



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:54 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 X-ray Structure Validation Summary 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	:	trunk28620
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)	:	recalc28949

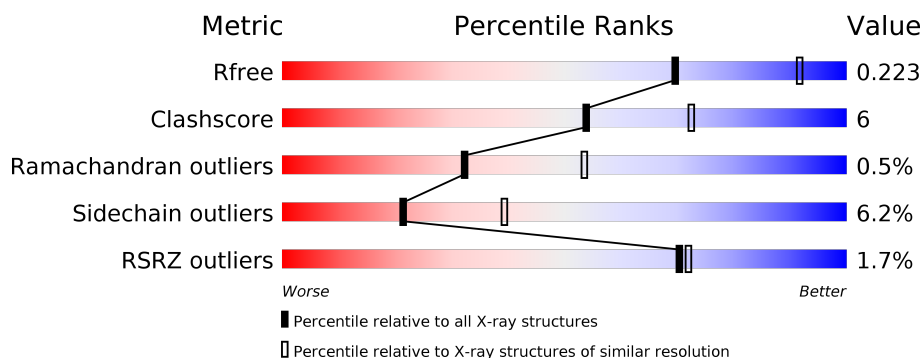
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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  $\geq 3$ , 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	678	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	B	678	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	C	678	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	D	678	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	E	678	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	F	678	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32414 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 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		

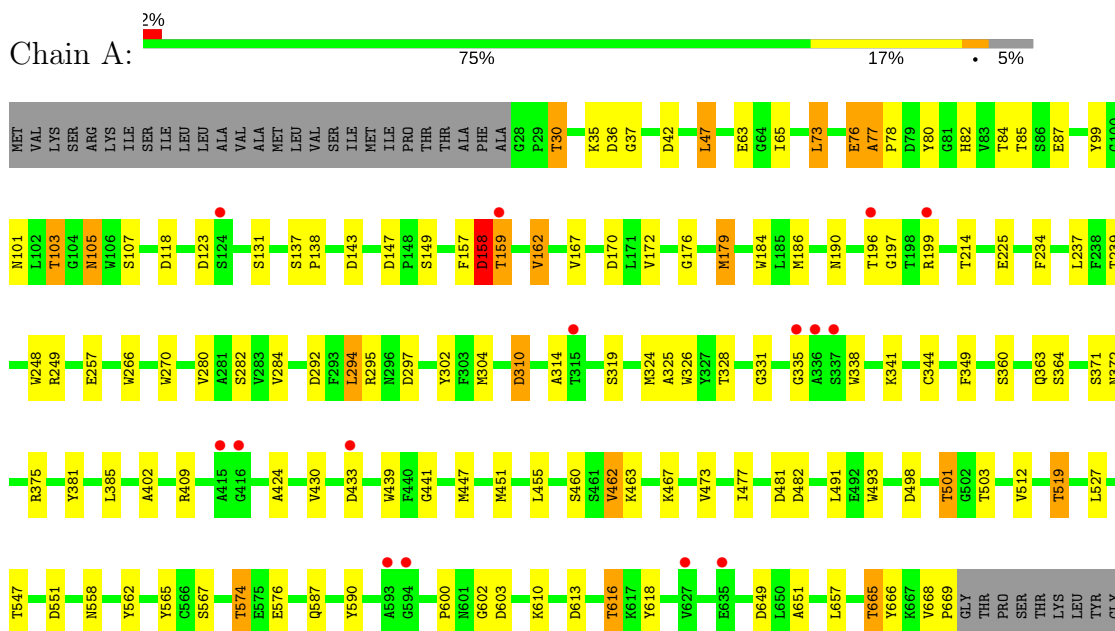
- Molecule 4 is water.

