



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 29, 2018 – 03:41 PM EST

PDB ID : 5XN1
Title : HIV-1 reverse transcriptase Q151M:DNA:entecavir-triphosphate ternary complex
Authors : Yasutake, Y.; Tamura, N.; Hayashi, H.; Maeda, K.
Deposited on : 2017-05-17
Resolution : 2.45 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

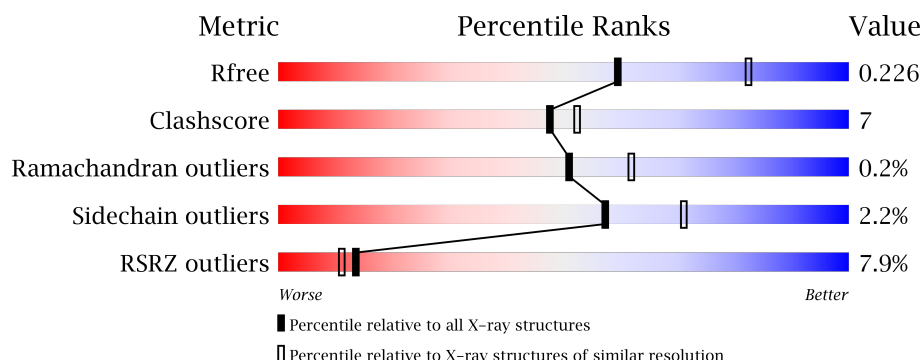
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	100719	1152 (2.46-2.42)
Clashscore	112137	1224 (2.46-2.42)
Ramachandran outliers	110173	1217 (2.46-2.42)
Sidechain outliers	110143	1217 (2.46-2.42)
RSRZ outliers	101464	1158 (2.46-2.42)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	557	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>
1	C	557	<div> <div>10%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
2	B	444	<div> <div>12%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 8%</div> </div> </div>
2	D	444	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>• 8%</div> </div> </div>
3	E	38	<div> <div></div> <div> <div></div> <div>74%</div> <div>16%</div> <div>• 8%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	38	

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
6	GOL	D	502	-	-	-	X
6	GOL	F	101	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17562 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 Pol protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	1	0
			4488	2903	748	829	8			
1	C	551	Total	C	N	O	S	0	0	0
			4483	2900	748	827	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP D3XFN7
A	0	VAL	-	expression tag	UNP D3XFN7
A	151	MET	GLN	engineered mutation	UNP D3XFN7
A	162	SER	CYS	engineered mutation	UNP D3XFN7
A	280	SER	CYS	engineered mutation	UNP D3XFN7
C	-1	MET	-	expression tag	UNP D3XFN7
C	0	VAL	-	expression tag	UNP D3XFN7
C	151	MET	GLN	engineered mutation	UNP D3XFN7
C	162	SER	CYS	engineered mutation	UNP D3XFN7
C	280	SER	CYS	engineered mutation	UNP D3XFN7

- Molecule 2 is a protein called Pol protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	407	Total	C	N	O	S	0	0	0
			3354	2183	558	607	6			
2	D	407	Total	C	N	O	S	0	0	0
			3354	2183	558	607	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	expression tag	UNP D3XFN7
B	-14	ALA	-	expression tag	UNP D3XFN7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP D3XFN7
B	-12	HIS	-	expression tag	UNP D3XFN7
B	-11	HIS	-	expression tag	UNP D3XFN7
B	-10	HIS	-	expression tag	UNP D3XFN7
B	-9	HIS	-	expression tag	UNP D3XFN7
B	-8	HIS	-	expression tag	UNP D3XFN7
B	-7	ALA	-	expression tag	UNP D3XFN7
B	-6	LEU	-	expression tag	UNP D3XFN7
B	-5	GLU	-	expression tag	UNP D3XFN7
B	-4	VAL	-	expression tag	UNP D3XFN7
B	-3	LEU	-	expression tag	UNP D3XFN7
B	-2	PHE	-	expression tag	UNP D3XFN7
B	-1	GLN	-	expression tag	UNP D3XFN7
B	0	GLY	-	expression tag	UNP D3XFN7
B	162	SER	CYS	engineered mutation	UNP D3XFN7
B	280	SER	CYS	engineered mutation	UNP D3XFN7
D	-15	MET	-	expression tag	UNP D3XFN7
D	-14	ALA	-	expression tag	UNP D3XFN7
D	-13	HIS	-	expression tag	UNP D3XFN7
D	-12	HIS	-	expression tag	UNP D3XFN7
D	-11	HIS	-	expression tag	UNP D3XFN7
D	-10	HIS	-	expression tag	UNP D3XFN7
D	-9	HIS	-	expression tag	UNP D3XFN7
D	-8	HIS	-	expression tag	UNP D3XFN7
D	-7	ALA	-	expression tag	UNP D3XFN7
D	-6	LEU	-	expression tag	UNP D3XFN7
D	-5	GLU	-	expression tag	UNP D3XFN7
D	-4	VAL	-	expression tag	UNP D3XFN7
D	-3	LEU	-	expression tag	UNP D3XFN7
D	-2	PHE	-	expression tag	UNP D3XFN7
D	-1	GLN	-	expression tag	UNP D3XFN7
D	0	GLY	-	expression tag	UNP D3XFN7
D	162	SER	CYS	engineered mutation	UNP D3XFN7
D	280	SER	CYS	engineered mutation	UNP D3XFN7

- Molecule 3 is a DNA chain called 38-MER DNA aptamer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			718	339	128	216	35			
3	F	38	Total	C	N	O	P	0	0	0
			777	369	140	231	37			

