



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:41 PM GMT

PDB ID : 3W7M
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with TT2-3-063
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 : 2013-03-02
Resolution : 2.40 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

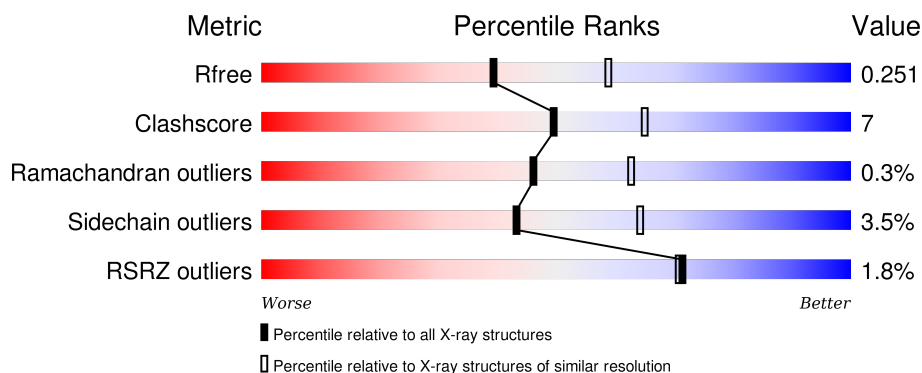
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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>86%13%</div> </div>
1	B	313	<div> <div>3%</div> <div>81%15%..</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	403	-	-	-	X
3	GOL	A	405	-	-	-	X
3	GOL	A	406	-	-	-	X
3	GOL	A	407	-	-	-	X
3	GOL	A	409	-	-	-	X
3	GOL	A	410	-	-	-	X
3	GOL	A	412	-	-	-	X

2 Entry composition [i](#)

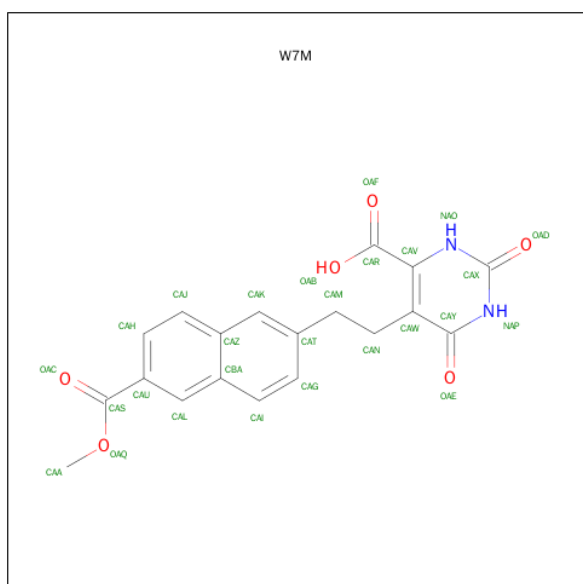
There are 6 unique types of molecules in this entry. The entry contains 5254 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-[6-(METHOXYCARBONYL)NAPHTHALEN-2-YL]ETHYL}-2,6-DI OXO-1,2,3,6-TETRAHYDOPYRIMIDINE-4-CARBOXYLIC ACID (three-letter code: W7M) (formula: C₁₉H₁₆N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	19	2	6		
2	B	1	Total	C	N	O	0	0
			27	19	2	6		

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



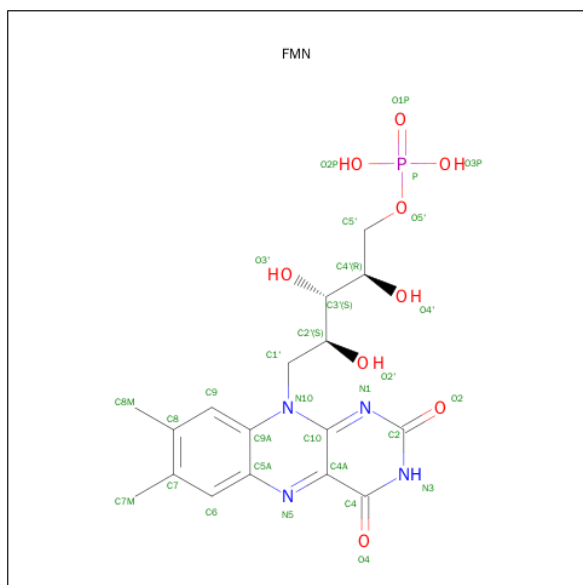
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

- 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	C	N	O	P	0	0
			31	17	4	9	1		
4	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 5 is COBALT HEXAMINE(III) (three-letter code: NCO) (formula: $CoH_{18}N_6$).



