



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:15 AM UTC

PDB ID : 7K98 / pdb_00007k98
Title : Preaminoacylation complex of M. tuberculosis PheRS with cognate precursor tRNA and 5'-O-(N-phenylalanyl)sulfamoyl-adenosine (F-AMS)
Authors : Michalska, K.; Chang, C.; Jedrzejczak, R.; Wower, J.; Baragana, B.; Forte, B.; Gilbert, I.H.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2020-09-28
Resolution : 2.19 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](#) ①) were used in the production of this report:

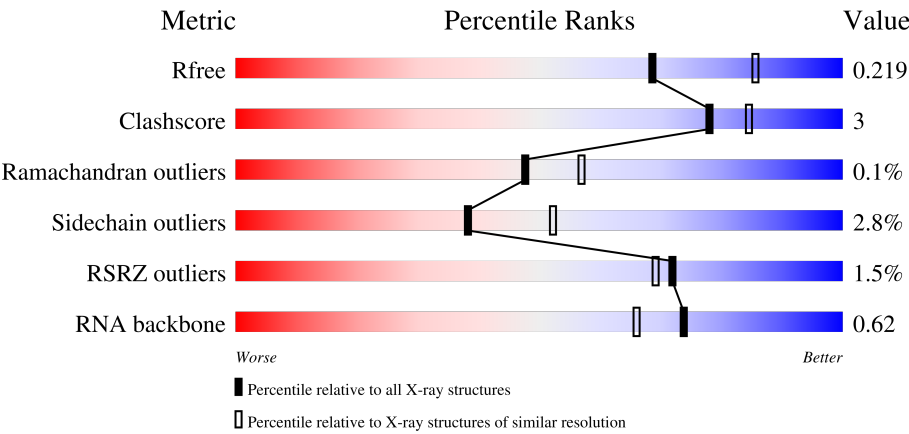
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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.



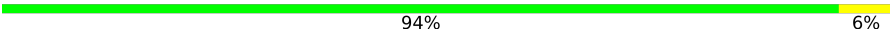
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)
RNA backbone	3983	1052 (2.50-1.90)

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	344	88%11%
1	D	344	88%10%
2	B	840	91%8%
2	E	840	92%7%

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Mol	Chain	Length	Quality of chain
3	C	77	 94%6%
3	F	77	 88%10%•

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22017 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 Phenylalanine–tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	2	0
			2667	1678	485	494	10			
1	D	343	Total	C	N	O	S	0	3	0
			2678	1684	489	495	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P9WUFU3
A	-1	ASN	-	expression tag	UNP P9WUFU3
A	0	ALA	-	expression tag	UNP P9WUFU3
D	-2	SER	-	expression tag	UNP P9WUFU3
D	-1	ASN	-	expression tag	UNP P9WUFU3
D	0	ALA	-	expression tag	UNP P9WUFU3

- Molecule 2 is a protein called Phenylalanine–tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	834	Total	C	N	O	S	0	4	0
			6281	3941	1146	1173	21			
2	E	836	Total	C	N	O	S	0	11	0
			6359	3986	1166	1186	21			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLU	-	expression tag	UNP P9WUFU1
B	-7	ASN	-	expression tag	UNP P9WUFU1
B	-6	LEU	-	expression tag	UNP P9WUFU1
B	-5	TYR	-	expression tag	UNP P9WUFU1
B	-4	PHE	-	expression tag	UNP P9WUFU1
B	-3	GLN	-	expression tag	UNP P9WUFU1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP P9WFU1
B	-1	ASN	-	expression tag	UNP P9WFU1
B	0	ALA	-	expression tag	UNP P9WFU1
E	-8	GLU	-	expression tag	UNP P9WFU1
E	-7	ASN	-	expression tag	UNP P9WFU1
E	-6	LEU	-	expression tag	UNP P9WFU1
E	-5	TYR	-	expression tag	UNP P9WFU1
E	-4	PHE	-	expression tag	UNP P9WFU1
E	-3	GLN	-	expression tag	UNP P9WFU1
E	-2	SER	-	expression tag	UNP P9WFU1
E	-1	ASN	-	expression tag	UNP P9WFU1
E	0	ALA	-	expression tag	UNP P9WFU1

- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------|---------|---------|-------|
| 3 | C | 77 | Total
1628 | C
724 | N
297 | O
531 | P
76 | 0 | 0 | 0 |
| 3 | F | 77 | Total
1628 | C
724 | N
297 | O
531 | P
76 | 0 | 0 | 0 |

-
- The chemical structure of W5Y is a complex molecule. It features a purine base (top) connected to a ribose sugar (middle). The purine base has atoms labeled N1, N3, N7, N9, C2, C4, C6, and C8. The ribose sugar has atoms labeled C1', C2', C3', C4', and C5'. The ribose is linked to a phosphate group (bottom left) via an oxygen atom. The phosphate group is connected to a tyrosine residue (bottom right) via a sulfur atom. The tyrosine residue has a carboxylate group (COO-) and a phenol group (OH). The tyrosine side chain is labeled with 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, C801, C802

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			34	19	7	7	1		
4	D	1	Total	C	N	O	S	0	0
			34	19	7	7	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Mg	0	0
			4	4		
5	B	1	Total	Mg	0	0
			1	1		
5	D	3	Total	Mg	0	0
			3	3		
5	C	2	Total	Mg	0	0
			2	2		
5	F	3	Total	Mg	0	0
			3	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	E	1	Total	Cl	0	0
			1	1		

