Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 05:52 PM EDT

PDB ID	:	3WJM
Title	:	Crystal structure of Bombyx mori Sp2/Sp3 heterohexamer
Authors	:	Yuan, Y.A.; Hou, Y.
Deposited on	:	2013-10-11
Resolution	:	2.80 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:

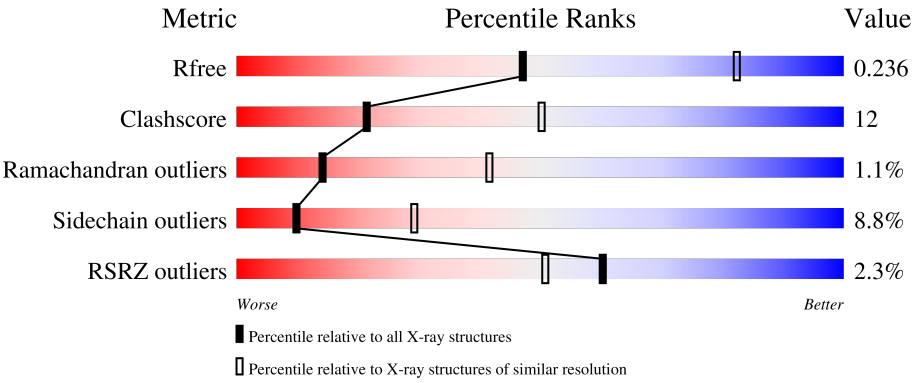
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	703	2% 71% 22% • 5%
1	E	703	3% 72% 20% • 5%
1	F	703	3% 67% 24% • 5%
2	B	696	2% 67% 24% 5% •
2	C	696	2% 68% 23% • •

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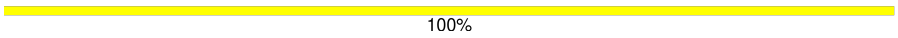
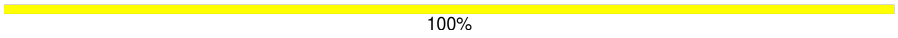
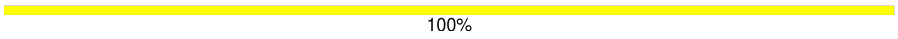
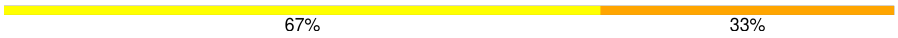
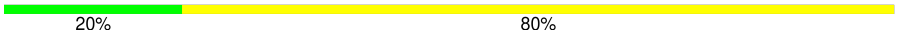
Mol	Chain	Length	Quality of chain
2	D	696	
3	G	5	
4	H	5	
5	I	6	
6	J	7	
7	K	6	
8	L	5	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 34590 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.

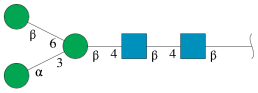
- Molecule 1 is a protein called Arylphorin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	670	Total	C	N	O	S	0	0	0
			5681	3734	892	1030	25			
1	E	669	Total	C	N	O	S	0	0	0
			5669	3725	891	1028	25			
1	F	669	Total	C	N	O	S	0	0	0
			5669	3725	891	1028	25			

- Molecule 2 is a protein called Silkworm storage protein.

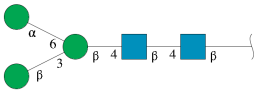
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	668	Total	C	N	O	S	0	0	0
			5669	3745	877	1021	26			
2	C	668	Total	C	N	O	S	0	0	0
			5669	3745	877	1021	26			
2	D	672	Total	C	N	O	S	0	0	0
			5703	3767	881	1029	26			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



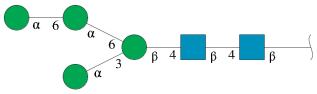
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



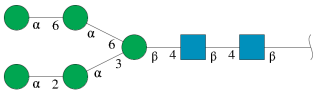
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	H	5	61	34	2	25	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



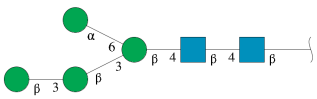
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	I	6	72	40	2	30	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



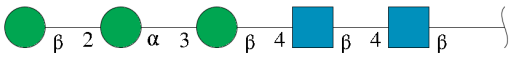
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	J	7	83	46	2	35	0	0	0

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	L	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 9 is water.

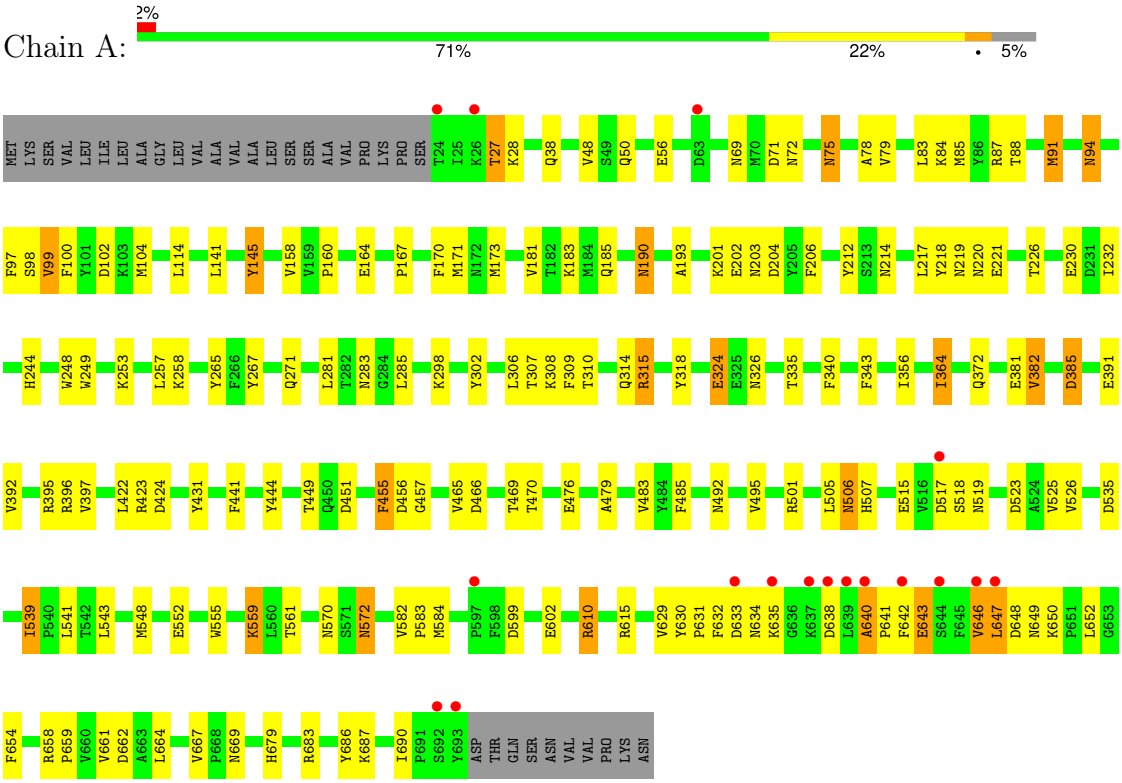
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	29	Total	O	0	0
			29	29		
9	B	14	Total	O	0	0
			14	14		
9	C	19	Total	O	0	0
			19	19		
9	D	27	Total	O	0	0
			27	27		
9	E	21	Total	O	0	0
			21	21		
9	F	10	Total	O	0	0
			10	10		

3 Residue-property plots (i)

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.

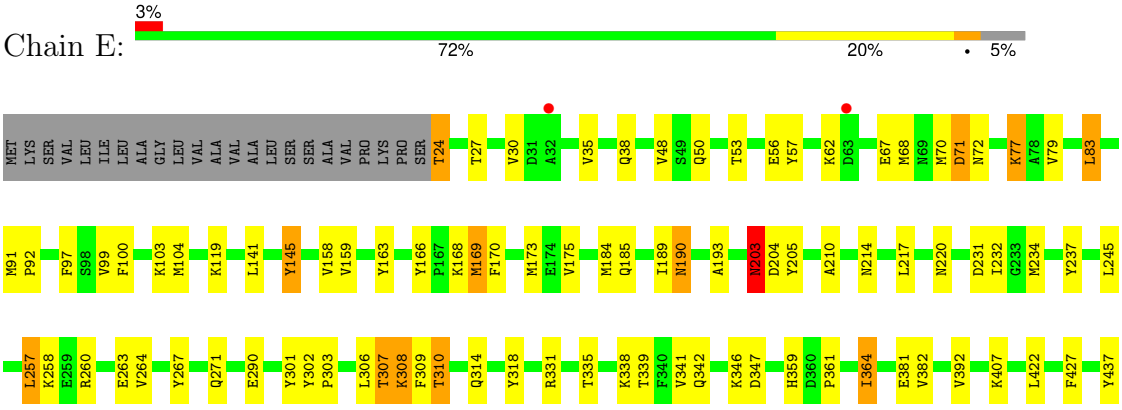
• Molecule 1: Arylphorin

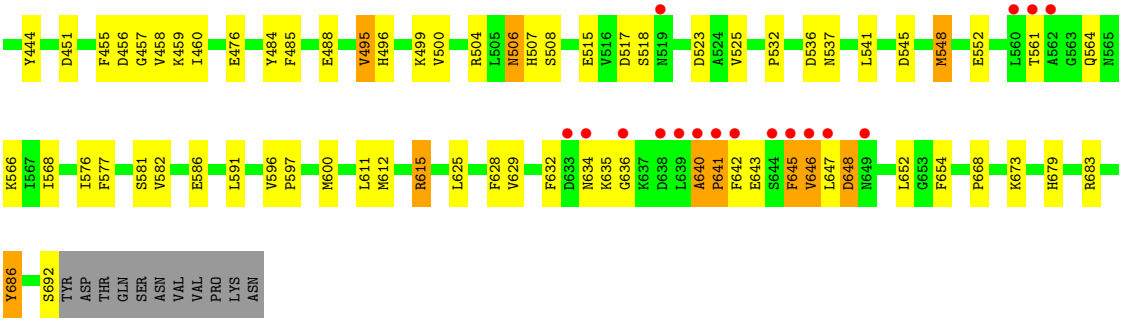
Chain A:



• Molecule 1: Arylphorin

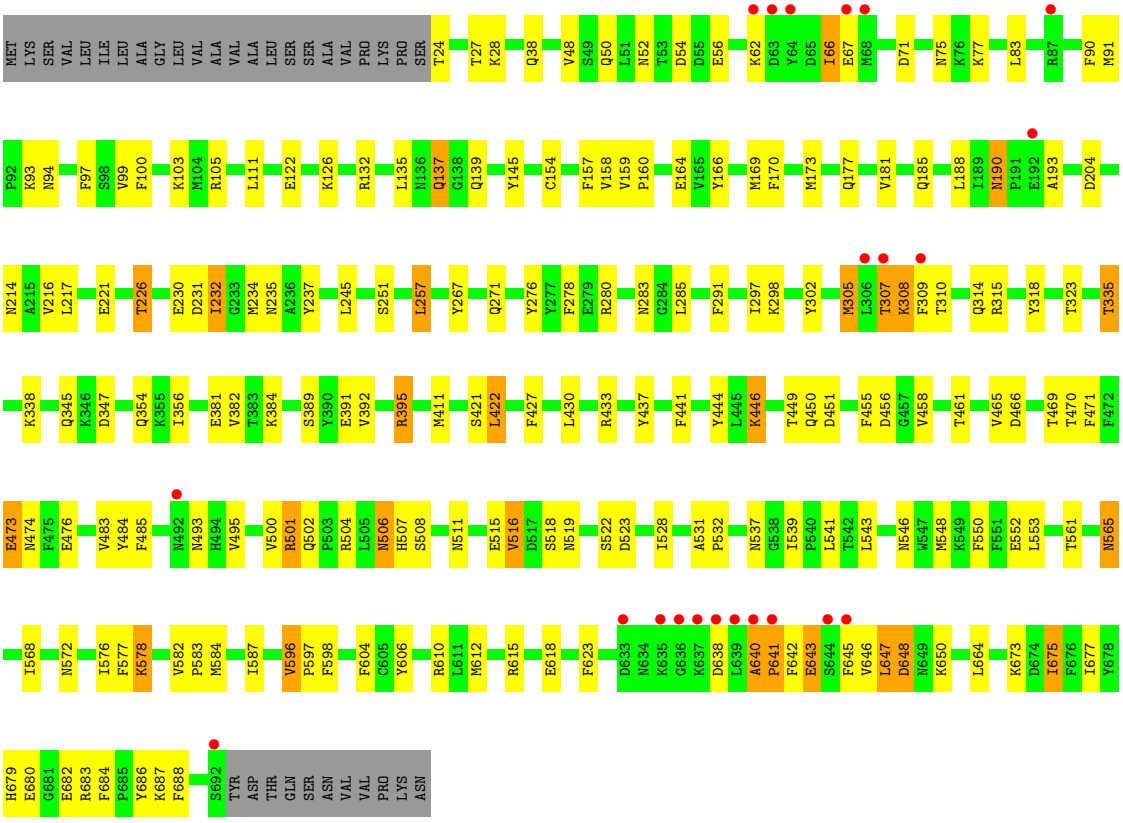
Chain E:





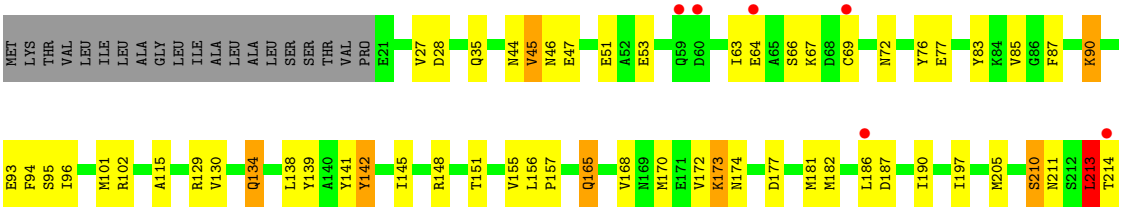
• Molecule 1: Arylphorin

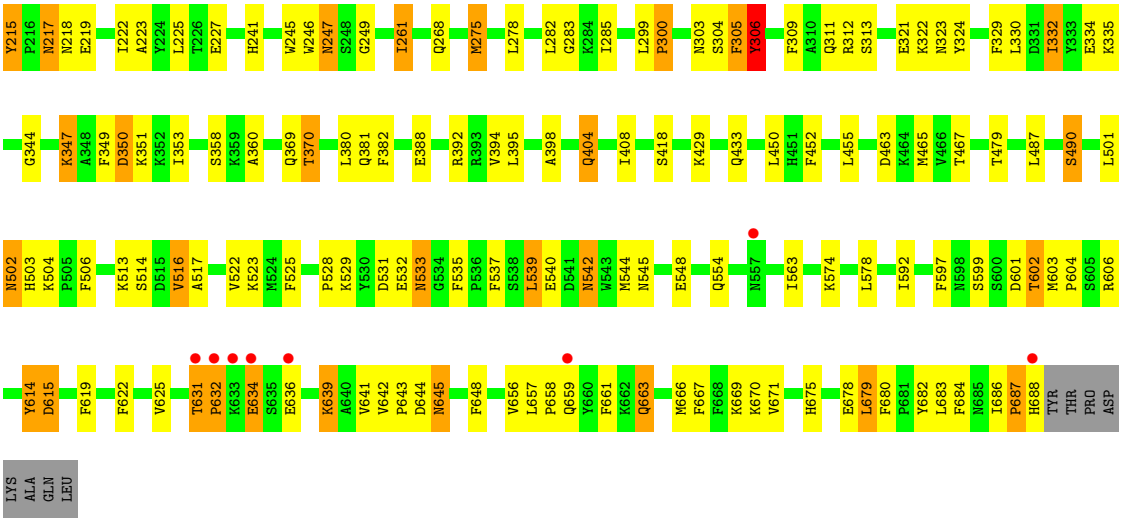
Chain F:



• Molecule 2: Silkworm storage protein

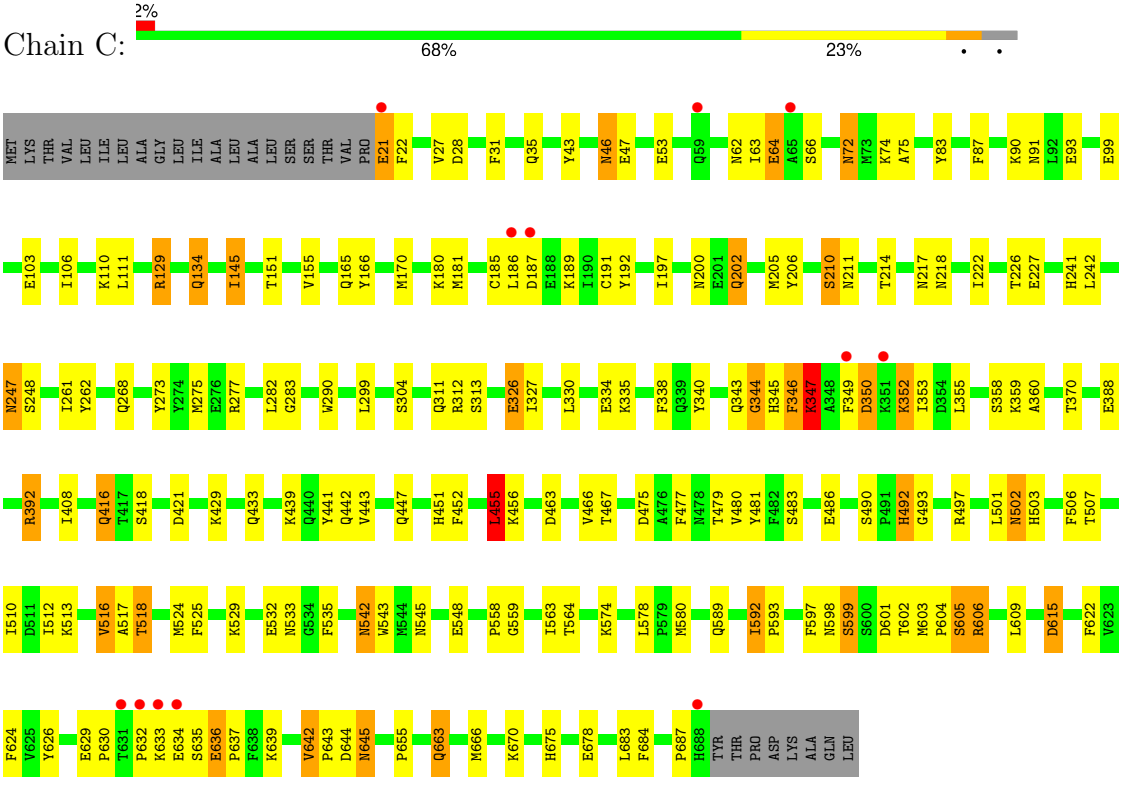
Chain B:





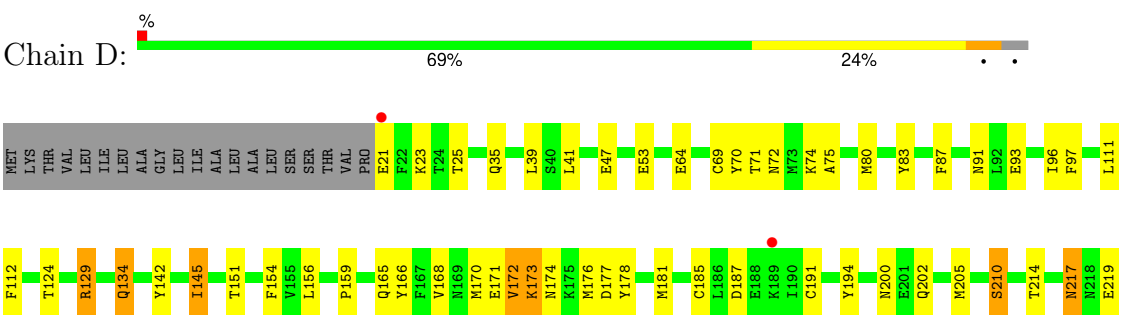
• Molecule 2: Silkworm storage protein

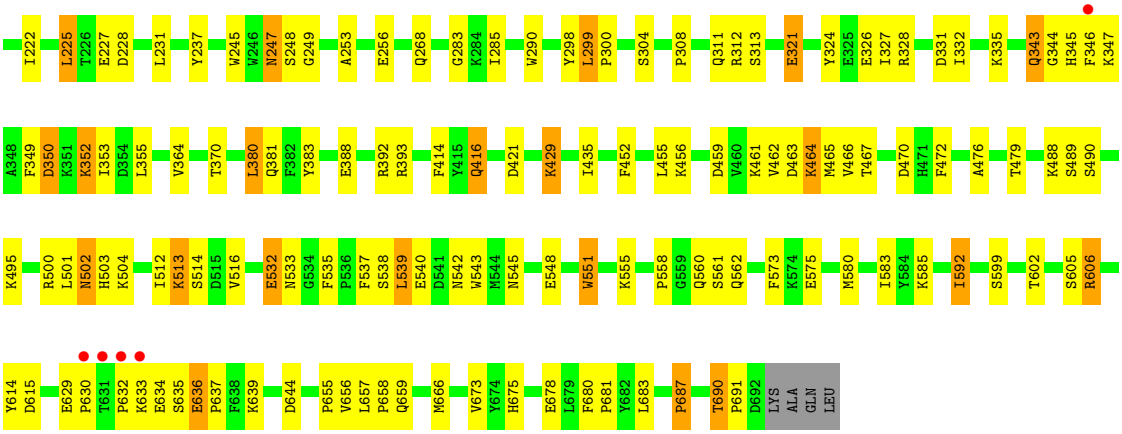
Chain C:



• Molecule 2: Silkworm storage protein

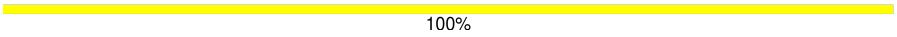
Chain D:





• Molecule 3: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

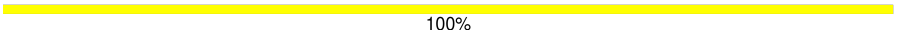


• Molecule 4: beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

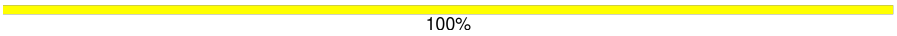
• Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 7: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamid

o-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 8: beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.06Å 205.02Å 119.71Å 90.00° 103.00° 90.00°	Depositor
Resolution (Å)	48.37 – 2.80 48.37 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.37-2.80) 96.5 (48.37-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.81 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.172 , 0.237 0.171 , 0.236	Depositor DCC
R_{free} test set	5121 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	50.2	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34590	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: BMA, MAN, NAG

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	0.62	0/5863	0.76	3/7934 (0.0%)
1	E	0.61	0/5850	0.74	1/7916 (0.0%)
1	F	0.58	0/5850	0.74	2/7916 (0.0%)
2	B	0.61	0/5865	0.76	1/7945 (0.0%)
2	C	0.64	0/5865	0.78	5/7945 (0.1%)
2	D	0.65	1/5901 (0.0%)	0.78	2/7996 (0.0%)
All	All	0.62	1/35194 (0.0%)	0.76	14/47652 (0.0%)

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
2	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	171	GLU	CD-OE2	-5.18	1.20	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	213	LEU	CA-CB-CG	9.09	136.20	115.30
1	A	315	ARG	NE-CZ-NH2	-8.73	115.93	120.30
2	C	392	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	F	315	ARG	NE-CZ-NH2	-6.68	116.96	120.30
2	D	171	GLU	OE1-CD-OE2	-6.65	115.32	123.30
2	C	455	LEU	CA-CB-CG	6.56	130.40	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	392	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	99	VAL	CB-CA-C	-6.05	99.90	111.40
1	E	541	LEU	CA-CB-CG	5.87	128.80	115.30
2	C	615	ASP	N-CA-CB	-5.80	100.15	110.60
2	D	470	ASP	CB-CG-OD1	5.65	123.39	118.30
1	F	395	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	395	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	C	187	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	246	TRP	Peptide
2	B	614	TYR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5681	0	5434	125	0
1	E	5669	0	5425	117	0
1	F	5669	0	5425	150	0
2	B	5669	0	5390	193	0
2	C	5669	0	5392	145	0
2	D	5703	0	5419	140	0
3	G	61	0	52	0	0
4	H	61	0	52	3	0
5	I	72	0	61	0	0
6	J	83	0	70	0	0
7	K	72	0	61	1	0
8	L	61	0	52	0	0
9	A	29	0	0	0	0
9	B	14	0	0	0	0
9	C	19	0	0	1	0
9	D	27	0	0	0	0
9	E	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	10	0	0	1	0
All	All	34590	0	32833	809	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 12.