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

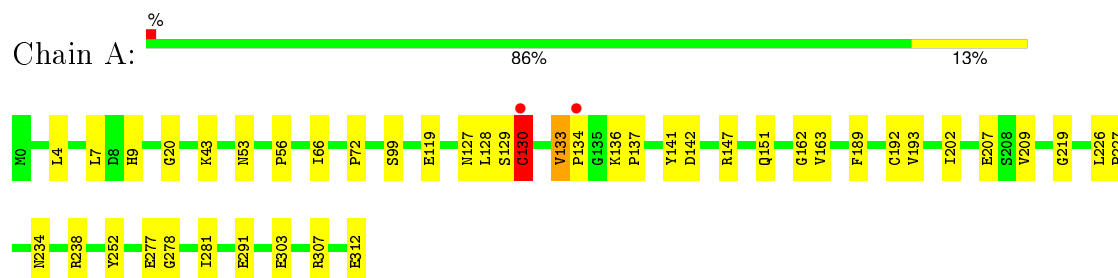
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	127	Total	O	0	0
			127	127		
6	B	126	Total	O	0	0
			126	126		

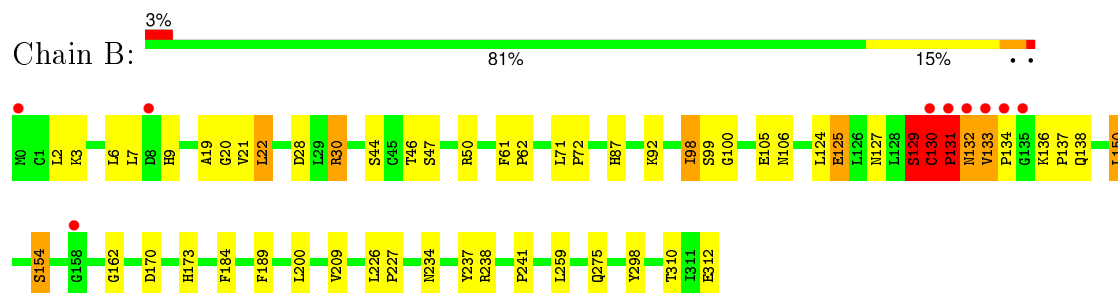
3 Residue-property plots

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 ($RSRZ > 2$). 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 72.01Å 129.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.18 – 2.40 48.18 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.8 (48.18-2.40) 89.8 (48.18-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.05 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.172 , 0.246 0.179 , 0.251	Depositor DCC
R_{free} test set	1180 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 23070 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5254	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 42.55 % 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 2.0059e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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, W7M, 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	0.83	2/2440 (0.1%)	0.86	4/3305 (0.1%)
1	B	0.79	2/2440 (0.1%)	0.85	5/3305 (0.2%)
All	All	0.81	4/4880 (0.1%)	0.85	9/6610 (0.1%)