-
- The ORTEP diagram shows the chemical structure of 2-amino-9-(4-hydroxy-3-((2S,3S,4S)-3-hydroxy-4-oxo-4-phosphonobut-2-en-1-yl)-5-oxo-1H-imidazo[4,5-b]pyridin-6-yl)imidazole-4-carboxamide. The molecule is shown with its symmetry-related counterparts, with atoms labeled with their respective coordinates (x, y, z). The structure features a central imidazo[4,5-b]pyridine core, a 2-amino group, and a 4-oxo-4-phosphonobut-2-en-1-yl side chain. The phosphorus atom is bonded to four oxygen atoms, and the carboxamide group is also shown. The diagram includes labels for atoms such as N11, N12, N13, C2, C4, C6, C8, 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,

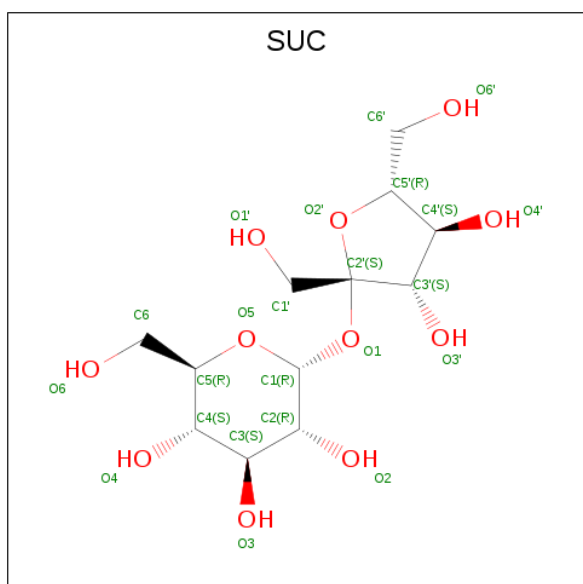
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		

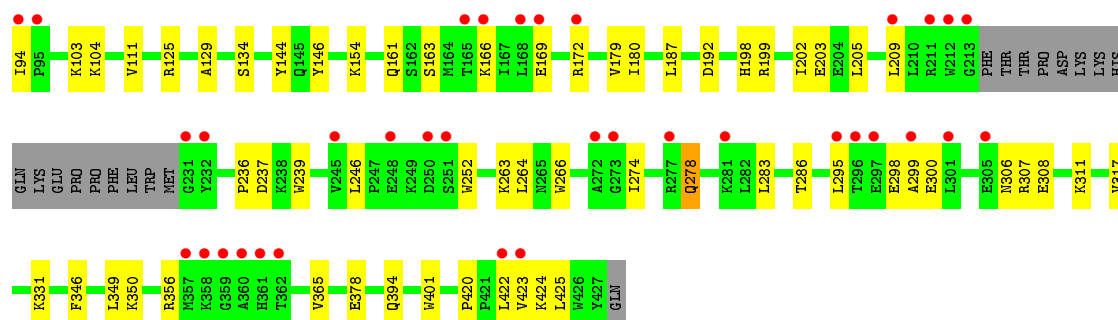
- Molecule 7 is SUCROSE (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



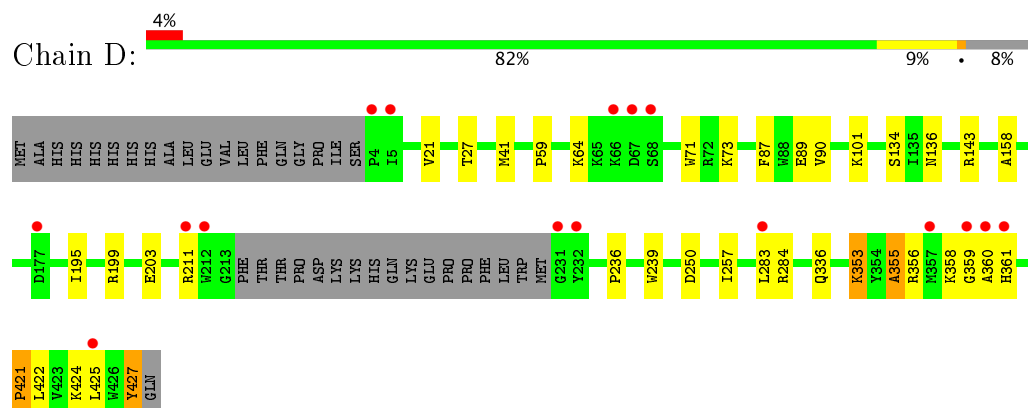
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			23	12	11		

- Molecule 8 is water.

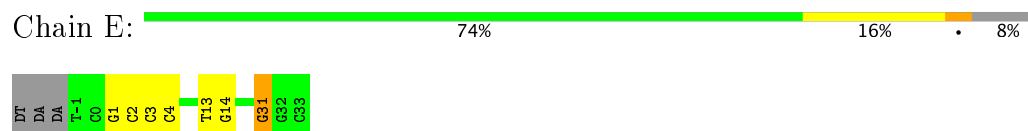
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	78	Total	O		0	0
			78	78			
8	B	28	Total	O		0	0
			28	28			
8	E	34	Total	O		0	0
			34	34			
8	C	56	Total	O		0	0
			56	56			
8	D	54	Total	O		0	0
			54	54			
8	F	19	Total	O		0	0
			19	19			



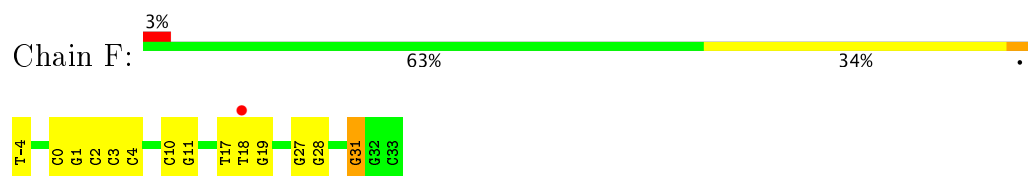
• Molecule 2: Pol protein



• Molecule 3: 38-MER DNA aptamer



• Molecule 3: 38-MER DNA aptamer



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	284.71 Å 284.71 Å 95.79 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.02 – 2.45 47.02 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.02-2.45) 99.9 (47.02-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.45 Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.188 , 0.227 0.186 , 0.226	Depositor DCC
R_{free} test set	5437 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17562	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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: OMC, GOL, MG, ET9, SUC

