Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 12:52 AM EDT

PDB ID	:	5VMK
Title	:	Crystal structure of a bifunctional GlmU UDP-N-acetylglucosamine diphosphorylase/glucosamine-1- phosphate N-acetyltransferase from Acinetobacter baumannii
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2017-04-27
Resolution	:	2.55 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

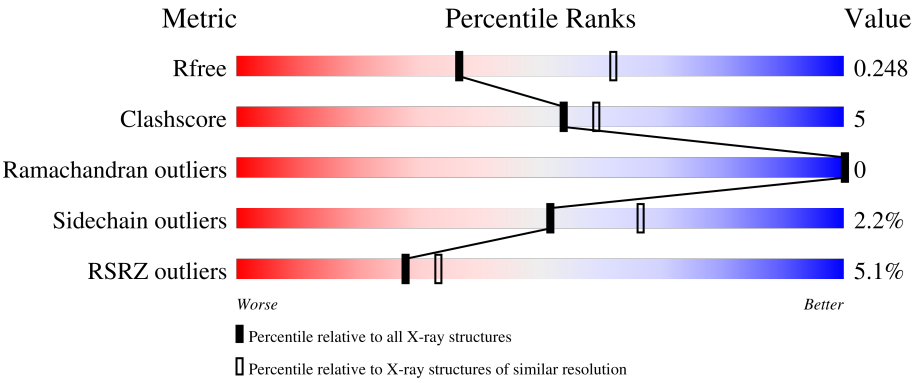
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	462	% 87% 10% • •
1	B	462	7% 82% 11% • 7%
1	C	462	7% 78% 11% • 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9670 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 Bifunctional protein GlmU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	1	0
			3294	2073	580	632	9			
1	B	430	Total	C	N	O	S	0	0	0
			3055	1920	544	583	8			
1	C	415	Total	C	N	O	S	0	0	0
			2930	1833	522	567	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP A0A0D5YCC7
A	-6	ALA	-	expression tag	UNP A0A0D5YCC7
A	-5	HIS	-	expression tag	UNP A0A0D5YCC7
A	-4	HIS	-	expression tag	UNP A0A0D5YCC7
A	-3	HIS	-	expression tag	UNP A0A0D5YCC7
A	-2	HIS	-	expression tag	UNP A0A0D5YCC7
A	-1	HIS	-	expression tag	UNP A0A0D5YCC7
A	0	HIS	-	expression tag	UNP A0A0D5YCC7
B	-7	MET	-	expression tag	UNP A0A0D5YCC7
B	-6	ALA	-	expression tag	UNP A0A0D5YCC7
B	-5	HIS	-	expression tag	UNP A0A0D5YCC7
B	-4	HIS	-	expression tag	UNP A0A0D5YCC7
B	-3	HIS	-	expression tag	UNP A0A0D5YCC7
B	-2	HIS	-	expression tag	UNP A0A0D5YCC7
B	-1	HIS	-	expression tag	UNP A0A0D5YCC7
B	0	HIS	-	expression tag	UNP A0A0D5YCC7
C	-7	MET	-	expression tag	UNP A0A0D5YCC7
C	-6	ALA	-	expression tag	UNP A0A0D5YCC7
C	-5	HIS	-	expression tag	UNP A0A0D5YCC7
C	-4	HIS	-	expression tag	UNP A0A0D5YCC7
C	-3	HIS	-	expression tag	UNP A0A0D5YCC7
C	-2	HIS	-	expression tag	UNP A0A0D5YCC7
C	-1	HIS	-	expression tag	UNP A0A0D5YCC7