All (809) 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)
2:B:631:THR:HB	2:B:632:PRO:CD	1.72	1.19
2:B:210:SER:HB2	2:B:214:THR:HG21	1.27	1.16
2:B:631:THR:CB	2:B:632:PRO:HD2	1.77	1.15
1:F:531:ALA:HB2	1:F:550:PHE:CD2	1.83	1.13
1:E:97:PHE:HA	1:E:104:MET:HE1	1.31	1.12
2:D:343:GLN:HA	2:D:343:GLN:HE21	1.15	1.11
2:B:95:SER:H	2:B:101:MET:CE	1.65	1.09
2:B:214:THR:HG23	2:B:215:TYR:HD2	1.14	1.08
1:F:531:ALA:HB2	1:F:550:PHE:CE2	1.95	1.01
2:B:631:THR:HB	2:B:632:PRO:HD2	1.01	1.00
2:B:332:ILE:HG12	2:C:335:LYS:HG2	1.42	1.00
1:F:640:ALA:N	1:F:641:PRO:HD3	1.77	1.00
1:A:314:GLN:HE22	2:D:311:GLN:H	1.08	1.00
2:D:134:GLN:H	2:D:134:GLN:HE21	1.04	0.99
1:F:232:ILE:HD13	1:F:232:ILE:H	1.26	0.98
2:B:615:ASP:H	2:D:615:ASP:HB3	1.28	0.98
1:E:640:ALA:H	1:E:641:PRO:HD3	1.30	0.97
2:C:340:TYR:HB3	2:C:346:PHE:HD2	1.31	0.95
1:F:531:ALA:CB	1:F:550:PHE:CE2	2.50	0.94
2:B:283:GLY:HA2	2:B:532:GLU:HG2	1.48	0.94
2:C:134:GLN:H	2:C:134:GLN:HE21	1.10	0.94
2:D:283:GLY:HA2	2:D:532:GLU:HG2	1.50	0.94
2:B:502:ASN:HD22	2:B:503:HIS:H	1.09	0.93
2:B:210:SER:HB2	2:B:214:THR:CG2	1.98	0.93
1:E:506:ASN:HD22	1:E:507:HIS:H	1.15	0.93
2:B:211:ASN:O	2:B:214:THR:HG22	1.67	0.93
2:C:72:ASN:HD22	2:C:75:ALA:H	1.12	0.93
1:F:99:VAL:HG22	1:F:105:ARG:HG3	1.49	0.92
2:B:663:GLN:HG2	2:B:666:MET:CE	1.98	0.92
1:F:66:ILE:HD12	1:F:66:ILE:H	1.35	0.92
2:B:134:GLN:H	2:B:134:GLN:NE2	1.68	0.92
2:D:134:GLN:H	2:D:134:GLN:NE2	1.67	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:GLN:HE22	1:E:485:PHE:H	1.19	0.91
2:C:165:GLN:HB3	2:C:479:THR:HG21	1.52	0.90
2:C:72:ASN:ND2	2:C:75:ALA:H	1.68	0.90
2:C:268:GLN:HE22	2:C:548:GLU:H	1.17	0.90
2:C:283:GLY:HA2	2:C:532:GLU:HG2	1.52	0.90
2:C:517:ALA:HB2	2:C:558:PRO:HD3	1.53	0.90
1:E:307:THR:HG22	1:E:310:THR:H	1.37	0.89
2:B:214:THR:HG23	2:B:215:TYR:CD2	2.06	0.89
2:B:134:GLN:H	2:B:134:GLN:HE21	0.89	0.88
2:B:247:ASN:ND2	2:B:249:GLY:H	1.72	0.88
2:B:210:SER:CB	2:B:214:THR:HG21	2.03	0.88
2:D:268:GLN:HE22	2:D:548:GLU:H	1.16	0.87
2:B:134:GLN:HE21	2:B:134:GLN:N	1.71	0.87
1:F:307:THR:HG22	1:F:310:THR:H	1.37	0.87
1:A:75:ASN:ND2	1:A:78:ALA:H	1.71	0.87
1:A:271:GLN:HE22	1:A:552:GLU:H	1.20	0.85
1:F:640:ALA:H	1:F:641:PRO:HD3	1.38	0.85
1:A:335:THR:OG1	2:B:335:LYS:HG2	1.75	0.85
2:C:615:ASP:OD1	1:F:618:GLU:HB3	1.75	0.85
2:C:134:GLN:HE21	2:C:134:GLN:N	1.75	0.84
1:F:190:ASN:HD22	1:F:193:ALA:H	1.24	0.84
1:A:212:TYR:HB3	1:A:226:THR:CG2	2.07	0.84
1:A:642:PHE:O	1:A:643:GLU:HG3	1.79	0.83
2:B:502:ASN:HD22	2:B:503:HIS:N	1.77	0.83
1:F:638:ASP:HB2	1:F:647:LEU:HA	1.59	0.82
2:B:663:GLN:HG2	2:B:666:MET:HE2	1.61	0.82
1:A:314:GLN:NE2	2:D:311:GLN:H	1.78	0.82
1:A:212:TYR:HB3	1:A:226:THR:HG21	1.60	0.82
1:E:97:PHE:HA	1:E:104:MET:CE	2.10	0.82
1:E:103:LYS:HG3	1:E:407:LYS:HB2	1.63	0.81
2:D:343:GLN:HA	2:D:343:GLN:NE2	1.93	0.80
1:A:298:LYS:HE2	1:E:318:TYR:OH	1.80	0.80
2:B:35:GLN:HE22	2:B:155:VAL:H	1.26	0.80
2:C:311:GLN:H	1:E:314:GLN:HE22	1.27	0.80
2:C:542:ASN:HD22	2:C:545:ASN:HD22	1.29	0.80
2:B:615:ASP:N	2:D:615:ASP:HB3	1.96	0.80
2:D:72:ASN:HD22	2:D:75:ALA:H	1.30	0.80
2:B:95:SER:N	2:B:101:MET:CE	2.45	0.80
2:D:573:PHE:HB3	2:D:605:SER:HB3	1.64	0.79
1:F:541:LEU:HD22	1:F:546:ASN:ND2	1.95	0.79
2:D:217:ASN:HD22	2:D:219:GLU:H	1.28	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:447:GLN:NE2	2:C:663:GLN:OE1	2.15	0.78
2:D:247:ASN:HD22	2:D:247:ASN:C	1.86	0.78
2:B:450:LEU:HB2	2:B:663:GLN:HE21	1.48	0.78
2:B:349:PHE:O	2:B:350:ASP:HB2	1.83	0.78
2:C:502:ASN:HD22	2:C:503:HIS:H	1.29	0.78
2:B:311:GLN:H	1:F:314:GLN:HE22	1.29	0.78
2:D:476:ALA:O	2:D:479:THR:HG22	1.84	0.78
1:E:271:GLN:HE22	1:E:552:GLU:H	1.29	0.78
2:C:134:GLN:H	2:C:134:GLN:NE2	1.82	0.78
2:C:211:ASN:HB3	9:C:919:HOH:O	1.84	0.78
2:B:663:GLN:HG2	2:B:666:MET:HE1	1.65	0.77
1:A:638:ASP:HB2	1:A:647:LEU:HA	1.66	0.77
1:F:450:GLN:HG2	1:F:664:LEU:HD23	1.66	0.77
2:B:165:GLN:HG3	2:B:479:THR:CG2	2.15	0.76
2:C:166:TYR:CD1	2:C:416:GLN:HG3	2.20	0.76
2:C:218:ASN:HB3	2:C:282:LEU:HD21	1.68	0.76
2:D:539:LEU:HG	2:D:656:VAL:HG11	1.66	0.76
2:B:275:MET:HE2	2:B:528:PRO:HD3	1.65	0.76
1:F:450:GLN:HG2	1:F:664:LEU:CD2	2.16	0.76
2:D:35:GLN:HE21	2:D:39:LEU:HG	1.51	0.75
2:B:268:GLN:HE22	2:B:548:GLU:H	1.31	0.75
2:C:542:ASN:ND2	2:C:545:ASN:HD22	1.84	0.75
2:B:95:SER:H	2:B:101:MET:HE2	1.52	0.75
2:C:599:SER:HB3	2:C:639:LYS:HD2	1.69	0.75
1:E:640:ALA:N	1:E:641:PRO:HD3	2.01	0.75
1:A:190:ASN:ND2	1:A:193:ALA:H	1.85	0.75
1:E:67:GLU:CG	1:E:83:LEU:HD21	2.17	0.75
2:B:222:ILE:HD11	2:B:282:LEU:HD12	1.69	0.74
2:D:25:THR:HB	2:D:592:ILE:HG22	1.68	0.74
1:F:231:ASP:O	1:F:235:ASN:ND2	2.19	0.74
1:F:307:THR:HG22	1:F:309:PHE:H	1.53	0.74
1:A:48:VAL:CG1	1:A:141:LEU:HD11	2.19	0.73
1:F:137:GLN:H	1:F:137:GLN:CD	1.91	0.73
1:F:640:ALA:N	1:F:641:PRO:CD	2.52	0.73
1:F:90:PHE:HD2	1:F:139:GLN:HE22	1.34	0.73
2:B:283:GLY:HA2	2:B:532:GLU:CG	2.19	0.73
2:B:615:ASP:OD1	2:D:614:TYR:HB2	1.88	0.72
1:E:307:THR:HG22	1:E:310:THR:N	2.03	0.72
1:A:75:ASN:HD22	1:A:78:ALA:H	1.36	0.72
1:F:474:ASN:HB3	1:F:501:ARG:HD3	1.69	0.72
1:A:298:LYS:HG2	1:A:318:TYR:CE2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:507:THR:HG21	2:C:564:THR:CG2	2.21	0.71
2:C:202:GLN:HG3	2:C:493:GLY:HA2	1.72	0.71
1:E:460:ILE:HD11	1:E:629:VAL:HG23	1.73	0.71
2:B:311:GLN:H	1:F:314:GLN:NE2	1.88	0.71
1:E:525:VAL:HG23	1:E:632:PHE:HB2	1.71	0.71
1:A:48:VAL:HG11	1:A:141:LEU:HD11	1.72	0.71
2:C:507:THR:HG21	2:C:564:THR:HG23	1.72	0.70
1:F:232:ILE:HD13	1:F:232:ILE:N	2.06	0.70
1:F:506:ASN:HD22	1:F:507:HIS:H	1.37	0.70
2:D:23:LYS:HG2	2:D:575:GLU:OE1	1.90	0.70
2:C:340:TYR:HB3	2:C:346:PHE:CD2	2.22	0.70
1:A:506:ASN:HD22	1:A:507:HIS:H	1.38	0.70
2:C:202:GLN:HG3	2:C:493:GLY:CA	2.22	0.70
2:B:303:ASN:HB2	1:F:173:MET:HE1	1.73	0.70
2:B:349:PHE:H	2:C:343:GLN:HE22	1.39	0.70
1:E:506:ASN:ND2	1:E:507:HIS:H	1.88	0.69
2:C:507:THR:CG2	2:C:564:THR:HG23	2.22	0.69
2:C:502:ASN:ND2	2:C:503:HIS:H	1.90	0.69
2:B:283:GLY:CA	2:B:532:GLU:HG2	2.22	0.69
1:A:470:THR:OG1	1:A:679:HIS:HD2	1.76	0.69
1:A:555:TRP:HH2	1:A:647:LEU:HD12	1.57	0.69
2:B:165:GLN:HG3	2:B:479:THR:HG22	1.73	0.69
2:B:210:SER:OG	2:B:227:GLU:OE2	2.10	0.69
2:C:21:GLU:OE1	2:C:21:GLU:HA	1.92	0.69
2:C:202:GLN:CG	2:C:493:GLY:HA2	2.23	0.69
2:C:512:ILE:HD12	2:C:563:ILE:HD12	1.75	0.69
1:A:307:THR:O	1:A:309:PHE:N	2.26	0.69
1:F:190:ASN:ND2	1:F:193:ALA:H	1.89	0.69
2:D:72:ASN:ND2	2:D:75:ALA:H	1.90	0.68
1:F:298:LYS:HG2	1:F:318:TYR:CE2	2.28	0.68
2:B:632:PRO:HB2	2:B:634:GLU:OE2	1.93	0.68
1:A:314:GLN:H	2:D:311:GLN:HE22	1.41	0.68
1:E:35:VAL:HG22	1:E:591:LEU:HD23	1.74	0.68
1:E:100:PHE:HD1	1:E:392:VAL:HG22	1.57	0.68
2:B:467:THR:OG1	2:B:675:HIS:HD2	1.77	0.68
2:D:299:LEU:HB3	2:D:311:GLN:HG2	1.76	0.68
1:F:91:MET:HE1	1:F:97:PHE:HB2	1.75	0.68
1:F:271:GLN:HE22	1:F:552:GLU:H	1.38	0.68
1:A:91:MET:HE1	1:A:97:PHE:HD2	1.58	0.68
2:B:645:ASN:H	2:B:645:ASN:ND2	1.91	0.68
1:E:234:MET:HE1	1:E:611:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:476:GLU:HG2	1:F:501:ARG:HG2	1.75	0.67
1:F:232:ILE:H	1:F:232:ILE:CD1	1.94	0.67
1:F:465:VAL:HG21	1:F:675:ILE:HD11	1.76	0.67
2:B:615:ASP:H	2:D:615:ASP:CB	2.05	0.67
2:D:247:ASN:C	2:D:247:ASN:ND2	2.46	0.67
1:E:67:GLU:HG2	1:E:83:LEU:HD21	1.77	0.67
2:D:91:ASN:H	2:D:134:GLN:HE22	1.43	0.67
2:B:450:LEU:CB	2:B:663:GLN:HE21	2.08	0.67
1:A:98:SER:O	1:A:104:MET:HE3	1.93	0.67
2:D:349:PHE:O	2:D:350:ASP:HB2	1.94	0.67
1:E:38:GLN:HE22	1:E:158:VAL:H	1.43	0.66
1:E:640:ALA:H	1:E:641:PRO:CD	2.06	0.66
2:D:134:GLN:HE21	2:D:134:GLN:N	1.84	0.66
2:D:247:ASN:HD22	2:D:248:SER:N	1.94	0.66
1:E:506:ASN:HD22	1:E:507:HIS:N	1.91	0.66
2:C:429:LYS:O	2:C:433:GLN:HG2	1.94	0.66
2:C:467:THR:OG1	2:C:675:HIS:HD2	1.79	0.66
1:F:531:ALA:HB3	1:F:550:PHE:CE2	2.30	0.66
2:C:35:GLN:HE21	2:C:592:ILE:HD11	1.60	0.66
1:E:640:ALA:N	1:E:641:PRO:CD	2.59	0.66
1:E:361:PRO:O	1:E:364:ILE:HG13	1.95	0.66
1:A:50:GLN:HE22	1:A:485:PHE:H	1.42	0.66
2:B:523:LYS:HE2	2:B:548:GLU:OE2	1.95	0.66
1:F:66:ILE:HB	1:F:83:LEU:HD21	1.78	0.66
2:B:539:LEU:HD13	2:B:656:VAL:HG11	1.77	0.65
1:F:38:GLN:HE22	1:F:158:VAL:H	1.44	0.65
1:F:506:ASN:ND2	1:F:507:HIS:H	1.93	0.65
1:F:470:THR:OG1	1:F:679:HIS:HD2	1.78	0.65
2:C:516:VAL:CG1	2:C:518:THR:HG22	2.27	0.65
2:C:99:GLU:O	2:C:103:GLU:HG2	1.97	0.65
2:B:95:SER:H	2:B:101:MET:HE1	1.56	0.65
2:B:502:ASN:ND2	2:B:503:HIS:H	1.88	0.65
1:F:584:MET:HA	1:F:587:ILE:HD12	1.79	0.65
2:D:210:SER:OG	2:D:227:GLU:OE2	2.14	0.65
2:B:408:ILE:HG21	1:F:302:TYR:OH	1.97	0.65
2:D:166:TYR:CD1	2:D:416:GLN:HG3	2.32	0.64
2:D:185:CYS:HG	2:D:191:CYS:HG	1.46	0.64
2:D:346:PHE:HB3	2:D:353:ILE:HD11	1.79	0.64
2:C:516:VAL:HG12	2:C:518:THR:HG22	1.80	0.64
2:D:93:GLU:HG2	2:D:304:SER:HB2	1.78	0.64
1:E:628:PHE:HE1	1:E:654:PHE:CE2	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:181:MET:CE	1:E:484:TYR:H	2.09	0.64
1:A:526:VAL:HG22	1:A:629:VAL:HG22	1.80	0.64
2:B:96:ILE:HD13	2:B:139:TYR:CE2	2.33	0.64
2:C:347:LYS:HB3	2:C:352:LYS:HA	1.80	0.64
2:C:529:LYS:NZ	2:C:670:LYS:HE3	2.12	0.64
2:B:181:MET:CE	1:F:483:VAL:HG13	2.29	0.63
1:E:91:MET:SD	1:E:104:MET:CE	2.86	0.63
2:C:35:GLN:HE22	2:C:155:VAL:H	1.46	0.63
2:D:35:GLN:NE2	2:D:39:LEU:HG	2.14	0.63
2:D:142:TYR:CD2	2:D:156:LEU:HD13	2.34	0.63
1:F:307:THR:CG2	1:F:309:PHE:H	2.11	0.63
1:A:687:LYS:HA	1:A:690:ILE:CD1	2.29	0.62
2:B:66:SER:HB2	2:B:69:CYS:SG	2.40	0.62
1:E:163:TYR:CD1	1:E:232:ILE:HG23	2.35	0.62
1:A:314:GLN:H	2:D:311:GLN:NE2	1.96	0.62
1:F:469:THR:HG21	1:F:680:GLU:HG3	1.81	0.62
2:B:408:ILE:CG2	1:F:302:TYR:OH	2.47	0.62
2:C:344:GLY:HA2	2:C:355:LEU:HD12	1.81	0.62
1:F:221:GLU:HB3	1:F:285:LEU:HD21	1.82	0.62
1:E:457:GLY:O	1:E:518:SER:HA	2.00	0.62
1:A:640:ALA:H	1:A:641:PRO:CD	2.13	0.62
1:F:307:THR:HG22	1:F:310:THR:N	2.14	0.62
1:F:173:MET:O	1:F:177:GLN:HG2	2.00	0.61
2:B:305:PHE:CD2	2:B:305:PHE:N	2.68	0.61
1:A:314:GLN:HE22	2:D:311:GLN:N	1.90	0.61
2:D:225:LEU:HD22	2:D:231:LEU:HD22	1.80	0.61
1:A:535:ASP:HB3	1:A:541:LEU:HD21	1.83	0.61
1:F:245:LEU:HD21	1:F:251:SER:HB3	1.83	0.61
1:E:50:GLN:NE2	1:E:485:PHE:H	1.96	0.61
1:A:98:SER:H	1:A:104:MET:HE3	1.65	0.61
2:B:213:LEU:HG	9:F:904:HOH:O	2.00	0.61
2:B:542:ASN:ND2	2:B:545:ASN:HD22	1.98	0.61
2:C:346:PHE:HE1	2:C:353:ILE:HB	1.65	0.61
2:D:459:ASP:OD1	2:D:461:LYS:HE3	2.00	0.61
2:B:165:GLN:HG3	2:B:479:THR:HG21	1.83	0.61
2:B:211:ASN:OD1	2:B:213:LEU:HB3	2.00	0.61
2:D:542:ASN:HD22	2:D:545:ASN:HD22	1.49	0.61
2:C:392:ARG:NH2	2:C:418:SER:OG	2.34	0.60
2:C:516:VAL:HG12	2:C:518:THR:CG2	2.31	0.60
1:F:347:ASP:OD1	1:F:444:TYR:HE2	1.84	0.60
2:B:247:ASN:ND2	2:B:249:GLY:N	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:LEU:HB2	2:B:663:GLN:NE2	2.15	0.60
2:B:531:ASP:OD2	2:B:533:ASN:HB2	2.01	0.60
2:C:206:TYR:CE2	2:C:497:ARG:HD2	2.36	0.60
1:A:94:ASN:ND2	2:D:194:TYR:OH	2.35	0.60
1:A:230:GLU:HG2	1:A:423:ARG:NH1	2.17	0.60
2:C:185:CYS:HG	2:C:191:CYS:HG	1.49	0.60
2:B:173:LYS:HE2	2:B:177:ASP:OD2	2.02	0.60
2:D:465:MET:CE	2:D:673:VAL:HG22	2.32	0.60
2:B:93:GLU:HG2	2:B:304:SER:HB2	1.83	0.60
2:D:145:ILE:HG21	2:D:156:LEU:HD21	1.82	0.60
1:A:630:TYR:HB2	1:A:631:PRO:CD	2.32	0.60
2:C:210:SER:OG	2:C:227:GLU:OE2	2.20	0.60
2:C:181:MET:HE1	1:E:484:TYR:H	1.66	0.59
2:B:217:ASN:HD21	2:B:219:GLU:HB2	1.66	0.59
2:C:507:THR:CG2	2:C:564:THR:CG2	2.78	0.59
2:B:502:ASN:ND2	2:B:503:HIS:N	2.49	0.59
1:F:422:LEU:HD22	1:F:427:PHE:CE2	2.37	0.59
2:B:305:PHE:HA	1:F:177:GLN:HG3	1.85	0.59
2:B:392:ARG:NH2	2:B:418:SER:OG	2.35	0.59
2:C:247:ASN:N	2:C:247:ASN:HD22	1.99	0.59
1:A:190:ASN:C	1:A:190:ASN:HD22	2.06	0.59
1:E:257:LEU:HD11	1:E:264:VAL:HG21	1.84	0.59
1:E:260:ARG:HD3	1:E:263:GLU:OE1	2.03	0.59
1:F:446:LYS:H	1:F:446:LYS:HD3	1.68	0.59
2:B:217:ASN:HD22	2:B:219:GLU:H	1.51	0.59
1:E:307:THR:O	1:E:309:PHE:N	2.36	0.59
2:C:663:GLN:HB2	2:C:666:MET:CE	2.32	0.58
2:B:531:ASP:CG	2:B:533:ASN:HB2	2.24	0.58
1:E:91:MET:SD	1:E:104:MET:HE3	2.44	0.58
1:F:643:GLU:HB3	1:F:645:PHE:HB2	1.84	0.58
1:F:646:VAL:C	1:F:648:ASP:H	2.06	0.58
1:A:267:TYR:OH	1:A:552:GLU:OE1	2.19	0.58
2:D:247:ASN:ND2	2:D:249:GLY:H	2.00	0.58
2:D:312:ARG:HH22	2:D:421:ASP:CG	2.07	0.58
