Full wwPDB X-ray Structure Validation Report (i)

Mar 21, 2016 – 05:06 PM EDT

PDB ID	:	5EJ1
Title	:	Pre-translocation state of bacterial cellulose synthase
Authors	:	Moragn, J.L.W.; Zimmer, J.
Deposited on	:	2015-10-30
Resolution	:	3.40 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:

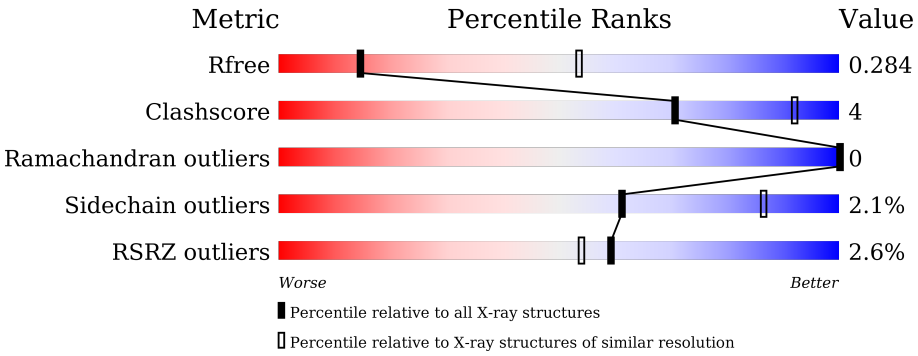
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	728	3% 85% 14%
2	B	669	2% 90% 7%
3	D	7	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
4	BGC	A	912	-	-	-	X
4	BGC	A	913	-	-	-	X
4	BGC	A	915	-	-	-	X
4	BGC	A	916	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10978 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	721	5684	3691	992	970	31	0	0	0

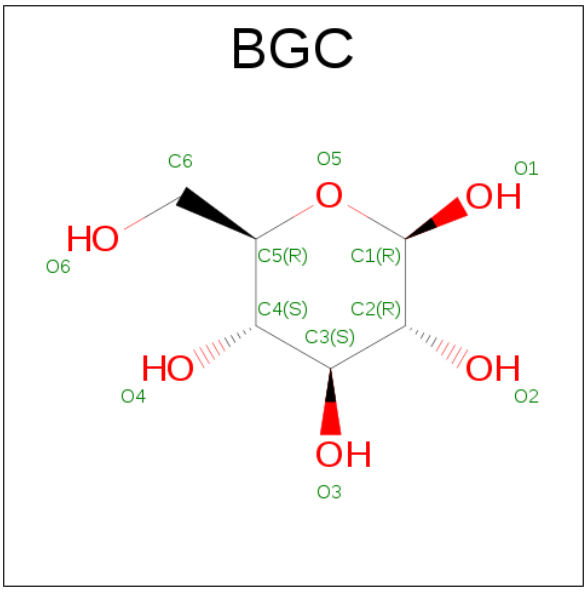
- Molecule 2 is a protein called Putative cellulose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	657	4899	3108	866	909	16	0	0	0

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

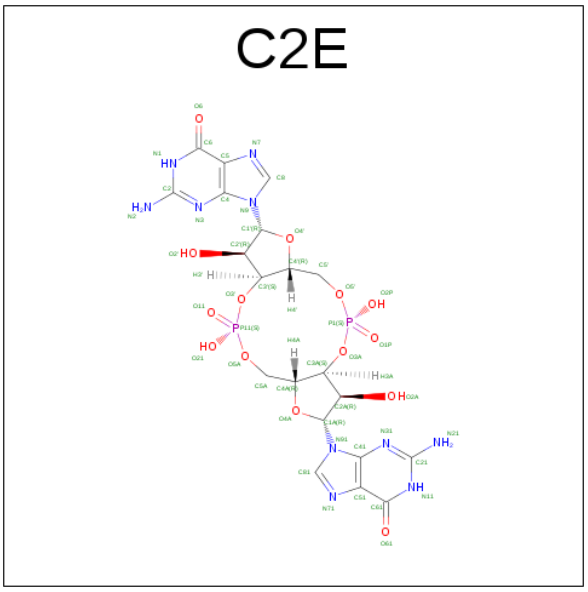
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	7	35	21	7	7	0	0	0

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



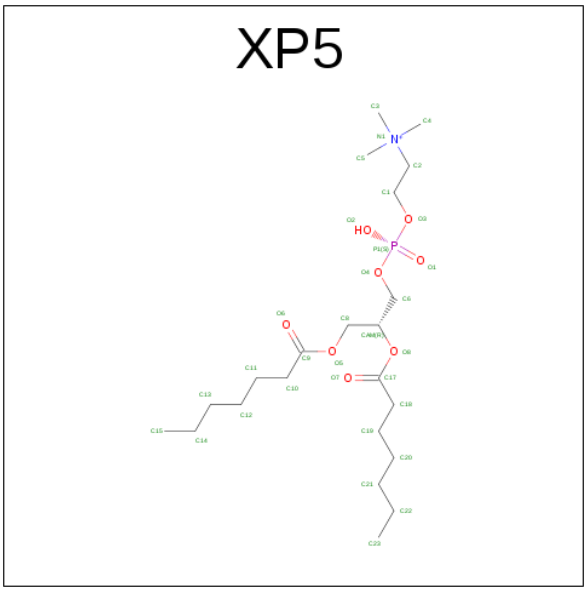
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 6 6	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11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

