Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:17 pm BST

PDB ID	:	1PM7
Title	:	RmlC (dTDP-6-DEOXY-D-XYLO-4-HEXULOSE 3,5-EPIMERASE)STRUCTURE FROM MYCOBACTERIUM TUBERCULOSIS AND INHIBITOR DESIGN. THE APO STRUCTURE.
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Deposited on	:	2003-06-10
Resolution	:	2.20 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

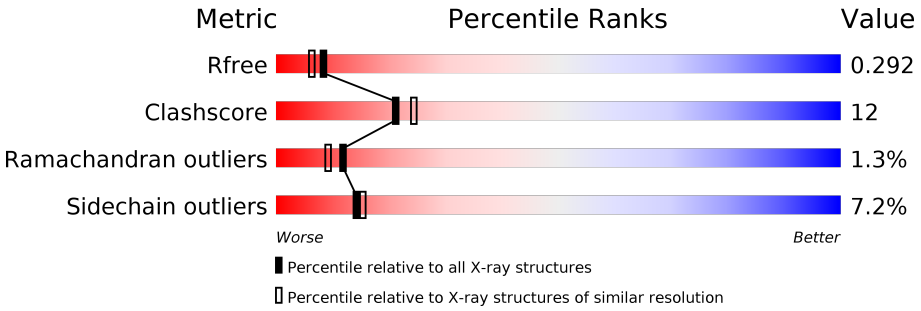
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 respectively. 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%

Mol	Chain	Length	Quality of chain
1	A	202	75% 16% 6% •
1	B	202	74% 18% 5% ••

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	B	251	-	-	X	-

2 Entry composition

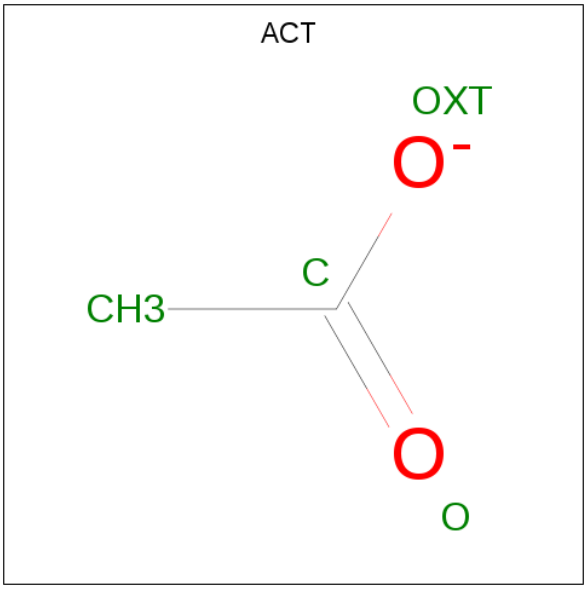
There are 4 unique types of molecules in this entry. The entry contains 3275 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RFBC.

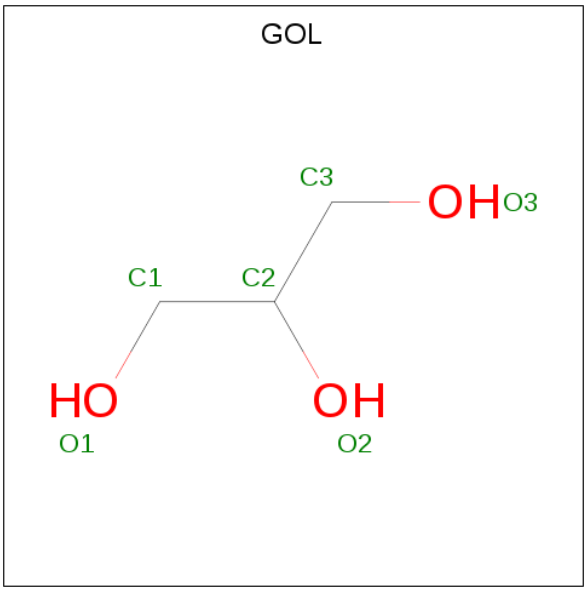
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1550	976	271	296	7			
1	B	199	Total	C	N	O	S	0	0	0
			1550	976	271	296	7			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