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		

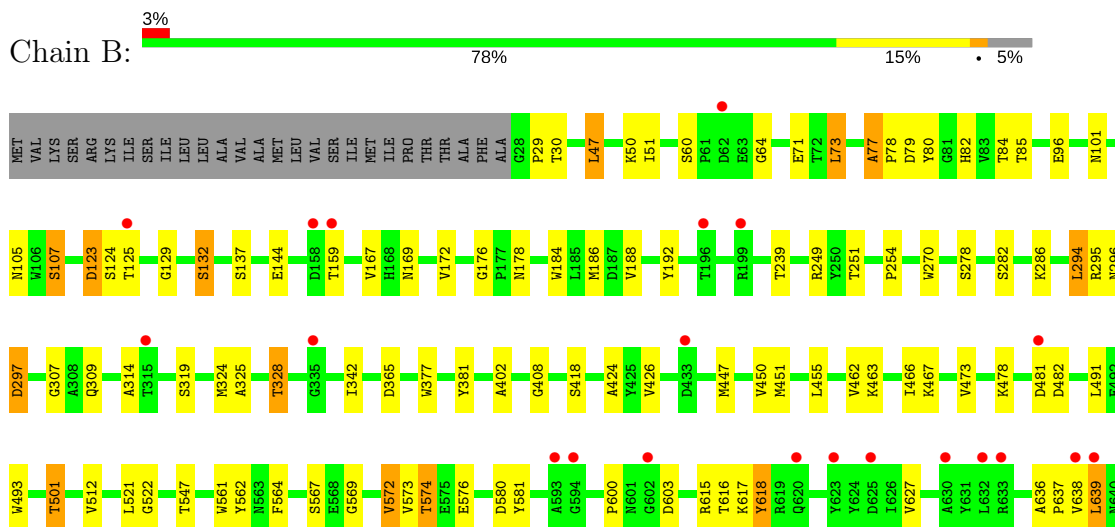
### 3 Residue-property plots

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.

#### • Molecule 1: cellobiohydrolase



#### • Molecule 1: cellobiohydrolase



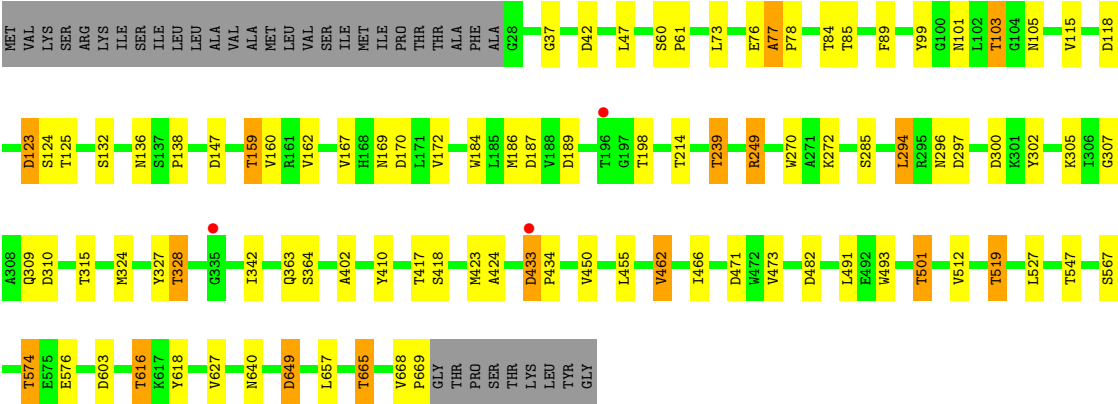
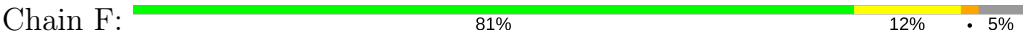
T501	P254	D123	S124	L125	SER	VAL
V512	N268	T125	T126	ARG	LYS	VAL
R513	K269	D127	D127	ARG	LYS	SER
T519	K271	P128	P128	LYS	LYS	ILE
T547	K272	N134	N134	ILE	ILE	SER
T574	L294	P135	P135	LEU	LEU	ILE
E576	D297	Y141	Y141	LEU	LEU	ALA
A577	D300	A142	A142	ALA	ALA	VAL
R578	K301	D143	D143	VAL	VAL	MET
F584	V302	E144	E144	MET	MET	LEU
G594	F303	D147	D147	LEU	LEU	VAL
D603	K311	P152	P152	SER	SER	SER
K604	T315	T159	T159	ILE	ILE	ILE
M609	G316	V160	V160	PRO	PRO	PRO
T616	V317	V161	V161	THR	THR	THR
K617	D318	G163	G163	THR	THR	ALA
Y618	M324	P166	P166	ALA	PHE	PHE
Y623	G335	N178	N178	ALA	ALA	G28
V627	A336	M179	M179	G28	G28	G37
R633	S337	M182	M182	L45	L45	L45
G634	F349	H183	H183	E46	E46	L47
P637	Q363	L185	L185	L47	L47	L47
Y641	S364	M186	M186	D62	D62	D62
D649	D385	T196	T196	E63	E63	G64
L650	Y381	G197	G197	G64	G64	I65
A651	V426	T198	T198	I65	I65	L73
L657	P427	P198	P198	L73	L73	L73
D663	V430	F226	F226	A77	A77	A77
T664	L455	K227	K227	Y80	Y80	G81
T665	S450	Y228	Y228	G81	G81	H82
V668	S461	G233	G233	H82	H82	H83
P669	V462	D236	D236	T84	T84	T84
GLY	L465	T239	T239	T85	T85	T85
PRO	I466	K240	K240	Y99	Y99	G100
SER	V473	D241	D241	G100	G100	N101
THR	D482	R242	R242	N101	N101	L102
LYS	P491	S243	S243	L102	L102	T103
LEU	D492	W248	W248	T103	T103	G104
TYR	L491	R249	R249	N105	N105	N105
GLY	F492	Y250	Y250	N105	N105	T120