- Molecule 5 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
5	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
5	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

- Molecule 6 is (4S,7R)-7-(heptanoyloxy)-4-hydroxy-N,N,N-trimethyl-10-oxo-3,5,9-trioxa-4-phosphahexadecan-1-aminium 4-oxide (three-letter code: XP5) (formula: $C_{22}H_{45}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			22	13	1	7	1		

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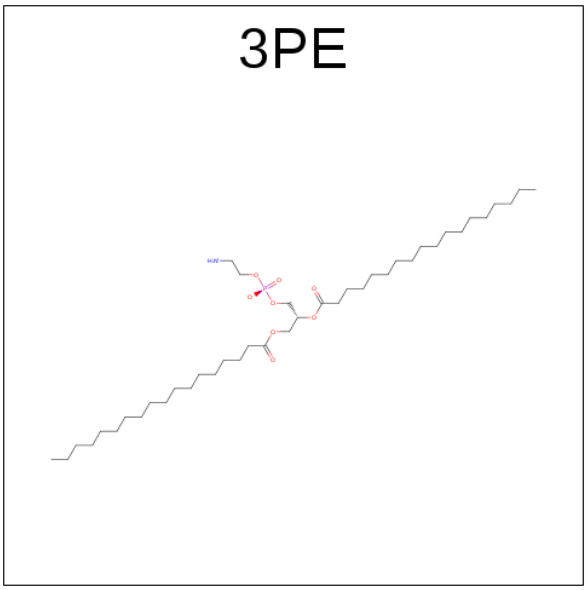
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			19	10	1	7	1		

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



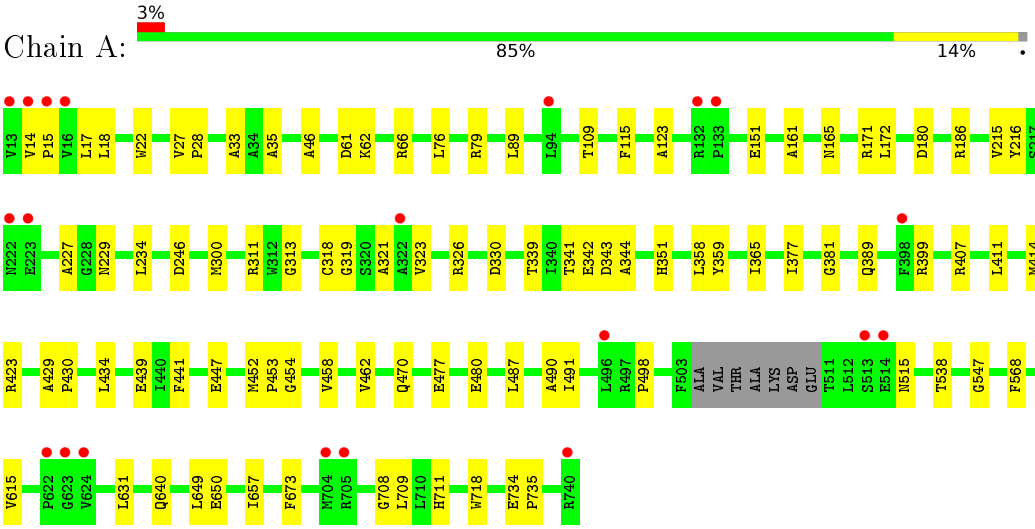
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			20	10	1	8	1		
7	A	1	Total	C				0	0
			8	8					

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.

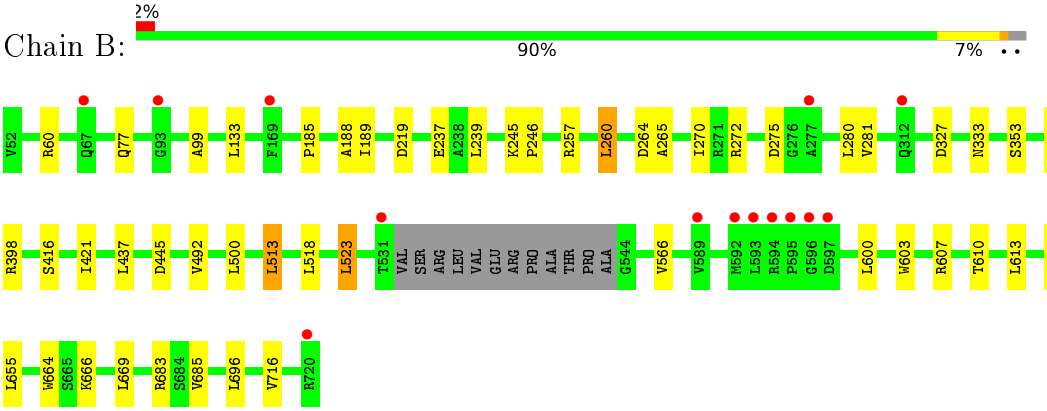
- Molecule 1: Putative cellulose synthase

Chain A:



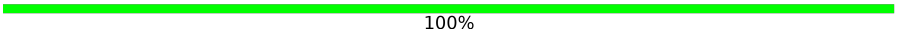
- Molecule 2: Putative cellulose synthase

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	67.36Å 218.23Å 220.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.86 – 3.40 29.48 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.86-3.40) 99.9 (29.48-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 3.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.233 , 0.277 0.248 , 0.284	Depositor DCC
R_{free} test set	2300 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	120.9	Xtriage
Anisotropy	0.798	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 69.2	EDS
Estimated twinning fraction	0.035 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 45653 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10978	wwPDB-VP
Average B, all atoms (Å^2)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: BGC, 3PE, XP5, 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	0.24	0/5829	0.44	0/7926
2	B	0.23	0/5018	0.45	1/6883 (0.0%)
All	All	0.23	0/10847	0.44	1/14809 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	260	LEU	CA-CB-CG	5.64	128.28	115.30

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	5684	0	5796	65	0
2	B	4899	0	4979	29	0
3	D	35	0	11	0	0
4	A	199	0	164	12	0
5	A	92	0	41	7	0
6	A	22	0	25	0	0
6	B	19	0	19	1	0
7	A	28	0	29	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10978	0	11064	97	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 4.

All (97) 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)
5:A:920:C2E:O4'	5:A:920:C2E:C4'	1.64	1.14
5:A:919:C2E:O4'	5:A:919:C2E:C4'	1.63	1.07
4:A:905:BGC:O2	2:B:566:VAL:HG21	1.69	0.93
2:B:513:LEU:HD21	2:B:523:LEU:HD22	1.61	0.83
1:A:319:GLY:HA3	4:A:918:BGC:H5	1.69	0.75
1:A:66:ARG:NH1	1:A:123:ALA:O	2.21	0.72
2:B:513:LEU:CD2	2:B:523:LEU:HD22	2.20	0.71
1:A:318:CYS:O	4:A:918:BGC:H5	1.95	0.67
1:A:76:LEU:HD21	1:A:454:GLY:C	2.15	0.66
1:A:480:GLU:OE1	4:A:914:BGC:O6	2.16	0.63
1:A:326:ARG:NH1	1:A:330:ASP:OD1	2.32	0.62
4:A:905:BGC:O2	2:B:566:VAL:CG2	2.46	0.61
1:A:341:THR:HG23	1:A:341:THR:O	2.00	0.61
1:A:161:ALA:O	1:A:165:ASN:ND2	2.33	0.60
1:A:411:LEU:HA	1:A:414:MET:HE2	1.83	0.60
2:B:60:ARG:NE	2:B:237:GLU:OE1	2.33	0.60
2:B:513:LEU:CD2	2:B:523:LEU:CD2	2.79	0.60
1:A:318:CYS:O	4:A:918:BGC:C5	2.52	0.58
2:B:264:ASP:OD1	2:B:265:ALA:N	2.37	0.57
1:A:613:SER:HG	5:A:919:C2E:HO2A	1.52	0.57
2:B:639:ALA:O	2:B:643:ARG:NH2	2.37	0.57
1:A:718:TRP:HE3	7:A:923:3PE:H2D1	1.69	0.57
5:A:920:C2E:H81	5:A:920:C2E:H512	1.85	0.57
1:A:547:GLY:HA3	4:A:906:BGC:H2	1.86	0.56
2:B:513:LEU:HD23	2:B:523:LEU:CD2	2.36	0.56
1:A:76:LEU:HD21	1:A:454:GLY:O	2.06	0.56
1:A:341:THR:O	1:A:341:THR:CG2	2.54	0.55
2:B:398:ARG:NH2	2:B:445:ASP:OD1	2.39	0.55
2:B:77:GLN:NE2	2:B:333:ASN:OD1	2.39	0.55
1:A:447:GLU:OE2	2:B:353:SER:OG	2.26	0.54
1:A:515:ASN:OD1	1:A:577:GLN:N	2.40	0.53
2:B:257:ARG:NH1	2:B:275:ASP:OD2	2.43	0.52
1:A:61:ASP:OD1	1:A:62:LYS:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:HIS:HB2	7:A:922:3PE:H122	1.92	0.51
2:B:603:TRP:O	2:B:607:ARG:NH1	2.44	0.51
5:A:920:C2E:C5A	5:A:920:C2E:H81	2.41	0.50
2:B:245:LYS:HB3	2:B:246:PRO:HD2	1.93	0.50
2:B:683:ARG:HE	6:B:801:XP5:H53C	1.76	0.50
