Full wwPDB X-ray Structure Validation Report (i)

Oct 14, 2023 – 10:54 PM EDT

PDB ID	:	8CZQ
Title	:	The crystal structure of MtbTOP1 in complex with both G- and T-segments
Authors	:	Tan, K.; Tse-Dinh, Y.-C.
Deposited on	:	2022-05-25
Resolution	:	2.78 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

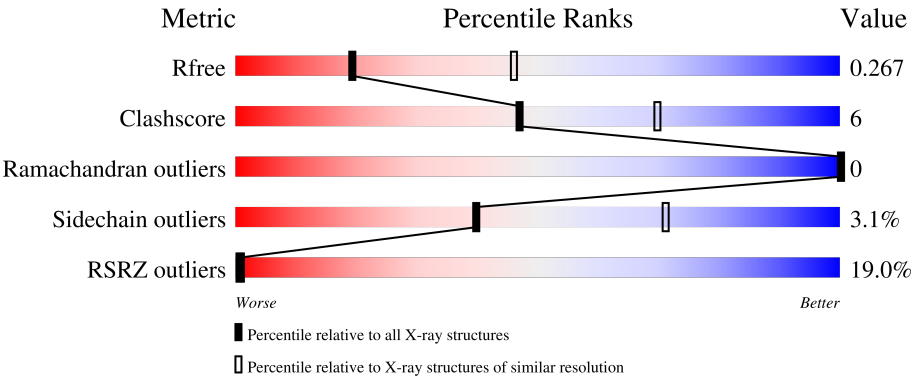
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 of 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% 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	706	18% 79% 13% 7%
2	B	12	50% 50%
2	C	12	8% 67% 33%
2	D	12	42% 50% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5690 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 DNA topoisomerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	0	0	0
			4930	3095	895	933	7			

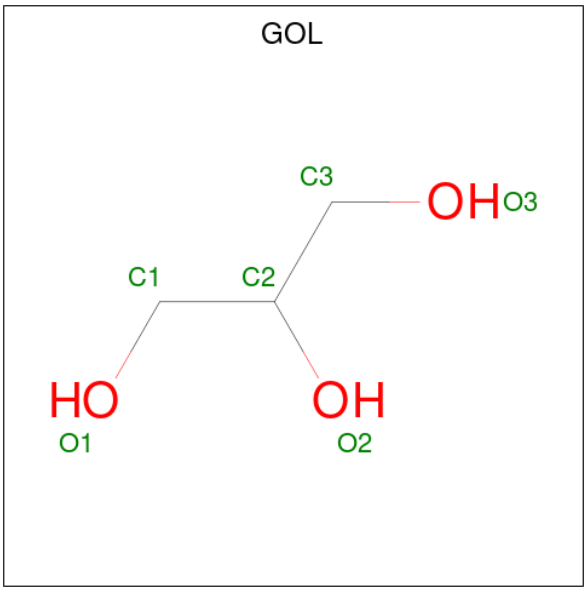
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0A0E8VY41
A	0	ASN	-	expression tag	UNP A0A0E8VY41
A	1	ALA	-	expression tag	UNP A0A0E8VY41

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*TP*TP*CP*CP*GP*CP*TP*TP*GP*AP*C)-3').

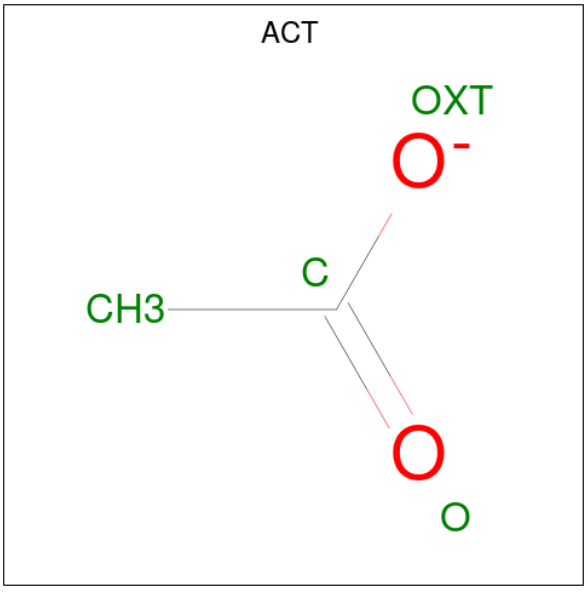
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	P	0	0	0
			237	115	38	73	11			
2	C	12	Total	C	N	O	P	0	0	0
			240	115	38	75	12			
2	D	11	Total	C	N	O	P	0	0	0
			221	106	35	69	11			

