



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 09:13 PM EDT

PDB ID : 4P00  
Title : Bacterial Cellulose Synthase in complex with cyclic-di-GMP and UDP  
Authors : Morgan, J.L.W.; McNamara, J.T.; Zimmer, J.  
Deposited on : 2014-02-19  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

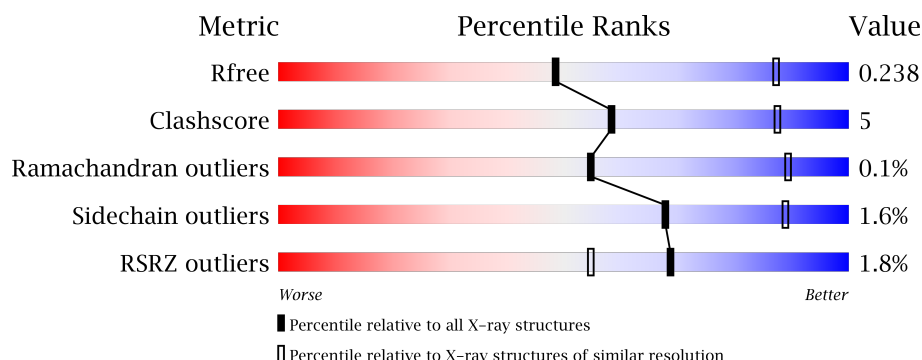
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	803	<div> <div>2%</div> <div>77%</div> <div>13%</div> <div>9%</div> </div>
2	B	724	<div> <div>%</div> <div>78%</div> <div>12%</div> <div>10%</div> </div>
3	D	9	<div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MG	A	921	-	-	-	X
8	PLC	A	922	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11070 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 Cellulose Synthase A subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	1	0
			5739	3725	1000	982	32			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	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

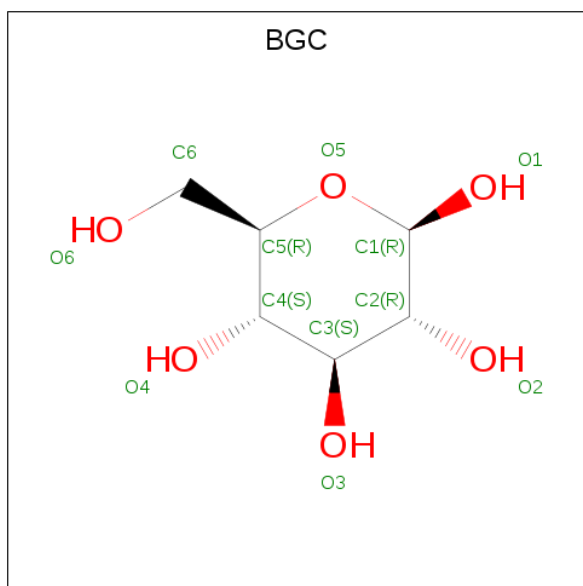
- Molecule 2 is a protein called Cellulose Synthase B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	655	Total	C	N	O	S	0	5	0
			4923	3120	872	915	16			

- Molecule 3 is a protein called unidentified peptide.

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

- Molecule 4 is BETA-D-GLUCOSE (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).



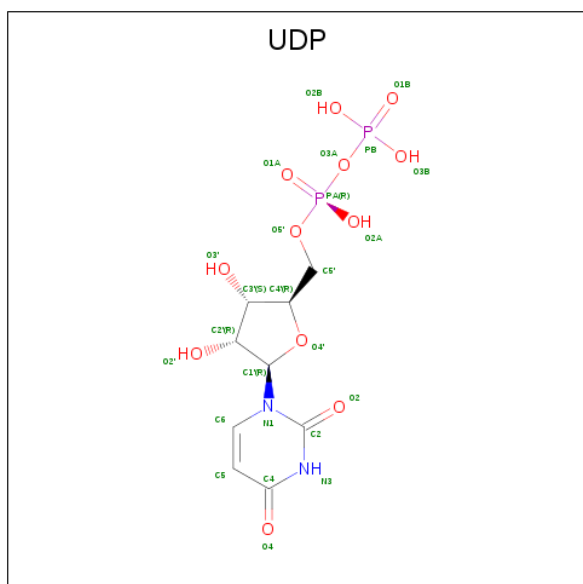
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