T609	G335	T125	MET
R615	I342	E126	VAL
T616	S360	K156	LYS
K617	Q363	T159	SER
Y618	S364	V162	ARG
L639	P368	M179	LYS
N640	Y381	M184	ILE
Y641	K412	L185	ILE
D649	V426	M196	LEU
L657	D433	D189	LEU
T665	M447	T198	ALA
V668	L455	R199	VAL
P669	V462	T214	SER
GLY	I466	H220	ILE
THR	V469	P221	ILE
PRO	T501	T239	PRO
SER	V512	R249	THR
THR	T519	T251	ALA
LYS	L491	N268	PHE
LEU	E492	K269	ALA
TYR	M493	W270	ALA
GLY	T601	E273	G28
	V512	S278	A32
	T519	S285	D36
	A537	D292	G37
	K544	F293	L43
	L545	L294	L47
	D546	D297	S60
	T547	Y302	E63
	Y565	G307	L73
	C566	F308	E76
	S567	L294	A77
	T574	Q309	P78
	E575	G316	T84
	E576	M324	Y99
	D603	T328	G100
			N101
			L102
			T103
			G104
			N105
			D123
			S124

R295	G307	T315	L323	G331	G335	S360	M423	V430	D433	L485	S460	S461	V462	K463	K467	D492	L491	S492	T501	G502	T503	V512	T519	D520	R540	T547	C566																								
Y133	M136	S137	P138	D147	D158	T159	V162	P166	V167	H168	M169	M179	M184	L185	M186	D187	G197	T198	R199	E210	W215	P221	E226	F226	K227	Y228	G233	T239	K240	D241	R242	W248	R249	Y250	T251	W266	W270	S278	T284	T285	E286	Y289	G100	N101	L102	T103	G104	N105	D123	S124	S131
VAL	SER	ARG	LYS	ILE	ILE	LEU	VAL	MET	LEU	VAL	SER	ILE	MET	ILE	PRO	THR	THR	ALA	PHE	ALA	G228	G37	L47	D53	P54	E63	L73	A77	P78	T84	T85	E86	Y89	G100	N101	L102	T103	G104	N105	D123	S124	S131									



● Molecule 1: cellobiohydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32414	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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 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	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
4	C	145	0	0	3	0
4	D	238	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	221	0	0	8	0
4	F	289	0	0	12	0
All	All	32414	0	28719	365	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 6.