- 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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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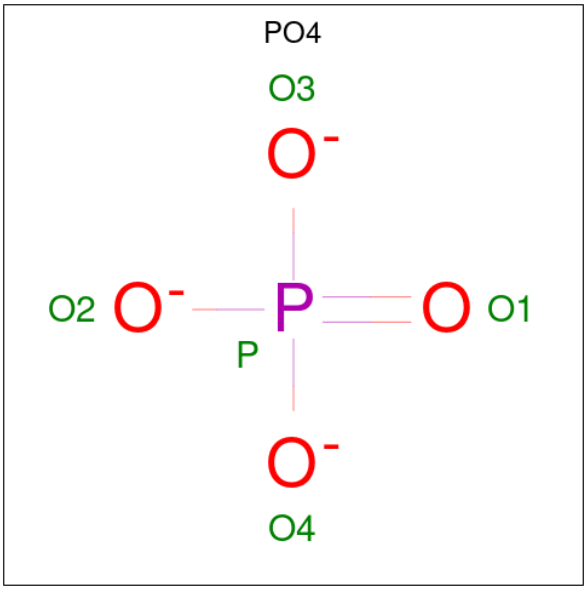
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	C	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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: DNA topoisomerase 1

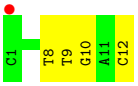
Chain A:

• Molecule 2: DNA (5'-D(*CP*TP*TP*CP*CP*GP*CP*TP*TP*GP*AP*C)-3')

Chain B:

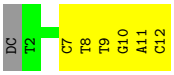
• Molecule 2: DNA (5'-D(*CP*TP*TP*CP*CP*GP*CP*TP*TP*GP*AP*C)-3')

Chain C:



• Molecule 2: DNA (5'-D(*CP*TP*TP*CP*CP*GP*CP*TP*TP*GP*AP*C)-3')

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	92.50Å 98.63Å 104.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.25 – 2.78 46.25 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.25-2.78) 99.2 (46.25-2.78)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.248 , 0.269 0.245 , 0.267	Depositor DCC
R_{free} test set	1198 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	82.8	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5690	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: ACT, PO4, GOL

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	0.25	0/5025	0.53	0/6832
2	B	0.54	0/263	0.97	0/403
2	C	0.52	0/266	0.98	0/407
2	D	0.54	0/245	1.00	0/375
All	All	0.30	0/5799	0.62	0/8017

There are no bond length outliers.

There are no bond angle outliers.

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	4930	0	4724	58	1
2	B	237	0	138	5	0
2	C	240	0	137	6	0
2	D	221	0	126	6	0
3	A	6	0	8	0	0
4	A	16	0	12	0	0
5	A	20	0	0	0	0
5	C	5	0	0	0	0
5	D	15	0	0	0	0
All	All	5690	0	5145	67	1