1:E:91:MET:SD	1:E:104:MET:HE2	2.44	0.58
2:B:217:ASN:ND2	2:B:219:GLU:H	2.00	0.58
2:B:463:ASP:HB2	2:B:506:PHE:HB2	1.85	0.58
2:D:268:GLN:NE2	2:D:548:GLU:H	1.96	0.58
2:C:502:ASN:HD22	2:C:503:HIS:N	1.97	0.58
2:B:145:ILE:HG23	2:B:151:THR:CG2	2.33	0.58
1:E:566:LYS:HD3	1:E:568:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:582:VAL:HG12	1:E:586:GLU:HB3	1.85	0.58
1:A:642:PHE:O	1:A:643:GLU:CG	2.51	0.57
2:C:290:TRP:HB3	2:C:327:ILE:HG12	1.86	0.57
1:F:50:GLN:HE22	1:F:485:PHE:H	1.52	0.57
2:C:93:GLU:HG2	2:C:304:SER:HB2	1.85	0.57
2:D:599:SER:HB3	2:D:639:LYS:HE3	1.86	0.57
2:B:332:ILE:CG1	2:C:335:LYS:HG2	2.27	0.57
2:B:388:GLU:O	2:B:392:ARG:HG3	2.05	0.57
2:C:525:PHE:CE2	2:C:548:GLU:HG3	2.39	0.57
1:F:283:ASN:OD1	1:F:615:ARG:NH2	2.38	0.57
1:E:67:GLU:HG3	1:E:83:LEU:HD21	1.87	0.57
1:F:267:TYR:OH	1:F:552:GLU:OE1	2.23	0.57
2:B:661:PHE:HA	2:B:666:MET:HE1	1.86	0.57
2:D:283:GLY:HA2	2:D:532:GLU:CG	2.31	0.57
2:D:503:HIS:HD2	2:D:504:LYS:O	1.88	0.57
1:E:495:VAL:HG23	1:E:496:HIS:CD2	2.40	0.56
1:A:687:LYS:HA	1:A:690:ILE:HD12	1.87	0.56
2:B:429:LYS:O	2:B:433:GLN:HG2	2.06	0.56
2:D:344:GLY:HA2	2:D:355:LEU:HD12	1.85	0.56
1:A:160:PRO:HB3	1:A:584:MET:HG3	1.86	0.56
1:A:257:LEU:HG	1:A:257:LEU:O	2.04	0.56
2:C:145:ILE:HG23	2:C:151:THR:HG22	1.85	0.56
2:D:388:GLU:O	2:D:392:ARG:HG3	2.05	0.56
1:E:347:ASP:OD1	1:E:444:TYR:HE2	1.89	0.56
1:E:615:ARG:HG2	1:E:679:HIS:CD2	2.41	0.56
1:F:24:THR:HG22	1:F:24:THR:O	2.05	0.56
1:F:170:PHE:HB3	1:F:232:ILE:HG22	1.86	0.56
2:B:358:SER:C	2:B:360:ALA:H	2.08	0.56
1:E:205:TYR:CE2	1:E:499:LYS:HE3	2.40	0.56
2:B:261:ILE:HG12	2:B:648:PHE:CE1	2.41	0.56
2:C:603:MET:HG2	2:C:604:PRO:HD2	1.88	0.56
2:D:177:ASP:O	2:D:181:MET:HG3	2.05	0.56
2:D:331:ASP:OD2	1:E:338:LYS:HE2	2.04	0.56
1:E:245:LEU:HB2	1:E:642:PHE:HE1	1.70	0.56
1:A:221:GLU:HB3	1:A:285:LEU:HD21	1.87	0.56
2:D:346:PHE:O	2:D:353:ILE:HG13	2.06	0.56
1:E:168:LYS:NZ	1:E:308:LYS:HE3	2.21	0.56
1:A:271:GLN:HE22	1:A:552:GLU:N	1.98	0.56
1:A:570:ASN:OD1	1:A:572:ASN:HB2	2.05	0.56
2:B:141:TYR:O	2:B:145:ILE:HD12	2.05	0.56
2:B:358:SER:C	2:B:360:ALA:N	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:222:ILE:O	2:D:222:ILE:CG2	2.54	0.55
1:F:638:ASP:HB2	1:F:647:LEU:HD22	1.87	0.55
2:C:222:ILE:HG22	2:C:226:THR:HG23	1.88	0.55
2:C:349:PHE:O	2:C:350:ASP:HB2	2.05	0.55
1:A:98:SER:H	1:A:104:MET:CE	2.19	0.55
1:E:628:PHE:HE1	1:E:654:PHE:HE2	1.52	0.55
1:A:212:TYR:HB3	1:A:226:THR:HG22	1.86	0.55
1:A:244:HIS:HD2	1:A:642:PHE:CE1	2.25	0.55
1:A:283:ASN:OD1	1:A:615:ARG:NH2	2.39	0.55
2:C:480:VAL:HA	1:E:184:MET:HE1	1.88	0.55
2:B:522:VAL:HG22	2:B:625:VAL:HG22	1.89	0.55
2:B:663:GLN:CG	2:B:666:MET:HE2	2.33	0.55
1:F:686:TYR:CE2	1:F:687:LYS:HD2	2.41	0.55
1:A:145:TYR:OH	1:A:160:PRO:O	2.24	0.55
2:D:551:TRP:C	2:D:551:TRP:CD1	2.80	0.55
2:B:667:PHE:HE2	2:B:669:LYS:HG3	1.72	0.55
2:C:268:GLN:HE22	2:C:548:GLU:N	1.95	0.55
1:E:581:SER:HB2	1:E:600:MET:SD	2.47	0.55
1:F:422:LEU:N	1:F:422:LEU:HD23	2.22	0.55
1:F:541:LEU:HD13	1:F:546:ASN:HB3	1.88	0.55
2:D:551:TRP:CH2	2:D:644:ASP:HB2	2.42	0.54
2:B:217:ASN:HD22	2:B:217:ASN:C	2.10	0.54
2:D:513:LYS:NZ	2:D:560:GLN:HE21	2.06	0.54
1:F:111:LEU:HD22	1:F:135:LEU:HD12	1.89	0.54
1:A:642:PHE:C	1:A:643:GLU:HG3	2.27	0.54
2:D:678:GLU:HG3	2:D:691:PRO:HB3	1.89	0.54
1:F:291:PHE:HB2	1:F:297:ILE:HG22	1.90	0.54
2:B:661:PHE:HA	2:B:666:MET:CE	2.37	0.54
1:F:395:ARG:NH2	1:F:421:SER:OG	2.41	0.54
2:D:145:ILE:HG23	2:D:151:THR:HG22	1.90	0.54
2:D:285:ILE:HD12	2:D:429:LYS:HG2	1.89	0.54
2:D:462:VAL:HG12	2:D:463:ASP:O	2.08	0.54
1:E:185:GLN:NE2	1:E:189:ILE:HD12	2.23	0.54
1:A:265:TYR:CE1	1:A:372:GLN:HB2	2.43	0.54
2:C:275:MET:CE	2:C:545:ASN:O	2.56	0.54
2:D:83:TYR:HA	2:D:87:PHE:CE1	2.43	0.53
1:E:190:ASN:HB3	1:E:193:ALA:HB3	1.90	0.53
1:A:75:ASN:ND2	1:A:78:ALA:N	2.50	0.53
1:A:173:MET:HE2	1:A:306:LEU:HD21	1.89	0.53
2:B:67:LYS:HG2	2:B:76:TYR:CE2	2.43	0.53
2:D:47:GLU:O	2:D:129:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:TYR:HB3	1:F:169:MET:HG3	1.89	0.53
2:D:636:GLU:CD	2:D:636:GLU:H	2.12	0.53
1:A:525:VAL:HG23	1:A:632:PHE:HB2	1.90	0.53
1:E:35:VAL:HG22	1:E:591:LEU:CD2	2.37	0.53
1:E:301:TYR:CD2	1:E:303:PRO:HD3	2.43	0.53
2:C:346:PHE:CE1	2:C:353:ILE:HB	2.43	0.53
1:E:335:THR:OG1	1:F:338:LYS:HG2	2.08	0.53
1:F:465:VAL:HG21	1:F:675:ILE:CD1	2.39	0.53
2:B:218:ASN:HB3	2:B:282:LEU:HD21	1.91	0.52
1:E:234:MET:CE	1:E:611:LEU:HD13	2.39	0.52
1:F:307:THR:HG22	1:F:309:PHE:N	2.23	0.52
2:B:94:PHE:HA	2:B:101:MET:HE3	1.91	0.52
2:C:624:PHE:CE1	2:C:626:TYR:CD2	2.98	0.52
2:B:174:ASN:ND2	1:F:308:LYS:HA	2.25	0.52
2:C:510:ILE:HD11	2:C:524:MET:CE	2.39	0.52
2:D:464:LYS:HD3	2:D:466:VAL:CG2	2.39	0.52
1:F:214:ASN:HA	1:F:217:LEU:O	2.08	0.52
1:A:190:ASN:HD22	1:A:193:ALA:H	1.55	0.52
2:C:83:TYR:HA	2:C:87:PHE:HE1	1.74	0.52
1:A:470:THR:OG1	1:A:679:HIS:CD2	2.61	0.52
1:A:476:GLU:HG2	1:A:501:ARG:HG3	1.91	0.52
2:C:502:ASN:ND2	2:C:503:HIS:N	2.58	0.52
2:B:303:ASN:HB2	1:F:173:MET:CE	2.39	0.52
2:B:304:SER:O	2:B:305:PHE:C	2.47	0.52
1:F:100:PHE:HD1	1:F:392:VAL:HG22	1.74	0.52
2:B:531:ASP:OD1	2:B:533:ASN:HB2	2.10	0.52
2:B:533:ASN:HB3	2:B:535:PHE:HB2	1.91	0.52
1:E:459:LYS:HG3	1:E:668:PRO:HB3	1.92	0.52
1:E:646:VAL:C	1:E:648:ASP:H	2.13	0.52
1:F:506:ASN:HD22	1:F:507:HIS:N	2.06	0.52
1:F:93:LYS:O	1:F:94:ASN:HB2	2.09	0.52
1:A:505:LEU:O	1:A:610:ARG:HD3	2.10	0.51
2:C:145:ILE:HG23	2:C:151:THR:CG2	2.40	0.51
2:D:455:LEU:C	2:D:455:LEU:HD23	2.31	0.51
1:E:70:MET:HG3	1:E:79:VAL:HG11	1.92	0.51
1:F:278:PHE:CE1	1:F:532:PRO:HG3	2.44	0.51
2:D:91:ASN:H	2:D:134:GLN:NE2	2.08	0.51
1:F:495:VAL:HG12	1:F:495:VAL:O	2.10	0.51
1:A:164:GLU:OE2	1:A:583:PRO:HA	2.11	0.51
2:D:222:ILE:O	2:D:222:ILE:HG22	2.09	0.51
2:D:465:MET:HE3	2:D:673:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:290:TRP:HB3	2:D:327:ILE:HG12	1.92	0.51
2:D:343:GLN:NE2	2:D:343:GLN:CA	2.68	0.51
4:H:2:NAG:H61	4:H:3:BMA:C1	2.41	0.51
2:B:615:ASP:HB2	2:D:615:ASP:HB3	1.92	0.51
1:E:686:TYR:C	1:E:686:TYR:CD2	2.84	0.51
1:A:444:TYR:N	1:A:444:TYR:HD1	2.09	0.51
2:D:214:THR:HB	2:D:299:LEU:O	2.11	0.51
2:B:645:ASN:ND2	2:B:645:ASN:N	2.56	0.51
2:C:312:ARG:NH2	2:C:421:ASP:OD2	2.43	0.51
2:D:349:PHE:O	2:D:350:ASP:CB	2.59	0.51
1:A:640:ALA:H	1:A:641:PRO:HD2	1.75	0.51
2:B:275:MET:HG2	2:B:619:PHE:CE1	2.45	0.51
1:F:94:ASN:H	1:F:137:GLN:HE22	1.58	0.51
2:B:217:ASN:HD22	2:B:219:GLU:N	2.09	0.50
2:B:245:TRP:HA	2:B:380:LEU:HG	1.93	0.50
2:C:47:GLU:O	2:C:129:ARG:NH2	2.44	0.50
2:C:330:LEU:O	2:C:334:GLU:HG3	2.10	0.50
2:C:533:ASN:HD21	1:F:214:ASN:HD22	1.58	0.50
2:C:578:LEU:HD12	2:C:593:PRO:HG3	1.94	0.50
2:C:475:ASP:OD1	2:C:477:PHE:HB3	2.10	0.50
1:F:190:ASN:ND2	1:F:193:ALA:N	2.60	0.50
1:A:181:VAL:O	1:A:185:GLN:HG3	2.12	0.50
1:A:217:LEU:HD21	1:A:302:TYR:HB3	1.93	0.50
1:E:615:ARG:HG2	1:E:679:HIS:HD2	1.74	0.50
2:B:222:ILE:HD11	2:B:282:LEU:CD1	2.39	0.50
2:B:663:GLN:H	2:B:666:MET:CE	2.25	0.50
1:E:234:MET:O	1:E:237:TYR:HB3	2.11	0.50
2:C:480:VAL:HG12	1:E:184:MET:HE1	1.93	0.50
2:D:533:ASN:OD1	2:D:535:PHE:HD1	1.95	0.49
1:F:278:PHE:HE1	1:F:532:PRO:HG3	1.76	0.49
2:B:44:ASN:HD22	2:B:487:LEU:HD21	1.76	0.49
2:C:180:LYS:HE3	2:C:481:TYR:O	2.12	0.49
2:C:529:LYS:HZ2	2:C:670:LYS:HE3	1.77	0.49
2:D:173:LYS:HA	2:D:176:MET:HE2	1.93	0.49
2:B:321:GLU:HA	2:B:324:TYR:CE1	2.47	0.49
2:D:502:ASN:HD22	2:D:503:HIS:H	1.59	0.49
2:B:94:PHE:HA	2:B:101:MET:CE	2.42	0.49
2:B:631:THR:HG21	2:B:645:ASN:OD1	2.13	0.49
2:C:678:GLU:OE1	2:C:683:LEU:HD13	2.12	0.49
2:D:332:ILE:HG21	1:E:341:VAL:HB	1.95	0.49
1:F:458:VAL:HG22	1:F:518:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:LEU:HD23	1:F:411:MET:SD	2.53	0.49
2:C:636:GLU:HB3	2:C:637:PRO:HD2	1.94	0.49
1:E:485:PHE:CD1	1:E:495:VAL:HG12	2.47	0.49
1:E:552:GLU:HG2	1:E:576:ILE:HD13	1.95	0.49
1:F:450:GLN:H	1:F:664:LEU:HD22	1.77	0.49
1:A:100:PHE:HD1	1:A:392:VAL:HG22	1.77	0.49
1:A:559:LYS:HD3	1:A:559:LYS:N	2.28	0.49
2:D:217:ASN:ND2	2:D:219:GLU:H	2.04	0.49
1:E:307:THR:HG23	1:E:309:PHE:H	1.76	0.49
1:A:444:TYR:N	1:A:444:TYR:CD1	2.80	0.49
2:C:31:PHE:CE2	2:C:592:ILE:HD12	2.48	0.49
1:A:202:GLU:O	1:A:203:ASN:HB2	2.12	0.49
1:A:646:VAL:C	1:A:648:ASP:H	2.16	0.49
2:B:210:SER:HB2	2:B:214:THR:CB	2.43	0.49
2:B:631:THR:O	2:B:632:PRO:O	2.29	0.49
2:C:214:THR:HB	2:C:299:LEU:O	2.13	0.49
2:C:678:GLU:HB2	2:C:684:PHE:CE1	2.47	0.49
1:E:267:TYR:OH	1:E:552:GLU:OE1	2.29	0.49
1:F:159:VAL:CG1	1:F:160:PRO:HD2	2.43	0.49
1:A:84:LYS:HG3	1:A:87:ARG:NH2	2.28	0.49
1:F:469:THR:CG2	1:F:680:GLU:HG3	2.43	0.49
2:B:145:ILE:HG23	2:B:151:THR:HG22	1.95	0.48
2:B:151:THR:HG22	2:B:151:THR:O	2.13	0.48
2:B:465:MET:HE3	2:B:671:VAL:HB	1.94	0.48
1:F:52:ASN:OD1	1:F:54:ASP:HB2	2.13	0.48
2:B:332:ILE:HD11	2:C:338:PHE:CD1	2.48	0.48
2:C:222:ILE:HG22	2:C:222:ILE:O	2.13	0.48
1:F:430:LEU:O	1:F:433:ARG:HB3	2.14	0.48
1:F:577:PHE:CZ	1:F:612:MET:HG3	2.47	0.48
2:C:241:HIS:CE1	2:C:601:ASP:HB3	2.48	0.48
2:C:663:GLN:HB2	2:C:666:MET:HE2	1.94	0.48
2:D:328:ARG:HD2	1:E:437:TYR:OH	2.13	0.48
1:F:67:GLU:HG2	1:F:83:LEU:HD13	1.95	0.48
1:A:214:ASN:O	1:E:537:ASN:ND2	2.36	0.48
2:B:168:VAL:HG13	2:B:172:VAL:HB	1.96	0.48
2:C:344:GLY:HA2	2:C:355:LEU:CD1	2.42	0.48
1:E:91:MET:HE3	1:E:97:PHE:HB2	1.96	0.48
1:E:190:ASN:C	1:E:190:ASN:HD22	2.17	0.48
1:E:231:ASP:OD2	1:E:504:ARG:NH1	2.46	0.48
2:B:529:LYS:HE2	2:B:670:LYS:HG2	1.96	0.48
2:B:615:ASP:CA	2:D:615:ASP:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:THR:HA	2:D:154:PHE:HD2	1.78	0.48
1:A:48:VAL:HG13	1:A:141:LEU:HD11	1.92	0.48
2:B:142:TYR:OH	2:B:157:PRO:O	2.26	0.48
2:B:404:GLN:HE21	2:B:404:GLN:HA	1.78	0.48
2:C:192:TYR:HD1	2:C:197:ILE:CG2	2.26	0.48
2:D:145:ILE:CG1	2:D:151:THR:HG21	2.44	0.48
2:B:181:MET:HE1	1:F:483:VAL:HA	1.96	0.48
2:B:304:SER:O	2:B:306:TYR:HB2	2.13	0.48
1:F:159:VAL:HG12	1:F:160:PRO:HD2	1.96	0.48
2:C:326:GLU:O	2:C:330:LEU:HG	2.14	0.48
1:F:234:MET:O	1:F:237:TYR:HB3	2.13	0.48
1:A:506:ASN:HD22	1:A:507:HIS:N	2.08	0.47
1:F:643:GLU:HG3	1:F:645:PHE:HD1	1.79	0.47
1:A:167:PRO:HB2	1:A:171:MET:CE	2.44	0.47
1:A:326:ASN:ND2	1:A:397:VAL:HG13	2.29	0.47
2:B:304:SER:O	2:B:306:TYR:N	2.46	0.47
2:D:513:LYS:HZ2	2:D:560:GLN:HG2	1.79	0.47
2:B:141:TYR:CZ	2:B:145:ILE:HD11	2.50	0.47
2:B:408:ILE:HG21	1:F:302:TYR:CZ	2.49	0.47
2:B:614:TYR:HE1	2:B:679:LEU:HD12	1.79	0.47
2:C:46:ASN:OD1	2:C:46:ASN:N	2.40	0.47
2:D:542:ASN:ND2	2:D:545:ASN:HD22	2.13	0.47
1:E:173:MET:CG	1:E:306:LEU:HG	2.44	0.47
1:E:517:ASP:OD1	1:E:564:GLN:HG2	2.14	0.47
1:F:638:ASP:CB	1:F:647:LEU:HA	2.39	0.47
2:C:483:SER:OG	2:C:486:GLU:HG3	2.14	0.47
1:A:492:ASN:HD22	1:A:492:ASN:N	2.11	0.47
2:B:285:ILE:HD12	2:B:429:LYS:HG3	1.97	0.47
2:D:298:TYR:CE2	2:D:300:PRO:HG3	2.49	0.47
2:D:335:LYS:HB3	1:F:335:THR:HG23	1.96	0.47
1:F:154:CYS:HA	1:F:157:PHE:HD1	1.78	0.47
1:A:457:GLY:O	1:A:518:SER:HA	2.15	0.47
1:A:667:VAL:HG13	1:A:669:ASN:OD1	2.15	0.47
2:B:503:HIS:HD2	2:B:504:LYS:O	1.98	0.47
2:B:657:LEU:HB3	2:B:659:GLN:HE22	1.79	0.47
2:D:168:VAL:CG1	2:D:172:VAL:HB	2.45	0.47
1:F:38:GLN:HE22	1:F:158:VAL:N	2.10	0.47
1:F:623:PHE:CD2	1:F:677:ILE:HD12	2.49	0.47
1:A:218:TYR:OH	1:E:536:ASP:HB3	2.15	0.47
2:B:680:PHE:HB2	2:B:683:LEU:HD12	1.96	0.47
2:C:451:HIS:ND1	2:C:663:GLN:NE2	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:TYR:CD1	1:E:57:TYR:C	2.88	0.47
1:F:305:MET:HE3	1:F:305:MET:HB3	1.63	0.47
1:A:171:MET:HE1	1:A:479:ALA:HB1	1.97	0.47
1:A:658:ARG:HB2	1:A:659:PRO:HD2	1.97	0.47
2:B:96:ILE:HD11	2:B:102:ARG:HG3	1.96	0.47
2:B:96:ILE:HG13	2:B:96:ILE:O	2.15	0.47
2:B:174:ASN:HD22	1:F:308:LYS:C	2.19	0.47
2:C:642:VAL:O	2:C:644:ASP:N	2.47	0.47
2:D:151:THR:HA	2:D:154:PHE:CD2	2.50	0.47
2:D:636:GLU:CB	2:D:637:PRO:CD	2.92	0.47
1:E:38:GLN:HE22	1:E:158:VAL:N	2.09	0.47
2:B:182:MET:HE2	2:B:186:LEU:HG	1.97	0.47
2:C:451:HIS:HA	2:C:663:GLN:HG3	1.97	0.47
2:D:346:PHE:CB	2:D:353:ILE:HD11	2.45	0.47
1:E:646:VAL:HG21	1:E:652:LEU:HD21	1.96	0.47
2:D:41:LEU:HD22	2:D:129:ARG:HG2	1.97	0.46
1:E:217:LEU:HD21	1:E:302:TYR:HB3	1.98	0.46
1:A:79:VAL:O	1:A:83:LEU:HG	2.14	0.46
1:A:219:ASN:O	1:A:220:ASN:HB3	2.15	0.46
1:F:648:ASP:C	1:F:650:LYS:H	2.19	0.46
