



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:40 PM GMT

PDB ID : 3W2U
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with MII-3-193
Authors : Inaoka, D.K.; Iida, M.; Tabuchi, T.; Lee, N.; Matsuoka, S.; Shiba, T.; Sakamoto, K.; Suzuki, S.; Balogun, E.O.; Nara, T.; Aoki, T.; Inoue, M.; Honma, T.; Tanaka, A.; Harada, S.; Kita, K.
Deposited on : 2012-12-05
Resolution : 2.25 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20026982

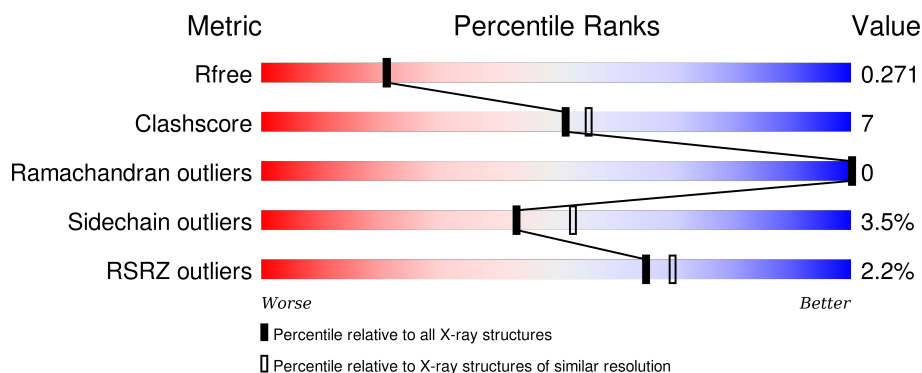
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

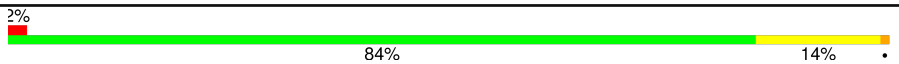
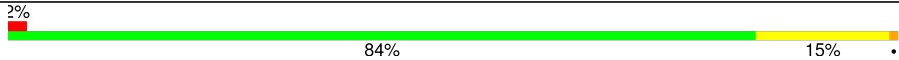
The reported resolution of this entry is 2.25 Å.

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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	313	
1	B	313	

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
3	GOL	A	402	-	-	-	X
3	GOL	A	404	-	-	-	X
3	GOL	A	406	-	-	-	X
3	GOL	A	407	-	-	-	X
3	GOL	A	409	-	-	-	X
3	GOL	A	410	-	-	-	X
3	GOL	A	411	-	-	-	X

2 Entry composition [i](#)

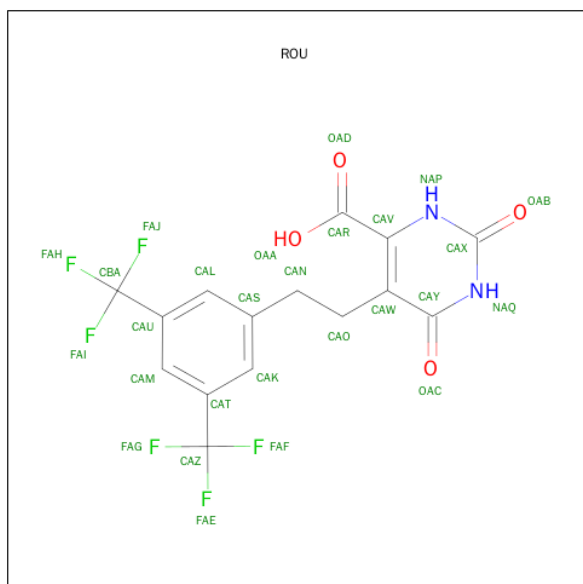
There are 6 unique types of molecules in this entry. The entry contains 5312 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydroorotate dehydrogenase (fumarate).