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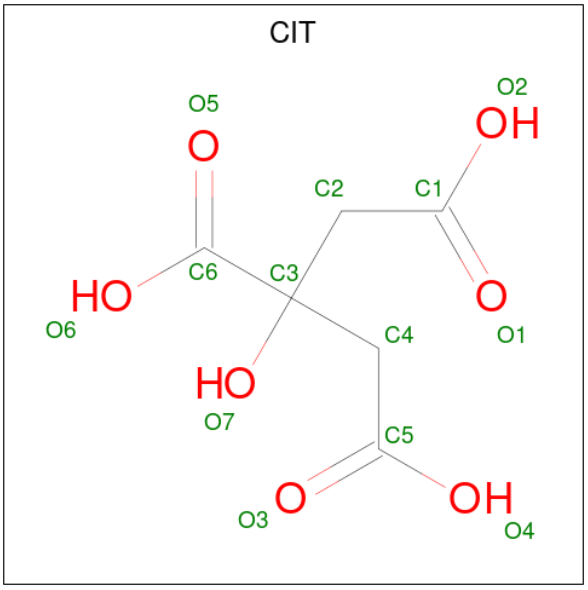
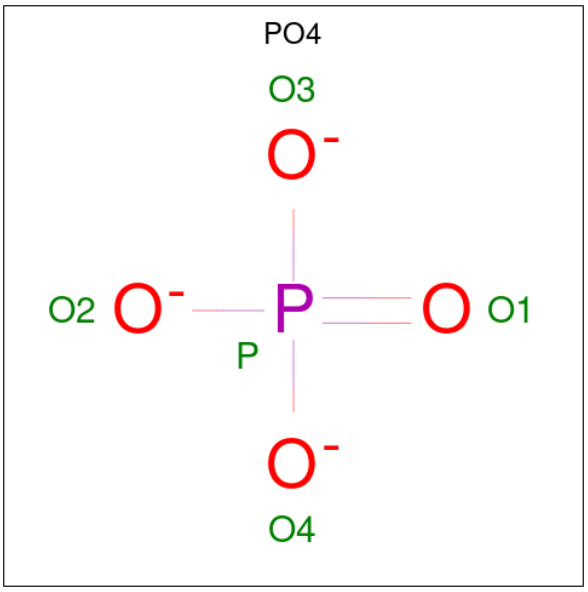
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP A0A0D5YCC7

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



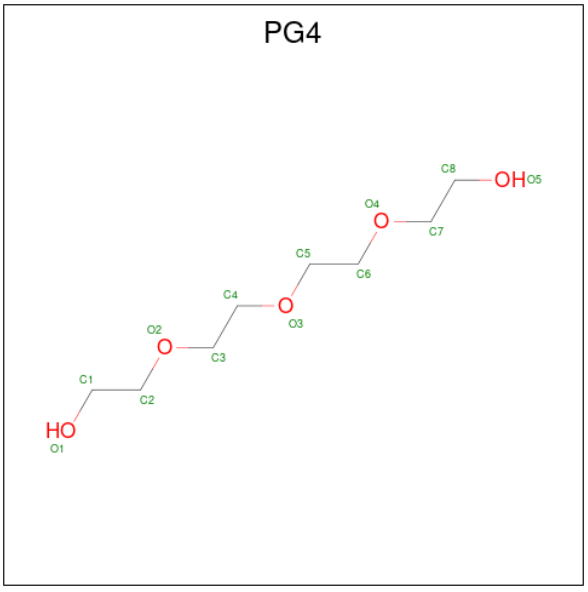
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 13 8 5	0	0
4	C	1	Total C O 13 8 5	0	0
4	C	1	Total C O 13 8 5	0	0

- Molecule 5 is water.

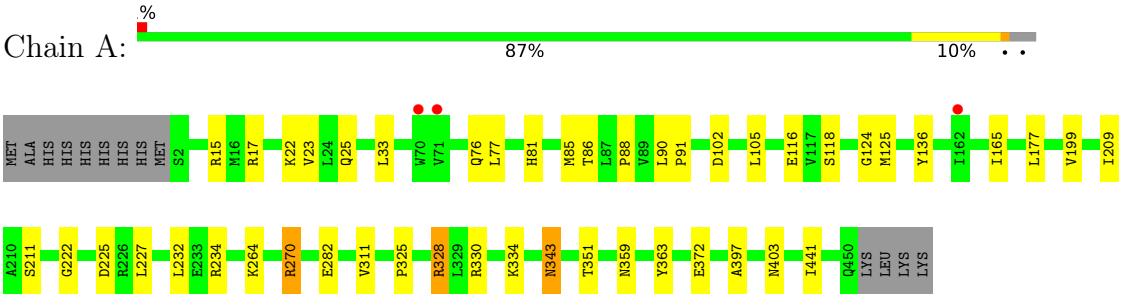
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	108	Total O 108 108	0	0
5	B	93	Total O 93 93	0	0
5	C	107	Total O 107 107	0	0

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.

