Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:37 PM 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 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:

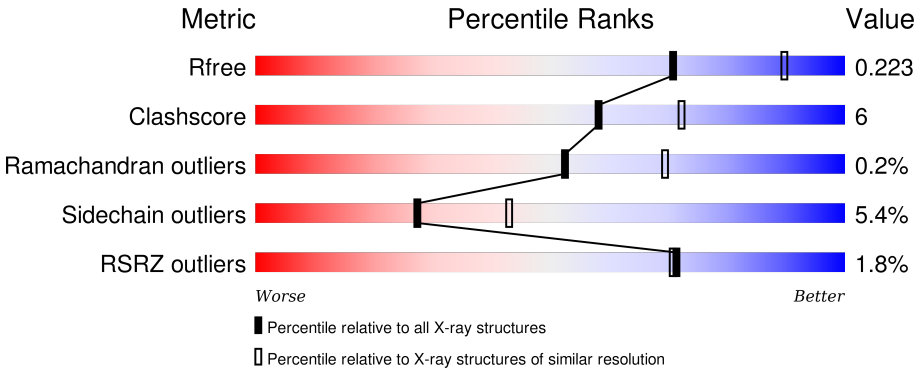
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 >=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	678	3% 78% 15% • 5%
1	B	678	2% 81% 11% • 5%
1	C	678	3% 78% 15% • 5%
1	D	678	% 81% 12% • 5%
1	E	678	% 81% 12% • 5%

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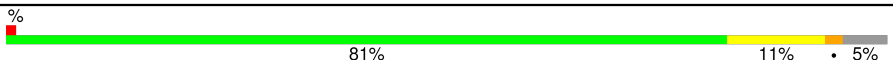
Mol	Chain	Length	Quality of chain
1	F	678	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32457 atoms, of which 0 are 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 water.

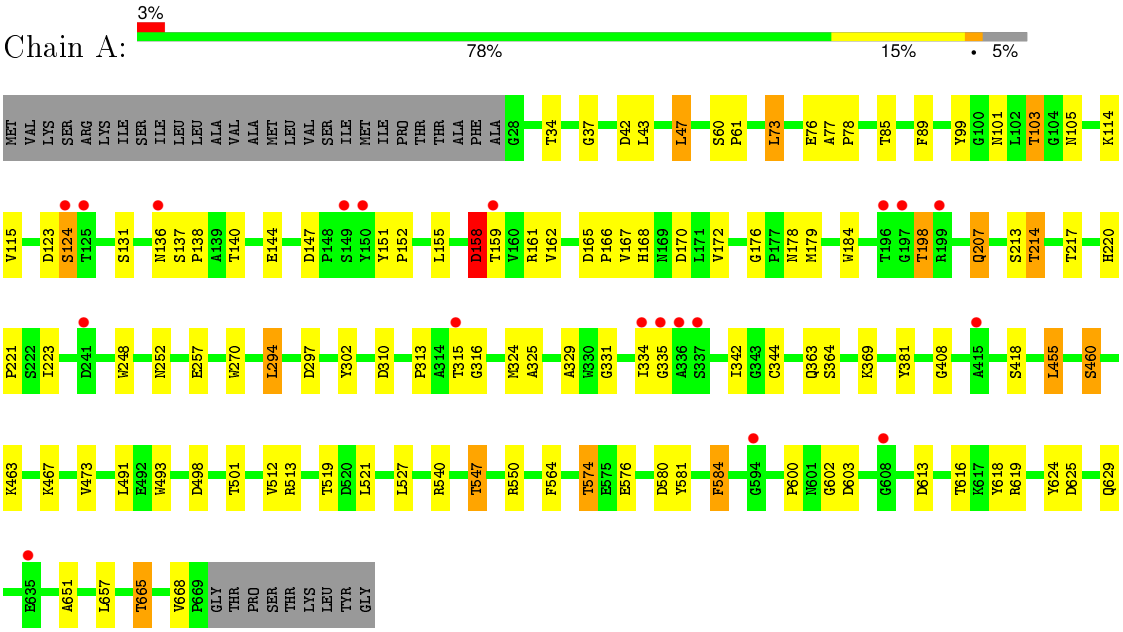
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	169	Total O 169 169	0	0
3	B	204	Total O 204 204	0	0
3	C	214	Total O 214 214	0	0
3	D	326	Total O 326 326	0	0
3	E	286	Total O 286 286	0	0
3	F	396	Total O 396 396	0	0

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.

