



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:30 PM GMT

PDB ID : 3W2J
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with MII-3-135
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 : 2012-11-28
Resolution : 1.42 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

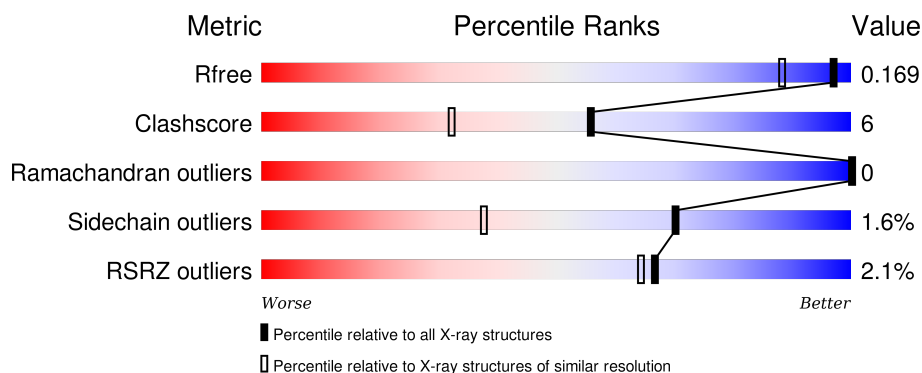
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.42 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	1632 (1.44-1.40)
Clashscore	102246	1743 (1.44-1.40)
Ramachandran outliers	100387	1698 (1.44-1.40)
Sidechain outliers	100360	1697 (1.44-1.40)
RSRZ outliers	91569	1632 (1.44-1.40)

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	<div> <div></div> <div>84%</div> <div>14%</div> <div>•</div> </div>
1	B	313	<div> <div>3%</div> <div>85%</div> <div>14%</div> <div>•</div> </div>

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	405	-	X	-	X
3	GOL	A	406	-	-	-	X
3	GOL	A	409	-	-	-	X
3	GOL	B	402	-	-	-	X
3	GOL	B	403	-	-	-	X
3	GOL	B	404	-	-	-	X
3	GOL	B	405	-	-	-	X
3	GOL	B	406	-	-	-	X
3	GOL	B	407	-	-	-	X
3	GOL	B	408	-	-	-	X
3	GOL	B	410	-	-	X	X
5	NCO	A	412	-	-	-	X

2 Entry composition [i](#)

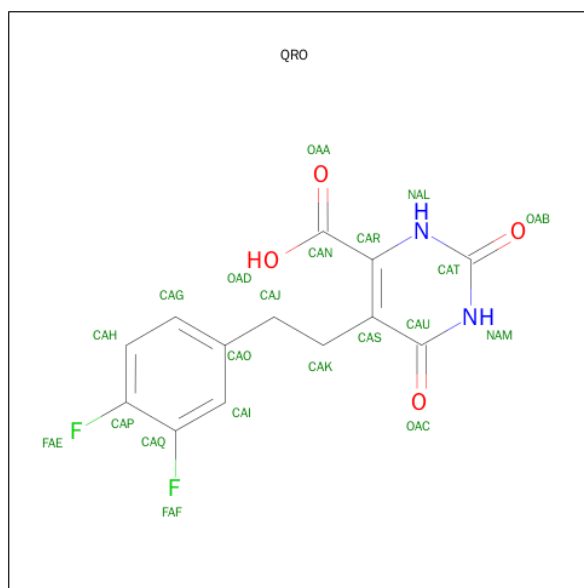
There are 6 unique types of molecules in this entry. The entry contains 5789 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-(3,4-DIFLUOROPHENYL)ETHYL]-2,6-DIOXO-1,2,3,6-TETRAHYDRO PYRIMIDINE-4-CARBOXYLIC ACID (three-letter code: QRO) (formula: C₁₃H₁₀F₂N₂O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			21	13	2	2	4		
2	B	1	Total	C	F	N	O	0	0
			21	13	2	2	4		