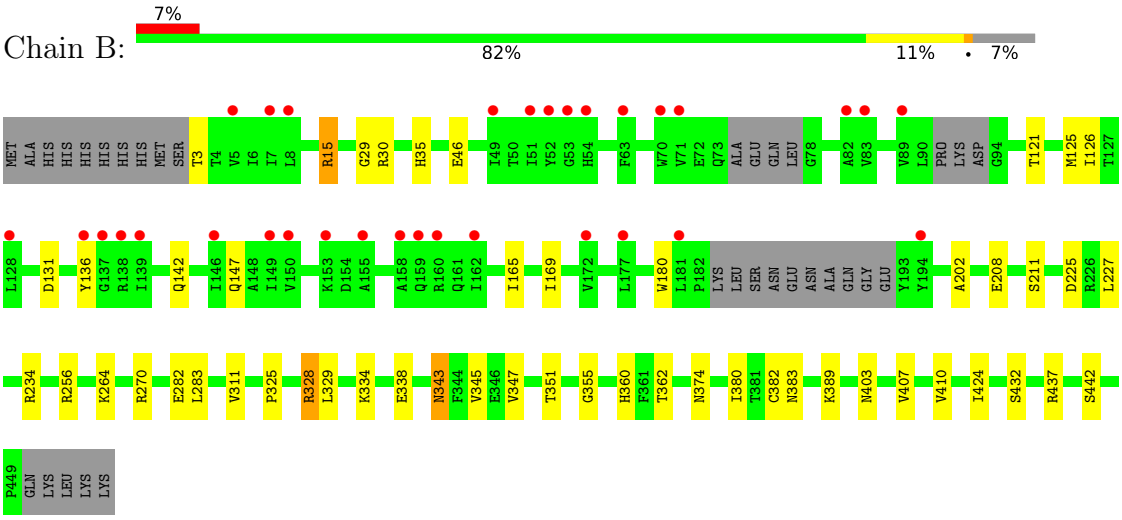
• Molecule 1: Bifunctional protein GlmU

Chain A:



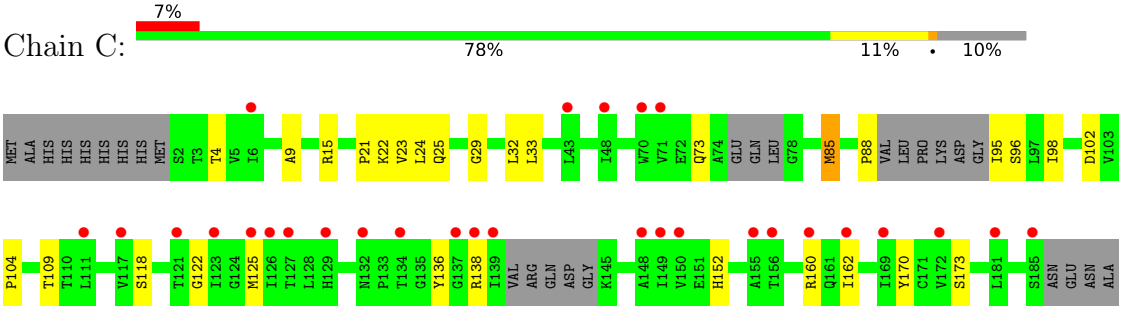
• Molecule 1: Bifunctional protein GlmU

Chain B:



• Molecule 1: Bifunctional protein GlmU

Chain C:




GLN
GLY
GLU
GLU
TYR
TYR
LEU
THR
ASP
ILE
VAL
ALA
M201
D205
GLY
LEU
GLU
I209
A210
S211
I212
N224
D225
R226
L227
R234
A252
R256
K264
D272
V273
E282
V311
P325
R328
K334
H340
N343
T351
K357
H360
N374
I380
N383
K389
S432
E436
ARG
ALA
Q439
Q450
LYS
LEU
LYS
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	96.62Å 96.62Å 262.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.51 – 2.55 47.51 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.51-2.55) 99.8 (47.51-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 2.54Å)	Xtriage
Refinement program	PHENIX (dev_2744: ???)	Depositor
R, R_{free}	0.185 , 0.248 0.185 , 0.248	Depositor DCC
R_{free} test set	1948 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9670	wwPDB-VP
Average B, all atoms (Å^2)	58.0	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 21.67 % 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 6.6796e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: PG4, PO4, CIT

