



Full wwPDB X-ray Structure Validation 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 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 ⓘ symbol.

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

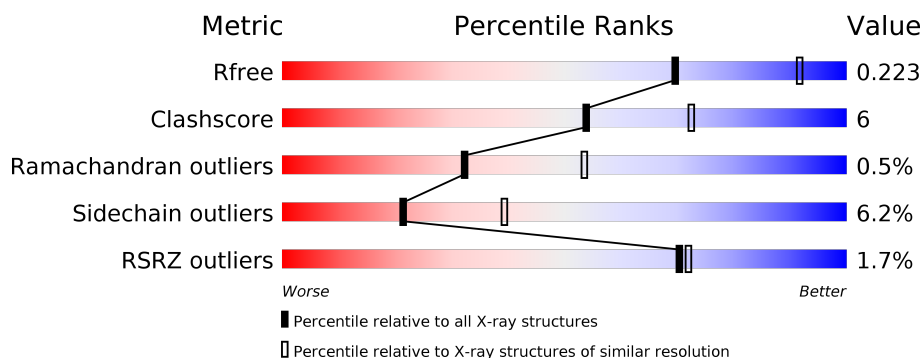
1 Overall quality at a glance

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 ≥ 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		

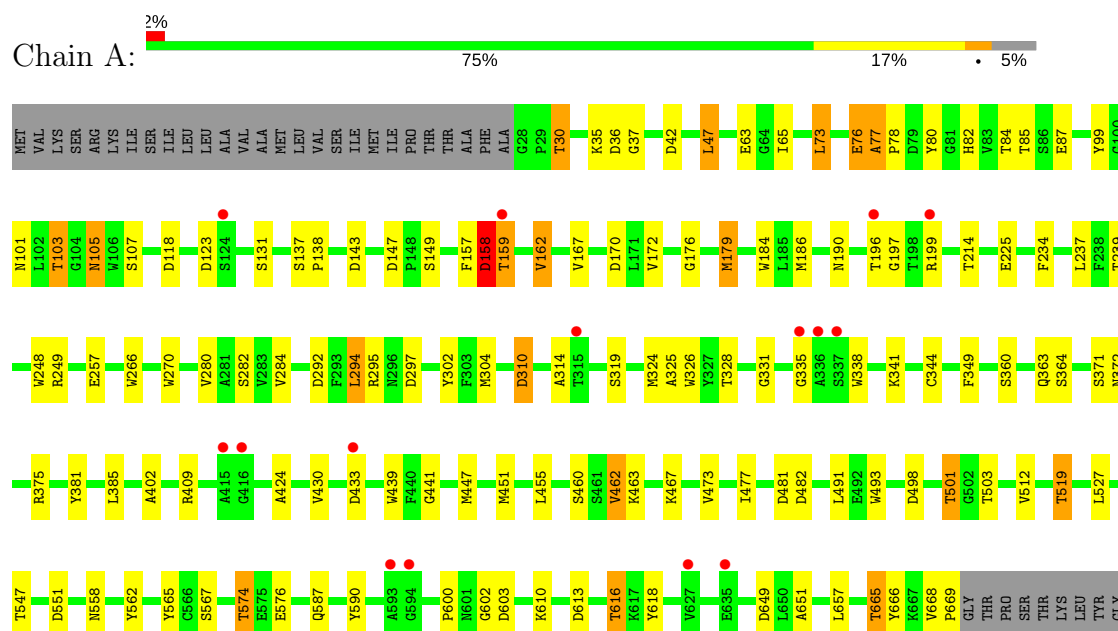
- Molecule 4 is water.

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		

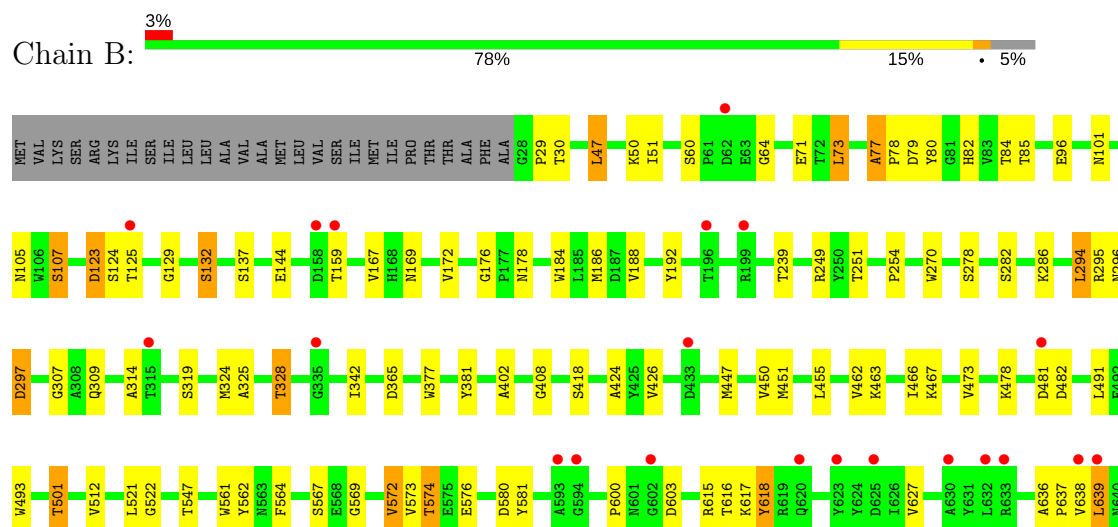
3 Residue-property plots

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

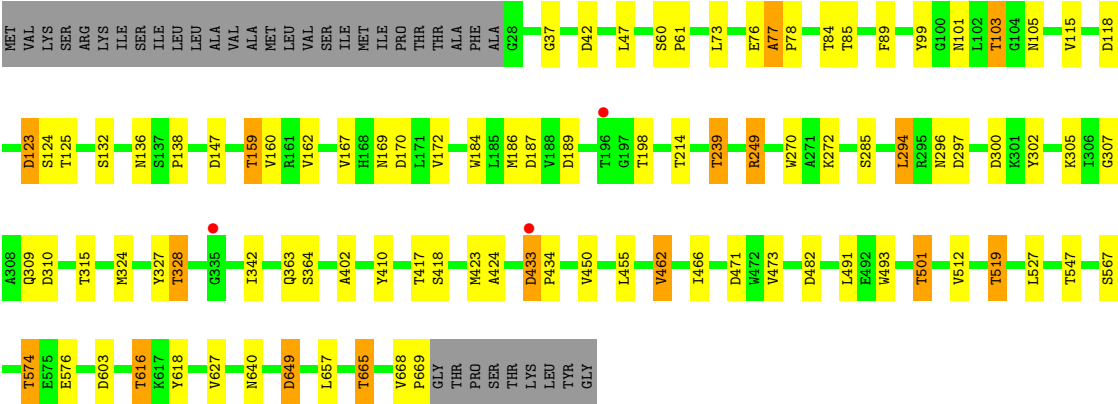
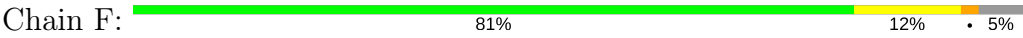


• Molecule 1: cellobiohydrolase





● Molecule 1: cellobiohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	148.03Å 207.64Å 215.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.5 (15.00-2.50) 95.5 (15.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.181 , 0.226 0.181 , 0.223	Depositor DCC
R_{free} test set	10814 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	35.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical 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

All (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

Continued on next page...