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 (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:DT:H2"	2:D:9:DT:H5"	1.71	0.72
1:A:321:ARG:O	1:A:321:ARG:HD2	1.92	0.70
1:A:222:LEU:HD13	1:A:242:ARG:HB3	1.75	0.67
2:C:8:DT:H2"	2:C:9:DT:H5"	1.79	0.64
1:A:100:LEU:HD12	1:A:127:LEU:HD13	1.80	0.63
1:A:432:MET:SD	1:A:467:PHE:HB3	2.42	0.60
1:A:661:LYS:HD3	1:A:661:LYS:N	2.17	0.59
1:A:669:LEU:HD23	1:A:679:PRO:HB3	1.82	0.59
1:A:25:SER:HA	2:B:8:DT:H4'	1.85	0.58
1:A:352:GLU:HA	1:A:355:ILE:HG22	1.85	0.58
1:A:31:LYS:HG2	1:A:141:ILE:HG21	1.86	0.57
1:A:26:PRO:HB3	2:B:10:DG:C8	2.40	0.57
1:A:315:GLU:OE2	1:A:426:ARG:NH1	2.40	0.54
1:A:320:LEU:HB3	1:A:322:PHE:CD1	2.42	0.54
1:A:301:ARG:HB3	1:A:435:ALA:HB3	1.90	0.53
1:A:142:THR:O	1:A:146:ILE:HG13	2.08	0.53
1:A:429:ALA:HB1	1:A:467:PHE:HB2	1.90	0.53
1:A:27:THR:OG1	2:B:9:DT:OP1	2.18	0.52
2:C:10:DG:H21	2:D:10:DG:H1'	1.74	0.52
1:A:330:ILE:HD11	1:A:415:ASP:HB3	1.92	0.52
1:A:296:GLU:HG3	1:A:440:LEU:HD13	1.90	0.52
1:A:307:PHE:HZ	1:A:315:GLU:OE2	1.93	0.51
1:A:307:PHE:CZ	1:A:315:GLU:OE2	2.63	0.51
2:D:7:DC:H2'	2:D:8:DT:C6	2.46	0.51
1:A:320:LEU:HB3	1:A:322:PHE:HD1	1.77	0.50
1:A:118:ALA:HB2	1:A:164:GLN:HG2	1.93	0.50
1:A:207:GLU:O	1:A:211:MET:HG3	2.12	0.50
1:A:17:GLY:N	1:A:104:ASP:OD2	2.34	0.50
1:A:376:ARG:NH1	1:A:432:MET:O	2.45	0.49
1:A:318:ARG:HB3	1:A:319:LYS:HE3	1.94	0.49
1:A:349:THR:HG22	1:A:379:THR:HA	1.96	0.47
2:B:2:DT:H5'	2:B:3:DT:H72	1.97	0.47
1:A:518:THR:OG1	2:C:9:DT:OP1	2.24	0.46
2:D:11:DA:H5"	2:D:11:DA:C8	2.51	0.46
1:A:53:PRO:HG2	1:A:59:VAL:HG12	1.99	0.44
1:A:288:GLN:HA	1:A:500:ASP:HA	1.99	0.44
1:A:301:ARG:NH1	2:C:12:DC:OP1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:ALA:HA	1:A:641:VAL:HG22	1.98	0.44
1:A:318:ARG:NH1	2:C:10:DG:OP1	2.29	0.44
1:A:669:LEU:CD2	1:A:679:PRO:HB3	2.47	0.44
1:A:195:VAL:HG12	1:A:540:ILE:HG12	2.00	0.44
1:A:355:ILE:HD11	1:A:431:GLN:OE1	2.18	0.44
1:A:318:ARG:HE	1:A:319:LYS:HE3	1.84	0.43
1:A:519:GLU:O	1:A:523:VAL:HG13	2.18	0.43
1:A:355:ILE:HD12	1:A:355:ILE:HA	1.76	0.43
1:A:214:ARG:HH11	1:A:214:ARG:HG3	1.84	0.43
1:A:328:MET:O	1:A:332:GLN:HG3	2.18	0.43
1:A:273:ASP:OD1	1:A:273:ASP:N	2.42	0.43
1:A:201:ARG:NH1	1:A:578:VAL:HG13	2.34	0.43
2:C:9:DT:H2"	2:C:10:DG:O4'	2.19	0.43
1:A:436:ARG:H	1:A:464:PHE:HB3	1.84	0.43
1:A:667:GLU:HG3	1:A:681:ARG:HG2	2.00	0.42
1:A:645:LYS:CE	1:A:654:PRO:HB3	2.49	0.42
1:A:54:ARG:NH1	1:A:55:ALA:HB2	2.33	0.42
1:A:211:MET:HG2	1:A:691:ASP:HA	2.02	0.42
1:A:665:TYR:CE2	1:A:681:ARG:HD3	2.55	0.42
2:B:1:DC:H2"	2:B:2:DT:O5'	2.20	0.42
1:A:53:PRO:HD3	1:A:82:LEU:O	2.20	0.42
1:A:309:THR:HG22	1:A:345:THR:O	2.19	0.42
1:A:653:ARG:NH1	1:A:670:VAL:HG13	2.35	0.41
1:A:255:ARG:HH22	2:D:12:DC:P	2.42	0.41
1:A:246:VAL:HA	1:A:453:VAL:HA	2.02	0.41
1:A:301:ARG:HG2	1:A:467:PHE:HZ	1.86	0.41
1:A:204:VAL:O	1:A:208:ARG:HG2	2.21	0.41
1:A:424:TRP:CE2	1:A:428:VAL:HG21	2.56	0.41
1:A:410:ASP:OD1	1:A:411:GLY:N	2.48	0.40
2:D:10:DG:H2"	2:D:11:DA:H8	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLU:OE2	1:A:621:ARG:NH1[4_556]	2.16	0.04