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



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

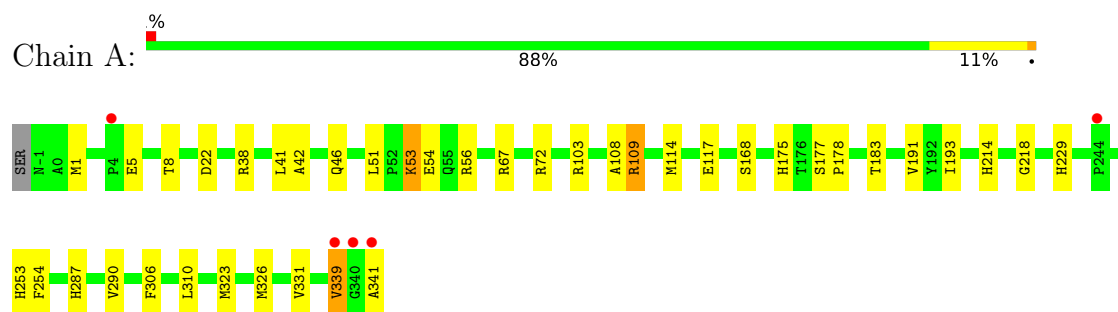
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	85	Total	O	0	0
			85	85		
8	B	219	Total	O	0	4
			221	221		
8	D	93	Total	O	0	0
			93	93		
8	E	188	Total	O	0	1
			189	189		
8	C	39	Total	O	0	0
			39	39		
8	F	48	Total	O	0	0
			48	48		

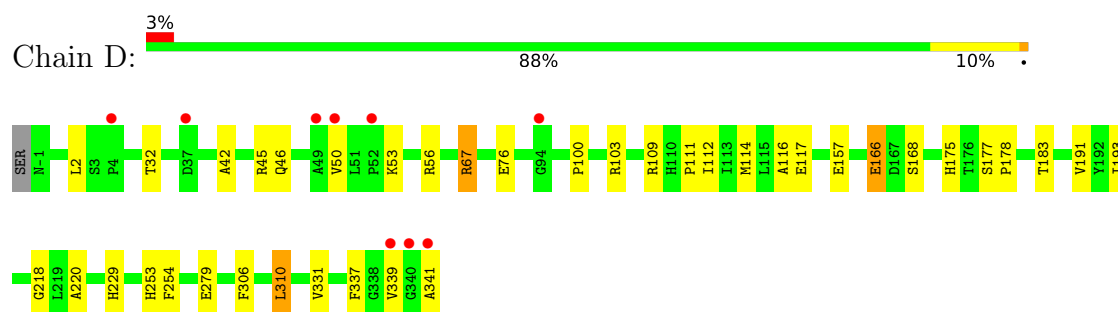
3 Residue-property plots [i](#)

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.

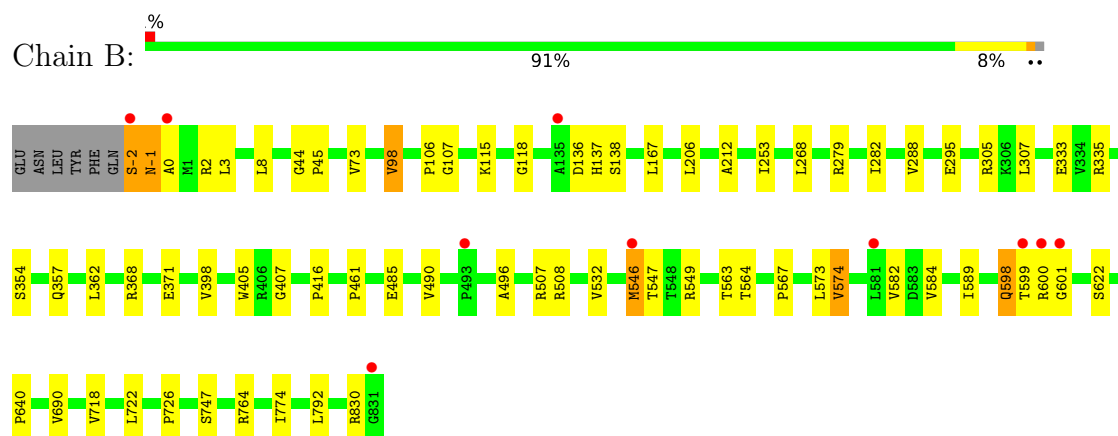
- Molecule 1: Phenylalanine-tRNA ligase alpha subunit



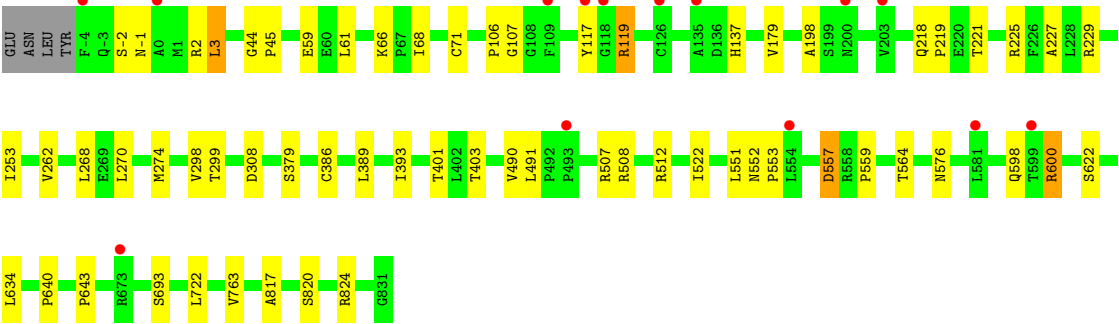
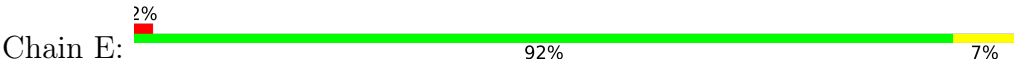
- Molecule 1: Phenylalanine-tRNA ligase alpha subunit



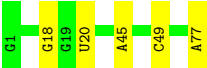
- Molecule 2: Phenylalanine-tRNA ligase beta subunit



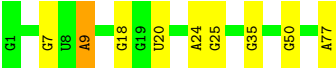
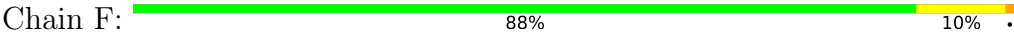
- Molecule 2: Phenylalanine-tRNA ligase beta subunit



• Molecule 3: tRNA(Phe)