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



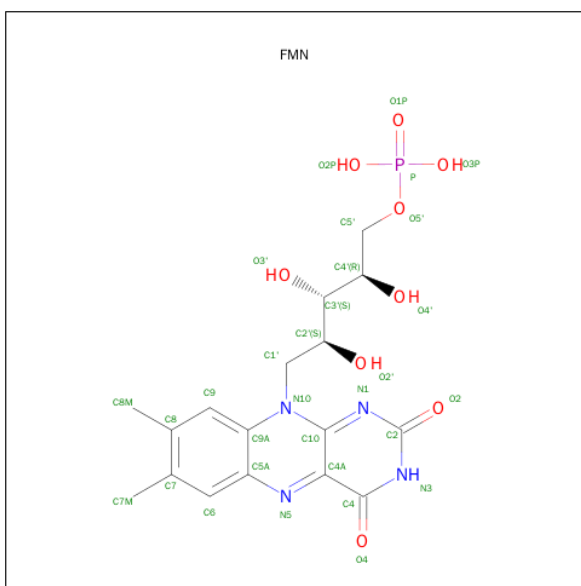
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

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

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

- 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	Co	N	0	0
			7	1	6		

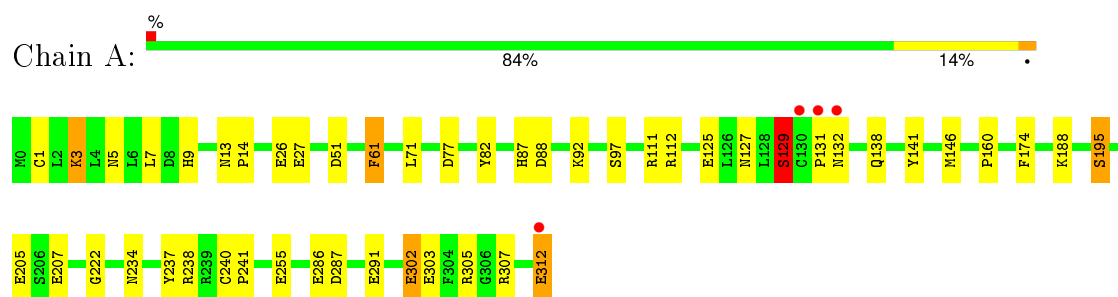
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	398	Total	O	0	0
			398	398		
6	B	390	Total	O	0	0
			390	390		

