



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:08 AM GMT

PDB ID : 1L2A
Title : The Crystal Structure and Catalytic Mechanism of Cellobiohydrolase CelS, the Major Enzymatic Component of the Clostridium thermocellum cellulosome
Authors : Guimaraes, B.G.; Souchon, H.; Lytle, B.L.; Wu, J.H.D.; Alzari, P.M.
Deposited on : 2002-02-20
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

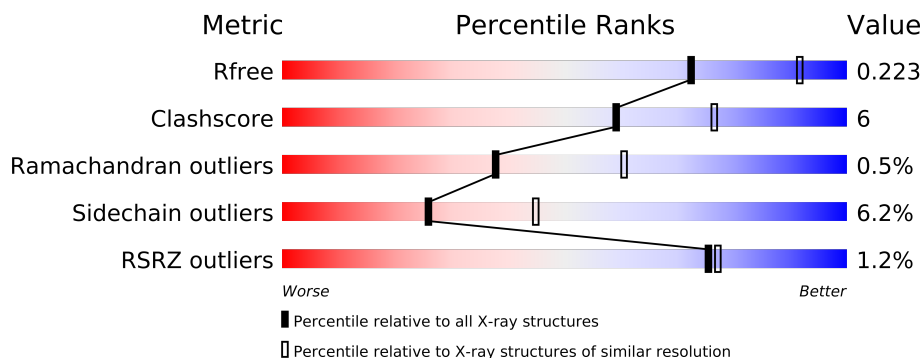
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	678	
1	B	678	
1	C	678	
1	D	678	
1	E	678	
1	F	678	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32414 atoms, of which 0 are hydrogen and 0 are deuterium.

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 cellobiohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5103	3285	825	973	20			
1	B	642	Total	C	N	O	S	0	0	0
			5128	3299	835	974	20			
1	C	642	Total	C	N	O	S	0	0	0
			5109	3287	832	970	20			
1	D	642	Total	C	N	O	S	0	0	0
			5136	3303	836	977	20			
1	E	642	Total	C	N	O	S	0	0	0
			5124	3298	832	974	20			
1	F	642	Total	C	N	O	S	0	0	0
			5130	3300	833	977	20			

- Molecule 2 is a polymer of unknown type called SUGAR (BGC-BGC).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	2	Total	C	O	0	0
			22	12	10		
2	B	2	Total	C	O	0	0
			22	12	10		
2	C	2	Total	C	O	0	0
			22	12	10		
2	D	2	Total	C	O	0	0
			22	12	10		
2	E	2	Total	C	O	0	0
			22	12	10		
2	F	2	Total	C	O	0	0
			22	12	10		

- Molecule 3 is a polymer of unknown type called SUGAR (BGC-BGC-BGC-BGC-BGC-BGC).

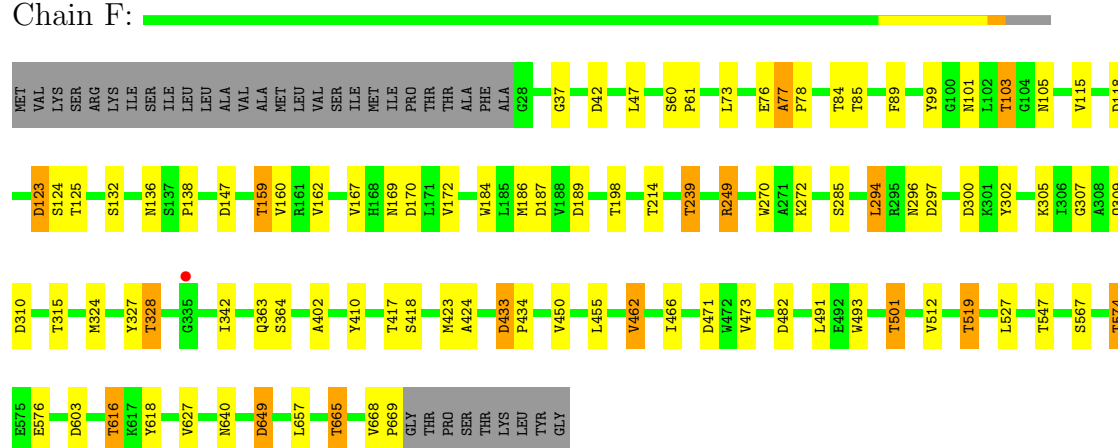
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	6	Total	C	O	0	0
			67	36	31		
3	B	6	Total	C	O	0	0
			67	36	31		
3	C	6	Total	C	O	0	0
			67	36	31		
3	D	6	Total	C	O	0	0
			67	36	31		
3	E	6	Total	C	O	0	0
			67	36	31		
3	F	6	Total	C	O	0	0
			67	36	31		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total	O	0	0
			130	130		
4	B	127	Total	O	0	0
			127	127		
4	C	145	Total	O	0	0
			145	145		
4	D	238	Total	O	0	0
			238	238		
4	E	221	Total	O	0	0
			221	221		
4	F	289	Total	O	0	0
			289	289		



Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	148.03Å 207.64Å 215.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.5 (15.00-2.50) 95.5 (15.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.181 , 0.226 0.181 , 0.223	Depositor DCC
R_{free} test set	10814 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 16.6	EDS
Estimated twinning fraction	0.004 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 217180 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32414	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC

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	0.59	0/5282	0.81	14/7213 (0.2%)
1	B	0.60	0/5307	0.78	8/7241 (0.1%)
1	C	0.59	0/5288	0.79	8/7218 (0.1%)
1	D	0.66	0/5315	0.81	8/7251 (0.1%)
1	E	0.66	1/5303 (0.0%)	0.82	12/7236 (0.2%)
1	F	0.68	0/5309	0.83	14/7244 (0.2%)
All	All	0.63	1/31804 (0.0%)	0.80	64/43403 (0.1%)

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	C	0	1
1	D	0	1
1	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	169	ASN	CB-CG	5.05	1.62	1.51

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	147	ASP	CB-CG-OD2	7.60	125.14	118.30
1	D	73	LEU	CA-CB-CG	7.27	132.01	115.30
1	C	663	ASP	CB-CG-OD2	6.62	124.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	315	THR	C-N-CA	-6.58	108.48	122.30
1	C	147	ASP	CB-CG-OD2	6.50	124.15	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	77	ALA	Peptide
1	D	316	GLY	Peptide
1	F	327	TYR	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5103	0	4667	82	0
1	B	5128	0	4727	65	0
1	C	5109	0	4686	57	0
1	D	5136	0	4737	54	0
1	E	5124	0	4720	62	0
1	F	5130	0	4726	69	0
2	A	22	0	19	0	0
2	B	22	0	19	0	0
2	C	22	0	19	0	0
2	D	22	0	19	0	0
2	E	22	0	19	0	0
2	F	22	0	19	0	0
3	A	67	0	57	2	0
3	B	67	0	57	1	0
3	C	67	0	57	2	0
3	D	67	0	57	4	0
3	E	67	0	57	1	0
3	F	67	0	57	0	0
4	A	130	0	0	6	0
4	B	127	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	145	0	0	3	0
4	D	238	0	0	7	0
4	E	221	0	0	8	0
4	F	289	0	0	12	0
All	All	32414	0	28719	365	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

The worst 5 of 365 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:638:VAL:HA	4:B:798:HOH:O	1.52	1.09
1:F:310:ASP:HB2	4:F:855:HOH:O	1.53	1.06
1:D:103:THR:HG22	1:D:105:ASN:H	1.26	1.01
1:F:423:MET:SD	4:F:968:HOH:O	2.19	0.99
1:B:574:THR:HG21	1:B:576:GLU:OE1	1.63	0.99