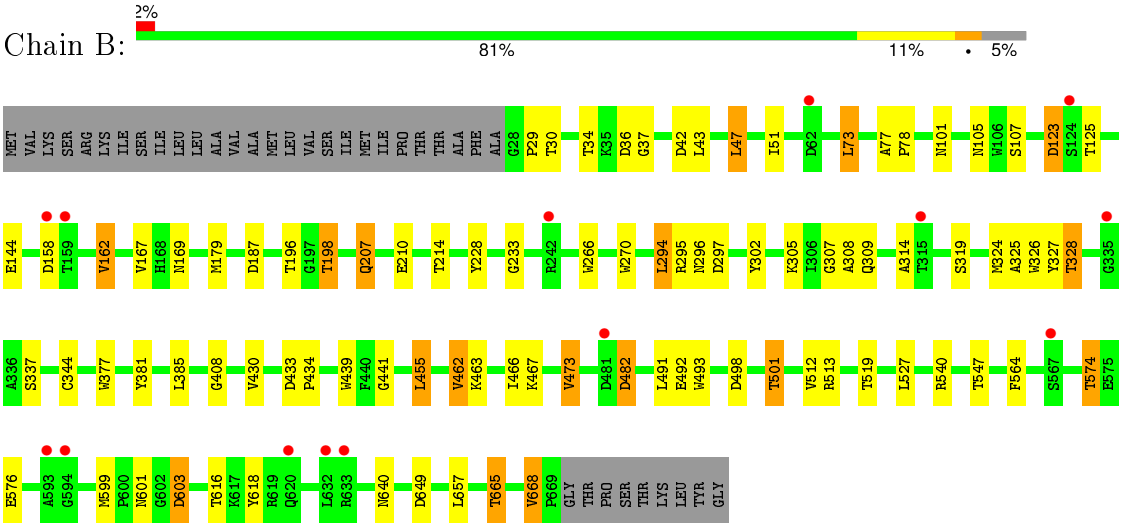
- Molecule 1: cellobiohydrolase

Chain A:



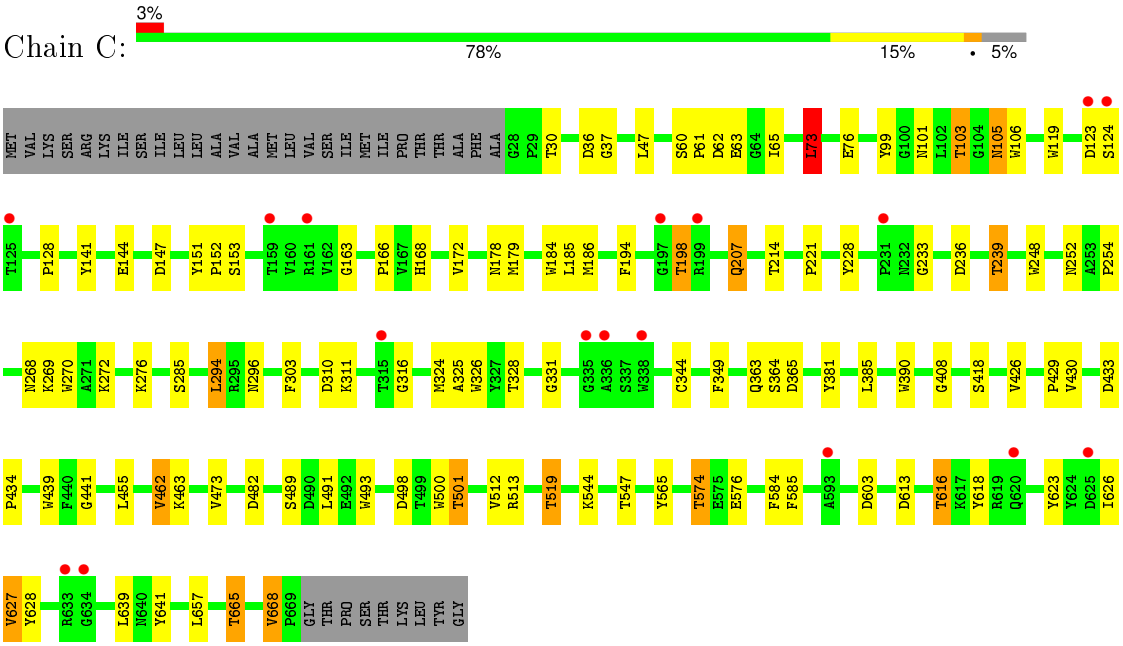
- Molecule 1: cellobiohydrolase

Chain B:



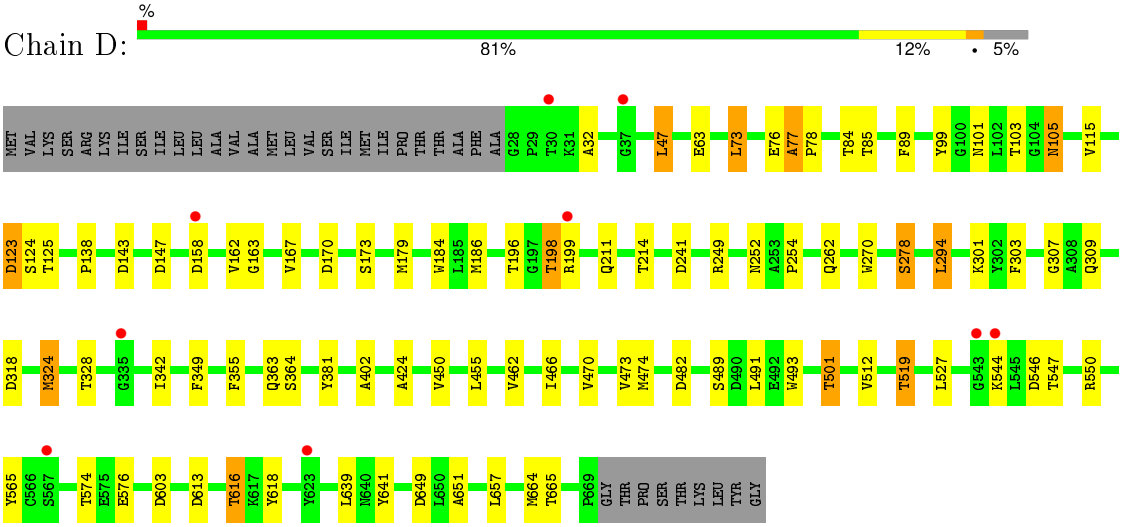
- Molecule 1: cellobiohydrolase

Chain C:



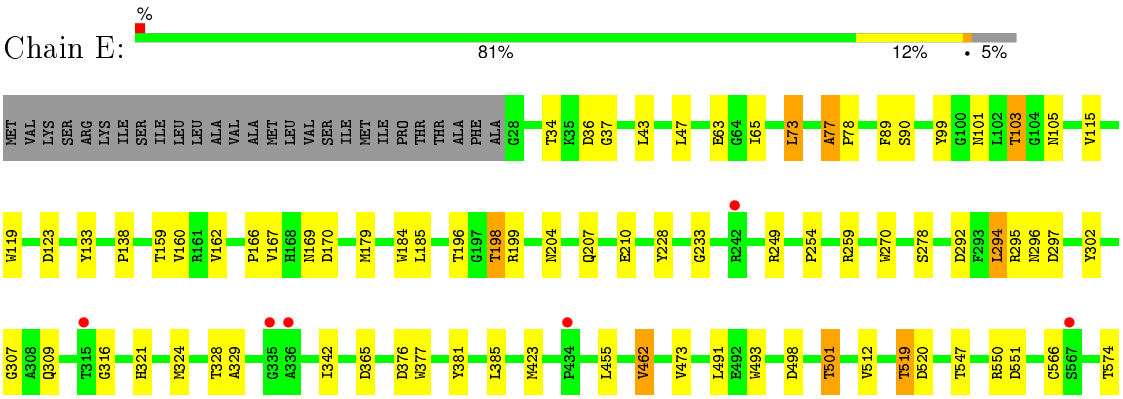
• Molecule 1: cellobiohydrolase

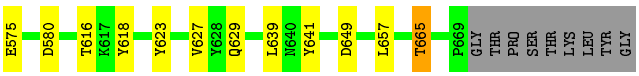
Chain D:



• Molecule 1: cellobiohydrolase

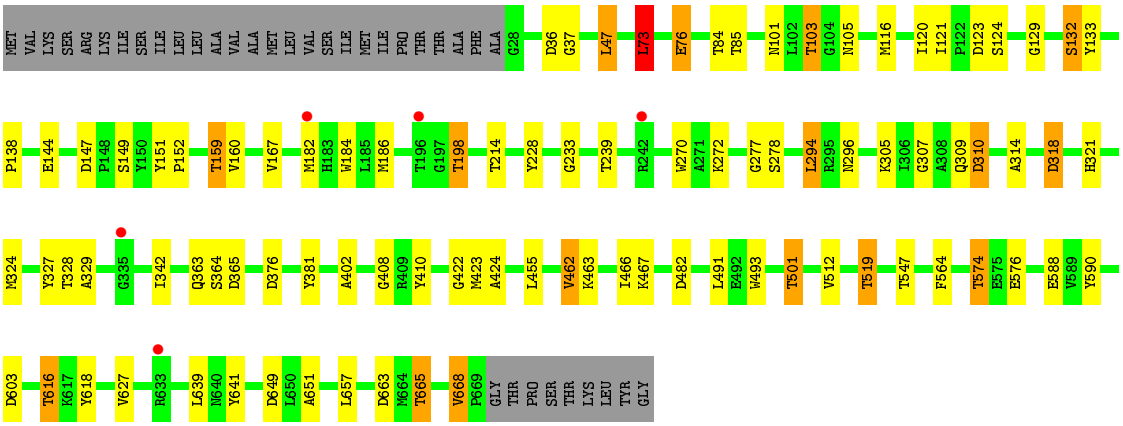
Chain E:





- Molecule 1: cellobiohydrolase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.53 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.189 , 0.224 0.188 , 0.223	Depositor DCC
R_{free} test set	12676 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 34.6	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	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^2)	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.*

[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

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 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	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
2	E	22	0	19	0	0
2	F	22	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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.

All (350) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLU:HB3	1:A:294:LEU:HD21	1.81	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	34 48
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%)	46 63
1	E	640/678 (94%)	623 (97%)	16 (2%)	1 (0%)	52 69
1	F	640/678 (94%)	623 (97%)	16 (2%)	1 (0%)	52 69
All	All	3840/4068 (94%)	3716 (97%)	117 (3%)	7 (0%)	52 69

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%)	22 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	519/556 (93%)	494 (95%)	25 (5%)	31 49
1	C	513/556 (92%)	481 (94%)	32 (6%)	23 35
1	D	521/556 (94%)	491 (94%)	30 (6%)	25 39
1	E	518/556 (93%)	494 (95%)	24 (5%)	33 51
1	F	520/556 (94%)	495 (95%)	25 (5%)	31 49
All	All	3103/3336 (93%)	2935 (95%)	168 (5%)	27 43

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

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Mol	Chain	Res	Type
1	F	268	ASN
1	F	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

