



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:48 AM UTC

PDB ID : 3QHM / pdb_00003qhm
Title : Crystal analysis of the complex structure, E342A-cellobetraose, of endocellulase from pyrococcus horikoshii
Authors : Kim, H.-W.; Ishikawa, K.
Deposited on : 2011-01-26
Resolution : 2.01 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

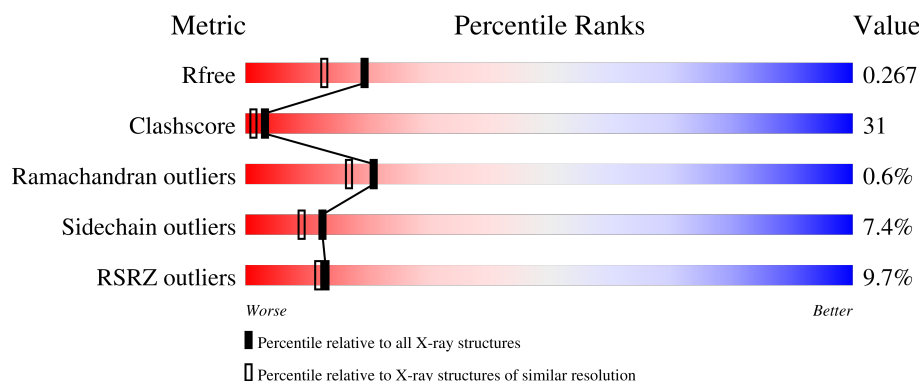
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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.



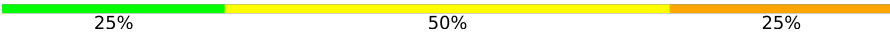
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	458	17% 38% 34% 8% 18%
1	B	458	% 64% 16% 18%
1	C	458	6% 47% 30% 5% 18%
2	D	4	50% 50%
2	E	4	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	4	 25% 50% 25%
3	F	2	 50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9565 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 458aa long hypothetical endo-1,4-beta-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3067	2000	502	555	10			
1	B	377	Total	C	N	O	S	0	0	0
			3067	2000	502	555	10			
1	C	377	Total	C	N	O	S	0	0	0
			3067	2000	502	555	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	342	ALA	GLU	engineered mutation	UNP O58925
B	342	ALA	GLU	engineered mutation	UNP O58925
C	342	ALA	GLU	engineered mutation	UNP O58925

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	4	Total	C	O	0	0	0
			45	24	21			
2	E	4	Total	C	O	0	0	0
			45	24	21			
2	G	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	F	2	Total	C	O	0	0	0
			23	12	11			

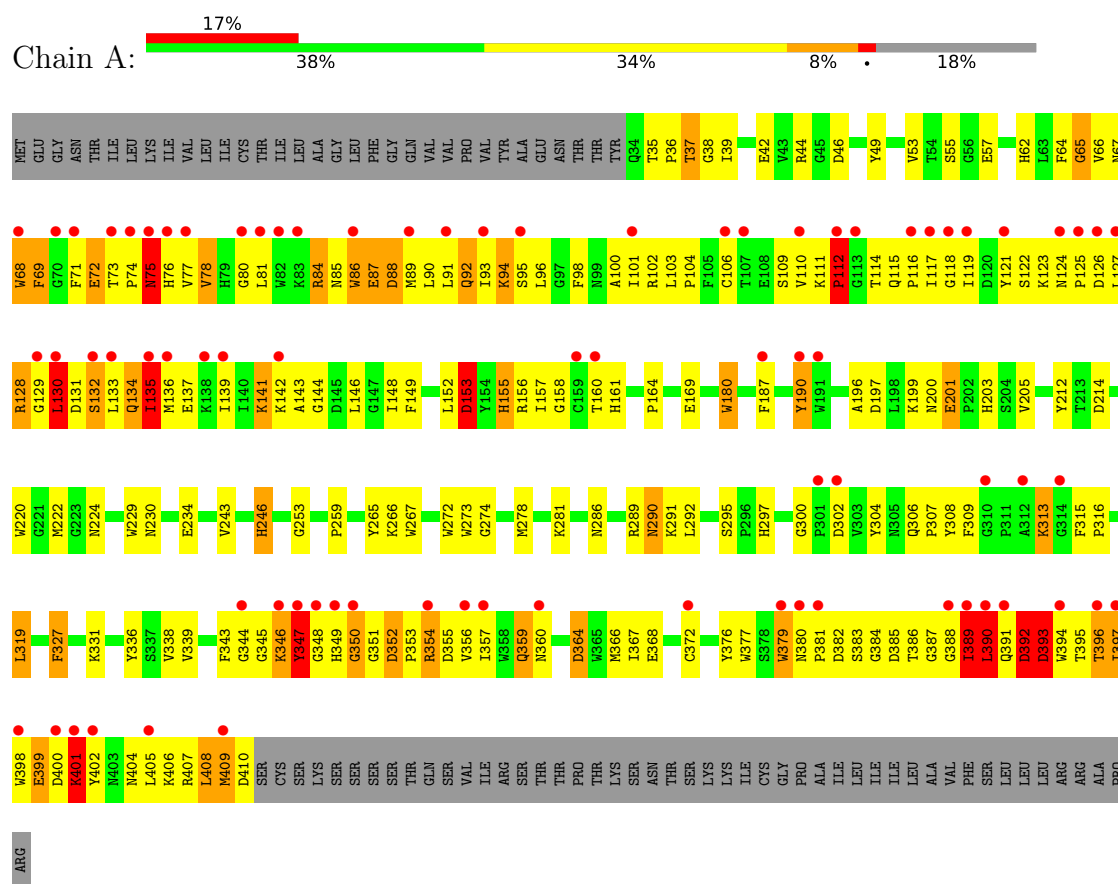
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total	O	0	0
			67	67		
4	B	97	Total	O	0	0
			97	97		
4	C	42	Total	O	0	0
			42	42		

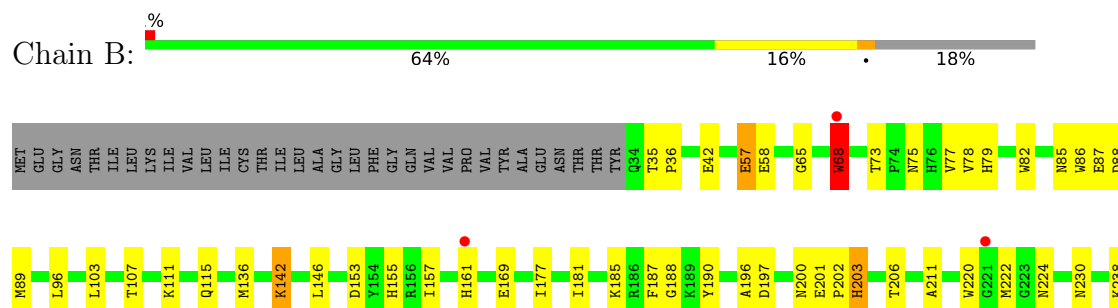
3 Residue-property plots

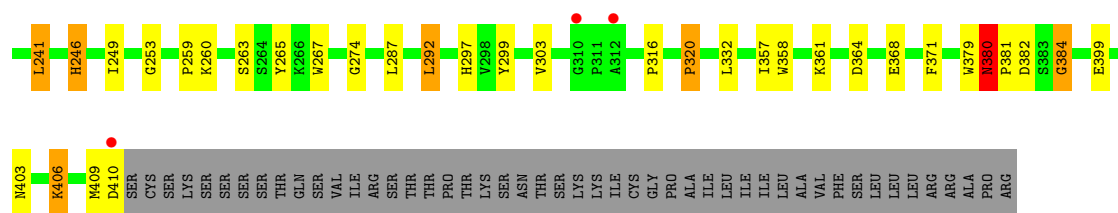
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 458aa long hypothetical endo-1,4-beta-glucanase

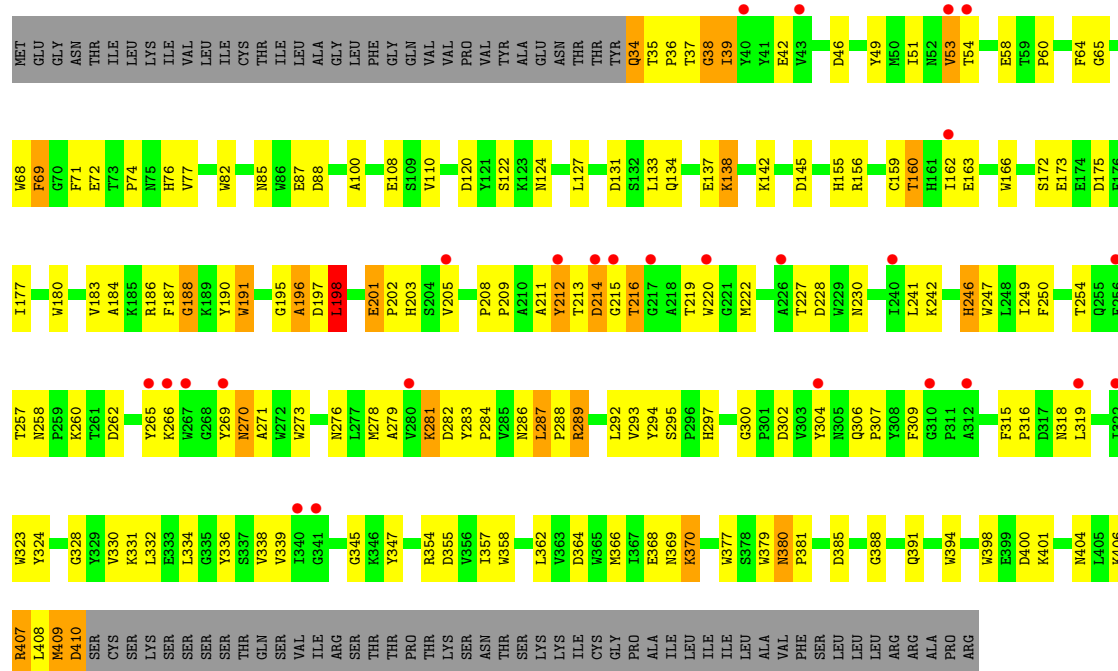


- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase

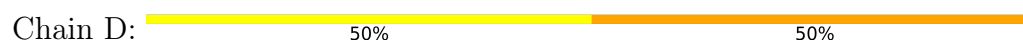




- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase



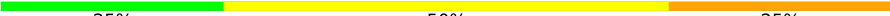
- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain G:  25% 50% 25%



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.53Å 58.60Å 139.06Å 90.00° 109.69° 90.00°	Depositor
Resolution (Å)	35.25 – 2.01 35.25 – 2.01	Depositor EDS
% Data completeness (in resolution range)	87.7 (35.25-2.01) 87.7 (35.25-2.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.261 0.236 , 0.267	Depositor DCC
R_{free} test set	3729 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9565	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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

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	0.46	0/3178	1.26	37/4339 (0.9%)
1	B	0.45	0/3178	1.02	18/4339 (0.4%)
1	C	0.37	0/3178	1.03	21/4339 (0.5%)
All	All	0.43	0/9534	1.11	76/13017 (0.6%)

