WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 06:46 PM GMT

PDB ID	:	3W7J
Title	:	Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with MII-6-040
Authors	:	Inaoka, D.K.; Iida, M.; Tabuchi, T.; Lee, N.; Hashimoto, S.; Matsuoka, S.; Kuranaga, T.; 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	:	2013-02-28
Resolution	:	1.58 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

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

The reported resolution of this entry is 1.58 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	Percentile Ranks	Value
Rfree		0.192
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		1.6%
RSRZ outliers		1.3%

Worse　　　　　　　　　　　　　　　　　　　　　　*Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
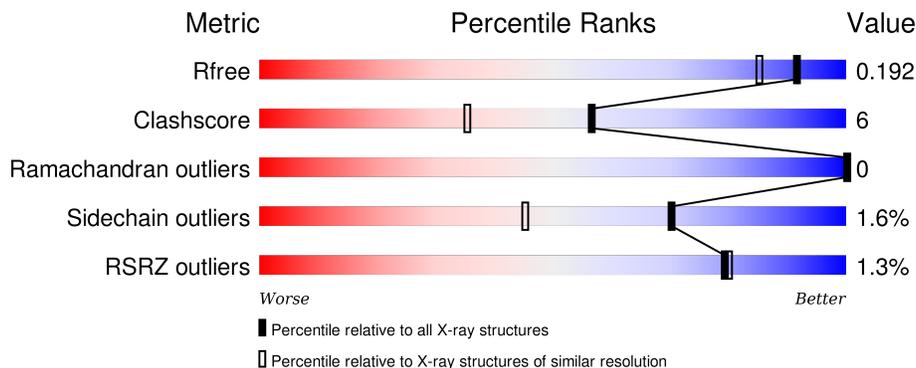
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3815 (1.60-1.56)
Clashscore	102246	4131 (1.60-1.56)
Ramachandran outliers	100387	4021 (1.60-1.56)
Sidechain outliers	100360	4018 (1.60-1.56)
RSRZ outliers	91569	3823 (1.60-1.56)

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 <=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	90%　　　　　　　9%　　•
1	B	313	2%　88%　　　　　　　12%

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	405	-	-	-	X
3	GOL	A	407	-	-	X	X
3	GOL	A	409	-	-	-	X
3	GOL	A	410	-	-	-	X
3	GOL	B	402	-	-	-	X
3	GOL	B	404	-	-	-	X
3	GOL	B	407	-	-	-	X
3	GOL	B	408	-	X	-	X
3	GOL	B	409	-	-	-	X
3	GOL	B	410	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5652 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	1	0
			2394	1535	397	444	18			
1	B	313	Total	C	N	O	S	0	0	0
			2388	1530	396	444	18			

- Molecule 2 is 5-[2-(6-CARBOXYNAPHTHALEN-2-YL)ETHYL]-2,6-DIOXO-1,2,3,6-TETRAHYDROPYRIMIDINE-4-CARBOXYLIC ACID (three-letter code: W7J) (formula: $C_{18}H_{14}N_2O_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	18	2	6		
2	B	1	Total	C	N	O	0	1
			52	36	4	12		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
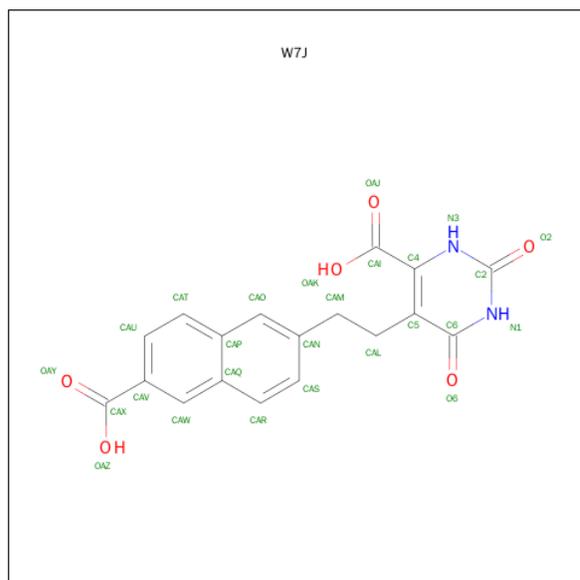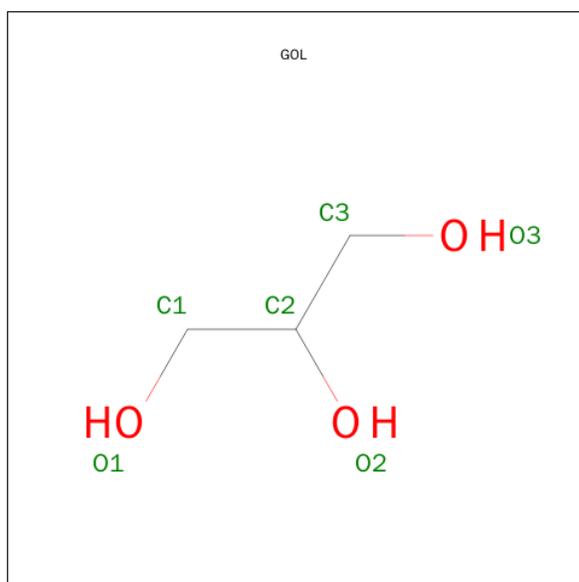
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	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
3	B	1	Total 6	C 3	O 3	0	0

