	A	3	VAL	3.5
1	A	108	ARG	3.4
1	B	299	VAL	3.4

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](#)

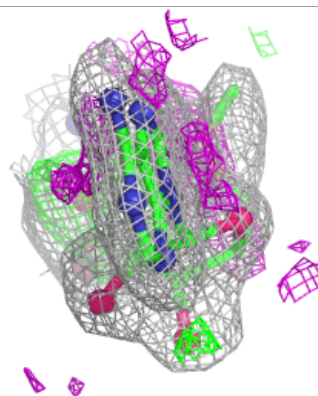
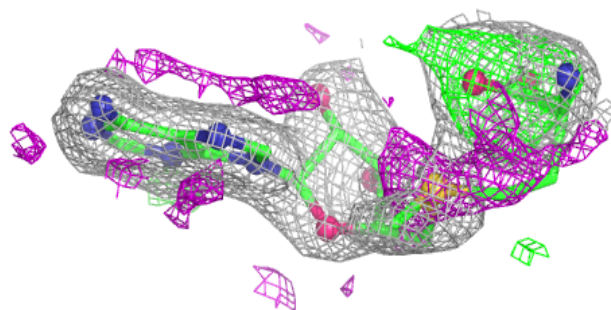
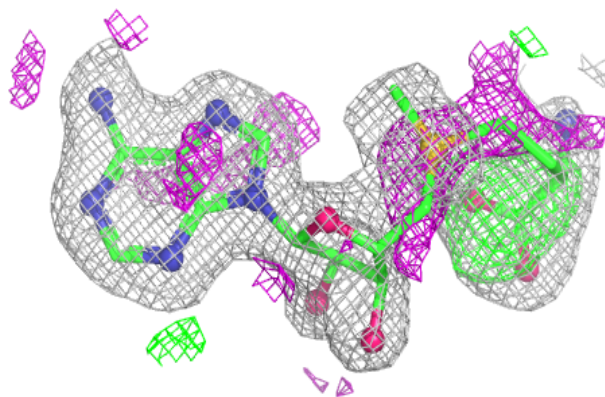
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
5	SO4	B	405	5/5	0.62	0.15	67,67,68,68	0
7	GOL	A	413	6/6	0.64	0.17	47,51,52,54	0
5	SO4	B	407	5/5	0.66	0.14	57,61,61,63	0
5	SO4	B	409	5/5	0.68	0.13	67,67,68,69	0
7	GOL	A	415	6/6	0.69	0.18	39,45,45,47	0
5	SO4	B	406	5/5	0.71	0.14	54,54,56,56	0
7	GOL	A	414	6/6	0.72	0.15	45,48,49,49	0
7	GOL	A	410	6/6	0.73	0.14	47,51,52,53	0
7	GOL	B	415	6/6	0.74	0.15	38,41,44,47	0
5	SO4	A	406	5/5	0.77	0.11	66,66,68,68	0
7	GOL	B	414	6/6	0.78	0.15	42,43,44,45	0
9	EDO	B	417	4/4	0.78	0.18	37,41,43,46	0
7	GOL	B	416	6/6	0.79	0.14	47,49,51,54	0
7	GOL	A	411	6/6	0.79	0.14	34,42,43,44	0
3	SAM	B	403	27/27	0.80	0.17	25,36,50,51	0
5	SO4	B	408	5/5	0.80	0.10	66,68,68,69	0
8	CL	A	416	1/1	0.81	0.14	68,68,68,68	0
7	GOL	A	409	6/6	0.81	0.14	40,43,44,44	0
4	7P8	B	404	23/23	0.85	0.12	24,32,41,47	0
7	GOL	A	412	6/6	0.85	0.12	34,39,39,40	0
3	SAM	A	403	27/27	0.86	0.12	27,33,45,49	0
4	7P8	A	404	23/23	0.87	0.12	27,36,47,48	0
7	GOL	A	408	6/6	0.88	0.11	31,35,38,38	0
6	NA	A	407	1/1	0.89	0.11	41,41,41,41	0
5	SO4	A	405	5/5	0.93	0.08	46,49,51,51	0
6	NA	B	410	1/1	0.95	0.08	31,31,31,31	0
6	NA	B	411	1/1	0.96	0.11	33,33,33,33	0
6	NA	B	412	1/1	0.97	0.12	32,32,32,32	0
6	NA	B	413	1/1	0.97	0.05	37,37,37,37	0
2	SF4	B	402	8/8	0.97	0.06	25,27,28,28	0
2	SF4	A	402	8/8	0.97	0.05	30,31,32,35	0
2	SF4	B	401	8/8	0.97	0.06	26,27,28,29	0
2	SF4	A	401	8/8	0.98	0.05	26,26,28,30	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.