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	A	0	1

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	ASP	N-CA-C	-14.70	88.06	109.96
1	A	352	ASP	CA-C-N	13.51	136.73	119.84
1	A	352	ASP	C-N-CA	13.51	136.73	119.84
1	A	130	LEU	N-CA-C	12.12	127.34	108.79
1	A	347	TYR	N-CA-C	-10.76	87.89	110.80
1	C	216	THR	N-CA-C	-9.59	100.70	111.82
1	A	115	GLN	CA-C-N	-9.51	107.95	119.84
1	A	115	GLN	C-N-CA	-9.51	107.95	119.84
1	C	379	TRP	N-CA-C	-9.19	101.16	111.82
1	A	135	ILE	N-CA-C	-9.01	100.35	110.62
1	A	157	ILE	N-CA-C	-8.84	101.36	111.00
1	C	213	THR	N-CA-C	8.43	123.76	112.88
1	A	379	TRP	N-CA-C	-8.21	102.97	113.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	TRP	N-CA-C	8.11	120.20	111.36
1	C	195	GLY	N-CA-C	7.91	120.74	110.45
1	B	379	TRP	N-CA-C	-7.86	102.80	111.36
1	A	401	LYS	N-CA-C	-7.66	102.93	111.28
1	A	128	ARG	N-CA-C	7.55	121.36	107.99
1	C	38	GLY	N-CA-C	-7.29	104.50	115.00
1	A	111	LYS	CA-C-N	7.23	128.88	119.84
1	A	111	LYS	C-N-CA	7.23	128.88	119.84
1	A	84	ARG	N-CA-C	7.19	118.08	108.38
1	A	72	GLU	N-CA-C	-6.95	104.72	112.57
1	A	75	ASN	N-CA-C	-6.94	104.08	112.54
1	B	82	TRP	N-CA-C	-6.68	105.13	113.28
1	C	202	PRO	N-CA-C	-6.67	100.73	111.14
1	B	155	HIS	N-CA-C	6.57	119.78	111.69
1	A	348	GLY	N-CA-C	6.48	128.53	113.18
1	C	82	TRP	N-CA-C	-6.39	105.49	113.28
1	C	201	GLU	N-CA-C	6.35	123.84	109.81
1	A	352	ASP	N-CA-C	6.30	123.73	109.81
1	B	157	ILE	N-CA-C	-6.29	104.14	111.00
1	A	155	HIS	N-CA-C	6.19	118.96	111.40
1	A	389	ILE	N-CA-C	-6.17	96.51	109.34
1	C	370	LYS	N-CA-C	6.16	119.74	111.24
1	A	409	MET	N-CA-C	-6.15	104.68	111.82
1	B	384	GLY	N-CA-C	6.15	120.08	112.64
1	A	292	LEU	N-CA-C	6.12	119.61	109.46
1	A	392	ASP	N-CA-C	6.09	118.42	111.11
1	A	197	ASP	N-CA-C	-6.08	97.28	107.99
1	A	69	PHE	N-CA-C	6.02	117.82	110.41
1	B	68	TRP	CA-CB-CG	5.91	124.83	113.60
1	B	202	PRO	N-CA-C	-5.84	102.03	111.14
1	C	300	GLY	CA-C-N	5.81	125.67	119.28
1	C	300	GLY	C-N-CA	5.81	125.67	119.28
1	B	65	GLY	N-CA-C	5.80	122.66	112.10
1	C	69	PHE	N-CA-C	5.80	119.10	110.52
1	C	188	GLY	N-CA-C	-5.80	107.14	114.16
1	C	155	HIS	N-CA-C	5.80	118.82	111.69
1	B	381	PRO	N-CA-C	-5.77	106.16	114.18
1	A	273	TRP	N-CA-C	-5.73	101.57	110.10
1	A	364	ASP	N-CA-C	-5.72	104.95	111.07
1	C	273	TRP	N-CA-C	-5.71	101.60	110.10
1	A	347	TYR	CA-CB-CG	5.70	124.16	113.90
1	C	212	TYR	N-CA-C	5.64	118.37	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	409	MET	N-CA-C	-5.50	105.83	112.54
1	A	122	SER	N-CA-C	-5.47	105.48	111.82
1	B	197	ASP	N-CA-C	-5.41	97.80	107.98
1	C	198	LEU	N-CA-C	5.40	120.23	111.37
1	A	65	GLY	N-CA-C	5.36	121.96	112.64
1	B	292	LEU	N-CA-C	5.35	118.33	109.46
1	B	371	PHE	N-CA-C	-5.32	99.31	108.56
1	C	191	TRP	N-CA-C	5.29	117.73	111.33
1	A	201	GLU	N-CA-C	5.28	121.48	109.81
1	C	160	THR	N-CA-C	5.26	119.93	112.93
1	B	332	LEU	N-CA-C	5.17	116.91	111.28
1	A	300	GLY	CA-C-N	5.16	124.96	119.28
1	A	300	GLY	C-N-CA	5.16	124.96	119.28
1	A	112	PRO	N-CA-C	5.12	123.02	112.47
1	B	196	ALA	N-CA-C	5.11	117.24	108.90
1	A	153	ASP	N-CA-C	5.07	116.67	108.41
1	B	224	ASN	CA-C-N	5.03	125.30	119.47
1	B	224	ASN	C-N-CA	5.03	125.30	119.47
1	B	203	HIS	N-CA-C	5.01	114.76	108.45
1	C	196	ALA	N-CA-C	5.01	117.23	108.76
1	B	380	ASN	CB-CA-C	-5.01	101.61	109.52

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347	TYR	Sidechain

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	3067	0	2909	338	1
1	B	3067	0	2909	69	0
1	C	3067	0	2909	160	0
2	D	45	0	38	3	0
2	E	45	0	39	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	45	0	39	2	0
3	F	23	0	21	2	0
4	A	67	0	0	18	0
4	B	97	0	0	10	2
4	C	42	0	0	5	2
All	All	9565	0	8864	564	3

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 31.