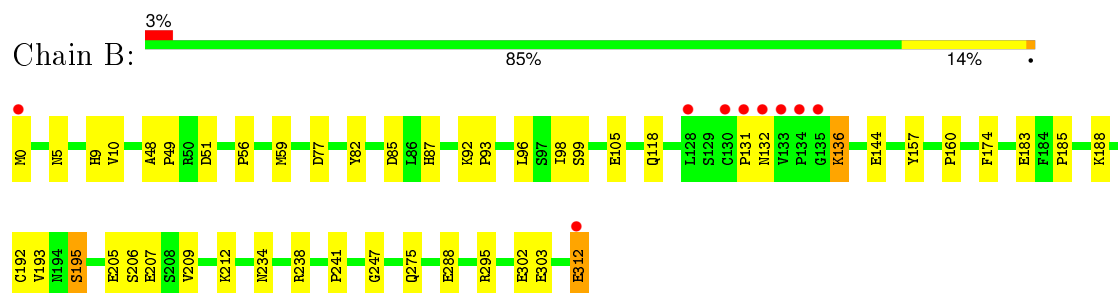
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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	68.10Å 71.82Å 129.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.87 – 1.42 46.87 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.87-1.42) 99.8 (46.87-1.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.142 , 0.168 0.145 , 0.169	Depositor DCC
R_{free} test set	5999 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	10.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 119392 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5789	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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 27.88 % 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 2.0316e-03. 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, QRO, 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	1.47	20/2440 (0.8%)	1.25	8/3305 (0.2%)
1	B	1.48	18/2440 (0.7%)	1.18	8/3305 (0.2%)
All	All	1.47	38/4880 (0.8%)	1.22	16/6610 (0.2%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	GLU	CD-OE1	-10.53	1.14	1.25
1	A	129	SER	CB-OG	9.22	1.54	1.42
1	A	3	LYS	CE-NZ	8.13	1.69	1.49
1	A	195	SER	CB-OG	-8.12	1.31	1.42
1	A	303	GLU	CD-OE1	-7.83	1.17	1.25
1	B	195	SER	CB-OG	-7.68	1.32	1.42
1	B	207	GLU	CD-OE1	-7.45	1.17	1.25
1	B	288	GLU	CD-OE1	-7.39	1.17	1.25
1	A	255	GLU	CD-OE2	-7.05	1.17	1.25
1	A	26	GLU	CD-OE2	-6.99	1.18	1.25
1	B	56	PRO	N-CD	6.85	1.57	1.47
1	B	49	PRO	N-CD	6.81	1.57	1.47
1	B	205	GLU	CD-OE2	-6.63	1.18	1.25
1	A	205	GLU	CD-OE2	6.61	1.32	1.25
1	B	183	GLU	CD-OE2	-6.59	1.18	1.25
1	A	27	GLU	CD-OE1	-6.37	1.18	1.25
1	A	302	GLU	CD-OE1	-6.30	1.18	1.25
1	B	99	SER	CB-OG	-6.26	1.34	1.42
1	B	288	GLU	CD-OE2	-6.14	1.18	1.25
1	B	131	PRO	N-CD	6.12	1.56	1.47
1	B	185	PRO	N-CD	6.07	1.56	1.47
1	A	3	LYS	CD-CE	5.93	1.66	1.51
1	B	303	GLU	CD-OE2	-5.85	1.19	1.25
1	A	131	PRO	N-CD	5.72	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	GLU	CD-OE1	5.68	1.31	1.25
1	B	247	GLY	C-O	-5.55	1.14	1.23
1	A	26	GLU	CD-OE1	-5.54	1.19	1.25
1	A	141	TYR	CE2-CZ	-5.44	1.31	1.38
1	A	222	GLY	N-CA	-5.42	1.38	1.46
1	B	144	GLU	CG-CD	5.33	1.59	1.51
1	B	183	GLU	CD-OE1	-5.32	1.19	1.25
1	B	295	ARG	CZ-NH2	-5.31	1.26	1.33
1	A	61	PHE	CB-CG	-5.31	1.42	1.51
1	B	48	ALA	C-O	-5.26	1.13	1.23
1	A	207	GLU	CD-OE1	-5.17	1.20	1.25
1	A	240	CYS	CB-SG	-5.11	1.73	1.81
1	B	207	GLU	CD-OE2	-5.07	1.20	1.25
1	A	127	ASN	C-O	-5.00	1.13	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	LYS	CD-CE-NZ	13.32	142.35	111.70
1	B	51	ASP	CB-CG-OD2	-8.93	110.26	118.30
1	B	174	PHE	CB-CG-CD2	-6.95	115.93	120.80
1	A	77	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	A	88	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	77	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	77	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	157	TYR	CB-CG-CD2	5.50	124.30	121.00
1	A	51	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	A	146	MET	CG-SD-CE	-5.38	91.58	100.20
1	A	287	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	71	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	174	PHE	CB-CG-CD1	5.23	124.46	120.80
1	B	174	PHE	CB-CG-CD1	5.17	124.42	120.80
1	B	105	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	B	85	ASP	CB-CG-OD2	-5.08	113.73	118.30

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	25	0
1	B	2388	0	2391	29	0
2	A	21	0	9	0	0
2	B	21	0	9	3	0
3	A	54	0	70	7	0
3	B	60	0	79	16	0
4	A	31	0	19	0	0
4	B	31	0	19	0	0
5	A	7	0	0	0	0
6	A	398	0	0	10	0
6	B	390	0	0	10	0
All	All	5789	0	4987	62	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 6.