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	0.38	0/4608	0.54	0/6257
1	C	0.35	0/4600	0.52	1/6246 (0.0%)
2	B	0.37	0/3449	0.54	0/4684
2	D	0.34	0/3449	0.52	0/4684
3	E	0.77	0/756	0.96	1/1165 (0.1%)
3	F	0.77	1/823 (0.1%)	0.88	2/1269 (0.2%)
All	All	0.41	1/17685 (0.0%)	0.58	4/24305 (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	2
1	C	0	3
2	D	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	-4	DT	O3'-P	-6.56	1.53	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	31	DG	O4'-C4'-C3'	-5.95	102.12	104.50
1	C	51	GLY	C-N-CD	5.45	139.84	128.40
3	F	31	DG	O4'-C4'-C3'	-5.26	102.40	104.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	31	DG	C4'-C3'-C2'	-5.01	98.59	103.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	TRP	Peptide
1	A	68	SER	Peptide
1	C	135	ILE	Peptide
1	C	138	GLU	Peptide
1	C	448	ARG	Sidechain
2	D	355	ALA	Peptide
2	D	421	PRO	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	4488	0	4536	87	0
1	C	4483	0	4532	58	0
2	B	3354	0	3387	50	0
2	D	3354	0	3387	35	0
3	E	718	0	397	5	0
3	F	777	0	432	12	0
4	A	32	0	0	0	0
4	C	32	0	0	2	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	12	0	16	2	0
6	D	12	0	16	0	0
6	F	6	0	8	0	0
7	B	23	0	22	1	0
8	A	78	0	0	0	0
8	B	28	0	0	0	0
8	C	56	0	0	0	0
8	D	54	0	0	1	0
8	E	34	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	19	0	0	0	0
All	All	17562	0	16733	237	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 7.