2:B:222:ILE:HG22	2:B:222:ILE:O	2.15	0.46
1:F:347:ASP:OD1	1:F:444:TYR:CE2	2.66	0.46
1:A:315:ARG:HH22	1:A:424:ASP:CG	2.17	0.46
1:F:596:VAL:HG12	1:F:597:PRO:HD2	1.98	0.46
2:B:83:TYR:HB2	2:B:87:PHE:HE1	1.81	0.46
2:C:83:TYR:HA	2:C:87:PHE:CE1	2.51	0.46
2:C:206:TYR:CZ	2:C:497:ARG:HD2	2.51	0.46
2:B:181:MET:HE2	1:F:484:TYR:H	1.81	0.46
2:B:501:LEU:HG	2:B:502:ASN:N	2.30	0.46
1:A:50:GLN:NE2	1:A:485:PHE:H	2.12	0.46
2:B:542:ASN:HD22	2:B:545:ASN:HD22	1.62	0.46
2:C:262:TYR:OH	2:C:388:GLU:OE1	2.26	0.46
2:D:185:CYS:SG	2:D:191:CYS:SG	3.02	0.46
1:F:231:ASP:OD1	1:F:504:ARG:HD2	2.14	0.46
1:E:339:THR:HG21	1:F:345:GLN:HE22	1.81	0.46
1:A:465:VAL:HG12	1:A:466:ASP:O	2.16	0.46
2:B:44:ASN:O	2:B:46:ASN:N	2.49	0.46
2:B:182:MET:CE	2:B:186:LEU:HG	2.46	0.46
1:F:682:GLU:HB2	1:F:688:PHE:CE1	2.51	0.46
1:A:615:ARG:HG3	1:A:679:HIS:CD2	2.51	0.46
2:B:145:ILE:HG23	2:B:151:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:678:GLU:OE1	2:D:683:LEU:HD13	2.16	0.46
1:A:535:ASP:OD1	1:A:539:ILE:HD12	2.16	0.45
2:B:93:GLU:CG	2:B:304:SER:HB2	2.46	0.45
2:B:599:SER:HA	2:B:639:LYS:HD3	1.98	0.45
2:C:62:ASN:OD1	2:C:64:GLU:HG3	2.15	0.45
1:A:102:ASP:HB3	1:A:385:ASP:OD2	2.16	0.45
1:A:667:VAL:CG1	1:A:669:ASN:OD1	2.64	0.45
1:F:232:ILE:HD12	1:F:502:GLN:OE1	2.17	0.45
1:F:476:GLU:HA	1:F:500:VAL:O	2.15	0.45
1:F:578:LYS:HG2	1:F:606:TYR:HB2	1.98	0.45
2:C:35:GLN:NE2	2:C:155:VAL:HB	2.31	0.45
2:C:72:ASN:HD21	2:C:74:LYS:HB3	1.81	0.45
2:C:349:PHE:O	2:C:350:ASP:CB	2.64	0.45
1:E:643:GLU:HB3	1:E:645:PHE:HB2	1.97	0.45
2:D:690:THR:HA	2:D:691:PRO:HD3	1.63	0.45
1:E:568:ILE:HD12	1:E:568:ILE:N	2.31	0.45
4:H:2:NAG:C6	4:H:3:BMA:C1	2.94	0.45
2:C:273:TYR:CE1	2:C:277:ARG:HD2	2.52	0.45
2:C:283:GLY:HA2	2:C:532:GLU:CG	2.34	0.45
2:C:542:ASN:HD22	2:C:545:ASN:ND2	2.05	0.45
2:C:513:LYS:HA	2:C:559:GLY:O	2.17	0.45
1:F:181:VAL:O	1:F:185:GLN:HG3	2.16	0.45
1:A:91:MET:HE1	1:A:97:PHE:CD2	2.44	0.45
2:B:347:LYS:HA	2:B:351:LYS:O	2.16	0.45
2:B:603:MET:HG2	2:B:604:PRO:HD2	1.99	0.45
2:C:529:LYS:HZ3	2:C:670:LYS:HE3	1.78	0.45
2:D:247:ASN:HD22	2:D:249:GLY:H	1.63	0.45
1:E:507:HIS:HD2	1:E:508:SER:O	2.00	0.45
1:A:582:VAL:HG12	1:A:583:PRO:HD2	1.98	0.45
2:B:27:VAL:HG21	2:B:592:ILE:HG12	1.98	0.45
2:B:467:THR:OG1	2:B:675:HIS:CD2	2.65	0.45
2:D:253:ALA:O	2:D:256:GLU:HG2	2.16	0.45
2:D:657:LEU:HB3	2:D:659:GLN:NE2	2.32	0.45
1:E:77:LYS:HD2	1:E:77:LYS:N	2.31	0.45
1:E:331:ARG:HD2	1:F:437:TYR:OH	2.16	0.45
1:A:38:GLN:NE2	1:A:158:VAL:HB	2.32	0.45
2:D:636:GLU:HB3	2:D:637:PRO:HD3	1.99	0.45
1:E:476:GLU:HA	1:E:500:VAL:O	2.17	0.45
2:C:480:VAL:HG12	1:E:184:MET:CE	2.47	0.45
2:D:467:THR:OG1	2:D:675:HIS:HD2	1.99	0.45
1:E:72:ASN:HA	1:E:119:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:HG23	1:A:28:LYS:N	2.32	0.44
1:A:391:GLU:OE2	1:A:431:TYR:OH	2.31	0.44
2:C:455:LEU:HD12	2:C:456:LYS:N	2.32	0.44
2:C:636:GLU:CD	2:C:636:GLU:H	2.19	0.44
1:A:632:PHE:CG	1:A:632:PHE:O	2.71	0.44
2:B:35:GLN:HE22	2:B:155:VAL:N	2.03	0.44
2:B:311:GLN:NE2	1:F:314:GLN:H	2.14	0.44
2:C:408:ILE:HG21	1:E:302:TYR:OH	2.17	0.44
2:D:202:GLN:OE1	2:D:495:LYS:HE3	2.18	0.44
1:E:234:MET:HB2	1:E:234:MET:HE2	1.78	0.44
2:C:180:LYS:HG2	1:E:184:MET:HE2	1.98	0.44
2:D:343:GLN:HE21	2:D:343:GLN:CA	2.03	0.44
1:E:141:LEU:O	1:E:145:TYR:HB2	2.17	0.44
1:F:541:LEU:HD13	1:F:546:ASN:CB	2.47	0.44
1:F:576:ILE:HG22	1:F:576:ILE:O	2.17	0.44
2:B:525:PHE:HB2	2:B:622:PHE:HB3	1.99	0.44
2:B:540:GLU:HG3	2:B:658:PRO:HD3	1.98	0.44
2:C:512:ILE:HD12	2:C:563:ILE:CD1	2.44	0.44
2:D:332:ILE:HG12	1:E:342:GLN:HG3	1.99	0.44
1:F:391:GLU:O	1:F:395:ARG:HG3	2.16	0.44
1:A:244:HIS:HD2	1:A:642:PHE:CZ	2.36	0.44
2:B:213:LEU:CD2	1:F:411:MET:HB2	2.48	0.44
2:B:299:LEU:HD23	1:F:411:MET:HE3	1.99	0.44
2:B:312:ARG:HD3	2:B:395:LEU:O	2.18	0.44
2:D:512:ILE:HD11	2:D:561:SER:OG	2.17	0.44
1:E:173:MET:HG2	1:E:306:LEU:HG	1.99	0.44
1:E:458:VAL:HA	1:E:517:ASP:O	2.18	0.44
1:A:648:ASP:C	1:A:650:LYS:H	2.21	0.44
2:D:112:PHE:HE1	2:D:124:THR:HG22	1.82	0.44
2:D:347:LYS:HE3	2:D:352:LYS:HE3	1.99	0.44
2:B:311:GLN:HE22	1:F:314:GLN:H	1.66	0.44
2:D:174:ASN:O	2:D:178:TYR:CD1	2.71	0.44
1:A:75:ASN:HD21	1:A:78:ALA:H	1.61	0.44
2:B:686:ILE:HA	2:B:687:PRO:HD2	1.70	0.44
2:C:106:ILE:HG22	2:C:110:LYS:HE3	1.99	0.44
1:E:203:ASN:HD22	1:E:204:ASP:H	1.66	0.44
1:F:122:GLU:O	1:F:126:LYS:HG3	2.18	0.44
1:F:226:THR:O	1:F:230:GLU:HB2	2.18	0.44
1:F:679:HIS:HE1	1:F:682:GLU:O	2.01	0.44
1:A:253:LYS:O	1:A:253:LYS:HG2	2.16	0.44
2:C:151:THR:HG22	2:C:151:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:93:GLU:CG	2:D:304:SER:HB2	2.45	0.44
1:A:364:ILE:O	1:A:364:ILE:HD13	2.17	0.43
2:B:329:PHE:HA	2:B:332:ILE:CD1	2.48	0.43
1:A:214:ASN:HA	1:A:217:LEU:O	2.18	0.43
1:A:340:PHE:O	1:A:343:PHE:HB2	2.17	0.43
2:B:211:ASN:C	2:B:213:LEU:H	2.22	0.43
1:E:24:THR:HG23	1:E:24:THR:O	2.17	0.43
2:B:35:GLN:NE2	2:B:155:VAL:H	2.04	0.43
2:B:322:LYS:NZ	2:B:398:ALA:O	2.50	0.43
2:D:321:GLU:HA	2:D:324:TYR:CE1	2.53	0.43
1:F:640:ALA:H	1:F:641:PRO:CD	2.18	0.43
2:B:678:GLU:HB2	2:B:684:PHE:CE1	2.53	0.43
2:C:35:GLN:HE22	2:C:155:VAL:HB	1.83	0.43
2:C:525:PHE:HB2	2:C:622:PHE:HB3	2.01	0.43
2:C:666:MET:HE2	2:C:666:MET:HB2	1.36	0.43
2:D:364:VAL:HG11	2:D:435:ILE:HG23	2.00	0.43
2:D:455:LEU:HD23	2:D:456:LYS:N	2.34	0.43
2:B:241:HIS:CE1	2:B:601:ASP:HB3	2.54	0.43
2:B:278:LEU:CD2	2:B:532:GLU:HG3	2.49	0.43
2:C:629:GLU:HA	2:C:630:PRO:HD3	1.87	0.43
2:D:159:PRO:HD3	2:D:237:TYR:OH	2.19	0.43
1:E:170:PHE:O	1:E:232:ILE:HD11	2.18	0.43
1:F:458:VAL:HG22	1:F:518:SER:CB	2.48	0.43
1:F:466:ASP:OD2	1:F:511:ASN:HB2	2.19	0.43
1:A:173:MET:HE2	1:A:306:LEU:CD2	2.48	0.43
1:F:28:LYS:HD2	1:F:598:PHE:HD1	1.84	0.43
1:F:276:TYR:CE1	1:F:280:ARG:HD2	2.54	0.43
2:B:531:ASP:OD1	2:B:533:ASN:CB	2.66	0.43
2:D:383:TYR:CZ	1:E:359:HIS:HE1	2.36	0.43
1:F:528:ILE:HG22	1:F:553:LEU:HD12	2.00	0.43
1:A:173:MET:CE	2:D:308:PRO:HD3	2.48	0.43
1:A:183:LYS:HG2	1:A:483:VAL:HG13	2.01	0.43
1:A:455:PHE:CD2	1:A:630:TYR:HA	2.53	0.43
2:B:115:ALA:HB3	2:B:148:ARG:NH1	2.34	0.43
2:B:323:ASN:ND2	2:B:394:VAL:HG13	2.33	0.43
2:C:21:GLU:OE1	2:C:21:GLU:CA	2.66	0.43
2:C:501:LEU:O	2:C:606:ARG:HB2	2.19	0.43
1:E:577:PHE:CZ	1:E:612:MET:HG3	2.53	0.43
2:C:247:ASN:N	2:C:247:ASN:ND2	2.66	0.43
1:E:71:ASP:OD1	1:E:71:ASP:N	2.40	0.43
1:F:543:LEU:HA	1:F:543:LEU:HD23	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASN:HB3	1:A:72:ASN:HD22	1.84	0.43
2:B:83:TYR:HB2	2:B:87:PHE:CE1	2.53	0.43
2:B:682:TYR:CD2	4:H:1:NAG:H62	2.53	0.43
2:C:574:LYS:O	2:C:605:SER:HB2	2.18	0.43
1:F:164:GLU:OE2	1:F:583:PRO:HA	2.19	0.43
1:A:298:LYS:HG2	1:A:318:TYR:HE2	1.78	0.42
2:B:329:PHE:O	2:B:332:ILE:HD12	2.19	0.42
2:D:501:LEU:O	2:D:606:ARG:HB2	2.19	0.42
2:D:543:TRP:CZ2	2:D:655:PRO:HD3	2.54	0.42
1:A:100:PHE:O	1:A:396:ARG:NH2	2.51	0.42
1:F:28:LYS:HZ2	1:F:598:PHE:HE1	1.66	0.42
1:F:516:VAL:HB	1:F:565:ASN:HD21	1.84	0.42
1:A:630:TYR:HB2	1:A:631:PRO:HD2	2.01	0.42
1:A:640:ALA:N	1:A:641:PRO:CD	2.82	0.42
2:C:64:GLU:H	2:C:64:GLU:HG2	1.24	0.42
2:C:439:LYS:HD2	2:C:442:GLN:OE1	2.18	0.42
2:D:64:GLU:HA	2:D:80:MET:HE1	2.01	0.42
2:D:174:ASN:HB3	2:D:178:TYR:CE1	2.54	0.42
2:D:636:GLU:HB3	2:D:637:PRO:CD	2.49	0.42
2:C:492:HIS:HB2	2:C:493:GLY:H	1.65	0.42
2:D:533:ASN:OD1	2:D:535:PHE:CD1	2.72	0.42
2:C:43:TYR:CE1	2:C:580:MET:HE1	2.55	0.42
2:D:228:ASP:OD2	2:D:500:ARG:NH1	2.52	0.42
2:D:245:TRP:HA	2:D:380:LEU:HB2	2.02	0.42
2:B:554:GLN:HG2	2:B:563:ILE:HD11	2.00	0.42
2:C:355:LEU:HD13	2:C:441:TYR:CD2	2.55	0.42
2:C:645:ASN:ND2	2:C:645:ASN:H	2.16	0.42
2:B:96:ILE:HD12	2:B:102:ARG:HA	2.02	0.42
2:D:580:MET:HA	2:D:583:ILE:HD12	2.00	0.42
1:A:686:TYR:CD2	1:A:686:TYR:C	2.92	0.42
2:B:329:PHE:HA	2:B:332:ILE:HD11	2.01	0.42
1:A:85:MET:O	1:A:88:THR:HB	2.20	0.42
1:A:315:ARG:NH2	1:A:424:ASP:OD2	2.53	0.42
2:C:463:ASP:HB2	2:C:506:PHE:HB2	2.02	0.42
2:B:332:ILE:HG12	2:C:335:LYS:CG	2.30	0.41
2:C:543:TRP:CZ2	2:C:655:PRO:HD3	2.55	0.41
2:D:69:CYS:HB2	2:D:70:TYR:CE2	2.55	0.41
1:F:111:LEU:HD22	1:F:135:LEU:CD1	2.49	0.41
1:F:354:GLN:HB2	1:F:356:ILE:CD1	2.50	0.41
1:A:541:LEU:HD23	1:A:541:LEU:HA	1.80	0.41
2:C:312:ARG:HH22	2:C:421:ASP:CG	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:352:LYS:HB2	2:D:352:LYS:NZ	2.34	0.41
2:D:472:PHE:HB3	2:D:500:ARG:HG3	2.01	0.41
2:B:90:LYS:HE3	2:B:130:VAL:O	2.20	0.41
2:B:181:MET:HE3	1:F:483:VAL:HG13	2.02	0.41
2:C:510:ILE:HD11	2:C:524:MET:HE2	2.01	0.41
2:D:332:ILE:HD13	1:E:338:LYS:HB3	2.02	0.41
2:D:344:GLY:O	2:D:355:LEU:HG	2.20	0.41
1:F:170:PHE:HD2	1:F:232:ILE:HG22	1.84	0.41
2:B:170:MET:HE2	2:B:170:MET:HB3	1.96	0.41
2:B:223:ALA:O	2:B:227:GLU:HG3	2.21	0.41
2:B:349:PHE:O	2:B:350:ASP:CB	2.62	0.41
2:C:261:ILE:HD13	2:C:261:ILE:HA	1.88	0.41
2:D:629:GLU:HA	2:D:630:PRO:HD2	1.93	0.41
2:D:666:MET:HB3	2:D:666:MET:HE3	1.69	0.41
1:F:471:PHE:HE1	1:F:473:GLU:HB3	1.85	0.41
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.82	0.41
1:A:248:TRP:O	1:A:382:VAL:HA	2.21	0.41
1:A:650:LYS:HD2	1:A:654:PHE:CE2	2.55	0.41
2:B:278:LEU:HD21	2:B:532:GLU:HG3	2.03	0.41
2:B:300:PRO:HG2	2:B:309:PHE:HB3	2.02	0.41
2:B:642:VAL:O	2:B:644:ASP:N	2.54	0.41
2:C:242:LEU:HD21	2:C:248:SER:HB3	2.02	0.41
2:C:510:ILE:HD11	2:C:524:MET:HE1	2.02	0.41
1:E:67:GLU:HG2	1:E:83:LEU:CD2	2.48	0.41
2:C:90:LYS:O	2:C:91:ASN:HB2	2.21	0.41
2:D:97:PHE:O	2:D:393:ARG:NH2	2.54	0.41
2:D:514:SER:O	2:D:558:PRO:HA	2.21	0.41
2:D:540:GLU:OE2	2:D:658:PRO:HG2	2.20	0.41
2:D:680:PHE:HA	2:D:681:PRO:HD3	1.85	0.41
1:F:278:PHE:HE1	1:F:532:PRO:CG	2.34	0.41
1:F:507:HIS:HD2	1:F:508:SER:O	2.03	0.41
1:A:214:ASN:HB2	1:E:537:ASN:OD1	2.21	0.41
2:B:661:PHE:C	2:B:666:MET:HE3	2.40	0.41
1:E:596:VAL:HA	1:E:597:PRO:HD3	1.95	0.41
1:E:634:ASN:HB3	1:E:635:LYS:H	1.78	0.41
1:A:201:LYS:HG3	1:A:206:PHE:CE2	2.55	0.41
1:A:634:ASN:HB3	1:A:635:LYS:H	1.76	0.41
2:B:574:LYS:HG2	2:B:602:THR:HG22	2.03	0.41
2:B:639:LYS:HD2	2:B:639:LYS:N	2.36	0.41
2:C:358:SER:C	2:C:360:ALA:N	2.73	0.41
2:C:455:LEU:HD12	2:C:455:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:545:ASP:O	1:E:548:MET:CE	2.69	0.41
1:F:137:GLN:H	1:F:137:GLN:NE2	2.19	0.41
1:A:646:VAL:CG2	1:A:652:LEU:HD21	2.51	0.41
1:A:646:VAL:HG22	1:A:652:LEU:HD21	2.03	0.41
2:B:138:LEU:HD23	2:B:138:LEU:HA	1.92	0.41
2:B:516:VAL:HG12	2:B:517:ALA:H	1.86	0.41
2:B:528:PRO:HA	2:B:619:PHE:HD1	1.85	0.41
2:C:145:ILE:HG13	2:C:151:THR:HG21	2.03	0.41
1:E:91:MET:HA	1:E:92:PRO:HD3	1.92	0.41
1:E:168:LYS:HE3	1:E:308:LYS:HE3	2.03	0.41
1:F:257:LEU:HG	1:F:257:LEU:O	2.20	0.41
1:F:537:ASN:HB3	1:F:539:ILE:HD13	2.03	0.41
1:F:623:PHE:CE2	1:F:677:ILE:HD12	2.55	0.41
2:B:44:ASN:C	2:B:46:ASN:H	2.24	0.41
2:B:155:VAL:CG1	2:B:156:LEU:N	2.84	0.41
2:C:181:MET:HE2	1:E:484:TYR:H	1.82	0.41
1:E:214:ASN:HA	1:E:217:LEU:O	2.21	0.41
1:F:170:PHE:CD2	1:F:232:ILE:HG22	2.55	0.41
1:F:267:TYR:O	1:F:271:GLN:HG2	2.20	0.41
7:K:4:BMA:O2	7:K:5:BMA:C1	2.69	0.41
1:A:190:ASN:ND2	1:A:190:ASN:C	2.74	0.40
1:A:248:TRP:CE3	1:A:249:TRP:HB2	2.56	0.40
2:B:95:SER:N	2:B:101:MET:HE3	2.32	0.40
2:B:330:LEU:O	2:B:334:GLU:HG3	2.20	0.40
2:C:222:ILE:O	2:C:222:ILE:CG2	2.69	0.40
1:E:307:THR:C	1:E:309:PHE:H	2.25	0.40
1:F:217:LEU:HD21	1:F:302:TYR:HB3	2.04	0.40
2:B:45:VAL:HG11	2:B:138:LEU:HD11	2.03	0.40
2:D:145:ILE:HG23	2:D:151:THR:CG2	2.52	0.40
2:D:170:MET:CE	2:D:174:ASN:HD21	2.34	0.40
2:D:675:HIS:HE1	2:D:678:GLU:O	2.04	0.40
1:A:218:TYR:CZ	1:E:536:ASP:HB3	2.56	0.40
2:D:222:ILE:HD13	2:D:222:ILE:HG21	1.42	0.40
1:E:422:LEU:HD22	1:E:427:PHE:CE2	2.56	0.40
1:F:684:PHE:O	1:F:687:LYS:HB2	2.21	0.40
1:A:170:PHE:HB3	1:A:232:ILE:HG22	2.03	0.40
2:B:369:GLN:O	2:B:370:THR:C	2.60	0.40
1:E:166:TYR:HB3	1:E:169:MET:HG3	2.03	0.40
1:E:175:VAL:HG21	1:E:210:ALA:HB2	2.04	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	668/703 (95%)	629 (94%)	33 (5%)	6 (1%)	17 46
1	E	667/703 (95%)	628 (94%)	32 (5%)	7 (1%)	15 44
1	F	667/703 (95%)	630 (94%)	34 (5%)	3 (0%)	34 66
2	B	666/696 (96%)	619 (93%)	33 (5%)	14 (2%)	7 23
2	C	666/696 (96%)	633 (95%)	24 (4%)	9 (1%)	11 34
2	D	670/696 (96%)	637 (95%)	27 (4%)	6 (1%)	17 46
All	All	4004/4197 (95%)	3776 (94%)	183 (5%)	45 (1%)	14 41