All (62) 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:3:LYS:NZ	1:A:3:LYS:CE	1.69	1.53
1:B:9:HIS:CE1	3:B:410:GOL:H11	1.88	1.09
1:B:9:HIS:ND1	3:B:410:GOL:H11	1.76	1.00
1:B:118:GLN:HG3	6:B:879:HOH:O	1.62	0.97
1:B:9:HIS:CE1	3:B:410:GOL:C1	2.56	0.89
1:B:136:LYS:HE2	6:B:864:HOH:O	1.84	0.76
1:B:195:SER:HB3	6:B:815:HOH:O	1.87	0.73
1:A:312:GLU:CD	1:A:312:GLU:C	2.48	0.72
1:A:195:SER:HB3	6:A:812:HOH:O	1.91	0.71
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.37	0.70
3:B:407:GOL:H11	6:B:873:HOH:O	1.91	0.70
1:B:9:HIS:HE1	3:B:410:GOL:C1	2.08	0.67
3:A:410:GOL:H32	6:A:703:HOH:O	1.94	0.67
1:B:5:ASN:OD1	1:B:10:VAL:HG22	1.93	0.67
2:B:401:QRO:FAF	3:B:403:GOL:H31	1.85	0.66
3:B:410:GOL:H31	6:B:799:HOH:O	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.44	0.65
3:B:410:GOL:H12	6:B:510:HOH:O	1.97	0.64
1:B:9:HIS:ND1	3:B:410:GOL:C1	2.58	0.63
1:A:7:LEU:O	1:A:9:HIS:HD2	1.82	0.62
1:A:61:PHE:CE1	3:A:407:GOL:H32	2.34	0.62
1:A:112:ARG:NH2	6:A:828:HOH:O	2.29	0.62
1:B:93:PRO:HG3	3:B:410:GOL:H32	1.81	0.61
1:A:129:SER:HA	1:A:138:GLN:OE1	2.00	0.61
1:B:241:PRO:HA	3:B:404:GOL:H12	1.83	0.60
1:B:96:LEU:CD2	1:B:98:ILE:HD11	2.31	0.60
1:B:132:ASN:HB2	6:B:589:HOH:O	2.02	0.60
1:B:206:SER:OG	3:B:407:GOL:H2	2.01	0.60
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.87	0.57
2:B:401:QRO:CAQ	3:B:403:GOL:H31	2.36	0.56
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.89	0.56
1:A:87:HIS:HE1	1:A:92:LYS:O	1.90	0.55
1:A:307:ARG:NH2	6:A:853:HOH:O	2.41	0.53
1:B:87:HIS:HE1	1:B:92:LYS:O	1.91	0.53
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.06	0.53
1:B:209:VAL:O	3:B:407:GOL:H31	2.10	0.52
2:B:401:QRO:CAI	3:B:403:GOL:H31	2.42	0.50
1:A:132:ASN:HB3	6:A:604:HOH:O	2.11	0.50
1:A:312:GLU:C	1:A:312:GLU:OE1	2.52	0.47
1:A:111:ARG:HD3	6:A:896:HOH:O	2.13	0.47
1:A:291:GLU:CD	6:A:804:HOH:O	2.54	0.46
1:B:275:GLN:NE2	6:B:611:HOH:O	2.48	0.44
1:B:59:MET:CE	6:B:622:HOH:O	2.65	0.44
1:A:13:ASN:HB2	1:A:14:PRO:HD2	2.00	0.44
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.11	0.44
1:A:241:PRO:HA	3:A:404:GOL:H32	1.99	0.43
1:B:160:PRO:HB3	1:B:188:LYS:HG3	1.99	0.43
1:B:96:LEU:CD2	1:B:98:ILE:CD1	2.97	0.43
1:A:302:GLU:CG	3:A:406:GOL:O2	2.66	0.43
1:A:312:GLU:HG3	1:B:212:LYS:NZ	2.34	0.43
1:A:237:TYR:O	3:A:404:GOL:H11	2.18	0.43
3:A:405:GOL:H11	6:A:532:HOH:O	2.19	0.43
1:A:160:PRO:HB3	1:A:188:LYS:HG3	2.01	0.42
1:B:59:MET:HB3	1:B:59:MET:HE3	1.91	0.42
1:A:302:GLU:HG3	1:A:305:ARG:HH12	1.84	0.41
1:A:9:HIS:HE1	6:A:527:HOH:O	2.03	0.41
1:B:312:GLU:N	1:B:312:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:MET:HE1	6:B:622:HOH:O	2.22	0.40
1:A:97:SER:HA	1:A:125:GLU:O	2.21	0.40
3:A:410:GOL:C3	6:A:703:HOH:O	2.61	0.40
1:B:192:CYS:HA	1:B:193:VAL:HA	1.87	0.40
1:B:9:HIS:HE1	3:B:410:GOL:O1	2.05	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%)	303 (97%)	8 (3%)	0	100	100
1	B	311/313 (99%)	304 (98%)	7 (2%)	0	100	100
All	All	622/626 (99%)	607 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/258 (100%)	254 (98%)	4 (2%)	70	38
1	B	258/258 (100%)	254 (98%)	4 (2%)	70	38
All	All	516/516 (100%)	508 (98%)	8 (2%)	70	38