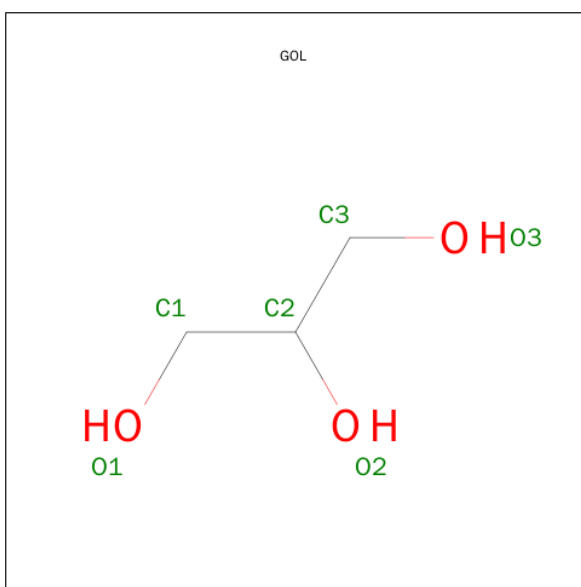
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2388	1530	396	444	18			
1	B	313	Total	C	N	O	S	0	0	0
			2388	1530	396	444	18			

- Molecule 2 is 5-{2-[3,5-BIS(TRIFLUOROMETHYL)PHENYL]ETHYL}-2,6-DIOXO-1,2,3,6-TETRAHYDOPYRIMIDINE-4-CARBOXYLIC ACID (three-letter code: ROU) (formula: C₁₅H₁₀F₆N₂O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			27	15	6	2	4		
2	B	1	Total	C	F	N	O	0	0
			27	15	6	2	4		

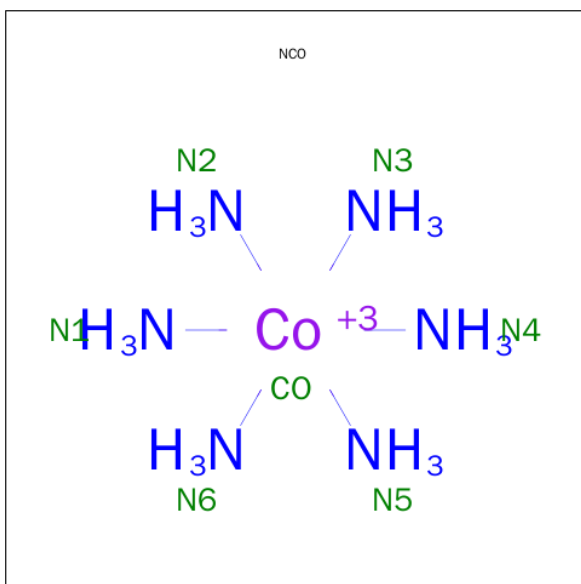
- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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- The chemical structure of FMN (Flavin Mononucleotide) is shown. It consists of an isoalloxazine ring system (a fused bicyclic system with two nitrogen atoms) and a ribityl side chain. The ribityl side chain is attached to the ring at the C10 position. The side chain consists of a ribose ring (C3', C4', C5') and a phosphate group (O1P, O2P, O3P, O4'). The ribose ring is shown in a chair conformation. The phosphate group is shown as a tetrahedral structure. The structure is labeled with atom names and numbers, including 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, C803, C804, C805,

- Molecule 5 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: $\text{CoH}_{18}\text{N}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 7	Co 1	N 6	0	0

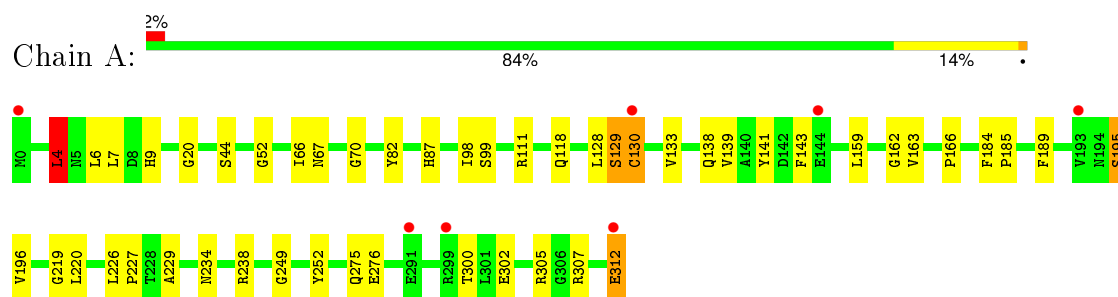
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	166	Total 166	O 166	0	0
6	B	163	Total 163	O 163	0	0