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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

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).
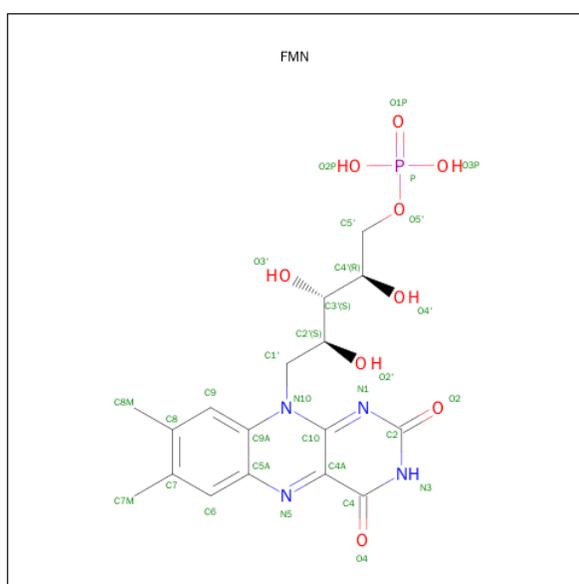
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 5 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: $CoH_{18}N_6$).
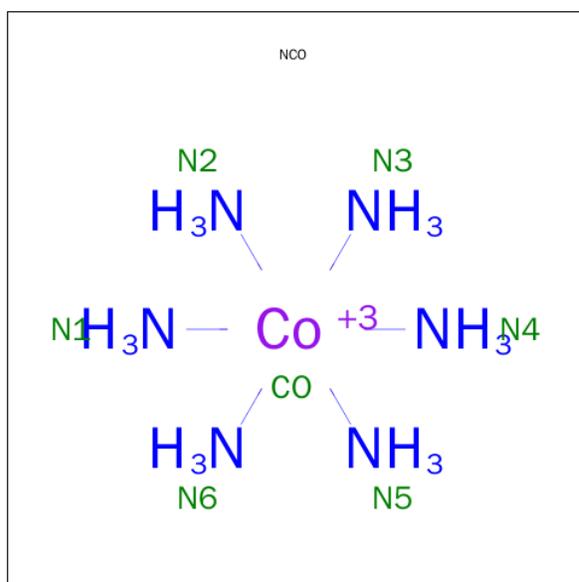
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total Co N 7 1 6		0	0
5	A	1	Total Co N 7 1 6		0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	309	Total O 309 309		0	0
6	B	299	Total O 299 299		0	0

