Full wwPDB X-ray Structure Validation Report (i)

Mar 20, 2016 – 05:00 AM EDT

PDB ID	:	5EIY
Title	:	Bacterial cellulose synthase bound to a substrate analogue
Authors	:	McNamara, J.T.; Zimmer, J.
Deposited on	:	2015-10-30
Resolution	:	2.95 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 (i) symbol.

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

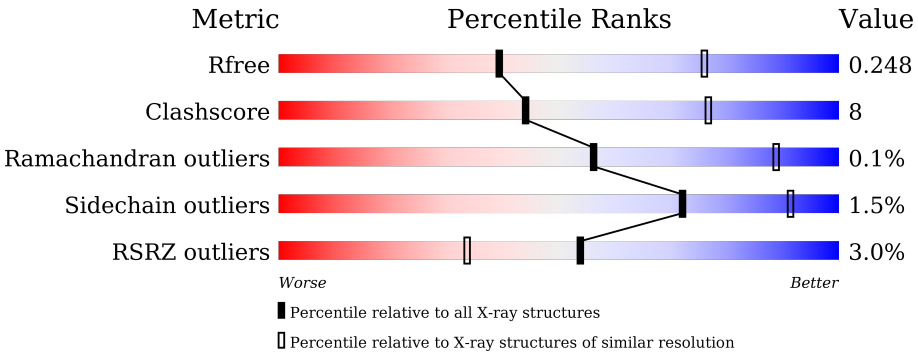
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	803	3% 73% 17% 9%
2	B	729	2% 77% 12% • 10%
3	D	9	100%

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
10	MG	A	924	-	-	-	X
4	PLC	A	901	-	-	-	X
5	43Y	A	902	-	-	-	X
6	BGC	A	915	-	-	-	X
9	LDA	A	922	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11144 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 Putative cellulose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	5734	3721	1000	982	31	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q3J125
A	1	GLY	-	expression tag	UNP Q3J125
A	789	HIS	-	expression tag	UNP Q3J125
A	790	HIS	-	expression tag	UNP Q3J125
A	791	HIS	-	expression tag	UNP Q3J125
A	792	HIS	-	expression tag	UNP Q3J125
A	793	HIS	-	expression tag	UNP Q3J125
A	794	HIS	-	expression tag	UNP Q3J125
A	795	LYS	-	expression tag	UNP Q3J125
A	796	LEU	-	expression tag	UNP Q3J125
A	797	HIS	-	expression tag	UNP Q3J125
A	798	HIS	-	expression tag	UNP Q3J125
A	799	HIS	-	expression tag	UNP Q3J125
A	800	HIS	-	expression tag	UNP Q3J125
A	801	HIS	-	expression tag	UNP Q3J125
A	802	HIS	-	expression tag	UNP Q3J125

- Molecule 2 is a protein called Putative cellulose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	658	4946	3134	878	918	16	0	5	0

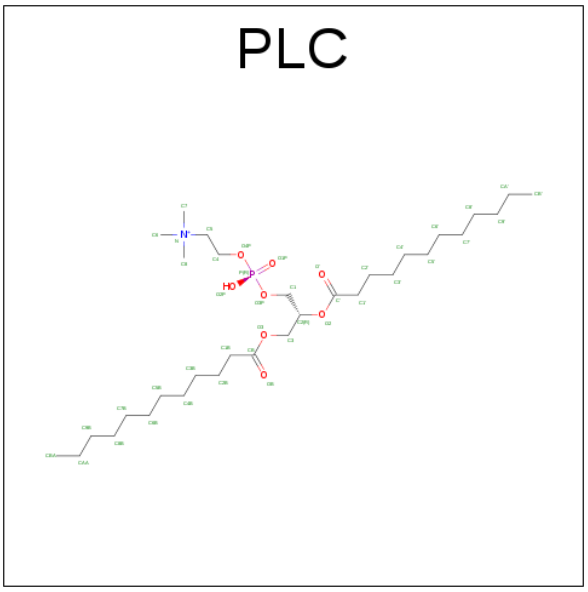
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	MET	-	initiating methionine	UNP Q3J126
B	-2	LYS	-	expression tag	UNP Q3J126
B	-1	TYR	-	expression tag	UNP Q3J126
B	0	LEU	-	expression tag	UNP Q3J126
B	1	LEU	-	expression tag	UNP Q3J126
B	2	PRO	-	expression tag	UNP Q3J126
B	3	THR	-	expression tag	UNP Q3J126
B	4	ALA	-	expression tag	UNP Q3J126
B	5	ALA	-	expression tag	UNP Q3J126
B	6	ALA	-	expression tag	UNP Q3J126
B	7	GLY	-	expression tag	UNP Q3J126
B	8	LEU	-	expression tag	UNP Q3J126
B	9	LEU	-	expression tag	UNP Q3J126
B	10	LEU	-	expression tag	UNP Q3J126
B	11	LEU	-	expression tag	UNP Q3J126
B	12	ALA	-	expression tag	UNP Q3J126
B	13	ALA	-	expression tag	UNP Q3J126
B	14	GLN	-	expression tag	UNP Q3J126
B	15	PRO	-	expression tag	UNP Q3J126
B	16	ALA	-	expression tag	UNP Q3J126
B	17	MET	-	expression tag	UNP Q3J126
B	18	ALA	-	expression tag	UNP Q3J126
B	19	MET	-	expression tag	UNP Q3J126
B	20	GLY	-	expression tag	UNP Q3J126

- Molecule 3 is a protein called poly(unk).

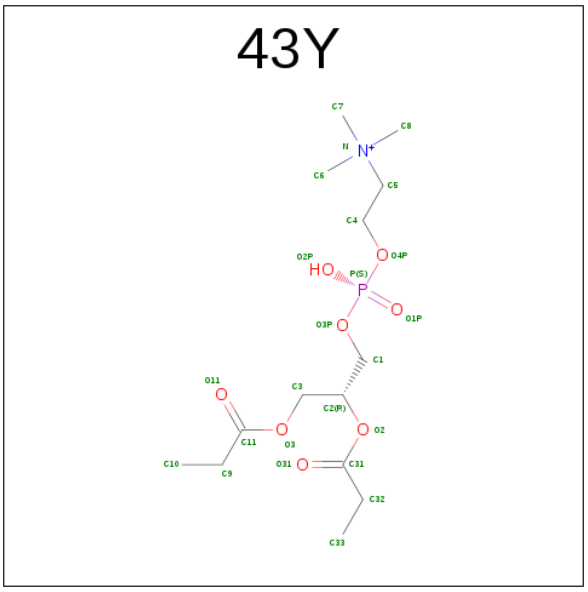
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	9	Total	C	N	O	0	0	0
			45	27	9	9			

- Molecule 4 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



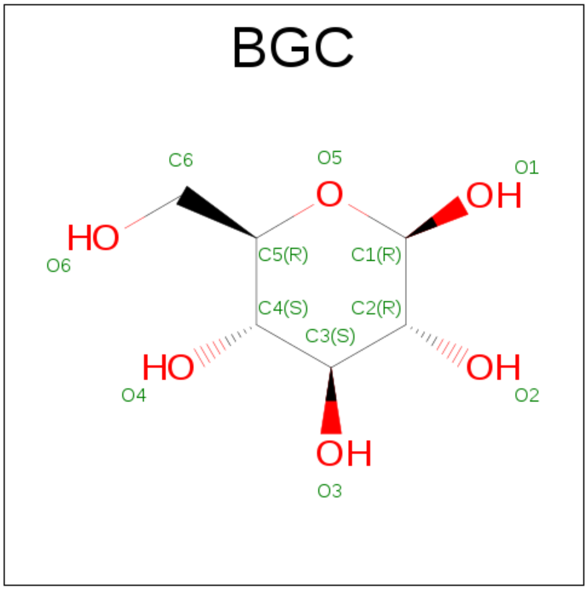
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			38	28	1	8	1		