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
1	A	5	ASN
1	A	129	SER
1	A	312	GLU
1	B	0	MET
1	B	136	LYS
1	B	302	GLU
1	B	312	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	9	HIS
1	A	87	HIS
1	A	152	GLN
1	A	234	ASN
1	B	9	HIS
1	B	87	HIS
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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

24 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	QRO	A	401	-	17,22,22	2.75	10 (58%)	18,31,31	3.88	7 (38%)
3	GOL	A	402	-	5,5,5	0.52	0	5,5,5	2.61	4 (80%)
3	GOL	A	403	-	5,5,5	0.62	0	5,5,5	0.76	0
3	GOL	A	404	-	5,5,5	0.64	0	5,5,5	0.73	0
3	GOL	A	405	-	5,5,5	2.48	3 (60%)	5,5,5	2.45	3 (60%)
3	GOL	A	406	-	5,5,5	0.91	0	5,5,5	0.86	0
3	GOL	A	407	-	5,5,5	1.36	1 (20%)	5,5,5	1.64	2 (40%)
3	GOL	A	408	-	5,5,5	0.66	0	5,5,5	1.37	0
3	GOL	A	409	-	5,5,5	1.13	1 (20%)	5,5,5	0.52	0
3	GOL	A	410	-	5,5,5	0.77	0	5,5,5	1.59	1 (20%)
4	FMN	A	411	-	32,33,33	1.18	2 (6%)	34,50,50	2.46	7 (20%)
5	NCO	A	412	-	6,6,6	3.34	6 (100%)	0,15,15	0.00	-
2	QRO	B	401	-	17,22,22	2.53	5 (29%)	18,31,31	3.00	6 (33%)
3	GOL	B	402	-	5,5,5	0.65	0	5,5,5	0.73	0
3	GOL	B	403	-	5,5,5	0.96	0	5,5,5	2.39	3 (60%)
3	GOL	B	404	-	5,5,5	1.04	1 (20%)	5,5,5	0.82	0
3	GOL	B	405	-	5,5,5	0.69	0	5,5,5	0.84	0
3	GOL	B	406	-	5,5,5	1.03	0	5,5,5	0.89	0
3	GOL	B	407	-	5,5,5	0.77	0	5,5,5	0.80	0
3	GOL	B	408	-	5,5,5	1.21	1 (20%)	5,5,5	1.17	1 (20%)
3	GOL	B	409	-	5,5,5	0.50	0	5,5,5	1.11	0
3	GOL	B	410	-	5,5,5	0.99	0	5,5,5	1.05	0
3	GOL	B	411	-	5,5,5	0.76	0	5,5,5	0.57	0
4	FMN	B	412	-	32,33,33	1.13	1 (3%)	34,50,50	2.70	7 (20%)