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)
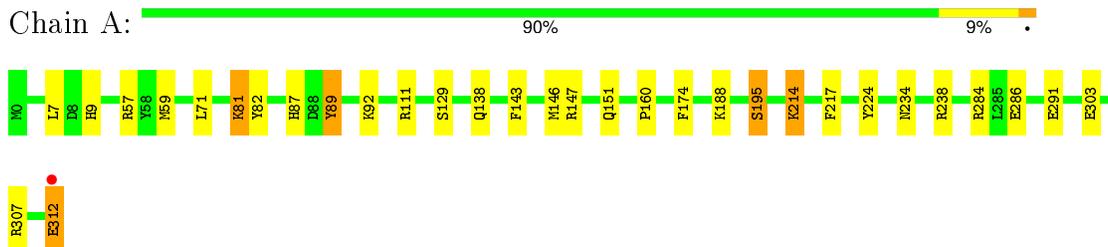
- Molecule 1: Dihydroorotate dehydrogenase (fumarate)
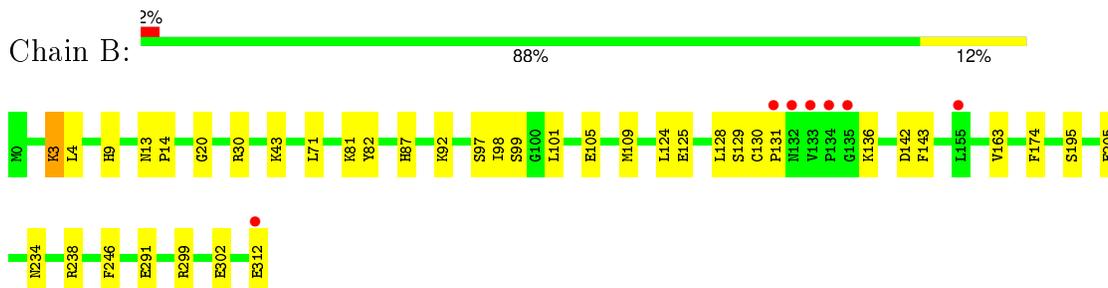
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.00Å 71.69Å 129.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.26 – 1.58 39.23 – 1.58	Depositor EDS
% Data completeness (in resolution range)	91.0 (39.26-1.58) 91.0 (39.23-1.58)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.07 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.147 , 0.182 0.161 , 0.192	Depositor DCC
R_{free} test set	3945 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	8.8	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 80122 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5652	wwPDB-VP
Average B, all atoms (Å^2)	12.0	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 29.95 % 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 1.4202e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FMN, GOL, W7J, 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	1.22	8/2449 (0.3%)	1.17	11/3316 (0.3%)
1	B	1.18	3/2440 (0.1%)	1.12	8/3305 (0.2%)
All	All	1.20	11/4889 (0.2%)	1.14	19/6621 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	SER	CB-OG	-7.62	1.32	1.42
1	A	195	SER	CB-OG	-6.46	1.33	1.42
1	A	291	GLU	CG-CD	6.10	1.61	1.51
1	A	89	TYR	CG-CD2	-5.64	1.31	1.39
1	A	286	GLU	CD-OE1	5.62	1.31	1.25
1	B	205	GLU	CD-OE1	5.46	1.31	1.25
1	A	224	TYR	CE1-CZ	-5.45	1.31	1.38
1	A	214[A]	LYS	CA-C	5.12	1.66	1.52
1	A	214[B]	LYS	CA-C	5.12	1.66	1.52
1	B	129	SER	CB-OG	5.06	1.48	1.42
1	A	303	GLU	CD-OE1	-5.03	1.20	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214[A]	LYS	CD-CE-NZ	8.46	131.17	111.70
1	A	214[B]	LYS	CD-CE-NZ	8.46	131.17	111.70
1	B	30	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	291	GLU	CA-CB-CG	6.07	126.76	113.40
1	A	147	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	174	PHE	CB-CG-CD2	-5.84	116.71	120.80
1	A	57	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	217	PHE	CB-CG-CD1	5.75	124.83	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	PHE	CB-CG-CD1	5.65	124.76	120.80
1	B	4	LEU	CB-CG-CD1	5.63	120.56	111.00
1	B	3	LYS	CA-CB-CG	5.61	125.74	113.40
1	A	217	PHE	CB-CG-CD2	-5.35	117.06	120.80
1	B	299	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	142	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	111	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	A	284	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	B	246	PHE	CB-CG-CD2	-5.15	117.20	120.80
1	A	146	MET	CG-SD-CE	-5.09	92.06	100.20
1	A	174	PHE	CB-CG-CD2	-5.05	117.26	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2394	0	2404	24	0
1	B	2388	0	2391	23	0
2	A	26	0	12	1	0
2	B	52	0	24	9	0
3	A	54	0	72	13	0
3	B	54	0	72	10	0
4	A	31	0	19	0	0
4	B	31	0	19	1	0
5	A	14	0	0	0	0
6	A	309	0	0	12	0
6	B	299	0	0	3	0
All	All	5652	0	5013	61	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 (61) 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:B:131:PRO:HB3	2:B:401[A]:W7J:CAU	1.98	0.93