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	0.40	0/3346	0.59	0/4555
1	B	0.37	0/3097	0.57	0/4215
1	C	0.39	0/2966	0.57	0/4033
All	All	0.38	0/9409	0.58	0/12803

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	3294	0	3249	34	0
1	B	3055	0	2918	34	0
1	C	2930	0	2771	34	0
2	A	13	0	5	0	0
2	B	13	0	5	3	0
2	C	13	0	5	1	0
3	A	5	0	0	1	0
4	B	13	0	18	3	0
4	C	26	0	36	4	0
5	A	108	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	93	0	0	3	0
5	C	107	0	0	2	0
All	All	9670	0	9007	98	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 5.

All (98) 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:29:GLY:H	4:B:502:PG4:H72	1.50	0.75
1:B:234:ARG:NH1	5:B:602:HOH:O	2.16	0.75
1:A:15[B]:ARG:NH1	3:A:502:PO4:O3	2.23	0.71
1:B:282:GLU:OE2	5:B:601:HOH:O	2.10	0.69
1:A:234:ARG:NH1	5:A:601:HOH:O	2.22	0.68
1:C:234:ARG:NH1	5:C:601:HOH:O	2.27	0.64
1:C:138:ARG:NH2	1:C:160:ARG:O	2.32	0.62
1:B:270:ARG:HB3	4:C:503:PG4:H42	1.82	0.61
1:B:15:ARG:HB3	1:B:225:ASP:HB3	1.83	0.61
1:A:15[B]:ARG:HB2	1:A:225:ASP:HB3	1.84	0.60
1:B:29:GLY:N	4:B:502:PG4:H72	2.19	0.57
1:A:270:ARG:HB3	4:B:502:PG4:H31	1.86	0.57
1:C:264:LYS:HB3	1:C:282:GLU:HG2	1.88	0.55
1:A:15[A]:ARG:HB3	1:A:225:ASP:HB3	1.89	0.54
1:A:264:LYS:HB3	1:A:282:GLU:HG2	1.88	0.54
1:C:23:VAL:HB	1:C:33:LEU:HB2	1.88	0.54
1:C:85:MET:O	1:C:88:PRO:HD2	2.08	0.54
1:B:30:ARG:NH1	5:B:608:HOH:O	2.41	0.53
1:B:360:HIS:NE2	2:C:502:CIT:O7	2.41	0.53
1:A:325:PRO:O	1:A:343:ASN:HA	2.09	0.52
1:B:227:LEU:HD12	1:B:227:LEU:H	1.75	0.52
1:C:311:VAL:HG22	1:C:328:ARG:HG2	1.92	0.52
1:C:340:HIS:HD2	5:C:686:HOH:O	1.93	0.51
1:A:334:LYS:HD2	1:A:351:THR:HG22	1.92	0.51
1:C:9:ALA:HB1	1:C:23:VAL:HG21	1.92	0.50
1:C:15:ARG:HB3	1:C:225:ASP:HB3	1.93	0.50
1:C:98:ILE:HD12	1:C:170:TYR:HB2	1.96	0.48
1:A:359:ASN:HD22	2:B:501:CIT:H42	1.78	0.48
1:A:359:ASN:ND2	2:B:501:CIT:H42	2.28	0.48
1:A:85:MET:O	1:A:88:PRO:HD2	2.15	0.47
1:C:227:LEU:H	1:C:227:LEU:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:VAL:CG2	1:A:328:ARG:HG2	2.44	0.47
1:A:199:VAL:HG13	1:A:209:ILE:CD1	2.44	0.47
1:B:125:MET:O	1:B:211:SER:HA	2.14	0.47
1:B:121:THR:HG21	1:B:208:GLU:O	2.14	0.47
1:C:118:SER:O	1:C:122:GLY:N	2.37	0.47
1:B:136:TYR:CD1	1:B:165:ILE:HD13	2.50	0.47
1:C:4:THR:O	1:C:96:SER:HA	2.14	0.47
1:C:29:GLY:H	4:C:503:PG4:H11	1.79	0.46
1:C:383:ASN:O	1:C:389:LYS:HA	2.16	0.46
1:A:136:TYR:CD1	1:A:165:ILE:HD13	2.50	0.46
1:C:21:PRO:HD2	1:C:24:LEU:HD12	1.97	0.46
1:A:227:LEU:HD12	1:A:227:LEU:H	1.79	0.46
1:B:180:TRP:CZ2	1:B:202:ALA:HA	2.51	0.46
1:A:118:SER:OG	1:A:124:GLY:HA3	2.16	0.45
1:C:138:ARG:NE	1:C:162:ILE:O	2.45	0.45
1:B:325:PRO:O	1:B:343:ASN:HA	2.16	0.45