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	640/678 (94%)	607 (95%)	28 (4%)	5 (1%)	27	46
1	B	640/678 (94%)	605 (94%)	33 (5%)	2 (0%)	50	73
1	C	640/678 (94%)	615 (96%)	20 (3%)	5 (1%)	27	46
1	D	640/678 (94%)	622 (97%)	16 (2%)	2 (0%)	50	73
1	E	640/678 (94%)	617 (96%)	20 (3%)	3 (0%)	38	60
1	F	640/678 (94%)	621 (97%)	18 (3%)	1 (0%)	56	79
All	All	3840/4068 (94%)	3687 (96%)	135 (4%)	18 (0%)	38	60

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	ALA
1	A	158	ASP
1	A	335	GLY
1	C	197	GLY
1	C	335	GLY

5.3.2 Protein sidechains ⓘ

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	512/556 (92%)	472 (92%)	40 (8%)	18	32
1	B	519/556 (93%)	490 (94%)	29 (6%)	30	51
1	C	513/556 (92%)	481 (94%)	32 (6%)	26	45
1	D	521/556 (94%)	491 (94%)	30 (6%)	28	49
1	E	518/556 (93%)	488 (94%)	30 (6%)	28	49
1	F	520/556 (94%)	490 (94%)	30 (6%)	28	49
All	All	3103/3336 (93%)	2912 (94%)	191 (6%)	26	45

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	462	VAL
1	D	124	SER
1	F	434	PRO
1	C	491	LEU
1	C	627	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	247	GLN
1	D	101	ASN
1	F	207	GLN
1	C	268	ASN
1	C	363	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