Continued from previous page...

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
1	E	73	LEU	CA-CB-CG	6.48	130.20	115.30
1	A	297	ASP	CB-CG-OD2	6.43	124.09	118.30
1	E	249	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	C	123	ASP	CB-CG-OD2	6.33	124.00	118.30
1	C	318	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	498	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	123	ASP	CB-CG-OD2	6.07	123.76	118.30
1	E	433	ASP	CB-CG-OD2	6.02	123.72	118.30
1	F	170	ASP	CB-CG-OD2	5.99	123.69	118.30
1	E	649	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	580	ASP	CB-CG-OD2	5.92	123.63	118.30
1	D	123	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	603	ASP	CB-CG-OD2	5.83	123.55	118.30
1	C	297	ASP	CB-CG-OD2	5.82	123.54	118.30
1	E	123	ASP	CB-CG-OD2	5.80	123.52	118.30
1	F	649	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	42	ASP	CB-CG-OD2	5.74	123.47	118.30
1	E	318	ASP	CB-CG-OD2	5.73	123.46	118.30
1	F	433	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	613	ASP	CB-CG-OD2	5.71	123.44	118.30
1	E	520	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	147	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	73	LEU	CA-CB-CG	5.69	128.38	115.30
1	F	482	ASP	CB-CG-OD2	5.69	123.42	118.30
1	F	187	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	310	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	481	ASP	CB-CG-OD2	5.64	123.37	118.30
1	D	189	ASP	CB-CG-OD2	5.62	123.36	118.30
1	E	187	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	482	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	123	ASP	CB-CG-OD2	5.59	123.33	118.30
1	F	471	ASP	CB-CG-OD2	5.56	123.30	118.30
1	F	297	ASP	CB-CG-OD2	5.52	123.26	118.30
1	C	482	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	118	ASP	CB-CG-OD2	5.49	123.24	118.30
1	F	189	ASP	CB-CG-OD2	5.49	123.24	118.30
1	E	482	ASP	CB-CG-OD2	5.45	123.21	118.30
1	F	42	ASP	CB-CG-OD2	5.45	123.20	118.30
1	F	123	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	79	ASP	CB-CG-OD2	5.42	123.17	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	147	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	297	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	62	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	36	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	546	ASP	CB-CG-OD2	5.28	123.05	118.30
1	E	297	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	481	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	433	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	76	GLU	N-CA-C	-5.22	96.89	111.00
1	D	433	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	300	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	297	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	482	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	73	LEU	CB-CG-CD1	5.17	119.79	111.00
1	F	118	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	551	ASP	CB-CG-OD2	5.15	122.94	118.30
1	E	315	THR	C-N-CA	-5.14	111.51	122.30
1	F	300	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	365	ASP	CB-CG-OD2	5.03	122.83	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

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

Continued on next page...

Continued from previous page...