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	B	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	PRO	N-CD	5.55	1.55	1.47
1	A	56	PRO	N-CD	5.34	1.55	1.47
1	B	137	PRO	N-CD	5.12	1.55	1.47
1	A	134	PRO	N-CD	5.08	1.54	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	PRO	CA-N-CD	-6.61	102.25	111.50
1	B	133	VAL	C-N-CD	6.02	141.04	128.40
1	A	130	CYS	C-N-CD	5.99	140.97	128.40
1	A	136	LYS	C-N-CD	5.79	140.55	128.40
1	B	136	LYS	C-N-CD	5.50	139.96	128.40
1	A	4	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	133	VAL	C-N-CD	5.35	139.64	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	LEU	CA-CB-CG	5.04	126.89	115.30
1	B	125	GLU	OE1-CD-OE2	-5.01	117.29	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	129	SER	Peptide
1	B	130	CYS	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	2388	0	2391	31	0
1	B	2388	0	2391	39	0
2	A	27	0	15	6	0
2	B	27	0	15	1	0
3	A	78	0	104	3	0
3	B	24	0	32	2	0
4	A	31	0	19	1	0
4	B	31	0	19	4	0
5	A	7	0	0	0	0
6	A	127	0	0	4	0
6	B	126	0	0	1	0
All	All	5254	0	4986	71	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 (71) 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:129:SER:HB3	6:A:615:HOH:O	1.70	0.90
1:A:53:ASN:HD21	2:A:401:W7M:H15	1.43	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:W7M:H11	2:A:401:W7M:H16	1.59	0.84
1:A:129:SER:CB	6:A:615:HOH:O	2.26	0.78
1:B:98:ILE:CD1	1:B:106:ASN:OD1	2.33	0.76
1:B:20:GLY:HA3	4:B:406:FMN:N5	2.07	0.70
1:A:53:ASN:ND2	2:A:401:W7M:H15	2.07	0.69
1:B:98:ILE:HD12	1:B:106:ASN:OD1	1.93	0.69
1:A:128:LEU:HD12	1:A:163:VAL:CG1	2.23	0.67
1:A:128:LEU:HD12	1:A:163:VAL:HG13	1.76	0.67
1:B:71:LEU:HD22	2:B:401:W7M:H9	1.79	0.63
1:A:141:TYR:CG	3:A:406:GOL:H2	2.34	0.63
1:B:20:GLY:HA3	4:B:406:FMN:C5A	2.28	0.63
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.46	0.62
1:A:53:ASN:HD21	2:A:401:W7M:CAA	2.12	0.62
1:A:226:LEU:HB3	1:A:227:PRO:HD3	1.84	0.60
1:B:21:VAL:HG13	1:B:275:GLN:HE21	1.71	0.56
1:B:87:HIS:HE1	1:B:92:LYS:O	1.90	0.55
1:A:7:LEU:O	1:A:9:HIS:HD2	1.89	0.55
1:B:7:LEU:O	1:B:9:HIS:HD2	1.91	0.54
2:A:401:W7M:H16	2:A:401:W7M:CAL	2.35	0.53
1:B:30:ARG:HB3	1:B:30:ARG:HH11	1.73	0.52
1:B:99:SER:HB2	1:B:127:ASN:HB3	1.92	0.52
1:A:147:ARG:O	1:A:151:GLN:HG3	2.11	0.51
1:B:162:GLY:HA3	1:B:189:PHE:CZ	2.47	0.50
1:B:124:LEU:HD12	1:B:125:GLU:N	2.27	0.50
1:B:226:LEU:HB3	1:B:227:PRO:HD3	1.94	0.50
1:B:150:LEU:O	1:B:154:SER:OG	2.26	0.50
1:B:100:GLY:HA3	1:B:105:GLU:HG2	1.93	0.50
1:B:237:TYR:CE2	3:B:405:GOL:H2	2.47	0.49
1:B:22:LEU:O	1:B:28:ASP:HB3	2.12	0.49
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.11	0.49
1:A:7:LEU:O	1:A:9:HIS:CD2	2.66	0.49
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.61	0.49
1:A:43:LYS:HE2	1:A:72:PRO:O	2.13	0.49
1:B:130:CYS:SG	1:B:131:PRO:HD3	2.52	0.49
1:B:20:GLY:CA	4:B:406:FMN:N5	2.74	0.48
1:A:99:SER:HB2	1:A:127:ASN:HB3	1.94	0.48
1:B:129:SER:O	1:B:138:GLN:NE2	2.47	0.47
1:B:241:PRO:HA	3:B:405:GOL:H32	1.96	0.47
1:A:162:GLY:HA3	1:A:189:PHE:CZ	2.49	0.47
1:B:132:ASN:HD22	1:B:132:ASN:N	2.13	0.46
1:A:129:SER:HB2	6:A:615:HOH:O	2.03	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:SER:HB3	1:B:99:SER:HB3	1.98	0.46
1:A:137:PRO:HG2	1:A:142:ASP:HB2	1.98	0.45
1:A:277:GLU:OE1	1:A:281:ILE:HD12	2.17	0.45
1:B:170:ASP:HB3	1:B:173:HIS:ND1	2.32	0.44
1:B:133:VAL:CG1	1:B:134:PRO:CD	2.96	0.44
1:A:209:VAL:HG22	1:B:310:THR:HA	1.98	0.44
3:A:405:GOL:H11	6:A:534:HOH:O	2.17	0.44
1:A:202:ILE:HB	1:B:259:LEU:HD22	1.99	0.44
1:A:20:GLY:HA3	4:A:415:FMN:N5	2.33	0.43
1:A:192:CYS:HA	1:A:193:VAL:HA	1.85	0.43
1:A:128:LEU:HD12	1:A:163:VAL:HG11	1.97	0.43
1:B:71:LEU:N	1:B:72:PRO:CD	2.80	0.43
1:A:207:GLU:OE1	1:B:298:TYR:OH	2.34	0.43
1:A:278:GLY:O	1:A:281:ILE:HG22	2.19	0.43
1:B:184:PHE:HB3	6:B:502:HOH:O	2.18	0.42
2:A:401:W7M:H11	2:A:401:W7M:CAA	2.41	0.42
1:B:162:GLY:HA3	1:B:189:PHE:CE1	2.54	0.42
1:A:66:ILE:HA	1:A:219:GLY:O	2.20	0.42
1:A:128:LEU:CD1	1:A:163:VAL:HG13	2.46	0.42
1:B:22:LEU:C	1:B:28:ASP:HB3	2.41	0.42
1:B:19:ALA:O	4:B:406:FMN:C10	2.69	0.41
1:B:46:THR:HG21	1:B:50:ARG:HD2	2.02	0.41
1:A:99:SER:HG	1:A:130:CYS:HG	1.68	0.41
1:B:200:LEU:HD11	1:B:209:VAL:HG12	2.03	0.41
1:A:128:LEU:HA	1:A:128:LEU:HD23	1.78	0.41
1:B:61:PHE:HB3	1:B:62:PRO:HD2	2.02	0.40
1:A:252:TYR:HB3	3:A:412:GOL:H2	2.02	0.40
1:B:133:VAL:HG13	1:B:134:PRO:HD3	2.03	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%)	301 (97%)	10 (3%)	0	100	100
1	B	311/313 (99%)	300 (96%)	9 (3%)	2 (1%)	30	43
All	All	622/626 (99%)	601 (97%)	19 (3%)	2 (0%)	46	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	131	PRO
1	B	130	CYS