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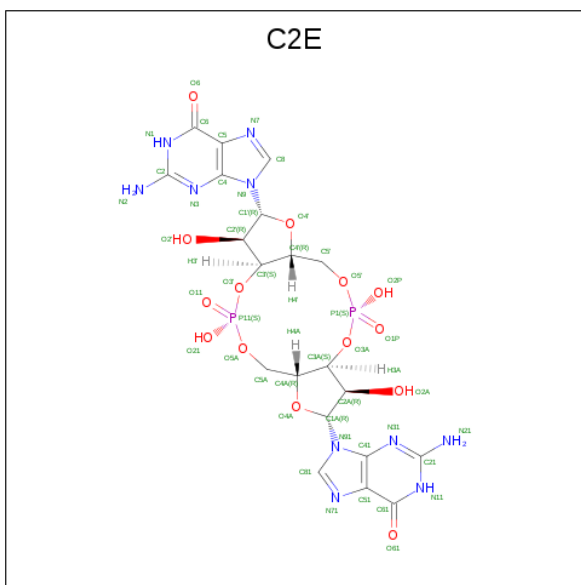
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 6 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-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:  $C_{20}H_{24}N_{10}O_{14}P_2$ ).

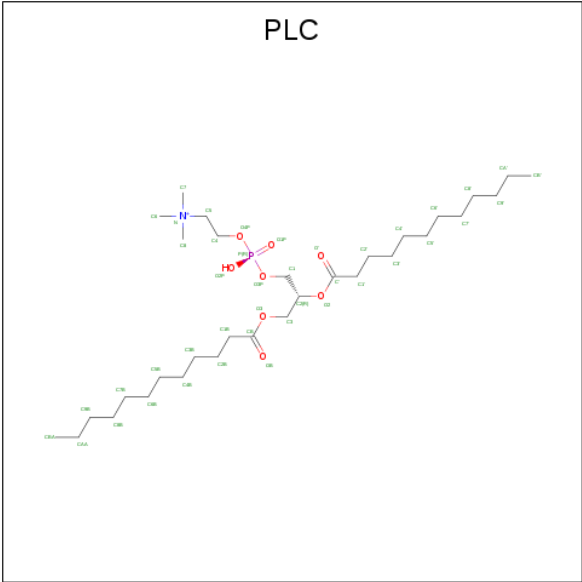


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	A	1	Total 46	C 20	N 10	O 14	P 2	0	0
6	A	1	Total 46	C 20	N 10	O 14	P 2	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

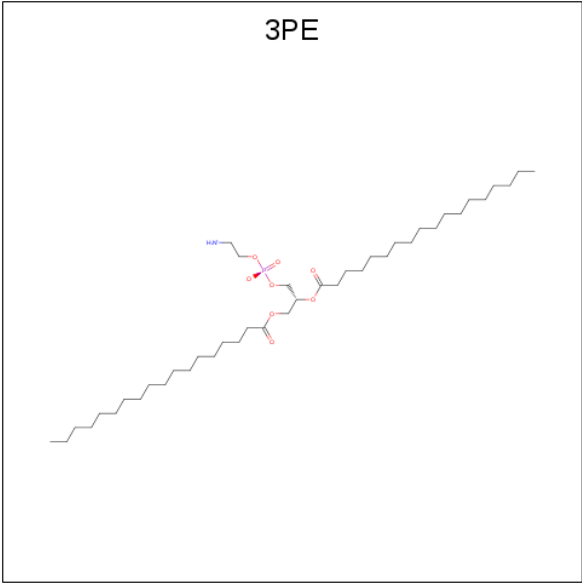
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0

- Molecule 8 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula:  $\text{C}_{32}\text{H}_{65}\text{NO}_8\text{P}$ ).



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

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



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



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 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.