- Molecule 5 is [(2R)-3-[oxidanyl-[2-(trimethyl-$l^{4}-azanyl)ethoxy]phosphoryl]oxy-2-propanoyloxy-propyl] propanoate (three-letter code: 43Y) (formula: $C_{14}H_{29}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			20	10	1	8	1		

- Molecule 6 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 12 6 6	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0

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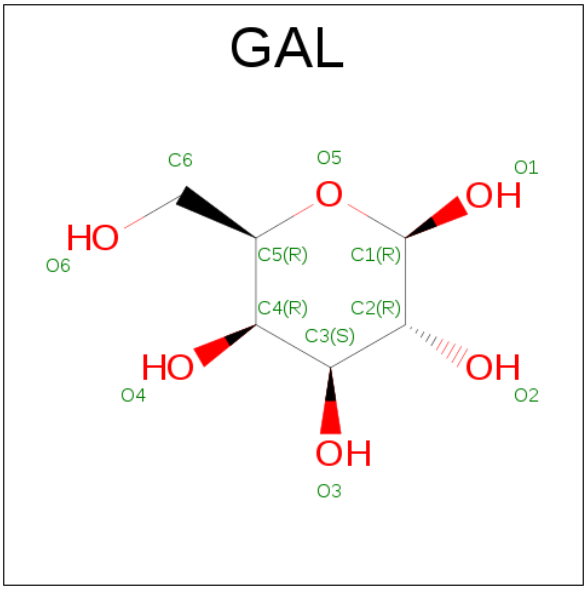
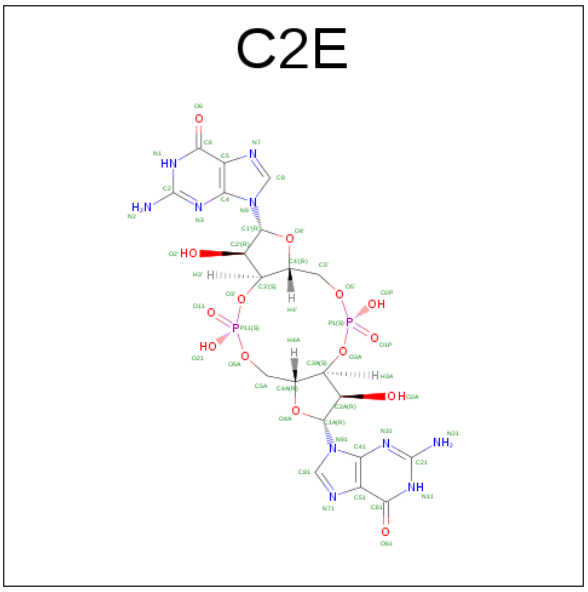
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0

- Molecule 7 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



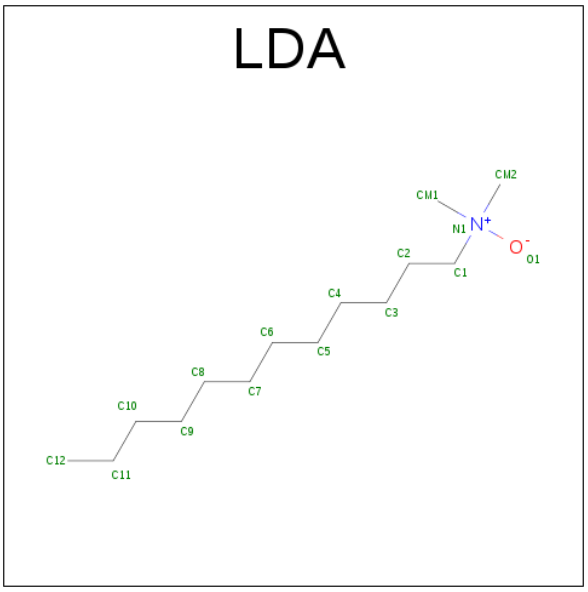
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 11 6 5	0	0

- Molecule 8 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidooctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: $C_{20}H_{24}N_{10}O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
8	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			16	14	1	1		

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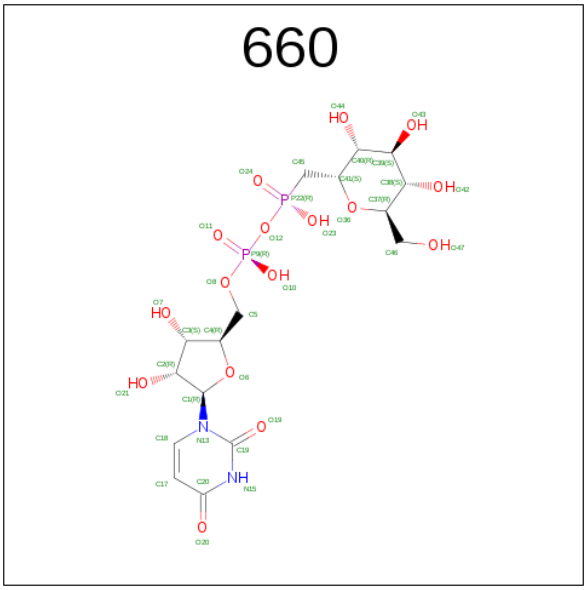
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 16 14 1 1	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Mg 1 1	0	0
10	A	1	Total Mg 1 1	0	0

- Molecule 11 is [[(2 {R},3 {S},4 {R},5 {R})-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-[[(2 {S},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]methyl]phosphinic acid (three-letter code: 660) (formula: $C_{16}H_{26}N_2O_{16}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C N O P 36 16 2 16 2	0	0

- Molecule 12 is water.

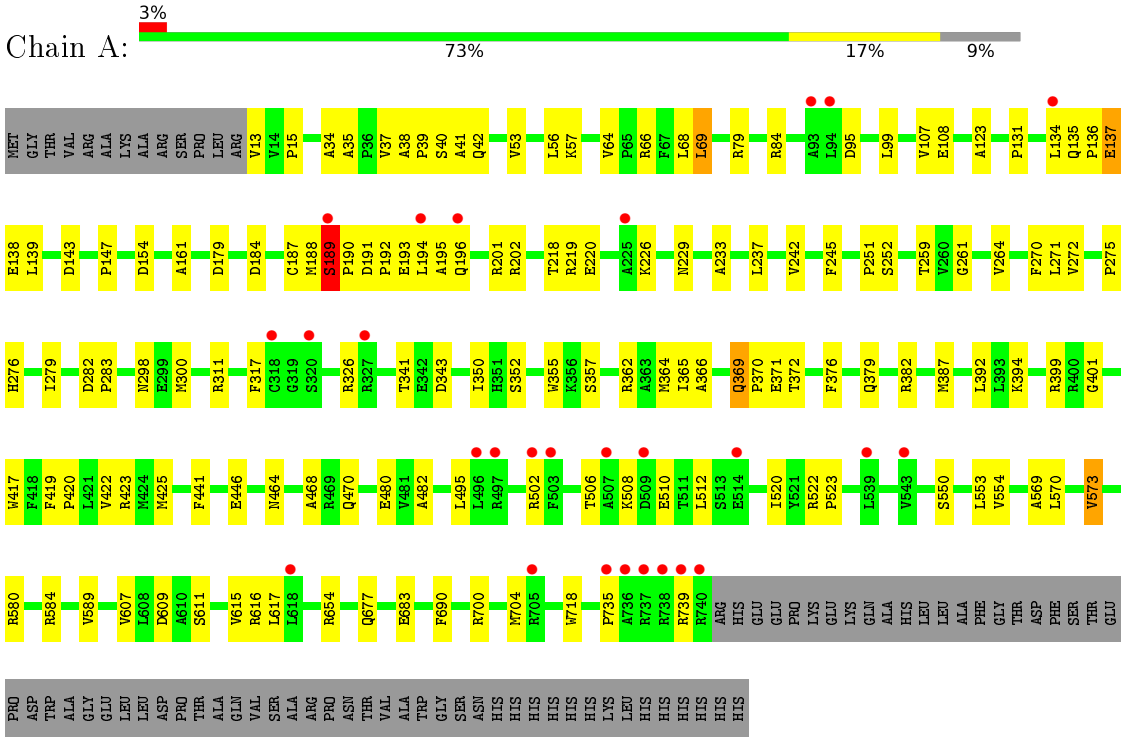
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	11	Total O 11 11	0	0

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.