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	643/706 (91%)	611 (95%)	32 (5%)	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	480/574 (84%)	465 (97%)	15 (3%)	40 71

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	63	TYR
1	A	64	LYS
1	A	174	TYR
1	A	264	ARG
1	A	319	LYS
1	A	321	ARG
1	A	361	GLN
1	A	407	ARG
1	A	416	ASP
1	A	426	ARG
1	A	539	SER
1	A	547	ARG

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Mol	Chain	Res	Type
1	A	605	ASN
1	A	647	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
5	PO4	A	807	-	4,4,4	0.91	0	6,6,6	0.43	0
4	ACT	A	802	-	3,3,3	1.29	0	3,3,3	1.39	0
5	PO4	A	809	-	4,4,4	0.91	0	6,6,6	0.43	0
3	GOL	A	801	-	5,5,5	0.92	0	5,5,5	1.01	0
4	ACT	A	805	-	3,3,3	1.32	0	3,3,3	1.40	0
5	PO4	A	808	-	4,4,4	0.91	0	6,6,6	0.43	0
5	PO4	D	101	-	4,4,4	0.91	0	6,6,6	0.43	0
4	ACT	A	803	-	3,3,3	1.31	0	3,3,3	1.38	0
5	PO4	D	103	-	4,4,4	0.92	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACT	A	804	-	3,3,3	1.34	0	3,3,3	1.39	0
5	PO4	C	101	-	4,4,4	0.91	0	6,6,6	0.43	0
5	PO4	D	102	-	4,4,4	0.91	0	6,6,6	0.43	0
5	PO4	A	806	-	4,4,4	0.91	0	6,6,6	0.43	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	A	801	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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