Chain A:

Chain B:

- Molecule 3: unidentified peptide

Chain D:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.49 Å   216.79 Å   219.62 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.98 – 3.20 49.62 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.98-3.20) 98.2 (49.62-3.20)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 3.19 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.208 , 0.238 0.208 , 0.238	Depositor DCC
$R_{free}$ test set	2715 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.0	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: UDP, BGC, MG, PLC, C2E, 3PE

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	0.21	0/5888	0.37	0/8007
2	B	0.20	0/5042	0.40	0/6913
All	All	0.21	0/10930	0.38	0/14920

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	5739	0	5855	64	0
2	B	4923	0	4997	51	0
3	D	45	0	12	0	0
4	A	187	0	154	9	0
5	A	25	0	11	1	0
6	A	92	0	44	11	0
7	A	1	0	0	0	0
8	A	38	0	53	1	0
9	A	20	0	14	1	0
All	All	11070	0	11140	122	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 (122) 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)
6:A:920:C2E:H81	6:A:920:C2E:H511	1.21	1.11
6:A:920:C2E:H81	6:A:920:C2E:C5A	1.93	0.98
1:A:578:GLN:OE1	6:A:920:C2E:N2	1.99	0.94
4:A:905:BGC:O6	2:B:390:ARG:NH2	2.05	0.88
1:A:57:LYS:NZ	9:A:923:3PE:O12	2.16	0.78
1:A:578:GLN:OE1	6:A:920:C2E:N1	2.20	0.74
4:A:904:BGC:O3	4:A:905:BGC:O5	2.06	0.73
1:A:578:GLN:OE1	6:A:920:C2E:C2	2.40	0.69
1:A:311:ARG:HH22	2:B:719:THR:HG23	1.59	0.68
1:A:312:TRP:HB3	1:A:405:ALA:HB1	1.80	0.63
1:A:42:GLN:OE1	1:A:79:ARG:NH1	2.32	0.63
1:A:385:THR:HG23	1:A:494:THR:HG21	1.80	0.63
1:A:419:PHE:HA	1:A:422:VAL:HG22	1.82	0.61
4:A:905:BGC:O3	4:A:906:BGC:O5	2.16	0.61
6:A:920:C2E:C81	6:A:920:C2E:H511	2.14	0.61
1:A:35:ALA:O	1:A:79:ARG:NH2	2.34	0.60
2:B:77[A]:GLN:HG3	2:B:157:HIS:H	1.67	0.59
2:B:377:LYS:HB2	2:B:416:SER:HB2	1.85	0.59
1:A:300:MET:HA	1:A:470:GLN:HB3	1.85	0.58
2:B:425:PRO:HG2	2:B:428:GLN:HB2	1.86	0.58
2:B:270:ILE:HG22	2:B:280:LEU:HA	1.85	0.58
1:A:432:ILE:HD11	1:A:440:ILE:HD13	1.85	0.58
2:B:360:ILE:HA	2:B:444:THR:HG23	1.85	0.57
2:B:328:THR:HG22	2:B:442:SER:H	1.69	0.57
4:A:904:BGC:HC	4:A:905:BGC:C5	2.16	0.57