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	QRO	A	401	-	-	0/5/9/9	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
4	FMN	A	411	-	-	0/18/18/18	0/3/3/3
5	NCO	A	412	-	-	0/0/0/0	0/0/0/0
2	QRO	B	401	-	-	0/5/9/9	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
3	GOL	B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	B	407	-	-	0/4/4/4	0/0/0/0
3	GOL	B	408	-	-	0/4/4/4	0/0/0/0
3	GOL	B	409	-	-	0/4/4/4	0/0/0/0
3	GOL	B	410	-	-	0/4/4/4	0/0/0/0
3	GOL	B	411	-	-	0/4/4/4	0/0/0/0
4	FMN	B	412	-	-	0/18/18/18	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	QRO	CAJ-CAO	-6.30	1.33	1.51
2	A	401	QRO	CAJ-CAO	-4.18	1.39	1.51
2	A	401	QRO	CAK-CAS	-4.14	1.46	1.52
2	A	401	QRO	CAR-CAS	-2.53	1.36	1.41
3	A	407	GOL	O2-C2	-2.34	1.36	1.43
4	A	411	FMN	C2'-C3'	-2.19	1.49	1.53
4	B	412	FMN	C5A-N5	-2.18	1.31	1.35
3	B	404	GOL	C3-C2	2.01	1.60	1.52
2	A	401	QRO	CAH-CAG	2.16	1.43	1.38
3	A	409	GOL	O3-C3	2.24	1.52	1.42
5	A	412	NCO	CO-N4	2.28	2.05	1.96
5	A	412	NCO	CO-N1	2.33	2.05	1.96
2	A	401	QRO	CAI-CAO	2.36	1.43	1.39
2	B	401	QRO	CAI-CAQ	2.38	1.41	1.37
2	A	401	QRO	FAE-CAP	2.40	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	GOL	C1-C2	2.45	1.61	1.52
3	B	408	GOL	O2-C2	2.55	1.51	1.43
2	B	401	QRO	FAE-CAP	2.63	1.42	1.35
5	A	412	NCO	CO-N2	2.79	2.07	1.96
2	A	401	QRO	CAI-CAQ	2.81	1.42	1.37
3	A	405	GOL	O2-C2	3.00	1.52	1.43
5	A	412	NCO	CO-N6	3.08	2.08	1.96
4	A	411	FMN	C9A-N10	3.42	1.43	1.38
3	A	405	GOL	O1-C1	3.75	1.58	1.42
2	B	401	QRO	CAU-NAM	3.82	1.39	1.33
5	A	412	NCO	CO-N5	3.93	2.11	1.96
2	A	401	QRO	CAG-CAO	4.14	1.47	1.38
2	A	401	QRO	CAU-NAM	4.46	1.41	1.33
2	A	401	QRO	CAR-NAL	4.56	1.41	1.34
5	A	412	NCO	CO-N3	4.86	2.14	1.96
2	B	401	QRO	CAR-NAL	5.18	1.42	1.34

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	412	FMN	C4-C4A-C10	-10.75	113.06	119.94
4	A	411	FMN	C4-C4A-C10	-8.06	114.78	119.94
2	A	401	QRO	NAM-CAT-NAL	-5.95	117.68	127.69
2	B	401	QRO	NAM-CAT-NAL	-5.00	119.27	127.69
4	B	412	FMN	C4A-C10-N10	-4.92	116.94	120.52
4	A	411	FMN	N3-C2-N1	-3.40	121.97	127.69
3	B	403	GOL	O2-C2-C3	-3.30	92.60	108.47
3	A	405	GOL	O2-C2-C3	-3.20	93.08	108.47
4	B	412	FMN	N3-C2-N1	-3.06	122.55	127.69
3	A	402	GOL	O2-C2-C3	-2.94	94.33	108.47
2	A	401	QRO	CAS-CAR-NAL	-2.88	118.38	122.66
3	A	410	GOL	O1-C1-C2	-2.80	95.78	109.97
3	A	402	GOL	O2-C2-C1	-2.79	95.08	108.47
4	A	411	FMN	C4A-C4-N3	-2.49	120.27	123.52
4	A	411	FMN	C4A-C10-N10	-2.44	118.75	120.52
2	B	401	QRO	CAS-CAR-NAL	-2.35	119.18	122.66
2	A	401	QRO	CAH-CAG-CAO	-2.12	118.05	121.02
4	B	412	FMN	C9-C8-C7	-2.08	115.90	119.97
3	A	407	GOL	O3-C3-C2	2.02	120.20	109.97
2	B	401	QRO	CAO-CAI-CAQ	2.03	120.83	119.45
3	A	402	GOL	O3-C3-C2	2.06	120.40	109.97
2	B	401	QRO	CAI-CAQ-CAP	2.12	123.00	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	405	GOL	O3-C3-C2	2.17	120.97	109.97
3	B	408	GOL	O2-C2-C3	2.36	119.78	108.47
4	B	412	FMN	C4A-N5-C5A	2.57	119.76	116.72
3	B	403	GOL	C3-C2-C1	2.59	121.97	111.06
3	A	407	GOL	C3-C2-C1	2.63	122.12	111.06
4	A	411	FMN	C4A-N5-C5A	2.68	119.89	116.72
3	B	403	GOL	O1-C1-C2	3.25	126.47	109.97
2	A	401	QRO	CAG-CAH-CAP	3.28	122.68	118.96
3	A	402	GOL	C3-C2-C1	3.49	125.77	111.06
3	A	405	GOL	O2-C2-C1	3.53	125.40	108.47
2	A	401	QRO	CAO-CAI-CAQ	3.72	121.99	119.45
4	B	412	FMN	C4-C4A-N5	3.83	123.36	118.70
4	A	411	FMN	C4-C4A-N5	4.26	123.88	118.70
2	B	401	QRO	CAT-NAL-CAR	4.67	120.36	115.68
4	B	412	FMN	C4-N3-C2	6.84	120.86	115.16
2	A	401	QRO	CAT-NAL-CAR	6.85	122.55	115.68
4	A	411	FMN	C4-N3-C2	8.75	122.45	115.16
2	B	401	QRO	CAU-NAM-CAT	9.46	123.05	115.16
2	A	401	QRO	CAU-NAM-CAT	11.63	124.86	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	GOL	2	0
3	A	405	GOL	1	0
3	A	406	GOL	1	0
3	A	407	GOL	1	0
3	A	410	GOL	2	0
2	B	401	QRO	3	0
3	B	403	GOL	3	0
3	B	404	GOL	1	0
3	B	407	GOL	3	0
3	B	410	GOL	9	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.19	4 (1%) 79 78	5, 9, 21, 41	0
1	B	313/313 (100%)	-0.05	9 (2%) 55 52	5, 10, 23, 44	0
All	All	626/626 (100%)	-0.12	13 (2%) 67 64	5, 10, 22, 44	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	PRO	4.9
1	A	130	CYS	4.7
1	A	131	PRO	4.5
1	B	133	VAL	4.3
1	B	312	GLU	3.9
1	B	135	GLY	3.6
1	A	312	GLU	3.3
1	B	134	PRO	3.0
1	B	130	CYS	2.6
1	B	132	ASN	2.5
1	B	0	MET	2.5
1	B	128	LEU	2.4
1	A	132	ASN	2.2