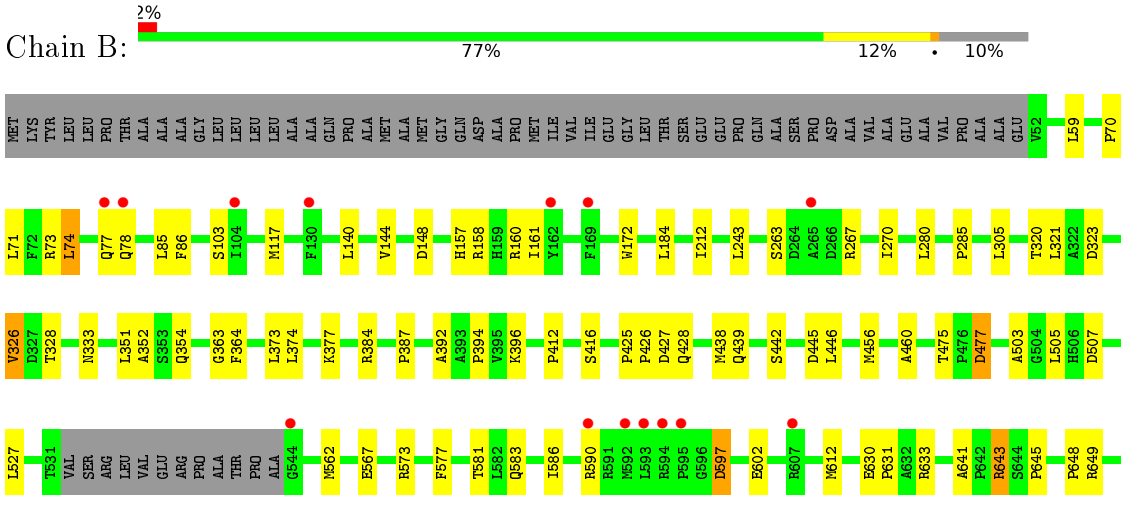
- Molecule 1: Putative cellulose synthase

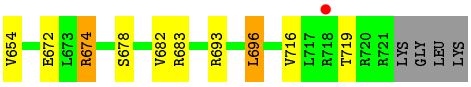
Chain A:



- Molecule 2: Putative cellulose synthase

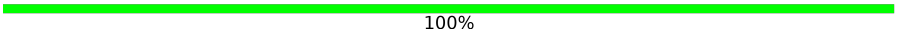
Chain B:





- Molecule 3: poly(unk)

Chain D:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.47Å 216.65Å 221.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.92 – 2.95 34.92 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.92-2.95) 99.8 (34.92-2.95)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.222 , 0.248 0.221 , 0.248	Depositor DCC
R_{free} test set	6608 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	75.5	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.7	EDS
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 70272 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11144	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, 0.375 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: MG, BGC, 43Y, LDA, 660, GAL, PLC, C2E

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	0/5880	0.45	1/7997 (0.0%)
2	B	0.22	0/5065	0.45	1/6945 (0.0%)
All	All	0.24	0/10945	0.45	2/14942 (0.0%)

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	1
2	B	0	3
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	SER	CB-CA-C	5.50	120.54	110.10
2	B	74	LEU	O-C-N	-5.19	114.40	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	GLN	Peptide
2	B	643	ARG	Sidechain
2	B	74	LEU	Mainchain

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	5734	0	5846	112	0
2	B	4946	0	5023	66	0
3	D	45	0	12	0	0
4	A	38	0	53	0	0
5	A	20	0	15	1	0
6	A	177	0	145	6	0
7	A	11	0	10	1	0
8	A	92	0	41	5	0
9	A	32	0	62	2	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	36	0	0	2	0
12	A	11	0	0	0	0
All	All	11144	0	11207	178	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 8.