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	258/258 (100%)	251 (97%)	7 (3%)	52	73
1	B	258/258 (100%)	247 (96%)	11 (4%)	35	55
All	All	516/516 (100%)	498 (96%)	18 (4%)	43	64

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

Mol	Chain	Res	Type
1	A	119	GLU
1	A	130	CYS
1	A	133	VAL
1	A	291	GLU
1	A	303	GLU
1	A	307	ARG
1	A	312	GLU
1	B	2	LEU
1	B	3	LYS
1	B	6	LEU
1	B	30	ARG
1	B	47	SER
1	B	98	ILE
1	B	129	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	132	ASN
1	B	150	LEU
1	B	154	SER
1	B	312	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	53	ASN
1	A	87	HIS
1	A	138	GLN
1	A	215	GLN
1	A	234	ASN
1	A	275	GLN
1	B	9	HIS
1	B	87	HIS
1	B	132	ASN
1	B	138	GLN
1	B	152	GLN
1	B	234	ASN
1	B	275	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

22 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	W7M	A	401	-	24,29,29	2.52	7 (29%)	28,41,41	2.58	7 (25%)
3	GOL	A	402	-	5,5,5	0.44	0	5,5,5	0.79	0
3	GOL	A	403	-	5,5,5	0.40	0	5,5,5	0.67	0
3	GOL	A	404	-	5,5,5	0.28	0	5,5,5	0.33	0
3	GOL	A	405	-	5,5,5	0.40	0	5,5,5	0.69	0
3	GOL	A	406	-	5,5,5	0.49	0	5,5,5	0.75	0
3	GOL	A	407	-	5,5,5	0.43	0	5,5,5	0.48	0
3	GOL	A	408	-	5,5,5	0.33	0	5,5,5	0.28	0
3	GOL	A	409	-	5,5,5	0.28	0	5,5,5	0.30	0
3	GOL	A	410	-	5,5,5	0.58	0	5,5,5	0.58	0
3	GOL	A	411	-	5,5,5	0.29	0	5,5,5	0.26	0
3	GOL	A	412	-	5,5,5	0.31	0	5,5,5	0.22	0
3	GOL	A	413	-	5,5,5	0.38	0	5,5,5	0.36	0
3	GOL	A	414	-	5,5,5	0.55	0	5,5,5	1.28	0
4	FMN	A	415	-	32,33,33	1.40	5 (15%)	34,50,50	2.11	8 (23%)
5	NCO	A	416	-	6,6,6	0.73	0	0,15,15	0.00	-
2	W7M	B	401	-	24,29,29	2.55	7 (29%)	28,41,41	2.35	5 (17%)
3	GOL	B	402	-	5,5,5	0.35	0	5,5,5	0.56	0
3	GOL	B	403	-	5,5,5	0.22	0	5,5,5	0.56	0
3	GOL	B	404	-	5,5,5	0.25	0	5,5,5	0.30	0
3	GOL	B	405	-	5,5,5	0.31	0	5,5,5	0.44	0
4	FMN	B	406	-	32,33,33	1.73	8 (25%)	34,50,50	2.69	11 (32%)