All (564) 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:406:LYS:HA	1:A:409:MET:HE3	1.23	1.19
1:A:381:PRO:HA	1:A:388:GLY:H	1.10	1.12
1:A:389:ILE:HD13	1:A:401:LYS:HE3	1.31	1.10
1:A:76:HIS:CD2	1:A:114:THR:HG21	1.90	1.05
1:A:402:TYR:HA	4:A:515:HOH:O	1.58	1.02
1:A:131:ASP:O	1:A:133:LEU:N	1.93	1.01
1:A:131:ASP:OD2	1:A:134:GLN:CG	2.11	0.99
1:A:112:PRO:O	1:A:131:ASP:HB3	1.62	0.99
1:A:131:ASP:OD2	1:A:134:GLN:HG2	1.62	0.99
1:A:87:GLU:HA	1:A:90:LEU:HD13	1.45	0.98
1:A:389:ILE:CD1	1:A:401:LYS:HE3	1.93	0.97
1:A:130:LEU:HB2	1:A:134:GLN:HG3	1.46	0.97
1:A:347:TYR:OH	1:A:360:ASN:CG	2.08	0.96
1:A:75:ASN:H	1:A:75:ASN:HD22	1.02	0.95
1:A:131:ASP:OD2	1:A:134:GLN:CD	2.10	0.95
1:A:133:LEU:O	1:A:137:GLU:HG3	1.66	0.95
1:A:89:MET:HE1	1:A:394:TRP:CE3	2.02	0.95
1:A:131:ASP:C	1:A:133:LEU:H	1.76	0.92
1:C:211:ALA:HA	1:C:216:THR:HG21	1.51	0.92
1:A:75:ASN:H	1:A:75:ASN:ND2	1.58	0.92
1:A:119:ILE:HG13	1:A:121:TYR:CE1	2.05	0.92
1:A:390:LEU:HA	1:A:397:ILE:HA	1.53	0.90
1:B:380:ASN:H	1:B:380:ASN:HD22	1.18	0.89
1:A:89:MET:HE1	1:A:394:TRP:HE3	1.37	0.88
1:C:269:TYR:C	1:C:270:ASN:HD22	1.80	0.88
1:A:88:ASP:O	1:A:92:GLN:HB2	1.74	0.88
1:A:381:PRO:HA	1:A:388:GLY:N	1.87	0.88
1:A:85:ASN:HD21	1:A:87:GLU:HG2	1.39	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:HA	4:A:513:HOH:O	1.72	0.87
1:A:77:VAL:HG23	1:A:116:PRO:HB3	1.56	0.86
1:A:68:TRP:CE2	1:A:78:VAL:HG11	2.11	0.86
1:A:75:ASN:HD22	1:A:75:ASN:N	1.75	0.85
1:A:146:LEU:HD11	4:A:473:HOH:O	1.76	0.85
1:C:201:GLU:OE2	1:C:297:HIS:HD2	1.58	0.85
1:C:318:ASN:OD1	1:C:319:LEU:HD12	1.75	0.85
1:A:224:ASN:HD21	1:B:75:ASN:HD21	1.27	0.83
1:A:78:VAL:HG12	4:A:502:HOH:O	1.80	0.82
1:C:198:LEU:HD21	1:C:249:ILE:CG2	2.10	0.82
1:B:146:LEU:HG	4:B:532:HOH:O	1.77	0.82
1:A:389:ILE:CG2	1:A:389:ILE:O	2.27	0.82
1:A:81:LEU:O	1:A:81:LEU:HD23	1.79	0.81
1:C:198:LEU:HD21	1:C:249:ILE:HG23	1.60	0.81
1:A:68:TRP:CZ2	1:A:78:VAL:HG11	2.15	0.81
1:A:129:GLY:C	1:A:130:LEU:HD22	2.06	0.81
1:A:364:ASP:O	1:A:368:GLU:HG3	1.81	0.81
1:A:131:ASP:O	1:A:134:GLN:N	2.14	0.80
1:B:384:GLY:HA3	4:B:524:HOH:O	1.81	0.80
1:C:85:ASN:HD22	1:C:88:ASP:H	1.29	0.80
1:C:214:ASP:OD1	1:C:216:THR:HB	1.82	0.80
1:C:254:THR:O	1:C:276:ASN:HB3	1.81	0.79
1:A:266:LYS:HE2	1:A:267:TRP:NE1	1.98	0.79
1:C:205:VAL:HG22	1:C:216:THR:O	1.83	0.78
1:C:270:ASN:HD22	1:C:270:ASN:N	1.80	0.78
1:A:131:ASP:C	1:A:133:LEU:N	2.38	0.77
1:A:85:ASN:HA	1:A:124:ASN:HD21	1.50	0.77
1:A:315:PHE:CE2	1:A:354:ARG:HG2	2.20	0.77
1:A:393:ASP:OD2	1:A:396:THR:HG22	1.85	0.77
1:A:290:ASN:H	1:A:290:ASN:HD22	1.31	0.76
1:C:214:ASP:C	1:C:216:THR:H	1.93	0.76
1:A:347:TYR:HH	1:A:360:ASN:CG	1.88	0.76
1:C:35:THR:HG22	1:C:38:GLY:H	1.49	0.76
1:C:35:THR:HG22	1:C:37:THR:H	1.51	0.75
1:A:381:PRO:HD2	1:A:394:TRP:CH2	2.20	0.75
1:A:347:TYR:CD1	1:A:356:VAL:HA	2.22	0.74
1:A:349:HIS:C	1:A:351:GLY:N	2.42	0.74
1:A:389:ILE:O	1:A:389:ILE:HG22	1.87	0.74
1:C:124:ASN:HB3	1:C:127:LEU:HD12	1.69	0.74
1:A:71:PHE:HB2	1:A:104:PRO:O	1.87	0.74
1:A:81:LEU:HD22	1:A:119:ILE:HB	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:TYR:N	1:A:190:TYR:HD2	1.85	0.74
1:A:347:TYR:OH	1:A:360:ASN:OD1	2.04	0.74
1:A:214:ASP:HB3	4:B:524:HOH:O	1.86	0.74
1:A:37:THR:HG22	1:A:39:ILE:H	1.53	0.74
1:A:75:ASN:HA	1:A:117:ILE:HB	1.70	0.74
1:B:253:GLY:O	1:B:274:GLY:HA2	1.87	0.74
1:C:64:PHE:HB3	1:C:409:MET:HE3	1.69	0.73
1:A:381:PRO:HD2	1:A:394:TRP:CZ2	2.24	0.73
1:A:73:THR:HB	1:A:74:PRO:HD2	1.69	0.73
1:A:71:PHE:HZ	1:A:135:ILE:HD11	1.52	0.73
1:A:89:MET:O	1:A:93:ILE:HG12	1.89	0.72
1:A:190:TYR:N	1:A:190:TYR:CD2	2.56	0.72
1:C:306:GLN:OE1	1:C:307:PRO:HD2	1.88	0.72
1:A:144:GLY:HA3	4:A:501:HOH:O	1.88	0.72
1:A:112:PRO:O	1:A:131:ASP:CB	2.37	0.72
1:C:35:THR:HG21	1:C:39:ILE:O	1.90	0.72
1:A:75:ASN:ND2	1:A:75:ASN:N	2.34	0.71
1:A:81:LEU:HB2	4:A:502:HOH:O	1.89	0.71
1:A:76:HIS:O	1:A:132:SER:HB3	1.89	0.71
1:A:76:HIS:CD2	1:A:114:THR:CG2	2.71	0.71
1:C:214:ASP:O	1:C:216:THR:N	2.19	0.71
1:B:380:ASN:HD22	1:B:380:ASN:N	1.89	0.71
1:A:349:HIS:C	1:A:351:GLY:H	1.97	0.70
1:B:241:LEU:HD13	1:B:249:ILE:HD11	1.74	0.70
1:C:35:THR:HG22	1:C:37:THR:N	2.06	0.70
1:C:35:THR:CG2	1:C:38:GLY:H	2.05	0.70
1:A:407:ARG:O	1:A:410:ASP:HB3	1.92	0.69
1:A:347:TYR:CD2	1:A:356:VAL:HG13	2.28	0.69
1:C:201:GLU:OE2	1:C:297:HIS:CD2	2.44	0.69
1:A:68:TRP:HH2	1:A:89:MET:HE3	1.58	0.69
1:B:96:LEU:O	1:B:409:MET:HE1	1.91	0.69
1:A:86:TRP:O	1:A:89:MET:HB2	1.92	0.68
1:A:345:GLY:O	1:A:346:LYS:HG3	1.92	0.68
1:A:390:LEU:HD23	1:A:391:GLN:H	1.57	0.68
1:A:349:HIS:O	1:A:351:GLY:N	2.26	0.68
1:A:86:TRP:O	1:A:90:LEU:HD12	1.94	0.67
1:A:87:GLU:HA	1:A:90:LEU:CD1	2.23	0.67
1:C:391:GLN:HG2	1:C:398:TRP:CE2	2.30	0.67
1:C:330:VAL:HG12	1:C:336:TYR:HB2	1.75	0.67
1:A:68:TRP:HE3	1:A:380:ASN:HD21	1.41	0.66
1:A:199:LYS:HE2	1:A:200:ASN:O	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:HB3	4:A:515:HOH:O	1.95	0.66
1:A:68:TRP:CG	1:A:78:VAL:HG21	2.30	0.66
1:A:390:LEU:O	1:A:391:GLN:HG3	1.96	0.66
1:C:316:PRO:O	1:C:319:LEU:HD13	1.95	0.66
1:A:84:ARG:NH1	1:A:394:TRP:O	2.28	0.66
1:A:91:LEU:HD23	4:A:473:HOH:O	1.94	0.66
1:C:289:ARG:NH1	1:C:336:TYR:CE1	2.64	0.66
1:A:346:LYS:HA	1:A:401:LYS:HG3	1.78	0.66
1:B:201:GLU:OE2	1:B:297:HIS:HD2	1.79	0.66
1:A:346:LYS:HE3	1:A:386:THR:C	2.20	0.65
1:B:403:ASN:HA	1:B:406:LYS:CD	2.26	0.65
1:B:85:ASN:HD22	1:B:88:ASP:H	1.44	0.65
1:A:397:ILE:HG22	4:A:478:HOH:O	1.97	0.65
1:A:93:ILE:HD11	1:A:379:TRP:CD2	2.32	0.65
1:A:71:PHE:CZ	1:A:135:ILE:HD11	2.31	0.64
1:B:246:HIS:CD2	1:B:246:HIS:H	2.15	0.64
1:B:364:ASP:O	1:B:368:GLU:HG3	1.97	0.64
1:A:81:LEU:HD22	1:A:119:ILE:CG2	2.27	0.64
1:A:399:GLU:CD	1:A:399:GLU:H	2.03	0.64
1:A:402:TYR:OH	1:A:406:LYS:NZ	2.31	0.64
1:A:84:ARG:HD3	1:A:89:MET:CE	2.28	0.64
1:C:354:ARG:HA	1:C:357:ILE:HD12	1.80	0.64
1:C:380:ASN:HD22	1:C:380:ASN:H	1.46	0.64
1:A:85:ASN:ND2	1:A:87:GLU:HG2	2.13	0.63
1:A:366:MET:HB2	1:A:408:LEU:HD11	1.81	0.63
1:B:403:ASN:HA	1:B:406:LYS:HD3	1.80	0.63
1:C:208:PRO:HA	1:C:211:ALA:H	1.64	0.63
1:A:84:ARG:HD3	1:A:89:MET:HE2	1.81	0.63
1:A:364:ASP:OD1	1:A:407:ARG:NH2	2.27	0.62
1:A:119:ILE:HG13	1:A:121:TYR:HE1	1.62	0.62
1:C:198:LEU:HD22	1:C:198:LEU:H	1.65	0.62
1:C:219:THR:HG22	1:C:227:THR:C	2.25	0.62
1:A:85:ASN:HA	1:A:124:ASN:ND2	2.14	0.62
1:A:77:VAL:HG12	1:A:78:VAL:O	1.99	0.62
1:A:380:ASN:C	1:A:388:GLY:HA3	2.24	0.62
1:A:392:ASP:O	1:A:393:ASP:C	2.41	0.62
1:A:246:HIS:H	1:A:246:HIS:CD2	2.16	0.61
1:A:347:TYR:CE1	1:A:356:VAL:O	2.53	0.61
1:C:306:GLN:HB2	1:C:309:PHE:CE2	2.35	0.61
1:C:246:HIS:H	1:C:246:HIS:CD2	2.17	0.61
1:A:62:HIS:CD2	1:A:372:CYS:SG	2.94	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:TYR:CE1	1:C:60:PRO:HG3	2.35	0.61
1:A:81:LEU:HD22	1:A:119:ILE:CB	2.30	0.61
1:B:142:LYS:HE2	1:B:146:LEU:HD11	1.83	0.61
1:C:316:PRO:HG3	1:C:357:ILE:CG2	2.31	0.61
1:A:160:THR:HB	1:A:161:HIS:HD2	1.66	0.60
1:C:39:ILE:HD13	1:C:191:TRP:HB2	1.83	0.60
1:C:76:HIS:NE2	1:C:159:CYS:SG	2.74	0.60
1:A:72:GLU:O	1:A:72:GLU:HG2	2.02	0.60
1:B:68:TRP:CH2	1:B:89:MET:HE3	2.36	0.60
1:A:352:ASP:OD2	1:A:352:ASP:C	2.43	0.60
1:A:392:ASP:O	1:A:394:TRP:N	2.35	0.60
1:C:276:ASN:OD1	1:C:278:MET:HG3	2.01	0.60
1:A:344:GLY:HA3	1:A:377:TRP:O	2.02	0.60
1:B:297:HIS:HE1	4:B:484:HOH:O	1.84	0.60
1:C:137:GLU:OE2	1:C:186:ARG:HD3	2.01	0.60
1:A:80:GLY:HA3	1:A:394:TRP:CE3	2.37	0.59
1:A:55:SER:OG	1:A:57:GLU:HG3	2.02	0.59
1:B:79:HIS:HD2	1:B:382:ASP:OD2	1.85	0.59
1:A:93:ILE:HD13	1:A:379:TRP:CE3	2.38	0.59
1:A:133:LEU:O	1:A:136:MET:HB3	2.03	0.59
1:C:219:THR:HG23	1:C:228:ASP:OD1	2.02	0.59
1:C:306:GLN:HB2	1:C:309:PHE:CD2	2.37	0.59
1:A:383:SER:O	1:A:385:ASP:N	2.36	0.59
1:C:271:ALA:CB	1:C:276:ASN:HB2	2.33	0.59
1:A:156:ARG:HB3	1:A:158:GLY:O	2.03	0.58
1:C:163:GLU:HB3	4:C:462:HOH:O	2.01	0.58
1:A:84:ARG:HD3	1:A:89:MET:SD	2.43	0.58
1:A:86:TRP:H	1:A:124:ASN:HD21	1.51	0.58
1:C:319:LEU:HD12	1:C:319:LEU:H	1.67	0.58
1:A:77:VAL:HG23	1:A:116:PRO:CB	2.30	0.58
1:C:34:GLN:HG3	1:C:53:VAL:HG21	1.84	0.58
1:A:90:LEU:O	1:A:93:ILE:HB	2.02	0.58
1:A:121:TYR:O	1:A:125:PRO:HG3	2.03	0.58
1:A:379:TRP:CE3	1:A:389:ILE:HG22	2.39	0.58
1:C:315:PHE:CE1	1:C:316:PRO:HB3	2.39	0.58
1:A:352:ASP:OD2	1:A:353:PRO:N	2.36	0.58
1:A:391:GLN:O	1:A:393:ASP:O	2.21	0.58
1:C:180:TRP:O	1:C:183:VAL:HG22	2.03	0.58
1:A:96:LEU:HD22	1:A:402:TYR:CZ	2.39	0.57
1:A:135:ILE:HG13	1:A:136:MET:N	2.19	0.57
1:A:68:TRP:CE3	1:A:68:TRP:HA	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LYS:HE2	1:B:146:LEU:CD1	2.34	0.57
1:C:138:LYS:HD2	4:C:471:HOH:O	2.03	0.57
1:C:407:ARG:HG2	1:C:407:ARG:HH11	1.69	0.57
1:C:120:ASP:OD1	1:C:122:SER:HB3	2.04	0.57
1:C:347:TYR:HB2	1:C:401:LYS:HD3	1.86	0.57
1:A:67:ASN:OD1	1:A:102:ARG:HB3	2.05	0.57
1:A:265:TYR:HB3	1:A:278:MET:HE1	1.87	0.57
1:A:352:ASP:OD2	1:A:354:ARG:N	2.38	0.57
1:A:400:ASP:OD1	1:A:400:ASP:N	2.38	0.57
1:A:391:GLN:OE1	1:A:396:THR:HG23	2.05	0.57
1:B:85:ASN:HD21	1:B:87:GLU:HB3	1.68	0.57
1:A:96:LEU:O	1:A:406:LYS:HE2	2.05	0.57
1:C:214:ASP:C	1:C:216:THR:N	2.59	0.57
1:A:66:VAL:CG2	1:A:101:ILE:HG22	2.34	0.57
1:C:324:TYR:HA	1:C:328:GLY:HA3	1.87	0.57
1:C:108:GLU:HG3	4:C:493:HOH:O	2.03	0.56
1:C:380:ASN:HD22	1:C:380:ASN:N	2.03	0.56
1:A:68:TRP:HE3	1:A:68:TRP:HA	1.71	0.56
1:A:135:ILE:C	1:A:135:ILE:HD12	2.30	0.56
1:A:376:TYR:HB3	4:A:517:HOH:O	2.06	0.56
1:C:35:THR:CG2	1:C:37:THR:H	2.18	0.56
1:C:180:TRP:CH2	1:C:196:ALA:HB1	2.41	0.56
1:A:72:GLU:HG3	1:A:155:HIS:CD2	2.40	0.56
1:C:297:HIS:HE1	4:C:474:HOH:O	1.89	0.56
1:A:347:TYR:OH	1:A:360:ASN:ND2	2.38	0.56
1:B:320:PRO:HD3	1:B:361:LYS:HZ3	1.71	0.56
1:B:403:ASN:O	1:B:406:LYS:HG2	2.06	0.56
1:A:65:GLY:HA2	1:A:100:ALA:O	2.06	0.56
1:A:267:TRP:CZ3	1:A:307:PRO:HG2	2.41	0.56
1:A:66:VAL:HG21	1:A:93:ILE:HD12	1.86	0.56
1:A:359:GLN:NE2	1:A:376:TYR:OH	2.39	0.56
1:C:220:TRP:CE2	1:C:230:ASN:HB3	2.41	0.56
1:C:209:PRO:HA	1:C:212:TYR:CD2	2.41	0.55
1:A:80:GLY:HA3	1:A:394:TRP:CD2	2.42	0.55
1:A:66:VAL:HG23	1:A:101:ILE:HG22	1.89	0.55
1:C:270:ASN:N	1:C:270:ASN:ND2	2.53	0.55
1:A:390:LEU:CD2	1:A:391:GLN:H	2.20	0.55
1:A:212:TYR:HB3	1:A:222:MET:HE2	1.89	0.54
1:A:93:ILE:CD1	1:A:379:TRP:CD2	2.90	0.54
1:A:404:ASN:O	1:A:407:ARG:HD3	2.06	0.54
1:C:201:GLU:O	1:C:203:HIS:HD2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:LYS:HB2	1:B:406:LYS:NZ	2.23	0.54
1:A:62:HIS:HD2	1:A:372:CYS:SG	2.30	0.54
1:A:102:ARG:O	1:A:104:PRO:HD3	2.08	0.54
1:A:297:HIS:HE1	4:A:489:HOH:O	1.89	0.54
1:A:94:LYS:NZ	1:A:146:LEU:HB3	2.23	0.53
1:A:180:TRP:CH2	1:A:196:ALA:HB1	2.43	0.53
1:C:219:THR:OG1	1:C:222:MET:HG2	2.08	0.53
1:C:400:ASP:OD1	1:C:401:LYS:N	2.41	0.53
1:C:404:ASN:O	1:C:407:ARG:HB2	2.08	0.53
1:A:76:HIS:HB3	1:A:132:SER:OG	2.08	0.53
1:A:117:ILE:CG2	1:A:118:GLY:N	2.72	0.53
1:C:409:MET:O	1:C:410:ASP:HB2	2.07	0.53
1:C:364:ASP:O	1:C:368:GLU:HG3	2.08	0.53
1:B:246:HIS:H	1:B:246:HIS:HD2	1.56	0.53
1:A:380:ASN:O	1:A:388:GLY:N	2.42	0.53
1:B:200:ASN:CG	1:B:201:GLU:HG3	2.34	0.53
1:C:262:ASP:HA	1:C:278:MET:HE1	1.90	0.53
1:A:380:ASN:C	1:A:388:GLY:CA	2.82	0.53
1:A:64:PHE:CZ	1:A:409:MET:HA	2.43	0.53
1:A:131:ASP:O	1:A:134:GLN:HG2	2.08	0.53
1:A:346:LYS:HE3	1:A:386:THR:CA	2.39	0.53
1:A:289:ARG:HB2	1:C:145:ASP:HA	1.91	0.52
1:A:161:HIS:HA	4:A:508:HOH:O	2.08	0.52
1:C:35:THR:OG1	1:C:246:HIS:HB3	2.09	0.52
1:A:94:LYS:HD3	4:A:499:HOH:O	2.08	0.52
1:C:219:THR:CG2	1:C:227:THR:OG1	2.57	0.52
1:C:220:TRP:HB3	1:C:257:THR:HB	1.90	0.52
1:C:246:HIS:H	1:C:246:HIS:HD2	1.57	0.52
1:A:347:TYR:CA	1:A:356:VAL:HG22	2.39	0.52
1:A:367:ILE:HG13	1:A:408:LEU:HG	1.91	0.52
1:C:37:THR:HG22	1:C:39:ILE:HD12	1.91	0.52
1:A:130:LEU:HD22	1:A:130:LEU:N	2.24	0.52
1:A:86:TRP:HD1	1:A:124:ASN:ND2	2.08	0.51
1:A:94:LYS:HE2	4:A:488:HOH:O	2.10	0.51
1:A:381:PRO:O	1:A:387:GLY:HA2	2.10	0.51
1:B:265:TYR:CE2	1:B:267:TRP:HB2	2.45	0.51
1:A:90:LEU:HD21	1:A:142:LYS:HB3	1.91	0.51
1:A:68:TRP:CZ2	1:A:78:VAL:CG1	2.89	0.51
1:A:87:GLU:O	1:A:91:LEU:N	2.37	0.51
1:A:128:ARG:C	1:A:130:LEU:HD22	2.36	0.51
1:A:379:TRP:CE3	1:A:389:ILE:CG2	2.94	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ILE:HD12	1:B:357:ILE:H	1.75	0.51
1:A:81:LEU:CD2	1:A:119:ILE:HB	2.39	0.51
1:C:198:LEU:HD22	1:C:250:PHE:O	2.09	0.51
1:A:347:TYR:CB	1:A:356:VAL:HG22	2.41	0.51
1:A:349:HIS:O	1:A:350:GLY:C	2.54	0.51
1:A:389:ILE:O	1:A:389:ILE:HG23	2.09	0.51
1:C:156:ARG:HG2	1:C:162:ILE:HG22	1.91	0.51
1:A:93:ILE:HD11	1:A:379:TRP:CG	2.45	0.51
1:A:73:THR:HB	1:A:75:ASN:ND2	2.25	0.51