All (237) 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:31:ILE:HB	1:A:132:ILE:HD11	1.18	1.09
1:A:24:TRP:CD1	1:A:25:PRO:HD3	2.11	0.86
1:C:450:THR:HG23	1:C:452:LEU:H	1.42	0.85
3:F:1:DG:H2'	3:F:2:OMC:C6	2.12	0.84
3:F:0:DC:H2''	3:F:1:DG:H5'	1.61	0.82
2:B:308:GLU:HA	2:B:311:LYS:HB2	1.61	0.81
2:B:394:GLN:HG2	6:B:501:GOL:H12	1.61	0.81
1:C:40:GLU:O	1:C:43:LYS:N	2.17	0.78
2:B:423:VAL:HB	2:B:425:LEU:CD1	2.15	0.77
1:C:195:ILE:O	1:C:199:ARG:HG3	1.86	0.76
1:C:136:ASN:O	1:C:138:GLU:N	2.19	0.74
1:A:31:ILE:HB	1:A:132:ILE:CD1	2.09	0.74
1:A:24:TRP:HD1	1:A:25:PRO:HD3	1.54	0.73
1:A:400:ALA:O	1:A:404:GLU:HG2	1.88	0.72
3:F:0:DC:C2'	3:F:1:DG:H5'	2.20	0.71
1:A:31:ILE:HD11	1:A:135:ILE:HA	1.72	0.71
1:A:31:ILE:CB	1:A:132:ILE:HD11	2.10	0.69
1:A:547:GLN:O	1:A:550:LYS:HB2	1.91	0.69
2:B:88:TRP:CD1	2:B:89:GLU:HG3	2.28	0.69
4:C:601:ET9:N2	3:F:0:DC:O2	2.25	0.69
1:A:34:LEU:HB3	1:A:132:ILE:HG13	1.75	0.69
2:B:423:VAL:HB	2:B:425:LEU:HD12	1.76	0.68
3:F:17:DT:H5''	3:F:17:DT:H6	1.58	0.67
2:D:422:LEU:N	2:D:422:LEU:HD22	2.09	0.67
1:C:372:VAL:HG11	1:C:411:ILE:HG23	1.77	0.66
2:D:90:VAL:HG11	2:D:158:ALA:HA	1.76	0.66
2:B:205:LEU:O	2:B:209:LEU:HD22	1.96	0.65
1:A:132:ILE:C	1:A:132:ILE:HD13	2.16	0.65
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.76	0.65
1:A:132:ILE:CG2	1:A:142:ILE:HB	2.28	0.64
1:C:134:SER:OG	1:C:135:ILE:N	2.30	0.64
2:B:350:LYS:NZ	2:B:378:GLU:OE2	2.27	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.81	0.62
1:A:543:GLY:HA2	2:B:283:LEU:O	1.99	0.62
3:F:3:DC:H2'	3:F:4:OMC:C6	2.35	0.62
1:A:131:THR:HG22	1:A:143:ARG:NE	2.14	0.62
1:A:193:LEU:HD13	1:A:197:GLN:HG3	1.80	0.61
1:A:132:ILE:HG23	1:A:142:ILE:HB	1.83	0.61
1:A:31:ILE:HA	1:A:34:LEU:HB2	1.83	0.61
1:A:131:THR:HG22	1:A:143:ARG:HE	1.64	0.61
2:B:394:GLN:CG	6:B:501:GOL:H12	2.32	0.60
2:B:163:SER:O	2:B:166:LYS:HG2	2.03	0.59
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.85	0.59
2:D:422:LEU:O	2:D:425:LEU:HD23	2.02	0.59
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.85	0.58
3:E:3:DC:H2'	3:E:4:OMC:C6	2.37	0.58
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.85	0.58
1:A:450:THR:HG22	1:A:452:LEU:HG	1.84	0.58
1:C:454:LYS:HB2	1:C:552:VAL:HG13	1.85	0.58
1:C:38:CYS:SG	1:C:132:ILE:HD11	2.44	0.58
1:C:284:ARG:HH12	1:C:357:MET:HE1	1.70	0.57
3:F:18:DT:H4'	3:F:19:DG:C8	2.39	0.57
2:B:252:TRP:CD1	2:B:295:LEU:HD21	2.40	0.57
1:C:60:VAL:HG12	1:C:75:VAL:HG22	1.87	0.56
1:A:24:TRP:HD1	1:A:25:PRO:CD	2.18	0.56
2:D:356:ARG:HA	2:D:361:HIS:CE1	2.41	0.56
2:B:172:ARG:HH11	2:B:180:ILE:HB	1.70	0.56
1:C:255:ASN:O	1:C:259:LYS:HG3	2.06	0.56
1:A:402:TRP:O	2:B:331:LYS:NZ	2.37	0.56
1:A:5:ILE:H	1:A:5:ILE:HD12	1.70	0.56
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.42	0.55
1:C:17:ASP:O	1:C:83:ARG:NH1	2.39	0.55
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.05	0.55
1:C:400:ALA:O	1:C:404:GLU:HG2	2.07	0.55
1:A:450:THR:O	1:A:451:LYS:HG2	2.06	0.55
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.87	0.55
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.87	0.55
2:D:421:PRO:C	2:D:422:LEU:HD22	2.27	0.55
1:A:276:VAL:HG22	1:A:353:LYS:HE2	1.89	0.55
4:C:601:ET9:N1	3:F:0:DC:N3	2.54	0.55
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.42	0.54
1:A:26:LEU:HD22	1:A:133:PRO:HG2	1.89	0.54
2:B:54:ASN:C	2:B:54:ASN:HD22	2.11	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ILE:HG22	1:C:64:LYS:H	1.72	0.54
2:D:421:PRO:HB3	2:D:424:LYS:HG3	1.88	0.53
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.38	0.53
1:A:450:THR:HG21	1:A:452:LEU:HB2	1.91	0.53
1:A:27:THR:HG22	1:A:29:GLU:N	2.24	0.53
1:C:125:ARG:HD3	1:C:147:ASN:HA	1.89	0.53
2:D:358:LYS:HB3	2:D:361:HIS:HB3	1.91	0.53