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	LYS
2	B	247	ASN
2	B	632	PRO
2	B	636	GLU
2	B	687	PRO
2	C	347	LYS
2	C	350	ASP
2	C	632	PRO
2	C	687	PRO
2	D	350	ASP
2	D	632	PRO
2	D	687	PRO
1	E	308	LYS
2	B	45	VAL
2	B	350	ASP
2	B	382	PHE
2	B	615	ASP
2	C	344	GLY
2	D	488	LYS
1	E	203	ASN

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Mol	Chain	Res	Type
1	F	308	LYS
1	F	641	PRO
1	A	94	ASN
1	A	647	LEU
2	D	635	SER
1	A	324	GLU
1	A	640	ALA
2	B	306	TYR
2	C	635	SER
1	E	640	ALA
2	B	344	GLY
2	C	186	LEU
2	C	599	SER
2	D	321	GLU
1	E	220	ASN
1	E	636	GLY
1	E	641	PRO
1	E	647	LEU
1	F	640	ALA
2	B	631	THR
2	B	85	VAL
2	B	490	SER
2	C	643	PRO
1	A	495	VAL
2	B	643	PRO

5.3.2 Protein sidechains (i)

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	610/638 (96%)	563 (92%)	47 (8%)	13 35
1	E	609/638 (96%)	563 (92%)	46 (8%)	13 36
1	F	609/638 (96%)	548 (90%)	61 (10%)	7 22
2	B	606/629 (96%)	548 (90%)	58 (10%)	8 24
2	C	606/629 (96%)	550 (91%)	56 (9%)	9 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	610/629 (97%)	556 (91%)	54 (9%)	9 28
All	All	3650/3801 (96%)	3328 (91%)	322 (9%)	10 29

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	56	GLU
1	A	71	ASP
1	A	75	ASN
1	A	91	MET
1	A	99	VAL
1	A	145	TYR
1	A	190	ASN
1	A	204	ASP
1	A	258	LYS
1	A	281	LEU
1	A	310	THR
1	A	324	GLU
1	A	356	ILE
1	A	364	ILE
1	A	381	GLU
1	A	382	VAL
1	A	385	ASP
1	A	422	LEU
1	A	441	PHE
1	A	449	THR
1	A	451	ASP
1	A	455	PHE
1	A	456	ASP
1	A	469	THR
1	A	506	ASN
1	A	515	GLU
1	A	517	ASP
1	A	519	ASN
1	A	523	ASP
1	A	539	ILE
1	A	543	LEU
1	A	548	MET
1	A	559	LYS
1	A	561	THR
1	A	572	ASN

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Mol	Chain	Res	Type
1	A	599	ASP
1	A	602	GLU
1	A	610	ARG
1	A	633	ASP
1	A	643	GLU
1	A	646	VAL
1	A	649	ASN
1	A	661	VAL
1	A	662	ASP
1	A	664	LEU
1	A	683	ARG
2	B	28	ASP
2	B	47	GLU
2	B	51	GLU
2	B	53	GLU
2	B	63	ILE
2	B	64	GLU
2	B	72	ASN
2	B	77	GLU
2	B	90	LYS
2	B	129	ARG
2	B	134	GLN
2	B	142	TYR
2	B	165	GLN
2	B	173	LYS
2	B	187	ASP
2	B	190	ILE
2	B	197	ILE
2	B	205	MET
2	B	210	SER
2	B	213	LEU
2	B	215	TYR
2	B	217	ASN
2	B	225	LEU
2	B	261	ILE
2	B	275	MET
2	B	300	PRO
2	B	305	PHE
2	B	306	TYR
2	B	313	SER
2	B	332	ILE
2	B	347	LYS

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Mol	Chain	Res	Type
2	B	353	ILE
2	B	370	THR
2	B	381	GLN
2	B	404	GLN
2	B	452	PHE
2	B	455	LEU
2	B	490	SER
2	B	502	ASN
2	B	513	LYS
2	B	514	SER
2	B	516	VAL
2	B	533	ASN
2	B	537	PHE
2	B	539	LEU
2	B	542	ASN
2	B	544	MET
2	B	578	LEU
2	B	597	PHE
2	B	602	THR
2	B	606	ARG
2	B	634	GLU
2	B	639	LYS
2	B	641	VAL
2	B	645	ASN
2	B	663	GLN
2	B	679	LEU
2	B	688	HIS
2	C	21	GLU
2	C	22	PHE
2	C	27	VAL
2	C	28	ASP
2	C	46	ASN
2	C	53	GLU
2	C	63	ILE
2	C	64	GLU
2	C	66	SER
2	C	72	ASN
2	C	111	LEU
2	C	129	ARG
2	C	134	GLN
2	C	145	ILE
2	C	170	MET

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Mol	Chain	Res	Type
2	C	189	LYS
2	C	200	ASN
2	C	202	GLN
2	C	205	MET
2	C	210	SER
2	C	217	ASN
2	C	247	ASN
2	C	313	SER
2	C	326	GLU
2	C	345	HIS
2	C	346	PHE
2	C	347	LYS
2	C	352	LYS
2	C	359	LYS
2	C	370	THR
2	C	416	GLN
2	C	443	VAL
2	C	452	PHE
2	C	455	LEU
2	C	466	VAL
2	C	490	SER
2	C	492	HIS
2	C	502	ASN
2	C	516	VAL
2	C	518	THR
2	C	535	PHE
2	C	542	ASN
2	C	589	GLN
2	C	592	ILE
2	C	597	PHE
2	C	598	ASN
2	C	602	THR
2	C	605	SER
2	C	606	ARG
2	C	609	LEU
2	C	633	LYS
2	C	634	GLU
2	C	636	GLU
2	C	642	VAL
2	C	645	ASN
2	C	663	GLN
2	D	21	GLU