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

All (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
1:A:35:LYS:HA	1:F:136:ASN:HD22	1.33	0.92
1:A:574:THR:HG21	1:A:576:GLU:OE1	1.72	0.89
1:E:103:THR:HG22	1:E:105:ASN:H	1.38	0.87
1:F:574:THR:HG21	1:F:576:GLU:OE1	1.75	0.85
1:A:76:GLU:O	1:A:78:PRO:O	1.96	0.84
1:C:574:THR:HG22	1:C:641:TYR:H	1.44	0.83
1:E:501:THR:CG2	1:F:307:GLY:O	2.28	0.82
1:C:294:LEU:HG	1:C:324:MET:CE	2.10	0.81
1:A:603:ASP:CB	4:A:806:HOH:O	2.28	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HG	1:A:324:MET:HE1	1.62	0.81
1:A:363:GLN:HE22	1:D:364:SER:H	1.29	0.80
1:C:99:TYR:O	1:C:103:THR:HB	1.82	0.79
1:A:669:PRO:C	4:A:714:HOH:O	2.20	0.79
1:E:307:GLY:O	1:F:501:THR:CG2	2.32	0.78
1:E:136:ASN:HB2	4:E:716:HOH:O	1.84	0.78
1:C:294:LEU:HG	1:C:324:MET:HE2	1.66	0.78
1:E:574:THR:HG21	4:E:774:HOH:O	1.84	0.77
1:F:37:GLY:HA2	1:F:665:THR:CG2	2.15	0.77
1:B:309:GLN:HE21	1:D:501:THR:HG21	1.49	0.76
1:B:501:THR:CG2	1:D:307:GLY:O	2.33	0.76
1:C:363:GLN:HE22	1:F:364:SER:H	1.33	0.75
1:B:129:GLY:O	1:B:132:SER:HB2	1.87	0.74
1:A:294:LEU:HG	1:A:324:MET:CE	2.17	0.74
1:B:328:THR:HG22	1:B:342:ILE:O	1.88	0.74
1:A:35:LYS:HA	1:F:136:ASN:ND2	2.04	0.73
1:E:278:SER:HB3	4:E:898:HOH:O	1.88	0.72
1:A:248:TRP:CZ3	1:A:331:GLY:HA2	2.23	0.72
1:A:616:THR:HB	4:A:806:HOH:O	1.89	0.71
1:C:103:THR:HG22	1:C:105:ASN:H	1.56	0.71
1:E:99:TYR:O	1:E:103:THR:HB	1.90	0.70
1:F:294:LEU:HG	1:F:324:MET:CE	2.21	0.70
1:F:294:LEU:HG	1:F:324:MET:HE1	1.71	0.69
1:B:600:PRO:HG2	4:B:797:HOH:O	1.91	0.69
1:A:103:THR:CG2	1:A:105:ASN:H	2.06	0.68
1:F:37:GLY:HA2	1:F:665:THR:HG21	1.75	0.68
1:B:47:LEU:O	1:B:51:ILE:HG13	1.93	0.68
1:B:50:LYS:HD3	1:B:569:GLY:O	1.93	0.67
1:C:124:SER:HB3	1:C:178:ASN:ND2	2.10	0.67
1:C:365:ASP:OD1	1:F:272:LYS:HE3	1.95	0.67
1:F:103:THR:HG22	1:F:105:ASN:H	1.61	0.66
1:D:99:TYR:O	1:D:103:THR:HB	1.95	0.66
1:B:447:MET:O	1:B:451:MET:HG2	1.96	0.66
1:D:574:THR:HG21	1:D:576:GLU:OE1	1.97	0.65
1:A:234:PHE:O	1:A:237:LEU:HB2	1.97	0.65
1:B:101:ASN:HB2	1:B:270:TRP:CE3	2.31	0.65
1:D:103:THR:HG22	1:D:105:ASN:N	2.06	0.65
1:B:192:TYR:C	4:B:797:HOH:O	2.35	0.65
1:B:573:VAL:HG23	1:B:641:TYR:O	1.96	0.65
1:B:296:ASN:HB3	1:B:328:THR:HG21	1.78	0.65
1:F:473:VAL:HG11	1:F:527:LEU:HD11	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:THR:HB	4:A:708:HOH:O	1.97	0.64
1:E:37:GLY:HA2	1:E:665:THR:CG2	2.28	0.64
1:D:519:THR:HG23	1:D:519:THR:O	1.98	0.63
1:A:63:GLU:HG3	1:A:65:ILE:HD12	1.81	0.63
1:B:77:ALA:H	1:B:78:PRO:HD2	1.63	0.63
1:C:37:GLY:HA2	1:C:665:THR:HG23	1.81	0.62
1:A:501:THR:CG2	1:A:501:THR:O	2.47	0.62
1:B:85:THR:HA	1:B:184:TRP:O	1.99	0.62
1:E:101:ASN:HB2	1:E:270:TRP:CE3	2.35	0.62
1:F:37:GLY:HA2	1:F:665:THR:HG23	1.81	0.62
1:C:294:LEU:HG	1:C:324:MET:HE1	1.81	0.62
1:A:36:ASP:H	1:F:136:ASN:HD21	1.46	0.62
1:C:101:ASN:HB2	1:C:270:TRP:CE3	2.34	0.62
1:D:254:PRO:HB2	1:D:324:MET:HE3	1.83	0.61
1:C:574:THR:HG21	1:C:576:GLU:OE1	2.01	0.61
1:D:462:VAL:HG13	1:D:466:ILE:HD12	1.82	0.61
1:F:462:VAL:HG13	1:F:466:ILE:HD12	1.82	0.60
1:C:603:ASP:OD2	1:C:616:THR:HB	2.00	0.60
1:E:158:ASP:CB	4:E:893:HOH:O	2.49	0.60
1:B:84:THR:HG22	1:B:186:MET:HB3	1.84	0.60
1:E:37:GLY:HA2	1:E:665:THR:HG23	1.82	0.60
1:F:76:GLU:O	1:F:214:THR:HG21	2.02	0.59
1:A:37:GLY:HA2	1:A:665:THR:HG23	1.84	0.59
1:E:162:VAL:HG22	1:E:302:TYR:HB3	1.84	0.59
1:F:296:ASN:HB3	1:F:328:THR:HG21	1.84	0.59
1:D:159:THR:HG22	4:D:688:HOH:O	2.02	0.59
1:A:473:VAL:HG11	1:A:527:LEU:HD11	1.84	0.59
1:F:328:THR:HG22	1:F:342:ILE:O	2.02	0.59
1:B:501:THR:HG21	1:D:309:GLN:HE21	1.67	0.58
1:E:625:ASP:O	1:E:629:GLN:HG3	2.03	0.58
1:C:128:PRO:HD2	1:C:248:TRP:NE1	2.18	0.58
1:E:296:ASN:HB3	1:E:328:THR:HG21	1.84	0.58
1:A:338:TRP:CH2	3:A:685:BGC:H6C1	2.39	0.58
1:D:84:THR:HG22	1:D:186:MET:HB3	1.84	0.57
1:A:473:VAL:CG1	1:A:527:LEU:HD11	2.34	0.57
1:B:251:THR:HG21	3:B:682:BGC:H3	1.86	0.57
1:A:138:PRO:HD2	1:A:162:VAL:CG1	2.34	0.57
1:D:76:GLU:O	1:D:77:ALA:C	2.42	0.57
1:E:501:THR:HG23	1:F:307:GLY:O	2.05	0.57
1:E:77:ALA:HB3	1:E:78:PRO:CD	2.35	0.57