1:A:380:ASN:O	1:A:388:GLY:CA	2.59	0.51
1:C:35:THR:HG21	1:C:39:ILE:H	1.75	0.51
1:C:131:ASP:OD1	1:C:134:GLN:HG3	2.11	0.51
1:A:130:LEU:HB3	1:A:134:GLN:HE21	1.76	0.51
1:A:77:VAL:CG1	1:A:78:VAL:N	2.74	0.50
1:C:110:VAL:HA	1:C:133:LEU:HD13	1.92	0.50
1:C:85:ASN:HD21	1:C:87:GLU:HB2	1.75	0.50
1:A:94:LYS:HG3	1:A:95:SER:N	2.25	0.50
1:C:208:PRO:HB2	1:C:212:TYR:CE2	2.46	0.50
1:C:163:GLU:CD	1:C:163:GLU:H	2.19	0.50
1:C:219:THR:HG22	1:C:227:THR:O	2.12	0.50
1:A:201:GLU:O	1:A:203:HIS:HD2	1.95	0.50
1:C:201:GLU:O	1:C:203:HIS:CD2	2.65	0.50
1:A:152:LEU:HD11	1:A:187:PHE:HB3	1.93	0.50
1:A:405:LEU:CB	4:A:515:HOH:O	2.56	0.50
1:C:316:PRO:HG3	1:C:357:ILE:HG21	1.94	0.50
1:C:377:TRP:CZ2	2:G:1:BGC:H3	2.47	0.50
1:A:84:ARG:CZ	1:A:394:TRP:O	2.59	0.49
1:A:156:ARG:CB	1:A:158:GLY:O	2.59	0.49
1:B:200:ASN:ND2	1:B:201:GLU:HG3	2.27	0.49
1:C:220:TRP:NE1	1:C:230:ASN:HB3	2.26	0.49
1:B:181:ILE:O	1:B:185:LYS:HG3	2.12	0.49
1:A:69:PHE:CD1	1:A:69:PHE:C	2.89	0.49
1:A:73:THR:OG1	1:A:75:ASN:ND2	2.45	0.49
1:A:89:MET:HE1	1:A:394:TRP:CZ3	2.44	0.49
1:A:347:TYR:CE2	1:A:356:VAL:HG13	2.48	0.49
1:A:87:GLU:O	1:A:91:LEU:HG	2.13	0.49
1:A:253:GLY:O	1:A:274:GLY:HA2	2.13	0.49
1:A:397:ILE:HD13	1:A:397:ILE:O	2.13	0.49
1:B:177:ILE:O	1:B:181:ILE:HG13	2.12	0.49
1:C:85:ASN:ND2	1:C:88:ASP:H	2.05	0.49
1:C:219:THR:HG23	1:C:228:ASP:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:TRP:HZ2	4:B:549:HOH:O	1.95	0.49
1:A:68:TRP:HB3	1:A:103:LEU:CD2	2.42	0.49
1:A:212:TYR:CD2	1:A:259:PRO:HD3	2.46	0.49
1:A:389:ILE:O	1:A:390:LEU:CB	2.57	0.49
1:A:393:ASP:O	1:A:395:THR:N	2.42	0.49
1:B:68:TRP:CZ3	1:B:79:HIS:O	2.66	0.49
1:A:266:LYS:HE2	1:A:267:TRP:HE1	1.77	0.49
1:A:135:ILE:HD12	1:A:139:ILE:HG13	1.95	0.49
1:B:203:HIS:HE1	4:B:512:HOH:O	1.96	0.49
1:B:259:PRO:O	1:B:263:SER:OG	2.26	0.49
1:B:380:ASN:HB3	1:B:382:ASP:OD1	2.13	0.49
1:A:90:LEU:HD22	1:A:142:LYS:CG	2.43	0.48
1:B:201:GLU:O	1:B:203:HIS:HD2	1.95	0.48
1:A:153:ASP:C	1:A:153:ASP:OD1	2.55	0.48
1:A:391:GLN:HE21	1:A:398:TRP:CD1	2.30	0.48
1:C:71:PHE:CE1	1:C:77:VAL:HA	2.48	0.48
1:A:94:LYS:NZ	1:A:94:LYS:HB2	2.28	0.48
1:A:134:GLN:O	1:A:135:ILE:C	2.54	0.48
1:C:270:ASN:OD1	1:C:307:PRO:HG3	2.14	0.48
1:A:85:ASN:CA	1:A:124:ASN:HD21	2.24	0.48
1:A:123:LYS:C	1:A:125:PRO:HD3	2.38	0.48
1:A:130:LEU:N	1:A:130:LEU:CD2	2.77	0.48
1:A:155:HIS:HA	1:A:200:ASN:CB	2.44	0.48
1:A:234:GLU:OE1	1:A:286:ASN:HB3	2.14	0.48
1:A:383:SER:C	1:A:385:ASP:N	2.70	0.48
1:A:77:VAL:HG12	1:A:78:VAL:N	2.28	0.48
1:A:331:LYS:HB2	1:A:338:VAL:CG2	2.44	0.48
1:A:73:THR:HB	1:A:75:ASN:HD21	1.77	0.47
1:C:187:PHE:HA	1:C:190:TYR:HD2	1.79	0.47
1:A:391:GLN:HB2	1:A:396:THR:HG23	1.95	0.47
1:C:332:LEU:HD21	1:C:369:ASN:HB3	1.97	0.47
1:A:376:TYR:CD2	1:A:389:ILE:HG12	2.50	0.47
1:B:86:TRP:CH2	1:B:142:LYS:HG3	2.50	0.47
1:C:166:TRP:NE1	1:C:173:GLU:OE1	2.43	0.47
1:A:69:PHE:CZ	1:A:382:ASP:OD1	2.67	0.47
1:A:73:THR:CB	1:A:75:ASN:ND2	2.77	0.47
1:A:347:TYR:HA	1:A:356:VAL:HA	1.96	0.47
1:A:385:ASP:OD1	2:D:3:BGC:H5	2.14	0.47
1:A:68:TRP:CE3	1:A:380:ASN:ND2	2.81	0.47
1:A:69:PHE:O	1:A:78:VAL:HA	2.13	0.47
1:A:132:SER:O	1:A:136:MET:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:HIS:HA	1:A:200:ASN:HB3	1.97	0.47
1:A:386:THR:C	1:A:387:GLY:O	2.57	0.47
1:B:107:THR:O	1:B:111:LYS:HG2	2.15	0.47
1:C:201:GLU:CD	2:G:1:BGC:O1	2.58	0.47
1:A:76:HIS:HB2	1:A:116:PRO:HA	1.96	0.47
1:A:89:MET:CE	1:A:394:TRP:CE3	2.88	0.47
1:A:366:MET:CB	1:A:408:LEU:HD11	2.43	0.47
1:B:75:ASN:ND2	4:B:516:HOH:O	2.47	0.47
1:C:381:PRO:HD2	1:C:394:TRP:CH2	2.49	0.47
1:A:49:TYR:OH	1:C:54:THR:HG21	2.15	0.47
1:A:69:PHE:CD2	1:A:377:TRP:CZ2	3.03	0.47
1:A:161:HIS:N	1:A:161:HIS:CD2	2.82	0.47
1:A:346:LYS:HE3	1:A:386:THR:HA	1.95	0.47
1:B:222:MET:SD	1:B:259:PRO:HD3	2.55	0.47
1:C:406:LYS:O	1:C:410:ASP:N	2.47	0.47
1:A:267:TRP:CE3	1:A:308:TYR:HD2	2.32	0.47
1:A:347:TYR:CG	1:A:356:VAL:HA	2.50	0.46
1:A:402:TYR:OH	1:A:406:LYS:CE	2.64	0.46
1:B:73:THR:OG1	1:B:79:HIS:HE1	1.98	0.46
1:A:94:LYS:HD3	1:A:94:LYS:C	2.40	0.46
1:A:42:GLU:OE2	1:A:44:ARG:NE	2.43	0.46
1:A:302:ASP:HB3	1:A:385:ASP:O	2.15	0.46
1:B:79:HIS:CD2	1:B:382:ASP:OD2	2.67	0.46
1:B:316:PRO:HG3	1:B:357:ILE:CG2	2.45	0.46
1:C:295:SER:HA	1:C:339:VAL:O	2.15	0.46
1:C:380:ASN:O	1:C:388:GLY:HA3	2.15	0.46
1:C:69:PHE:HB2	1:C:72:GLU:OE2	2.16	0.46
1:C:315:PHE:HD1	1:C:319:LEU:HD11	1.79	0.46
1:A:69:PHE:HZ	1:A:382:ASP:OD1	1.99	0.46
1:B:238:LYS:NZ	4:B:514:HOH:O	2.48	0.46
1:B:409:MET:O	1:B:410:ASP:OD1	2.33	0.46
1:C:366:MET:HE2	1:C:408:LEU:HD21	1.96	0.46
1:A:91:LEU:N	4:A:473:HOH:O	2.47	0.46
1:A:135:ILE:O	1:A:139:ILE:HG12	2.15	0.46
1:A:352:ASP:HA	1:A:353:PRO:HD3	1.28	0.46
1:B:380:ASN:N	1:B:380:ASN:ND2	2.60	0.46
1:A:72:GLU:HG3	1:A:155:HIS:HD2	1.81	0.46
1:A:80:GLY:HA3	1:A:394:TRP:CZ3	2.51	0.46
1:A:316:PRO:O	1:A:319:LEU:HB2	2.15	0.46
1:B:77:VAL:O	1:B:78:VAL:C	2.59	0.46
1:C:315:PHE:HA	1:C:316:PRO:HA	1.70	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:THR:HG22	1:A:39:ILE:N	2.27	0.46
1:A:71:PHE:CD2	1:A:103:LEU:HD22	2.51	0.46
1:C:246:HIS:CD2	1:C:246:HIS:N	2.84	0.46
1:A:135:ILE:HD12	1:A:139:ILE:CG1	2.46	0.45
1:C:68:TRP:HD1	1:C:380:ASN:HD21	1.63	0.45
1:A:331:LYS:HB2	1:A:338:VAL:HG23	1.99	0.45
1:B:287:LEU:HD12	1:B:292:LEU:HD13	1.98	0.45
1:C:281:LYS:NZ	1:C:281:LYS:CB	2.79	0.45
1:C:209:PRO:HA	1:C:212:TYR:HD2	1.82	0.45
1:A:93:ILE:CD1	1:A:379:TRP:CE3	2.99	0.45
1:A:123:LYS:O	1:A:125:PRO:HD3	2.16	0.45
1:B:75:ASN:ND2	1:B:79:HIS:CE1	2.84	0.45
1:B:299:TYR:HE2	4:B:529:HOH:O	1.99	0.45
1:A:291:LYS:HA	1:A:291:LYS:HE2	1.97	0.45
1:C:74:PRO:HD3	1:C:159:CYS:O	2.17	0.45
1:A:103:LEU:HA	1:A:103:LEU:HD23	1.81	0.45
1:C:35:THR:HG21	1:C:39:ILE:N	2.32	0.45
1:C:46:ASP:OD1	1:C:46:ASP:C	2.60	0.45
1:C:304:TYR:CD2	3:F:1:BGC:H5	2.51	0.45
1:B:85:ASN:ND2	1:B:87:GLU:HB3	2.31	0.45
1:C:219:THR:HG21	1:C:227:THR:OG1	2.16	0.45
1:C:281:LYS:HZ2	1:C:281:LYS:HB2	1.81	0.45
1:C:331:LYS:HB2	1:C:338:VAL:HG23	1.99	0.45
1:A:100:ALA:HA	1:A:148:ILE:HG23	1.98	0.45
1:B:57:GLU:HG3	1:B:58:GLU:N	2.32	0.45
1:A:94:LYS:HE3	1:A:98:PHE:O	2.17	0.45
1:A:143:ALA:O	1:A:148:ILE:HB	2.17	0.45
1:A:220:TRP:CE2	1:A:230:ASN:HB3	2.52	0.44
1:C:319:LEU:HD12	1:C:319:LEU:N	2.30	0.44
1:A:77:VAL:HG22	1:A:135:ILE:HG12	1.99	0.44
1:C:162:ILE:O	1:C:162:ILE:HG13	2.16	0.44
1:C:292:LEU:HG	1:C:293:VAL:N	2.31	0.44
1:A:383:SER:C	1:A:385:ASP:H	2.25	0.44
1:B:357:ILE:HD12	1:B:357:ILE:N	2.32	0.44
1:A:64:PHE:CG	1:A:409:MET:HG2	2.53	0.44
1:A:86:TRP:N	1:A:124:ASN:HD21	2.14	0.44
1:A:134:GLN:HG2	1:A:134:GLN:H	1.55	0.44
1:A:306:GLN:O	1:A:309:PHE:HB2	2.16	0.44
1:A:383:SER:HB3	1:A:387:GLY:N	2.32	0.44
1:B:406:LYS:HB2	1:B:406:LYS:HZ2	1.81	0.44
1:A:36:PRO:HG2	1:A:37:THR:H	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:GLU:C	1:C:370:LYS:H	2.24	0.44
1:A:65:GLY:CA	1:A:100:ALA:O	2.66	0.44
1:A:68:TRP:CH2	1:A:89:MET:HE3	2.46	0.44
1:C:330:VAL:HG12	1:C:336:TYR:CB	2.45	0.44
1:A:144:GLY:CA	4:A:501:HOH:O	2.56	0.44
1:A:152:LEU:HD11	1:A:187:PHE:CB	2.48	0.44
1:C:219:THR:HG22	1:C:227:THR:OG1	2.17	0.44
1:A:71:PHE:O	1:A:109:SER:OG	2.33	0.44
1:A:267:TRP:CZ2	1:A:313:LYS:HG2	2.52	0.44
1:C:316:PRO:HA	1:C:319:LEU:CD1	2.48	0.44
1:A:295:SER:HA	1:A:339:VAL:O	2.18	0.44
1:A:389:ILE:O	1:A:390:LEU:HB2	2.11	0.44
1:A:86:TRP:H	1:A:124:ASN:ND2	2.14	0.43
1:A:397:ILE:HG12	1:A:398:TRP:N	2.32	0.43
1:C:316:PRO:CA	1:C:319:LEU:HD13	2.48	0.43
1:A:272:TRP:CZ3	1:A:304:TYR:HB3	2.52	0.43
1:A:381:PRO:HD2	1:A:394:TRP:CZ3	2.53	0.43
1:B:103:LEU:HD23	1:B:136:MET:HE3	2.00	0.43
1:C:188:GLY:O	1:C:246:HIS:HE1	2.00	0.43
1:A:121:TYR:N	1:A:121:TYR:CD1	2.86	0.43
1:A:327:PHE:CD1	1:A:327:PHE:C	2.96	0.43
1:C:35:THR:CG2	1:C:39:ILE:O	2.60	0.43
1:A:68:TRP:CD2	1:A:78:VAL:HG21	2.54	0.43
1:B:406:LYS:NZ	1:B:406:LYS:CB	2.82	0.43
1:A:36:PRO:HG2	1:A:37:THR:N	2.34	0.43
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.57	0.43
1:C:37:THR:HG21	1:C:191:TRP:CB	2.49	0.43
1:C:316:PRO:C	1:C:319:LEU:HD13	2.43	0.43
1:A:346:LYS:HG2	4:A:492:HOH:O	2.18	0.43
1:A:354:ARG:HG3	1:A:357:ILE:HD12	2.01	0.43
1:C:286:ASN:ND2	4:C:464:HOH:O	2.42	0.43
1:A:164:PRO:HG3	1:A:205:VAL:CG1	2.49	0.43
1:A:289:ARG:NH2	1:A:336:TYR:CZ	2.87	0.43
1:C:35:THR:HA	1:C:36:PRO:HD3	1.83	0.43
1:A:119:ILE:HD11	1:A:121:TYR:OH	2.19	0.43
1:A:379:TRP:CG	1:A:379:TRP:O	2.72	0.43
1:A:141:LYS:HD3	1:A:141:LYS:HA	1.83	0.43
1:A:398:TRP:HB3	1:A:401:LYS:CB	2.49	0.43
1:B:220:TRP:CE2	1:B:230:ASN:HB3	2.54	0.43
1:C:287:LEU:O	1:C:288:PRO:C	2.61	0.43
1:C:289:ARG:O	1:C:289:ARG:CG	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLY:CA	1:A:394:TRP:CE2	3.02	0.42
1:C:65:GLY:HA2	1:C:100:ALA:O	2.18	0.42
1:C:302:ASP:HB3	1:C:385:ASP:O	2.18	0.42
1:A:346:LYS:CE	1:A:386:THR:C	2.88	0.42
1:B:188:GLY:O	1:B:246:HIS:HE1	2.02	0.42
1:C:265:TYR:CD1	1:C:266:LYS:N	2.87	0.42
1:A:90:LEU:CD2	1:A:142:LYS:HB3	2.49	0.42
1:A:381:PRO:CG	1:A:394:TRP:CE2	3.02	0.42
1:B:142:LYS:O	1:B:146:LEU:HD13	2.19	0.42
1:C:49:TYR:HE1	1:C:60:PRO:HG3	1.82	0.42
1:A:38:GLY:O	1:A:53:VAL:HG22	2.20	0.42
1:A:68:TRP:HE3	1:A:380:ASN:ND2	2.14	0.42
1:A:93:ILE:HG22	1:A:94:LYS:N	2.34	0.42
1:A:379:TRP:CZ3	1:A:389:ILE:CG2	3.03	0.42
1:A:381:PRO:CA	1:A:388:GLY:N	2.72	0.42
1:C:34:GLN:OE1	1:C:34:GLN:HA	2.19	0.42
1:A:68:TRP:HB3	1:A:103:LEU:HD23	2.01	0.42
1:A:110:VAL:O	1:A:133:LEU:HD22	2.19	0.42
1:A:316:PRO:HG3	1:A:357:ILE:CG2	2.50	0.42
1:B:86:TRP:CZ3	1:B:142:LYS:HG3	2.55	0.42
1:B:187:PHE:HA	1:B:190:TYR:HD2	1.84	0.42
1:A:84:ARG:CD	1:A:89:MET:HE2	2.48	0.42
1:B:87:GLU:OE2	1:B:142:LYS:NZ	2.47	0.42
1:C:292:LEU:HD21	1:C:294:TYR:CE2	2.54	0.42
1:B:35:THR:HA	1:B:36:PRO:HD3	1.76	0.42
1:B:161:HIS:HE1	4:B:508:HOH:O	2.02	0.42
1:C:42:GLU:OE2	1:C:51:ILE:CD1	2.68	0.42
1:C:172:SER:O	1:C:175:ASP:HB2	2.20	0.42
1:C:319:LEU:H	1:C:319:LEU:CD1	2.33	0.42
1:C:319:LEU:HD21	1:C:358:TRP:HD1	1.85	0.42
1:A:72:GLU:OE2	2:D:4:BGC:O6	2.25	0.42
1:A:73:THR:HB	1:A:74:PRO:CD	2.45	0.42
1:A:265:TYR:CB	1:A:278:MET:HE1	2.49	0.42
1:C:198:LEU:CD2	1:C:250:PHE:O	2.68	0.42
1:C:242:LYS:HE3	1:C:242:LYS:HB2	1.86	0.42
1:C:283:TYR:N	1:C:284:PRO:CD	2.83	0.42
1:C:345:GLY:HA3	1:C:355:ASP:OD2	2.20	0.42
1:A:35:THR:HB	1:A:246:HIS:HB3	2.01	0.41
1:A:131:ASP:O	1:A:133:LEU:CA	2.67	0.41
1:A:222:MET:SD	1:A:259:PRO:HD2	2.60	0.41
1:A:346:LYS:HA	1:A:401:LYS:CG	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:HIS:CD2	1:B:246:HIS:N	2.86	0.41
1:C:271:ALA:HB1	1:C:276:ASN:HB2	2.01	0.41
1:C:316:PRO:HG3	1:C:357:ILE:HG22	2.02	0.41
1:A:74:PRO:O	1:A:76:HIS:ND1	2.39	0.41
1:A:353:PRO:C	1:A:355:ASP:N	2.78	0.41
1:C:241:LEU:HD23	1:C:241:LEU:HA	1.83	0.41
1:A:81:LEU:HB3	1:A:119:ILE:HG22	2.02	0.41
1:A:199:LYS:HB3	1:A:229:TRP:CH2	2.55	0.41
1:A:376:TYR:OH	1:A:401:LYS:HD3	2.21	0.41
1:C:279:ALA:O	1:C:283:TYR:HB2	2.21	0.41
1:A:68:TRP:CD1	1:A:78:VAL:HG21	2.55	0.41
1:A:93:ILE:O	1:A:96:LEU:HB2	2.20	0.41
1:A:106:CYS:HA	1:A:156:ARG:O	2.20	0.41
1:A:135:ILE:HD12	1:A:135:ILE:O	2.21	0.41
1:A:267:TRP:CE2	1:A:308:TYR:HB3	2.55	0.41
1:B:42:GLU:OE2	1:B:58:GLU:OE2	2.38	0.41
1:A:379:TRP:CZ3	1:A:389:ILE:HG22	2.55	0.41
1:C:257:THR:OG1	1:C:258:ASN:N	2.52	0.41
1:C:323:TRP:CH2	1:C:362:LEU:HA	2.55	0.41
1:A:131:ASP:OD2	1:A:134:GLN:NE2	2.49	0.41
1:C:304:TYR:CE2	3:F:1:BGC:H5	2.56	0.41
1:A:72:GLU:OE1	1:A:72:GLU:N	2.44	0.41
1:A:100:ALA:HA	1:A:149:PHE:O	2.21	0.41
1:A:344:GLY:HA2	1:A:376:TYR:CE1	2.56	0.41
1:A:383:SER:OG	1:A:385:ASP:OD2	2.37	0.41
1:A:398:TRP:HB3	1:A:401:LYS:HB3	2.01	0.41
1:B:206:THR:O	1:B:211:ALA:HB2	2.21	0.41
1:C:180:TRP:CE3	1:C:183:VAL:HG21	2.56	0.41
1:C:205:VAL:CG2	1:C:216:THR:O	2.63	0.41
1:A:130:LEU:CB	1:A:134:GLN:HE21	2.34	0.41
1:C:184:ALA:HA	1:C:247:TRP:CH2	2.55	0.41
1:A:316:PRO:HG3	1:A:357:ILE:HG21	2.04	0.40
1:B:299:TYR:C	1:B:358:TRP:CZ2	2.99	0.40
1:A:72:GLU:OE2	2:D:4:BGC:C6	2.70	0.40
1:A:133:LEU:HD12	1:A:133:LEU:HA	1.70	0.40
1:A:343:PHE:O	1:A:377:TRP:N	2.40	0.40
1:A:347:TYR:CG	1:A:356:VAL:HG13	2.56	0.40
1:C:198:LEU:HD21	1:C:249:ILE:HG22	1.98	0.40
1:A:315:PHE:HA	1:A:316:PRO:HA	1.85	0.40
1:C:173:GLU:O	1:C:177:ILE:HG13	2.22	0.40
1:C:197:ASP:HA	1:C:250:PHE:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:TYR:CD1	1:B:303:VAL:HG21	2.56	0.40
1:C:331:LYS:HB2	1:C:338:VAL:CG2	2.51	0.40
1:C:131:ASP:OD1	1:C:134:GLN:CG	2.70	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:554:HOH:O	4:C:500:HOH:O[4_545]	2.03	0.17
4:B:553:HOH:O	4:C:553:HOH:O[4_545]	2.10	0.10
1:A:95:SER:OG	1:A:354:ARG:NH1[4_556]	2.16	0.04