1:C:325:PRO:O	1:C:343:ASN:HA	2.16	0.44
1:A:372:GLU:O	1:A:397:ALA:HA	2.16	0.44
1:B:3:THR:O	1:B:46:GLU:N	2.46	0.44
1:B:30:ARG:HG3	1:B:35:HIS:NE2	2.32	0.44
4:C:503:PG4:H32	4:C:503:PG4:H51	1.85	0.44
1:B:383:ASN:O	1:B:389:LYS:HA	2.18	0.44
1:B:142:GLN:H	1:B:147:GLN:HE21	1.65	0.44
1:C:95:ILE:HA	1:C:173:SER:HA	2.00	0.43
1:C:252:ALA:HB2	4:C:501:PG4:H41	2.00	0.43
1:A:125:MET:O	1:A:211:SER:HA	2.17	0.43
1:B:345:VAL:HG13	1:B:362:THR:HG23	1.99	0.43
1:A:311:VAL:HG22	1:A:328:ARG:HG2	2.01	0.43
1:B:382:CYS:HB2	1:B:407:VAL:HA	2.00	0.43
1:B:227:LEU:HD12	1:B:227:LEU:N	2.33	0.43
1:B:264:LYS:HB3	1:B:282:GLU:HG2	2.00	0.43
1:C:125:MET:O	1:C:211:SER:HA	2.19	0.43
1:A:105:LEU:HD12	1:A:232:LEU:HD11	2.01	0.42
1:B:311:VAL:HG22	1:B:328:ARG:HG2	2.01	0.42
1:C:22:LYS:O	1:C:25:GLN:HG2	2.19	0.42
1:A:77:LEU:HB2	1:A:81:HIS:ND1	2.35	0.42
1:B:126:ILE:HD12	1:B:169:ILE:HG21	2.01	0.42
1:C:32:LEU:HD22	1:C:104:PRO:HG3	1.99	0.42
1:B:410:VAL:HG21	1:B:424:ILE:HG22	2.01	0.42
1:B:329:LEU:HD22	1:B:347:VAL:HB	2.01	0.42
1:A:102:ASP:O	1:A:222:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ILE:HD11	1:B:437:ARG:HB2	2.02	0.42
1:C:340:HIS:HB2	1:C:357:LYS:HB3	2.02	0.42
1:B:256:ARG:HD3	1:C:256:ARG:HG2	2.01	0.41
1:C:22:LYS:HD3	1:C:102:ASP:CB	2.50	0.41
1:A:77:LEU:HD12	1:A:81:HIS:CE1	2.55	0.41
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.90	0.41
1:A:403:ASN:CG	1:B:380:ILE:HD12	2.40	0.41
1:B:282:GLU:O	1:B:283:LEU:HD23	2.19	0.41
1:B:334:LYS:HB2	1:B:351:THR:HG22	2.01	0.41
1:A:22:LYS:O	1:A:25:GLN:HG2	2.20	0.41
1:A:90:LEU:HA	1:A:91:PRO:HD3	1.94	0.41
1:A:76:GLN:O	1:A:77:LEU:HD23	2.21	0.41
1:A:227:LEU:HD12	1:A:227:LEU:N	2.36	0.41
1:A:328:ARG:NH1	1:A:330:ARG:HD2	2.35	0.41
1:B:389:LYS:HE3	2:B:501:CIT:O6	2.20	0.41
1:C:272:ASP:OD1	1:C:273:VAL:N	2.51	0.41
1:A:363:TYR:CZ	1:C:360:HIS:CE1	3.09	0.40
1:B:403:ASN:CG	1:C:380:ILE:HD12	2.42	0.40
1:A:86:THR:O	1:A:90:LEU:HB2	2.22	0.40
1:C:15:ARG:HE	1:C:224:ASN:HB3	1.86	0.40
1:B:338:GLU:HB2	1:B:355:GLY:HA2	2.04	0.40
1:C:334:LYS:HB2	1:C:351:THR:HG22	2.02	0.40
1:A:23:VAL:HB	1:A:33:LEU:HB2	2.04	0.40
1:C:22:LYS:HD3	1:C:102:ASP:HB3	2.03	0.40
1:C:136:TYR:O	1:C:152:HIS:HB2	2.21	0.40
1:C:311:VAL:CG2	1:C:328:ARG:HG2	2.51	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	448/462 (97%)	437 (98%)	11 (2%)	0	100	100
1	B	422/462 (91%)	413 (98%)	9 (2%)	0	100	100
1	C	401/462 (87%)	393 (98%)	8 (2%)	0	100	100
All	All	1271/1386 (92%)	1243 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/372 (90%)	329 (98%)	5 (2%)	65	77
1	B	289/372 (78%)	282 (98%)	7 (2%)	49	64
1	C	278/372 (75%)	270 (97%)	8 (3%)	42	57
All	All	901/1116 (81%)	881 (98%)	20 (2%)	52	66