1:F:272:LYS:HD2	4:F:912:HOH:O	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:ARG:HB3	4:E:897:HOH:O	2.05	0.56
1:A:63:GLU:CG	1:A:65:ILE:HD12	2.36	0.56
1:B:463:LYS:O	1:B:467:LYS:HG2	2.05	0.56
1:F:101:ASN:HB2	1:F:270:TRP:CE3	2.40	0.56
1:A:447:MET:O	1:A:451:MET:HG2	2.06	0.56
1:F:249:ARG:HD2	4:F:958:HOH:O	2.05	0.56
1:B:73:LEU:HD12	1:B:627:VAL:HG21	1.87	0.55
1:A:103:THR:HG23	1:A:105:ASN:H	1.70	0.55
1:B:616:THR:O	1:B:618:TYR:N	2.39	0.55
1:B:64:GLY:O	4:B:767:HOH:O	2.17	0.55
1:F:501:THR:HB	4:F:689:HOH:O	2.05	0.55
1:E:166:PRO:HG3	1:E:316:GLY:O	2.06	0.55
1:E:297:ASP:CB	1:E:324:MET:HE3	2.36	0.55
1:A:76:GLU:O	1:A:77:ALA:C	2.45	0.55
1:B:616:THR:C	1:B:618:TYR:H	2.09	0.55
1:E:77:ALA:HB3	1:E:78:PRO:HD3	1.89	0.55
1:D:76:GLU:O	1:D:78:PRO:O	2.25	0.54
1:E:297:ASP:HB2	1:E:324:MET:HE3	1.88	0.54
1:B:307:GLY:O	1:D:501:THR:CG2	2.55	0.54
1:B:294:LEU:HG	1:B:324:MET:HE1	1.89	0.54
1:B:501:THR:HG23	1:D:307:GLY:CA	2.37	0.54
1:A:460:SER:HB2	4:A:800:HOH:O	2.07	0.54
1:E:323:LEU:HD12	1:E:423:MET:HE1	1.90	0.54
1:A:103:THR:HG22	1:A:105:ASN:H	1.72	0.54
1:A:85:THR:HA	1:A:184:TRP:O	2.08	0.54
1:B:615:ARG:O	1:B:618:TYR:HB2	2.08	0.53
1:A:587:GLN:O	1:A:610:LYS:HA	2.08	0.53
1:A:77:ALA:HB3	1:A:78:PRO:CD	2.38	0.53
1:B:107:SER:HA	4:B:807:HOH:O	2.08	0.53
1:B:169:ASN:HB2	4:B:727:HOH:O	2.08	0.53
1:E:307:GLY:O	1:F:501:THR:HG22	2.07	0.53
1:A:99:TYR:O	1:A:103:THR:HB	2.09	0.53
1:E:85:THR:HA	1:E:184:TRP:O	2.08	0.53
1:F:493:TRP:CZ3	1:F:512:VAL:HB	2.44	0.53
1:D:101:ASN:HB2	1:D:270:TRP:CE3	2.44	0.53
1:A:172:VAL:HA	1:A:176:GLY:O	2.09	0.53
1:E:73:LEU:HD13	1:E:584:PHE:HZ	1.74	0.52
1:B:574:THR:CG2	1:B:576:GLU:OE1	2.48	0.52
1:A:47:LEU:HD13	1:A:651:ALA:HB2	1.92	0.52
1:F:76:GLU:O	1:F:77:ALA:C	2.47	0.52
1:A:364:SER:H	1:D:363:GLN:HE22	1.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:PRO:HB3	1:B:564:PHE:HA	1.91	0.52
1:F:450:VAL:HG12	1:F:466:ILE:HD11	1.92	0.52
1:C:462:VAL:HG13	1:C:466:ILE:HD12	1.92	0.52
1:E:225:GLU:O	1:E:226:PHE:HB2	2.10	0.52
1:A:77:ALA:HB3	1:A:78:PRO:HD2	1.92	0.52
1:D:251:THR:HG21	3:D:682:BGC:H3	1.92	0.52
1:B:71:GLU:OE2	1:B:642:HIS:ND1	2.38	0.51
1:C:268:ASN:HD21	1:C:272:LYS:NZ	2.08	0.51
1:D:294:LEU:HG	1:D:324:MET:CE	2.40	0.51
1:E:228:TYR:O	1:E:233:GLY:HA2	2.10	0.51
1:C:152:PRO:HG3	1:C:236:ASP:O	2.10	0.51
1:C:37:GLY:HA2	1:C:665:THR:CG2	2.39	0.51
1:F:162:VAL:HG22	1:F:302:TYR:HB3	1.93	0.51
1:F:249:ARG:NH2	4:F:756:HOH:O	2.43	0.51
1:B:124:SER:HB3	1:B:178:ASN:ND2	2.26	0.51
1:F:433:ASP:C	1:F:433:ASP:OD1	2.48	0.51
1:A:149:SER:HA	1:A:590:TYR:CD2	2.45	0.51
1:A:87:GLU:HG3	4:A:715:HOH:O	2.10	0.51
1:B:123:ASP:OD2	1:B:125:THR:HB	2.11	0.51
1:A:101:ASN:HB2	1:A:270:TRP:CE3	2.46	0.51
1:C:162:VAL:HG22	1:C:302:TYR:HB3	1.92	0.51
1:E:503:THR:HG21	4:F:966:HOH:O	2.11	0.51
1:A:473:VAL:O	1:A:477:ILE:HG13	2.11	0.51
1:D:60:SER:HB2	4:D:917:HOH:O	2.10	0.51
1:E:239:THR:HG22	4:E:873:HOH:O	2.10	0.51
1:B:450:VAL:HG12	1:B:466:ILE:HD11	1.93	0.50
1:B:562:TYR:CE1	1:B:668:VAL:HG23	2.46	0.50
1:C:144:GLU:HG2	4:C:826:HOH:O	2.10	0.50
1:C:623:TYR:O	1:C:627:VAL:HG12	2.11	0.50
1:E:603:ASP:OD1	1:E:616:THR:HB	2.11	0.50
1:A:463:LYS:O	1:A:467:LYS:HG2	2.12	0.50
1:C:364:SER:H	1:F:363:GLN:HE22	1.59	0.50
1:F:76:GLU:O	1:F:78:PRO:O	2.29	0.50
1:B:167:VAL:HG22	1:B:295:ARG:NH1	2.26	0.50
1:C:578:ARG:O	1:C:637:PRO:HD2	2.11	0.50
1:E:133:TYR:OH	1:E:138:PRO:HB3	2.12	0.50
1:D:360:SER:HB3	4:D:742:HOH:O	2.12	0.50
1:E:221:PRO:O	1:E:249:ARG:NH2	2.45	0.49
1:A:385:LEU:HD22	1:A:462:VAL:HG21	1.93	0.49
1:E:324:MET:HA	1:E:324:MET:CE	2.42	0.49
1:B:501:THR:HG22	1:D:307:GLY:O	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:GLU:HA	4:D:913:HOH:O	2.12	0.49
1:F:99:TYR:O	1:F:103:THR:HB	2.12	0.49
1:E:307:GLY:CA	1:F:501:THR:HG23	2.43	0.49
1:A:325:ALA:HB1	1:A:344:CYS:HB3	1.95	0.49
1:D:239:THR:HG22	4:D:816:HOH:O	2.12	0.49
1:F:239:THR:CG2	4:F:696:HOH:O	2.59	0.49
1:A:149:SER:HA	1:A:590:TYR:CE2	2.48	0.49
1:D:37:GLY:HA2	1:D:665:THR:CG2	2.42	0.49
1:B:80:TYR:CE2	1:B:82:HIS:HB2	2.48	0.48
1:B:294:LEU:HB3	1:B:377:TRP:HZ2	1.78	0.48