• Molecule 3: tRNA(Phe)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	147.42Å 65.30Å 193.48Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	29.85 – 2.19 29.85 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.85-2.19) 96.4 (29.85-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.18rc1_3777	Depositor
R, R_{free}	0.177 , 0.224 (Not available) , 0.219	Depositor DCC
R_{free} test set	3499 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22017	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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, MG, W5Y, CL

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	0.33	0/2727	0.52	0/3708
1	D	0.34	0/2738	0.52	0/3722
2	B	0.34	0/6417	0.54	0/8783
2	E	0.33	0/6496	0.52	0/8889
3	C	0.26	0/1818	0.45	0/2831
3	F	0.26	0/1818	0.43	0/2831
All	All	0.32	0/22014	0.51	0/30764

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	2667	0	2622	21	0
1	D	2678	0	2634	23	0
2	B	6281	0	6311	40	0
2	E	6359	0	6387	39	0
3	C	1628	0	827	2	0
3	F	1628	0	827	5	0
4	A	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	34	0	0	0	0
5	A	4	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	3	0	0	0	0
5	F	3	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
7	B	6	0	8	0	0
7	C	6	0	8	0	0
7	E	6	0	8	0	0
8	A	85	0	0	0	0
8	B	221	0	0	2	0
8	C	39	0	0	0	0
8	D	93	0	0	0	0
8	E	189	0	0	0	0
8	F	48	0	0	1	0
All	All	22017	0	19632	115	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 (115) 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:109[A]:ARG:NH2	1:A:117:GLU:OE1	2.07	0.87
1:D:46:GLN:HG2	3:C:20:U:H5''	1.62	0.80
1:A:46:GLN:HG2	3:F:20:U:H5''	1.63	0.79
1:D:166:GLU:HA	2:E:551:LEU:HD11	1.63	0.78
2:B:-1:ASN:OD1	2:B:2:ARG:NH1	2.22	0.71
2:B:764:ARG:NH2	8:B:1001:HOH:O	2.25	0.67
3:F:7:G:O2'	3:F:50:G:OP2	2.12	0.65
1:D:117:GLU:OE1	2:E:512[B]:ARG:NH1	2.30	0.64
2:B:3:LEU:HD11	2:B:8:LEU:HD13	1.81	0.62
2:E:-2:SER:HB2	2:E:2:ARG:NH2	2.15	0.61
2:B:599:THR:HA	2:B:622:SER:O	2.01	0.60
2:E:59:GLU:OE1	2:E:119:ARG:NH2	2.35	0.58
2:E:-2:SER:HB2	2:E:2:ARG:HH22	1.67	0.58
2:E:198[A]:ALA:HB2	2:E:270:LEU:HD22	1.87	0.56
1:A:114[B]:MET:HE2	1:A:341:ALA:H	1.69	0.56
2:E:-1:ASN:H	2:E:2:ARG:HH22	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:830:ARG:NH2	3:F:35:G:N7	2.50	0.54
2:E:225:ARG:HD3	2:E:379:SER:HB2	1.89	0.53
1:A:42:ALA:O	1:A:46:GLN:HG3	2.08	0.53
1:A:108:ALA:HA	1:A:339:VAL:HA	1.91	0.53
1:D:112:ILE:HG23	1:D:310:LEU:HD13	1.91	0.53
2:E:598:GLN:HG2	2:E:600:ARG:NH2	2.24	0.52
1:D:117:GLU:HG3	2:E:508:ARG:CZ	2.39	0.52
1:A:41:LEU:HD13	1:A:67:ARG:HA	1.90	0.52
1:A:229:HIS:HA	2:B:490:VAL:O	2.10	0.51
2:E:68:ILE:HG21	2:E:117:TYR:HD1	1.75	0.51
2:B:253:ILE:HD12	2:B:268:LEU:HD11	1.93	0.51
1:A:53:LYS:HA	1:A:56:ARG:HD2	1.92	0.51
2:E:508:ARG:O	2:E:512[A]:ARG:HG3	2.10	0.51
2:B:305:ARG:CZ	2:B:362:LEU:HD21	2.41	0.50
2:E:137:HIS:O	2:E:137:HIS:ND1	2.43	0.50
2:E:61:LEU:N	2:E:68:ILE:O	2.45	0.50
1:D:183:THR:HG21	1:D:193:ILE:HG12	1.94	0.50
1:D:177:SER:N	1:D:178:PRO:HD2	2.27	0.49
2:B:690:VAL:HG11	2:B:726:PRO:HD2	1.95	0.49
2:B:206:LEU:HD13	2:B:398:VAL:HG11	1.95	0.49
2:B:0:ALA:O	2:B:2:ARG:NH2	2.45	0.49
2:B:136:ASP:HB3	2:B:138:SER:H	1.77	0.49
2:B:-1:ASN:H	2:B:2:ARG:HH12	1.60	0.49
1:D:229:HIS:HA	2:E:490:VAL:O	2.13	0.48
2:B:115:LYS:HE3	2:B:118:GLY:HA2	1.95	0.48
2:E:262:VAL:HG12	2:E:386:CYS:SG	2.53	0.48
1:A:114[B]:MET:HE2	1:A:341:ALA:N	2.29	0.48
1:A:287:HIS:HB3	1:A:290:VAL:HG23	1.96	0.48
1:A:183:THR:HG21	1:A:193:ILE:HG12	1.95	0.48
3:F:24:A:H2'	3:F:25:G:C8	2.48	0.47
2:B:405:TRP:CH2	2:B:407:GLY:HA2	2.49	0.47