2:B:693:ARG:HG2	2:B:695:PRO:HD2	1.85	0.57
2:B:358:ILE:HG12	2:B:446:LEU:HD23	1.87	0.56
1:A:343:ASP:N	1:A:343:ASP:OD1	2.38	0.56
2:B:320:THR:HA	2:B:445:ASP:HA	1.86	0.56
2:B:59:LEU:HD13	2:B:85:LEU:HD13	1.86	0.56
1:A:480:GLU:OE2	4:A:914:BGC:O6	2.21	0.55
1:A:654:ARG:O	1:A:677:GLN:NE2	2.39	0.55
1:A:161:ALA:HB1	1:A:683:GLU:HG2	1.88	0.55
1:A:394:LYS:O	1:A:399:ARG:NH1	2.40	0.55
1:A:372:THR:HG22	1:A:512:LEU:HD21	1.90	0.54
1:A:151:GLU:O	1:A:201:ARG:NH2	2.42	0.53
2:B:185:PRO:HG2	2:B:188:ALA:HB2	1.89	0.53
2:B:101:ARG:NE	2:B:174:GLU:OE1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLU:OE2	1:A:399:ARG:NH2	2.42	0.52
1:A:66:ARG:NH1	1:A:123:ALA:O	2.42	0.52
1:A:547:GLY:O	4:A:907:BGC:O6	2.27	0.52
1:A:84:ARG:NH1	1:A:108:GLU:OE1	2.42	0.52
2:B:475:THR:HG22	2:B:477:ASP:H	1.73	0.52
2:B:606:THR:HG23	2:B:607:ARG:HE	1.74	0.51
1:A:219:ARG:HD3	1:A:229:ASN:HA	1.93	0.51
1:A:57:LYS:HG3	1:A:465:ALA:HB2	1.92	0.51
1:A:587:MET:N	1:A:608:LEU:O	2.41	0.51
2:B:287:GLU:OE1	2:B:287:GLU:N	2.44	0.51
6:A:919:C2E:H2'	6:A:920:C2E:N11	2.26	0.50
1:A:296:PRO:HG2	1:A:299:GLU:HB2	1.93	0.50
1:A:446:GLU:OE2	2:B:573:ARG:NH2	2.41	0.50
1:A:402:LEU:O	1:A:407:ARG:NH2	2.45	0.49
1:A:274:THR:OG1	1:A:321:ALA:O	2.21	0.49
1:A:183:THR:H	1:A:186:ARG:HB2	1.78	0.49
1:A:276:HIS:O	1:A:298:ASN:ND2	2.46	0.49
1:A:515:ASN:OD1	1:A:577:GLN:N	2.46	0.49
2:B:57:ILE:HD13	2:B:184:LEU:HD21	1.95	0.48
1:A:482:ALA:HB2	1:A:569:ALA:HB1	1.95	0.47
1:A:272:VAL:HG22	1:A:358:LEU:HD21	1.96	0.47
1:A:369:GLN:HG3	1:A:370:PRO:HD2	1.96	0.47
1:A:580:ARG:NH2	6:A:920:C2E:H2'	2.31	0.46
1:A:534:GLY:O	1:A:538:THR:HG23	2.16	0.46
1:A:579:ARG:O	6:A:919:C2E:H5'1	2.15	0.46
1:A:419:PHE:CD2	1:A:420:PRO:HD3	2.50	0.46
1:A:382:ARG:NH2	5:A:918:UDP:O2A	2.49	0.46
4:A:906:BGC:O3	8:A:922:PLC:H71	2.16	0.46
1:A:152:PRO:HB2	1:A:154:ASP:OD1	2.16	0.46
2:B:78[A]:GLN:HE21	2:B:333:ASN:HD21	1.63	0.46
1:A:29:PHE:HZ	1:A:75:MET:HA	1.80	0.46
2:B:77[A]:GLN:HE22	2:B:158:ARG:CZ	2.28	0.46
2:B:396:LYS:HG3	2:B:397:PRO:HD2	1.97	0.46
1:A:607:VAL:HG13	1:A:615:VAL:HG13	1.98	0.45
1:A:394:LYS:HA	1:A:394:LYS:HD3	1.75	0.45
1:A:616:ARG:HB2	6:A:919:C2E:HN11	1.81	0.45
2:B:103:SER:HB2	2:B:172:TRP:CD2	2.52	0.45
2:B:200:LEU:HD13	2:B:239:LEU:HD21	1.98	0.45
2:B:148:ASP:HB3	2:B:305:LEU:HG	1.98	0.45
