



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:58 AM GMT

PDB ID : 1L1Y  
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 : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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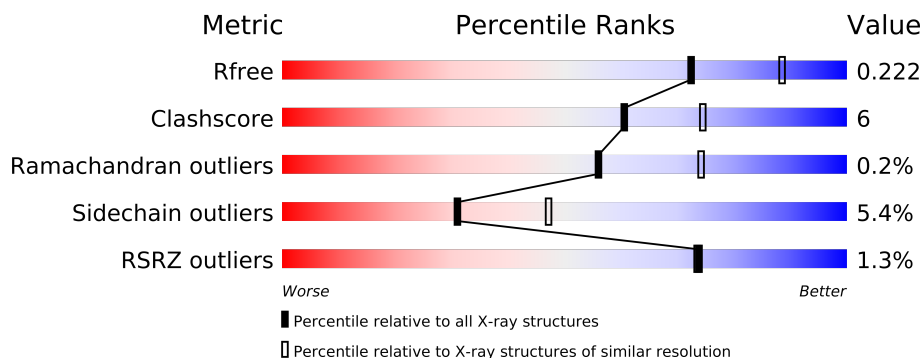
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. 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 3 unique types of molecules in this entry. The entry contains 32457 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 water.

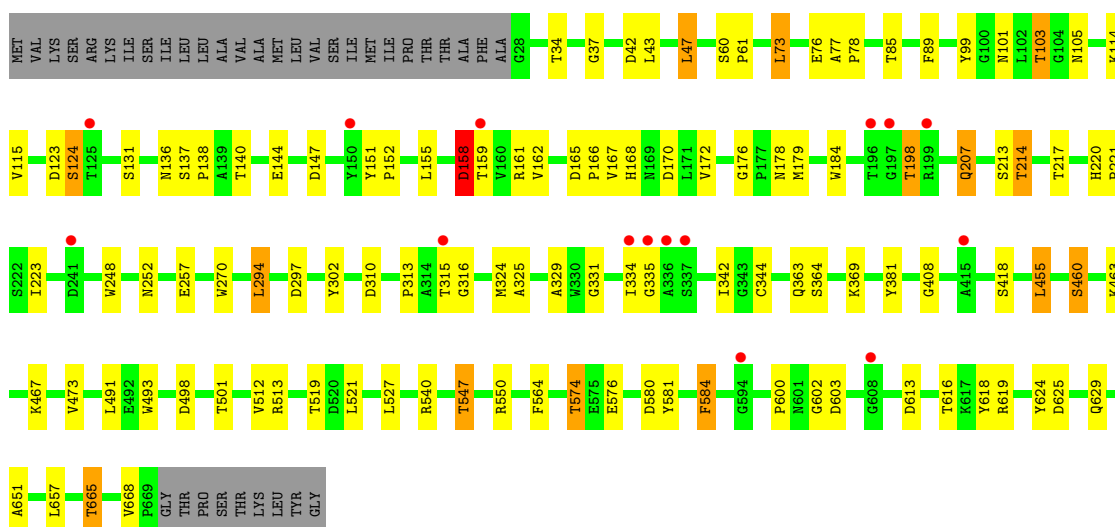
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	169	Total 169	O 169	0	0
3	B	204	Total 204	O 204	0	0
3	C	214	Total 214	O 214	0	0
3	D	326	Total 326	O 326	0	0
3	E	286	Total 286	O 286	0	0
3	F	396	Total 396	O 396	0	0

### 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 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.

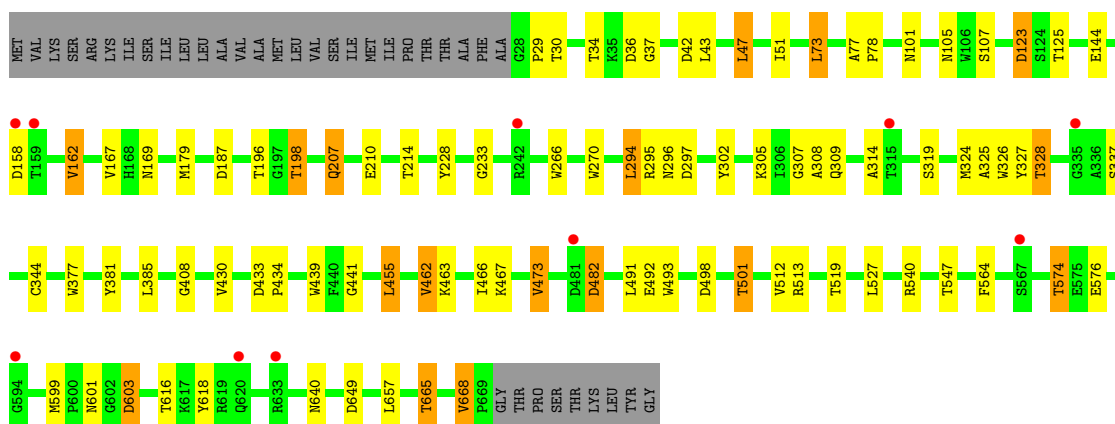
- Molecule 1: cellobiohydrolase

Chain A: 



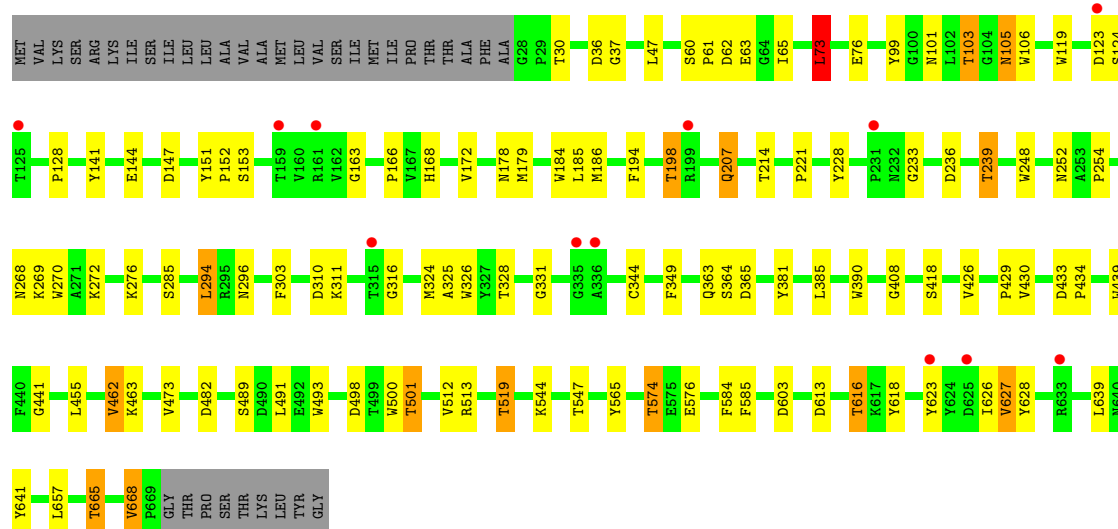
- Molecule 1: cellobiohydrolase

Chain B: 