48 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BGC	A	679	2	10,11,12	0.64	0	11,15,17	1.00	1 (9%)
2	BGC	A	680	2	10,11,12	0.91	1 (10%)	11,15,17	1.18	2 (18%)
3	BGC	A	681	3	12,12,12	0.45	0	17,17,17	1.74	5 (29%)
3	BGC	A	682	3	10,11,12	0.90	1 (10%)	11,15,17	0.88	1 (9%)
3	BGC	A	683	3	10,11,12	0.92	1 (10%)	11,15,17	0.81	0
3	BGC	A	684	3	10,11,12	0.69	0	11,15,17	2.05	5 (45%)
3	BGC	A	685	3	10,11,12	0.89	1 (10%)	11,15,17	1.13	1 (9%)
3	BGC	A	686	3	10,11,12	0.74	0	11,15,17	1.01	0
2	BGC	B	679	2	10,11,12	0.62	0	11,15,17	1.35	1 (9%)
2	BGC	B	680	2	10,11,12	0.77	0	11,15,17	1.73	3 (27%)
3	BGC	B	681	3	12,12,12	0.62	0	17,17,17	1.23	3 (17%)
3	BGC	B	682	3	10,11,12	0.85	0	11,15,17	1.63	2 (18%)
3	BGC	B	683	3	10,11,12	0.72	0	11,15,17	0.85	1 (9%)
3	BGC	B	684	3	10,11,12	0.79	0	11,15,17	1.74	2 (18%)
3	BGC	B	685	3	10,11,12	0.92	1 (10%)	11,15,17	1.20	2 (18%)
3	BGC	B	686	3	10,11,12	0.70	0	11,15,17	1.45	2 (18%)
2	BGC	C	679	2	10,11,12	0.84	0	11,15,17	1.49	1 (9%)
2	BGC	C	680	2	10,11,12	0.75	0	11,15,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	C	681	3	12,12,12	0.54	0	17,17,17	1.09	1 (5%)
3	BGC	C	682	3	10,11,12	0.83	0	11,15,17	1.57	2 (18%)
3	BGC	C	683	3	10,11,12	0.79	0	11,15,17	0.92	0
3	BGC	C	684	3	10,11,12	0.81	0	11,15,17	1.60	2 (18%)
3	BGC	C	685	3	10,11,12	0.83	0	11,15,17	1.21	2 (18%)
3	BGC	C	686	3	10,11,12	0.75	0	11,15,17	1.25	2 (18%)
2	BGC	D	679	2	10,11,12	0.81	0	11,15,17	0.97	1 (9%)
2	BGC	D	680	2	10,11,12	0.74	0	11,15,17	1.27	1 (9%)
3	BGC	D	681	3	12,12,12	0.73	0	17,17,17	2.30	6 (35%)
3	BGC	D	682	3	10,11,12	0.95	1 (10%)	11,15,17	1.51	1 (9%)
3	BGC	D	683	3	10,11,12	1.02	1 (10%)	11,15,17	1.22	0
3	BGC	D	684	3	10,11,12	0.97	1 (10%)	11,15,17	2.63	6 (54%)
3	BGC	D	685	3	10,11,12	0.80	0	11,15,17	1.26	1 (9%)
3	BGC	D	686	3	10,11,12	0.66	0	11,15,17	1.41	1 (9%)
2	BGC	E	679	2	10,11,12	0.80	0	11,15,17	1.53	2 (18%)
2	BGC	E	680	2	10,11,12	0.96	1 (10%)	11,15,17	0.74	0
3	BGC	E	681	3	12,12,12	0.52	0	17,17,17	1.07	1 (5%)
3	BGC	E	682	3	10,11,12	0.94	1 (10%)	11,15,17	1.28	2 (18%)
3	BGC	E	683	3	10,11,12	0.95	1 (10%)	11,15,17	0.76	0
3	BGC	E	684	3	10,11,12	0.74	0	11,15,17	1.91	3 (27%)
3	BGC	E	685	3	10,11,12	0.88	1 (10%)	11,15,17	1.10	1 (9%)
3	BGC	E	686	3	10,11,12	0.80	0	11,15,17	1.16	1 (9%)
2	BGC	F	679	2	10,11,12	0.69	0	11,15,17	1.57	1 (9%)
2	BGC	F	680	2	10,11,12	0.67	0	11,15,17	0.67	0
3	BGC	F	681	3	12,12,12	0.76	0	17,17,17	1.38	4 (23%)
3	BGC	F	682	3	10,11,12	0.85	0	11,15,17	1.59	4 (36%)
3	BGC	F	683	3	10,11,12	0.84	0	11,15,17	1.16	1 (9%)
3	BGC	F	684	3	10,11,12	0.74	0	11,15,17	0.97	0
3	BGC	F	685	3	10,11,12	0.79	0	11,15,17	1.02	0
3	BGC	F	686	3	10,11,12	0.71	0	11,15,17	1.29	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	A	679	2	-	0/2/19/22	0/1/1/1
2	BGC	A	680	2	-	0/2/19/22	0/1/1/1
3	BGC	A	681	3	-	0/2/22/22	0/1/1/1
3	BGC	A	682	3	-	0/2/19/22	0/1/1/1
3	BGC	A	683	3	-	0/2/19/22	0/1/1/1
3	BGC	A	684	3	-	0/2/19/22	0/1/1/1
3	BGC	A	685	3	-	0/2/19/22	0/1/1/1
3	BGC	A	686	3	-	0/2/19/22	0/1/1/1
2	BGC	B	679	2	-	0/2/19/22	0/1/1/1
2	BGC	B	680	2	-	0/2/19/22	0/1/1/1
3	BGC	B	681	3	-	0/2/22/22	0/1/1/1
3	BGC	B	682	3	-	0/2/19/22	0/1/1/1
3	BGC	B	683	3	-	0/2/19/22	0/1/1/1
3	BGC	B	684	3	-	0/2/19/22	0/1/1/1
3	BGC	B	685	3	-	0/2/19/22	0/1/1/1
3	BGC	B	686	3	-	0/2/19/22	0/1/1/1
2	BGC	C	679	2	-	0/2/19/22	0/1/1/1
2	BGC	C	680	2	-	0/2/19/22	0/1/1/1
3	BGC	C	681	3	-	0/2/22/22	0/1/1/1
3	BGC	C	682	3	-	0/2/19/22	0/1/1/1
3	BGC	C	683	3	-	0/2/19/22	0/1/1/1
3	BGC	C	684	3	-	0/2/19/22	0/1/1/1
3	BGC	C	685	3	-	0/2/19/22	0/1/1/1
3	BGC	C	686	3	-	0/2/19/22	0/1/1/1
2	BGC	D	679	2	-	0/2/19/22	0/1/1/1
2	BGC	D	680	2	-	0/2/19/22	0/1/1/1
3	BGC	D	681	3	-	0/2/22/22	0/1/1/1
3	BGC	D	682	3	-	0/2/19/22	0/1/1/1
3	BGC	D	683	3	-	0/2/19/22	0/1/1/1
3	BGC	D	684	3	-	0/2/19/22	0/1/1/1
3	BGC	D	685	3	-	0/2/19/22	0/1/1/1
3	BGC	D	686	3	-	0/2/19/22	0/1/1/1
2	BGC	E	679	2	-	0/2/19/22	0/1/1/1
2	BGC	E	680	2	-	0/2/19/22	0/1/1/1
3	BGC	E	681	3	-	0/2/22/22	0/1/1/1
3	BGC	E	682	3	-	0/2/19/22	0/1/1/1
3	BGC	E	683	3	-	0/2/19/22	0/1/1/1
3	BGC	E	684	3	-	0/2/19/22	0/1/1/1
3	BGC	E	685	3	-	0/2/19/22	0/1/1/1
3	BGC	E	686	3	-	0/2/19/22	0/1/1/1
2	BGC	F	679	2	-	0/2/19/22	0/1/1/1
2	BGC	F	680	2	-	0/2/19/22	0/1/1/1
3	BGC	F	681	3	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	F	682	3	-	0/2/19/22	0/1/1/1
3	BGC	F	683	3	-	0/2/19/22	0/1/1/1
3	BGC	F	684	3	-	0/2/19/22	0/1/1/1
3	BGC	F	685	3	-	0/2/19/22	0/1/1/1
3	BGC	F	686	3	-	0/2/19/22	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	683	BGC	O5-C5	-2.48	1.40	1.45
3	D	684	BGC	O5-C5	-2.38	1.41	1.45
3	D	683	BGC	O5-C5	-2.33	1.41	1.45
2	E	680	BGC	O5-C5	-2.25	1.41	1.45
3	E	685	BGC	O5-C5	-2.23	1.41	1.45