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Mol	Chain	Res	Type
2	D	53	GLU
2	D	71	THR
2	D	74	LYS
2	D	96	ILE
2	D	111	LEU
2	D	129	ARG
2	D	134	GLN
2	D	145	ILE
2	D	165	GLN
2	D	172	VAL
2	D	173	LYS
2	D	187	ASP
2	D	200	ASN
2	D	205	MET
2	D	210	SER
2	D	217	ASN
2	D	225	LEU
2	D	247	ASN
2	D	299	LEU
2	D	313	SER
2	D	326	GLU
2	D	343	GLN
2	D	345	HIS
2	D	352	LYS
2	D	370	THR
2	D	380	LEU
2	D	381	GLN
2	D	414	PHE
2	D	416	GLN
2	D	429	LYS
2	D	452	PHE
2	D	464	LYS
2	D	489	SER
2	D	490	SER
2	D	502	ASN
2	D	513	LYS
2	D	516	VAL
2	D	532	GLU
2	D	537	PHE
2	D	538	SER
2	D	539	LEU
2	D	551	TRP

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Mol	Chain	Res	Type
2	D	555	LYS
2	D	562	GLN
2	D	585	LYS
2	D	592	ILE
2	D	602	THR
2	D	606	ARG
2	D	633	LYS
2	D	634	GLU
2	D	636	GLU
2	D	687	PRO
2	D	690	THR
1	E	24	THR
1	E	27	THR
1	E	30	VAL
1	E	48	VAL
1	E	53	THR
1	E	56	GLU
1	E	62	LYS
1	E	68	MET
1	E	71	ASP
1	E	77	LYS
1	E	83	LEU
1	E	99	VAL
1	E	145	TYR
1	E	159	VAL
1	E	169	MET
1	E	190	ASN
1	E	203	ASN
1	E	257	LEU
1	E	258	LYS
1	E	290	GLU
1	E	307	THR
1	E	310	THR
1	E	346	LYS
1	E	364	ILE
1	E	381	GLU
1	E	382	VAL
1	E	451	ASP
1	E	455	PHE
1	E	456	ASP
1	E	488	GLU
1	E	495	VAL

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Mol	Chain	Res	Type
1	E	506	ASN
1	E	515	GLU
1	E	523	ASP
1	E	532	PRO
1	E	548	MET
1	E	561	THR
1	E	615	ARG
1	E	625	LEU
1	E	645	PHE
1	E	646	VAL
1	E	648	ASP
1	E	673	LYS
1	E	683	ARG
1	E	686	TYR
1	E	692	SER
1	F	27	THR
1	F	48	VAL
1	F	56	GLU
1	F	62	LYS
1	F	66	ILE
1	F	71	ASP
1	F	75	ASN
1	F	77	LYS
1	F	103	LYS
1	F	132	ARG
1	F	137	GLN
1	F	145	TYR
1	F	188	LEU
1	F	190	ASN
1	F	204	ASP
1	F	216	VAL
1	F	226	THR
1	F	232	ILE
1	F	257	LEU
1	F	305	MET
1	F	307	THR
1	F	323	THR
1	F	335	THR
1	F	381	GLU
1	F	382	VAL
1	F	384	LYS
1	F	389	SER

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Mol	Chain	Res	Type
1	F	422	LEU
1	F	441	PHE
1	F	446	LYS
1	F	449	THR
1	F	451	ASP
1	F	455	PHE
1	F	456	ASP
1	F	461	THR
1	F	473	GLU
1	F	493	ASN
1	F	501	ARG
1	F	506	ASN
1	F	515	GLU
1	F	516	VAL
1	F	519	ASN
1	F	522	SER
1	F	523	ASP
1	F	548	MET
1	F	561	THR
1	F	565	ASN
1	F	568	ILE
1	F	572	ASN
1	F	578	LYS
1	F	582	VAL
1	F	596	VAL
1	F	604	PHE
1	F	610	ARG
1	F	642	PHE
1	F	643	GLU
1	F	647	LEU
1	F	648	ASP
1	F	673	LYS
1	F	675	ILE
1	F	683	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	50	GLN
1	A	69	ASN
1	A	72	ASN

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Mol	Chain	Res	Type
1	A	75	ASN
1	A	94	ASN
1	A	190	ASN
1	A	244	HIS
1	A	271	GLN
1	A	314	GLN
1	A	359	HIS
1	A	492	ASN
1	A	494	HIS
1	A	506	ASN
1	A	507	HIS
1	A	513	ASN
1	A	546	ASN
1	A	679	HIS
2	B	35	GLN
2	B	44	ASN
2	B	59	GLN
2	B	134	GLN
2	B	217	ASN
2	B	232	ASN
2	B	247	ASN
2	B	268	GLN
2	B	303	ASN
2	B	311	GLN
2	B	404	GLN
2	B	433	GLN
2	B	502	ASN
2	B	503	HIS
2	B	542	ASN
2	B	645	ASN
2	B	663	GLN
2	B	675	HIS
2	C	35	GLN
2	C	72	ASN
2	C	134	GLN
2	C	217	ASN
2	C	232	ASN
2	C	247	ASN
2	C	268	GLN
2	C	311	GLN
2	C	343	GLN
2	C	447	GLN

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Mol	Chain	Res	Type
2	C	471	HIS
2	C	502	ASN
2	C	503	HIS
2	C	533	ASN
2	C	542	ASN
2	C	645	ASN
2	C	663	GLN
2	C	675	HIS
2	C	688	HIS
2	D	72	ASN
2	D	134	GLN
2	D	174	ASN
2	D	217	ASN
2	D	232	ASN
2	D	247	ASN
2	D	268	GLN
2	D	311	GLN
2	D	343	GLN
2	D	447	GLN
2	D	502	ASN
2	D	503	HIS
2	D	542	ASN
2	D	560	GLN
2	D	663	GLN
2	D	675	HIS
1	E	38	GLN
1	E	50	GLN
1	E	139	GLN
1	E	177	GLN
1	E	190	ASN
1	E	203	ASN
1	E	235	ASN
1	E	244	HIS
1	E	271	GLN
1	E	314	GLN
1	E	359	HIS
1	E	506	ASN
1	E	507	HIS
1	E	513	ASN
1	E	679	HIS
1	F	38	GLN
1	F	50	GLN

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Mol	Chain	Res	Type
1	F	137	GLN
1	F	139	GLN
1	F	190	ASN
1	F	271	GLN
1	F	314	GLN
1	F	345	GLN
1	F	359	HIS
1	F	493	ASN
1	F	506	ASN
1	F	507	HIS
1	F	519	ASN
1	F	546	ASN
1	F	565	ASN
1	F	649	ASN
1	F	679	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

34 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	$\#\|Z\| > 2$
3	NAG	G	1	1,3	14,14,15	1.01	2 (14%)	17,19,21	1.89	5 (29%)
3	NAG	G	2	3	14,14,15	0.83	1 (7%)	17,19,21	2.15	6 (35%)
3	BMA	G	3	3	11,11,12	0.84	0	15,15,17	2.29	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	G	4	3	11,11,12	0.73	0	15,15,17	1.13	1 (6%)
3	BMA	G	5	3	11,11,12	1.02	1 (9%)	15,15,17	3.31	4 (26%)
4	NAG	H	1	4,2	14,14,15	0.75	1 (7%)	17,19,21	1.33	1 (5%)
4	NAG	H	2	4	14,14,15	0.64	0	17,19,21	1.45	2 (11%)
4	BMA	H	3	4	11,11,12	1.27	1 (9%)	15,15,17	1.37	3 (20%)
4	BMA	H	4	4	11,11,12	0.62	0	15,15,17	1.14	1 (6%)
4	MAN	H	5	4	11,11,12	0.69	0	15,15,17	1.13	1 (6%)
5	NAG	I	1	2,5	14,14,15	0.60	0	17,19,21	1.80	4 (23%)
5	NAG	I	2	5	14,14,15	0.78	1 (7%)	17,19,21	1.42	1 (5%)
5	BMA	I	3	5	11,11,12	0.67	0	15,15,17	1.98	5 (33%)
5	MAN	I	4	5	11,11,12	0.89	1 (9%)	15,15,17	1.86	3 (20%)
5	MAN	I	5	5	11,11,12	0.65	0	15,15,17	2.42	4 (26%)
5	MAN	I	6	5	11,11,12	0.74	0	15,15,17	1.79	3 (20%)
6	NAG	J	1	2,6	14,14,15	0.57	0	17,19,21	1.28	1 (5%)
6	NAG	J	2	6	14,14,15	0.87	1 (7%)	17,19,21	1.52	3 (17%)
6	BMA	J	3	6	11,11,12	0.47	0	15,15,17	1.67	3 (20%)
6	MAN	J	4	6	11,11,12	0.54	0	15,15,17	1.37	1 (6%)
6	MAN	J	5	6	11,11,12	0.79	0	15,15,17	1.29	3 (20%)
6	MAN	J	6	6	11,11,12	0.63	0	15,15,17	1.17	2 (13%)
6	MAN	J	7	6	11,11,12	0.67	0	15,15,17	2.45	3 (20%)
7	NAG	K	1	7,1	14,14,15	0.69	0	17,19,21	1.42	3 (17%)
7	NAG	K	2	7	14,14,15	0.54	0	17,19,21	1.09	1 (5%)
7	BMA	K	3	7	11,11,12	0.65	0	15,15,17	2.10	3 (20%)
7	BMA	K	4	7	11,11,12	0.68	0	15,15,17	2.26	4 (26%)
7	BMA	K	5	7	11,11,12	0.90	1 (9%)	15,15,17	2.10	2 (13%)
7	MAN	K	6	7	11,11,12	0.80	0	15,15,17	1.52	2 (13%)
8	NAG	L	1	1,8	14,14,15	0.52	0	17,19,21	1.72	4 (23%)
8	NAG	L	2	8	14,14,15	0.55	0	17,19,21	1.29	0
8	BMA	L	3	8	11,11,12	0.46	0	15,15,17	1.11	2 (13%)
8	MAN	L	4	8	11,11,12	0.78	1 (9%)	15,15,17	1.49	4 (26%)
8	BMA	L	5	8	11,11,12	0.67	0	15,15,17	2.32	3 (20%)

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
3	NAG	G	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	BMA	G	5	3	-	1/2/19/22	0/1/1/1
4	NAG	H	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
4	BMA	H	4	4	-	2/2/19/22	0/1/1/1
4	MAN	H	5	4	-	0/2/19/22	0/1/1/1
5	NAG	I	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
5	BMA	I	3	5	-	2/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1
5	MAN	I	5	5	-	2/2/19/22	0/1/1/1
5	MAN	I	6	5	-	1/2/19/22	0/1/1/1
6	NAG	J	1	2,6	-	1/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	2/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
6	MAN	J	6	6	-	2/2/19/22	0/1/1/1
6	MAN	J	7	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	BMA	K	3	7	-	2/2/19/22	0/1/1/1
7	BMA	K	4	7	-	2/2/19/22	0/1/1/1
7	BMA	K	5	7	-	0/2/19/22	0/1/1/1
7	MAN	K	6	7	-	2/2/19/22	0/1/1/1
8	NAG	L	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	L	2	8	-	0/6/23/26	0/1/1/1
8	BMA	L	3	8	-	0/2/19/22	0/1/1/1
8	MAN	L	4	8	-	2/2/19/22	0/1/1/1
8	BMA	L	5	8	-	2/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	3	BMA	O5-C1	-3.72	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	O5-C1	-2.59	1.39	1.43
3	G	5	BMA	C2-C3	2.50	1.56	1.52
6	J	2	NAG	O5-C1	-2.25	1.39	1.43
4	H	1	NAG	O5-C1	-2.21	1.40	1.43
3	G	1	NAG	O5-C5	-2.20	1.39	1.43
8	L	4	MAN	C2-C3	2.15	1.55	1.52
5	I	4	MAN	C2-C3	2.14	1.55	1.52
5	I	2	NAG	O5-C1	-2.13	1.40	1.43
3	G	2	NAG	O3-C3	-2.06	1.37	1.43
7	K	5	BMA	C2-C3	2.01	1.55	1.52

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	5	BMA	C1-O5-C5	-9.13	99.95	112.19
6	J	7	MAN	C1-O5-C5	8.11	123.06	112.19
8	L	5	BMA	C1-O5-C5	7.51	122.25	112.19
3	G	3	BMA	O5-C5-C6	6.81	120.93	107.66
3	G	5	BMA	O5-C5-C6	6.79	120.87	107.66
7	K	4	BMA	C1-O5-C5	6.26	120.58	112.19
5	I	5	MAN	C1-O5-C5	6.13	120.41	112.19
7	K	5	BMA	C1-C2-C3	5.72	117.98	109.64
7	K	3	BMA	C1-O5-C5	5.66	119.78	112.19
5	I	1	NAG	C1-O5-C5	5.53	119.60	112.19
3	G	1	NAG	C2-N2-C7	-5.28	115.82	122.90
5	I	4	MAN	C1-C2-C3	5.04	116.98	109.64
5	I	6	MAN	C1-O5-C5	4.93	118.79	112.19
5	I	3	BMA	C1-C2-C3	4.84	116.69	109.64
6	J	4	MAN	C1-O5-C5	4.69	118.47	112.19
3	G	2	NAG	C3-C4-C5	-4.61	101.87	110.23
5	I	2	NAG	C1-O5-C5	4.59	118.33	112.19
7	K	5	BMA	C1-O5-C5	4.49	118.20	112.19
3	G	5	BMA	C3-C4-C5	-4.41	102.24	110.23
5	I	5	MAN	C1-C2-C3	4.40	116.05	109.64
4	H	1	NAG	C1-O5-C5	4.29	117.93	112.19
4	H	2	NAG	C1-O5-C5	4.25	117.88	112.19
8	L	1	NAG	C1-O5-C5	4.17	117.77	112.19
6	J	2	NAG	C2-N2-C7	-4.10	117.41	122.90
3	G	2	NAG	O3-C3-C2	-3.81	101.48	109.40
3	G	2	NAG	C1-C2-N2	-3.58	104.79	110.43
6	J	3	BMA	C1-C2-C3	3.56	114.83	109.64
7	K	1	NAG	C1-O5-C5	3.55	116.95	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	6	MAN	C1-C2-C3	3.53	114.78	109.64
7	K	6	MAN	C1-O5-C5	3.46	116.83	112.19
7	K	3	BMA	O3-C3-C2	3.46	117.11	110.05
7	K	4	BMA	C3-C4-C5	3.45	116.49	110.23
6	J	3	BMA	C1-O5-C5	3.40	116.74	112.19
3	G	4	MAN	C3-C4-C5	3.35	116.31	110.23
5	I	5	MAN	C3-C4-C5	3.33	116.26	110.23
5	I	4	MAN	C1-O5-C5	3.28	116.59	112.19
7	K	4	BMA	O5-C5-C4	3.28	118.80	110.83
7	K	6	MAN	C1-C2-C3	3.26	114.40	109.64
3	G	3	BMA	O6-C6-C5	3.17	122.13	111.33
8	L	1	NAG	C2-N2-C7	3.15	127.13	122.90
8	L	5	BMA	C1-C2-C3	3.08	114.13	109.64
5	I	3	BMA	C3-C4-C5	3.07	115.81	110.23
4	H	5	MAN	C1-O5-C5	3.04	116.26	112.19
7	K	1	NAG	C1-C2-N2	-3.00	105.71	110.43
3	G	2	NAG	O5-C5-C6	2.97	113.44	107.66
5	I	5	MAN	C2-C3-C4	2.96	116.07	110.86
5	I	3	BMA	C1-O5-C5	2.90	116.07	112.19
4	H	3	BMA	C3-C4-C5	2.88	115.46	110.23
6	J	6	MAN	C1-O5-C5	2.83	115.98	112.19
6	J	6	MAN	O5-C5-C6	2.69	112.90	107.66
8	L	4	MAN	C2-C3-C4	2.61	115.45	110.86
8	L	4	MAN	C1-C2-C3	2.59	113.42	109.64
8	L	4	MAN	C1-O5-C5	2.59	115.65	112.19
4	H	3	BMA	O3-C3-C2	2.54	115.24	110.05
4	H	4	BMA	C3-C4-C5	2.53	114.82	110.23
5	I	6	MAN	C2-C3-C4	2.49	115.24	110.86
3	G	5	BMA	C6-C5-C4	2.49	119.12	113.02
8	L	1	NAG	O7-C7-N2	2.48	126.37	121.98
7	K	4	BMA	O3-C3-C2	2.48	115.11	110.05
5	I	1	NAG	C1-C2-N2	-2.46	106.56	110.43
3	G	1	NAG	O6-C6-C5	-2.44	103.01	111.33
6	J	5	MAN	C1-C2-C3	2.38	113.12	109.64
6	J	3	BMA	O5-C1-C2	2.38	116.46	110.79
5	I	3	BMA	C2-C3-C4	2.36	115.01	110.86
3	G	3	BMA	C1-C2-C3	2.36	113.08	109.64
8	L	1	NAG	O7-C7-C8	-2.35	117.86	122.05
5	I	1	NAG	O4-C4-C5	-2.35	103.53	109.32
3	G	1	NAG	C3-C4-C5	-2.35	105.98	110.23
5	I	4	MAN	C2-C3-C4	2.34	114.98	110.86
6	J	7	MAN	C1-C2-C3	2.31	113.01	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	C1-O5-C5	2.28	115.24	112.19
8	L	5	BMA	O5-C1-C2	2.24	116.14	110.79
3	G	1	NAG	C8-C7-N2	2.24	119.83	116.12
6	J	2	NAG	O5-C1-C2	-2.20	107.88	111.29
7	K	1	NAG	C3-C4-C5	-2.16	106.31	110.23
6	J	5	MAN	O5-C5-C4	-2.15	105.60	110.83
5	I	3	BMA	O5-C1-C2	2.14	115.89	110.79
6	J	1	NAG	C3-C4-C5	-2.14	106.36	110.23
6	J	7	MAN	C3-C4-C5	-2.12	106.39	110.23
6	J	5	MAN	C1-O5-C5	2.10	115.01	112.19
7	K	3	BMA	O3-C3-C4	2.07	115.25	110.38
4	H	3	BMA	C1-O5-C5	-2.07	109.42	112.19
3	G	2	NAG	C6-C5-C4	2.06	118.09	113.02
8	L	3	BMA	O2-C2-C1	-2.06	104.52	109.22
5	I	1	NAG	O7-C7-C8	-2.05	118.40	122.05
4	H	2	NAG	C3-C4-C5	-2.04	106.53	110.23
7	K	2	NAG	O5-C5-C6	2.04	111.64	107.66
3	G	2	NAG	C1-O5-C5	-2.03	109.46	112.19
6	J	2	NAG	C1-O5-C5	2.03	114.91	112.19
8	L	4	MAN	O5-C5-C6	2.02	111.60	107.66
8	L	3	BMA	C3-C4-C5	2.01	113.88	110.23
3	G	3	BMA	O4-C4-C3	-2.00	105.66	110.38