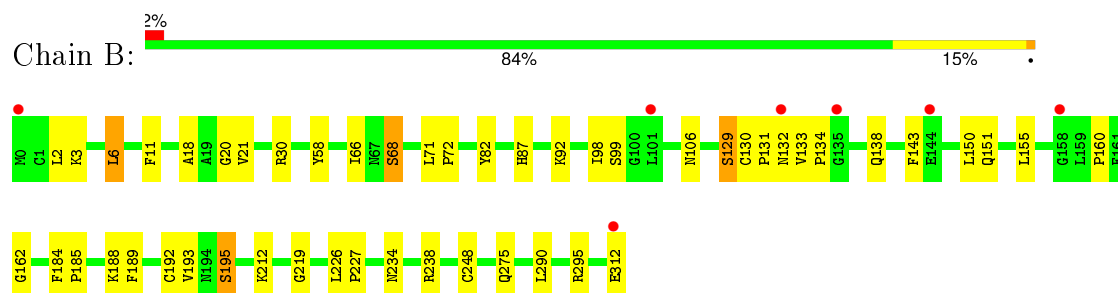
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Dihydroorotate dehydrogenase (fumarate)



- Molecule 1: Dihydroorotate dehydrogenase (fumarate)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.22Å 71.67Å 129.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.51 – 2.25 36.51 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (36.51-2.25) 99.6 (36.51-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.05 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.205 , 0.270 0.211 , 0.271	Depositor DCC
R_{free} test set	1562 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.1	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	6 of 30947 reflections (0.019%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5312	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 42.79 % 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 1.9375e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FMN, GOL, ROU, NCO