All (178) 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)
8:A:921:C2E:O4'	8:A:921:C2E:C4'	1.64	1.21
8:A:920:C2E:O4'	8:A:920:C2E:C4'	1.64	1.20
1:A:134:LEU:O	1:A:134:LEU:HD12	1.58	1.04
2:B:140:LEU:HB3	2:B:144:VAL:HG11	1.42	1.00
2:B:643:ARG:HD3	2:B:643:ARG:N	1.82	0.94
1:A:189:SER:HB3	1:A:191:ASP:N	1.83	0.93
1:A:189:SER:HB3	1:A:191:ASP:H	1.32	0.93
2:B:140:LEU:HB3	2:B:144:VAL:CG1	1.98	0.92
1:A:134:LEU:HD22	1:A:264:VAL:HG21	1.55	0.88
1:A:189:SER:CB	1:A:190:PRO:HA	2.08	0.84
1:A:95:ASP:O	1:A:99:LEU:HD13	1.83	0.78
2:B:270:ILE:HG22	2:B:280:LEU:HA	1.67	0.76
1:A:189:SER:HB2	1:A:190:PRO:HA	1.68	0.73
2:B:643:ARG:HD3	2:B:643:ARG:H	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:VAL:O	1:A:68:LEU:HD13	1.91	0.70
2:B:377:LYS:HB2	2:B:416:SER:HB2	1.73	0.70
2:B:643:ARG:CD	2:B:643:ARG:N	2.54	0.70
2:B:630:GLU:OE1	2:B:633:ARG:NH1	2.24	0.69
1:A:179:ASP:OD1	1:A:201:ARG:NH1	2.25	0.69
1:A:300:MET:HA	1:A:470:GLN:HB3	1.74	0.69
1:A:341:THR:HG23	1:A:341:THR:O	1.91	0.69
1:A:134:LEU:HD22	1:A:264:VAL:CG2	2.24	0.68
2:B:693:ARG:HD2	2:B:696:LEU:HD13	1.74	0.68
1:A:369:GLN:HG3	1:A:370:PRO:HD2	1.76	0.67
1:A:143:ASP:CG	1:A:237:LEU:HD23	2.15	0.67
1:A:341:THR:CG2	1:A:341:THR:O	2.42	0.67
1:A:191:ASP:HB3	1:A:194:LEU:HD12	1.77	0.66
1:A:508:LYS:NZ	11:A:925:660:O23	2.27	0.66
1:A:35:ALA:O	1:A:79:ARG:NH2	2.29	0.65
1:A:189:SER:CB	1:A:191:ASP:H	2.08	0.65
2:B:364:PHE:HE1	2:B:396:LYS:HD2	1.61	0.65
1:A:57:LYS:NZ	5:A:902:43Y:O2P	2.30	0.64
1:A:134:LEU:CD1	1:A:139:LEU:HD12	2.27	0.64
2:B:672:GLU:OE1	2:B:674:ARG:NH1	2.30	0.64
1:A:191:ASP:CB	1:A:194:LEU:HD12	2.28	0.63
1:A:382:ARG:HH12	1:A:506:THR:HG23	1.63	0.63
6:A:908:BGC:H6C2	2:B:384:ARG:HH11	1.64	0.62
2:B:73:ARG:NH2	2:B:172:TRP:CE2	2.67	0.62
1:A:134:LEU:HD11	1:A:139:LEU:HD12	1.82	0.62
6:A:908:BGC:H6C2	2:B:384:ARG:NH1	2.14	0.61
1:A:40:SER:HA	2:B:581:THR:HG22	1.83	0.60
1:A:187:CYS:SG	1:A:202:ARG:NH1	2.74	0.60
1:A:352:SER:O	1:A:401:GLY:HA3	2.01	0.60
1:A:84:ARG:NH1	1:A:108:GLU:OE1	2.33	0.60
1:A:53:VAL:HG13	1:A:69:LEU:HD13	1.84	0.59
1:A:42:GLN:OE1	1:A:79:ARG:NH1	2.36	0.59
2:B:77[A]:GLN:HG3	2:B:157:HIS:H	1.67	0.59
1:A:350:ILE:HG22	1:A:355:TRP:HB2	1.86	0.58
2:B:475:THR:HG22	2:B:477:ASP:H	1.68	0.58
1:A:196:GLN:OE1	1:A:196:GLN:HA	2.05	0.57
2:B:612:MET:HG2	2:B:654:VAL:HG22	1.85	0.57
1:A:184:ASP:O	1:A:188:MET:HG2	2.05	0.56
1:A:419:PHE:HA	1:A:422:VAL:HG22	1.88	0.56
1:A:193:GLU:O	1:A:196:GLN:HB2	2.06	0.55
1:A:189:SER:CB	1:A:190:PRO:CA	2.81	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77[A]:GLN:HE22	2:B:158:ARG:NE	2.05	0.55
1:A:161:ALA:HB1	1:A:683:GLU:HG2	1.90	0.54
1:A:66:ARG:NH1	1:A:123:ALA:O	2.40	0.54
1:A:271:LEU:HD23	1:A:357:SER:HB2	1.89	0.54
2:B:328:THR:HG22	2:B:442:SER:H	1.72	0.54
1:A:654:ARG:O	1:A:677:GLN:NE2	2.41	0.54
1:A:134:LEU:CD1	1:A:134:LEU:O	2.46	0.53
1:A:107:VAL:HG21	1:A:425:MET:HG2	1.89	0.53
1:A:37:VAL:HG13	1:A:41:ALA:HB3	1.91	0.53
1:A:387:MET:HG3	1:A:417:TRP:CD1	2.45	0.52
2:B:412:PRO:HB2	2:B:645:PRO:HA	1.92	0.52
1:A:589:VAL:HB	1:A:607:VAL:HB	1.92	0.52
1:A:520:ILE:O	1:A:523:PRO:HD2	2.10	0.52
1:A:735:PRO:O	1:A:739:ARG:NH1	2.44	0.51
1:A:482:ALA:HB2	1:A:569:ALA:HB1	1.91	0.51
1:A:270:PHE:CG	1:A:350:ILE:HG21	2.46	0.51
2:B:140:LEU:HB3	2:B:144:VAL:HG13	1.86	0.50
2:B:438:MET:HG2	2:B:439:GLN:N	2.25	0.50
1:A:13:VAL:HG13	1:A:15:PRO:HD2	1.93	0.50
2:B:425:PRO:HG2	2:B:428:GLN:HB2	1.93	0.50
1:A:134:LEU:HD13	1:A:138:GLU:HB2	1.94	0.50
1:A:193:GLU:O	1:A:196:GLN:N	2.44	0.50
1:A:609:ASP:OD2	1:A:616:ARG:HD2	2.12	0.49
1:A:276:HIS:O	1:A:298:ASN:ND2	2.45	0.49
1:A:134:LEU:CD2	1:A:264:VAL:CG2	2.90	0.49
2:B:364:PHE:CZ	2:B:392:ALA:HA	2.48	0.49
2:B:78[A]:GLN:HE21	2:B:333:ASN:ND2	2.11	0.49
2:B:59:LEU:HD12	2:B:85:LEU:HD13	1.93	0.49
1:A:464:ASN:O	1:A:468:ALA:HB2	2.13	0.48
1:A:718:TRP:HE3	9:A:923:LDA:H62	1.78	0.48
1:A:394:LYS:O	1:A:399:ARG:NH1	2.46	0.48
1:A:446:GLU:OE2	2:B:573:ARG:NH2	2.39	0.48
2:B:364:PHE:CE1	2:B:396:LYS:HD2	2.47	0.48
1:A:219:ARG:HD3	1:A:229:ASN:HA	1.96	0.48
6:A:908:BGC:C6	2:B:384:ARG:NH1	2.77	0.48
2:B:363:GLY:HA3	2:B:394:PRO:O	2.14	0.47
1:A:419:PHE:CD2	1:A:420:PRO:HD3	2.48	0.47
2:B:148:ASP:HB3	2:B:305:LEU:HG	1.96	0.47
1:A:259:THR:HG23	1:A:272:VAL:HG11	1.95	0.47
2:B:321:LEU:HB3	2:B:326:VAL:HG22	1.96	0.47
2:B:503:ALA:HB1	2:B:507:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:678:SER:O	2:B:682:VAL:HG23	2.15	0.47
2:B:716:VAL:HA	2:B:719:THR:HG22	1.97	0.47
1:A:570:LEU:O	1:A:573:VAL:HB	2.15	0.47
1:A:341:THR:OG1	1:A:343:ASP:OD1	2.33	0.47
1:A:226:LYS:HG2	1:A:226:LYS:O	2.14	0.46
1:A:584:ARG:HG2	1:A:611:SER:HB3	1.97	0.46
1:A:580:ARG:NH2	8:A:921:C2E:H2'	2.30	0.46
1:A:311:ARG:NH2	2:B:716:VAL:O	2.49	0.46
1:A:189:SER:HB3	1:A:190:PRO:HA	1.94	0.46
6:A:906:BGC:O3	6:A:907:BGC:O5	2.22	0.46
2:B:351:LEU:HD11	2:B:456:MET:HE1	1.98	0.46
1:A:282:ASP:HA	1:A:369:GLN:HG2	1.98	0.45
2:B:70:PRO:HG2	2:B:71:LEU:HD13	1.98	0.45
1:A:187:CYS:O	1:A:195:ALA:HB1	2.16	0.45
2:B:320:THR:HA	2:B:445:ASP:HA	1.98	0.45
1:A:251:PRO:HA	1:A:365:ILE:HG22	1.98	0.45
2:B:373:LEU:HD23	2:B:387:PRO:HA	1.97	0.45
2:B:583:GLN:HA	2:B:586:ILE:HG12	1.99	0.45
1:A:480:GLU:OE2	6:A:916:BGC:O6	2.30	0.45
2:B:117:MET:HB3	2:B:117:MET:HE2	1.77	0.44
2:B:460:ALA:HB2	2:B:649:ARG:HG2	1.99	0.44
1:A:134:LEU:CD1	1:A:139:LEU:CD1	2.95	0.44
1:A:252:SER:N	1:A:364:MET:O	2.40	0.44
1:A:218:THR:OG1	1:A:219:ARG:N	2.50	0.44
1:A:34:ALA:O	2:B:683:ARG:NH1	2.51	0.44
1:A:379:GLN:HB2	1:A:506:THR:HG21	2.00	0.44
1:A:13:VAL:HG22	1:A:15:PRO:HD2	2.00	0.44
1:A:275:PRO:HD2	1:A:362:ARG:O	2.18	0.43
1:A:233:ALA:O	1:A:237:LEU:HD13	2.18	0.43
1:A:283:PRO:HG2	1:A:376:PHE:HB2	2.01	0.43
1:A:700:ARG:O	1:A:704:MET:HG3	2.18	0.43
2:B:602:GLU:H	2:B:602:GLU:HG2	1.67	0.43
1:A:154:ASP:N	1:A:154:ASP:OD1	2.51	0.43
2:B:427:ASP:OD1	2:B:427:ASP:N	2.50	0.43
1:A:341:THR:OG1	7:A:919:GAL:O6	2.34	0.42
1:A:189:SER:HB3	1:A:190:PRO:CA	2.46	0.42
1:A:134:LEU:CD2	1:A:264:VAL:HG21	2.37	0.42
1:A:38:ALA:HA	1:A:39:PRO:HD3	1.93	0.42
2:B:212:ILE:HB	2:B:243:LEU:HD23	2.01	0.42
2:B:630:GLU:HA	2:B:631:PRO:HD3	1.89	0.42
1:A:366:ALA:HB3	1:A:690:PHE:HD1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:ARG:HG3	2:B:161:ILE:HG12	2.01	0.42
2:B:320:THR:HG22	2:B:323:ASP:CG	2.40	0.42
1:A:136:PRO:O	1:A:137:GLU:HG2	2.20	0.42
1:A:184:ASP:HB2	1:A:220:GLU:HA	2.00	0.42
1:A:242:VAL:HG23	1:A:326:ARG:HG2	2.02	0.42
1:A:553:LEU:HA	1:A:553:LEU:HD12	1.87	0.42
2:B:477:ASP:OD1	2:B:477:ASP:N	2.52	0.42
1:A:550:SER:OG	2:B:567:GLU:HG3	2.19	0.42
9:A:923:LDA:H22	9:A:923:LDA:HM23	1.76	0.42
1:A:143:ASP:CB	1:A:237:LEU:HD23	2.50	0.42
1:A:64:VAL:O	1:A:68:LEU:CD1	2.65	0.42
1:A:317:PHE:O	1:A:343:ASP:HB2	2.20	0.41
1:A:392:LEU:HD11	1:A:495:LEU:HD23	2.02	0.41
2:B:505:LEU:HD21	2:B:527:LEU:HD12	2.01	0.41
1:A:143:ASP:HB3	1:A:237:LEU:HD23	2.02	0.41
1:A:143:ASP:OD2	1:A:237:LEU:HB3	2.20	0.41
1:A:441:PHE:CD2	6:A:912:BGC:H2	2.55	0.41
1:A:372:THR:HG22	1:A:512:LEU:HD11	2.01	0.41
2:B:425:PRO:HA	2:B:426:PRO:HD3	1.84	0.41
2:B:562:MET:HE2	2:B:562:MET:HB3	1.99	0.41
2:B:641:ALA:HB1	2:B:648:PRO:HD2	2.02	0.41
1:A:371:GLU:HG2	1:A:510:GLU:O	2.20	0.41
2:B:103:SER:HB2	2:B:172:TRP:CD2	2.56	0.41
2:B:374:LEU:HD13	2:B:438:MET:SD	2.61	0.41
2:B:597:ASP:OD1	2:B:597:ASP:N	2.52	0.41
1:A:56:LEU:HD13	1:A:68:LEU:HB3	2.03	0.41
2:B:78[A]:GLN:HE21	2:B:333:ASN:HD22	1.67	0.41
1:A:382:ARG:NH2	11:A:925:660:O12	2.54	0.41
2:B:263:SER:O	2:B:285:PRO:HA	2.20	0.41
2:B:78[A]:GLN:HB2	2:B:333:ASN:ND2	2.36	0.41
8:A:920:C2E:H2'	8:A:921:C2E:N11	2.36	0.41
1:A:279:ILE:HG23	1:A:366:ALA:HB1	2.03	0.41
1:A:522:ARG:HB2	1:A:523:PRO:HD3	2.02	0.41
1:A:423:ARG:HD3	1:A:423:ARG:HA	1.93	0.41
1:A:131:PRO:HB3	1:A:261:GLY:HA3	2.01	0.41
2:B:352:ALA:HB3	2:B:354:GLN:NE2	2.36	0.41
2:B:586:ILE:O	2:B:590:ARG:HG2	2.21	0.40
1:A:147:PRO:HD2	1:A:245:PHE:O	2.21	0.40
1:A:616:ARG:HH22	8:A:921:C2E:H511	1.87	0.40
2:B:577:PHE:O	2:B:581:THR:HG23	2.21	0.40
1:A:192:PRO:HA	1:A:193:GLU:HA	1.80	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	726/803 (90%)	700 (96%)	25 (3%)	1 (0%)	56 89
2	B	659/729 (90%)	646 (98%)	13 (2%)	0	100 100
All	All	1385/1532 (90%)	1346 (97%)	38 (3%)	1 (0%)	56 89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	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	598/661 (90%)	590 (99%)	8 (1%)	76 92
2	B	525/573 (92%)	516 (98%)	9 (2%)	68 90
All	All	1123/1234 (91%)	1106 (98%)	17 (2%)	72 91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	137	GLU