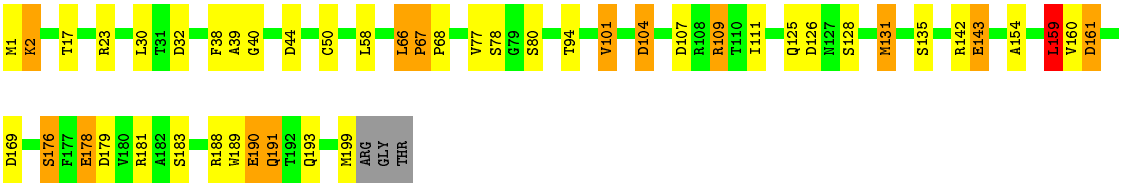
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	84	Total O 84 84	0	0
4	B	71	Total O 71 71	0	0

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

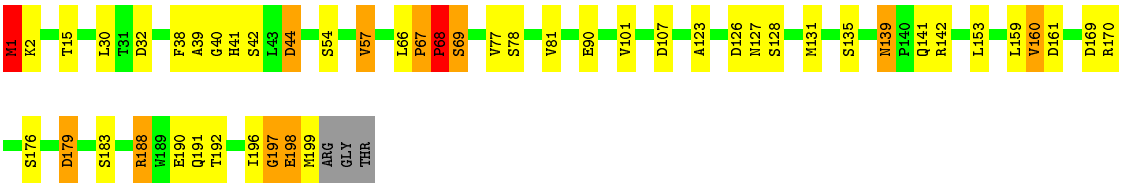
- Molecule 1: RFBC

Chain A:



- Molecule 1: RFBC

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	66.07Å 66.07Å 87.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.80 – 2.20 34.78 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (56.80-2.20) 99.8 (34.78-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.207 , 0.283 0.296 , 0.292	Depositor DCC
R_{free} test set	1110 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 10.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l 0.488 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3275	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, ACT

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	0.81	1/1590 (0.1%)	1.01	8/2168 (0.4%)
1	B	0.89	2/1590 (0.1%)	1.03	14/2168 (0.6%)
All	All	0.85	3/3180 (0.1%)	1.02	22/4336 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	N-CA	14.91	1.76	1.46
1	A	143	GLU	CD-OE2	6.54	1.32	1.25
1	B	44	ASP	CB-CG	-5.79	1.39	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1	MET	N-CA-CB	8.04	125.08	110.60
1	B	44	ASP	CB-CG-OD2	7.30	124.87	118.30
1	B	68	PRO	N-CD-CG	-6.45	93.52	103.20
1	A	107	ASP	CB-CG-OD2	6.36	124.03	118.30
1	A	169	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	44	ASP	CB-CG-OD1	-6.10	112.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	179	ASP	CB-CG-OD1	5.95	123.66	118.30
1	B	170	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	109	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	104	ASP	CB-CG-OD1	5.77	123.49	118.30
1	B	126	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	68	PRO	N-CA-C	5.32	125.94	112.10
1	B	107	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	160	VAL	CB-CA-C	5.29	121.45	111.40
1	A	126	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	32	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	197	GLY	O-C-N	5.16	130.96	122.70
1	A	161	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	169	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	131	MET	CG-SD-CE	-5.11	92.03	100.20
1	B	32	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	198	GLU	CA-C-N	-5.03	106.14	117.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	LEU	Peptide
1	A	66	LEU	Peptide
1	B	67	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1550	0	1482	32	0
1	B	1550	0	1482	42	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	6	0	8	3	0
3	B	6	0	8	5	0
4	A	84	0	0	6	0
4	B	71	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3275	0	2986	74	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 12.