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, 95^{th} 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	655/706 (92%)	1.36	130 (19%) 1 0	49, 85, 178, 206	0
2	B	12/12 (100%)	0.54	0 100 100	52, 76, 129, 153	0
2	C	12/12 (100%)	0.15	1 (8%) 11 7	90, 112, 135, 142	0
2	D	11/12 (91%)	0.00	0 100 100	92, 114, 142, 152	0
All	All	690/742 (92%)	1.30	131 (18%) 1 1	49, 87, 177, 206	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	ALA	15.2
1	A	225	LEU	14.3
1	A	453	VAL	11.5
1	A	454	VAL	10.7
1	A	446	GLY	9.0
1	A	471	TYR	8.7
1	A	506	PRO	8.5
1	A	223	ALA	8.5
1	A	472	VAL	7.7
1	A	291	VAL	7.6
1	A	292	ALA	7.6
1	A	246	VAL	7.6
1	A	279	ALA	7.6
1	A	458	THR	7.6
1	A	455	PHE	7.1
1	A	220	ASP	7.0
1	A	239	PHE	7.0
1	A	442	LEU	6.9
1	A	249	ARG	6.7
1	A	468	LEU	6.6
1	A	505	THR	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	217	ALA	6.5
1	A	444	ILE	6.4
1	A	252	ALA	6.1
1	A	224	LYS	6.1
1	A	504	LEU	6.1
1	A	433	ALA	5.9
1	A	278	THR	5.4
1	A	221	ILE	5.3
1	A	495	PRO	5.2
1	A	218	TYR	5.2
1	A	467	PHE	5.0
1	A	509	HIS	5.0
1	A	503	GLU	4.9
1	A	502	VAL	4.8
1	A	222	LEU	4.8
1	A	253	THR	4.8
1	A	61	ALA	4.6
1	A	373	PRO	4.6
1	A	501	ILE	4.6
1	A	271	VAL	4.6
1	A	263	LEU	4.5
1	A	250	ARG	4.5
1	A	377	GLN	4.5
1	A	498	ARG	4.5
1	A	440	LEU	4.5
1	A	290	THR	4.4
1	A	443	ARG	4.3
1	A	457	ALA	4.3
1	A	386	GLN	4.3
1	A	355	ILE	4.3
1	A	242	ARG	4.2
1	A	492	HIS	4.2
1	A	431	GLN	4.2
1	A	456	SER	4.2
1	A	697	VAL	4.0
1	A	447	MET	4.0
1	A	102	ASP	3.8
1	A	251	VAL	3.8
1	A	296	GLU	3.8
1	A	672	GLY	3.7
1	A	383	LYS	3.7
1	A	670	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	369	GLU	3.5
1	A	63	TYR	3.5
1	A	382	VAL	3.5
1	A	243	LEU	3.5
1	A	41	ILE	3.5
1	A	257	PHE	3.5
1	A	133	VAL	3.5
1	A	130	ARG	3.4
1	A	465	PRO	3.4
1	A	241	ALA	3.3
1	A	277	ALA	3.3
1	A	693	LEU	3.3
1	A	280	LEU	3.3
1	A	273	ASP	3.3
1	A	434	ASP	3.3
1	A	240	SER	3.2
2	C	1	DC	3.2
1	A	260	LEU	3.2
1	A	248	GLY	3.2
1	A	270	ILE	3.1
1	A	445	THR	3.1
1	A	244	THR	3.0
1	A	272	LEU	2.9
1	A	376	ARG	2.9
1	A	405	VAL	2.9
1	A	430	SER	2.8
1	A	141	ILE	2.8
1	A	464	PHE	2.8
1	A	256	ASP	2.8
1	A	304	TYR	2.8
1	A	370	TYR	2.8
1	A	436	ARG	2.7
1	A	432	MET	2.7
1	A	101	LYS	2.7
1	A	300	ALA	2.7
1	A	254	GLY	2.7
1	A	399	PHE	2.6
1	A	276	SER	2.6
1	A	238	THR	2.6
1	A	374	ALA	2.5
1	A	511	THR	2.4
1	A	345	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	371	VAL	2.4
1	A	17	GLY	2.4
1	A	419	LEU	2.3
1	A	500	ASP	2.3
1	A	392	ILE	2.3
1	A	294	ALA	2.3
1	A	32	LEU	2.3
1	A	262	THR	2.2
1	A	210	ARG	2.2
1	A	19	ARG	2.2
1	A	651	HIS	2.2
1	A	362	ALA	2.2
1	A	675	GLY	2.1
1	A	20	LEU	2.1
1	A	106	LEU	2.1
1	A	307	PHE	2.1
1	A	417	PHE	2.1
1	A	375	PRO	2.1
1	A	489	ARG	2.1
1	A	422	LEU	2.1
1	A	424	TRP	2.1
1	A	107	TYR	2.0
1	A	494	THR	2.0
1	A	281	ALA	2.0
1	A	103	VAL	2.0
1	A	359	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
5	PO4	C	101	5/5	0.70	0.14	133,134,137,139	0
5	PO4	A	806	5/5	0.77	0.12	149,150,153,155	0
5	PO4	D	101	5/5	0.77	0.28	137,137,141,142	0
4	ACT	A	804	4/4	0.81	0.51	63,67,69,71	0
4	ACT	A	803	4/4	0.82	0.25	84,87,87,88	0
5	PO4	D	102	5/5	0.82	0.12	132,134,137,137	0
3	GOL	A	801	6/6	0.83	0.34	65,69,71,72	0
5	PO4	A	809	5/5	0.84	0.14	116,122,125,125	0
4	ACT	A	802	4/4	0.84	0.28	79,82,83,86	0
4	ACT	A	805	4/4	0.85	0.20	61,64,66,67	0
5	PO4	A	807	5/5	0.85	0.12	122,124,130,130	0
5	PO4	D	103	5/5	0.89	0.10	123,124,126,127	0
5	PO4	A	808	5/5	0.90	0.09	125,127,128,132	0

6.5 Other polymers (i)

There are no such residues in this entry.