The worst 5 of 365 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B: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 [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	640/678 (94%)	607 (95%)	28 (4%)	5 (1%)	22	39
1	B	640/678 (94%)	605 (94%)	33 (5%)	2 (0%)	44	66
1	C	640/678 (94%)	615 (96%)	20 (3%)	5 (1%)	22	39
1	D	640/678 (94%)	622 (97%)	16 (2%)	2 (0%)	44	66
1	E	640/678 (94%)	617 (96%)	20 (3%)	3 (0%)	32	53
1	F	640/678 (94%)	621 (97%)	18 (3%)	1 (0%)	51	73
All	All	3840/4068 (94%)	3687 (96%)	135 (4%)	18 (0%)	32	53

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%)	15	28
1	B	519/556 (93%)	490 (94%)	29 (6%)	25	45
1	C	513/556 (92%)	481 (94%)	32 (6%)	21	39
1	D	521/556 (94%)	491 (94%)	30 (6%)	23	43
1	E	518/556 (93%)	488 (94%)	30 (6%)	23	43
1	F	520/556 (94%)	490 (94%)	30 (6%)	23	43
All	All	3103/3336 (93%)	2912 (94%)	191 (6%)	21	39

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

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Mol	Chain	Res	Type
1	F	207	GLN
1	C	268	ASN
1	C	363	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 ⓘ

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	11,11,12	0.60	0	13,15,17	1.28	2 (15%)
2	BGC	A	680	2	11,11,12	0.73	0	13,15,17	0.93	0
3	BGC	A	681	3	12,12,12	0.48	0	17,17,17	1.76	5 (29%)
3	BGC	A	682	3	11,11,12	0.74	0	13,15,17	0.68	0
3	BGC	A	683	3	11,11,12	0.79	0	13,15,17	1.10	1 (7%)
3	BGC	A	684	3	11,11,12	0.59	0	13,15,17	1.98	6 (46%)
3	BGC	A	685	3	11,11,12	0.73	0	13,15,17	0.96	0
3	BGC	A	686	3	11,11,12	0.66	0	13,15,17	1.69	2 (15%)
2	BGC	B	679	2	11,11,12	0.67	0	13,15,17	1.49	2 (15%)
2	BGC	B	680	2	11,11,12	0.73	0	13,15,17	1.11	1 (7%)
3	BGC	B	681	3	12,12,12	0.64	0	17,17,17	1.24	3 (17%)
3	BGC	B	682	3	11,11,12	0.91	1 (9%)	13,15,17	1.67	3 (23%)
3	BGC	B	683	3	11,11,12	0.53	0	13,15,17	0.78	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BGC	B	684	3	11,11,12	0.62	0	13,15,17	1.29	2 (15%)
3	BGC	B	685	3	11,11,12	0.76	0	13,15,17	0.75	0
3	BGC	B	686	3	11,11,12	0.58	0	13,15,17	1.78	2 (15%)
2	BGC	C	679	2	11,11,12	0.81	0	13,15,17	1.20	1 (7%)
2	BGC	C	680	2	11,11,12	0.54	0	13,15,17	0.55	0
3	BGC	C	681	3	12,12,12	0.57	0	17,17,17	1.12	1 (5%)
3	BGC	C	682	3	11,11,12	0.76	0	13,15,17	1.25	1 (7%)
3	BGC	C	683	3	11,11,12	0.69	0	13,15,17	1.29	2 (15%)
3	BGC	C	684	3	11,11,12	0.69	0	13,15,17	1.28	2 (15%)
3	BGC	C	685	3	11,11,12	0.63	0	13,15,17	1.15	1 (7%)
3	BGC	C	686	3	11,11,12	0.69	0	13,15,17	1.15	2 (15%)
2	BGC	D	679	2	11,11,12	0.71	0	13,15,17	1.51	2 (15%)
2	BGC	D	680	2	11,11,12	0.75	0	13,15,17	0.98	1 (7%)
3	BGC	D	681	3	12,12,12	0.73	0	17,17,17	2.33	5 (29%)
3	BGC	D	682	3	11,11,12	0.96	1 (9%)	13,15,17	1.70	2 (15%)
3	BGC	D	683	3	11,11,12	0.85	0	13,15,17	1.29	1 (7%)
3	BGC	D	684	3	11,11,12	1.03	1 (9%)	13,15,17	2.40	5 (38%)
3	BGC	D	685	3	11,11,12	0.54	0	13,15,17	0.82	0
3	BGC	D	686	3	11,11,12	0.65	0	13,15,17	1.85	2 (15%)
2	BGC	E	679	2	11,11,12	0.87	1 (9%)	13,15,17	1.82	3 (23%)
2	BGC	E	680	2	11,11,12	0.87	0	13,15,17	1.45	2 (15%)
3	BGC	E	681	3	12,12,12	0.52	0	17,17,17	1.05	1 (5%)
3	BGC	E	682	3	11,11,12	0.89	0	13,15,17	1.50	3 (23%)
3	BGC	E	683	3	11,11,12	0.71	0	13,15,17	0.88	0
3	BGC	E	684	3	11,11,12	0.73	0	13,15,17	1.33	3 (23%)
3	BGC	E	685	3	11,11,12	0.77	0	13,15,17	1.24	1 (7%)
3	BGC	E	686	3	11,11,12	0.70	0	13,15,17	1.57	3 (23%)
2	BGC	F	679	2	11,11,12	0.86	0	13,15,17	1.27	1 (7%)
2	BGC	F	680	2	11,11,12	0.53	0	13,15,17	0.66	0
3	BGC	F	681	3	12,12,12	0.80	0	17,17,17	1.38	3 (17%)
3	BGC	F	682	3	11,11,12	0.95	0	13,15,17	1.77	4 (30%)
3	BGC	F	683	3	11,11,12	0.66	0	13,15,17	1.24	1 (7%)
3	BGC	F	684	3	11,11,12	0.68	0	13,15,17	1.21	1 (7%)
3	BGC	F	685	3	11,11,12	0.65	0	13,15,17	1.42	2 (15%)
3	BGC	F	686	3	11,11,12	0.67	0	13,15,17	1.70	3 (23%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	684	BGC	O5-C1	-2.56	1.39	1.43
3	D	682	BGC	O5-C1	-2.19	1.40	1.43
3	B	682	BGC	O5-C1	-2.09	1.40	1.43
2	E	679	BGC	C2-C3	2.23	1.55	1.52