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.91	0.53
1:C:542:ILE:O	1:C:546:GLU:N	2.34	0.53
1:A:139:THR:HB	1:A:140:PRO:CD	2.38	0.53
2:B:199:ARG:O	2:B:203:GLU:HG2	2.10	0.52
1:C:447:ASN:OD1	1:C:449:GLU:N	2.38	0.52
2:B:278:GLN:HG2	2:B:299:ALA:N	2.25	0.52
1:A:447:ASN:HB3	1:A:450:THR:HB	1.90	0.52
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.90	0.52
1:C:440:PHE:HZ	1:C:463:ARG:HH21	1.58	0.52
2:D:421:PRO:HB3	2:D:424:LYS:HE2	1.92	0.52
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.90	0.52
2:B:266:TRP:CZ2	2:B:346:PHE:HE2	2.28	0.52
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.44	0.52
2:D:358:LYS:HE2	2:D:366:LYS:NZ	2.25	0.51
2:B:94:ILE:HG12	2:B:161:GLN:NE2	2.26	0.51
2:D:101:LYS:O	2:D:236:PRO:HB2	2.11	0.51
1:A:450:THR:HG22	1:A:452:LEU:CG	2.41	0.51
2:B:274:ILE:HG23	2:B:306:ASN:OD1	2.10	0.51
1:C:31:ILE:O	1:C:35:VAL:HG23	2.11	0.51
2:B:263:LYS:HB2	2:B:423:VAL:HG11	1.93	0.51
1:C:298:GLU:OE2	1:C:298:GLU:N	2.29	0.51
1:A:38:CYS:HB3	1:A:47:ILE:HD11	1.93	0.51
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.38	0.50
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.92	0.50
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.46	0.50
1:C:157:PRO:O	1:C:161:GLN:HG3	2.11	0.50
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.93	0.50
1:A:110[A]:ASP:HB2	1:A:220:LYS:HB3	1.93	0.50
1:A:23:GLN:HA	1:A:59:PRO:HB3	1.93	0.50
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.94	0.50
1:A:466:VAL:CG2	1:A:551:LEU:HG	2.42	0.49
1:A:450:THR:CG2	1:A:452:LEU:HB2	2.42	0.49
2:B:266:TRP:CE2	2:B:425:LEU:HD21	2.46	0.49
2:B:88:TRP:HD1	2:B:89:GLU:N	2.10	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ALA:O	1:C:37:ILE:HG22	2.12	0.49
1:A:135:ILE:HG13	1:A:136:ASN:OD1	2.12	0.48
2:B:125:ARG:HB3	2:B:146:TYR:O	2.13	0.48
2:B:54:ASN:HD22	2:B:55:PRO:N	2.12	0.48
1:A:26:LEU:HD22	1:A:133:PRO:CG	2.44	0.48
1:A:24:TRP:CD1	1:A:25:PRO:CD	2.91	0.48
1:A:31:ILE:O	1:A:35:VAL:HG23	2.14	0.48
1:A:541:GLY:HA2	1:A:546:GLU:HG3	1.96	0.48
1:C:130:PHE:CZ	1:C:144:TYR:HB2	2.49	0.48
3:F:1:DG:H2'	3:F:2:OMC:H6	1.75	0.48
1:A:466:VAL:HG21	1:A:551:LEU:HG	1.95	0.47
1:A:23:GLN:OE1	1:A:59:PRO:HA	2.14	0.47
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.48	0.47
2:D:336:GLN:HG3	2:D:427:TYR:OH	2.14	0.47
2:D:358:LYS:O	2:D:360:ALA:N	2.47	0.47
2:D:87:PHE:HB3	2:D:89:GLU:OE2	2.15	0.47
1:A:132:ILE:O	1:A:132:ILE:HG23	2.15	0.47
1:C:91:GLN:HB2	1:C:161:GLN:HE22	1.80	0.47
1:C:406:TRP:HB3	2:D:421:PRO:HG3	1.96	0.47
1:A:57:ASN:OD1	1:A:131:THR:HG23	2.14	0.46
1:A:132:ILE:N	1:A:142:ILE:O	2.42	0.46
2:B:88:TRP:NE1	2:B:89:GLU:HG3	2.29	0.46
1:C:450:THR:CG2	1:C:452:LEU:HB2	2.45	0.46
3:F:10:DC:H2''	3:F:11:DG:C8	2.50	0.46
1:A:27:THR:HB	1:A:30:LYS:HG3	1.98	0.46
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.51	0.46
1:A:266:TRP:CE2	3:E:31:DG:H4'	2.51	0.46
1:A:23:GLN:HG3	1:A:24:TRP:N	2.30	0.46
1:A:33:ALA:O	1:A:37:ILE:HG13	2.16	0.46
2:B:198:HIS:O	2:B:202:ILE:HG12	2.16	0.46
1:A:473:THR:O	1:A:477:THR:HG23	2.16	0.46
2:D:257:ILE:HG22	2:D:283:LEU:HD11	1.98	0.46
1:C:325:LEU:HD23	1:C:325:LEU:HA	1.77	0.46
1:C:380:ILE:HD12	2:D:27:THR:HG22	1.97	0.46
1:A:28:GLU:HG2	1:A:135:ILE:HD11	1.98	0.46
2:D:421:PRO:O	2:D:422:LEU:HD13	2.16	0.46
1:C:65:LYS:HG3	1:C:70:LYS:O	2.16	0.45
2:B:179:VAL:O	2:B:180:ILE:HD13	2.17	0.45
2:B:88:TRP:CD1	2:B:89:GLU:N	2.84	0.45
1:A:34:LEU:CB	1:A:132:ILE:HG13	2.44	0.45
1:A:40:GLU:O	1:A:44:GLU:HG3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TRP:NE1	2:B:425:LEU:HD21	2.31	0.45
1:C:451:LYS:N	1:C:451:LYS:HD3	2.32	0.45
1:A:34:LEU:HD11	1:A:60:VAL:HG11	1.99	0.45
2:B:111:VAL:HG11	2:B:187:LEU:HD12	1.98	0.45
1:C:516:GLU:O	1:C:520:GLN:HG3	2.17	0.45
2:B:278:GLN:CD	2:B:298:GLU:HB3	2.37	0.44