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	375/458 (82%)	338 (90%)	31 (8%)	6 (2%)	7	3
1	B	375/458 (82%)	361 (96%)	14 (4%)	0	100	100
1	C	375/458 (82%)	354 (94%)	20 (5%)	1 (0%)	36	35
All	All	1125/1374 (82%)	1053 (94%)	65 (6%)	7 (1%)	21	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	A	384	GLY
1	A	390	LEU
1	A	112	PRO
1	C	215	GLY
1	A	327	PHE
1	A	350	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/395 (82%)	284 (88%)	39 (12%)	5	3
1	B	323/395 (82%)	310 (96%)	13 (4%)	28	27
1	C	323/395 (82%)	303 (94%)	20 (6%)	16	13
All	All	969/1185 (82%)	897 (93%)	72 (7%)	13	9

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	46	ASP
1	A	68	TRP
1	A	75	ASN
1	A	78	VAL
1	A	87	GLU
1	A	88	ASP
1	A	92	GLN
1	A	94	LYS
1	A	112	PRO
1	A	126	ASP
1	A	127	LEU
1	A	130	LEU
1	A	134	GLN
1	A	135	ILE
1	A	141	LYS
1	A	153	ASP
1	A	169	GLU
1	A	180	TRP
1	A	190	TYR
1	A	243	VAL
1	A	246	HIS
1	A	281	LYS
1	A	290	ASN
1	A	313	LYS
1	A	319	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	346	LYS
1	A	347	TYR
1	A	354	ARG
1	A	359	GLN
1	A	389	ILE
1	A	390	LEU
1	A	392	ASP
1	A	393	ASP
1	A	396	THR
1	A	397	ILE
1	A	399	GLU
1	A	401	LYS
1	A	408	LEU
1	B	57	GLU
1	B	68	TRP
1	B	115	GLN
1	B	142	LYS
1	B	153	ASP
1	B	169	GLU
1	B	241	LEU
1	B	246	HIS
1	B	260	LYS
1	B	320	PRO
1	B	380	ASN
1	B	399	GLU
1	B	406	LYS
1	C	34	GLN
1	C	39	ILE
1	C	53	VAL
1	C	58	GLU
1	C	138	LYS
1	C	142	LYS
1	C	160	THR
1	C	198	LEU
1	C	214	ASP
1	C	246	HIS
1	C	260	LYS
1	C	270	ASN
1	C	281	LYS
1	C	282	ASP
1	C	287	LEU
1	C	289	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	334	LEU
1	C	380	ASN
1	C	407	ARG
1	C	410	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	75	ASN
1	A	85	ASN
1	A	124	ASN
1	A	134	GLN
1	A	161	HIS
1	A	203	HIS
1	A	246	HIS
1	A	290	ASN
1	A	297	HIS
1	A	359	GLN
1	A	380	ASN
1	B	62	HIS
1	B	75	ASN
1	B	79	HIS
1	B	85	ASN
1	B	161	HIS
1	B	178	ASN
1	B	203	HIS
1	B	246	HIS
1	B	270	ASN
1	B	297	HIS
1	B	325	HIS
1	B	326	HIS
1	B	349	HIS
1	B	359	GLN
1	B	380	ASN
1	B	391	GLN
1	C	34	GLN
1	C	62	HIS
1	C	75	ASN
1	C	79	HIS
1	C	85	ASN
1	C	203	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	246	HIS
1	C	255	GLN
1	C	270	ASN
1	C	297	HIS
1	C	349	HIS
1	C	359	GLN
1	C	360	ASN
1	C	380	ASN