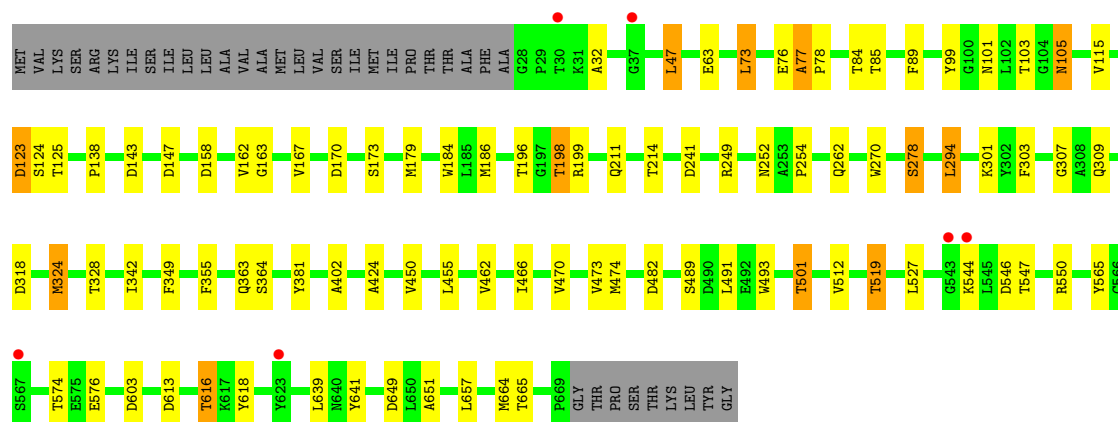
- Molecule 1: cellobiohydrolase

Chain C: 



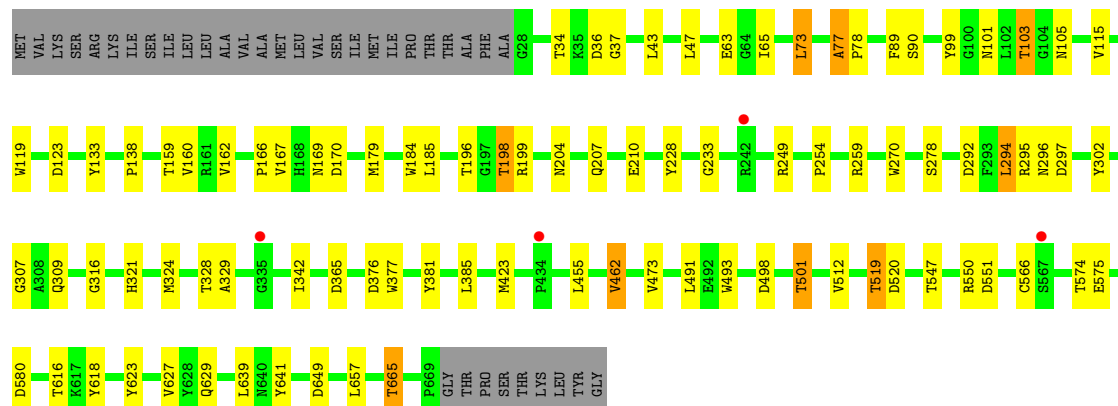
• Molecule 1: cellobiohydrolase

Chain D:



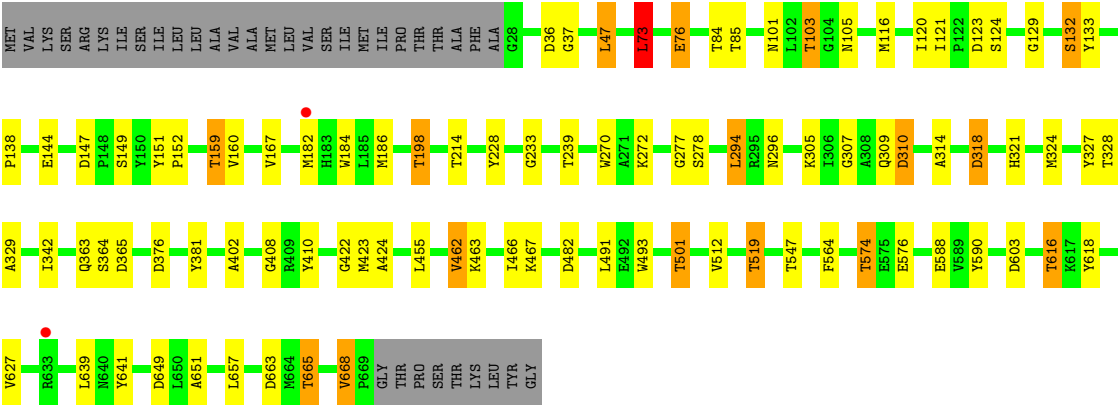
• Molecule 1: cellobiohydrolase

Chain E:



• Molecule 1: cellobiohydrolase

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.24Å 207.20Å 213.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 14.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.00-2.40) 99.9 (14.99-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.189 , 0.224 0.188 , 0.222	Depositor DCC
$R_{free}$ test set	12676 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 22.4	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 252098 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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	0.56	0/5282	0.77	11/7213 (0.2%)
1	B	0.55	0/5307	0.75	9/7241 (0.1%)
1	C	0.54	0/5288	0.76	8/7218 (0.1%)
1	D	0.62	1/5315 (0.0%)	0.79	11/7251 (0.2%)
1	E	0.60	0/5303	0.78	12/7236 (0.2%)
1	F	0.64	0/5309	0.79	8/7244 (0.1%)
All	All	0.59	1/31804 (0.0%)	0.77	59/43403 (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	B	0	1
1	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	324	MET	SD-CE	-5.16	1.49	1.77