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	W7M	A	401	-	-	0/11/15/15	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	GOL	A	414	-	-	0/4/4/4	0/0/0/0
4	FMN	A	415	-	-	0/18/18/18	0/3/3/3
5	NCO	A	416	-	-	0/0/0/0	0/0/0/0
2	W7M	B	401	-	-	0/11/15/15	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
4	FMN	B	406	-	-	0/18/18/18	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	W7M	CAN-CAW	-9.02	1.40	1.52
2	B	401	W7M	CAN-CAW	-6.83	1.43	1.52
2	B	401	W7M	CAM-CAT	-3.96	1.40	1.51
2	B	401	W7M	CAU-CAS	-3.85	1.40	1.49
4	A	415	FMN	C1'-N10	-3.57	1.44	1.48
2	A	401	W7M	CAM-CAT	-3.06	1.42	1.51
4	B	406	FMN	C1'-N10	-2.64	1.45	1.48
4	B	406	FMN	P-O2P	-2.38	1.46	1.54
4	B	406	FMN	C6-C5A	-2.30	1.38	1.41
2	A	401	W7M	CAU-CAS	-2.21	1.44	1.49
2	A	401	W7M	CAI-CAG	2.02	1.40	1.36
2	B	401	W7M	CAI-CAG	2.15	1.41	1.36
2	B	401	W7M	CAX-NAO	2.30	1.43	1.38
4	B	406	FMN	C9A-N10	2.42	1.42	1.38
2	A	401	W7M	CAL-CAU	2.46	1.41	1.37
4	A	415	FMN	C4-C4A	2.53	1.46	1.41
4	A	415	FMN	C8-C7	2.55	1.47	1.41
4	A	415	FMN	C4A-C10	2.81	1.46	1.40
4	A	415	FMN	C9A-C5A	3.06	1.49	1.42
4	B	406	FMN	C4-C4A	3.22	1.47	1.41
4	B	406	FMN	C8-C7	3.36	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	W7M	CAV-NAO	3.38	1.40	1.34
4	B	406	FMN	C9A-C5A	3.59	1.50	1.42
2	A	401	W7M	CAY-NAP	4.12	1.40	1.33
4	B	406	FMN	C4A-C10	4.12	1.48	1.40
2	B	401	W7M	CAY-NAP	4.74	1.41	1.33
2	B	401	W7M	CAV-NAO	5.40	1.43	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	406	FMN	C4-C4A-C10	-6.98	115.47	119.94
2	B	401	W7M	NAP-CAX-NAO	-5.52	118.39	127.69
2	A	401	W7M	NAP-CAX-NAO	-5.43	118.54	127.69
2	B	401	W7M	CAM-CAN-CAW	-4.34	104.85	112.47
4	B	406	FMN	C4A-C4-N3	-4.25	117.96	123.52
4	A	415	FMN	C4A-C4-N3	-4.24	117.98	123.52
4	B	406	FMN	N3-C2-N1	-3.51	121.79	127.69
2	A	401	W7M	CAM-CAN-CAW	-2.95	107.29	112.47
4	A	415	FMN	C4-C4A-C10	-2.92	118.07	119.94
4	A	415	FMN	N3-C2-N1	-2.91	122.79	127.69
2	A	401	W7M	OAQ-CAS-OAC	-2.81	117.62	123.45
4	A	415	FMN	O5'-P-O1P	-2.66	100.40	107.08
4	B	406	FMN	O5'-P-O1P	-2.63	100.47	107.08
2	A	401	W7M	CAH-CAU-CAL	-2.62	115.82	119.26
4	A	415	FMN	C4A-C10-N10	-2.47	118.72	120.52
4	B	406	FMN	O2'-C2'-C1'	-2.20	104.50	109.93
4	B	406	FMN	C5A-C9A-N10	2.03	119.10	117.58
2	B	401	W7M	CAK-CAZ-CBA	2.29	121.95	118.92
4	B	406	FMN	C1'-N10-C9A	2.38	121.59	118.83
4	A	415	FMN	O2P-P-O1P	2.68	119.36	110.63
4	B	406	FMN	O3P-P-O1P	2.68	119.39	110.63
4	B	406	FMN	C4A-N5-C5A	3.58	120.94	116.72
4	B	406	FMN	C4-C4A-N5	3.90	123.44	118.70
4	A	415	FMN	C4A-N5-C5A	4.00	121.44	116.72
2	B	401	W7M	CAX-NAO-CAV	4.22	119.91	115.68
2	A	401	W7M	CAX-NAO-CAV	4.70	120.39	115.68
2	A	401	W7M	OAQ-CAS-CAU	4.93	120.73	112.37
4	A	415	FMN	C4-N3-C2	7.67	121.56	115.16
2	B	401	W7M	CAY-NAP-CAX	7.73	121.61	115.16
2	A	401	W7M	CAY-NAP-CAX	8.47	122.22	115.16
4	B	406	FMN	C4-N3-C2	9.84	123.37	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	W7M	6	0
3	A	405	GOL	1	0
3	A	406	GOL	1	0
3	A	412	GOL	1	0
4	A	415	FMN	1	0
2	B	401	W7M	1	0
3	B	405	GOL	2	0
4	B	406	FMN	4	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%)	-0.35	2 (0%) 90 90	15, 25, 46, 66	0
1	B	313/313 (100%)	-0.23	9 (2%) 55 54	16, 27, 47, 97	0
All	All	626/626 (100%)	-0.29	11 (1%) 71 71	15, 26, 47, 97	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	GLY	5.6
1	B	133	VAL	3.8
1	B	131	PRO	2.9
1	B	158	GLY	2.8
1	B	132	ASN	2.8
1	A	130	CYS	2.6
1	B	130	CYS	2.6
1	A	134	PRO	2.5
1	B	8	ASP	2.4
1	B	0	MET	2.2
1	B	134	PRO	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 ⓘ