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	0.90	1/2440 (0.0%)	0.90	3/3305 (0.1%)
1	B	0.88	1/2440 (0.0%)	0.91	3/3305 (0.1%)
All	All	0.89	2/4880 (0.0%)	0.91	6/6610 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	GLU	C-O	-6.60	1.10	1.23
1	B	58	TYR	CB-CG	5.19	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	307	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	B	295	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	4	LEU	CA-CB-CG	5.56	128.09	115.30
1	B	68	SER	CB-CA-C	5.19	119.95	110.10
1	B	30	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2391	36	0
1	B	2388	0	2391	31	0
2	A	27	0	9	1	0
2	B	27	0	9	1	0
3	A	72	0	96	7	0
3	B	12	0	16	0	0
4	A	31	0	19	1	0
4	B	31	0	19	4	0
5	A	7	0	0	0	0
6	A	166	0	0	3	0
6	B	163	0	0	0	0
All	All	5312	0	4950	67	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 (67) 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:7:LEU:O	1:A:9:HIS:HD2	1.57	0.86
1:A:7:LEU:O	1:A:9:HIS:CD2	2.42	0.73
1:B:20:GLY:HA3	4:B:404:FMN:N5	2.06	0.70
1:B:98:ILE:CD1	1:B:106:ASN:OD1	2.40	0.70
1:B:129:SER:HA	1:B:138:GLN:NE2	2.06	0.69
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.43	0.64
1:B:20:GLY:HA3	4:B:404:FMN:C5A	2.28	0.63
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.84	0.60
1:A:118:GLN:CG	1:A:159:LEU:HD11	2.31	0.60
1:A:129:SER:HB2	6:A:649:HOH:O	2.01	0.59
1:B:162:GLY:HA3	1:B:189:PHE:CZ	2.37	0.59
1:B:98:ILE:HD12	1:B:106:ASN:OD1	2.04	0.57
1:B:66:ILE:HA	1:B:219:GLY:O	2.07	0.54
1:A:44:SER:HB3	1:A:99:SER:HB2	1.89	0.53
1:B:162:GLY:HA3	1:B:189:PHE:CE2	2.43	0.53
1:A:129:SER:O	1:A:130:CYS:C	2.47	0.52
1:A:129:SER:CB	6:A:649:HOH:O	2.58	0.52
1:A:118:GLN:HG2	1:A:159:LEU:HD11	1.91	0.52
1:A:129:SER:HA	1:A:138:GLN:NE2	2.25	0.51
1:A:226:LEU:HB3	1:A:227:PRO:HD3	1.92	0.51
1:B:160:PRO:HB3	1:B:188:LYS:HG3	1.92	0.51
1:A:128:LEU:HD12	1:A:163:VAL:HG11	1.92	0.50
1:A:128:LEU:HG	1:A:163:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TYR:HB3	3:A:413:GOL:H2	1.93	0.50
1:B:133:VAL:HG12	1:B:134:PRO:O	2.12	0.50
1:B:2:LEU:HG	1:B:290:LEU:HD21	1.93	0.49
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.11	0.49
1:B:226:LEU:HB3	1:B:227:PRO:HD3	1.95	0.49
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.60	0.49
1:A:143:PHE:HB2	3:A:412:GOL:C1	2.42	0.48
1:B:195:SER:OG	2:B:401:ROU:OAB	2.31	0.48
1:B:131:PRO:HA	1:B:138:GLN:HA	1.96	0.48
1:A:312:GLU:OE2	1:A:312:GLU:N	2.46	0.48
1:A:143:PHE:HB2	3:A:412:GOL:H11	1.96	0.47
1:B:87:HIS:HE1	1:B:92:LYS:O	1.97	0.47
1:B:162:GLY:HA3	1:B:189:PHE:CE1	2.49	0.47
1:A:300:THR:HB	1:A:302:GLU:OE1	2.14	0.47
1:B:99:SER:OG	1:B:130:CYS:SG	2.72	0.47
3:A:408:GOL:H11	1:B:143:PHE:CE2	2.50	0.46
1:A:312:GLU:HB2	1:B:212:LYS:HE3	1.96	0.46
1:B:21:VAL:HG13	1:B:275:GLN:HE21	1.79	0.46
1:A:196:VAL:HB	1:A:220:LEU:HB2	1.98	0.46
1:B:82:TYR:CE2	1:B:87:HIS:HB2	2.52	0.45
2:A:401:ROU:H5	2:A:401:ROU:OAA	2.15	0.45
1:A:20:GLY:HA3	4:A:414:FMN:N5	2.31	0.45
1:A:82:TYR:CE2	1:A:87:HIS:HB2	2.52	0.45
1:B:18:ALA:HB1	4:B:404:FMN:O2'	2.18	0.44
1:A:138:GLN:HE22	1:A:166:PRO:HB3	1.82	0.43
1:A:66:ILE:HA	1:A:219:GLY:O	2.18	0.43
1:A:111:ARG:CD	3:A:409:GOL:O1	2.66	0.43
1:A:52:GLY:HA2	1:A:70:GLY:O	2.19	0.43
1:A:4:LEU:HD12	1:A:6:LEU:CD2	2.49	0.43
1:B:71:LEU:N	1:B:72:PRO:CD	2.82	0.42
1:A:118:GLN:HG3	1:A:159:LEU:HD11	2.00	0.42
1:A:130:CYS:O	1:A:139:VAL:HG23	2.19	0.42
1:A:195:SER:HB3	6:A:664:HOH:O	2.19	0.42
1:B:6:LEU:HD12	1:B:11:PHE:CE1	2.55	0.41
1:A:275:GLN:HE22	3:A:410:GOL:C1	2.34	0.41
1:B:129:SER:HA	1:B:138:GLN:HE22	1.84	0.41
1:B:184:PHE:HA	1:B:185:PRO:HD2	1.95	0.41
1:A:141:TYR:HB3	3:A:407:GOL:H2	2.02	0.41
1:B:192:CYS:HA	1:B:193:VAL:HA	1.79	0.41
1:B:248:CYS:SG	4:B:404:FMN:H3'	2.61	0.40
1:A:229:ALA:CB	1:A:249:GLY:HA3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLY:HA3	1:A:189:PHE:CE1	2.56	0.40
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.20	0.40
1:A:184:PHE:HA	1:A:185:PRO:HD2	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	311/313 (99%)	299 (96%)	12 (4%)	0	100	100
1	B	311/313 (99%)	301 (97%)	10 (3%)	0	100	100
All	All	622/626 (99%)	600 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/258 (100%)	250 (97%)	8 (3%)	47	58
1	B	258/258 (100%)	248 (96%)	10 (4%)	39	48
All	All	516/516 (100%)	498 (96%)	18 (4%)	43	53