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	123	ASP	CB-CG-OD2	7.01	124.61	118.30
1	C	62	ASP	CB-CG-OD2	6.96	124.56	118.30
1	A	147	ASP	CB-CG-OD2	6.65	124.28	118.30
1	C	73	LEU	CA-CB-CG	6.59	130.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	170	ASP	CB-CG-OD2	6.48	124.13	118.30
1	C	482	ASP	CB-CG-OD2	6.46	124.12	118.30
1	B	482	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	123	ASP	CB-CG-OD2	6.22	123.90	118.30
1	E	297	ASP	CB-CG-OD2	6.21	123.89	118.30
1	F	482	ASP	CB-CG-OD2	6.17	123.85	118.30
1	F	663	ASP	CB-CG-OD2	6.17	123.85	118.30
1	F	147	ASP	CB-CG-OD2	6.14	123.83	118.30
1	F	73	LEU	CA-CB-CG	6.11	129.35	115.30
1	B	498	ASP	CB-CG-OD2	6.10	123.79	118.30
1	E	498	ASP	CB-CG-OD2	6.06	123.76	118.30
1	D	147	ASP	CB-CG-OD2	6.05	123.74	118.30
1	C	498	ASP	CB-CG-OD2	6.01	123.71	118.30
1	D	158	ASP	CB-CG-OD2	6.00	123.70	118.30
1	F	123	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	170	ASP	CB-CG-OD2	5.95	123.66	118.30
1	B	603	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	158	ASP	CB-CG-OD2	5.91	123.61	118.30
1	A	123	ASP	CB-CG-OD2	5.88	123.60	118.30
1	A	550	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	498	ASP	CB-CG-OD2	5.77	123.50	118.30
1	D	546	ASP	CB-CG-OD2	5.77	123.50	118.30
1	C	123	ASP	CB-CG-OD2	5.76	123.49	118.30
1	E	73	LEU	CA-CB-CG	5.72	128.46	115.30
1	A	73	LEU	CA-CB-CG	5.70	128.42	115.30
1	B	42	ASP	CB-CG-OD2	5.69	123.42	118.30
1	F	310	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	297	ASP	CB-CG-OD2	5.64	123.38	118.30
1	E	170	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	613	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	73	LEU	CA-CB-CG	5.59	128.15	115.30
1	C	147	ASP	CB-CG-OD2	5.51	123.26	118.30
1	D	613	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	73	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	42	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	613	ASP	CB-CG-OD2	5.40	123.16	118.30
1	E	580	ASP	CB-CG-OD2	5.36	123.12	118.30
1	E	376	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	143	ASP	CB-CG-OD1	5.29	123.06	118.30
1	E	520	ASP	CB-CG-OD2	5.28	123.06	118.30
1	E	649	ASP	CB-CG-OD2	5.26	123.04	118.30
1	E	365	ASP	CB-CG-OD2	5.21	122.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	318	ASP	CB-CG-OD2	5.21	122.99	118.30
1	E	36	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	187	ASP	CB-CG-OD2	5.18	122.96	118.30
1	F	318	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	297	ASP	CB-CG-OD2	5.17	122.96	118.30
1	E	551	ASP	CB-CG-OD2	5.15	122.94	118.30
1	D	482	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	580	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	365	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	123	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	158	ASP	CB-CG-OD2	5.09	122.88	118.30
1	F	376	ASP	CB-CG-OD2	5.01	122.81	118.30
1	D	241	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	327	TYR	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	67	0
1	B	5128	0	4727	58	0
1	C	5109	0	4686	64	0
1	D	5136	0	4737	54	0
1	E	5124	0	4720	55	0
1	F	5130	0	4726	73	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	22	0	19	0	0
2	F	22	0	19	0	0
3	A	169	0	0	8	0
3	B	204	0	0	4	0
3	C	214	0	0	10	0
3	D	326	0	0	5	0
3	E	286	0	0	7	0
3	F	396	0	0	13	0
All	All	32457	0	28377	350	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.