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	116	GLU
1	A	270	ARG
1	A	328	ARG
1	A	343	ASN
1	B	15	ARG
1	B	131	ASP
1	B	328	ARG
1	B	343	ASN
1	B	374	ASN
1	B	432	SER
1	B	442	SER
1	C	73	GLN
1	C	85	MET
1	C	109	THR

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Mol	Chain	Res	Type
1	C	328	ARG
1	C	343	ASN
1	C	357	LYS
1	C	374	ASN
1	C	432	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	ASN

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)

7 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	CIT	B	501	-	12,12,12	1.19	1 (8%)	17,17,17	1.73	5 (29%)
2	CIT	A	501	-	12,12,12	1.17	1 (8%)	17,17,17	1.71	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PG4	C	501	-	12,12,12	0.54	0	11,11,11	0.41	0
2	CIT	C	502	-	12,12,12	1.12	0	17,17,17	1.53	3 (17%)
4	PG4	B	502	-	12,12,12	0.53	0	11,11,11	0.31	0
3	PO4	A	502	-	4,4,4	0.78	0	6,6,6	0.61	0
4	PG4	C	503	-	12,12,12	0.53	0	11,11,11	0.46	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
2	CIT	B	501	-	-	3/16/16/16	-
2	CIT	A	501	-	-	0/16/16/16	-
4	PG4	C	501	-	-	5/10/10/10	-
2	CIT	C	502	-	-	3/16/16/16	-
4	PG4	B	502	-	-	4/10/10/10	-
4	PG4	C	503	-	-	5/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	CIT	C3-C6	-2.25	1.51	1.53
2	A	501	CIT	C3-C6	-2.03	1.51	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	CIT	O6-C6-C3	4.40	120.69	113.05
2	A	501	CIT	O6-C6-C3	3.96	119.92	113.05
2	C	502	CIT	O6-C6-C3	3.74	119.54	113.05
2	B	501	CIT	O5-C6-C3	-2.83	118.25	122.25
2	A	501	CIT	C3-C2-C1	-2.26	108.34	113.81
2	A	501	CIT	O4-C5-O3	-2.20	117.82	123.30
2	B	501	CIT	O7-C3-C6	-2.15	105.84	108.86
2	C	502	CIT	O4-C5-O3	-2.15	117.94	123.30
2	B	501	CIT	O2-C1-C2	2.14	121.23	114.35
2	C	502	CIT	O2-C1-C2	2.10	121.09	114.35
2	B	501	CIT	O4-C5-O3	-2.07	118.13	123.30