1:D:253:HIS:CD2	1:D:254:PHE:H	2.33	0.47
1:D:253:HIS:CG	1:D:254:PHE:H	2.31	0.47
2:B:507:ARG:HG2	2:B:589:ILE:HG21	1.97	0.47
2:E:722:LEU:HD23	2:E:722:LEU:HA	1.72	0.47
2:B:532:VAL:HG21	2:B:567:PRO:HB3	1.97	0.47
1:A:177:SER:N	1:A:178:PRO:HD2	2.30	0.47
1:D:32:THR:HG21	3:C:45:A:H5''	1.95	0.47
2:E:218:GLN:OE1	2:E:219:PRO:HD2	2.15	0.47
2:B:599:THR:O	2:B:600:ARG:NH1	2.49	0.46
2:B:368:ARG:HA	2:B:371:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114[A]:MET:HE2	1:D:341:ALA:N	2.30	0.46
2:E:227:ALA:HA	2:E:403:THR:O	2.15	0.46
2:E:274:MET:HE3	2:E:274:MET:HB3	1.82	0.46
1:D:53:LYS:HA	1:D:56:ARG:NE	2.30	0.46
1:A:253:HIS:CG	1:A:254:PHE:H	2.33	0.46
2:B:547:THR:HG22	2:B:563:THR:HG23	1.98	0.46
2:E:557:ASP:OD1	2:E:557:ASP:N	2.42	0.46
1:A:22:ASP:OD1	1:A:22:ASP:N	2.41	0.46
2:B:496:ALA:HB3	2:E:491:LEU:HD13	1.99	0.45
2:B:333:GLU:O	2:B:335:ARG:HD2	2.17	0.45
1:A:323:MET:O	1:A:326:MET:HB3	2.16	0.45
2:B:106:PRO:HA	2:B:107:GLY:HA2	1.56	0.45
2:B:295:GLU:O	2:B:307:LEU:HB2	2.17	0.45
1:A:214:HIS:HB2	1:A:310:LEU:HB3	1.99	0.44
1:D:116:ALA:HB2	1:D:310:LEU:HD11	1.99	0.44
1:D:45:ARG:HH22	1:D:67:ARG:HD2	1.82	0.44
1:A:117:GLU:HG2	2:B:508:ARG:CZ	2.47	0.44
1:D:218:GLY:HA3	1:D:306:PHE:CZ	2.52	0.44
1:D:331:VAL:HG13	2:E:576:ASN:OD1	2.18	0.44
2:B:574:VAL:HG22	8:B:1170:HOH:O	2.17	0.43
2:E:44:GLY:HA3	2:E:45:PRO:HA	1.71	0.43
2:B:44:GLY:HA3	2:B:45:PRO:HA	1.75	0.43
1:D:103:ARG:O	2:E:640:PRO:HD2	2.18	0.43
2:E:553:PRO:HG3	2:E:559:PRO:HB3	2.00	0.43
2:E:598:GLN:O	2:E:622:SER:HA	2.18	0.43
1:A:218:GLY:HA3	1:A:306:PHE:CZ	2.53	0.43
1:D:100:PRO:HD2	2:E:643:PRO:HG3	1.99	0.43
1:D:42:ALA:O	1:D:46:GLN:HG3	2.18	0.43
1:D:109[A]:ARG:NH1	1:D:117:GLU:OE2	2.50	0.43
2:E:106:PRO:HA	2:E:107:GLY:HA2	1.48	0.43
2:B:0:ALA:HB1	2:B:167:LEU:O	2.19	0.42
2:E:253:ILE:HD12	2:E:268:LEU:HD11	2.01	0.42
2:B:73:VAL:HG11	2:B:98:VAL:HG11	2.00	0.42
2:E:61:LEU:HD21	2:E:119:ARG:NH2	2.34	0.42
2:B:-2:SER:HB3	2:B:368:ARG:HH22	1.84	0.42
2:E:229:ARG:HG3	2:E:401:THR:O	2.20	0.42
2:B:416:PRO:HD2	2:B:461:PRO:O	2.19	0.42
2:E:68:ILE:HG21	2:E:117:TYR:CD1	2.54	0.42
2:B:747:SER:HA	2:B:792:LEU:O	2.20	0.41
2:B:354:SER:HB2	2:B:371:GLU:HB2	2.03	0.41
2:B:722:LEU:HD23	2:B:722:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3:LEU:HD23	2:E:179:VAL:HG22	2.01	0.41
2:E:820:SER:O	2:E:824:ARG:HG3	2.21	0.41
2:B:598:GLN:H	2:B:598:GLN:HG2	1.50	0.41
1:D:111:PRO:HG3	1:D:337:PHE:CD2	2.55	0.41
2:B:279:ARG:HA	2:B:282:ILE:HD12	2.03	0.41
1:D:191:VAL:O	1:D:220:ALA:HA	2.20	0.41
2:E:66:LYS:HD3	2:E:66:LYS:HA	1.75	0.41
2:E:763:VAL:HG13	2:E:817:ALA:HB1	2.03	0.40
3:F:9:A:H2'	8:F:217:HOH:O	2.20	0.40
1:A:1:MET:HE3	1:A:1:MET:HB2	1.95	0.40
2:B:485:GLU:H	2:B:485:GLU:CD	2.29	0.40
1:A:38:ARG:HE	1:A:38:ARG:HB3	1.75	0.40
2:E:389:LEU:O	2:E:393:ILE:HG13	2.22	0.40
2:E:552:ASN:OD1	2:E:552:ASN:N	2.53	0.40
1:A:103:ARG:O	2:B:640:PRO:HD2	2.21	0.40
2:B:573:LEU:HG	2:B:584:VAL:HG11	2.04	0.40
2:B:600:ARG:HB3	2:B:601:GLY:H	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	343/344 (100%)	336 (98%)	7 (2%)	0	100	100
1	D	344/344 (100%)	333 (97%)	11 (3%)	0	100	100
2	B	836/840 (100%)	807 (96%)	27 (3%)	2 (0%)	43	51
2	E	845/840 (101%)	816 (97%)	29 (3%)	0	100	100
All	All	2368/2368 (100%)	2292 (97%)	74 (3%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	212	ALA
2	B	546	MET

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	271/270 (100%)	258 (95%)	13 (5%)	23	30
1	D	272/270 (101%)	261 (96%)	11 (4%)	28	38
2	B	655/657 (100%)	641 (98%)	14 (2%)	47	63
2	E	663/657 (101%)	649 (98%)	14 (2%)	47	63
All	All	1861/1854 (100%)	1809 (97%)	52 (3%)	38	52