All (350) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:574:THR:HG21	1:A:576:GLU:OE1	1.58	1.03
1:A:105:ASN:HB2	3:A:840:HOH:O	1.62	0.97
3:C:703:HOH:O	1:E:169:ASN:HB3	1.66	0.95
1:C:103:THR:HG22	1:C:105:ASN:H	1.35	0.91
1:C:294:LEU:HG	1:C:324:MET:HE1	1.55	0.86
1:F:278:SER:HB3	3:F:1064:HOH:O	1.76	0.86
1:C:294:LEU:HG	1:C:324:MET:CE	2.05	0.85
1:C:574:THR:HG21	1:C:576:GLU:OE1	1.76	0.85
1:F:574:THR:HG21	1:F:576:GLU:OE1	1.74	0.85
1:F:116:MET:HG3	1:F:182:MET:SD	2.16	0.85
1:A:76:GLU:O	1:A:214:THR:HG21	1.77	0.84
1:E:103:THR:HG22	1:E:105:ASN:H	1.42	0.84
1:F:120:ILE:CG2	1:F:182:MET:SD	2.68	0.82
1:F:76:GLU:O	1:F:214:THR:HG21	1.78	0.82
1:B:37:GLY:HA2	1:B:665:THR:HG21	1.63	0.81
1:B:599:MET:HB2	1:B:603:ASP:HB2	1.63	0.80
1:D:254:PRO:HB2	1:D:324:MET:HE3	1.66	0.77
1:B:501:THR:HG21	1:D:309:GLN:HE21	1.49	0.77
1:F:310:ASP:HB2	3:F:842:HOH:O	1.85	0.76
1:E:501:THR:HG23	1:F:307:GLY:O	1.86	0.76
1:A:460:SER:HB2	3:A:829:HOH:O	1.85	0.76
1:E:99:TYR:O	1:E:103:THR:HB	1.86	0.75
1:F:519:THR:HG22	3:F:715:HOH:O	1.87	0.75
1:B:37:GLY:HA2	1:B:665:THR:CG2	2.17	0.75
1:E:574:THR:HG23	3:E:814:HOH:O	1.87	0.74
1:C:363:GLN:HE22	1:F:364:SER:H	1.31	0.74
1:F:120:ILE:HG23	1:F:182:MET:SD	2.28	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:501:THR:HG21	1:F:309:GLN:HE21	1.54	0.72
1:D:574:THR:HG22	1:D:641:TYR:H	1.53	0.72
1:C:268:ASN:HD21	1:C:272:LYS:HZ2	1.38	0.72
1:D:198:THR:HB	3:D:834:HOH:O	1.89	0.72
1:E:629:GLN:HB3	3:E:859:HOH:O	1.90	0.72
1:A:162:VAL:HG23	1:A:302:TYR:HB3	1.72	0.71
1:A:103:THR:HG22	1:A:105:ASN:H	1.56	0.70
1:F:37:GLY:HA2	1:F:665:THR:CG2	2.20	0.70
1:B:307:GLY:O	1:D:501:THR:CG2	2.40	0.70
1:A:47:LEU:HD13	1:A:651:ALA:HB2	1.74	0.69
1:E:254:PRO:HB2	1:E:324:MET:CE	2.22	0.69
1:B:574:THR:HG21	1:B:576:GLU:OE1	1.93	0.69
1:A:103:THR:CG2	1:A:105:ASN:H	2.06	0.69
1:B:501:THR:CG2	1:D:307:GLY:O	2.41	0.69
1:D:76:GLU:O	1:D:214:THR:HG21	1.93	0.69
1:E:101:ASN:HB2	1:E:270:TRP:CE3	2.28	0.69
1:F:121:ILE:HG13	1:F:182:MET:HG2	1.76	0.68
1:C:364:SER:H	1:F:363:GLN:HE22	1.41	0.68
1:E:37:GLY:HA2	1:E:665:THR:CG2	2.24	0.68
1:B:47:LEU:O	1:B:51:ILE:HG13	1.94	0.67
1:A:37:GLY:HA2	1:A:665:THR:CG2	2.24	0.67
1:C:623:TYR:O	1:C:627:VAL:HG12	1.93	0.67
1:C:513:ARG:HD3	3:C:878:HOH:O	1.94	0.66
1:C:99:TYR:O	1:C:103:THR:HB	1.94	0.66
1:D:473:VAL:HG11	1:D:527:LEU:HD11	1.78	0.66
1:C:513:ARG:CD	3:C:878:HOH:O	2.44	0.66
1:E:307:GLY:O	1:F:501:THR:CG2	2.43	0.66
1:E:199:ARG:HD2	3:E:961:HOH:O	1.96	0.65
1:C:152:PRO:HG3	1:C:236:ASP:O	1.96	0.65
1:B:307:GLY:O	1:D:501:THR:HG23	1.96	0.65
1:A:364:SER:H	1:D:363:GLN:HE22	1.45	0.65
1:F:198:THR:CG2	3:F:924:HOH:O	2.44	0.64
1:C:269:LYS:HE3	3:C:889:HOH:O	1.97	0.64
1:A:363:GLN:HE22	1:D:364:SER:H	1.44	0.64
1:B:207:GLN:HE21	1:B:207:GLN:HA	1.62	0.64
1:A:101:ASN:HB2	1:A:270:TRP:CE3	2.33	0.63
1:E:254:PRO:HB2	1:E:324:MET:HE2	1.79	0.63
1:E:37:GLY:HA2	1:E:665:THR:HG21	1.81	0.63
1:C:144:GLU:HB2	1:C:408:GLY:HA3	1.79	0.63
1:B:309:GLN:HE21	1:D:501:THR:HG21	1.64	0.63
1:A:625:ASP:O	1:A:629:GLN:HG2	1.99	0.63
1:A:257:GLU:HB3	1:A:294:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:305:LYS:HD2	3:F:1066:HOH:O	1.98	0.63
1:C:76:GLU:O	1:C:214:THR:HG21	1.99	0.63
1:F:101:ASN:HB2	1:F:270:TRP:CE3	2.34	0.62
1:D:254:PRO:HB2	1:D:324:MET:CE	2.29	0.62
1:E:309:GLN:HE21	1:F:501:THR:HG21	1.63	0.62
1:C:119:TRP:O	1:C:186:MET:HE1	2.00	0.62
1:E:501:THR:CG2	1:F:307:GLY:O	2.47	0.61
1:D:103:THR:HG22	1:D:105:ASN:H	1.65	0.61
1:C:603:ASP:OD2	1:C:616:THR:HB	2.01	0.61
1:F:37:GLY:HA2	1:F:665:THR:HG21	1.81	0.61
1:E:196:THR:O	1:E:199:ARG:HG3	2.01	0.60
1:F:294:LEU:HG	1:F:324:MET:CE	2.31	0.60
1:D:101:ASN:HB2	1:D:270:TRP:CE3	2.36	0.60
1:C:101:ASN:HB2	1:C:270:TRP:CE3	2.36	0.60
1:B:101:ASN:HB2	1:B:270:TRP:CE3	2.37	0.60
1:F:121:ILE:CG1	1:F:182:MET:HG2	2.32	0.60
1:F:37:GLY:HA2	1:F:665:THR:HG23	1.84	0.59
1:D:550:ARG:HD2	1:D:664:MET:SD	2.42	0.59
1:A:248:TRP:CZ3	1:A:331:GLY:HA2	2.38	0.59
1:B:169:ASN:HB2	3:B:873:HOH:O	2.02	0.58
1:A:124:SER:HB3	1:A:178:ASN:HD21	1.68	0.58
1:B:294:LEU:HG	1:B:324:MET:CE	2.33	0.58
1:A:37:GLY:HA2	1:A:665:THR:HG23	1.84	0.58
1:D:294:LEU:HG	1:D:324:MET:CE	2.33	0.58
1:B:296:ASN:HB3	1:B:328:THR:HG21	1.86	0.58
1:A:223:ILE:HG23	1:A:334:ILE:HD11	1.86	0.57
1:B:77:ALA:H	1:B:78:PRO:HD2	1.70	0.57
1:C:124:SER:HB3	1:C:178:ASN:ND2	2.19	0.57
1:A:124:SER:HB3	1:A:178:ASN:ND2	2.20	0.57
1:F:103:THR:CG2	1:F:105:ASN:H	2.17	0.57
1:F:588:GLU:HG3	3:F:942:HOH:O	2.03	0.56
1:C:207:GLN:HE21	1:C:207:GLN:HA	1.69	0.56
1:C:385:LEU:HD22	1:C:462:VAL:HG21	1.86	0.56
1:D:99:TYR:O	1:D:103:THR:HB	2.06	0.56
1:A:114:LYS:HE3	3:A:838:HOH:O	2.05	0.56
1:C:36:ASP:OD1	1:C:668:VAL:HG12	2.06	0.56
1:A:547:THR:CG2	3:A:831:HOH:O	2.54	0.55
1:B:198:THR:HG22	3:B:806:HOH:O	2.06	0.55
1:B:105:ASN:ND2	1:B:107:SER:OG	2.37	0.55
1:B:162:VAL:HG22	1:B:302:TYR:HB3	1.87	0.55
1:A:519:THR:HG23	3:A:731:HOH:O	2.07	0.55
1:B:493:TRP:CZ3	1:B:512:VAL:HB	2.41	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:574:THR:HG21	1:D:576:GLU:OE1	2.07	0.55
1:A:294:LEU:HG	1:A:324:MET:CE	2.36	0.55
1:F:493:TRP:CZ3	1:F:512:VAL:HB	2.42	0.55
1:C:294:LEU:HG	1:C:324:MET:HE3	1.88	0.55
1:B:601:ASN:HD21	1:B:616:THR:HB	1.71	0.54
1:A:37:GLY:HA2	1:A:665:THR:HG21	1.89	0.54
1:A:581:TYR:O	1:A:584:PHE:HB2	2.08	0.54
1:B:439:TRP:CE2	1:B:441:GLY:HA3	2.43	0.53
1:A:463:LYS:O	1:A:467:LYS:HG2	2.09	0.53
1:D:76:GLU:O	1:D:77:ALA:C	2.47	0.53
1:B:325:ALA:HB1	1:B:344:CYS:HB3	1.90	0.53
1:E:574:THR:HG22	1:E:575:GLU:N	2.24	0.53
1:E:77:ALA:H	1:E:78:PRO:HD2	1.74	0.53
1:C:272:LYS:HE2	3:F:863:HOH:O	2.09	0.53
1:B:574:THR:O	1:B:640:ASN:HA	2.09	0.53
1:F:463:LYS:O	1:F:467:LYS:HG2	2.08	0.53
1:A:89:PHE:HE2	1:A:115:VAL:HG12	1.74	0.53
1:D:519:THR:CG2	3:D:999:HOH:O	2.56	0.52
1:F:84:THR:HG22	1:F:186:MET:HB3	1.89	0.52
1:A:213:SER:O	1:A:217:THR:HG23	2.09	0.52
1:D:294:LEU:HG	1:D:324:MET:HE2	1.91	0.52
1:F:294:LEU:HG	1:F:324:MET:HE3	1.91	0.52
1:E:37:GLY:HA2	1:E:665:THR:HG23	1.91	0.52
1:F:574:THR:CG2	1:F:576:GLU:OE1	2.52	0.52
1:A:473:VAL:HG11	1:A:527:LEU:HD11	1.92	0.52
1:B:294:LEU:HG	1:B:324:MET:HE1	1.92	0.52
1:C:198:THR:HG22	3:C:876:HOH:O	2.09	0.52
1:E:296:ASN:HB3	1:E:328:THR:HG21	1.90	0.52
1:F:47:LEU:HD13	1:F:651:ALA:HB2	1.91	0.51
1:D:47:LEU:HD13	1:D:651:ALA:HB2	1.93	0.51
1:F:310:ASP:HB3	3:F:717:HOH:O	2.11	0.51
1:D:574:THR:HG22	1:D:641:TYR:N	2.25	0.51
1:B:324:MET:CE	1:B:377:TRP:HH2	2.24	0.51
1:E:103:THR:CG2	1:E:105:ASN:H	2.19	0.50
1:F:198:THR:HG23	3:F:924:HOH:O	2.09	0.50
1:A:166:PRO:HG3	1:A:316:GLY:O	2.11	0.50
1:F:103:THR:HG23	1:F:105:ASN:H	1.76	0.50
1:B:501:THR:HG23	1:D:307:GLY:O	2.10	0.50
1:D:262:GLN:HG3	1:D:355:PHE:CD2	2.45	0.50
1:F:272:LYS:HD2	1:F:277:GLY:HA3	1.93	0.50
1:B:519:THR:HG23	3:B:783:HOH:O	2.11	0.50
1:B:492:GLU:OE1	1:B:513:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:619:ARG:HG2	1:A:624:TYR:CZ	2.45	0.50
1:B:36:ASP:OD1	1:B:668:VAL:HG12	2.12	0.50
1:A:140:THR:HB	1:A:155:LEU:HD22	1.93	0.50
1:A:77:ALA:HB3	1:A:78:PRO:HD3	1.94	0.50
1:F:272:LYS:HD2	1:F:277:GLY:CA	2.41	0.50
1:C:296:ASN:HB3	1:C:328:THR:HG21	1.94	0.49
1:E:34:THR:HG21	1:E:43:LEU:HD21	1.94	0.49
1:C:639:LEU:HD22	1:C:641:TYR:OH	2.13	0.49
1:E:249:ARG:HD3	3:E:883:HOH:O	2.11	0.49
1:B:34:THR:HG21	1:B:43:LEU:HD21	1.95	0.49
1:A:144:GLU:HB2	1:A:408:GLY:HA3	1.93	0.49
1:B:228:TYR:O	1:B:233:GLY:HA2	2.12	0.49
1:F:116:MET:CG	1:F:182:MET:SD	2.97	0.49
1:A:161:ARG:O	1:A:313:PRO:HG3	2.12	0.49
1:C:493:TRP:CZ3	1:C:512:VAL:HB	2.47	0.49
1:E:294:LEU:HG	1:E:324:MET:HE1	1.93	0.49
1:E:77:ALA:HB3	1:E:78:PRO:CD	2.43	0.49
1:E:159:THR:HG23	1:E:160:VAL:HG23	1.94	0.49
1:B:210:GLU:HG2	3:B:879:HOH:O	2.11	0.49
1:A:99:TYR:O	1:A:103:THR:HB	2.12	0.49
1:F:310:ASP:HA	1:F:410:TYR:HB3	1.95	0.49