2:B:401[B]:W7J:CAT	3:B:410:GOL:H12	2.02	0.90
1:A:89:TYR:HB3	3:A:407:GOL:H2	1.58	0.84
3:A:409:GOL:O1	3:B:408:GOL:H2	1.81	0.80
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.35	0.74
1:A:214[A]:LYS:HE2	6:A:629:HOH:O	1.86	0.73
2:B:401[B]:W7J:CAT	3:B:410:GOL:C1	2.67	0.73
1:A:81:LYS:HE3	6:A:783:HOH:O	1.94	0.67
1:B:128:LEU:HD12	1:B:163:VAL:HG11	1.80	0.64
1:B:98:ILE:HD12	1:B:124:LEU:CD1	2.29	0.63
1:A:9:HIS:ND1	3:A:407:GOL:H11	2.13	0.63
3:A:410:GOL:H12	6:A:516:HOH:O	1.98	0.62
1:B:98:ILE:HD12	1:B:124:LEU:HD13	1.82	0.61
3:A:407:GOL:H31	6:A:647:HOH:O	2.00	0.60
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.48	0.60
1:B:128:LEU:HD12	1:B:163:VAL:CG1	2.32	0.59
1:A:9:HIS:CE1	3:A:407:GOL:H11	2.37	0.58
1:B:128:LEU:CD1	1:B:163:VAL:HG11	2.32	0.58
1:B:195:SER:HB3	6:B:702:HOH:O	2.03	0.58
1:A:87:HIS:HE1	1:A:92:LYS:O	1.84	0.58
1:A:89:TYR:HD2	3:A:407:GOL:H12	1.67	0.58
1:A:7:LEU:O	1:A:9:HIS:HD2	1.85	0.57
1:B:128:LEU:CD1	1:B:163:VAL:CG1	2.83	0.57
2:B:401[B]:W7J:C2	3:B:410:GOL:O1	2.52	0.57
1:B:71:LEU:HD22	2:B:401[A]:W7J:H8	1.85	0.57
1:A:195:SER:HB3	6:A:701:HOH:O	2.05	0.56
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.88	0.56
2:B:401[B]:W7J:CAP	3:B:410:GOL:H12	2.35	0.55
1:A:129:SER:HA	1:A:138:GLN:OE1	2.07	0.55
1:B:87:HIS:HE1	1:B:92:LYS:O	1.91	0.54
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.91	0.53
1:A:312:GLU:CD	1:A:312:GLU:C	2.68	0.53
3:A:407:GOL:H12	6:A:521:HOH:O	2.13	0.49
6:A:718:HOH:O	3:B:406:GOL:H12	2.13	0.49
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.05	0.48
1:A:143:PHE:CE2	3:A:409:GOL:C3	2.96	0.48
1:A:59:MET:HE1	6:A:705:HOH:O	2.13	0.47
1:B:101:LEU:HD12	6:B:703:HOH:O	2.14	0.47
2:B:401[B]:W7J:CAP	3:B:410:GOL:C1	2.93	0.46
1:A:59:MET:CE	6:A:705:HOH:O	2.63	0.46
1:B:105:GLU:HG2	1:B:109:MET:HE2	1.98	0.46
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:SER:HA	1:B:125:GLU:O	2.18	0.44
1:A:160:PRO:HB3	1:A:188:LYS:HG3	1.99	0.44
1:A:307:ARG:NH2	6:A:787:HOH:O	2.41	0.44
3:A:407:GOL:C1	6:A:521:HOH:O	2.65	0.43
1:A:143:PHE:CE2	3:A:409:GOL:H31	2.52	0.43
1:B:13:ASN:HB2	1:B:14:PRO:HD2	2.01	0.43
1:B:143:PHE:CE2	3:B:407:GOL:H12	2.54	0.42
1:B:20:GLY:HA2	1:B:43:LYS:HD2	2.01	0.42
3:B:407:GOL:O3	3:B:408:GOL:H2	2.20	0.42
1:B:128:LEU:HG	1:B:163:VAL:HG13	2.02	0.41
2:B:401[B]:W7J:CAO	3:B:410:GOL:H11	2.51	0.41
1:A:89:TYR:CD2	3:A:407:GOL:H12	2.53	0.41
1:B:9:HIS:HE1	6:B:650:HOH:O	2.03	0.41
1:A:59:MET:HB3	1:A:59:MET:HE3	1.93	0.41
1:B:131:PRO:HB3	2:B:401[A]:W7J:CAT	2.50	0.40
3:A:408:GOL:O1	3:A:410:GOL:H11	2.21	0.40
1:A:71:LEU:HD22	2:A:401:W7J:H8	2.04	0.40
1:B:20:GLY:HA3	4:B:411:FMN:N5	2.36	0.40
1:A:151:GLN:NE2	6:A:710:HOH:O	2.47	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	312/313 (100%)	302 (97%)	10 (3%)	0	100	100
1	B	311/313 (99%)	305 (98%)	6 (2%)	0	100	100
All	All	623/626 (100%)	607 (97%)	16 (3%)	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	259/258 (100%)	257 (99%)	2 (1%)	86	74
1	B	258/258 (100%)	252 (98%)	6 (2%)	58	28
All	All	517/516 (100%)	509 (98%)	8 (2%)	70	48