1:A:313:GLY:O	1:A:351:HIS:NE2	2.44	0.50
1:A:487:LEU:O	1:A:490:ALA:N	2.43	0.50
1:A:300:MET:HA	1:A:470:GLN:HB3	1.93	0.49
1:A:640:GLN:NE2	1:A:650:GLU:OE2	2.46	0.49
2:B:365:ALA:N	2:B:437:LEU:O	2.46	0.49
1:A:14:VAL:N	1:A:15:PRO:HD2	2.28	0.49
2:B:189:ILE:O	2:B:272:ARG:NH1	2.46	0.48
1:A:46:ALA:HA	1:A:76:LEU:HD13	1.94	0.48
1:A:389:GLN:NE2	1:A:498:PRO:O	2.47	0.48
1:A:423:ARG:NH1	4:A:912:BGC:O6	2.47	0.47
1:A:477:GLU:N	1:A:477:GLU:OE1	2.44	0.47
2:B:664:TRP:CH2	2:B:666:LYS:HA	2.49	0.47
1:A:439:GLU:HB2	4:A:908:BGC:H6C2	1.96	0.47
1:A:76:LEU:HD23	1:A:458:VAL:HG22	1.95	0.47
1:A:14:VAL:O	1:A:17:LEU:N	2.45	0.47
1:A:708:GLY:HA3	7:A:922:3PE:H111	1.97	0.47
2:B:610:THR:N	2:B:655:LEU:O	2.45	0.47
1:A:246:ASP:OD2	4:A:918:BGC:O6	2.29	0.46
1:A:76:LEU:HD23	1:A:458:VAL:CG2	2.45	0.46
1:A:18:LEU:O	1:A:22:TRP:N	2.47	0.46
2:B:185:PRO:HG2	2:B:188:ALA:HB2	1.98	0.45
1:A:115:PHE:HE1	1:A:462:VAL:HG11	1.81	0.45
2:B:600:LEU:N	2:B:600:LEU:HD12	2.32	0.44
1:A:377:ILE:O	1:A:381:GLY:N	2.48	0.44
1:A:76:LEU:CD2	1:A:454:GLY:O	2.65	0.44
1:A:709:LEU:N	7:A:922:3PE:O14	2.46	0.44
1:A:180:ASP:OD1	1:A:229:ASN:ND2	2.49	0.43
1:A:441:PHE:HB3	4:A:909:BGC:H3	2.01	0.43
1:A:734:GLU:N	1:A:735:PRO:HD2	2.34	0.42
1:A:33:ALA:HA	1:A:79:ARG:HD2	2.02	0.42
1:A:180:ASP:O	1:A:186:ARG:NE	2.52	0.42
5:A:920:C2E:H3'	5:A:920:C2E:H511	2.02	0.42
1:A:419:PHE:N	1:A:420:PRO:CD	2.83	0.42
1:A:35:ALA:O	1:A:79:ARG:NH2	2.50	0.42
1:A:452:MET:HB3	1:A:453:PRO:HD3	2.01	0.42
1:A:343:ASP:OD1	1:A:344:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ARG:O	1:A:407:ARG:NH2	2.53	0.42
1:A:434:LEU:HD22	1:A:538:THR:HG22	2.02	0.41
1:A:311:ARG:NH2	2:B:716:VAL:O	2.53	0.41
1:A:358:LEU:HD13	1:A:359:TYR:N	2.35	0.41
2:B:99:ALA:HB1	2:B:133:LEU:HD11	2.01	0.41
1:A:171:ARG:HG3	1:A:172:LEU:HD22	2.02	0.41
1:A:151:GLU:OE1	1:A:151:GLU:N	2.52	0.41
1:A:227:ALA:HB2	1:A:342:GLU:HB2	2.02	0.41
1:A:429:ALA:HB3	1:A:430:PRO:HD3	2.02	0.41
1:A:215:VAL:HG12	1:A:216:TYR:H	1.84	0.41
2:B:270:ILE:HG22	2:B:280:LEU:HA	2.01	0.41
2:B:359:GLY:HA3	2:B:398:ARG:NH2	2.36	0.41
2:B:327:ASP:N	2:B:327:ASP:OD1	2.51	0.41
1:A:218:THR:HG22	1:A:219:ARG:N	2.35	0.41
1:A:613:SER:OG	5:A:919:C2E:O2A	2.28	0.41
1:A:321:ALA:HB2	1:A:365:ILE:HG13	2.02	0.41
2:B:600:LEU:HG	2:B:664:TRP:CH2	2.56	0.41
1:A:487:LEU:O	1:A:491:ILE:N	2.54	0.40
1:A:439:GLU:CG	4:A:908:BGC:H6C2	2.51	0.40
2:B:219:ASP:N	2:B:219:ASP:OD1	2.51	0.40
1:A:234:LEU:O	1:A:326:ARG:NH2	2.54	0.40
1:A:27:VAL:N	1:A:28:PRO:HD2	2.37	0.40
1:A:615:VAL:HG23	1:A:673:PHE:CZ	2.57	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	717/728 (98%)	683 (95%)	34 (5%)	0	100	100
2	B	653/669 (98%)	638 (98%)	15 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1370/1397 (98%)	1321 (96%)	49 (4%)	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	593/598 (99%)	585 (99%)	8 (1%)	76 91
2	B	521/531 (98%)	506 (97%)	15 (3%)	50 82
All	All	1114/1129 (99%)	1091 (98%)	23 (2%)	61 86

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	109	THR
1	A	323	VAL
1	A	339	THR
1	A	568	PHE
1	A	631	LEU
1	A	649	LEU
1	A	657	ILE
2	B	239	LEU
2	B	260	LEU
2	B	281	VAL
2	B	416	SER
2	B	421	ILE
2	B	492	VAL
2	B	500	LEU
2	B	513	LEU
2	B	518	LEU
2	B	523	LEU
2	B	613	LEU
2	B	643	ARG