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	8	THR
1	A	51	LEU
1	A	53	LYS
1	A	54	GLU
1	A	72	ARG
1	A	109[A]	ARG
1	A	109[B]	ARG
1	A	168	SER
1	A	175	HIS
1	A	191	VAL
1	A	331	VAL
1	A	339	VAL
2	B	-2	SER
2	B	-1	ASN
2	B	98	VAL
2	B	137	HIS
2	B	288	VAL
2	B	357	GLN
2	B	546	MET

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Mol	Chain	Res	Type
2	B	549	ARG
2	B	564	THR
2	B	574	VAL
2	B	582	VAL
2	B	598	GLN
2	B	718	VAL
2	B	774	ILE
1	D	2	LEU
1	D	50	VAL
1	D	67	ARG
1	D	76	GLU
1	D	157	GLU
1	D	166	GLU
1	D	168	SER
1	D	175	HIS
1	D	279	GLU
1	D	310	LEU
1	D	339	VAL
2	E	3	LEU
2	E	71	CYS
2	E	119	ARG
2	E	221	THR
2	E	298	VAL
2	E	299	THR
2	E	308	ASP
2	E	507	ARG
2	E	522	ILE
2	E	557	ASP
2	E	564	THR
2	E	600	ARG
2	E	634	LEU
2	E	693	SER

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

Mol	Chain	Res	Type
2	B	28	GLN
2	B	120	ASN
2	B	137	HIS
2	B	598	GLN
1	D	289	ASN
2	E	35	HIS

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Mol	Chain	Res	Type
2	E	452	HIS
2	E	687	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	74/77 (96%)	3 (4%)	0
3	F	74/77 (96%)	3 (4%)	0
All	All	148/154 (96%)	6 (4%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	18	G
3	C	49	C
3	C	77	A
3	F	9	A
3	F	18	G
3	F	77	A

There are no RNA pucker outliers to report.

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 20 ligands modelled in this entry, 15 are monoatomic - leaving 5 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	$\# Z > 2$
7	GOL	E	902	-	5,5,5	1.01	0	5,5,5	0.92	0
7	GOL	C	103	-	5,5,5	0.90	0	5,5,5	1.08	0
4	W5Y	D	401	-	37,37,37	1.50	8 (21%)	51,54,54	1.86	11 (21%)
4	W5Y	A	401	-	37,37,37	1.36	4 (10%)	51,54,54	1.90	10 (19%)
7	GOL	B	903	-	5,5,5	0.83	0	5,5,5	1.16	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
7	GOL	E	902	-	-	4/4/4/4	-
7	GOL	C	103	-	-	0/4/4/4	-
4	W5Y	D	401	-	-	2/22/39/39	0/4/4/4
4	W5Y	A	401	-	-	0/22/39/39	0/4/4/4
7	GOL	B	903	-	-	4/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	W5Y	C5-C4	4.58	1.47	1.39
4	D	401	W5Y	C5-C4	4.49	1.47	1.39
4	D	401	W5Y	O5'-SBI	-3.74	1.52	1.60
4	A	401	W5Y	C-NAT	-2.82	1.32	1.37
4	D	401	W5Y	C-NAT	-2.63	1.32	1.37
4	D	401	W5Y	C5-C6	2.60	1.48	1.41
4	A	401	W5Y	C5-N7	-2.60	1.34	1.39
4	D	401	W5Y	SBI-NAT	-2.48	1.55	1.59
4	A	401	W5Y	C5-C6	2.46	1.47	1.41
4	D	401	W5Y	C4-N9	-2.21	1.33	1.37
4	D	401	W5Y	C5-N7	-2.18	1.35	1.39
4	D	401	W5Y	C8-N7	2.15	1.35	1.31

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	W5Y	OAE-SBI-OAD	-6.63	110.93	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	W5Y	OAE-SBI-OAD	-6.39	111.28	120.85
4	A	401	W5Y	C5-C4-N3	-5.51	119.14	126.72
4	D	401	W5Y	C5-C4-N3	-5.11	119.68	126.72
4	A	401	W5Y	N3-C4-N9	4.24	134.38	127.17
4	D	401	W5Y	N3-C4-N9	3.86	133.73	127.17
4	D	401	W5Y	C4-C5-N7	-3.75	106.30	110.58
4	A	401	W5Y	C4-C5-N7	-3.59	106.47	110.58
4	A	401	W5Y	C2-N3-C4	3.54	120.47	111.83
4	D	401	W5Y	C2-N3-C4	3.44	120.22	111.83
4	A	401	W5Y	N1-C2-N3	-3.28	123.62	128.58
4	D	401	W5Y	N1-C2-N3	-3.21	123.72	128.58
4	D	401	W5Y	C4-N9-C8	2.78	108.65	105.74
4	D	401	W5Y	C5-N7-C8	2.66	107.63	103.45
4	A	401	W5Y	C5-N7-C8	2.61	107.56	103.45
4	D	401	W5Y	O5'-SBI-OAD	2.53	113.13	105.48
4	D	401	W5Y	C6-C5-N7	2.33	136.59	132.09
4	A	401	W5Y	O5'-SBI-NAT	2.28	111.58	105.69
4	A	401	W5Y	C2-N1-C6	2.22	122.38	118.73
4	A	401	W5Y	C4-N9-C8	2.21	108.06	105.74
4	D	401	W5Y	N9-C8-N7	-2.19	110.83	113.94

There are no chirality outliers.