2:B:78[A]:GLN:HE21	2:B:333:ASN:ND2	2.15	0.45
2:B:350:LEU:HD23	2:B:354:GLN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:SER:HA	1:A:77:VAL:HG22	1.99	0.45
1:A:243:VAL:HG22	1:A:323:VAL:HG12	2.00	0.44
2:B:285:PRO:HA	2:B:286:PRO:HD3	1.90	0.44
2:B:272:ARG:NH2	2:B:276:GLY:O	2.44	0.44
1:A:144:ILE:HG13	1:A:243:VAL:HB	2.00	0.43
1:A:203:ARG:NH1	1:A:207:GLN:HB2	2.33	0.43
2:B:310:LEU:HB2	2:B:343:GLN:HG2	1.99	0.43
1:A:392:LEU:HD11	1:A:495:LEU:HD23	2.00	0.43
6:A:920:C2E:C5A	6:A:920:C2E:C81	2.82	0.43
2:B:261:LEU:HD12	2:B:262:PRO:HD2	2.01	0.43
4:A:901:BGC:H6C1	4:A:902:BGC:O2	2.19	0.43
1:A:389:GLN:NE2	1:A:498:PRO:O	2.51	0.43
2:B:234:LEU:HD12	2:B:239:LEU:HD11	2.01	0.43
2:B:70:PRO:HG2	2:B:71:LEU:HD12	2.01	0.43
2:B:262:PRO:HB3	2:B:286:PRO:HG3	2.01	0.43
2:B:117:MET:HE2	2:B:122:ILE:HG21	2.01	0.42
2:B:641:ALA:HB1	2:B:648:PRO:HD2	2.01	0.42
1:A:384:ALA:O	1:A:388:MET:HG2	2.20	0.42
2:B:73:ARG:NH1	2:B:174:GLU:OE2	2.53	0.42
1:A:387:MET:HG3	1:A:417:TRP:CD1	2.54	0.42
2:B:157:HIS:CE1	2:B:173:THR:HG22	2.55	0.42
1:A:147:PRO:HG3	1:A:230:MET:HE3	2.01	0.42
2:B:350:LEU:HD21	2:B:449:PRO:HB2	2.02	0.42
2:B:55:TRP:CE3	2:B:189:ILE:HG13	2.54	0.41
2:B:266:ASP:OD1	2:B:266:ASP:N	2.53	0.41
1:A:464:ASN:O	1:A:468:ALA:HB2	2.19	0.41
2:B:369:PRO:HB2	2:B:422:PRO:HG2	2.02	0.41
1:A:441:PHE:HB3	4:A:909:BGC:O4	2.21	0.41
1:A:40:SER:HA	2:B:581:THR:HG22	2.02	0.41
2:B:307:PRO:HA	2:B:308:PRO:HD3	1.91	0.41
1:A:184:ASP:HB2	1:A:220:GLU:HA	2.03	0.41
2:B:76[A]:GLY:HA2	2:B:168:GLU:O	2.20	0.41
1:A:448:VAL:O	1:A:453:PRO:HD3	2.20	0.41
2:B:238:ALA:HB2	2:B:488:ALA:HB2	2.03	0.41
1:A:218:THR:OG1	1:A:219:ARG:N	2.54	0.41
2:B:267:ARG:HG2	2:B:283:GLU:HB2	2.03	0.41
1:A:677:GLN:HB3	1:A:681:VAL:HG21	2.03	0.41
2:B:263:SER:OG	2:B:264:ASP:N	2.50	0.41
1:A:271:LEU:HD11	1:A:317:PHE:HB2	2.02	0.40
2:B:425:PRO:HA	2:B:426:PRO:HD3	1.85	0.40
2:B:678:SER:O	2:B:682:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ILE:HG12	1:A:637:ILE:HG13	2.02	0.40
2:B:321:LEU:HB3	2:B:326:VAL:HG22	2.02	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	727/803 (90%)	689 (95%)	36 (5%)	2 (0%)	44	81
2	B	656/724 (91%)	632 (96%)	24 (4%)	0	100	100
All	All	1383/1527 (91%)	1321 (96%)	60 (4%)	2 (0%)	55	89