1:B:616:THR:C	1:B:618:TYR:N	2.67	0.48
1:C:120:ILE:HG23	1:C:182:MET:HG2	1.94	0.48
1:E:73:LEU:HD13	1:E:584:PHE:CZ	2.48	0.48
1:A:326:TRP:CD2	1:A:430:VAL:HG21	2.49	0.48
1:B:581:TYR:CE2	1:B:639:LEU:HD21	2.49	0.48
1:D:269:LYS:HE2	1:D:273:GLU:OE2	2.13	0.48
1:F:603:ASP:OD1	1:F:616:THR:HB	2.14	0.48
1:B:501:THR:HG23	1:D:307:GLY:O	2.11	0.48
1:D:519:THR:CG2	1:D:519:THR:O	2.61	0.48
1:A:501:THR:HG22	1:A:501:THR:O	2.14	0.48
3:D:681:BGC:H6C1	4:D:767:HOH:O	2.14	0.48
1:F:305:LYS:HD2	4:F:812:HOH:O	2.14	0.48
1:F:310:ASP:HB3	4:F:770:HOH:O	2.14	0.48
1:E:501:THR:HG22	1:F:307:GLY:O	2.12	0.48
1:B:144:GLU:HB2	1:B:408:GLY:HA3	1.95	0.48
1:F:294:LEU:HG	1:F:324:MET:HE3	1.95	0.48
1:F:310:ASP:HA	1:F:410:TYR:HB3	1.96	0.48
1:A:76:GLU:O	1:A:78:PRO:N	2.47	0.47
1:D:603:ASP:OD2	1:D:616:THR:HB	2.14	0.47
1:E:501:THR:HG21	1:F:309:GLN:HE21	1.78	0.47
1:A:372:ASN:HD22	1:A:375:ARG:NH2	2.12	0.47
1:E:248:TRP:CZ3	1:E:331:GLY:HA2	2.50	0.47
1:F:85:THR:HA	1:F:184:TRP:O	2.13	0.47
1:A:162:VAL:HG22	1:A:302:TYR:HB3	1.96	0.47
1:A:562:TYR:HB2	1:A:666:TYR:OH	2.14	0.47
1:C:85:THR:HA	1:C:184:TRP:O	2.14	0.47
1:C:462:VAL:HG22	1:C:465:LEU:HD23	1.96	0.47
1:B:314:ALA:HB3	1:B:319:SER:HB3	1.97	0.47
1:C:249:ARG:N	1:C:249:ARG:HD3	2.30	0.47
3:D:681:BGC:H6C2	3:D:682:BGC:C1	2.45	0.47
1:A:257:GLU:HB2	1:A:294:LEU:HD11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:THR:HG21	3:C:682:BGC:H3	1.97	0.47
1:C:63:GLU:HG3	1:C:65:ILE:HD12	1.96	0.47
1:D:76:GLU:O	1:D:214:THR:HG21	2.15	0.47
1:C:128:PRO:HD2	1:C:248:TRP:CD1	2.50	0.47
1:F:305:LYS:HG3	4:F:812:HOH:O	2.14	0.47
1:B:254:PRO:HG2	1:B:325:ALA:O	2.15	0.46
1:A:36:ASP:H	1:F:136:ASN:ND2	2.14	0.46
1:A:63:GLU:HG3	1:A:65:ILE:CD1	2.46	0.46
1:C:134:ASN:HA	1:C:135:PRO:HD2	1.76	0.46
1:D:268:ASN:ND2	4:D:785:HOH:O	2.47	0.46
1:E:501:THR:HB	4:E:697:HOH:O	2.15	0.46
1:A:143:ASP:HB3	1:A:409:ARG:HG2	1.98	0.46
1:A:493:TRP:CZ3	1:A:512:VAL:HB	2.50	0.46
1:C:268:ASN:HD21	1:C:272:LYS:HZ2	1.64	0.46
1:C:47:LEU:HD13	1:C:651:ALA:HB2	1.98	0.46
1:F:473:VAL:CG1	1:F:527:LEU:HD11	2.43	0.46
1:B:521:LEU:HD13	1:B:572:VAL:HG23	1.98	0.46
1:D:493:TRP:CZ3	1:D:512:VAL:HB	2.51	0.46
1:F:462:VAL:CG1	1:F:466:ILE:HD12	2.46	0.46
1:A:558:ASN:HA	1:A:666:TYR:HE1	1.81	0.46
1:B:478:LYS:HE3	4:B:803:HOH:O	2.14	0.46
1:D:455:LEU:HD23	1:D:537:ALA:HA	1.97	0.46
1:A:239:THR:HG21	3:A:684:BGC:H2	1.97	0.46
1:B:493:TRP:CZ3	1:B:512:VAL:HB	2.51	0.46
1:D:184:TRP:CZ2	1:D:185:LEU:HD22	2.51	0.45
1:E:37:GLY:HA2	1:E:665:THR:HG21	1.97	0.45
1:E:210:GLU:HB2	1:E:430:VAL:O	2.16	0.45
1:E:463:LYS:O	1:E:467:LYS:HG2	2.16	0.45
1:B:105:ASN:ND2	1:B:107:SER:OG	2.47	0.45
1:C:426:VAL:HA	1:C:427:PRO:HD3	1.83	0.45
1:D:162:VAL:HG22	1:D:302:TYR:HB3	1.99	0.45
1:C:254:PRO:HB2	1:C:324:MET:HE3	1.99	0.45
1:A:439:TRP:CE2	1:A:441:GLY:HA3	2.51	0.45
1:D:220:HIS:HB2	1:D:221:PRO:HD2	1.98	0.45
1:A:77:ALA:CB	1:A:78:PRO:CD	2.94	0.45
1:F:89:PHE:HE2	1:F:115:VAL:HG12	1.81	0.45
1:F:84:THR:HG22	1:F:186:MET:HB3	1.98	0.45
1:B:294:LEU:HG	1:B:324:MET:CE	2.46	0.45
1:C:73:LEU:HD13	1:C:584:PHE:HZ	1.80	0.45
1:F:519:THR:HG23	1:F:519:THR:O	2.17	0.45
1:A:292:ASP:OD1	1:A:295:ARG:NH2	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:GLY:HA3	1:B:645:TRP:CZ3	2.52	0.45
1:E:251:THR:HG21	3:E:682:BGC:H3	1.99	0.45
1:A:372:ASN:HD22	1:A:375:ARG:HH22	1.65	0.44
1:A:519:THR:HG23	1:A:519:THR:O	2.17	0.44
1:C:228:TYR:O	1:C:233:GLY:HA2	2.17	0.44
1:C:166:PRO:HG3	1:C:316:GLY:O	2.18	0.44
1:D:328:THR:HG23	1:D:342:ILE:O	2.17	0.44
1:C:669:PRO:C	4:C:706:HOH:O	2.56	0.44
1:D:294:LEU:HG	1:D:324:MET:HE1	1.99	0.44
1:E:668:VAL:HA	1:E:669:PRO:HD3	1.73	0.44
1:F:668:VAL:HA	1:F:669:PRO:HD3	1.80	0.44
1:A:190:ASN:HB2	1:A:199:ARG:O	2.18	0.44
1:E:84:THR:HG22	1:E:186:MET:HB3	1.98	0.44
1:C:80:TYR:CE2	1:C:82:HIS:HB2	2.53	0.44
1:A:105:ASN:HD22	1:A:105:ASN:C	2.20	0.44
1:A:162:VAL:HA	1:A:304:MET:HE2	1.99	0.44
1:E:47:LEU:HD13	1:E:651:ALA:HB2	2.00	0.44
1:F:462:VAL:HG13	1:F:466:ILE:CD1	2.47	0.44
1:A:294:LEU:HG	1:A:324:MET:HE3	1.99	0.44
1:C:239:THR:HG21	3:C:684:BGC:H2	1.99	0.44