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Mol	Chain	Res	Type
1	A	369	GLN
1	A	502	ARG
1	A	554	VAL
1	A	573	VAL
1	A	615	VAL
1	A	617	LEU
2	B	86	PHE
2	B	184	LEU
2	B	267	ARG
2	B	326	VAL
2	B	446	LEU
2	B	477	ASP
2	B	597	ASP
2	B	674	ARG
2	B	696	LEU

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

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

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 for Mogul analysis.

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	$\#\|Z\| > 2$
4	PLC	A	901	-	37,37,41	1.10	4 (10%)	41,45,49	1.06	2 (4%)
5	43Y	A	902	-	19,19,23	1.36	4 (21%)	21,24,31	1.44	2 (9%)
6	BGC	A	903	6	12,12,12	2.34	3 (25%)	17,17,17	1.64	4 (23%)
6	BGC	A	904	6	11,11,12	2.58	4 (36%)	15,15,17	1.94	5 (33%)
6	BGC	A	905	6	11,11,12	2.61	2 (18%)	15,15,17	2.37	6 (40%)
6	BGC	A	906	6	11,11,12	2.66	4 (36%)	15,15,17	2.19	5 (33%)
6	BGC	A	907	6	11,11,12	2.50	3 (27%)	15,15,17	2.14	4 (26%)
6	BGC	A	908	6	11,11,12	2.89	5 (45%)	15,15,17	1.12	2 (13%)
6	BGC	A	909	6	11,11,12	2.62	3 (27%)	15,15,17	1.39	2 (13%)
6	BGC	A	910	6	11,11,12	2.48	3 (27%)	15,15,17	1.99	6 (40%)
6	BGC	A	911	6	11,11,12	2.56	2 (18%)	15,15,17	1.56	1 (6%)
6	BGC	A	912	6	11,11,12	2.56	2 (18%)	15,15,17	1.94	4 (26%)
6	BGC	A	913	6	11,11,12	2.59	2 (18%)	15,15,17	1.26	2 (13%)
6	BGC	A	914	6	11,11,12	2.64	2 (18%)	15,15,17	1.21	2 (13%)
6	BGC	A	915	6	11,11,12	2.51	2 (18%)	15,15,17	1.41	2 (13%)
6	BGC	A	916	6	11,11,12	2.57	3 (27%)	15,15,17	2.00	2 (13%)
6	BGC	A	917	6	11,11,12	2.58	3 (27%)	15,15,17	1.47	3 (20%)
6	BGC	A	918	7,6	11,11,12	2.69	3 (27%)	15,15,17	1.99	4 (26%)
7	GAL	A	919	6	11,11,12	0.56	0	15,15,17	0.92	0
8	C2E	A	920	-	44,52,52	4.92	29 (65%)	50,82,82	3.22	11 (22%)
8	C2E	A	921	-	44,52,52	4.91	29 (65%)	50,82,82	3.27	11 (22%)
9	LDA	A	922	-	15,15,15	3.97	2 (13%)	16,17,17	0.54	0
9	LDA	A	923	-	15,15,15	3.96	2 (13%)	16,17,17	0.62	0
11	660	A	925	-	32,38,38	3.16	12 (37%)	39,58,58	1.60	5 (12%)