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	574	ALA
1	A	167	ILE

### 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	599/661 (91%)	591 (99%)	8 (1%)	73	91
2	B	523/572 (91%)	513 (98%)	10 (2%)	62	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1122/1233 (91%)	1104 (98%)	18 (2%)	68 89

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

Mol	Chain	Res	Type
1	A	37	VAL
1	A	175	VAL
1	A	341	THR
1	A	358	LEU
1	A	369	GLN
1	A	446	GLU
1	A	568	PHE
1	A	627	PRO
2	B	87	LEU
2	B	144	VAL
2	B	148	ASP
2	B	266	ASP
2	B	326	VAL
2	B	378	VAL
2	B	523	LEU
2	B	575	GLN
2	B	643	ARG
2	B	672	GLU

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	BGC	A	901	4	11,11,12	0.30	0	13,15,17	0.82	0
4	BGC	A	902	4	11,11,12	0.34	0	13,15,17	0.99	0
4	BGC	A	903	4	11,11,12	0.30	0	13,15,17	0.83	0
4	BGC	A	904	4	11,11,12	0.39	0	13,15,17	1.27	1 (7%)
4	BGC	A	905	4	11,11,12	0.44	0	13,15,17	1.68	2 (15%)
4	BGC	A	906	4	11,11,12	0.26	0	13,15,17	0.65	0
4	BGC	A	907	4	11,11,12	0.27	0	13,15,17	0.91	1 (7%)
4	BGC	A	908	4	11,11,12	0.36	0	13,15,17	1.21	1 (7%)
4	BGC	A	909	4	11,11,12	0.30	0	13,15,17	0.71	0
4	BGC	A	910	4	11,11,12	0.32	0	13,15,17	0.86	1 (7%)
4	BGC	A	911	4	11,11,12	0.29	0	13,15,17	0.69	0
4	BGC	A	912	4	11,11,12	0.30	0	13,15,17	0.75	1 (7%)
4	BGC	A	913	4	11,11,12	0.30	0	13,15,17	0.64	0
4	BGC	A	914	4	11,11,12	0.33	0	13,15,17	1.26	1 (7%)
4	BGC	A	915	4	11,11,12	0.31	0	13,15,17	0.87	1 (7%)
4	BGC	A	916	4	11,11,12	0.29	0	13,15,17	0.77	0
4	BGC	A	917	4	11,11,12	0.25	0	13,15,17	0.60	0
5	UDP	A	918	7	21,26,26	1.06	1 (4%)	22,40,40	1.64	1 (4%)
6	C2E	A	919	-	44,52,52	1.21	4 (9%)	50,82,82	1.97	13 (26%)
6	C2E	A	920	-	44,52,52	1.20	4 (9%)	50,82,82	1.95	13 (26%)
8	PLC	A	922	-	37,37,41	1.10	2 (5%)	42,45,49	1.14	3 (7%)
9	3PE	A	923	-	19,19,50	1.56	2 (10%)	21,24,55	1.65	3 (14%)

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	BGC	A	901	4	-	0/2/19/22	0/1/1/1
4	BGC	A	902	4	-	0/2/19/22	0/1/1/1
4	BGC	A	903	4	-	0/2/19/22	0/1/1/1
4	BGC	A	904	4	-	0/2/19/22	0/1/1/1
4	BGC	A	905	4	-	0/2/19/22	0/1/1/1
4	BGC	A	906	4	-	0/2/19/22	0/1/1/1
4	BGC	A	907	4	-	0/2/19/22	0/1/1/1
4	BGC	A	908	4	-	0/2/19/22	0/1/1/1
4	BGC	A	909	4	-	0/2/19/22	0/1/1/1
4	BGC	A	910	4	-	0/2/19/22	0/1/1/1
4	BGC	A	911	4	-	0/2/19/22	0/1/1/1
4	BGC	A	912	4	-	0/2/19/22	0/1/1/1
4	BGC	A	913	4	-	0/2/19/22	0/1/1/1
4	BGC	A	914	4	-	0/2/19/22	0/1/1/1
4	BGC	A	915	4	-	0/2/19/22	0/1/1/1
4	BGC	A	916	4	-	0/2/19/22	0/1/1/1
4	BGC	A	917	4	-	0/2/19/22	0/1/1/1
5	UDP	A	918	7	-	0/12/32/32	0/2/2/2
6	C2E	A	919	-	-	0/22/62/62	0/6/7/7
6	C2E	A	920	-	-	0/22/62/62	0/6/7/7
8	PLC	A	922	-	-	0/41/41/45	0/0/0/0
9	3PE	A	923	-	-	0/22/22/54	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	918	UDP	C4-N3	2.91	1.38	1.33
6	A	919	C2E	C51-C41	2.95	1.47	1.40
6	A	919	C2E	C5-C4	2.97	1.47	1.40
6	A	920	C2E	C51-C41	3.01	1.47	1.40
6	A	920	C2E	C5-C4	3.03	1.47	1.40
6	A	920	C2E	C61-C51	3.73	1.48	1.41
6	A	919	C2E	C6-C5	3.76	1.48	1.41
6	A	920	C2E	C6-C5	3.84	1.48	1.41
6	A	919	C2E	C61-C51	3.86	1.48	1.41
8	A	922	PLC	O2-C'	4.02	1.46	1.34
8	A	922	PLC	O3-CB	4.27	1.45	1.33
9	A	923	3PE	O31-C31	4.28	1.45	1.33
9	A	923	3PE	O21-C21	4.63	1.45	1.35