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	67	ASN
1	A	98	ILE
1	A	129	SER
1	A	130	CYS
1	A	133	VAL
1	A	195	SER
1	A	312	GLU
1	B	3	LYS
1	B	6	LEU
1	B	68	SER
1	B	129	SER
1	B	132	ASN
1	B	150	LEU
1	B	151	GLN
1	B	155	LEU
1	B	195	SER
1	B	312	GLU

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	9	HIS
1	A	87	HIS
1	A	138	GLN
1	A	234	ASN
1	A	275	GLN
1	B	9	HIS
1	B	87	HIS
1	B	138	GLN
1	B	152	GLN
1	B	234	ASN
1	B	275	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ROU	A	401	-	23,28,28	3.33	11 (47%)	30,43,43	2.26	4 (13%)
3	GOL	A	402	-	5,5,5	0.52	0	5,5,5	0.78	0
3	GOL	A	403	-	5,5,5	0.31	0	5,5,5	0.82	0
3	GOL	A	404	-	5,5,5	0.52	0	5,5,5	0.45	0
3	GOL	A	405	-	5,5,5	0.17	0	5,5,5	0.19	0
3	GOL	A	406	-	5,5,5	0.52	0	5,5,5	0.85	0
3	GOL	A	407	-	5,5,5	0.50	0	5,5,5	0.67	0
3	GOL	A	408	-	5,5,5	0.54	0	5,5,5	0.69	0
3	GOL	A	409	-	5,5,5	0.30	0	5,5,5	0.59	0
3	GOL	A	410	-	5,5,5	0.61	0	5,5,5	0.68	0
3	GOL	A	411	-	5,5,5	0.59	0	5,5,5	0.63	0
3	GOL	A	412	-	5,5,5	0.21	0	5,5,5	0.49	0
3	GOL	A	413	-	5,5,5	0.50	0	5,5,5	0.34	0
4	FMN	A	414	-	32,33,33	1.43	6 (18%)	34,50,50	2.52	11 (32%)
5	NCO	A	415	-	6,6,6	1.50	1 (16%)	0,15,15	0.00	-
2	ROU	B	401	-	23,28,28	2.72	8 (34%)	30,43,43	2.16	7 (23%)
3	GOL	B	402	-	5,5,5	0.42	0	5,5,5	0.91	0
3	GOL	B	403	-	5,5,5	0.33	0	5,5,5	0.32	0
4	FMN	B	404	-	32,33,33	1.58	4 (12%)	34,50,50	3.06	9 (26%)