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Mol	Chain	Res	Type
2	B	669	LEU
2	B	685	VAL
2	B	696	LEU

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

Mol	Chain	Res	Type
2	B	77	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

24 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	$\#\|Z\| > 2$
4	BGC	A	901	4	12,12,12	1.39	1 (8%)	17,17,17	1.46	3 (17%)
4	BGC	A	902	4	11,11,12	1.75	3 (27%)	15,15,17	1.67	4 (26%)
4	BGC	A	903	4	11,11,12	1.69	2 (18%)	15,15,17	2.08	3 (20%)
4	BGC	A	904	4	11,11,12	1.70	2 (18%)	15,15,17	2.21	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BGC	A	905	4	11,11,12	1.58	2 (18%)	15,15,17	1.88	4 (26%)
4	BGC	A	906	4	11,11,12	2.12	3 (27%)	15,15,17	1.07	1 (6%)
4	BGC	A	907	4	11,11,12	1.71	3 (27%)	15,15,17	1.05	0
4	BGC	A	908	4	11,11,12	1.65	2 (18%)	15,15,17	1.74	4 (26%)
4	BGC	A	909	4	11,11,12	1.66	2 (18%)	15,15,17	1.27	1 (6%)
4	BGC	A	910	4	11,11,12	1.76	2 (18%)	15,15,17	1.80	3 (20%)
4	BGC	A	911	4	11,11,12	1.60	2 (18%)	15,15,17	1.11	2 (13%)
4	BGC	A	912	4	11,11,12	1.70	2 (18%)	15,15,17	0.85	0
4	BGC	A	913	4	11,11,12	1.62	2 (18%)	15,15,17	1.25	2 (13%)
4	BGC	A	914	4	11,11,12	1.62	2 (18%)	15,15,17	1.51	2 (13%)
4	BGC	A	915	4	11,11,12	1.64	2 (18%)	15,15,17	1.50	4 (26%)
4	BGC	A	916	4	11,11,12	1.54	2 (18%)	15,15,17	2.06	3 (20%)
4	BGC	A	917	4	11,11,12	1.76	3 (27%)	15,15,17	1.08	1 (6%)
4	BGC	A	918	4	11,11,12	1.67	2 (18%)	15,15,17	1.05	1 (6%)
5	C2E	A	919	-	44,52,52	5.39	28 (63%)	50,82,82	2.55	11 (22%)
5	C2E	A	920	-	44,52,52	5.39	29 (65%)	50,82,82	2.52	10 (20%)
6	XP5	A	921	-	21,21,31	1.22	2 (9%)	24,28,39	1.14	1 (4%)
7	3PE	A	922	-	19,19,50	1.36	4 (21%)	21,24,55	1.60	3 (14%)
7	3PE	A	923	-	7,7,50	0.31	0	6,6,55	0.77	0
6	XP5	B	801	-	18,18,31	1.22	1 (5%)	21,25,39	0.77	1 (4%)

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	-	0/2/22/22	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
4	BGC	A	918	4	-	0/2/19/22	0/1/1/1
5	C2E	A	919	-	-	0/22/62/62	0/6/7/7
5	C2E	A	920	-	-	0/22/62/62	0/6/7/7
6	XP5	A	921	-	-	0/24/24/35	0/0/0/0
7	3PE	A	922	-	-	0/22/22/54	0/0/0/0
7	3PE	A	923	-	-	0/5/5/54	0/0/0/0
6	XP5	B	801	-	-	0/19/19/35	0/0/0/0