All (74) 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:1:MET:N	1:B:1:MET:CA	1.76	1.47
1:B:2:LYS:NZ	4:B:322:HOH:O	1.95	0.98
1:B:1:MET:N	1:B:15:THR:O	1.98	0.96
1:B:196:ILE:O	1:B:198:GLU:O	1.96	0.83
1:B:160:VAL:HG12	1:B:161:ASP:OD1	1.77	0.82
1:A:40:GLY:O	1:A:199:MET:CE	2.41	0.68
1:B:197:GLY:HA2	4:B:328:HOH:O	1.95	0.67
1:A:40:GLY:O	1:A:199:MET:HE2	1.96	0.66
1:A:109:ARG:HD3	4:A:287:HOH:O	1.94	0.66
1:B:1:MET:HB2	4:B:301:HOH:O	1.98	0.64
1:A:178:GLU:HG2	4:A:271:HOH:O	1.99	0.63
1:A:30:LEU:HD22	4:B:324:HOH:O	1.97	0.62
1:B:30:LEU:HA	3:B:251:GOL:H31	1.82	0.62
1:A:50:CYS:HB2	1:A:131:MET:CE	2.30	0.61
1:A:101:VAL:CG1	1:A:111:ILE:HD12	2.30	0.61
1:A:44:ASP:O	1:A:135:SER:HA	2.00	0.61
1:B:66:LEU:O	1:B:69:SER:N	2.34	0.60
1:B:139:ASN:HD21	1:B:141:GLN:HB3	1.66	0.59
1:B:54:SER:O	1:B:57:VAL:HG13	2.03	0.58
1:A:101:VAL:HG13	1:A:111:ILE:HD12	1.86	0.58
1:B:1:MET:HG2	3:B:251:GOL:C1	2.33	0.58
1:A:2:LYS:CE	3:A:250:GOL:O1	2.51	0.57
1:B:1:MET:HG2	3:B:251:GOL:H12	1.85	0.57
1:B:66:LEU:O	1:B:68:PRO:C	2.44	0.56
3:B:251:GOL:H2	4:B:309:HOH:O	2.06	0.56
1:A:159:LEU:C	1:A:161:ASP:H	2.09	0.55
1:B:139:ASN:HD22	1:B:142:ARG:H	1.55	0.54
1:B:66:LEU:HA	1:B:69:SER:HB2	1.89	0.54
1:B:1:MET:HA	1:B:1:MET:N	2.08	0.53
1:A:190:GLU:HA	1:A:190:GLU:OE1	2.08	0.53
1:B:153:LEU:HB2	4:B:270:HOH:O	2.08	0.53
1:B:44:ASP:O	1:B:44:ASP:OD1	2.26	0.52
1:A:80:SER:OG	1:A:125:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HD13	4:B:324:HOH:O	2.10	0.52
1:B:81:VAL:HG12	1:B:123:ALA:HA	1.92	0.52
1:B:66:LEU:O	1:B:67:PRO:C	2.46	0.52
1:A:2:LYS:HE2	3:A:250:GOL:O1	2.11	0.51
1:A:40:GLY:O	1:A:199:MET:HE3	2.11	0.51
1:B:198:GLU:O	1:B:199:MET:HG3	2.11	0.50
1:A:66:LEU:HG	1:A:67:PRO:CD	2.41	0.50
1:A:17:THR:OG1	3:A:250:GOL:H2	2.12	0.50
1:A:189:TRP:O	1:A:193:GLN:HG3	2.12	0.49
1:A:159:LEU:HD21	4:A:338:HOH:O	2.12	0.48
1:B:66:LEU:O	1:B:66:LEU:HD12	2.13	0.48
1:A:181:ARG:HD3	4:A:306:HOH:O	2.13	0.48
1:A:66:LEU:HD23	1:A:191:GLN:HG3	1.94	0.48
1:B:160:VAL:HG12	1:B:161:ASP:N	2.29	0.48
1:A:77:VAL:HG21	1:B:77:VAL:HG21	1.94	0.48
1:A:154:ALA:HA	4:A:315:HOH:O	2.16	0.46
1:B:41:HIS:HD2	1:B:42:SER:O	1.99	0.45
1:A:50:CYS:HB2	1:A:131:MET:HE1	1.96	0.45
1:A:68:PRO:HD2	4:A:322:HOH:O	2.15	0.45
1:A:38:PHE:CD1	1:A:39:ALA:N	2.85	0.45
1:A:176:SER:O	1:A:179:ASP:HB2	2.17	0.44
1:B:40:GLY:O	1:B:199:MET:CE	2.66	0.44
1:B:142:ARG:NE	4:B:325:HOH:O	2.50	0.43
1:B:190:GLU:OE1	1:B:190:GLU:HA	2.18	0.43
1:B:38:PHE:CD1	1:B:38:PHE:C	2.92	0.42
1:B:40:GLY:O	1:B:199:MET:HE3	2.19	0.42
1:B:78:SER:O	1:B:128:SER:HA	2.20	0.42
1:A:159:LEU:C	1:A:161:ASP:N	2.72	0.42
1:B:139:ASN:HD22	1:B:139:ASN:C	2.23	0.42
1:A:78:SER:O	1:A:128:SER:HA	2.19	0.42
1:B:1:MET:H2	1:B:15:THR:C	2.06	0.41
1:A:80:SER:HB3	1:A:104:ASP:HB3	2.02	0.41
1:B:66:LEU:HD23	1:B:191:GLN:HG3	2.01	0.41
1:B:188:ARG:O	1:B:192:THR:HG23	2.21	0.41
1:B:54:SER:O	1:B:57:VAL:CG1	2.69	0.41
1:A:67:PRO:O	1:A:142:ARG:NH2	2.46	0.40
1:B:176:SER:O	1:B:179:ASP:HB2	2.20	0.40
1:B:1:MET:HG2	3:B:251:GOL:H11	2.03	0.40
1:B:38:PHE:CD1	1:B:39:ALA:N	2.89	0.40
1:B:41:HIS:HE1	4:B:273:HOH:O	2.03	0.40
1:B:44:ASP:O	1:B:135:SER:HA	2.22	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	197/202 (98%)	188 (95%)	7 (4%)	2 (1%)	15 14
1	B	197/202 (98%)	191 (97%)	3 (2%)	3 (2%)	10 8
All	All	394/404 (98%)	379 (96%)	10 (2%)	5 (1%)	12 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	PRO
1	A	159	LEU
1	B	68	PRO
1	B	160	VAL
1	B	69	SER