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	681	BGC	C6-C5-C4	-6.15	98.60	113.00
2	E	679	BGC	O5-C1-C2	-5.25	102.56	110.79
2	B	679	BGC	O5-C1-C2	-4.32	104.02	110.79
2	E	680	BGC	O5-C1-C2	-4.16	104.28	110.79
2	F	679	BGC	O5-C1-C2	-4.11	104.34	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	684	BGC	1	0
3	A	685	BGC	1	0
3	B	682	BGC	1	0
3	C	682	BGC	1	0
3	C	684	BGC	1	0
3	D	681	BGC	2	0
3	D	682	BGC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	684	BGC	1	0
3	E	682	BGC	1	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	642/678 (94%)	-0.35	15 (2%) 61 63	20, 39, 62, 68	0
1	B	642/678 (94%)	-0.28	22 (3%) 46 48	23, 41, 61, 79	0
1	C	642/678 (94%)	-0.46	15 (2%) 61 63	21, 37, 61, 74	0
1	D	642/678 (94%)	-0.67	5 (0%) 86 86	20, 30, 45, 55	0
1	E	642/678 (94%)	-0.69	4 (0%) 89 89	18, 29, 42, 52	0
1	F	642/678 (94%)	-0.79	3 (0%) 90 91	17, 26, 38, 51	0
All	All	3852/4068 (94%)	-0.54	64 (1%) 70 72	17, 32, 58, 79	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	638	VAL	6.8
1	B	639	LEU	6.0
1	A	315	THR	4.3
1	A	159	THR	4.3
1	A	336	ALA	4.3