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	920	C2E	C2A-C1A	-14.79	1.30	1.53
5	A	919	C2E	C2A-C1A	-14.57	1.30	1.53
5	A	919	C2E	C3'-C4'	-10.04	1.24	1.52
5	A	920	C2E	C3'-C4'	-9.89	1.25	1.52
5	A	919	C2E	O4'-C1'	-7.29	1.30	1.41
5	A	920	C2E	O4'-C1'	-7.27	1.30	1.41
5	A	919	C2E	O4A-C4A	-5.90	1.31	1.45
5	A	920	C2E	O4A-C4A	-5.77	1.31	1.45
4	A	906	BGC	C2-C3	-3.22	1.48	1.52
5	A	919	C2E	O3A-C3A	-3.04	1.34	1.44
5	A	920	C2E	O3A-C3A	-3.04	1.34	1.44
4	A	917	BGC	C2-C3	-3.00	1.48	1.52
4	A	902	BGC	C2-C3	-2.97	1.48	1.52
4	A	913	BGC	C2-C3	-2.75	1.48	1.52
5	A	919	C2E	O2'-C2'	-2.74	1.36	1.43
4	A	912	BGC	C2-C3	-2.72	1.48	1.52
4	A	915	BGC	C2-C3	-2.69	1.48	1.52
4	A	910	BGC	C2-C3	-2.68	1.48	1.52
5	A	920	C2E	O2'-C2'	-2.66	1.36	1.43
4	A	907	BGC	C2-C3	-2.63	1.49	1.52
4	A	903	BGC	C2-C3	-2.62	1.49	1.52
4	A	918	BGC	C2-C3	-2.57	1.49	1.52
5	A	919	C2E	C2'-C1'	-2.56	1.49	1.53
4	A	908	BGC	C2-C3	-2.44	1.49	1.52
4	A	909	BGC	C2-C3	-2.40	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	920	C2E	C2'-C1'	-2.39	1.49	1.53
4	A	914	BGC	C2-C3	-2.38	1.49	1.52
6	A	921	XP5	O8-CAM	-2.37	1.40	1.46
4	A	904	BGC	C2-C3	-2.37	1.49	1.52
4	A	911	BGC	C2-C3	-2.35	1.49	1.52
4	A	916	BGC	C2-C3	-2.25	1.49	1.52
7	A	922	3PE	O21-C2	-2.24	1.40	1.46
6	B	801	XP5	O5-C8	-2.16	1.40	1.45
7	A	922	3PE	O31-C3	-2.14	1.40	1.45
5	A	920	C2E	O6-C6	-2.03	1.19	1.24
4	A	917	BGC	O5-C5	2.02	1.47	1.43
6	A	921	XP5	O8-C17	2.04	1.40	1.34
4	A	902	BGC	O5-C5	2.05	1.48	1.43
4	A	907	BGC	O5-C5	2.07	1.48	1.43
5	A	919	C2E	C21-N31	2.14	1.46	1.35
5	A	920	C2E	C21-N31	2.17	1.46	1.35
4	A	905	BGC	O2-C2	2.20	1.48	1.43
7	A	922	3PE	O21-C21	2.33	1.40	1.35
4	A	906	BGC	O5-C5	2.39	1.48	1.43
5	A	920	C2E	P11-O5A	2.41	1.69	1.59
5	A	919	C2E	C2'-C3'	2.42	1.58	1.53
5	A	920	C2E	C2-N3	2.42	1.47	1.35
7	A	922	3PE	O31-C31	2.42	1.40	1.33
5	A	920	C2E	C2'-C3'	2.43	1.58	1.53
5	A	919	C2E	P11-O5A	2.46	1.69	1.59
5	A	919	C2E	C2-N3	2.49	1.48	1.35
5	A	919	C2E	P1-O5'	3.00	1.71	1.59
5	A	920	C2E	P1-O5'	3.09	1.72	1.59
5	A	919	C2E	O2A-C2A	3.47	1.51	1.43
5	A	920	C2E	O2A-C2A	3.54	1.51	1.43
5	A	919	C2E	O3'-C3'	3.77	1.56	1.44
4	A	905	BGC	O5-C1	3.85	1.50	1.43
5	A	920	C2E	O3'-C3'	3.89	1.56	1.44
4	A	901	BGC	O5-C1	3.92	1.50	1.43
4	A	913	BGC	O5-C1	3.93	1.50	1.43
4	A	916	BGC	O5-C1	3.94	1.50	1.43
4	A	915	BGC	O5-C1	3.98	1.50	1.43
4	A	911	BGC	O5-C1	4.04	1.50	1.43
4	A	908	BGC	O5-C1	4.10	1.50	1.43
4	A	902	BGC	O5-C1	4.14	1.50	1.43
4	A	914	BGC	O5-C1	4.16	1.50	1.43
4	A	917	BGC	O5-C1	4.22	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	918	BGC	O5-C1	4.23	1.50	1.43
4	A	903	BGC	O5-C1	4.24	1.50	1.43
4	A	907	BGC	O5-C1	4.25	1.50	1.43
4	A	912	BGC	O5-C1	4.25	1.50	1.43
4	A	909	BGC	O5-C1	4.29	1.50	1.43
4	A	904	BGC	O5-C1	4.29	1.50	1.43
4	A	910	BGC	O5-C1	4.36	1.50	1.43
5	A	920	C2E	P1-O3A	4.42	1.72	1.60
5	A	919	C2E	P1-O3A	4.45	1.72	1.60
5	A	920	C2E	C2-N1	4.82	1.44	1.35
5	A	919	C2E	C21-N21	4.96	1.44	1.34
5	A	919	C2E	C2-N1	4.96	1.44	1.35
5	A	920	C2E	C21-N21	5.11	1.44	1.34
5	A	919	C2E	P11-O3'	5.16	1.74	1.60
5	A	920	C2E	P11-O3'	5.21	1.74	1.60
5	A	919	C2E	C21-N11	5.26	1.45	1.35
4	A	906	BGC	O5-C1	5.42	1.52	1.43
5	A	920	C2E	C21-N11	5.46	1.45	1.35
5	A	919	C2E	C61-N11	5.61	1.43	1.33
5	A	920	C2E	C61-N11	5.68	1.43	1.33
5	A	920	C2E	C61-C51	6.11	1.53	1.41
5	A	919	C2E	C61-C51	6.19	1.53	1.41
5	A	920	C2E	C2-N2	6.24	1.47	1.34
5	A	920	C2E	C6-N1	6.26	1.44	1.33
5	A	919	C2E	C2-N2	6.38	1.47	1.34
5	A	919	C2E	C6-N1	6.50	1.44	1.33
5	A	920	C2E	C6-C5	6.54	1.54	1.41
5	A	919	C2E	C6-C5	6.61	1.54	1.41
5	A	919	C2E	O4'-C4'	8.18	1.63	1.45
5	A	920	C2E	O4'-C4'	8.31	1.64	1.45
5	A	919	C2E	C41-N31	8.49	1.49	1.35
5	A	920	C2E	C41-N31	8.59	1.49	1.35
5	A	920	C2E	C4-N3	9.02	1.50	1.35
5	A	919	C2E	C4-N3	9.06	1.50	1.35
5	A	920	C2E	O4A-C1A	15.14	1.62	1.41
5	A	919	C2E	O4A-C1A	15.25	1.63	1.41