All (10) torsion outliers are listed below:

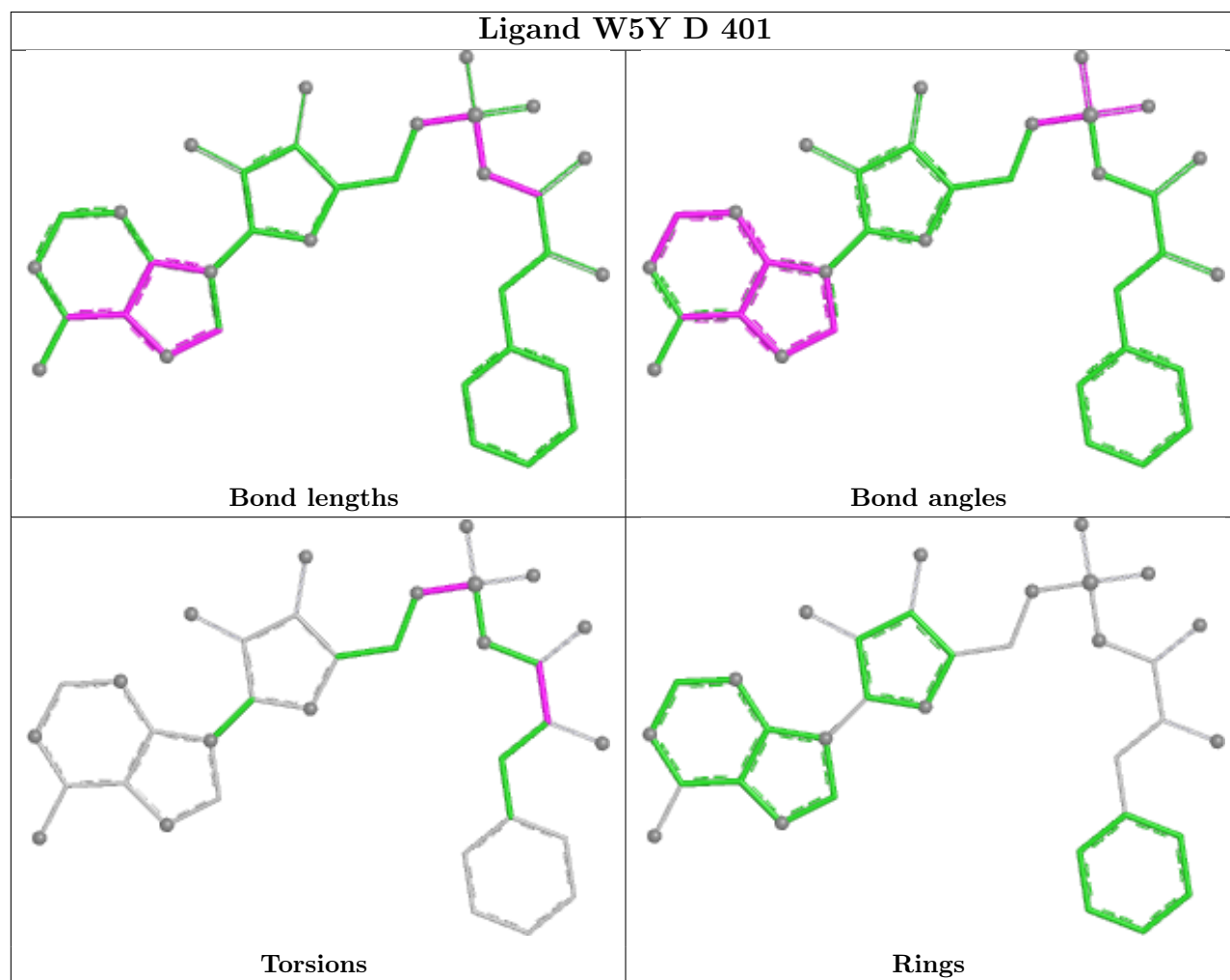
Mol	Chain	Res	Type	Atoms
7	E	902	GOL	O1-C1-C2-O2
7	E	902	GOL	O1-C1-C2-C3
7	E	902	GOL	C1-C2-C3-O3
7	B	903	GOL	O1-C1-C2-C3
7	B	903	GOL	C1-C2-C3-O3
7	B	903	GOL	O1-C1-C2-O2
7	B	903	GOL	O2-C2-C3-O3
7	E	902	GOL	O2-C2-C3-O3
4	D	401	W5Y	O-C-CA-CB
4	D	401	W5Y	C5'-O5'-SBI-NAT

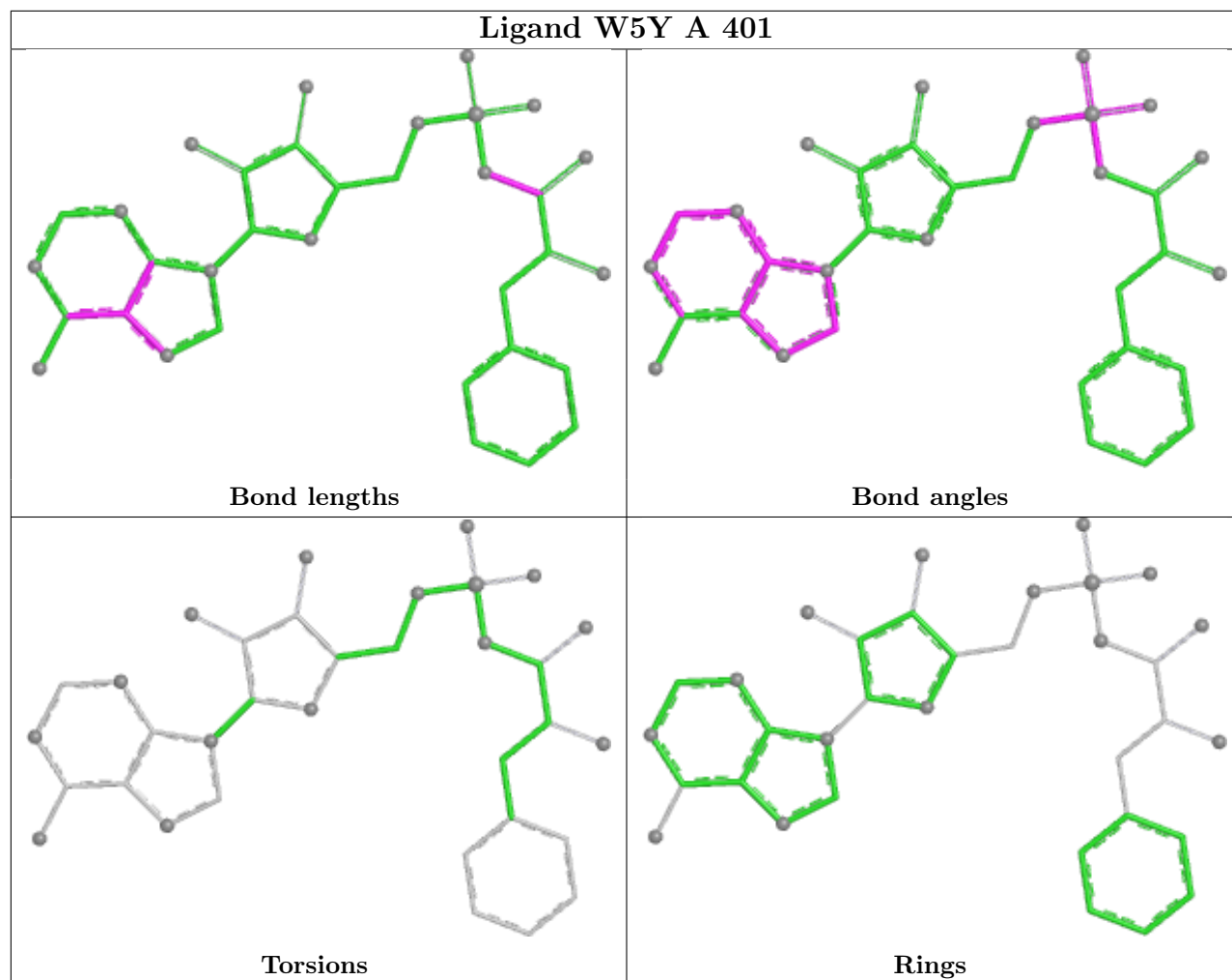
There are no ring outliers.