1:D:574:THR:CG2	1:D:641:TYR:H	2.25	0.49
1:B:324:MET:HE1	1:B:377:TRP:HH2	1.78	0.49
1:A:172:VAL:HA	1:A:176:GLY:O	2.13	0.48
1:F:133:TYR:OH	1:F:138:PRO:HB3	2.13	0.48
1:D:493:TRP:CZ3	1:D:512:VAL:HB	2.48	0.48
1:A:493:TRP:CZ3	1:A:512:VAL:HB	2.49	0.48
1:E:307:GLY:O	1:F:501:THR:HG22	2.13	0.48
1:B:144:GLU:HB2	1:B:408:GLY:HA3	1.95	0.48
1:A:665:THR:HG22	3:A:811:HOH:O	2.13	0.48
1:C:426:VAL:HG23	1:C:429:PRO:HG3	1.95	0.48
1:F:36:ASP:OD1	1:F:668:VAL:HG13	2.14	0.48
1:A:76:GLU:O	1:A:77:ALA:C	2.51	0.48
1:F:294:LEU:HG	1:F:324:MET:HE1	1.95	0.48
1:E:89:PHE:HE2	1:E:115:VAL:HG12	1.77	0.48
1:A:165:ASP:OD2	1:A:168:HIS:HB2	2.14	0.48
1:C:30:THR:O	1:C:565:TYR:HB3	2.13	0.48
1:F:519:THR:HG21	1:F:564:PHE:CZ	2.48	0.48
1:D:77:ALA:HB3	1:D:78:PRO:HD3	1.94	0.48
1:B:294:LEU:HB3	1:B:377:TRP:HZ2	1.79	0.48
1:B:105:ASN:ND2	1:B:107:SER:H	2.12	0.48
1:F:314:ALA:HB1	1:F:318:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:519:THR:HG22	3:E:814:HOH:O	2.15	0.47
1:A:329:ALA:HB3	1:A:342:ILE:HD11	1.96	0.47
1:D:103:THR:HG22	1:D:105:ASN:N	2.29	0.47
1:B:463:LYS:O	1:B:467:LYS:HG2	2.14	0.47
1:C:63:GLU:HG3	1:C:65:ILE:CD1	2.44	0.47
1:B:266:TRP:HB3	1:B:270:TRP:CZ3	2.49	0.47
1:D:76:GLU:O	1:D:78:PRO:O	2.33	0.47
1:E:133:TYR:OH	1:E:138:PRO:HB3	2.14	0.47
1:B:473:VAL:HG11	1:B:527:LEU:HD11	1.96	0.47
1:F:321:HIS:HB2	1:F:423:MET:HE1	1.96	0.47
1:F:296:ASN:HB3	1:F:328:THR:HG21	1.97	0.47
1:F:519:THR:CG2	1:F:519:THR:O	2.62	0.47
1:F:151:TYR:HA	1:F:152:PRO:C	2.36	0.47
1:A:136:ASN:HB3	3:A:844:HOH:O	2.14	0.47
1:E:254:PRO:CB	1:E:324:MET:CE	2.92	0.46
1:E:162:VAL:HG13	1:E:302:TYR:O	2.14	0.46
1:B:37:GLY:HA2	1:B:665:THR:HG23	1.97	0.46
1:D:294:LEU:HG	1:D:324:MET:HE1	1.97	0.46
1:E:166:PRO:HG3	1:E:316:GLY:O	2.16	0.46
1:D:574:THR:CG2	1:D:641:TYR:HB2	2.45	0.46
1:A:547:THR:HG23	3:A:831:HOH:O	2.16	0.46
1:F:120:ILE:HG21	1:F:182:MET:SD	2.55	0.46
1:C:272:LYS:HD2	1:F:365:ASP:OD1	2.16	0.46
1:C:37:GLY:HA2	1:C:665:THR:CG2	2.45	0.46
1:B:123:ASP:OD2	1:B:125:THR:HB	2.16	0.46
1:A:37:GLY:CA	1:A:665:THR:HG23	2.46	0.46
3:C:769:HOH:O	1:F:272:LYS:HE2	2.15	0.46
1:D:211:GLN:HG3	3:D:815:HOH:O	2.14	0.46
1:E:196:THR:HG22	1:E:199:ARG:HE	1.81	0.46
1:B:305:LYS:HB2	1:B:308:ALA:HB2	1.98	0.46
1:B:439:TRP:CZ2	1:B:441:GLY:HA3	2.51	0.46
1:E:329:ALA:HB3	1:E:342:ILE:CG1	2.46	0.46
1:E:385:LEU:HD22	1:E:462:VAL:HG21	1.98	0.46
1:D:138:PRO:HD2	1:D:162:VAL:HG12	1.97	0.45
1:E:184:TRP:CZ2	1:E:185:LEU:HD22	2.50	0.45
1:E:204:ASN:HB2	3:E:740:HOH:O	2.16	0.45
1:B:455:LEU:HD22	1:B:540:ARG:NH1	2.31	0.45
1:A:501:THR:HG22	1:A:501:THR:O	2.16	0.45
1:A:455:LEU:HD22	1:A:540:ARG:NH1	2.31	0.45
1:D:603:ASP:OD2	1:D:616:THR:HB	2.16	0.45
1:A:207:GLN:HG3	1:A:220:HIS:CE1	2.51	0.45
1:F:228:TYR:O	1:F:233:GLY:HA2	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:268:ASN:HD21	1:C:272:LYS:NZ	2.11	0.45
1:D:519:THR:O	1:D:519:THR:HG23	2.17	0.45
1:D:123:ASP:OD2	1:D:125:THR:HB	2.17	0.45
1:C:166:PRO:HG3	1:C:316:GLY:O	2.16	0.45
1:B:385:LEU:HD22	1:B:462:VAL:HG21	1.98	0.45
1:E:493:TRP:CZ3	1:E:512:VAL:HB	2.52	0.45
1:E:307:GLY:CA	1:F:501:THR:HG23	2.47	0.45
1:B:167:VAL:HG23	1:B:295:ARG:NH1	2.31	0.45
1:E:65:ILE:HD11	1:E:119:TRP:CG	2.52	0.45
1:A:602:GLY:O	1:A:603:ASP:C	2.55	0.45
1:E:294:LEU:HB3	1:E:377:TRP:HZ2	1.81	0.45
1:D:84:THR:HG22	1:D:186:MET:HB3	1.99	0.45
1:D:450:VAL:HG12	1:D:466:ILE:HD11	1.99	0.45
1:F:73:LEU:HD12	1:F:73:LEU:C	2.37	0.45
1:F:519:THR:CG2	1:F:564:PHE:CZ	3.00	0.45
1:C:228:TYR:O	1:C:233:GLY:HA2	2.17	0.44
1:A:85:THR:HA	1:A:184:TRP:O	2.16	0.44
1:C:585:PHE:CZ	1:C:628:TYR:HD1	2.34	0.44
1:A:151:TYR:HA	1:A:152:PRO:C	2.38	0.44
1:B:37:GLY:CA	1:B:665:THR:HG23	2.47	0.44
1:E:254:PRO:HB2	1:E:324:MET:HE3	1.98	0.44
1:C:153:SER:O	1:C:239:THR:HA	2.17	0.44
1:F:329:ALA:HB3	1:F:342:ILE:HG12	1.99	0.44
1:C:198:THR:O	1:C:198:THR:CG2	2.66	0.44
1:F:639:LEU:HD22	1:F:641:TYR:OH	2.17	0.44
1:B:326:TRP:CG	1:B:430:VAL:HG21	2.53	0.44
1:A:198:THR:HG23	1:A:198:THR:O	2.18	0.44
1:A:138:PRO:HD2	1:A:162:VAL:HG11	1.99	0.44
1:A:89:PHE:CE2	1:A:115:VAL:HG12	2.52	0.44
1:C:73:LEU:HD13	1:C:584:PHE:CZ	2.52	0.44
1:B:294:LEU:HG	1:B:324:MET:HE3	1.98	0.44
1:C:198:THR:CG2	3:C:876:HOH:O	2.65	0.44
1:B:433:ASP:HA	1:B:434:PRO:HA	1.87	0.44
1:C:326:TRP:CD2	1:C:430:VAL:HG21	2.53	0.44
1:C:60:SER:HA	1:C:61:PRO:HD3	1.88	0.44
1:B:37:GLY:CA	1:B:665:THR:CG2	2.94	0.44
1:F:37:GLY:CA	1:F:665:THR:HG23	2.46	0.44
1:E:501:THR:OG1	1:F:422:GLY:HA2	2.18	0.43
1:D:519:THR:HG22	3:D:999:HOH:O	2.16	0.43
1:C:128:PRO:HD2	1:C:248:TRP:NE1	2.33	0.43
1:C:105:ASN:HD22	1:C:106:TRP:N	2.16	0.43
1:A:77:ALA:HB3	1:A:78:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:141:TYR:CZ	1:C:311:LYS:HE3	2.53	0.43
1:E:37:GLY:CA	1:E:665:THR:HG23	2.49	0.43
1:C:163:GLY:HA3	1:C:303:PHE:O	2.19	0.43
1:A:363:GLN:NE2	1:D:364:SER:H	2.15	0.43
1:B:482:ASP:OD1	1:B:482:ASP:C	2.57	0.43
1:D:519:THR:CG2	1:D:519:THR:O	2.66	0.43
1:A:521:LEU:HD21	1:A:564:PHE:CD1	2.54	0.43
1:D:328:THR:HG23	1:D:342:ILE:O	2.19	0.43
1:A:325:ALA:HB1	1:A:344:CYS:HB3	2.01	0.43
1:F:149:SER:HA	1:F:590:TYR:CE2	2.54	0.42
1:D:32:ALA:HB2	1:D:565:TYR:HB2	2.00	0.42
1:E:639:LEU:HD22	1:E:641:TYR:OH	2.20	0.42
1:E:294:LEU:HG	1:E:324:MET:CE	2.49	0.42
1:C:124:SER:CB	1:C:178:ASN:ND2	2.82	0.42
1:F:462:VAL:HG12	1:F:466:ILE:HD12	2.00	0.42
1:D:89:PHE:HE2	1:D:115:VAL:HG12	1.85	0.42
1:A:99:TYR:CE2	1:A:103:THR:HG21	2.54	0.42
1:C:254:PRO:HB2	1:C:324:MET:HE2	2.01	0.42
1:E:90:SER:HB2	1:E:259:ARG:HB3	2.02	0.42
1:C:194:PHE:CD1	1:C:221:PRO:HD3	2.54	0.42
1:B:501:THR:HG22	1:D:307:GLY:O	2.18	0.42
1:F:519:THR:CG2	3:F:715:HOH:O	2.55	0.42
1:C:439:TRP:CE2	1:C:441:GLY:HA3	2.55	0.42
1:F:129:GLY:O	1:F:132:SER:HB2	2.20	0.42
1:C:276:LYS:HA	3:C:720:HOH:O	2.20	0.42
1:F:278:SER:CA	3:F:1061:HOH:O	2.67	0.42
1:F:501:THR:HB	3:F:708:HOH:O	2.20	0.42
1:D:163:GLY:HA3	1:D:303:PHE:O	2.18	0.42
1:C:519:THR:HG23	3:C:877:HOH:O	2.20	0.42
1:A:574:THR:CG2	1:A:576:GLU:OE1	2.48	0.41
1:A:60:SER:HA	1:A:61:PRO:HD3	1.96	0.41
1:E:198:THR:O	1:E:198:THR:CG2	2.69	0.41
1:D:470:VAL:O	1:D:474:MET:HG2	2.20	0.41
1:B:314:ALA:HB3	1:B:319:SER:HB3	2.01	0.41
1:A:220:HIS:HB2	1:A:221:PRO:HD2	2.01	0.41
1:C:390:TRP:CD1	1:C:500:TRP:HB2	2.56	0.41
1:F:85:THR:HA	1:F:184:TRP:O	2.20	0.41
1:A:76:GLU:C	1:A:214:THR:HG21	2.40	0.41
1:D:639:LEU:HD22	1:D:641:TYR:OH	2.21	0.41
1:F:665:THR:HG21	3:F:948:HOH:O	2.21	0.41
1:A:473:VAL:CG1	1:A:527:LEU:HD11	2.51	0.41
1:C:626:ILE:HG13	3:C:890:HOH:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:292:ASP:O	1:E:295:ARG:HD3	2.20	0.41
1:A:138:PRO:HD2	1:A:162:VAL:CG1	2.51	0.41
1:F:103:THR:HG22	1:F:105:ASN:H	1.85	0.41
1:A:501:THR:CG2	1:A:501:THR:O	2.68	0.41
1:C:248:TRP:CZ3	1:C:331:GLY:HA2	2.56	0.41
1:D:301:LYS:HE3	1:D:342:ILE:HD12	2.02	0.41
1:D:402:ALA:HA	1:D:424:ALA:O	2.21	0.41
1:E:228:TYR:O	1:E:233:GLY:HA2	2.21	0.41
1:B:29:PRO:HB3	1:B:564:PHE:HA	2.02	0.41
1:E:547:THR:HG23	1:E:550:ARG:NH2	2.36	0.41
1:E:321:HIS:HB2	1:E:423:MET:HE1	2.02	0.41
1:D:198:THR:CB	3:D:834:HOH:O	2.60	0.41
1:C:151:TYR:HA	1:C:152:PRO:C	2.41	0.41
1:F:402:ALA:HA	1:F:424:ALA:O	2.21	0.41
1:F:159:THR:HG22	1:F:160:VAL:HG23	2.03	0.41
1:A:34:THR:HG21	1:A:43:LEU:HD21	2.03	0.40
1:F:603:ASP:OD2	1:F:616:THR:HB	2.22	0.40
1:C:194:PHE:CE1	1:C:221:PRO:HD3	2.56	0.40
1:C:168:HIS:O	1:C:172:VAL:HG23	2.21	0.40
1:C:325:ALA:HB1	1:C:344:CYS:HB3	2.03	0.40
1:D:85:THR:HA	1:D:184:TRP:O	2.21	0.40
1:F:144:GLU:HB2	1:F:408:GLY:HA3	2.04	0.40
1:C:184:TRP:CE2	1:C:185:LEU:HB2	2.56	0.40
1:C:268:ASN:ND2	1:C:272:LYS:HZ2	2.14	0.40
1:B:36:ASP:OD1	1:B:668:VAL:CG1	2.70	0.40
1:B:462:VAL:HG12	1:B:466:ILE:HD12	2.03	0.40
1:C:433:ASP:HA	1:C:434:PRO:HA	1.91	0.40
1:C:501:THR:O	1:C:501:THR:CG2	2.69	0.40
1:E:278:SER:HB3	3:E:957:HOH:O	2.22	0.40