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	920	C2E	C1'-N9-C4	-12.63	112.71	126.81
5	A	919	C2E	C1'-N9-C4	-12.60	112.75	126.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	920	C2E	N3-C2-N1	-5.60	119.94	127.56
5	A	919	C2E	N3-C2-N1	-5.57	119.98	127.56
5	A	920	C2E	N31-C21-N11	-5.38	120.23	127.56
5	A	919	C2E	N31-C21-N11	-5.31	120.33	127.56
5	A	920	C2E	C5-C6-N1	-2.77	119.90	123.52
5	A	919	C2E	C5-C6-N1	-2.77	119.90	123.52
5	A	919	C2E	C4A-O4A-C1A	-2.77	106.71	109.64
5	A	920	C2E	C51-C61-N11	-2.69	120.01	123.52
5	A	919	C2E	C51-C61-N11	-2.66	120.05	123.52
7	A	922	3PE	C2-O21-C21	-2.64	112.96	117.93
4	A	905	BGC	O4-C4-C5	-2.37	102.98	109.23
4	A	905	BGC	C1-O5-C5	-2.35	108.69	112.14
4	A	910	BGC	O3-C3-C2	-2.28	105.83	110.01
4	A	904	BGC	C6-C5-C4	-2.25	107.34	112.99
4	A	904	BGC	O3-C3-C4	-2.09	105.64	110.36
6	B	801	XP5	C1-C2-N1	-2.08	109.23	116.04
4	A	911	BGC	C3-C4-C5	2.02	113.83	110.23
4	A	913	BGC	C1-C2-C3	2.03	112.01	109.55
4	A	915	BGC	C2-C3-C4	2.06	114.64	111.05
4	A	911	BGC	C1-C2-C3	2.09	112.08	109.55
4	A	910	BGC	C2-C3-C4	2.10	114.72	111.05
4	A	915	BGC	O5-C5-C4	2.11	113.62	110.13
4	A	915	BGC	C1-C2-C3	2.13	112.13	109.55
4	A	902	BGC	C1-C2-C3	2.14	112.15	109.55
4	A	901	BGC	C4-C3-C2	2.17	114.78	110.79
4	A	904	BGC	C3-C4-C5	2.23	114.21	110.23
4	A	904	BGC	O5-C5-C4	2.24	113.84	110.13
5	A	920	C2E	C3'-C2'-C1'	2.27	105.00	100.06
4	A	914	BGC	O5-C1-C2	2.27	114.53	110.89
4	A	916	BGC	C3-C4-C5	2.28	114.29	110.23
4	A	913	BGC	O5-C5-C4	2.29	113.92	110.13
4	A	908	BGC	O5-C5-C4	2.32	113.98	110.13
4	A	917	BGC	O5-C5-C4	2.34	114.02	110.13
4	A	902	BGC	C2-C3-C4	2.44	115.30	111.05
5	A	920	C2E	O21-P11-O3'	2.46	116.88	106.76
4	A	918	BGC	C1-C2-C3	2.48	112.55	109.55
4	A	906	BGC	C1-C2-C3	2.51	112.59	109.55
5	A	920	C2E	C3A-C2A-C1A	2.53	105.58	100.06
5	A	919	C2E	C3'-C2'-C1'	2.56	105.63	100.06
5	A	919	C2E	O21-P11-O3'	2.59	117.44	106.76
4	A	908	BGC	C2-C3-C4	2.72	115.79	111.05
4	A	915	BGC	C3-C4-C5	2.75	115.13	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	908	BGC	C3-C4-C5	2.87	115.35	110.23
4	A	903	BGC	C3-C4-C5	2.95	115.48	110.23
5	A	919	C2E	C3A-C2A-C1A	2.98	106.56	100.06
4	A	901	BGC	O5-C5-C4	3.04	115.47	109.67
4	A	902	BGC	C3-C4-C5	3.05	115.67	110.23
4	A	902	BGC	O5-C5-C4	3.05	115.19	110.13
7	A	922	3PE	O31-C31-C32	3.08	120.33	111.16
4	A	908	BGC	C1-C2-C3	3.10	113.31	109.55
4	A	916	BGC	C2-C3-C4	3.21	116.65	111.05
4	A	901	BGC	C3-C4-C5	3.30	116.12	110.23
5	A	920	C2E	C61-N11-C21	3.31	119.76	115.88
5	A	919	C2E	C61-N11-C21	3.31	119.77	115.88
5	A	919	C2E	C6-N1-C2	3.43	119.91	115.88
5	A	920	C2E	C6-N1-C2	3.55	120.05	115.88
4	A	903	BGC	C2-C3-C4	3.61	117.35	111.05
4	A	909	BGC	C1-C2-C3	3.78	114.14	109.55
4	A	904	BGC	C2-C3-C4	3.79	117.66	111.05
4	A	905	BGC	C2-C3-C4	4.00	118.03	111.05
6	A	921	XP5	O8-C17-C18	4.05	120.06	111.53
4	A	905	BGC	C1-C2-C3	4.39	114.88	109.55
4	A	914	BGC	C1-C2-C3	4.44	114.93	109.55
7	A	922	3PE	O21-C21-C22	4.98	120.57	111.09
4	A	903	BGC	C1-C2-C3	5.04	115.65	109.55
4	A	910	BGC	C1-C2-C3	5.21	115.86	109.55
4	A	916	BGC	C1-C2-C3	5.65	116.39	109.55
4	A	904	BGC	C1-C2-C3	5.73	116.49	109.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	905	BGC	2	0
4	A	906	BGC	1	0
4	A	908	BGC	2	0
4	A	909	BGC	1	0
4	A	912	BGC	1	0
4	A	914	BGC	1	0
4	A	918	BGC	4	0
5	A	919	C2E	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	920	C2E	4	0
7	A	922	3PE	3	0
7	A	923	3PE	1	0
6	B	801	XP5	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	173:UNK	C	175:UNK	N	4.64