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 ⓘ

14 monosaccharides 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	D	1	2	12,12,12	1.22	1 (8%)	17,17,17	1.56	4 (23%)
2	BGC	D	2	2	11,11,12	0.76	0	15,15,17	1.03	2 (13%)
2	BGC	D	3	2	11,11,12	0.88	0	15,15,17	1.35	2 (13%)
2	BGC	D	4	2	11,11,12	0.65	0	15,15,17	1.18	2 (13%)
2	BGC	E	1	2	12,12,12	1.24	0	17,17,17	1.74	2 (11%)
2	BGC	E	2	2	11,11,12	0.87	0	15,15,17	1.05	1 (6%)
2	BGC	E	3	2	11,11,12	1.01	1 (9%)	15,15,17	1.12	0
2	BGC	E	4	2	11,11,12	0.73	0	15,15,17	0.90	1 (6%)
3	BGC	F	1	3	12,12,12	0.51	0	17,17,17	0.92	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	F	2	3	11,11,12	0.32	0	15,15,17	0.83	0
2	BGC	G	1	2	12,12,12	1.38	0	17,17,17	2.15	5 (29%)
2	BGC	G	2	2	11,11,12	0.86	0	15,15,17	1.00	0
2	BGC	G	3	2	11,11,12	0.86	1 (9%)	15,15,17	1.09	2 (13%)
2	BGC	G	4	2	11,11,12	0.79	0	15,15,17	0.96	1 (6%)