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

Mol	Chain	Res	Type
1	A	81	LYS
1	A	312	GLU
1	B	3	LYS
1	B	81	LYS
1	B	130	CYS
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	87	HIS
1	A	132	ASN
1	A	151	GLN
1	A	152	GLN
1	A	215	GLN
1	A	234	ASN
1	B	9	HIS
1	B	87	HIS
1	B	152	GLN
1	B	215	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 ⓘ

25 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	W7J	A	401	-	20,28,28	2.61	7 (35%)	24,40,40	3.80	11 (45%)
3	GOL	A	402	-	5,5,5	0.52	0	5,5,5	0.95	0
3	GOL	A	403	-	5,5,5	0.58	0	5,5,5	1.08	1 (20%)
3	GOL	A	404	-	5,5,5	0.51	0	5,5,5	0.42	0
3	GOL	A	405	-	5,5,5	1.05	0	5,5,5	0.99	0
3	GOL	A	406	-	5,5,5	0.34	0	5,5,5	0.65	0
3	GOL	A	407	-	5,5,5	0.29	0	5,5,5	0.68	0
3	GOL	A	408	-	5,5,5	0.43	0	5,5,5	0.60	0
3	GOL	A	409	-	5,5,5	0.59	0	5,5,5	0.34	0
3	GOL	A	410	-	5,5,5	2.12	3 (60%)	5,5,5	1.67	2 (40%)
4	FMN	A	411	-	32,33,33	1.73	9 (28%)	34,50,50	1.95	4 (11%)
5	NCO	A	412	-	6,6,6	2.56	4 (66%)	0,15,15	0.00	-
5	NCO	A	413	-	6,6,6	1.63	2 (33%)	0,15,15	0.00	-
2	W7J	B	401[A]	-	20,28,28	2.48	8 (40%)	24,40,40	3.27	9 (37%)
2	W7J	B	401[B]	-	20,28,28	2.43	5 (25%)	24,40,40	2.94	8 (33%)
3	GOL	B	402	-	5,5,5	0.84	0	5,5,5	1.88	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	GOL	B	403	-	5,5,5	0.37	0	5,5,5	0.36	0
3	GOL	B	404	-	5,5,5	0.78	0	5,5,5	0.61	0
3	GOL	B	405	-	5,5,5	0.37	0	5,5,5	0.60	0
3	GOL	B	406	-	5,5,5	0.36	0	5,5,5	0.50	0
3	GOL	B	407	-	5,5,5	0.45	0	5,5,5	0.34	0
3	GOL	B	408	-	5,5,5	2.88	4 (80%)	5,5,5	3.33	3 (60%)
3	GOL	B	409	-	5,5,5	0.81	0	5,5,5	0.82	0
3	GOL	B	410	-	5,5,5	0.42	0	5,5,5	0.53	0
4	FMN	B	411	-	32,33,33	1.71	8 (25%)	34,50,50	2.36	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	W7J	A	401	-	-	0/5/13/13	0/3/3/3
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
5	NCO	A	413	-	-	0/0/0/0	0/0/0/0
2	W7J	B	401[A]	-	-	0/5/13/13	0/3/3/3
2	W7J	B	401[B]	-	-	0/5/13/13	0/3/3/3
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