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	721/728 (99%)	-0.06	22 (3%) 52 48	95, 145, 232, 335	0
2	B	657/669 (98%)	-0.16	14 (2%) 67 61	93, 139, 213, 325	0
3	D	0/7	-	-	-	-
All	All	1378/1404 (98%)	-0.10	36 (2%) 59 54	93, 142, 227, 335	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	593	LEU	5.6
2	B	531	THR	3.9
1	A	496	LEU	3.8
2	B	589	VAL	3.7
2	B	597	ASP	3.6
1	A	15	PRO	3.4
1	A	624	VAL	3.4
2	B	594	ARG	3.2
1	A	222	ASN	3.1
2	B	596	GLY	3.1
2	B	592	MET	3.0
1	A	13	VAL	2.9
2	B	312	GLN	2.9
2	B	595	PRO	2.7
1	A	16	VAL	2.7
1	A	221	ARG	2.7
1	A	14	VAL	2.7
1	A	514	GLU	2.6
1	A	513	SER	2.6
1	A	223	GLU	2.6
1	A	623	GLY	2.4
1	A	704	MET	2.4
1	A	705	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	93	GLY	2.3
2	B	720	ARG	2.2
1	A	740	ARG	2.2
1	A	132	ARG	2.2
2	B	67	GLN	2.2
1	A	133	PRO	2.2
1	A	94	LEU	2.1
1	A	622	PRO	2.1
2	B	277	ALA	2.1
2	B	169	PHE	2.1
1	A	322	ALA	2.1
1	A	220	GLU	2.0
1	A	398	PHE	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
4	BGC	A	912	11/12	0.93	0.35	2.79	150,155,158,161	0
4	BGC	A	913	11/12	0.92	0.47	2.49	148,153,155,155	0
4	BGC	A	916	11/12	0.94	0.25	2.09	168,168,169,170	0
4	BGC	A	915	11/12	0.94	0.27	2.04	146,146,147,148	0
7	3PE	A	922	20/51	0.86	0.33	1.90	162,167,172,172	0
4	BGC	A	914	11/12	0.87	0.37	1.46	132,133,134,134	0
6	XP5	A	921	22/32	0.88	0.29	1.28	215,221,227,228	0
4	BGC	A	918	11/12	0.80	0.33	1.19	160,161,162,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	BGC	A	911	11/12	0.93	0.23	1.16	136,138,142,142	0
4	BGC	A	917	11/12	0.93	0.23	1.06	142,144,146,147	0
4	BGC	A	906	11/12	0.88	0.32	0.74	149,158,183,204	0
4	BGC	A	908	11/12	0.83	0.29	0.46	153,158,185,206	0
4	BGC	A	905	11/12	0.89	0.27	0.34	111,114,128,173	0
6	XP5	B	801	19/32	0.79	0.32	0.33	208,212,214,215	0
4	BGC	A	909	11/12	0.98	0.15	-0.92	112,117,123,127	0
4	BGC	A	910	11/12	0.97	0.14	-1.07	117,125,144,150	0
4	BGC	A	904	11/12	0.94	0.14	-1.07	119,127,169,194	0
5	C2E	A	919	46/46	0.93	0.12	-1.38	133,138,143,144	0
5	C2E	A	920	46/46	0.94	0.10	-1.93	143,147,150,151	0
4	BGC	A	903	11/12	0.85	0.22	-	181,200,213,215	0
4	BGC	A	902	11/12	0.81	0.23	-	185,200,214,230	0
4	BGC	A	907	11/12	0.82	0.43	-	118,136,142,154	0
4	BGC	A	901	12/12	0.70	0.27	-	267,272,285,306	0
7	3PE	A	923	8/51	0.80	0.19	-	118,120,122,123	0

6.5 Other polymers (i)

There are no such residues in this entry.