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	CIT	C1-C2-C3-O7
2	B	501	CIT	C1-C2-C3-C4
2	B	501	CIT	C1-C2-C3-C6
2	C	502	CIT	C1-C2-C3-C4
2	C	502	CIT	C1-C2-C3-C6
4	C	501	PG4	O2-C3-C4-O3
2	C	502	CIT	C1-C2-C3-O7
4	C	503	PG4	O3-C5-C6-O4
4	C	501	PG4	C5-C6-O4-C7
4	C	503	PG4	O4-C7-C8-O5
4	B	502	PG4	O4-C7-C8-O5
4	C	503	PG4	C5-C6-O4-C7
4	B	502	PG4	C8-C7-O4-C6
4	C	501	PG4	C1-C2-O2-C3
4	C	501	PG4	C4-C3-O2-C2
4	C	503	PG4	C8-C7-O4-C6
4	C	501	PG4	O4-C7-C8-O5
4	B	502	PG4	O3-C5-C6-O4
4	B	502	PG4	C5-C6-O4-C7
4	C	503	PG4	C3-C4-O3-C5

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	CIT	3	0
4	C	501	PG4	1	0
2	C	502	CIT	1	0
4	B	502	PG4	3	0
3	A	502	PO4	1	0
4	C	503	PG4	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

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	449/462 (97%)	-0.17	3 (0%)	87	90	24, 51, 89, 114	0
1	B	430/462 (93%)	0.18	32 (7%)	14	18	25, 60, 108, 134	0
1	C	415/462 (89%)	0.20	31 (7%)	14	17	25, 53, 124, 165	0
All	All	1294/1386 (93%)	0.07	66 (5%)	28	33	24, 54, 110, 165	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	TRP	5.1
1	C	139	ILE	5.0
1	B	136	TYR	4.2
1	C	125	MET	4.2
1	C	123	ILE	4.1
1	B	162	ILE	4.0
1	B	149	ILE	3.8
1	B	146	ILE	3.8
1	C	150	VAL	3.5
1	C	132	ASN	3.4
1	C	212	ILE	3.4
1	C	181	LEU	3.4
1	B	82	ALA	3.3
1	C	149	ILE	3.3
1	B	153	LYS	3.2
1	C	156	THR	3.2
1	B	49	ILE	3.1
1	B	194	TYR	3.1
1	B	139	ILE	3.1
1	B	172	VAL	3.1
1	B	159	GLN	3.0
1	B	51	ILE	3.0
1	B	155	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	172	VAL	3.0
1	B	5	VAL	2.9
1	C	71	VAL	2.8
1	B	181	LEU	2.8
1	C	138	ARG	2.8
1	C	48	ILE	2.8
1	C	134	THR	2.8
1	B	71	VAL	2.7
1	C	210	ALA	2.7
1	B	63	PHE	2.7
1	C	6	ILE	2.6
1	A	70	TRP	2.6
1	C	117	VAL	2.5
1	B	89	VAL	2.5
1	C	162	ILE	2.5
1	B	137	GLY	2.5
1	B	83	VAL	2.4
1	B	150	VAL	2.4
1	B	160	ARG	2.4
1	B	53	GLY	2.4
1	B	54	HIS	2.4
1	C	129	HIS	2.4
1	B	128	LEU	2.4
1	B	177	LEU	2.4
1	C	160	ARG	2.3
1	C	70	TRP	2.3
1	A	71	VAL	2.3
1	C	155	ALA	2.3
1	C	43	LEU	2.2
1	B	138	ARG	2.2
1	B	158	ALA	2.2
1	B	8	LEU	2.2
1	B	52	TYR	2.1
1	C	121	THR	2.1
1	C	137	GLY	2.1
1	C	148	ALA	2.1
1	C	127	THR	2.1
1	B	7	ILE	2.1
1	A	162	ILE	2.0
1	C	111	LEU	2.0
1	C	185	SER	2.0
1	C	126	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	169	ILE	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
3	PO4	A	502	5/5	0.84	0.14	115,117,119,120	0
2	CIT	A	501	13/13	0.91	0.15	61,66,83,83	0
2	CIT	B	501	13/13	0.94	0.14	58,66,70,74	0
4	PG4	C	501	13/13	0.94	0.19	45,55,62,64	0
4	PG4	B	502	13/13	0.95	0.17	47,53,71,75	0
2	CIT	C	502	13/13	0.95	0.10	55,60,64,65	0
4	PG4	C	503	13/13	0.95	0.20	52,57,76,79	0

6.5 Other polymers (i)

There are no such residues in this entry.