No monomer is involved in short contacts.

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	343/344 (99%)	-0.20	5 (1%) 72 69	21, 53, 103, 123	2 (0%)
1	D	343/344 (99%)	-0.19	9 (2%) 57 54	20, 50, 115, 166	3 (0%)
2	B	834/840 (99%)	-0.27	10 (1%) 76 74	22, 51, 87, 142	4 (0%)
2	E	836/840 (99%)	-0.21	14 (1%) 69 66	22, 53, 94, 145	11 (1%)
3	C	77/77 (100%)	-0.59	0 100 100	55, 84, 116, 152	0
3	F	77/77 (100%)	-0.63	0 100 100	50, 78, 104, 150	0
All	All	2510/2522 (99%)	-0.25	38 (1%) 72 69	20, 53, 99, 166	20 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	341	ALA	8.1
1	A	341	ALA	5.3
2	E	200[A]	ASN	5.0
2	E	109	PHE	4.2
1	D	340	GLY	4.1
2	E	-4	PHE	3.4
1	A	339	VAL	3.2
2	E	493	PRO	3.2
2	B	581	LEU	3.1
1	A	340	GLY	3.0
2	E	0	ALA	2.9
2	E	117	TYR	2.7
1	A	4	PRO	2.7
2	E	135	ALA	2.6
1	D	339	VAL	2.6
1	A	244	PRO	2.6
2	B	601	GLY	2.6
2	B	599	THR	2.6
2	B	0	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	135	ALA	2.6
1	D	4	PRO	2.6
2	B	-2	SER	2.5
2	E	673[A]	ARG	2.5
2	E	118	GLY	2.5
2	E	203	VAL	2.5
2	E	581	LEU	2.4
2	B	600	ARG	2.3
1	D	94	GLY	2.3
2	E	554	LEU	2.2
1	D	52	PRO	2.2
1	D	37	ASP	2.2
2	B	546	MET	2.1
2	B	831	GLY	2.1
2	B	493	PRO	2.0
2	E	599	THR	2.0
1	D	50	VAL	2.0
1	D	49	ALA	2.0
2	E	126	CYS	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.

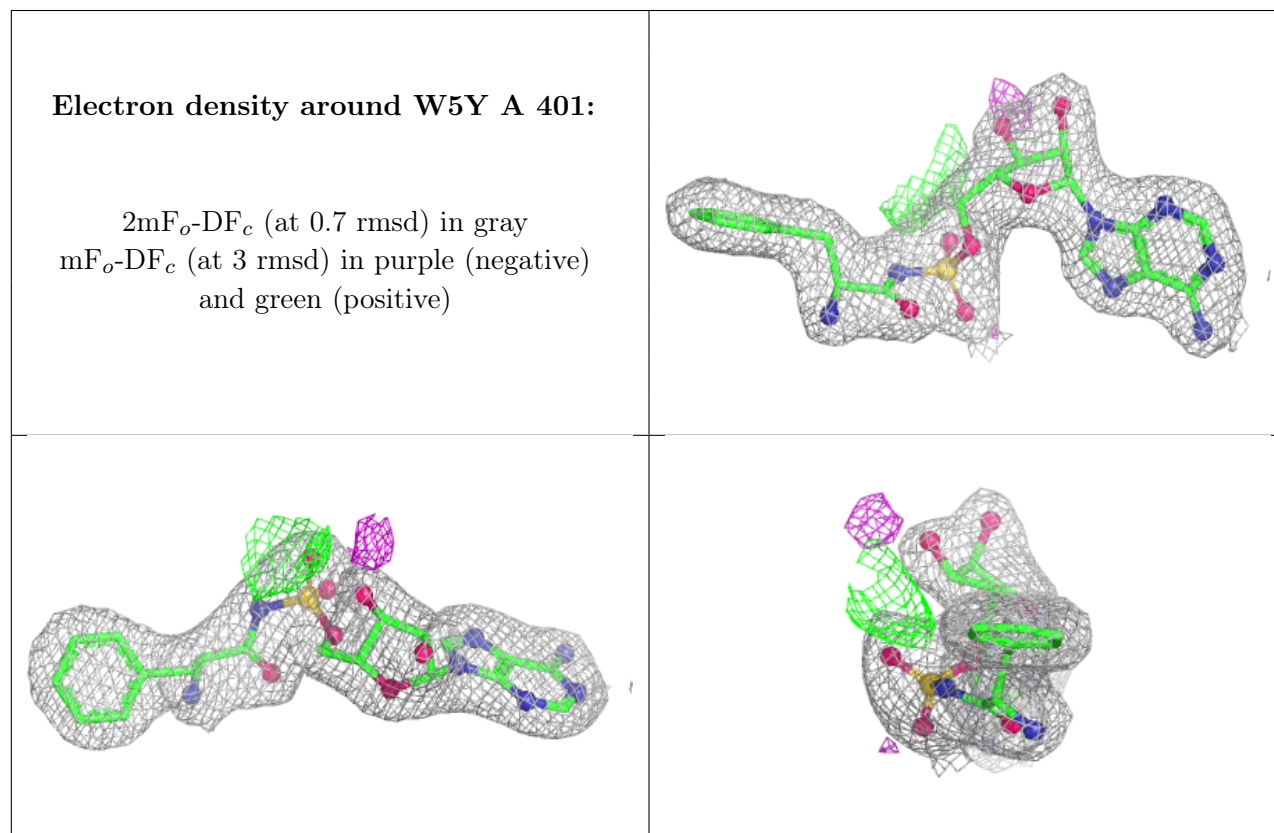
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	A	405	1/1	0.83	0.11	69,69,69,69	0
5	MG	D	404	1/1	0.83	0.10	61,61,61,61	0
7	GOL	E	902	6/6	0.86	0.10	73,82,88,91	0
7	GOL	C	103	6/6	0.86	0.15	79,83,84,84	0