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	919	C2E	C5-C6-N1	-3.78	118.10	123.48
6	A	920	C2E	C5-C6-N1	-3.78	118.10	123.48
6	A	919	C2E	C51-C61-N11	-3.77	118.11	123.48
6	A	919	C2E	C61-C51-C41	-3.75	117.12	120.84
6	A	920	C2E	C51-C61-N11	-3.67	118.25	123.48
6	A	920	C2E	C6-C5-C4	-3.64	117.22	120.84
6	A	920	C2E	C61-C51-C41	-3.58	117.29	120.84
6	A	919	C2E	C6-C5-C4	-3.54	117.32	120.84
6	A	920	C2E	C4-C5-N7	-3.15	106.37	109.41
6	A	919	C2E	C41-C51-N71	-3.07	106.45	109.41
6	A	920	C2E	N31-C21-N11	-2.99	123.09	127.46
9	A	923	3PE	C2-O21-C21	-2.98	112.18	117.94
6	A	919	C2E	N31-C21-N11	-2.98	123.11	127.46
6	A	919	C2E	C4-C5-N7	-2.96	106.55	109.41
6	A	920	C2E	C41-C51-N71	-2.95	106.56	109.41
6	A	919	C2E	N3-C2-N1	-2.91	123.20	127.46
6	A	920	C2E	N3-C2-N1	-2.89	123.23	127.46
4	A	907	BGC	O5-C1-C2	-2.37	107.08	110.79
8	A	922	PLC	C2-O2-C'	-2.37	112.28	117.88
4	A	915	BGC	O5-C1-C2	-2.14	107.44	110.79
4	A	912	BGC	C1-C2-C3	2.19	112.42	109.65
6	A	920	C2E	C3'-C2'-C1'	2.29	105.08	99.95
4	A	908	BGC	C3-C4-C5	2.32	114.30	110.22
6	A	919	C2E	C3'-C2'-C1'	2.37	105.27	99.95
4	A	905	BGC	C2-C3-C4	2.53	115.28	110.88
4	A	910	BGC	C1-C2-C3	2.59	112.93	109.65
8	A	922	PLC	O3-CB-C1B	2.89	120.30	111.90
9	A	923	3PE	O31-C31-C32	3.26	120.10	111.35
4	A	904	BGC	C1-C2-C3	3.61	114.23	109.65
6	A	920	C2E	C61-N11-C21	4.04	121.86	116.06
4	A	914	BGC	C1-C2-C3	4.05	114.79	109.65
6	A	919	C2E	C6-N1-C2	4.07	121.91	116.06
6	A	920	C2E	C6-N1-C2	4.08	121.93	116.06
6	A	919	C2E	C61-N11-C21	4.12	121.98	116.06
8	A	922	PLC	O2-C'-C1'	4.21	120.30	111.55
4	A	905	BGC	C1-C2-C3	4.38	115.20	109.65
6	A	919	C2E	C2-N3-C4	4.80	120.77	115.16
6	A	920	C2E	C2-N3-C4	4.81	120.77	115.16
6	A	919	C2E	C21-N31-C41	4.84	120.82	115.16
9	A	923	3PE	O21-C21-C22	4.90	120.29	111.10
6	A	920	C2E	C21-N31-C41	4.97	120.96	115.16
5	A	918	UDP	C4-N3-C2	6.62	119.81	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	BGC	1	0
4	A	902	BGC	1	0
4	A	904	BGC	2	0
4	A	905	BGC	4	0
4	A	906	BGC	2	0
4	A	907	BGC	1	0
4	A	909	BGC	1	0
4	A	914	BGC	1	0
5	A	918	UDP	1	0
6	A	919	C2E	3	0
6	A	920	C2E	9	0