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	ROU	A	401	-	-	0/17/21/21	0/2/2/2
3	GOL	A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	A	404	-	-	0/4/4/4	0/0/0/0
3	GOL	A	405	-	-	0/4/4/4	0/0/0/0
3	GOL	A	406	-	-	0/4/4/4	0/0/0/0
3	GOL	A	407	-	-	0/4/4/4	0/0/0/0
3	GOL	A	408	-	-	0/4/4/4	0/0/0/0
3	GOL	A	409	-	-	0/4/4/4	0/0/0/0
3	GOL	A	410	-	-	0/4/4/4	0/0/0/0
3	GOL	A	411	-	-	0/4/4/4	0/0/0/0
3	GOL	A	412	-	-	0/4/4/4	0/0/0/0
3	GOL	A	413	-	-	0/4/4/4	0/0/0/0
4	FMN	A	414	-	-	0/18/18/18	0/3/3/3
5	NCO	A	415	-	-	0/0/0/0	0/0/0/0
2	ROU	B	401	-	-	0/17/21/21	0/2/2/2
3	GOL	B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	B	403	-	-	0/4/4/4	0/0/0/0
4	FMN	B	404	-	-	0/18/18/18	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ROU	CAO-CAW	-10.92	1.37	1.52
2	B	401	ROU	CAO-CAW	-7.35	1.42	1.52
2	A	401	ROU	FAE-CAZ	-6.34	1.09	1.32
2	A	401	ROU	CAN-CAS	-4.06	1.39	1.51
2	B	401	ROU	CAN-CAS	-3.55	1.41	1.51
4	A	414	FMN	C2-N3	-2.61	1.32	1.38
2	B	401	ROU	CBA-CAU	-2.50	1.44	1.49
2	A	401	ROU	CAZ-CAT	-2.40	1.44	1.49
2	A	401	ROU	FAF-CAZ	-2.19	1.24	1.32
2	A	401	ROU	CBA-CAU	-2.11	1.45	1.49
4	A	414	FMN	P-O5'	2.12	1.66	1.59
2	A	401	ROU	FAI-CBA	2.21	1.40	1.32
4	A	414	FMN	C4-C4A	2.37	1.46	1.41
4	B	404	FMN	C4-C4A	2.51	1.46	1.41
2	A	401	ROU	FAJ-CBA	2.54	1.42	1.32
2	B	401	ROU	FAH-CBA	2.70	1.42	1.32
4	A	414	FMN	C8-C7	2.72	1.48	1.41
2	B	401	ROU	FAJ-CBA	2.77	1.42	1.32
2	A	401	ROU	CAV-NAP	2.84	1.39	1.34
4	A	414	FMN	C9A-C5A	2.94	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	404	FMN	C8-C7	3.07	1.49	1.41
5	A	415	NCO	CO-N5	3.20	2.08	1.96
4	A	414	FMN	C4A-C10	3.23	1.46	1.40
2	B	401	ROU	CAY-NAQ	3.46	1.39	1.33
2	B	401	ROU	CAV-NAP	3.86	1.40	1.34
4	B	404	FMN	C9A-C5A	3.95	1.50	1.42
2	A	401	ROU	FAH-CBA	4.16	1.47	1.32
2	A	401	ROU	CAY-NAQ	4.29	1.40	1.33
4	B	404	FMN	C4A-C10	5.16	1.50	1.40
2	B	401	ROU	FAI-CBA	6.18	1.55	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	FMN	C4-C4A-C10	-5.95	116.14	119.94
4	B	404	FMN	C4A-C4-N3	-5.68	116.10	123.52
2	A	401	ROU	NAQ-CAX-NAP	-5.28	118.80	127.69
4	A	414	FMN	C4-C4A-C10	-4.93	116.78	119.94
2	B	401	ROU	NAQ-CAX-NAP	-4.64	119.87	127.69
4	A	414	FMN	C4A-C4-N3	-4.57	117.55	123.52
4	B	404	FMN	O2P-P-O5'	-3.34	96.98	106.72
4	B	404	FMN	N3-C2-N1	-3.22	122.27	127.69
4	A	414	FMN	N3-C2-N1	-2.95	122.72	127.69
2	B	401	ROU	FAJ-CBA-CAU	-2.90	106.80	112.92
4	B	404	FMN	C4A-C10-N10	-2.36	118.81	120.52
4	A	414	FMN	C4A-C10-N10	-2.33	118.83	120.52
4	A	414	FMN	O5'-P-O1P	-2.15	101.69	107.08
4	A	414	FMN	O4'-C4'-C5'	-2.09	105.53	110.09
2	B	401	ROU	FAH-CBA-CAU	-2.03	108.63	112.92