4	FMN	B	411	-	-	0/18/18/18	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	W7J	CAL-C5	-5.97	1.44	1.52
2	A	401	W7J	CAR-CAQ	-4.08	1.32	1.42
2	B	401[B]	W7J	CAL-C5	-3.73	1.47	1.52
2	B	401[A]	W7J	CAM-CAN	-3.65	1.41	1.51
4	A	411	FMN	C1'-N10	-3.46	1.44	1.48
2	B	401[B]	W7J	CAM-CAN	-3.28	1.42	1.51
4	A	411	FMN	C10-N10	-3.18	1.35	1.39
4	B	411	FMN	C10-N10	-3.11	1.35	1.39
2	B	401[A]	W7J	CAW-CAQ	-2.98	1.35	1.42
4	B	411	FMN	C4-N3	-2.87	1.27	1.33
4	B	411	FMN	C2-N1	-2.83	1.32	1.38
2	A	401	W7J	CAW-CAV	-2.65	1.32	1.38
4	B	411	FMN	C9-C9A	-2.55	1.35	1.40
2	A	401	W7J	C2-N1	-2.42	1.33	1.38
2	B	401[A]	W7J	CAR-CAQ	-2.41	1.36	1.42
4	A	411	FMN	C2-N1	-2.31	1.33	1.38
2	B	401[A]	W7J	CAW-CAV	-2.27	1.32	1.38
4	A	411	FMN	C10-N1	-2.17	1.31	1.35
4	A	411	FMN	C8M-C8	-2.07	1.46	1.51
2	A	401	W7J	CAT-CAP	-2.06	1.37	1.42
2	B	401[A]	W7J	CAL-C5	-2.05	1.49	1.52
4	A	411	FMN	C9A-N10	2.11	1.41	1.38
3	A	410	GOL	O2-C2	2.11	1.49	1.43
5	A	413	NCO	CO-N6	2.17	2.04	1.96
5	A	413	NCO	CO-N1	2.19	2.05	1.96
4	A	411	FMN	C8-C7	2.24	1.47	1.41
5	A	412	NCO	CO-N2	2.32	2.05	1.96
2	B	401[A]	W7J	CAO-CAN	2.36	1.43	1.37
3	B	408	GOL	C3-C2	2.39	1.61	1.52
4	B	411	FMN	P-O5'	2.40	1.66	1.59
5	A	412	NCO	CO-N5	2.65	2.06	1.96
4	B	411	FMN	C4A-C10	2.70	1.45	1.40
3	A	410	GOL	O1-C1	2.71	1.54	1.42
4	A	411	FMN	C4A-C10	2.78	1.46	1.40
4	B	411	FMN	C5'-C4'	2.83	1.56	1.51
2	B	401[B]	W7J	CAR-CAS	3.00	1.42	1.36
3	A	410	GOL	O3-C3	3.14	1.56	1.42
3	B	408	GOL	C1-C2	3.17	1.64	1.52
3	B	408	GOL	O1-C1	3.24	1.56	1.42
5	A	412	NCO	CO-N6	3.27	2.09	1.96
5	A	412	NCO	CO-N3	3.31	2.09	1.96
4	B	411	FMN	C4-C4A	3.47	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	408	GOL	O3-C3	3.60	1.57	1.42
4	A	411	FMN	C5'-C4'	3.81	1.57	1.51
2	A	401	W7J	C4-N3	4.03	1.41	1.34
2	A	401	W7J	C6-N1	5.22	1.42	1.33
2	B	401[B]	W7J	C4-N3	5.26	1.43	1.34
2	B	401[A]	W7J	C4-N3	5.51	1.43	1.34
2	B	401[A]	W7J	C6-N1	6.26	1.44	1.33
2	B	401[B]	W7J	C6-N1	6.77	1.45	1.33