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	D	1	2	-	0/2/22/22	0/1/1/1
2	BGC	D	2	2	-	0/2/19/22	0/1/1/1
2	BGC	D	3	2	-	0/2/19/22	0/1/1/1
2	BGC	D	4	2	-	0/2/19/22	0/1/1/1
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	E	4	2	-	0/2/19/22	0/1/1/1
3	BGC	F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	F	2	3	-	0/2/19/22	0/1/1/1
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	BGC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	G	3	2	-	0/2/19/22	0/1/1/1
2	BGC	G	4	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	BGC	C4-C5	2.13	1.57	1.53
2	D	1	BGC	O5-C5	2.06	1.49	1.44
2	G	3	BGC	O5-C1	2.06	1.47	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	BGC	C1-C2-C3	-4.90	100.37	110.36
2	G	1	BGC	C1-O5-C5	-4.26	105.40	113.65
2	E	1	BGC	C1-C2-C3	-3.88	102.44	110.36
2	E	1	BGC	C1-O5-C5	-3.75	106.39	113.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	BGC	C1-O5-C5	-3.63	106.62	113.65
2	D	3	BGC	C1-C2-C3	-3.38	104.72	109.64
2	D	1	BGC	C1-C2-C3	-2.96	104.32	110.36
2	G	1	BGC	O4-C4-C5	-2.57	103.00	109.32
3	F	1	BGC	C1-O5-C5	-2.45	108.91	113.65
2	D	4	BGC	C1-C2-C3	-2.41	106.14	109.64
2	G	3	BGC	C1-C2-C3	-2.36	106.20	109.64
2	D	1	BGC	C6-C5-C4	-2.34	107.28	113.02
2	D	2	BGC	C6-C5-C4	-2.25	107.50	113.02
2	D	3	BGC	C1-O5-C5	-2.14	109.31	112.19
2	G	4	BGC	C6-C5-C4	-2.12	107.82	113.02
2	G	3	BGC	C6-C5-C4	-2.10	107.86	113.02
2	D	2	BGC	C1-C2-C3	-2.08	106.62	109.64
3	F	1	BGC	C3-C4-C5	-2.08	106.46	110.23
2	D	4	BGC	C1-O5-C5	-2.04	109.46	112.19
2	D	1	BGC	O2-C2-C3	-2.03	105.59	110.38
2	G	1	BGC	O4-C4-C3	2.02	115.14	110.38
2	E	4	BGC	C2-C3-C4	-2.01	107.32	110.86
2	E	2	BGC	C6-C5-C4	-2.01	108.09	113.02
2	G	1	BGC	O2-C2-C3	-2.00	105.66	110.38

There are no chirality outliers.

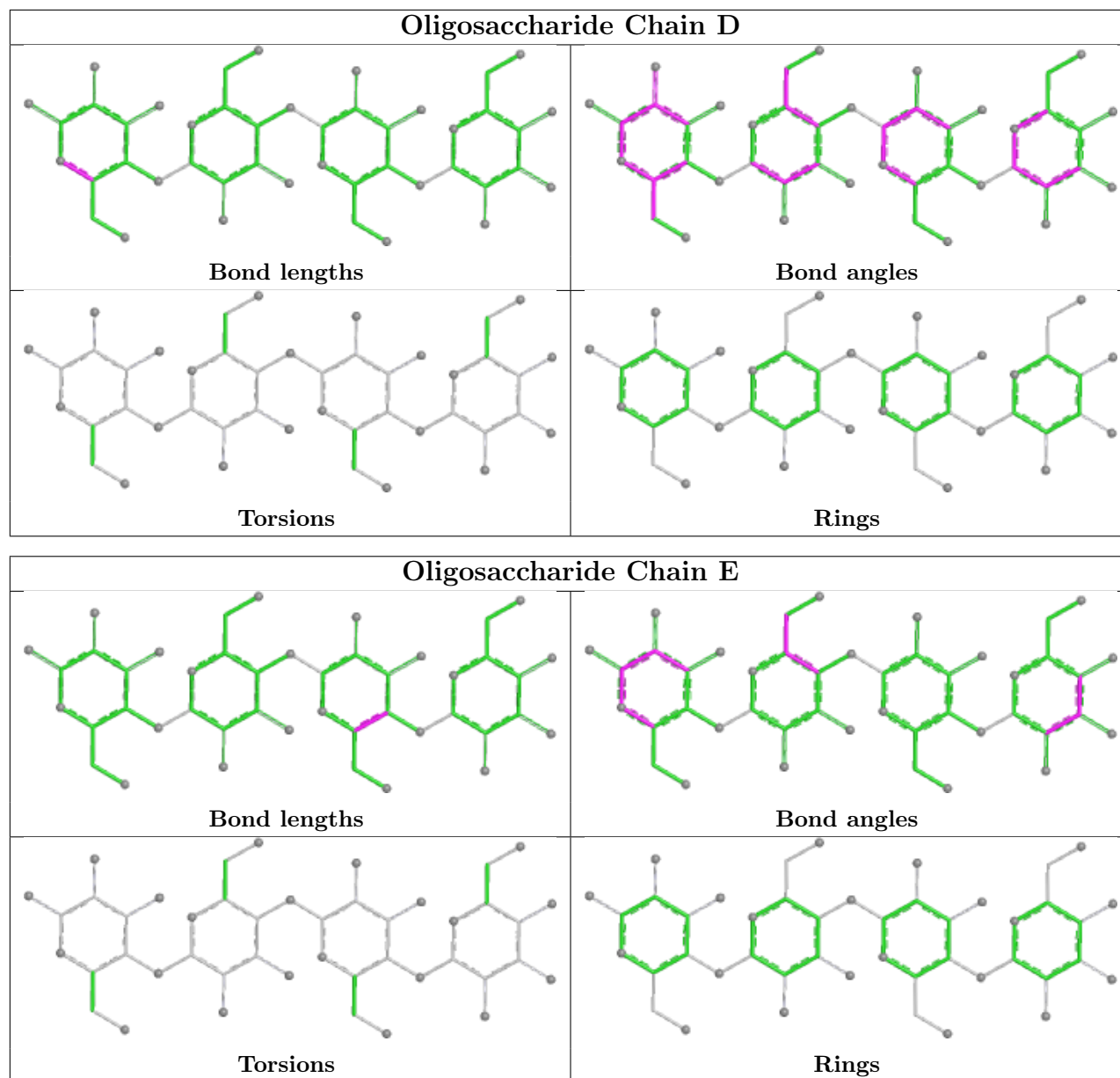
There are no torsion outliers.