1:C:84:THR:HG22	1:C:186:MET:HB3	2.00	0.43
1:C:668:VAL:HG23	1:C:669:PRO:HD2	2.00	0.43
1:F:159:THR:HG22	1:F:160:VAL:HG23	1.99	0.43
1:F:169:ASN:HA	1:F:172:VAL:HB	2.00	0.43
1:B:60:SER:HB3	1:B:188:VAL:HG11	1.99	0.43
1:E:324:MET:HB3	1:E:324:MET:HE2	1.88	0.43
1:A:402:ALA:HA	1:A:424:ALA:O	2.19	0.43
1:F:138:PRO:HD2	1:F:162:VAL:CG1	2.48	0.43
1:A:84:THR:HG22	1:A:186:MET:HB3	1.99	0.43
1:C:519:THR:HG23	1:C:519:THR:O	2.17	0.43
1:A:314:ALA:HB3	1:A:319:SER:HB3	2.01	0.43
1:B:172:VAL:HA	1:B:176:GLY:O	2.19	0.43
1:B:254:PRO:HG3	1:B:297:ASP:OD1	2.19	0.43
1:F:402:ALA:HA	1:F:424:ALA:O	2.19	0.43
1:A:248:TRP:CE3	1:A:331:GLY:HA2	2.54	0.43
1:D:32:ALA:HB2	1:D:565:TYR:HB2	2.01	0.43
1:E:493:TRP:CZ3	1:E:512:VAL:HB	2.53	0.43
1:A:158:ASP:N	1:A:158:ASP:OD1	2.52	0.43
1:A:30:THR:HG21	1:A:567:SER:HB3	1.99	0.43
1:E:198:THR:CG2	4:E:902:HOH:O	2.66	0.43
1:D:156:LYS:HB3	1:D:159:THR:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:THR:O	1:A:565:TYR:HB3	2.19	0.42
1:A:80:TYR:CE2	1:A:82:HIS:HB2	2.54	0.42
1:D:239:THR:HG21	3:D:684:BGC:H2	2.02	0.42
1:F:574:THR:O	1:F:640:ASN:HA	2.19	0.42
1:A:37:GLY:HA2	1:A:665:THR:CG2	2.49	0.42
1:D:324:MET:HE3	1:D:324:MET:HB3	1.97	0.42
1:C:184:TRP:CE2	1:C:185:LEU:HB2	2.54	0.42
1:D:606:GLN:O	1:D:609:ILE:HG12	2.19	0.42
1:A:280:VAL:O	1:A:284:VAL:HG23	2.19	0.42
1:B:96:GLU:HA	1:B:96:GLU:OE1	2.19	0.42
1:C:363:GLN:NE2	1:F:364:SER:H	2.09	0.42
1:B:77:ALA:HB3	1:B:78:PRO:CD	2.50	0.42
1:C:163:GLY:HA3	1:C:303:PHE:O	2.20	0.42
1:C:668:VAL:HA	1:C:669:PRO:HD3	1.84	0.42
1:B:636:ALA:HA	1:B:637:PRO:HD3	1.93	0.42
1:C:249:ARG:NH2	4:C:784:HOH:O	2.52	0.42
1:D:309:GLN:O	1:D:412:LYS:HE3	2.20	0.42
1:E:241:ASP:OD1	1:E:242:ARG:N	2.52	0.42
1:C:45:LEU:HA	1:C:45:LEU:HD23	1.80	0.41
1:E:99:TYR:CE2	1:E:103:THR:HG21	2.55	0.41
1:E:53:ASP:HA	1:E:54:PRO:HD2	1.95	0.41
1:D:292:ASP:CG	1:D:368:PRO:HB3	2.40	0.41
1:B:307:GLY:O	1:D:501:THR:HG23	2.20	0.41
1:E:324:MET:HA	1:E:324:MET:HE3	2.02	0.41
1:E:501:THR:HG23	1:F:307:GLY:CA	2.49	0.41
1:D:37:GLY:HA2	1:D:665:THR:HG23	2.01	0.41
1:E:297:ASP:HB2	1:E:324:MET:CE	2.50	0.41
1:E:297:ASP:HB3	1:E:324:MET:HE3	2.02	0.41
1:B:402:ALA:HA	1:B:424:ALA:O	2.20	0.41
1:F:103:THR:CG2	1:F:105:ASN:H	2.32	0.41
1:A:105:ASN:ND2	1:A:107:SER:H	2.19	0.41
1:D:668:VAL:HA	1:D:669:PRO:HD3	1.81	0.41
1:C:241:ASP:HB3	1:C:243:SER:O	2.21	0.41
1:F:37:GLY:CA	1:F:665:THR:HG23	2.48	0.41
1:A:266:TRP:HB3	1:A:270:TRP:CH2	2.55	0.41
1:A:266:TRP:HB3	1:A:270:TRP:CZ3	2.56	0.41
1:B:47:LEU:HG	1:B:561:TRP:CZ3	2.56	0.41
1:B:73:LEU:CD1	1:B:627:VAL:HG21	2.51	0.41
1:B:77:ALA:H	1:B:78:PRO:CD	2.33	0.41
1:D:447:MET:HG3	1:D:469:TRP:CE2	2.56	0.41
1:E:96:GLU:OE1	1:E:96:GLU:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:ASP:HB2	4:F:947:HOH:O	2.21	0.41
1:A:158:ASP:HB2	1:A:159:THR:H	1.73	0.41
1:A:602:GLY:O	1:A:603:ASP:C	2.59	0.41
1:B:282:SER:O	1:B:286:LYS:HG3	2.20	0.41
1:C:126:GLU:C	1:C:128:PRO:HD3	2.41	0.40
1:D:639:LEU:HD22	1:D:641:TYR:OH	2.21	0.40
1:E:167:VAL:HG22	1:E:295:ARG:NH1	2.35	0.40
1:F:417:THR:HG21	1:F:424:ALA:HB1	2.02	0.40
1:F:60:SER:HA	1:F:61:PRO:HD3	1.97	0.40
1:C:141:TYR:CZ	1:C:311:LYS:HE2	2.56	0.40
1:D:615:ARG:O	1:D:618:TYR:HB2	2.21	0.40
1:E:248:TRP:C	1:E:249:ARG:HG3	2.40	0.40
1:E:266:TRP:HB3	1:E:270:TRP:CZ3	2.57	0.40
1:E:455:LEU:HD22	1:E:540:ARG:NH1	2.37	0.40
1:C:63:GLU:HG3	1:C:65:ILE:CD1	2.52	0.40
1:D:43:LEU:HA	1:D:43:LEU:HD23	1.90	0.40
1:E:215:TRP:HB3	1:E:587:GLN:HG2	2.04	0.40
1:A:179:MET:HE1	1:A:341:LYS:HE2	2.02	0.40
1:C:141:TYR:CG	1:C:142:ALA:N	2.89	0.40
1:F:310:ASP:HA	1:F:410:TYR:O	2.22	0.40
1:F:574:THR:CG2	1:F:576:GLU:OE1	2.59	0.40
1:C:103:THR:HG22	1:C:105:ASN:N	2.31	0.40
1:C:493:TRP:CZ3	1:C:512:VAL:HB	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	640/678 (94%)	607 (95%)	28 (4%)	5 (1%)	22 39
1	B	640/678 (94%)	605 (94%)	33 (5%)	2 (0%)	44 66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	D	278	SER
1	E	278	SER
1	B	617	LYS
1	C	77	ALA
1	D	77	ALA
1	E	77	ALA
1	B	77	ALA
1	C	226	PHE
1	E	197	GLY
1	F	77	ALA
1	A	600	PRO
1	A	197	GLY
1	C	430	VAL