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	B	407	6/6	0.81	0.25	19.88	30,37,40,43	0
3	GOL	B	404	6/6	0.79	0.15	17.65	29,32,35,43	0
3	GOL	B	410	6/6	0.88	0.28	11.02	21,31,33,33	0
3	GOL	B	403	6/6	0.86	0.19	9.18	18,22,31,35	0
3	GOL	A	402	6/6	0.94	0.11	8.38	13,16,18,18	0
3	GOL	B	406	6/6	0.87	0.18	7.84	22,30,31,31	0
3	GOL	B	405	6/6	0.75	0.18	5.97	35,41,47,50	0
3	GOL	B	408	6/6	0.81	0.15	5.20	24,27,34,41	0
3	GOL	A	409	6/6	0.59	0.30	4.66	29,47,50,52	0
3	GOL	A	405	6/6	0.75	0.23	2.79	17,22,27,28	0
3	GOL	B	402	6/6	0.90	0.09	2.38	16,17,20,22	0
5	NCO	A	412	7/7	0.99	0.09	2.25	8,8,9,9	0
3	GOL	A	406	6/6	0.84	0.18	2.13	20,24,25,29	0
3	GOL	A	407	6/6	0.92	0.11	1.88	24,27,29,29	0
2	QRO	A	401	21/21	0.94	0.11	0.14	6,10,21,23	0
4	FMN	A	411	31/31	0.98	0.07	-0.12	4,5,7,10	0
2	QRO	B	401	21/21	0.96	0.09	-0.14	6,10,23,36	0
3	GOL	A	403	6/6	0.95	0.07	-0.31	15,16,17,18	0
4	FMN	B	412	31/31	0.99	0.07	-0.59	4,5,7,9	0
3	GOL	B	411	6/6	0.72	0.24	-	28,33,37,41	0
3	GOL	A	404	6/6	0.76	0.14	-	36,44,46,55	0
3	GOL	A	408	6/6	0.73	0.17	-	28,35,35,40	0
3	GOL	B	409	6/6	0.78	0.15	-	27,39,43,49	0
3	GOL	A	410	6/6	0.85	0.17	-	30,39,39,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.