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.52	0.44
2:B:64:LYS:HD2	2:B:71:TRP:CZ2	2.53	0.44
1:C:448:ARG:O	1:C:451:LYS:NZ	2.31	0.44
1:C:22:LYS:HA	1:C:22:LYS:HD2	1.76	0.44
1:C:136:ASN:N	1:C:136:ASN:OD1	2.50	0.44
1:C:475:GLN:N	1:C:475:GLN:OE1	2.42	0.44
2:D:211:ARG:HG3	2:D:211:ARG:O	2.18	0.44
1:A:57:ASN:OD1	1:A:131:THR:N	2.48	0.44
1:A:56:TYR:O	1:A:143:ARG:NH2	2.50	0.44
3:E:1:DG:H2'	3:E:2:OMC:C6	2.52	0.44
1:C:266:TRP:CE2	3:F:31:DG:H4'	2.53	0.44
1:A:132:ILE:HD13	1:A:133:PRO:N	2.32	0.44
1:C:175:ASN:HB3	1:C:178:ILE:HG13	2.00	0.44
1:C:207:GLN:O	1:C:211:ARG:HG3	2.17	0.44
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.53	0.44
1:A:44:GLU:HB2	1:A:46:LYS:HG2	1.99	0.44
2:B:104:LYS:HB2	2:B:192:ASP:HA	2.00	0.44
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.99	0.44
1:A:22:LYS:HZ2	1:A:23:GLN:H	1.64	0.43
1:C:442:VAL:HB	1:C:481:ALA:HB1	2.00	0.43
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.53	0.43
1:C:136:ASN:C	1:C:138:GLU:N	2.72	0.43
1:C:406:TRP:CE3	2:D:421:PRO:HD3	2.53	0.43
1:A:22:LYS:NZ	1:A:23:GLN:H	2.16	0.43
1:A:173:LYS:HE2	1:A:173:LYS:HB2	1.62	0.43
2:B:103:LYS:HE3	2:B:179:VAL:CG2	2.48	0.43
1:C:202:ILE:O	1:C:206:ARG:HG3	2.19	0.43
2:D:163:SER:O	2:D:167:ILE:HG12	2.19	0.43
1:C:463:ARG:NH2	1:C:488:ASP:O	2.52	0.43
2:B:84:THR:HB	2:B:154:LYS:HE2	2.01	0.42
1:C:195:ILE:HD12	1:C:195:ILE:HA	1.85	0.42
2:D:195:ILE:O	2:D:199:ARG:HG3	2.19	0.42
2:D:355:ALA:HB1	2:D:356:ARG:HG3	2.01	0.42
1:C:326:ILE:CG2	1:C:390:LYS:HD2	2.49	0.42
2:D:64:LYS:HE3	2:D:71:TRP:CZ2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASN:OD1	1:A:130:PHE:HA	2.19	0.42
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.55	0.42
1:A:63:ILE:O	1:A:72:ARG:N	2.40	0.42
1:C:96:HIS:CG	1:C:97:PRO:HD2	2.54	0.42
2:D:358:LYS:HE3	2:D:358:LYS:HB3	1.81	0.42
2:D:361:HIS:HB2	8:D:643:HOH:O	2.20	0.42
3:E:13:DT:H2''	3:E:14:DG:C8	2.55	0.42
1:C:23:GLN:OE1	1:C:59:PRO:HA	2.20	0.42
2:D:422:LEU:N	2:D:422:LEU:CD2	2.80	0.42
2:B:103:LYS:HD3	2:B:103:LYS:HA	1.77	0.42
3:F:27:DG:H2'	3:F:28:DG:C8	2.55	0.42
1:A:33:ALA:O	1:A:36:GLU:HG2	2.20	0.42
2:D:353:LYS:HE2	2:D:427:TYR:CD1	2.55	0.42
1:A:429:LEU:HD11	1:A:506:ILE:HG22	2.02	0.41
2:B:172:ARG:NH1	2:B:180:ILE:HB	2.35	0.41
1:C:201:LYS:HA	1:C:201:LYS:HD3	1.76	0.41
2:D:143:ARG:HH11	2:D:143:ARG:HG2	1.84	0.41
1:A:404:GLU:H	1:A:404:GLU:HG2	1.71	0.41
2:B:129:ALA:HA	2:B:144:TYR:O	2.20	0.41
1:C:382:ILE:O	2:D:136:ASN:HB2	2.20	0.41
1:A:340:GLN:HE21	1:A:340:GLN:HB3	1.66	0.41
1:C:450:THR:HG23	1:C:452:LEU:HB2	2.02	0.41
1:A:447:ASN:HB3	1:A:450:THR:CB	2.51	0.41
2:B:278:GLN:HG2	2:B:298:GLU:C	2.41	0.41
1:A:19:PRO:HG3	1:A:80:LEU:HB2	2.03	0.41
3:E:4:OMC:H1'	3:E:4:OMC:HM23	1.93	0.41
2:D:236:PRO:HA	2:D:239:TRP:CD2	2.56	0.41
1:C:63:ILE:O	1:C:72:ARG:N	2.40	0.41
2:D:358:LYS:HE2	2:D:366:LYS:HZ2	1.86	0.41
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.56	0.40
2:B:54:ASN:ND2	2:B:56:TYR:H	2.20	0.40
2:B:79:GLU:OE1	7:B:503:SUC:O3	2.23	0.40
1:A:139:THR:HB	1:A:140:PRO:HD3	2.01	0.40
2:D:41:MET:SD	2:D:73:LYS:HE2	2.61	0.40
1:A:38:CYS:HB3	1:A:47:ILE:CD1	2.51	0.40
1:A:450:THR:O	1:A:451:LYS:CB	2.69	0.40
1:C:132:ILE:HD12	1:C:144:TYR:HE2	1.86	0.40
1:A:211:ARG:O	1:A:211:ARG:HD2	2.21	0.40
2:B:13:LYS:HB2	2:B:16:MET:HE3	2.04	0.40
1:C:136:ASN:C	1:C:138:GLU:H	2.16	0.40
1:C:363:ASN:HA	1:C:511:ASP:OD1	2.21	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	550/557 (99%)	531 (96%)	18 (3%)	1 (0%)	51	62
1	C	549/557 (99%)	524 (95%)	25 (5%)	0	100	100
2	B	403/444 (91%)	391 (97%)	11 (3%)	1 (0%)	51	62
2	D	403/444 (91%)	388 (96%)	14 (4%)	1 (0%)	51	62
All	All	1905/2002 (95%)	1834 (96%)	68 (4%)	3 (0%)	51	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	359	GLY
1	A	24	TRP
2	B	237	ASP