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%)	30 (5%)	3 (0%)	38	53
1	B	640/678 (94%)	623 (97%)	17 (3%)	0	100	100
1	C	640/678 (94%)	618 (97%)	22 (3%)	0	100	100
1	D	640/678 (94%)	622 (97%)	16 (2%)	2 (0%)	50	68
1	E	640/678 (94%)	623 (97%)	16 (2%)	1 (0%)	56	74
1	F	640/678 (94%)	623 (97%)	16 (2%)	1 (0%)	56	74
All	All	3840/4068 (94%)	3716 (97%)	117 (3%)	7 (0%)	56	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
1	A	335	GLY
1	E	77	ALA
1	A	600	PRO
1	D	278	SER
1	F	76	GLU
1	D	77	ALA

### 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%)	480 (94%)	32 (6%)	25	38
1	B	519/556 (93%)	494 (95%)	25 (5%)	35	53
1	C	513/556 (92%)	481 (94%)	32 (6%)	26	39
1	D	521/556 (94%)	491 (94%)	30 (6%)	28	43
1	E	518/556 (93%)	494 (95%)	24 (5%)	37	55
1	F	520/556 (94%)	495 (95%)	25 (5%)	35	53
All	All	3103/3336 (93%)	2935 (95%)	168 (5%)	31	47