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
4	PLC	A	901	-	-	0/41/41/45	0/0/0/0
5	43Y	A	902	-	-	0/22/22/27	0/0/0/0
6	BGC	A	903	6	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BGC	A	904	6	-	0/2/19/22	0/1/1/1
6	BGC	A	905	6	-	0/2/19/22	0/1/1/1
6	BGC	A	906	6	-	0/2/19/22	0/1/1/1
6	BGC	A	907	6	-	0/2/19/22	0/1/1/1
6	BGC	A	908	6	-	0/2/19/22	0/1/1/1
6	BGC	A	909	6	-	0/2/19/22	0/1/1/1
6	BGC	A	910	6	-	0/2/19/22	0/1/1/1
6	BGC	A	911	6	-	0/2/19/22	0/1/1/1
6	BGC	A	912	6	-	0/2/19/22	0/1/1/1
6	BGC	A	913	6	-	0/2/19/22	0/1/1/1
6	BGC	A	914	6	-	0/2/19/22	0/1/1/1
6	BGC	A	915	6	-	0/2/19/22	0/1/1/1
6	BGC	A	916	6	-	0/2/19/22	0/1/1/1
6	BGC	A	917	6	-	0/2/19/22	0/1/1/1
6	BGC	A	918	7,6	-	0/2/19/22	0/1/1/1
7	GAL	A	919	6	-	0/2/19/22	0/1/1/1
8	C2E	A	920	-	-	0/22/62/62	0/6/7/7
8	C2E	A	921	-	-	0/22/62/62	0/6/7/7
9	LDA	A	922	-	-	0/13/13/13	0/0/0/0
9	LDA	A	923	-	-	0/13/13/13	0/0/0/0
11	660	A	925	-	-	0/16/59/59	0/3/3/3

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	922	LDA	O1-N1	-14.99	1.25	1.39
9	A	923	LDA	O1-N1	-14.94	1.25	1.39
8	A	920	C2E	C2A-C3A	-13.71	1.22	1.53
8	A	921	C2E	C2A-C3A	-13.63	1.22	1.53
8	A	921	C2E	C3'-C4'	-9.42	1.26	1.52
8	A	920	C2E	C3'-C4'	-9.25	1.26	1.52
8	A	921	C2E	O4'-C1'	-8.22	1.29	1.41
8	A	920	C2E	O4'-C1'	-8.11	1.29	1.41
8	A	920	C2E	O4A-C4A	-6.54	1.30	1.45
8	A	921	C2E	O4A-C4A	-6.42	1.30	1.45
11	A	925	660	P22-O23	-4.24	1.46	1.56
6	A	918	BGC	C2-C3	-3.18	1.48	1.52
11	A	925	660	C2-C1	-3.06	1.48	1.53
6	A	908	BGC	C2-C3	-3.06	1.48	1.52
9	A	923	LDA	C1-N1	-2.99	1.45	1.51
6	A	903	BGC	O1-C1	-2.99	1.28	1.39
9	A	922	LDA	C1-N1	-2.93	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	906	BGC	C2-C3	-2.80	1.48	1.52
6	A	904	BGC	C2-C3	-2.74	1.48	1.52
6	A	917	BGC	C2-C3	-2.66	1.48	1.52
6	A	914	BGC	C2-C3	-2.61	1.49	1.52
6	A	905	BGC	C2-C3	-2.51	1.49	1.52
6	A	910	BGC	C2-C3	-2.47	1.49	1.52
6	A	913	BGC	C2-C3	-2.47	1.49	1.52
8	A	921	C2E	O2'-C2'	-2.43	1.37	1.43
6	A	912	BGC	C2-C3	-2.42	1.49	1.52
6	A	909	BGC	C2-C3	-2.42	1.49	1.52
8	A	920	C2E	O2'-C2'	-2.42	1.37	1.43
11	A	925	660	C2-C3	-2.38	1.47	1.53
6	A	915	BGC	C2-C3	-2.38	1.49	1.52
8	A	921	C2E	O61-C61	-2.36	1.18	1.24
8	A	920	C2E	O61-C61	-2.35	1.18	1.24
4	A	901	PLC	O2-C2	-2.32	1.40	1.46
5	A	902	43Y	O2-C2	-2.28	1.40	1.46
6	A	911	BGC	C2-C3	-2.15	1.49	1.52
4	A	901	PLC	O3-C3	-2.13	1.40	1.45
11	A	925	660	O20-C20	-2.11	1.19	1.24
5	A	902	43Y	O3-C3	-2.07	1.40	1.45
11	A	925	660	P22-O24	-2.02	1.46	1.51
11	A	925	660	P9-O10	-2.01	1.46	1.55
6	A	904	BGC	O3-C3	2.02	1.47	1.43
6	A	917	BGC	O3-C3	2.03	1.47	1.43
6	A	908	BGC	C1-C2	2.03	1.57	1.52
8	A	921	C2E	P1-O5'	2.03	1.67	1.59
6	A	909	BGC	O3-C3	2.03	1.47	1.43
6	A	903	BGC	O3-C3	2.04	1.47	1.43
6	A	908	BGC	O4-C4	2.05	1.47	1.43
8	A	920	C2E	P1-O5'	2.07	1.68	1.59
6	A	916	BGC	O3-C3	2.08	1.47	1.43
6	A	910	BGC	O3-C3	2.08	1.47	1.43
6	A	906	BGC	O3-C3	2.11	1.47	1.43
6	A	904	BGC	O5-C5	2.11	1.48	1.43
11	A	925	660	C19-N15	2.12	1.42	1.38
4	A	901	PLC	O2-C'	2.12	1.40	1.34
6	A	916	BGC	C1-C2	2.14	1.57	1.52
6	A	907	BGC	O3-C3	2.17	1.48	1.43
6	A	908	BGC	O5-C5	2.17	1.48	1.43
8	A	920	C2E	C21-N31	2.21	1.46	1.35
8	A	921	C2E	C21-N31	2.24	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	907	BGC	C1-C2	2.26	1.57	1.52
6	A	918	BGC	O5-C5	2.27	1.48	1.43
4	A	901	PLC	O3-CB	2.38	1.40	1.33
5	A	902	43Y	O2-C31	2.39	1.40	1.35
6	A	906	BGC	O4-C4	2.43	1.48	1.43
8	A	921	C2E	C2-N3	2.51	1.48	1.35
5	A	902	43Y	O3-C11	2.52	1.40	1.33
8	A	920	C2E	C2-N3	2.54	1.48	1.35
8	A	920	C2E	P11-O5A	2.70	1.70	1.59
8	A	921	C2E	P11-O5A	2.76	1.70	1.59
8	A	920	C2E	O3A-C3A	2.80	1.53	1.44
8	A	921	C2E	O3A-C3A	2.87	1.53	1.44
8	A	920	C2E	P1-O3A	3.70	1.70	1.60
8	A	921	C2E	P1-O3A	3.88	1.71	1.60
8	A	920	C2E	C21-N21	3.98	1.42	1.34
8	A	921	C2E	C21-N21	4.00	1.42	1.34
8	A	921	C2E	O3'-C3'	4.00	1.56	1.44
8	A	921	C2E	C2-N2	4.12	1.42	1.34
8	A	920	C2E	O3'-C3'	4.14	1.57	1.44
8	A	920	C2E	C2-N2	4.19	1.43	1.34
8	A	920	C2E	O2A-C2A	4.21	1.52	1.43
8	A	921	C2E	O2A-C2A	4.21	1.52	1.43
8	A	921	C2E	P11-O3'	4.21	1.71	1.60
8	A	920	C2E	P11-O3'	4.51	1.72	1.60
8	A	920	C2E	C21-N11	4.93	1.44	1.35
8	A	921	C2E	C21-N11	5.01	1.44	1.35
11	A	925	660	O6-C1	5.08	1.48	1.41
11	A	925	660	C20-N15	5.10	1.42	1.33
8	A	921	C2E	C2-N1	5.26	1.45	1.35
8	A	920	C2E	C2-N1	5.27	1.45	1.35
8	A	921	C2E	C61-N11	5.36	1.42	1.33
8	A	920	C2E	C61-N11	5.39	1.42	1.33
8	A	920	C2E	C3A-C4A	5.61	1.68	1.52
8	A	920	C2E	C2A-C1A	5.66	1.62	1.53
8	A	921	C2E	C2A-C1A	5.68	1.62	1.53
8	A	921	C2E	C3A-C4A	5.79	1.69	1.52
8	A	921	C2E	C6-N1	5.91	1.43	1.33
8	A	920	C2E	C6-N1	5.94	1.43	1.33
8	A	921	C2E	C61-C51	6.11	1.53	1.41
11	A	925	660	P22-O12	6.16	1.65	1.58
8	A	920	C2E	C61-C51	6.18	1.53	1.41
6	A	903	BGC	O5-C1	6.28	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	921	C2E	C6-C5	6.43	1.54	1.41
8	A	920	C2E	C6-C5	6.49	1.54	1.41
6	A	910	BGC	O5-C1	6.66	1.54	1.43
6	A	915	BGC	O5-C1	6.79	1.54	1.43
6	A	907	BGC	O5-C1	6.87	1.54	1.43
6	A	904	BGC	O5-C1	6.90	1.55	1.43
6	A	917	BGC	O5-C1	6.93	1.55	1.43
6	A	912	BGC	O5-C1	6.93	1.55	1.43
8	A	921	C2E	O4A-C1A	7.01	1.51	1.41
6	A	911	BGC	O5-C1	7.03	1.55	1.43
6	A	916	BGC	O5-C1	7.09	1.55	1.43
6	A	918	BGC	O5-C1	7.09	1.55	1.43
8	A	920	C2E	O4A-C1A	7.09	1.51	1.41
6	A	913	BGC	O5-C1	7.13	1.55	1.43
6	A	906	BGC	O5-C1	7.13	1.55	1.43
6	A	905	BGC	O5-C1	7.16	1.55	1.43
6	A	909	BGC	O5-C1	7.19	1.55	1.43
6	A	914	BGC	O5-C1	7.20	1.55	1.43
11	A	925	660	P22-C45	7.31	1.86	1.80
6	A	908	BGC	O5-C1	7.84	1.56	1.43
8	A	920	C2E	C4-N3	8.28	1.48	1.35
8	A	921	C2E	C4-N3	8.30	1.48	1.35
8	A	921	C2E	C41-N31	8.39	1.49	1.35
8	A	921	C2E	O4'-C4'	8.44	1.64	1.45
8	A	920	C2E	C41-N31	8.47	1.49	1.35
8	A	920	C2E	O4'-C4'	8.58	1.64	1.45
11	A	925	660	C18-N13	10.30	1.49	1.35