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	47	LEU
1	A	73	LEU
1	A	103	THR
1	A	105	ASN
1	A	131	SER
1	A	137	SER
1	A	157	PHE
1	A	158	ASP
1	A	159	THR
1	A	162	VAL
1	A	167	VAL
1	A	170	ASP
1	A	179	MET
1	A	196	THR
1	A	214	THR
1	A	225	GLU
1	A	249	ARG
1	A	282	SER
1	A	294	LEU
1	A	310	ASP
1	A	328	THR
1	A	349	PHE
1	A	360	SER
1	A	371	SER
1	A	381	TYR
1	A	455	LEU
1	A	462	VAL
1	A	491	LEU
1	A	501	THR
1	A	503	THR
1	A	519	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	547	THR
1	A	574	THR
1	A	616	THR
1	A	618	TYR
1	A	649	ASP
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	107	SER
1	B	132	SER
1	B	137	SER
1	B	159	THR
1	B	239	THR
1	B	249	ARG
1	B	278	SER
1	B	294	LEU
1	B	328	THR
1	B	381	TYR
1	B	418	SER
1	B	426	VAL
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	567	SER
1	B	572	VAL
1	B	574	THR
1	B	618	TYR
1	B	639	LEU
1	B	649	ASP
1	B	657	LEU
1	B	665	THR
1	C	47	LEU
1	C	63	GLU
1	C	73	LEU
1	C	103	THR
1	C	124	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	125	THR
1	C	159	THR
1	C	161	ARG
1	C	179	MET
1	C	198	THR
1	C	249	ARG
1	C	294	LEU
1	C	349	PHE
1	C	381	TYR
1	C	426	VAL
1	C	455	LEU
1	C	460	SER
1	C	462	VAL
1	C	473	VAL
1	C	491	LEU
1	C	501	THR
1	C	513	ARG
1	C	519	THR
1	C	547	THR
1	C	574	THR
1	C	616	THR
1	C	618	TYR
1	C	627	VAL
1	C	649	ASP
1	C	657	LEU
1	C	665	THR
1	C	668	VAL
1	D	36	ASP
1	D	47	LEU
1	D	63	GLU
1	D	73	LEU
1	D	103	THR
1	D	124	SER
1	D	159	THR
1	D	179	MET
1	D	198	THR
1	D	239	THR
1	D	249	ARG
1	D	285	SER
1	D	294	LEU
1	D	381	TYR
1	D	426	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	455	LEU
1	D	462	VAL
1	D	473	VAL
1	D	491	LEU
1	D	501	THR
1	D	519	THR
1	D	544	LYS
1	D	547	THR
1	D	566	CYS
1	D	574	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	124	SER
1	E	131	SER
1	E	159	THR
1	E	162	VAL
1	E	167	VAL
1	E	179	MET
1	E	198	THR
1	E	239	THR
1	E	278	SER
1	E	294	LEU
1	E	328	THR
1	E	360	SER
1	E	455	LEU
1	E	460	SER
1	E	462	VAL
1	E	491	LEU
1	E	501	THR
1	E	519	THR
1	E	547	THR
1	E	566	CYS
1	E	616	THR
1	E	618	TYR
1	E	623	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	125	THR
1	F	132	SER
1	F	159	THR
1	F	167	VAL
1	F	198	THR
1	F	239	THR
1	F	249	ARG
1	F	285	SER
1	F	294	LEU
1	F	328	THR
1	F	418	SER
1	F	434	PRO
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	567	SER
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	105	ASN
1	A	207	GLN
1	A	363	GLN
1	A	372	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	169	ASN
1	B	178	ASN
1	B	268	ASN
1	B	309	GLN
1	C	105	ASN
1	C	178	ASN
1	C	247	GLN
1	C	268	ASN
1	C	363	GLN
1	D	101	ASN
1	D	105	ASN
1	D	268	ASN
1	D	363	GLN
1	E	101	ASN
1	E	178	ASN
1	E	640	ASN
1	F	101	ASN
1	F	105	ASN
1	F	136	ASN
1	F	207	GLN
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 ⓘ