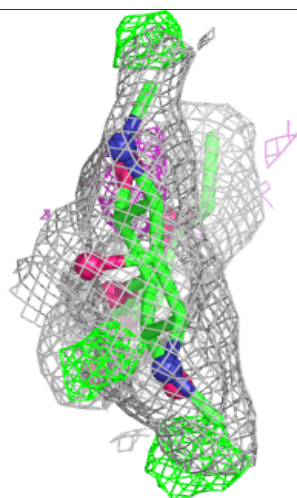
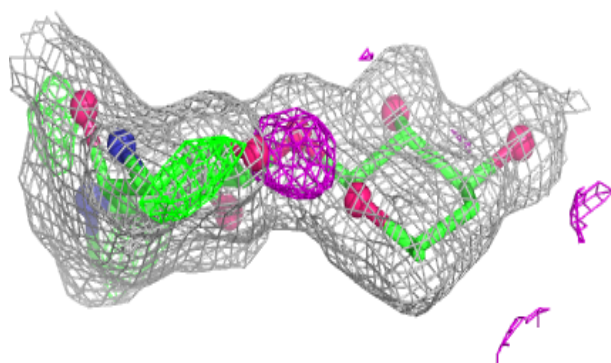
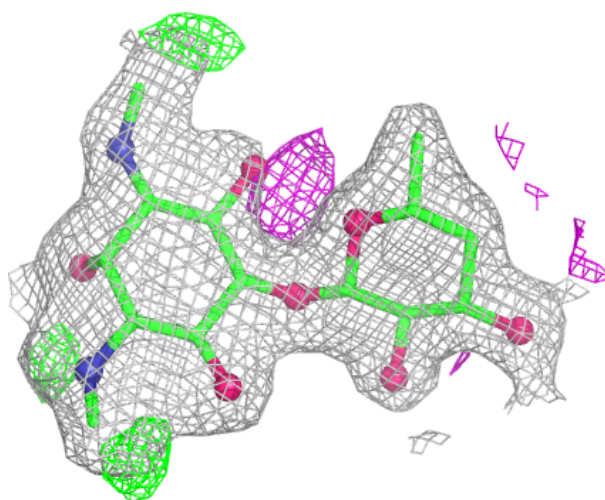
Electron density around SAM B 403:

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



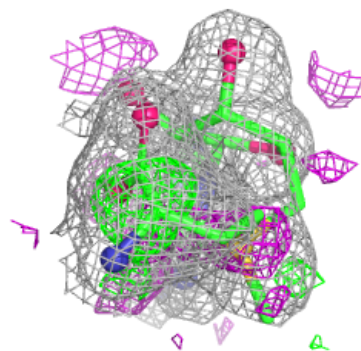
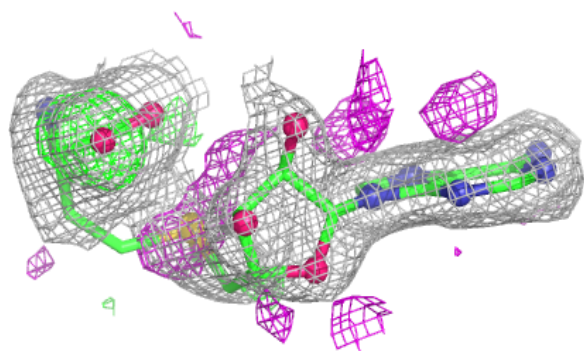
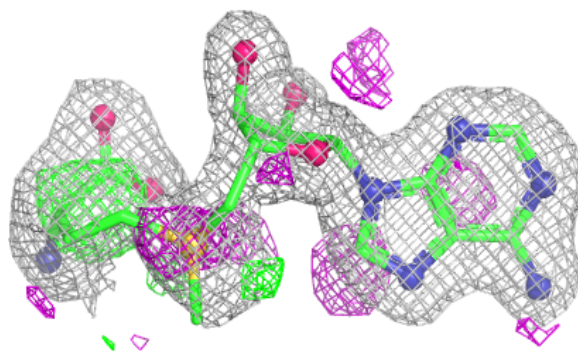
Electron density around 7P8 B 404:

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



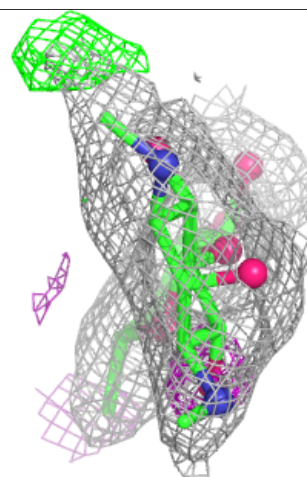
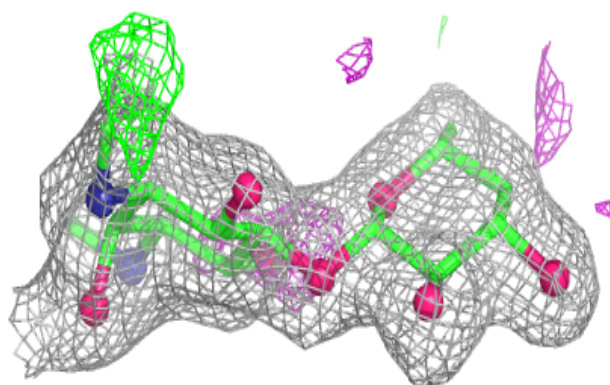
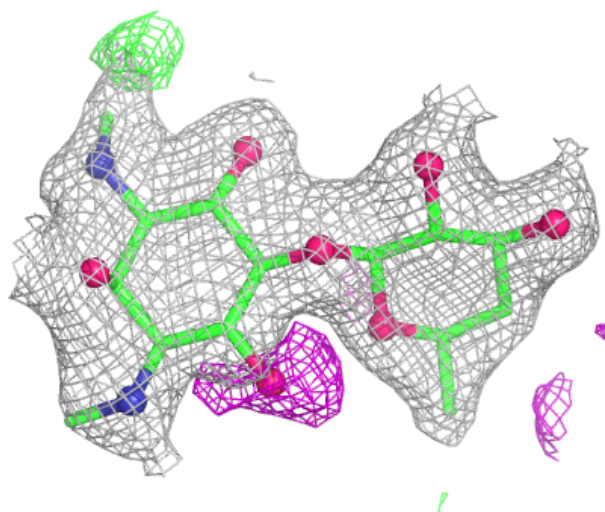
Electron density around SAM A 403:

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



Electron density around 7P8 A 404:

$2mF_o-DF_c$ (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.