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	921	C2E	C1'-N9-C4	-17.68	107.07	126.81
8	A	920	C2E	C1'-N9-C4	-17.26	107.54	126.81
8	A	921	C2E	C1A-N91-C41	-8.51	117.31	126.81
8	A	920	C2E	C1A-N91-C41	-8.14	117.72	126.81
8	A	920	C2E	N3-C2-N1	-5.40	120.20	127.56
8	A	920	C2E	N31-C21-N11	-5.39	120.22	127.56
8	A	921	C2E	N3-C2-N1	-5.39	120.22	127.56
8	A	921	C2E	N31-C21-N11	-5.35	120.28	127.56
11	A	925	660	C4-O6-C1	-4.51	104.87	109.64
6	A	904	BGC	O5-C1-C2	-3.58	105.17	110.89
8	A	921	C2E	C4A-O4A-C1A	-3.10	106.35	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	909	BGC	O5-C1-C2	-3.10	105.94	110.89
8	A	920	C2E	C4A-O4A-C1A	-3.01	106.45	109.64
8	A	920	C2E	C5-C6-N1	-3.01	119.59	123.52
11	A	925	660	O23-P22-O24	-2.99	100.69	110.24
6	A	910	BGC	O5-C1-C2	-2.94	106.19	110.89
6	A	912	BGC	O3-C3-C2	-2.90	104.69	110.01
6	A	913	BGC	O5-C1-C2	-2.82	106.39	110.89
6	A	907	BGC	O5-C1-C2	-2.81	106.40	110.89
8	A	921	C2E	C5-C6-N1	-2.75	119.92	123.52
8	A	921	C2E	C51-C61-N11	-2.73	119.95	123.52
6	A	917	BGC	O5-C1-C2	-2.73	106.53	110.89
6	A	907	BGC	O4-C4-C5	-2.63	102.28	109.23
8	A	920	C2E	C51-C61-N11	-2.63	120.09	123.52
6	A	903	BGC	O5-C1-C2	-2.60	105.45	110.00
6	A	918	BGC	C6-C5-C4	-2.35	107.11	112.99
6	A	914	BGC	O3-C3-C2	-2.30	105.79	110.01
6	A	905	BGC	O5-C1-C2	-2.28	107.24	110.89
6	A	906	BGC	O3-C3-C2	-2.26	105.87	110.01
6	A	905	BGC	O4-C4-C3	-2.26	105.27	110.36
6	A	908	BGC	O5-C1-C2	-2.25	107.30	110.89
6	A	915	BGC	O3-C3-C2	-2.18	106.01	110.01
6	A	906	BGC	O5-C1-C2	-2.17	107.42	110.89
11	A	925	660	O10-P9-O11	-2.16	101.30	112.56
6	A	910	BGC	C1-O5-C5	-2.04	109.14	112.14
6	A	912	BGC	C3-C4-C5	2.17	114.10	110.23
8	A	921	C2E	C3'-C2'-C1'	2.19	104.83	100.06
6	A	905	BGC	O5-C5-C4	2.19	113.76	110.13
6	A	913	BGC	C3-C4-C5	2.19	114.14	110.23
6	A	908	BGC	O5-C5-C4	2.21	113.79	110.13
6	A	909	BGC	C3-C4-C5	2.30	114.32	110.23
8	A	921	C2E	O21-P11-O3'	2.33	116.36	106.76
6	A	904	BGC	C1-C2-C3	2.39	112.44	109.55
8	A	920	C2E	C3'-C2'-C1'	2.45	105.39	100.06
6	A	914	BGC	C1-C2-C3	2.47	112.55	109.55
6	A	910	BGC	O5-C5-C4	2.51	114.29	110.13
4	A	901	PLC	O3-CB-C1B	2.60	119.84	111.85
6	A	903	BGC	C4-C3-C2	2.63	115.63	110.79
6	A	917	BGC	O5-C5-C4	2.66	114.54	110.13
8	A	920	C2E	O21-P11-O3'	2.66	117.72	106.76
6	A	904	BGC	C2-C3-C4	2.70	115.75	111.05
6	A	910	BGC	C1-C2-C3	2.74	112.87	109.55
6	A	917	BGC	C3-C4-C5	2.76	115.15	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	906	BGC	C3-C4-C5	2.77	115.16	110.23
6	A	903	BGC	O5-C5-C4	2.85	115.11	109.67
6	A	915	BGC	C1-C2-C3	2.89	113.05	109.55
6	A	916	BGC	C2-C3-C4	2.91	116.13	111.05
6	A	918	BGC	C3-C4-C5	2.92	115.44	110.23
6	A	910	BGC	C2-C3-C4	2.95	116.20	111.05
6	A	912	BGC	C2-C3-C4	2.98	116.24	111.05
11	A	925	660	O23-P22-C45	2.99	111.54	105.39
5	A	902	43Y	O3-C11-C9	3.06	120.27	111.16
8	A	920	C2E	C61-N11-C21	3.08	119.50	115.88
6	A	904	BGC	C3-C4-C5	3.11	115.77	110.23
6	A	904	BGC	O5-C5-C4	3.12	115.31	110.13
8	A	921	C2E	C61-N11-C21	3.16	119.58	115.88
8	A	921	C2E	C6-N1-C2	3.19	119.62	115.88
6	A	907	BGC	C2-C3-C4	3.30	116.81	111.05
8	A	920	C2E	C6-N1-C2	3.39	119.86	115.88
6	A	905	BGC	C3-C4-C5	3.47	116.41	110.23
4	A	901	PLC	O2-C'-C1'	3.56	119.03	111.53
6	A	903	BGC	C3-C4-C5	3.56	116.58	110.23
6	A	910	BGC	C3-C4-C5	3.62	116.67	110.23
6	A	905	BGC	C2-C3-C4	4.09	118.19	111.05
6	A	918	BGC	C1-O5-C5	4.23	118.36	112.14
6	A	918	BGC	O5-C5-C4	4.24	117.16	110.13
6	A	911	BGC	C1-C2-C3	4.37	114.85	109.55
6	A	906	BGC	C1-C2-C3	4.53	115.05	109.55
6	A	906	BGC	C2-C3-C4	4.66	119.17	111.05
5	A	902	43Y	O2-C31-C32	4.68	120.00	111.09
6	A	912	BGC	C1-C2-C3	5.19	115.84	109.55
11	A	925	660	C20-N15-C19	5.23	119.72	114.21
6	A	905	BGC	C1-C2-C3	5.39	116.08	109.55
6	A	907	BGC	C1-C2-C3	5.75	116.52	109.55
6	A	916	BGC	C1-C2-C3	6.38	117.28	109.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	902	43Y	1	0
6	A	906	BGC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	907	BGC	1	0
6	A	908	BGC	3	0
6	A	912	BGC	1	0
6	A	916	BGC	1	0
7	A	919	GAL	1	0
8	A	920	C2E	2	0
8	A	921	C2E	4	0
9	A	923	LDA	2	0
11	A	925	660	2	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