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	681	BGC	C6-C5-C4	-5.96	98.60	113.00
3	D	684	BGC	O5-C5-C4	5.56	117.70	110.65
3	E	684	BGC	O5-C5-C6	5.03	112.26	106.98
2	F	679	BGC	O5-C5-C6	4.92	112.14	106.98
3	B	684	BGC	O5-C5-C6	4.63	111.84	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 95th 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	642/678 (94%)	-0.35	12 (1%) 64 66	20, 39, 62, 68	0
1	B	642/678 (94%)	-0.28	20 (3%) 47 48	23, 41, 61, 79	0
1	C	642/678 (94%)	-0.46	10 (1%) 68 71	21, 37, 61, 74	0
1	D	642/678 (94%)	-0.65	3 (0%) 88 90	20, 30, 45, 55	0
1	E	642/678 (94%)	-0.68	2 (0%) 91 93	18, 29, 42, 52	0
1	F	642/678 (94%)	-0.78	1 (0%) 93 94	17, 26, 38, 51	0
All	All	3852/4068 (94%)	-0.53	48 (1%) 75 77	17, 32, 58, 79	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	638	VAL	5.8
1	B	639	LEU	5.2
1	A	315	THR	4.3
1	A	159	THR	3.9
1	A	336	ALA	3.8