8	A	922	PLC	1	0
9	A	923	3PE	1	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	728/803 (90%)	-0.11	15 (2%) 64 49	45, 69, 116, 196	0
2	B	655/724 (90%)	-0.20	10 (1%) 74 61	42, 64, 112, 169	0
3	D	0/9	-	-	-	-
All	All	1383/1536 (90%)	-0.16	25 (1%) 69 55	42, 67, 115, 196	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	595	PRO	3.7
1	A	15	PRO	3.5
1	A	496	LEU	3.1
2	B	169	PHE	3.1
1	A	188	MET	3.1
2	B	593	LEU	3.0
2	B	168	GLU	2.8
2	B	592	MET	2.8
1	A	137	GLU	2.8
1	A	740	ARG	2.7
1	A	133	PRO	2.6
2	B	77[A]	GLN	2.4
2	B	596	GLY	2.3
2	B	589	VAL	2.3
1	A	16	VAL	2.3
1	A	190	PRO	2.2
1	A	221	ARG	2.2
1	A	136	PRO	2.2
1	A	192	PRO	2.2
1	A	13	VAL	2.2
2	B	78[A]	GLN	2.1
1	A	735	PRO	2.1
1	A	223	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	187	CYS	2.0
2	B	494	ASP	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	MG	A	921	1/1	0.90	0.41	6.28	36,36,36,36	0
8	PLC	A	922	38/42	0.85	0.39	2.56	87,120,154,168	0
9	3PE	A	923	20/51	0.90	0.22	1.38	71,90,113,120	0
4	BGC	A	917	11/12	0.96	0.23	1.35	71,78,85,93	0
5	UDP	A	918	25/25	0.92	0.23	1.32	54,80,92,126	0
4	BGC	A	914	11/12	0.95	0.28	0.74	60,71,82,88	0
4	BGC	A	913	11/12	0.96	0.27	0.61	69,73,89,101	0
4	BGC	A	916	11/12	0.96	0.24	0.50	69,75,100,117	0
4	BGC	A	905	11/12	0.93	0.22	0.37	37,52,58,107	0
4	BGC	A	912	11/12	0.97	0.20	0.17	56,65,81,98	0
4	BGC	A	908	11/12	0.93	0.17	-0.63	62,72,97,133	0
4	BGC	A	915	11/12	0.96	0.20	-0.89	49,55,75,75	0
4	BGC	A	906	11/12	0.96	0.15	-1.01	41,43,71,105	0
4	BGC	A	910	11/12	0.96	0.16	-1.12	61,76,94,99	0
6	C2E	A	919	46/46	0.97	0.12	-1.38	31,51,63,76	0
4	BGC	A	911	11/12	0.97	0.14	-1.39	56,75,96,98	0
4	BGC	A	907	11/12	0.93	0.14	-1.43	43,54,65,80	0
6	C2E	A	920	46/46	0.97	0.11	-2.21	35,56,70,91	0
4	BGC	A	909	11/12	0.97	0.13	-2.38	61,68,81,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BGC	A	904	11/12	0.93	0.20	-	52,60,88,145	0
4	BGC	A	903	11/12	0.93	0.19	-	79,90,124,128	0
4	BGC	A	902	11/12	0.85	0.24	-	97,117,134,144	0
4	BGC	A	901	11/12	0.72	0.35	-	103,136,174,199	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.