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	0.57	0.78	17.47	52,57,61,63	0
3	GOL	A	406	6/6	0.69	0.49	17.37	58,63,64,65	0
3	GOL	A	407	6/6	0.68	0.38	8.52	56,63,65,74	0
3	GOL	A	409	6/6	0.83	0.22	7.76	43,48,50,51	0
3	GOL	A	405	6/6	0.92	0.35	7.18	45,50,51,56	0
3	GOL	A	412	6/6	0.85	0.24	6.38	49,52,55,56	0
3	GOL	A	403	6/6	0.85	0.33	5.37	59,61,62,64	0
3	GOL	A	402	6/6	0.92	0.20	4.34	29,30,32,32	0
3	GOL	A	408	6/6	0.89	0.18	1.46	59,60,61,65	0
3	GOL	B	403	6/6	0.94	0.17	0.92	38,41,43,46	0
5	NCO	A	416	7/7	0.98	0.14	0.69	23,25,26,26	0
3	GOL	B	402	6/6	0.93	0.16	0.57	31,33,36,39	0
2	W7M	A	401	27/27	0.93	0.16	0.56	22,27,40,41	0
2	W7M	B	401	27/27	0.92	0.20	0.54	20,32,51,54	0
4	FMN	A	415	31/31	0.97	0.14	0.34	15,20,24,25	0
4	FMN	B	406	31/31	0.97	0.12	-0.33	15,20,23,23	0
3	GOL	A	414	6/6	0.83	0.23	-	39,43,47,53	0
3	GOL	B	405	6/6	0.91	0.19	-	48,54,56,61	0
3	GOL	B	404	6/6	0.80	0.40	-	71,71,76,81	0
3	GOL	A	404	6/6	0.89	0.20	-	52,57,58,58	0
3	GOL	A	411	6/6	0.78	0.19	-	71,74,75,77	0
3	GOL	A	413	6/6	0.86	0.19	-	50,52,53,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.