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

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

6.3 Carbohydrates ⓘ

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, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BGC	A	686	11/12	0.29	7.29	76,77,78,79	0
3	BGC	B	686	11/12	0.23	6.83	64,66,67,69	0
3	BGC	F	686	11/12	0.19	6.25	43,46,52,57	0
3	BGC	E	686	11/12	0.17	3.19	45,48,49,50	0
3	BGC	C	686	11/12	0.26	2.44	75,77,78,78	0
3	BGC	D	686	11/12	0.15	2.24	40,44,46,47	0
3	BGC	D	681	12/12	0.10	2.04	29,30,33,40	0
3	BGC	F	681	12/12	0.10	1.35	23,25,28,30	0
3	BGC	E	681	12/12	0.09	0.95	25,27,28,32	0
3	BGC	D	684	11/12	0.09	0.57	28,31,33,36	0
2	BGC	E	679	11/12	0.10	0.46	27,30,32,32	0
2	BGC	A	679	11/12	0.11	0.35	33,36,38,40	0
3	BGC	B	681	12/12	0.09	0.13	33,35,37,38	0
2	BGC	C	679	11/12	0.10	0.06	34,36,37,38	0
3	BGC	E	682	11/12	0.08	0.01	27,28,29,29	0
3	BGC	A	685	11/12	0.16	-0.00	67,68,71,74	0
2	BGC	B	679	11/12	0.11	-0.28	42,44,45,46	0
2	BGC	D	679	11/12	0.09	-0.28	32,35,37,38	0
3	BGC	C	682	11/12	0.09	-0.43	39,42,44,44	0
3	BGC	C	685	11/12	0.13	-0.44	61,64,67,72	0
2	BGC	F	680	11/12	0.07	-0.49	23,24,25,26	0
3	BGC	D	685	11/12	0.07	-0.53	33,34,38,38	0
3	BGC	F	682	11/12	0.08	-0.56	21,26,27,27	0
2	BGC	F	679	11/12	0.08	-0.64	25,27,31,32	0
3	BGC	F	685	11/12	0.08	-0.76	32,35,37,40	0
3	BGC	C	683	11/12	0.09	-0.77	43,44,45,48	0
2	BGC	E	680	11/12	0.06	-0.78	23,25,27,28	0
3	BGC	A	684	11/12	0.10	-0.79	56,58,61,64	0
3	BGC	B	682	11/12	0.08	-0.86	29,35,39,42	0
3	BGC	C	684	11/12	0.10	-0.88	45,51,54,59	0
3	BGC	A	681	12/12	0.09	-0.96	38,42,44,47	0
3	BGC	D	683	11/12	0.07	-1.02	26,28,31,32	0
3	BGC	B	684	11/12	0.09	-1.10	39,42,46,51	0
3	BGC	F	684	11/12	0.07	-1.16	28,29,31,31	0
2	BGC	A	680	11/12	0.06	-1.26	30,31,32,32	0
3	BGC	C	681	12/12	0.07	-1.32	33,38,39,40	0
3	BGC	B	683	11/12	0.08	-1.32	35,37,40,41	0
3	BGC	A	683	11/12	0.09	-1.44	43,47,50,53	0
3	BGC	E	685	11/12	0.07	-1.46	32,35,37,42	0
3	BGC	B	685	11/12	0.08	-1.49	53,54,56,60	0
2	BGC	D	680	11/12	0.06	-1.61	28,30,31,32	0
3	BGC	E	683	11/12	0.06	-1.73	23,28,29,29	0
2	BGC	C	680	11/12	0.06	-1.78	29,30,32,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BGC	A	682	11/12	0.09	-1.79	40,43,44,45	0
2	BGC	B	680	11/12	0.07	-1.96	34,40,41,41	0
3	BGC	E	684	11/12	0.06	-2.01	25,29,30,31	0
3	BGC	D	682	11/12	0.06	-2.21	27,29,30,30	0
3	BGC	F	683	11/12	0.05	-2.71	26,27,29,29	0

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.