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	W7J	N1-C2-N3	-6.51	116.73	127.69
2	B	401[A]	W7J	CAW-CAV-CAX	-6.17	112.42	120.46
4	B	411	FMN	C4-C4A-C10	-5.68	116.31	119.94
4	B	411	FMN	C4A-C10-N10	-5.40	116.60	120.52
2	B	401[B]	W7J	N1-C2-N3	-5.07	119.15	127.69
2	A	401	W7J	CAR-CAQ-CAW	-4.96	113.46	122.05
2	B	401[A]	W7J	N1-C2-N3	-4.96	119.34	127.69
2	B	401[A]	W7J	CAR-CAQ-CAW	-4.28	114.64	122.05
4	A	411	FMN	C4-C4A-C10	-4.23	117.24	119.94
4	A	411	FMN	C4A-C4-N3	-4.01	118.28	123.52
4	B	411	FMN	C4A-C4-N3	-3.21	119.33	123.52
4	A	411	FMN	N3-C2-N1	-3.02	122.60	127.69
2	B	401[B]	W7J	CAS-CAN-CAO	-2.92	114.02	118.79
2	A	401	W7J	CAN-CAO-CAP	-2.90	116.01	121.32
3	B	402	GOL	O2-C2-C1	-2.66	95.70	108.47
4	B	411	FMN	N3-C2-N1	-2.44	123.58	127.69
2	A	401	W7J	CAS-CAR-CAQ	-2.44	116.99	120.82
4	B	411	FMN	C9-C8-C7	-2.29	115.50	119.97
2	B	401[B]	W7J	CAU-CAV-CAX	-2.23	117.49	120.43
3	A	403	GOL	O3-C3-C2	-2.20	98.83	109.97
2	A	401	W7J	CAT-CAP-CAQ	-2.15	114.85	118.93
2	B	401[A]	W7J	CAU-CAT-CAP	-2.11	117.51	120.82
3	B	402	GOL	C3-C2-C1	2.01	119.52	111.06
2	B	401[B]	W7J	CAM-CAN-CAS	2.04	126.40	121.24
3	A	410	GOL	O1-C1-C2	2.14	120.84	109.97
2	B	401[B]	W7J	CAN-CAO-CAP	2.31	125.55	121.32
2	A	401	W7J	CAR-CAS-CAN	2.40	126.21	121.22
3	A	410	GOL	O2-C2-C1	2.46	120.29	108.47
2	B	401[B]	W7J	CAW-CAV-CAX	2.46	123.67	120.46
2	A	401	W7J	CAM-CAL-C5	2.57	116.98	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401[B]	W7J	C2-N3-C4	2.88	118.57	115.68
4	B	411	FMN	C4A-N5-C5A	2.89	120.13	116.72
2	B	401[A]	W7J	CAU-CAV-CAW	2.96	122.47	118.14
4	B	411	FMN	C1'-N10-C9A	3.13	122.46	118.83
2	A	401	W7J	CAO-CAP-CAQ	3.16	123.10	118.92
3	B	408	GOL	O1-C1-C2	3.26	126.50	109.97
2	B	401[A]	W7J	C2-N3-C4	3.43	119.11	115.68
2	B	401[A]	W7J	CAU-CAV-CAX	3.50	125.04	120.43
4	B	411	FMN	C4-C4A-N5	3.57	123.04	118.70
2	B	401[A]	W7J	CAW-CAQ-CAP	3.59	123.67	118.92
3	B	408	GOL	O3-C3-C2	4.34	132.00	109.97
3	B	408	GOL	C3-C2-C1	4.75	131.07	111.06
2	A	401	W7J	CAW-CAQ-CAP	4.90	125.41	118.92
2	A	401	W7J	C2-N3-C4	5.32	121.01	115.68
4	A	411	FMN	C4-N3-C2	7.28	121.23	115.16
4	B	411	FMN	C4-N3-C2	7.38	121.32	115.16
2	B	401[A]	W7J	C6-N1-C2	10.48	123.90	115.16
2	B	401[B]	W7J	C6-N1-C2	11.81	125.01	115.16
2	A	401	W7J	C6-N1-C2	12.84	125.88	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	W7J	1	0
3	A	407	GOL	8	0
3	A	408	GOL	1	0
3	A	409	GOL	3	0
3	A	410	GOL	2	0
2	B	401[A]	W7J	3	0
2	B	401[B]	W7J	6	0
3	B	406	GOL	1	0
3	B	407	GOL	2	0
3	B	408	GOL	2	0
3	B	410	GOL	6	0
4	B	411	FMN	1	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%)	-0.42	1 (0%)	94 94	4, 8, 18, 42	0
1	B	313/313 (100%)	-0.23	7 (2%)	65 66	4, 10, 26, 46	0
All	All	626/626 (100%)	-0.33	8 (1%)	79 80	4, 9, 21, 46	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	PRO	11.6
1	A	312	GLU	4.1
1	B	135	GLY	3.9
1	B	312	GLU	3.6
1	B	133	VAL	3.4
1	B	132	ASN	3.1
1	B	134	PRO	2.5
1	B	155	LEU	2.1