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	728/803 (90%)	0.06	27 (3%) 45 27	47, 80, 140, 234	0
2	B	658/729 (90%)	-0.09	15 (2%) 64 43	47, 74, 123, 188	0
3	D	0/9	-	-	-	-
All	All	1386/1541 (89%)	-0.01	42 (3%) 54 33	47, 77, 132, 234	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	502	ARG	5.5
1	A	496	LEU	5.0
2	B	77[A]	GLN	4.8
1	A	509	ASP	4.1
2	B	592	MET	3.8
1	A	318	CYS	3.8
2	B	169	PHE	3.7
2	B	593	LEU	3.7
2	B	544	GLY	3.6
2	B	78[A]	GLN	3.5
1	A	705	ARG	3.2
1	A	739	ARG	3.2
2	B	607	ARG	3.2
1	A	94	LEU	3.1
2	B	594	ARG	3.0
1	A	539	LEU	3.0
2	B	265	ALA	3.0
2	B	595	PRO	2.9
1	A	503	PHE	2.6
1	A	507	ALA	2.6
2	B	130	PHE	2.6
1	A	93	ALA	2.5
1	A	320	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	196	GLN	2.4
1	A	497	ARG	2.3
1	A	738	ARG	2.3
1	A	327	ARG	2.3
1	A	189	SER	2.3
1	A	618	LEU	2.2
1	A	134	LEU	2.2
1	A	736	ALA	2.2
2	B	590	ARG	2.2
2	B	162	TYR	2.1
1	A	514	GLU	2.1
1	A	740	ARG	2.1
1	A	737	ARG	2.1
1	A	194	LEU	2.1
2	B	104	ILE	2.1
1	A	735	PRO	2.1
2	B	718	ARG	2.0
1	A	543	VAL	2.0
1	A	225	ALA	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 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, 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	LLDF	B-factors(Å^2)	Q<0.9
10	MG	A	924	1/1	0.88	1.46	19.71	83,83,83,83	0
9	LDA	A	922	16/16	0.61	0.48	7.80	52,67,83,85	16

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	PLC	A	901	38/42	0.82	0.42	3.54	106,129,151,152	0
5	43Y	A	902	20/24	0.93	0.28	2.15	88,105,122,129	0
6	BGC	A	915	11/12	0.95	0.30	2.05	63,80,85,85	0
9	LDA	A	923	16/16	0.62	0.28	1.90	76,91,111,119	16
6	BGC	A	914	11/12	0.96	0.24	1.53	63,73,83,87	0
6	BGC	A	916	11/12	0.94	0.28	1.41	65,81,86,87	0
7	GAL	A	919	11/12	0.96	0.33	1.10	65,80,96,98	0
6	BGC	A	910	11/12	0.93	0.21	1.04	72,76,97,117	0
6	BGC	A	918	11/12	0.97	0.30	1.04	59,69,86,93	0
11	660	A	925	36/36	0.92	0.33	0.90	67,78,89,95	36
10	MG	B	801	1/1	0.73	0.19	0.67	54,54,54,54	0
6	BGC	A	912	11/12	0.96	0.23	0.53	71,77,92,98	0
6	BGC	A	917	11/12	0.97	0.27	0.41	59,68,73,73	0
6	BGC	A	913	11/12	0.96	0.21	0.39	82,89,93,95	0
6	BGC	A	911	11/12	0.97	0.20	0.14	69,74,79,88	0
6	BGC	A	907	11/12	0.93	0.18	-0.21	49,55,64,105	0
6	BGC	A	906	11/12	0.94	0.19	-0.28	56,69,114,142	0
6	BGC	A	908	11/12	0.88	0.19	-0.45	53,63,85,108	0
6	BGC	A	909	11/12	0.91	0.17	-0.58	49,65,72,81	0
8	C2E	A	920	46/46	0.96	0.13	-0.94	51,67,82,82	0
8	C2E	A	921	46/46	0.95	0.12	-1.26	53,76,86,95	0
6	BGC	A	905	11/12	0.90	0.20	-	92,109,121,126	0
6	BGC	A	904	11/12	0.84	0.25	-	105,120,134,148	0
6	BGC	A	903	12/12	0.72	0.34	-	161,171,185,205	0

6.5 Other polymers

There are no such residues in this entry.