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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

Continued on next page...

Continued from previous page...

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

All (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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
3	D	682	BGC	O4-C4-C5	-4.03	99.12	109.28
2	D	679	BGC	O5-C1-C2	-3.92	104.64	110.79
2	C	679	BGC	O5-C1-C2	-3.47	105.36	110.79
2	A	679	BGC	O5-C1-C2	-3.24	105.71	110.79
3	D	684	BGC	C6-C5-C4	-3.23	105.44	113.00
3	D	684	BGC	O6-C6-C5	-3.20	100.57	111.34
3	E	682	BGC	O5-C1-C2	-3.02	106.06	110.79
3	F	681	BGC	O4-C4-C3	-2.91	104.03	110.36
3	C	681	BGC	O4-C4-C3	-2.86	104.13	110.36
3	B	682	BGC	O5-C1-C2	-2.80	106.41	110.79
3	D	684	BGC	O4-C4-C5	-2.76	102.33	109.28
3	A	681	BGC	C6-C5-C4	-2.72	106.63	113.00
3	E	684	BGC	O3-C3-C2	-2.69	105.14	110.02
3	B	684	BGC	O3-C3-C2	-2.67	105.17	110.02
3	D	681	BGC	O3-C3-C4	-2.64	104.62	110.36
3	C	682	BGC	O4-C4-C5	-2.62	102.68	109.28
3	C	685	BGC	O3-C3-C2	-2.54	105.40	110.02
2	E	679	BGC	C3-C4-C5	-2.52	105.77	110.22
3	A	681	BGC	O3-C3-C4	-2.41	105.11	110.36
3	E	681	BGC	C1-C2-C3	-2.40	106.31	110.65
3	F	686	BGC	O5-C1-C2	-2.39	107.04	110.79
3	F	682	BGC	O4-C4-C5	-2.39	103.25	109.28
3	C	684	BGC	O3-C3-C2	-2.38	105.70	110.02
3	B	682	BGC	O4-C4-C5	-2.36	103.34	109.28
3	F	682	BGC	O2-C2-C3	-2.35	105.55	110.17
3	E	684	BGC	O4-C4-C5	-2.30	103.48	109.28
3	F	681	BGC	O5-C1-C2	-2.30	106.22	110.04
3	B	683	BGC	O4-C4-C3	-2.26	105.44	110.36
3	E	682	BGC	O4-C4-C5	-2.23	103.67	109.28
3	A	684	BGC	C6-C5-C4	-2.20	107.85	113.00
3	A	684	BGC	O3-C3-C2	-2.16	106.10	110.02
3	E	686	BGC	O3-C3-C4	-2.15	105.67	110.36
3	B	684	BGC	O5-C1-C2	-2.15	107.42	110.79
3	B	681	BGC	O4-C4-C3	-2.07	105.86	110.36
3	D	683	BGC	O4-C4-C5	-2.02	104.19	109.28
3	D	686	BGC	O4-C4-C3	-2.01	105.97	110.36
3	F	685	BGC	O4-C4-C5	-2.00	104.24	109.28
3	C	686	BGC	C1-O5-C5	2.00	114.93	112.17
2	B	679	BGC	C1-O5-C5	2.01	114.94	112.17
3	E	684	BGC	C1-O5-C5	2.01	114.94	112.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	680	BGC	C1-C2-C3	2.03	112.22	109.65
3	C	683	BGC	O3-C3-C4	2.03	114.77	110.36
3	C	684	BGC	O2-C2-C1	2.09	113.42	109.18
2	E	679	BGC	O2-C2-C3	2.11	114.31	110.17
3	E	685	BGC	C1-O5-C5	2.12	115.08	112.17
3	F	684	BGC	C1-C2-C3	2.13	112.36	109.65
3	D	684	BGC	C3-C4-C5	2.17	114.05	110.22
2	D	679	BGC	C1-O5-C5	2.26	115.28	112.17
2	E	680	BGC	C1-O5-C5	2.35	115.40	112.17
3	C	686	BGC	C1-C2-C3	2.35	112.64	109.65
3	F	681	BGC	O5-C5-C6	2.38	112.11	106.41
2	D	680	BGC	C1-O5-C5	2.43	115.52	112.17
3	F	682	BGC	O3-C3-C4	2.48	115.75	110.36
2	A	679	BGC	C1-O5-C5	2.50	115.62	112.17
3	B	686	BGC	C3-C4-C5	2.51	114.64	110.22
3	D	681	BGC	O5-C5-C4	2.52	114.30	109.66
3	A	684	BGC	C3-C4-C5	2.60	114.80	110.22
3	E	686	BGC	C1-C2-C3	2.67	113.04	109.65
3	E	682	BGC	O3-C3-C4	2.70	116.22	110.36
3	B	681	BGC	O5-C5-C4	2.77	114.76	109.66
3	B	681	BGC	C1-O5-C5	2.81	118.46	113.39
3	F	686	BGC	C1-C2-C3	2.82	113.23	109.65
3	A	684	BGC	C1-O5-C5	2.89	116.16	112.17
3	A	681	BGC	C1-O5-C5	2.95	118.72	113.39
3	A	683	BGC	C1-O5-C5	2.97	116.26	112.17
3	C	683	BGC	C1-O5-C5	2.99	116.29	112.17
3	A	684	BGC	C1-C2-C3	3.03	113.49	109.65
3	A	684	BGC	C2-C3-C4	3.17	116.41	110.88
3	A	681	BGC	C3-C4-C5	3.25	115.94	110.22
3	D	682	BGC	C1-O5-C5	3.28	116.69	112.17
3	B	682	BGC	C1-O5-C5	3.31	116.73	112.17
3	F	686	BGC	C1-O5-C5	3.48	116.97	112.17
3	A	686	BGC	C1-C2-C3	3.53	114.13	109.65
3	F	683	BGC	C1-O5-C5	3.56	117.08	112.17
3	E	686	BGC	C1-O5-C5	3.58	117.10	112.17
3	A	686	BGC	C1-O5-C5	3.66	117.21	112.17
3	A	681	BGC	O5-C5-C4	3.70	116.47	109.66
3	D	681	BGC	C1-O5-C5	3.79	120.23	113.39
3	F	682	BGC	C1-O5-C5	4.02	117.70	112.17
3	D	681	BGC	C3-C4-C5	4.03	117.33	110.22
3	F	685	BGC	C1-O5-C5	4.26	118.04	112.17
3	D	686	BGC	C1-O5-C5	5.33	119.51	112.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	686	BGC	C1-O5-C5	5.45	119.67	112.17
3	D	684	BGC	C1-O5-C5	6.13	120.61	112.17

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
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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	642/678 (94%)	-0.35	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

All (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
1	B	433	ASP	3.5
1	A	196	THR	3.4
1	B	158	ASP	3.3
1	C	196	THR	3.3
1	B	315	THR	3.1
1	E	567	SER	3.1
1	B	159	THR	3.0
1	C	159	THR	3.0
1	B	633	ARG	3.0
1	B	623	TYR	2.9
1	A	124	SER	2.8
1	A	335	GLY	2.8
1	D	544	LYS	2.8
1	C	199	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	593	ALA	2.7
1	C	623	TYR	2.7
1	B	620	GLN	2.7
1	B	125	THR	2.6
1	A	635	GLU	2.6
1	D	433	ASP	2.6
1	B	630	ALA	2.6
1	B	602	GLY	2.5
1	B	481	ASP	2.5
1	C	594	GLY	2.5
1	C	335	GLY	2.5
1	C	336	ALA	2.5
1	B	594	GLY	2.5
1	B	593	ALA	2.5
1	B	62	ASP	2.4
1	A	416	GLY	2.4
1	B	335	GLY	2.3
1	B	199	ARG	2.3
1	E	433	ASP	2.3
1	B	632	LEU	2.3
1	C	337	SER	2.3
1	B	196	THR	2.3
1	C	161	ARG	2.3
1	A	337	SER	2.3
1	F	433	ASP	2.3
1	C	125	THR	2.3
1	C	604	LYS	2.2
1	A	627	VAL	2.2
1	C	315	THR	2.2
1	A	199	ARG	2.2
1	C	633	ARG	2.2
1	F	335	GLY	2.2
1	D	567	SER	2.2
1	E	315	THR	2.1
1	A	433	ASP	2.1
1	C	197	GLY	2.1
1	A	415	ALA	2.1
1	A	594	GLY	2.1
1	F	196	THR	2.1
1	B	625	ASP	2.1
1	C	634	GLY	2.1
1	E	335	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	199	ARG	2.0
1	B	663	ASP	2.0
1	D	335	GLY	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å 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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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.