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	491/494 (99%)	481 (98%)	10 (2%)	60	74
1	C	490/494 (99%)	480 (98%)	10 (2%)	60	74
2	B	366/400 (92%)	354 (97%)	12 (3%)	43	58
2	D	366/400 (92%)	360 (98%)	6 (2%)	68	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1713/1788 (96%)	1675 (98%)	38 (2%)	57 71

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	126	LYS
1	A	132	ILE
1	A	136	ASN
1	A	221	HIS
1	A	334	GLN
1	A	340	GLN
1	A	356	ARG
1	A	451	LYS
1	A	503	LEU
2	B	54	ASN
2	B	65	LYS
2	B	70	LYS
2	B	88	TRP
2	B	134	SER
2	B	169	GLU
2	B	278	GLN
2	B	300	GLU
2	B	307	ARG
2	B	356	ARG
2	B	422	LEU
2	B	424	LYS
1	C	42	GLU
1	C	64	LYS
1	C	83	ARG
1	C	136	ASN
1	C	191	SER
1	C	277	ARG
1	C	283	LEU
1	C	287	LYS
1	C	390	LYS
1	C	503	LEU
2	D	134	SER
2	D	203	GLU
2	D	250	ASP
2	D	284	ARG
2	D	353	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	427	TYR

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

Mol	Chain	Res	Type
1	A	334	GLN
1	A	464	GLN
2	B	54	ASN
2	B	137	ASN
2	B	161	GLN
1	C	161	GLN
1	C	221	HIS
1	C	265	ASN
2	D	182	GLN
2	D	336	GLN
2	D	361	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	E	2	3	15,22,23	4.66	10 (66%)	19,31,34	1.05	0
3	OMC	E	4	3	15,22,23	3.02	5 (33%)	19,31,34	0.63	0
3	OMC	F	2	3	15,22,23	4.62	10 (66%)	19,31,34	1.05	1 (5%)
3	OMC	F	4	3	15,22,23	3.04	5 (33%)	19,31,34	0.77	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
3	OMC	E	2	3	-	0/5/27/28	0/2/2/2
3	OMC	E	4	3	-	0/5/27/28	0/2/2/2
3	OMC	F	2	3	-	0/5/27/28	0/2/2/2
3	OMC	F	4	3	-	0/5/27/28	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	OMC	O4'-C1'	-9.04	1.28	1.41
3	F	2	OMC	O4'-C1'	-8.77	1.29	1.41
3	F	2	OMC	C3'-C4'	-8.00	1.32	1.53
3	E	2	OMC	C3'-C4'	-7.79	1.32	1.53
3	F	2	OMC	O5'-C5'	-6.23	1.36	1.44
3	E	2	OMC	O5'-C5'	-5.72	1.36	1.44
3	F	2	OMC	O2'-C2'	-3.29	1.33	1.42
3	E	2	OMC	O2'-C2'	-3.21	1.34	1.42
3	F	2	OMC	C5-C4	2.23	1.46	1.41
3	E	2	OMC	C5-C4	2.49	1.47	1.41
3	F	4	OMC	C5-C4	3.04	1.48	1.41
3	E	4	OMC	C5-C4	3.19	1.49	1.41
3	F	2	OMC	C2-N3	3.70	1.45	1.38
3	F	2	OMC	C4-N3	3.75	1.41	1.35
3	E	2	OMC	C2-N3	3.80	1.45	1.38
3	F	2	OMC	C6-C5	3.97	1.46	1.38
3	E	2	OMC	C4-N3	4.04	1.42	1.35
3	E	2	OMC	C6-C5	4.11	1.46	1.38
3	E	4	OMC	C4-N3	4.70	1.43	1.35
3	E	4	OMC	C6-C5	4.86	1.48	1.38
3	E	4	OMC	C2-N3	4.93	1.47	1.38
3	F	4	OMC	C2-N3	5.01	1.48	1.38
3	F	4	OMC	C4-N3	5.08	1.44	1.35
3	F	4	OMC	C6-C5	5.08	1.49	1.38
3	F	2	OMC	C6-N1	5.96	1.43	1.35
3	E	2	OMC	C6-N1	6.22	1.44	1.35
3	F	2	OMC	O4'-C4'	6.28	1.59	1.45
3	E	2	OMC	O4'-C4'	6.39	1.59	1.45
3	F	4	OMC	C6-N1	6.78	1.45	1.35
3	E	4	OMC	C6-N1	7.04	1.45	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	OMC	C4'-O4'-C1'	-3.09	106.48	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	OMC	1	0
3	E	4	OMC	2	0
3	F	2	OMC	2	0
3	F	4	OMC	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
4	ET9	A	601	5	26,34,34	1.30	1 (3%)	19,54,54	2.39	8 (42%)
6	GOL	B	501	-	5,5,5	0.34	0	5,5,5	0.68	0
6	GOL	B	502	-	5,5,5	0.42	0	5,5,5	0.29	0
7	SUC	B	503	-	24,24,24	0.43	0	36,36,36	0.60	0
4	ET9	C	601	5	26,34,34	1.18	3 (11%)	19,54,54	2.38	8 (42%)
6	GOL	D	501	-	5,5,5	0.31	0	5,5,5	0.55	0
6	GOL	D	502	-	5,5,5	0.44	0	5,5,5	0.48	0
6	GOL	F	101	-	5,5,5	0.29	0	5,5,5	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
4	ET9	A	601	5	-	0/18/38/38	0/3/3/3
6	GOL	B	501	-	-	0/4/4/4	0/0/0/0
6	GOL	B	502	-	-	0/4/4/4	0/0/0/0
7	SUC	B	503	-	-	0/12/51/51	0/2/2/2
4	ET9	C	601	5	-	0/18/38/38	0/3/3/3
6	GOL	D	501	-	-	0/4/4/4	0/0/0/0
6	GOL	D	502	-	-	0/4/4/4	0/0/0/0
6	GOL	F	101	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	ET9	C2'-C1'	-2.35	1.51	1.54
4	C	601	ET9	C5-C4	2.12	1.45	1.40
4	C	601	ET9	C6-C5	2.87	1.46	1.41
4	A	601	ET9	C6-C5	3.24	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	ET9	C4-C5-N7	-4.14	105.41	109.41
4	A	601	ET9	C6-C5-C4	-3.82	117.05	120.84
4	C	601	ET9	C5-C6-N1	-3.76	118.12	123.48
4	A	601	ET9	C5-C6-N1	-3.67	118.26	123.48
4	C	601	ET9	C4-C5-N7	-3.23	106.29	109.41
4	C	601	ET9	C4'-C6'-C44	-3.14	121.77	127.90
4	C	601	ET9	C6-C5-C4	-3.10	117.76	120.84
4	C	601	ET9	N3-C2-N1	-2.68	123.55	127.46
4	A	601	ET9	N3-C2-N1	-2.55	123.74	127.46
4	A	601	ET9	C4'-C6'-C44	-2.40	123.23	127.90
4	A	601	ET9	C3'-C2'-C1'	2.52	107.26	104.00
4	C	601	ET9	C3'-C2'-C1'	3.78	108.89	104.00
4	A	601	ET9	C6-N1-C2	3.90	121.66	116.06
4	C	601	ET9	C6-N1-C2	3.92	121.70	116.06
4	C	601	ET9	C2-N3-C4	4.91	120.89	115.16
4	A	601	ET9	C2-N3-C4	5.09	121.10	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	GOL	2	0
7	B	503	SUC	1	0
4	C	601	ET9	2	0