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	167/169 (99%)	152 (91%)	15 (9%)	9 9
1	B	167/169 (99%)	158 (95%)	9 (5%)	22 26
All	All	334/338 (99%)	310 (93%)	24 (7%)	14 15

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	23	ARG
1	A	58	LEU
1	A	94	THR
1	A	101	VAL
1	A	131	MET
1	A	143	GLU
1	A	159	LEU
1	A	176	SER
1	A	178	GLU
1	A	183	SER
1	A	188	ARG
1	A	190	GLU
1	A	191	GLN
1	B	1	MET
1	B	57	VAL
1	B	90	GLU
1	B	101	VAL
1	B	127	ASN
1	B	139	ASN
1	B	159	LEU
1	B	183	SER
1	B	188	ARG

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	41	HIS
1	A	62	HIS
1	A	125	GLN
1	A	141	GLN
1	A	191	GLN
1	A	193	GLN
1	B	41	HIS
1	B	62	HIS
1	B	70	GLN
1	B	125	GLN
1	B	127	ASN
1	B	139	ASN
1	B	141	GLN
1	B	191	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

4 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	$\#\|Z\| > 2$
3	GOL	B	251	-	5,5,5	0.51	0	5,5,5	0.82	0
2	ACT	B	261	-	1,3,3	1.32	0	0,3,3	0.00	-
2	ACT	A	260	-	1,3,3	1.29	0	0,3,3	0.00	-
3	GOL	A	250	-	5,5,5	0.30	0	5,5,5	0.66	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	251	-	-	4/4/4/4	-
3	GOL	A	250	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	251	GOL	O1-C1-C2-C3
3	B	251	GOL	C1-C2-C3-O3
3	A	250	GOL	O1-C1-C2-C3
3	B	251	GOL	O1-C1-C2-O2
3	B	251	GOL	O2-C2-C3-O3
3	A	250	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	251	GOL	5	0
3	A	250	GOL	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.