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	73	LEU
1	A	103	THR
1	A	124	SER
1	A	131	SER
1	A	137	SER
1	A	158	ASP
1	A	159	THR
1	A	167	VAL
1	A	179	MET
1	A	198	THR
1	A	207	GLN
1	A	214	THR
1	A	252	ASN
1	A	294	LEU
1	A	310	ASP
1	A	315	THR
1	A	369	LYS
1	A	381	TYR
1	A	418	SER
1	A	455	LEU
1	A	460	SER
1	A	491	LEU
1	A	513	ARG
1	A	547	THR
1	A	574	THR
1	A	584	PHE
1	A	616	THR
1	A	618	TYR
1	A	657	LEU
1	A	665	THR
1	A	668	VAL
1	B	30	THR
1	B	47	LEU
1	B	73	LEU
1	B	162	VAL
1	B	179	MET
1	B	196	THR
1	B	198	THR
1	B	207	GLN
1	B	214	THR
1	B	294	LEU
1	B	328	THR

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Mol	Chain	Res	Type
1	B	337	SER
1	B	381	TYR
1	B	455	LEU
1	B	462	VAL
1	B	473	VAL
1	B	491	LEU
1	B	501	THR
1	B	547	THR
1	B	574	THR
1	B	618	TYR
1	B	649	ASP
1	B	657	LEU
1	B	665	THR
1	B	668	VAL
1	C	47	LEU
1	C	73	LEU
1	C	103	THR
1	C	105	ASN
1	C	179	MET
1	C	198	THR
1	C	207	GLN
1	C	239	THR
1	C	252	ASN
1	C	285	SER
1	C	294	LEU
1	C	310	ASP
1	C	349	PHE
1	C	381	TYR
1	C	418	SER
1	C	455	LEU
1	C	462	VAL
1	C	463	LYS
1	C	473	VAL
1	C	489	SER
1	C	491	LEU
1	C	501	THR
1	C	519	THR
1	C	544	LYS
1	C	547	THR
1	C	574	THR
1	C	616	THR
1	C	618	TYR

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Mol	Chain	Res	Type
1	C	627	VAL
1	C	657	LEU
1	C	665	THR
1	C	668	VAL
1	D	47	LEU
1	D	63	GLU
1	D	73	LEU
1	D	105	ASN
1	D	124	SER
1	D	167	VAL
1	D	173	SER
1	D	179	MET
1	D	196	THR
1	D	198	THR
1	D	199	ARG
1	D	249	ARG
1	D	252	ASN
1	D	278	SER
1	D	294	LEU
1	D	349	PHE
1	D	381	TYR
1	D	455	LEU
1	D	462	VAL
1	D	489	SER
1	D	491	LEU
1	D	501	THR
1	D	519	THR
1	D	544	LYS
1	D	547	THR
1	D	616	THR
1	D	618	TYR
1	D	649	ASP
1	D	657	LEU
1	D	665	THR
1	E	47	LEU
1	E	63	GLU
1	E	73	LEU
1	E	103	THR
1	E	167	VAL
1	E	179	MET
1	E	198	THR
1	E	207	GLN