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	11,11,12	0.64	0	14,15,17	1.35	2 (14%)
2	BGC	A	680	2	11,11,12	0.49	0	14,15,17	0.85	1 (7%)
2	BGC	B	679	2	11,11,12	0.45	0	14,15,17	1.27	2 (14%)
2	BGC	B	680	2	11,11,12	0.58	0	14,15,17	0.84	0
2	BGC	C	679	2	11,11,12	0.82	0	14,15,17	1.29	1 (7%)
2	BGC	C	680	2	11,11,12	0.67	0	14,15,17	0.95	1 (7%)
2	BGC	D	679	2	11,11,12	0.74	0	14,15,17	1.94	2 (14%)
2	BGC	D	680	2	11,11,12	0.74	0	14,15,17	1.16	1 (7%)
2	BGC	E	679	2	11,11,12	0.75	0	14,15,17	1.18	1 (7%)
2	BGC	E	680	2	11,11,12	0.73	0	14,15,17	1.15	1 (7%)
2	BGC	F	679	2	11,11,12	0.71	0	14,15,17	1.56	1 (7%)
2	BGC	F	680	2	11,11,12	0.68	0	14,15,17	0.71	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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	679	BGC	O5-C1-C2	-5.85	101.37	110.86
2	F	679	BGC	O5-C1-C2	-4.93	102.87	110.86
2	E	679	BGC	O5-C1-C2	-3.78	104.72	110.86
2	A	679	BGC	O5-C1-C2	-3.69	104.87	110.86
2	C	679	BGC	O5-C1-C2	-3.43	105.29	110.86
2	B	679	BGC	O5-C1-C2	-3.02	105.96	110.86
2	D	679	BGC	O2-C2-C1	2.04	113.30	109.21
2	C	680	BGC	C1-O5-C5	2.23	115.07	112.25
2	A	679	BGC	C1-O5-C5	2.24	115.09	112.25
2	A	680	BGC	C1-O5-C5	2.59	115.54	112.25
2	B	679	BGC	C1-O5-C5	2.63	115.58	112.25
2	E	680	BGC	C1-O5-C5	3.16	116.25	112.25
2	D	680	BGC	C1-O5-C5	3.79	117.06	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{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	642/678 (94%)	-0.18	19 (2%)	54	53	23, 40, 65, 73	0
1	B	642/678 (94%)	-0.43	14 (2%)	65	64	23, 37, 55, 69	0
1	C	642/678 (94%)	-0.36	17 (2%)	59	58	20, 37, 63, 73	0
1	D	642/678 (94%)	-0.53	9 (1%)	78	77	20, 31, 47, 55	0
1	E	642/678 (94%)	-0.67	6 (0%)	85	85	18, 29, 43, 56	0
1	F	642/678 (94%)	-0.79	5 (0%)	87	87	17, 26, 38, 53	0
All	All	3852/4068 (94%)	-0.49	70 (1%)	71	71	17, 32, 58, 73	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	336	ALA	6.1
1	A	336	ALA	5.0
1	A	335	GLY	4.2
1	D	567	SER	3.6
1	A	415	ALA	3.6
1	C	125	THR	3.4
1	A	315	THR	3.3
1	B	594	GLY	3.3
1	E	335	GLY	3.3
1	E	567	SER	3.2
1	D	543	GLY	3.0
1	B	242	ARG	3.0
1	B	633	ARG	3.0
1	B	567	SER	3.0
1	A	608	GLY	2.9
1	A	159	THR	2.9
1	C	199	ARG	2.9
1	B	315	THR	2.9
1	D	544	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	335	GLY	2.8
1	A	196	THR	2.8
1	B	158	ASP	2.8
1	C	231	PRO	2.7
1	C	161	ARG	2.7
1	C	315	THR	2.7
1	A	124	SER	2.7
1	C	159	THR	2.6
1	A	125	THR	2.6
1	B	481	ASP	2.5
1	D	37	GLY	2.5
1	D	30	THR	2.5
1	F	182	MET	2.5
1	C	123	ASP	2.5
1	A	149	SER	2.4
1	E	336	ALA	2.4
1	C	625	ASP	2.4
1	A	150	TYR	2.4
1	A	197	GLY	2.4
1	A	199	ARG	2.4
1	A	241	ASP	2.4
1	E	242	ARG	2.4
1	C	633	ARG	2.4
1	D	623	TYR	2.3
1	A	337	SER	2.3
1	A	334	ILE	2.3
1	F	633	ARG	2.3
1	A	594	GLY	2.3
1	B	335	GLY	2.3
1	C	634	GLY	2.3
1	E	434	PRO	2.3
1	C	593	ALA	2.3
1	D	199	ARG	2.2
1	B	593	ALA	2.2
1	D	335	GLY	2.2
1	B	620	GLN	2.2
1	B	159	THR	2.2
1	B	124	SER	2.1
1	C	620	GLN	2.1
1	C	197	GLY	2.1
1	F	196	THR	2.1
1	F	335	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	338	TRP	2.1
1	A	635	GLU	2.1
1	E	315	THR	2.1
1	D	158	ASP	2.1
1	C	124	SER	2.0
1	A	136	ASN	2.0
1	B	632	LEU	2.0
1	F	242	ARG	2.0
1	B	62	ASP	2.0

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

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

6.3 Carbohydrates (i)

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
2	BGC	E	679	11/12	0.93	0.11	1.04	26,29,34,34	0
2	BGC	B	679	11/12	0.93	0.12	0.75	38,38,41,41	0
2	BGC	F	679	11/12	0.95	0.10	0.46	28,31,36,37	0
2	BGC	C	679	11/12	0.95	0.11	0.43	30,36,39,40	0
2	BGC	D	679	11/12	0.93	0.12	0.39	35,37,43,44	0
2	BGC	A	679	11/12	0.93	0.11	-0.12	34,35,37,37	0
2	BGC	A	680	11/12	0.94	0.10	-0.22	33,34,35,35	0
2	BGC	E	680	11/12	0.97	0.08	-0.41	24,25,26,27	0
2	BGC	F	680	11/12	0.98	0.07	-0.48	24,27,29,30	0
2	BGC	C	680	11/12	0.98	0.08	-0.87	31,32,33,35	0
2	BGC	D	680	11/12	0.97	0.07	-1.13	30,31,32,33	0
2	BGC	B	680	11/12	0.97	0.06	-1.70	31,33,34,35	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.