2	B	401	ROU	CAM-CAT-CAZ	2.15	122.46	119.58
2	B	401	ROU	CAT-CAK-CAS	2.22	123.84	121.33
4	A	414	FMN	O2P-P-O1P	2.31	118.16	110.63
2	A	401	ROU	CAM-CAT-CAZ	2.46	122.88	119.58
4	A	414	FMN	O3P-P-O1P	2.54	118.91	110.63
4	A	414	FMN	C1'-N10-C9A	2.73	122.00	118.83
4	B	404	FMN	O3P-P-O2P	2.79	117.69	107.44
4	A	414	FMN	C4A-N5-C5A	2.98	120.23	116.72
4	B	404	FMN	C5A-C9A-N10	3.52	120.22	117.58
2	B	401	ROU	CAX-NAP-CAV	3.91	119.60	115.68
2	A	401	ROU	CAX-NAP-CAV	4.69	120.38	115.68
4	B	404	FMN	C1'-N10-C9A	5.07	124.71	118.83
2	B	401	ROU	CAY-NAQ-CAX	8.13	121.94	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ROU	CAY-NAQ-CAX	8.83	122.53	115.16
4	A	414	FMN	C4-N3-C2	10.01	123.51	115.16
4	B	404	FMN	C4-N3-C2	12.25	125.38	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ROU	1	0
3	A	407	GOL	1	0
3	A	408	GOL	1	0
3	A	409	GOL	1	0
3	A	410	GOL	1	0
3	A	412	GOL	2	0
3	A	413	GOL	1	0
4	A	414	FMN	1	0
2	B	401	ROU	1	0
4	B	404	FMN	4	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 [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	313/313 (100%)	0.17	7 (2%) 65 70	10, 21, 36, 50	0
1	B	313/313 (100%)	0.21	7 (2%) 65 70	10, 21, 43, 67	0
All	All	626/626 (100%)	0.19	14 (2%) 65 70	10, 21, 38, 67	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	GLY	6.8
1	B	0	MET	4.0
1	B	312	GLU	3.8
1	A	0	MET	3.3
1	B	132	ASN	3.0
1	A	130	CYS	2.8
1	A	193	VAL	2.4
1	A	144	GLU	2.2
1	A	291	GLU	2.2
1	A	312	GLU	2.2
1	A	299	ARG	2.1
1	B	144	GLU	2.1
1	B	101	LEU	2.1
1	B	158	GLY	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 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(Å ²)	Q<0.9
3	GOL	A	411	6/6	0.71	0.40	8.76	35,39,41,41	0
3	GOL	A	402	6/6	0.85	0.25	7.53	25,31,32,33	0
3	GOL	A	410	6/6	0.79	0.24	5.99	28,30,33,33	0
3	GOL	A	407	6/6	0.75	0.30	4.47	53,60,63,68	0
3	GOL	A	404	6/6	0.84	0.26	2.92	39,42,42,43	0
3	GOL	A	409	6/6	0.79	0.22	2.49	42,47,49,53	0
3	GOL	A	406	6/6	0.82	0.24	2.40	33,40,42,43	0
3	GOL	A	403	6/6	0.93	0.15	0.26	28,29,30,30	0
3	GOL	B	402	6/6	0.93	0.16	0.14	23,25,26,27	0
4	FMN	B	404	31/31	0.95	0.14	0.06	11,18,23,27	0
2	ROU	B	401	27/27	0.89	0.14	-0.22	12,22,29,34	0
2	ROU	A	401	27/27	0.90	0.12	-0.40	15,22,27,32	0
4	FMN	A	414	31/31	0.94	0.14	-0.44	9,16,20,24	0
5	NCO	A	415	7/7	0.98	0.10	-1.18	10,11,12,12	0
3	GOL	B	403	6/6	0.66	0.41	-	54,56,61,62	0
3	GOL	A	412	6/6	0.80	0.20	-	63,66,70,70	0
3	GOL	A	408	6/6	0.80	0.28	-	46,47,49,51	0
3	GOL	A	405	6/6	0.79	0.19	-	47,52,58,58	0
3	GOL	A	413	6/6	0.82	0.42	-	35,38,40,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.