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	551/557 (98%)	0.15	31 (5%) 25 22	26, 48, 92, 175	0
1	C	551/557 (98%)	0.34	54 (9%) 8 6	29, 56, 111, 166	0
2	B	407/444 (91%)	0.74	53 (13%) 4 3	30, 65, 118, 164	0
2	D	407/444 (91%)	0.10	17 (4%) 37 34	29, 53, 94, 150	0
3	E	33/38 (86%)	-0.38	0 100 100	27, 43, 78, 117	0
3	F	36/38 (94%)	-0.28	1 (2%) 53 49	33, 57, 113, 148	0
All	All	1985/2078 (95%)	0.30	156 (7%) 13 11	26, 54, 110, 175	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4	PRO	12.3
2	D	67	ASP	9.8
2	B	301	LEU	9.7
2	B	92	LEU	8.7
2	B	88	TRP	8.7
1	C	138	GLU	8.0
1	A	69	THR	7.9
1	C	133	PRO	7.7
1	C	34	LEU	7.5
1	A	34	LEU	7.2
2	D	360	ALA	6.6
2	B	94	ILE	6.6
1	A	137	ASN	6.5
2	B	212	TRP	6.5
2	D	4	PRO	6.5
2	B	360	ALA	6.3
1	A	136	ASN	6.3
1	C	132	ILE	6.3
2	B	5	ILE	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	93	GLY	6.2
1	C	135	ILE	6.2
1	A	139	THR	6.1
2	B	209	LEU	6.1
1	A	66	LYS	5.9
1	A	68	SER	5.9
2	B	359	GLY	5.8
2	B	91	GLN	5.7
1	C	67	ASP	5.6
2	B	90	VAL	5.6
2	B	361	HIS	5.6
1	C	141	GLY	5.5
1	C	62	ALA	5.5
1	C	50	ILE	5.5
1	C	142	ILE	5.3
1	A	141	GLY	5.1
2	B	232	TYR	5.1
1	C	69	THR	5.0
1	C	28	GLU	4.9
1	A	140	PRO	4.9
2	B	213	GLY	4.7
2	D	231	GLY	4.7
1	A	67	ASP	4.6
1	C	35	VAL	4.4
1	A	25	PRO	4.4
1	C	140	PRO	4.4
2	D	232	TYR	4.3
1	A	62	ALA	4.3
2	B	89	GLU	4.3
1	A	61	PHE	4.2
1	C	51	GLY	4.2
1	C	452	LEU	4.1
1	C	68	SER	4.1
1	A	32	LYS	4.1
1	C	32	LYS	4.1
2	B	231	GLY	4.0
2	B	168	LEU	4.0
1	C	139	THR	4.0
2	B	95	PRO	4.0
1	C	551	LEU	4.0
2	B	295	LEU	3.9
2	B	7	THR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	37	ILE	3.8
2	D	212	TRP	3.8
1	C	71	TRP	3.7
1	A	63	ILE	3.7
1	C	553	SER	3.7
2	B	68	SER	3.7
2	B	357	MET	3.6
1	C	52	PRO	3.6
1	A	64	LYS	3.6
2	B	305	GLU	3.6
1	C	144	TYR	3.6
2	D	5	ILE	3.5
2	D	66	LYS	3.5
2	B	67	ASP	3.5
2	D	359	GLY	3.4
2	B	423	VAL	3.4
1	A	26	LEU	3.3
1	C	70	LYS	3.3
2	B	250	ASP	3.3
1	C	26	LEU	3.3
2	B	297	GLU	3.3
1	A	60	VAL	3.3
1	A	132	ILE	3.3
2	D	361	HIS	3.2
1	C	33	ALA	3.2
2	D	68	SER	3.2
1	C	39	THR	3.1
1	A	134	SER	3.1
2	B	6	GLU	3.1
2	D	283	LEU	3.1
2	B	245	VAL	3.1
1	A	27	THR	3.1
2	B	172	ARG	3.1
1	C	49	LYS	3.0
1	A	71	TRP	2.9
1	A	35	VAL	2.9
2	B	87	PHE	2.9
1	C	66	LYS	2.8
1	A	131	THR	2.8
1	C	552	VAL	2.8
2	B	272	ALA	2.7
1	C	136	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	24	TRP	2.7
1	C	65	LYS	2.7
2	D	357	MET	2.7
2	B	281	LYS	2.7
2	B	277	ARG	2.6
2	B	299	ALA	2.6
1	A	24	TRP	2.6
1	C	15	GLY	2.6
1	C	134	SER	2.5
1	C	544	GLY	2.5
1	C	469	LEU	2.5
1	C	550	LYS	2.5
1	C	36	GLU	2.5
2	B	8	VAL	2.4
1	A	142	ILE	2.4
2	B	362	THR	2.4
3	F	18	DT	2.4
1	C	29	GLU	2.4
2	B	422	LEU	2.4
2	D	177	ASP	2.4
2	B	166	LYS	2.4
1	A	133	PRO	2.4
1	A	29	GLU	2.4
1	C	450	THR	2.3
1	C	59	PRO	2.3
1	A	65	LYS	2.3
2	B	251	SER	2.3
2	D	174	GLN	2.3
1	C	448	ARG	2.3
1	C	54	ASN	2.3
2	B	211	ARG	2.3
2	D	211	ARG	2.3
1	C	547	GLN	2.3
2	B	169	GLU	2.3
2	B	296	THR	2.3
1	C	143	ARG	2.2
2	B	9	PRO	2.2
2	B	10	VAL	2.2
2	B	248	GLU	2.2
2	B	66	LYS	2.2
1	C	457	TYR	2.2
2	B	165	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	138	GLU	2.1
1	C	30	LYS	2.1
1	C	131	THR	2.1
1	C	128	THR	2.1
1	C	449	GLU	2.1
2	B	358	LYS	2.1
1	A	36	GLU	2.1
2	B	273	GLY	2.1
1	C	63	ILE	2.0
2	B	11	LYS	2.0
2	D	425	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	OMC	F	2	21/22	0.97	0.16	-	45,49,56,59	0
3	OMC	E	2	21/22	0.97	0.17	-	27,33,40,44	0
3	OMC	E	4	21/22	0.99	0.18	-	26,29,33,34	0
3	OMC	F	4	21/22	0.98	0.19	-	30,35,40,41	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
6	GOL	D	502	6/6	0.92	0.20	3.73	40,44,53,55	0
6	GOL	F	101	6/6	0.88	0.23	3.42	54,60,62,67	0
6	GOL	B	501	6/6	0.86	0.24	1.75	41,47,51,58	0
7	SUC	B	503	23/23	0.81	0.24	1.56	47,84,103,105	0
6	GOL	B	502	6/6	0.95	0.23	1.41	40,46,48,51	0
6	GOL	D	501	6/6	0.93	0.18	0.05	40,44,44,46	0
4	ET9	A	601	32/32	0.90	0.18	-0.16	47,56,72,73	0
4	ET9	C	601	32/32	0.91	0.14	-0.55	62,67,84,86	0
5	MG	A	602	1/1	0.82	0.11	-1.65	32,32,32,32	1
5	MG	C	602	1/1	0.89	0.11	-3.45	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.