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Mol	Chain	Res	Type
1	E	210	GLU
1	E	294	LEU
1	E	381	TYR
1	E	455	LEU
1	E	462	VAL
1	E	473	VAL
1	E	491	LEU
1	E	501	THR
1	E	519	THR
1	E	566	CYS
1	E	616	THR
1	E	618	TYR
1	E	623	TYR
1	E	627	VAL
1	E	657	LEU
1	E	665	THR
1	F	47	LEU
1	F	73	LEU
1	F	103	THR
1	F	124	SER
1	F	132	SER
1	F	159	THR
1	F	167	VAL
1	F	198	THR
1	F	239	THR
1	F	294	LEU
1	F	381	TYR
1	F	455	LEU
1	F	462	VAL
1	F	491	LEU
1	F	501	THR
1	F	519	THR
1	F	547	THR
1	F	574	THR
1	F	616	THR
1	F	618	TYR
1	F	627	VAL
1	F	649	ASP
1	F	657	LEU
1	F	665	THR
1	F	668	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	105	ASN
1	A	178	ASN
1	A	207	GLN
1	A	268	ASN
1	A	363	GLN
1	B	105	ASN
1	B	178	ASN
1	B	207	GLN
1	B	509	ASN
1	C	101	ASN
1	C	105	ASN
1	C	178	ASN
1	C	207	GLN
1	C	268	ASN
1	C	363	GLN
1	D	101	ASN
1	D	105	ASN
1	D	309	GLN
1	D	363	GLN
1	D	509	ASN
1	E	101	ASN
1	E	309	GLN
1	E	509	ASN
1	E	640	ASN
1	F	101	ASN
1	F	268	ASN
1	F	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 ⓘ

12 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	0.74	0	11,15,17	0.97	1 (9%)
2	BGC	A	680	2	10,11,12	0.67	0	11,15,17	0.79	1 (9%)
2	BGC	B	679	2	10,11,12	0.65	0	11,15,17	1.02	1 (9%)
2	BGC	B	680	2	10,11,12	0.82	1 (10%)	11,15,17	0.90	0
2	BGC	C	679	2	10,11,12	0.87	0	11,15,17	1.49	2 (18%)
2	BGC	C	680	2	10,11,12	0.85	1 (10%)	11,15,17	0.89	0
2	BGC	D	679	2	10,11,12	0.82	0	11,15,17	1.36	2 (18%)
2	BGC	D	680	2	10,11,12	0.77	0	11,15,17	0.76	0
2	BGC	E	679	2	10,11,12	0.88	1 (10%)	11,15,17	1.20	1 (9%)
2	BGC	E	680	2	10,11,12	0.82	0	11,15,17	1.19	2 (18%)
2	BGC	F	679	2	10,11,12	0.83	0	11,15,17	1.02	1 (9%)
2	BGC	F	680	2	10,11,12	0.79	0	11,15,17	0.65	0

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
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
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
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
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
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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	680	BGC	O5-C5	-2.05	1.41	1.45
2	E	679	BGC	O5-C5	-2.01	1.41	1.45
2	C	680	BGC	O5-C5	-2.00	1.41	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	679	BGC	O5-C5-C6	3.53	110.68	106.98
2	E	679	BGC	O5-C5-C6	3.38	110.52	106.98
2	D	679	BGC	O5-C5-C6	3.26	110.40	106.98
2	C	679	BGC	C4-C3-C2	2.86	114.34	110.50
2	E	680	BGC	O5-C5-C6	2.76	109.88	106.98
2	F	679	BGC	O5-C5-C6	2.74	109.86	106.98
2	A	679	BGC	O5-C5-C6	2.50	109.61	106.98
2	B	679	BGC	O5-C5-C6	2.28	109.37	106.98
2	E	680	BGC	O5-C5-C4	-2.16	107.92	110.65
2	A	680	BGC	O5-C5-C4	-2.06	108.04	110.65
2	D	679	BGC	C4-C3-C2	-2.04	107.77	110.50

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, 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%)	-0.19	15 (2%) 57 55	23, 40, 65, 73	0
1	B	642/678 (94%)	-0.43	10 (1%) 68 67	23, 37, 55, 69	0
1	C	642/678 (94%)	-0.36	12 (1%) 64 61	20, 37, 63, 73	0
1	D	642/678 (94%)	-0.51	6 (0%) 81 81	20, 31, 47, 55	0
1	E	642/678 (94%)	-0.65	4 (0%) 86 86	18, 29, 43, 56	0
1	F	642/678 (94%)	-0.77	2 (0%) 91 92	17, 26, 38, 53	0
All	All	3852/4068 (94%)	-0.49	49 (1%) 74 73	17, 32, 58, 73	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	336	ALA	5.5
1	A	336	ALA	4.7
1	A	335	GLY	3.5
1	A	415	ALA	3.4
1	D	567	SER	3.2
1	B	594	GLY	3.2
1	C	125	THR	3.0
1	B	567	SER	2.9
1	E	335	GLY	2.9
1	A	315	THR	2.9
1	A	608	GLY	2.9
1	E	567	SER	2.8
1	B	315	THR	2.7
1	C	335	GLY	2.7
1	D	544	LYS	2.7
1	A	159	THR	2.6
1	B	242	ARG	2.6
1	B	158	ASP	2.6
1	B	633	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	150	TYR	2.5
1	A	199	ARG	2.5
1	D	543	GLY	2.5
1	D	37	GLY	2.4
1	C	199	ARG	2.4
1	B	335	GLY	2.4
1	C	315	THR	2.3
1	B	481	ASP	2.3
1	C	231	PRO	2.3
1	C	159	THR	2.3
1	A	125	THR	2.3
1	C	161	ARG	2.2
1	F	182	MET	2.2
1	D	623	TYR	2.2
1	A	196	THR	2.2
1	A	334	ILE	2.2
1	B	620	GLN	2.2
1	C	625	ASP	2.1
1	A	241	ASP	2.1
1	C	633	ARG	2.1
1	E	434	PRO	2.1
1	A	594	GLY	2.1
1	D	30	THR	2.1
1	E	242	ARG	2.1
1	C	623	TYR	2.0
1	A	337	SER	2.0
1	F	633	ARG	2.0
1	B	159	THR	2.0
1	C	123	ASP	2.0
1	A	197	GLY	2.0

## 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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	B	679	11/12	0.12	1.08	38,38,41,41	0
2	BGC	E	679	11/12	0.11	1.06	26,29,34,34	0
2	BGC	F	679	11/12	0.10	0.98	28,31,36,37	0
2	BGC	C	679	11/12	0.11	0.64	30,36,39,40	0
2	BGC	D	679	11/12	0.12	0.33	35,37,43,44	0
2	BGC	A	679	11/12	0.11	-0.09	34,35,37,37	0
2	BGC	A	680	11/12	0.10	-0.20	33,34,35,35	0
2	BGC	F	680	11/12	0.07	-0.40	24,27,29,30	0
2	BGC	E	680	11/12	0.07	-0.52	24,25,26,27	0
2	BGC	C	680	11/12	0.08	-0.77	31,32,33,35	0
2	BGC	D	680	11/12	0.07	-1.09	30,31,32,33	0
2	BGC	B	680	11/12	0.06	-1.96	31,33,34,35	0

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.