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	410	6/6	0.62	0.26	19.32	7,18,21,21	0
3	GOL	B	407	6/6	0.76	0.22	12.87	37,40,42,44	0
3	GOL	A	409	6/6	0.84	0.18	11.95	30,34,34,35	0
3	GOL	B	404	6/6	0.88	0.17	6.40	25,30,31,32	0
3	GOL	A	407	6/6	0.90	0.25	4.77	20,34,35,36	0
3	GOL	B	408	6/6	0.91	0.17	4.18	12,20,23,30	0
3	GOL	B	402	6/6	0.95	0.11	3.60	14,17,17,18	0
3	GOL	A	405	6/6	0.90	0.12	3.25	25,27,27,28	0
3	GOL	B	409	6/6	0.87	0.13	2.27	25,27,30,32	0
5	NCO	A	412	7/7	0.99	0.08	1.83	8,8,9,9	0
3	GOL	A	406	6/6	0.86	0.14	1.62	30,40,49,54	0
3	GOL	A	402	6/6	0.90	0.11	1.34	20,22,23,25	0
4	FMN	B	411	31/31	0.99	0.09	1.30	3,5,6,7	0
3	GOL	A	403	6/6	0.94	0.08	1.27	17,18,20,28	0
3	GOL	B	410	6/6	0.85	0.14	1.16	19,21,26,31	0
4	FMN	A	411	31/31	0.98	0.08	0.63	3,4,5,7	0
2	W7J	A	401	26/26	0.96	0.07	0.16	5,9,17,21	0
2	W7J	B	401[A]	26/26	0.95	0.12	0.07	5,8,16,16	26
2	W7J	B	401[B]	26/26	0.95	0.12	0.06	4,7,14,16	26
5	NCO	A	413	7/7	0.88	0.29	-	30,31,33,34	0
3	GOL	B	406	6/6	0.88	0.13	-	27,30,33,34	0
3	GOL	A	408	6/6	0.73	0.17	-	34,37,40,41	0
3	GOL	B	405	6/6	0.79	0.22	-	38,40,42,50	0
3	GOL	A	404	6/6	0.83	0.14	-	39,41,43,49	0
3	GOL	B	403	6/6	0.78	0.14	-	35,41,44,45	0

6.5 Other polymers (i)

There are no such residues in this entry.