### 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](#)

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( $\text{\AA}^2$ )	Q<0.9
3	BGC	F	681	12/12	0.98	0.10	1.44	23,25,28,30	0
3	BGC	D	681	12/12	0.96	0.10	1.19	29,30,33,40	0
3	BGC	E	681	12/12	0.99	0.10	0.76	25,27,28,32	0
2	BGC	E	679	11/12	0.95	0.11	0.55	27,30,32,32	0
2	BGC	C	679	11/12	0.96	0.11	0.40	34,36,37,38	0
2	BGC	A	679	11/12	0.94	0.12	0.35	33,36,38,40	0
2	BGC	D	679	11/12	0.96	0.10	0.27	32,35,37,38	0
3	BGC	A	685	11/12	0.86	0.17	0.25	67,68,71,74	0
3	BGC	D	684	11/12	0.96	0.09	0.15	28,31,33,36	0
3	BGC	B	681	12/12	0.98	0.10	0.06	33,35,37,38	0
3	BGC	C	685	11/12	0.90	0.15	0.02	61,64,67,72	0
3	BGC	E	682	11/12	0.98	0.09	-0.06	27,28,29,29	0
3	BGC	C	683	11/12	0.96	0.10	-0.33	43,44,45,48	0
2	BGC	B	679	11/12	0.94	0.11	-0.46	42,44,45,46	0
3	BGC	C	684	11/12	0.94	0.11	-0.49	45,51,54,59	0
3	BGC	A	684	11/12	0.93	0.11	-0.54	56,58,61,64	0
2	BGC	F	679	11/12	0.96	0.08	-0.73	25,27,31,32	0
3	BGC	C	682	11/12	0.97	0.09	-0.78	39,42,44,44	0
3	BGC	D	685	11/12	0.98	0.07	-0.79	33,34,38,38	0
3	BGC	F	685	11/12	0.98	0.09	-0.87	32,35,37,40	0
3	BGC	A	681	12/12	0.96	0.09	-0.87	38,42,44,47	0
3	BGC	F	684	11/12	0.97	0.08	-0.92	28,29,31,31	0
3	BGC	B	685	11/12	0.94	0.10	-0.95	53,54,56,60	0
2	BGC	E	680	11/12	0.98	0.06	-0.96	23,25,27,28	0
3	BGC	B	684	11/12	0.96	0.10	-0.99	39,42,46,51	0
3	BGC	A	683	11/12	0.96	0.10	-1.02	43,47,50,53	0
2	BGC	F	680	11/12	0.98	0.07	-1.07	23,24,25,26	0
3	BGC	D	683	11/12	0.98	0.07	-1.08	26,28,31,32	0
3	BGC	D	682	11/12	0.97	0.07	-1.31	27,29,30,30	0
3	BGC	C	681	12/12	0.98	0.08	-1.33	33,38,39,40	0
3	BGC	B	682	11/12	0.98	0.07	-1.35	29,35,39,42	0
2	BGC	B	680	11/12	0.95	0.08	-1.36	34,40,41,41	0
3	BGC	F	682	11/12	0.98	0.08	-1.39	21,26,27,27	0
3	BGC	B	683	11/12	0.94	0.09	-1.41	35,37,40,41	0
3	BGC	E	683	11/12	0.98	0.07	-1.42	23,28,29,29	0
2	BGC	A	680	11/12	0.98	0.06	-1.48	30,31,32,32	0
3	BGC	E	685	11/12	0.97	0.07	-1.68	32,35,37,42	0
2	BGC	D	680	11/12	0.98	0.06	-1.73	28,30,31,32	0
2	BGC	C	680	11/12	0.98	0.06	-1.75	29,30,32,33	0
3	BGC	A	682	11/12	0.97	0.09	-1.76	40,43,44,45	0
3	BGC	E	684	11/12	0.98	0.06	-2.06	25,29,30,31	0
3	BGC	F	683	11/12	0.98	0.06	-3.09	26,27,29,29	0
3	BGC	D	686	11/12	0.91	0.16	-	40,44,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BGC	E	686	11/12	0.92	0.17	-	45,48,49,50	0
3	BGC	F	686	11/12	0.91	0.21	-	43,46,52,57	0
3	BGC	B	686	11/12	0.88	0.24	-	64,66,67,69	0
3	BGC	A	686	11/12	0.87	0.31	-	76,77,78,79	0
3	BGC	C	686	11/12	0.84	0.28	-	75,77,78,78	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.