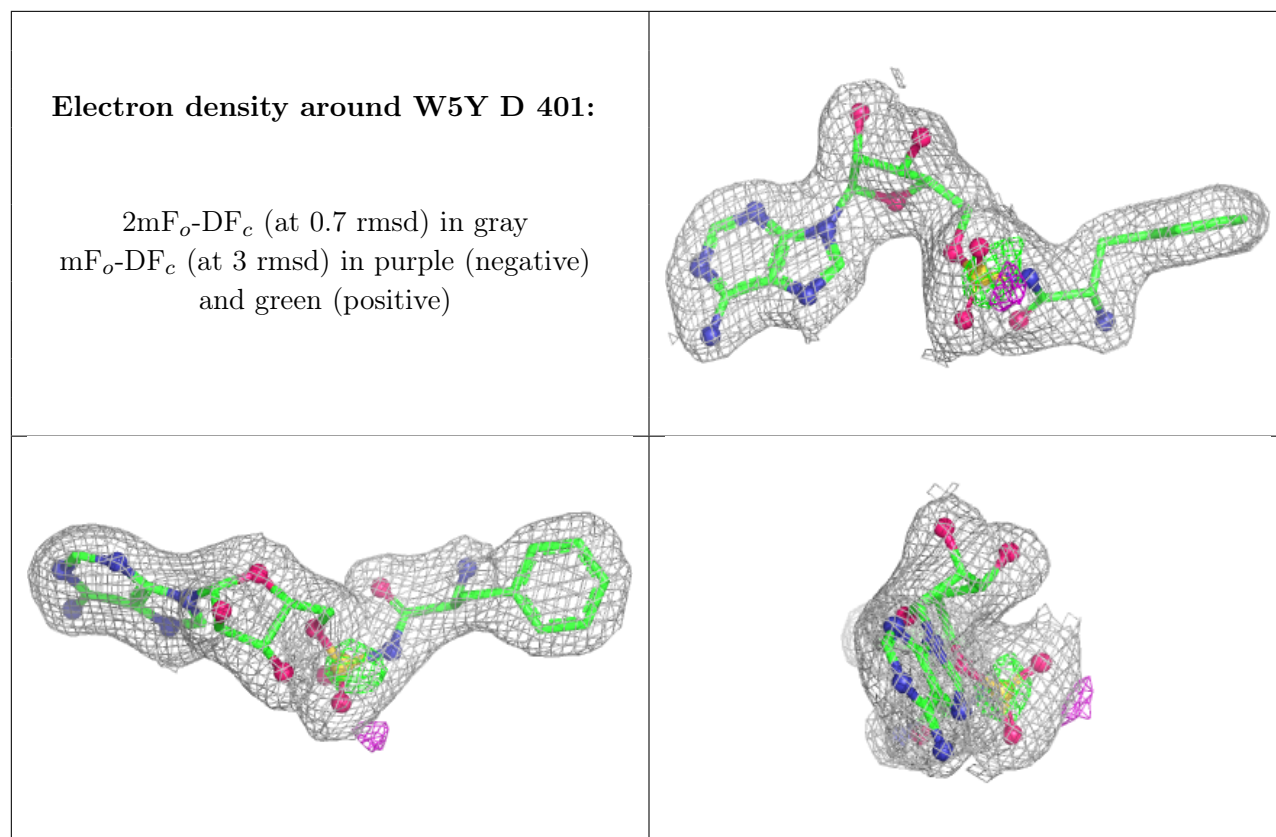
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	C	102	1/1	0.88	0.09	64,64,64,64	0
7	GOL	B	903	6/6	0.88	0.10	65,73,78,84	0
5	MG	C	101	1/1	0.90	0.10	65,65,65,65	0
5	MG	F	103	1/1	0.92	0.06	93,93,93,93	0
5	MG	B	901	1/1	0.92	0.08	54,54,54,54	0
5	MG	F	102	1/1	0.94	0.08	74,74,74,74	0
6	CL	E	901	1/1	0.96	0.07	51,51,51,51	0
4	W5Y	A	401	34/34	0.97	0.06	31,40,45,47	0
6	CL	B	902	1/1	0.97	0.08	57,57,57,57	0
5	MG	A	404	1/1	0.97	0.04	71,71,71,71	0
5	MG	F	101	1/1	0.98	0.06	67,67,67,67	0
4	W5Y	D	401	34/34	0.98	0.05	31,37,40,56	0
5	MG	D	402	1/1	0.99	0.03	46,46,46,46	0
5	MG	A	402	1/1	0.99	0.03	48,48,48,48	0
5	MG	D	403	1/1	1.00	0.02	41,41,41,41	0
5	MG	A	403	1/1	1.00	0.01	40,40,40,40	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.