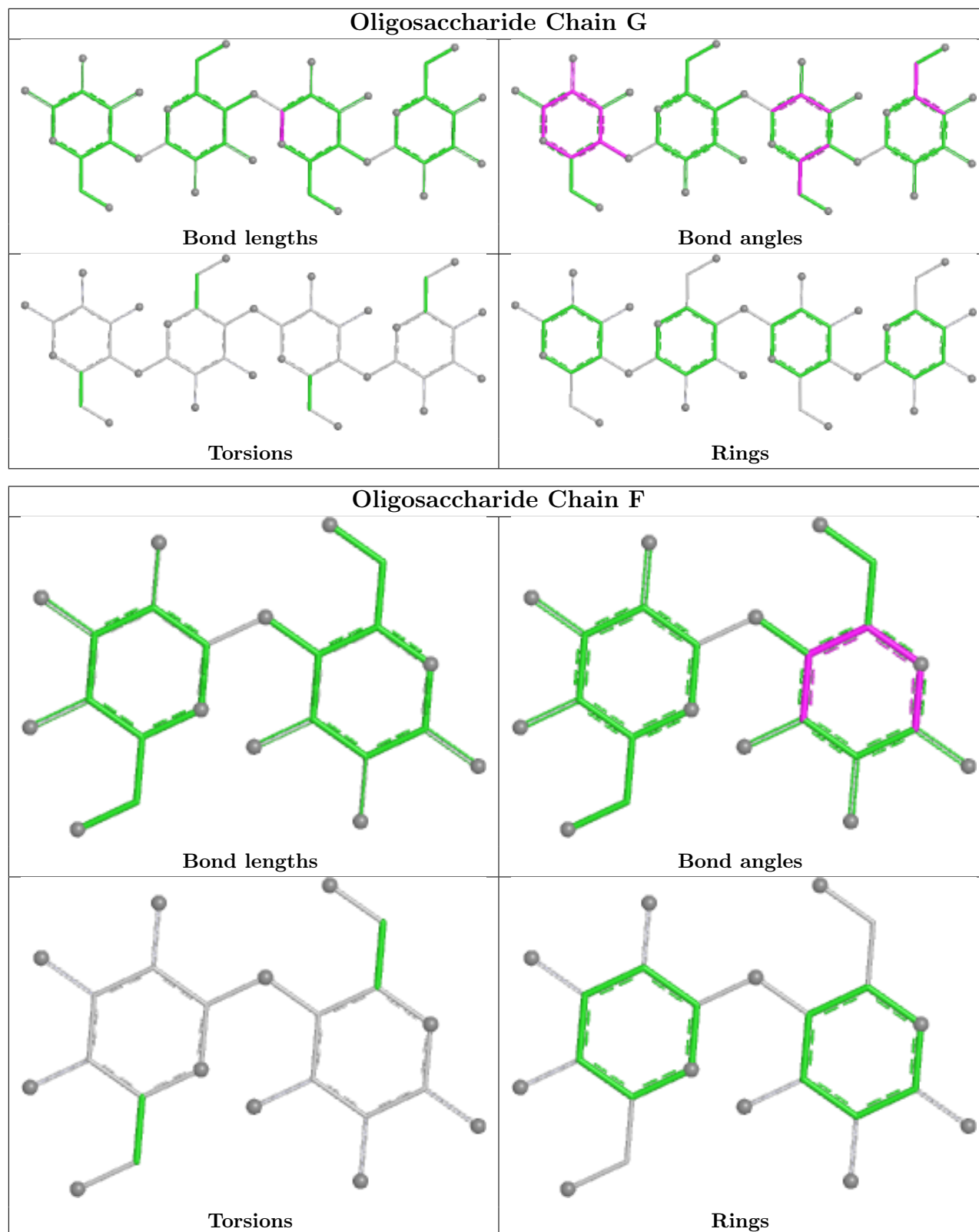
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	BGC	2	0
2	D	4	BGC	2	0
3	F	1	BGC	2	0
2	D	3	BGC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	377/458 (82%)	1.08	78 (20%) 2 2	24, 52, 84, 113	2 (0%)
1	B	377/458 (82%)	-0.03	6 (1%) 70 70	10, 33, 55, 85	3 (0%)
1	C	377/458 (82%)	0.67	26 (6%) 23 21	29, 56, 81, 101	2 (0%)
All	All	1131/1374 (82%)	0.57	110 (9%) 13 12	10, 45, 79, 113	7 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	310	GLY	8.4
1	B	312	ALA	7.4
1	A	310	GLY	7.1
1	A	312	ALA	6.9
1	C	312	ALA	6.4
1	A	135	ILE	5.1
1	B	310	GLY	5.1
1	A	127	LEU	4.9
1	A	347	TYR	4.7
1	A	71	PHE	4.6
1	A	118	GLY	4.3
1	A	379	TRP	4.1
1	A	394	TRP	4.1
1	A	390	LEU	4.1
1	A	388	GLY	4.0
1	A	349	HIS	3.8
1	A	119	ILE	3.8
1	C	217	GLY	3.6
1	A	380	ASN	3.6
1	A	350	GLY	3.5
1	A	89	MET	3.5
1	A	117	ILE	3.3
1	B	68	TRP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	93	ILE	3.3
1	A	397	ILE	3.2
1	A	91	LEU	3.2
1	A	80	GLY	3.2
1	A	398	TRP	3.2
1	A	346	LYS	3.2
1	A	389	ILE	3.2
1	A	70	GLY	3.2
1	A	302	ASP	3.1
1	C	267	TRP	3.0
1	A	77	VAL	3.0
1	A	130	LEU	3.0
1	A	187	PHE	3.0
1	A	101	ILE	3.0
1	A	82	TRP	3.0
1	A	348	GLY	2.9
1	A	139	ILE	2.9
1	A	125	PRO	2.9
1	A	81	LEU	2.8
1	A	142	LYS	2.8
1	A	74	PRO	2.8
1	A	86	TRP	2.8
1	A	110	VAL	2.8
1	C	319	LEU	2.8
1	C	162	ILE	2.8
1	A	356	VAL	2.7
1	A	95	SER	2.7
1	A	159	CYS	2.7
1	A	129	GLY	2.7
1	A	401	LYS	2.6
1	A	136	MET	2.6
1	C	215	GLY	2.6
1	A	76	HIS	2.6
1	A	68	TRP	2.5
1	A	126	ASP	2.5
1	B	161	HIS	2.5
1	A	357	ILE	2.5
1	C	53	VAL	2.5
1	A	121	TYR	2.5
1	A	402	TYR	2.5
1	C	265	TYR	2.5
1	A	400	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	214	ASP	2.4
1	A	381	PRO	2.4
1	B	221	GLY	2.4
1	C	240	ILE	2.4
1	C	280	VAL	2.4
1	C	220	TRP	2.4
1	A	83	LYS	2.4
1	A	372	CYS	2.4
1	C	40	TYR	2.4
1	C	322	ILE	2.4
1	C	340	ILE	2.4
1	A	138	LYS	2.4
1	A	360	ASN	2.3
1	A	409	MET	2.3
1	A	132	SER	2.3
1	C	205	VAL	2.3
1	C	226	ALA	2.3
1	A	133	LEU	2.3
1	A	191	TRP	2.3
1	C	256	PHE	2.3
1	B	410	ASP	2.3
1	A	113	GLY	2.3
1	C	54	THR	2.2
1	A	396	THR	2.2
1	C	266	LYS	2.2
1	A	190	TYR	2.2
1	A	116	PRO	2.2
1	C	43	VAL	2.2
1	A	405	LEU	2.2
1	A	112	PRO	2.1
1	A	124	ASN	2.1
1	A	106	CYS	2.1
1	C	269	TYR	2.1
1	C	304	TYR	2.1
1	A	391	GLN	2.1
1	A	314	GLY	2.1
1	A	344	GLY	2.1
1	A	301	PRO	2.1
1	A	107	THR	2.0
1	C	212	TYR	2.0
1	A	75	ASN	2.0
1	A	354	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	73	THR	2.0
1	A	160	THR	2.0
1	C	341	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](#)

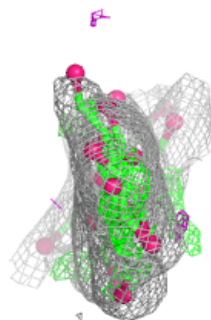
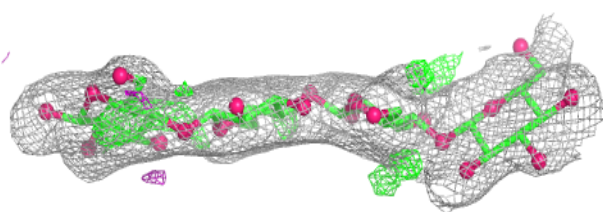
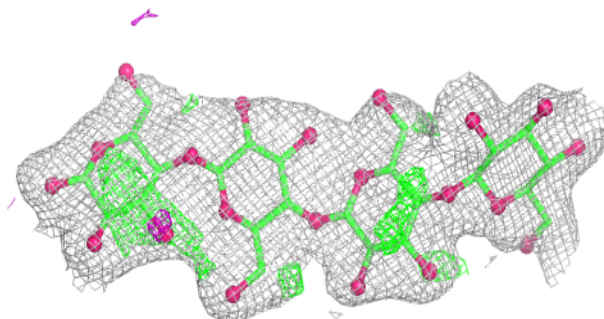
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	D	3	11/12	0.80	0.12	56,61,65,71	0
2	BGC	G	1	12/12	0.81	0.14	50,57,67,68	0
2	BGC	G	4	11/12	0.82	0.13	49,58,69,76	0
2	BGC	E	1	12/12	0.83	0.14	36,42,49,66	0
3	BGC	F	2	11/12	0.83	0.14	63,68,75,77	0
2	BGC	D	1	12/12	0.87	0.13	38,48,59,71	0
3	BGC	F	1	12/12	0.88	0.10	58,68,75,78	0
2	BGC	G	2	11/12	0.88	0.10	40,46,51,52	0
2	BGC	G	3	11/12	0.89	0.09	53,61,67,68	0
2	BGC	D	2	11/12	0.90	0.11	39,44,60,64	0
2	BGC	E	2	11/12	0.90	0.09	28,35,42,47	0
2	BGC	D	4	11/12	0.91	0.12	46,56,70,72	0
2	BGC	E	3	11/12	0.92	0.09	23,26,37,55	0
2	BGC	E	4	11/12	0.94	0.10	31,33,41,43	0

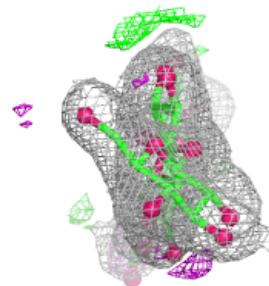
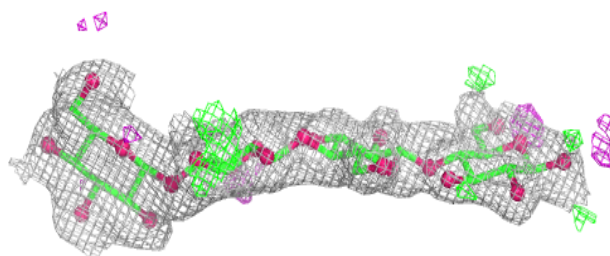
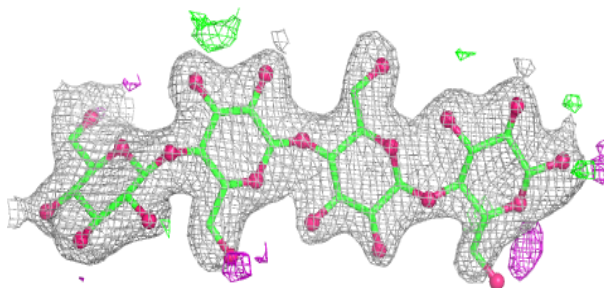
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

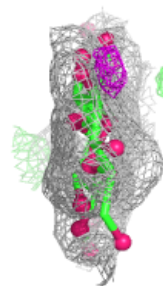
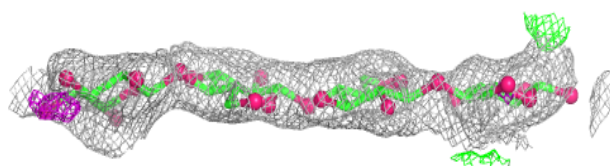
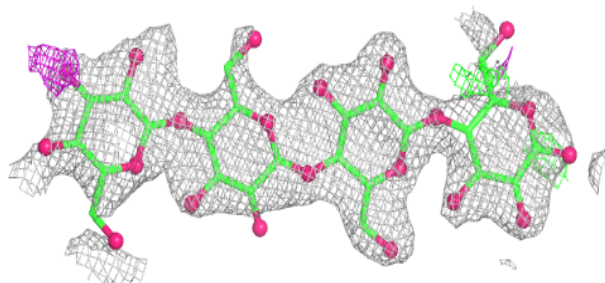
**Electron density around Chain E:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

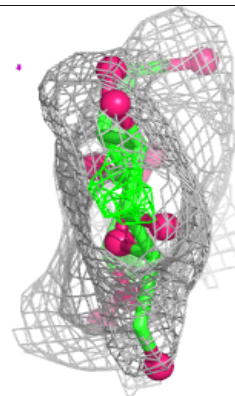
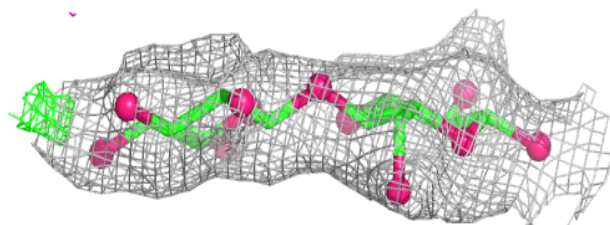
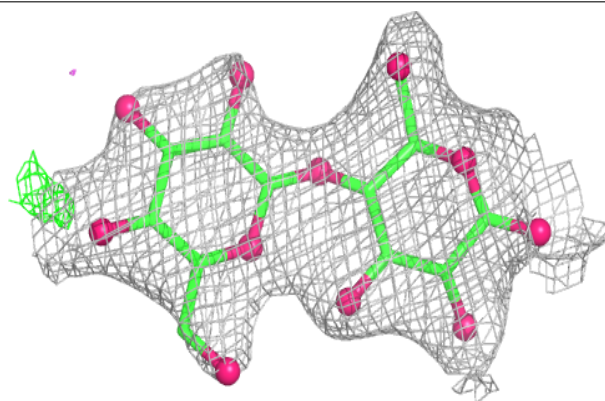


Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain F:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.