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	K	6	MAN	O5-C5-C6-O6
6	J	6	MAN	O5-C5-C6-O6
6	J	4	MAN	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
8	L	4	MAN	O5-C5-C6-O6
6	J	6	MAN	C4-C5-C6-O6
5	I	5	MAN	C4-C5-C6-O6
4	H	4	BMA	O5-C5-C6-O6
5	I	5	MAN	O5-C5-C6-O6
7	K	6	MAN	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
8	L	5	BMA	O5-C5-C6-O6
7	K	4	BMA	C4-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6
8	L	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	L	5	BMA	C4-C5-C6-O6
6	J	4	MAN	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
5	I	3	BMA	C4-C5-C6-O6
5	I	3	BMA	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
7	K	3	BMA	O5-C5-C6-O6
7	K	3	BMA	C4-C5-C6-O6
7	K	4	BMA	O5-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
3	G	5	BMA	O5-C5-C6-O6
4	H	4	BMA	C4-C5-C6-O6
5	I	6	MAN	O5-C5-C6-O6
3	G	4	MAN	C4-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
6	J	1	NAG	C1-C2-N2-C7
7	K	1	NAG	O5-C5-C6-O6
7	K	1	NAG	C4-C5-C6-O6
7	K	2	NAG	C4-C5-C6-O6

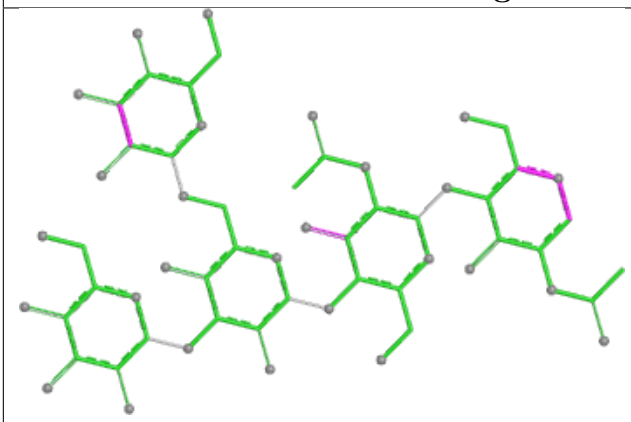
There are no ring outliers.

5 monomers are involved in 4 short contacts:

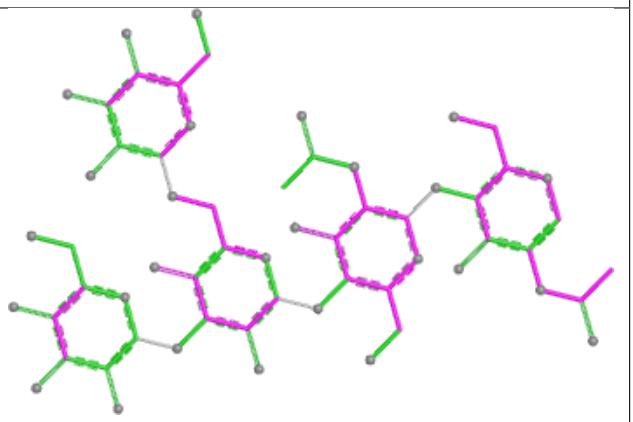
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	NAG	2	0
4	H	1	NAG	1	0
7	K	4	BMA	1	0
4	H	3	BMA	2	0
7	K	5	BMA	1	0

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

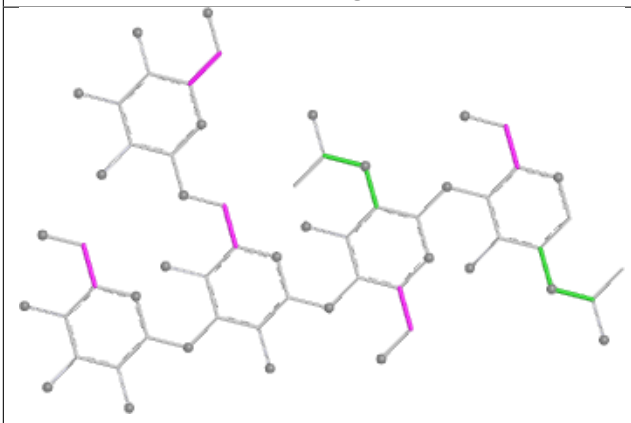
Oligosaccharide Chain G



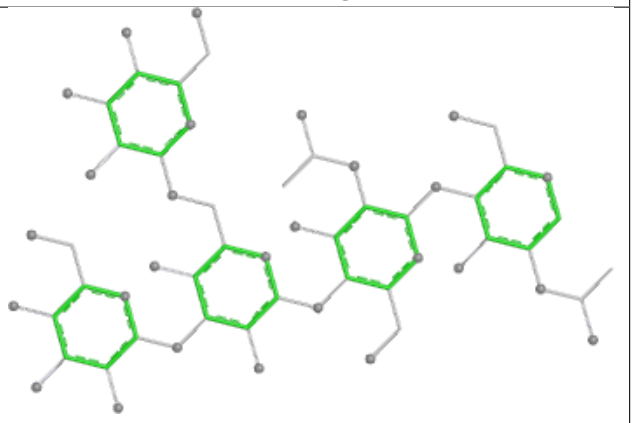
Bond lengths



Bond angles

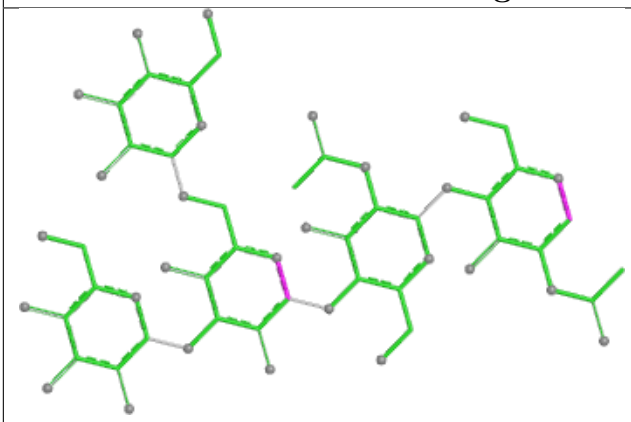


Torsions

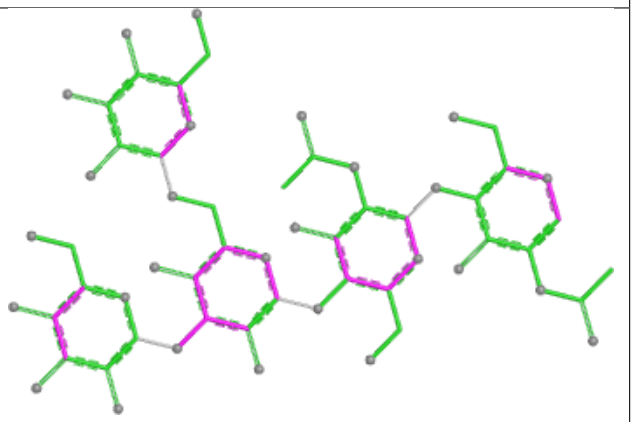


Rings

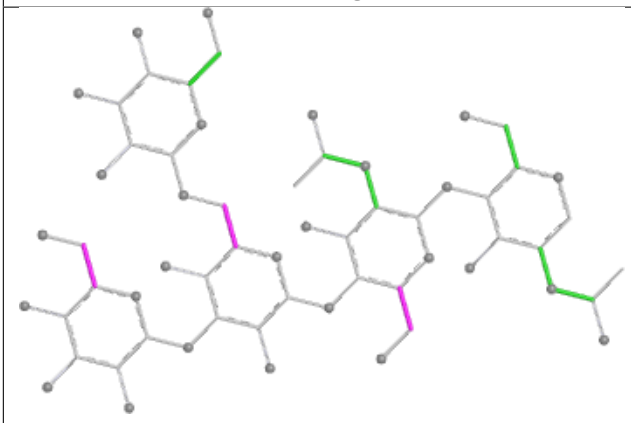
Oligosaccharide Chain H



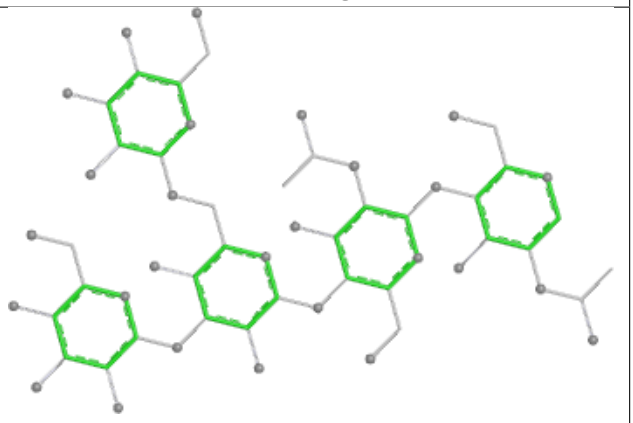
Bond lengths



Bond angles

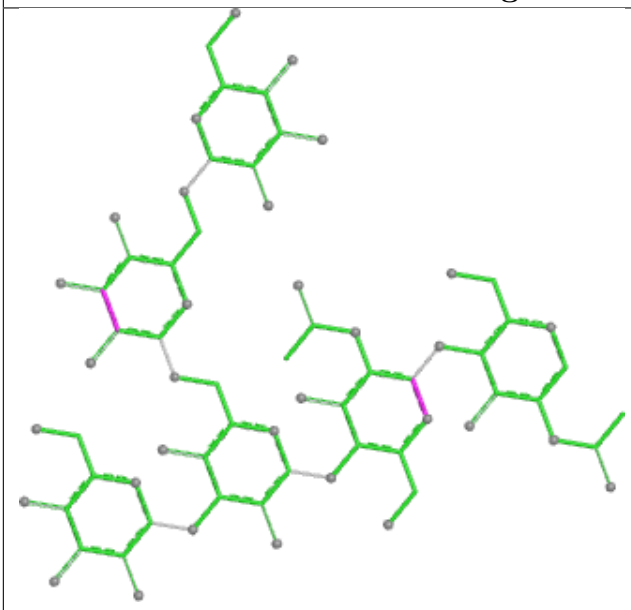


Torsions

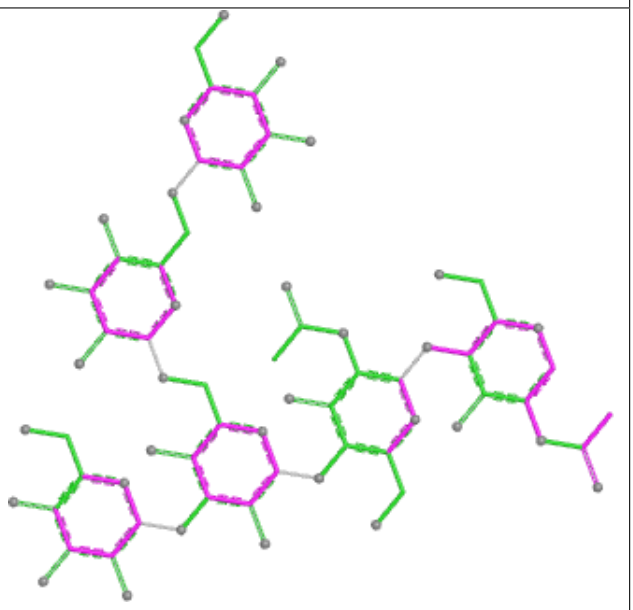


Rings

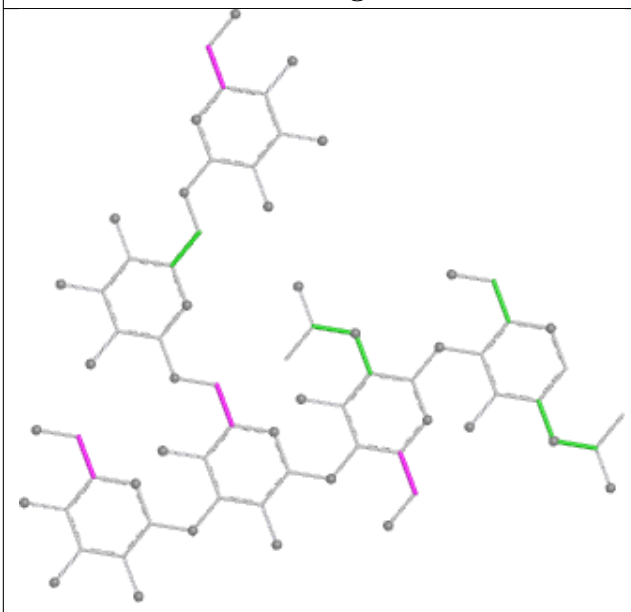
Oligosaccharide Chain I



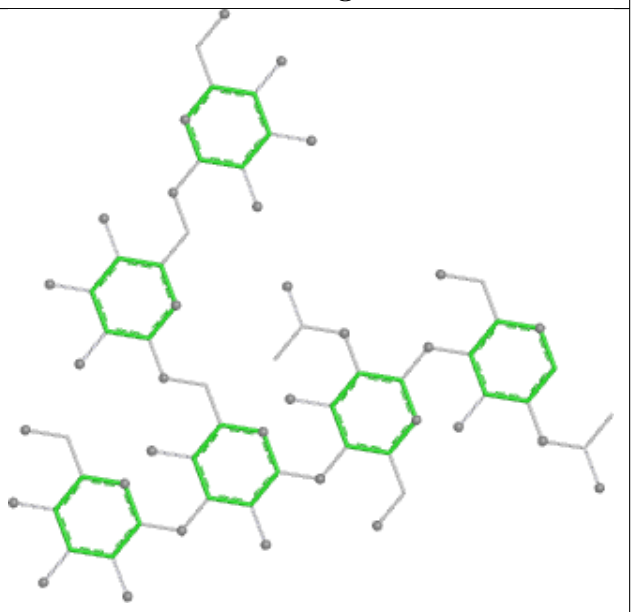
Bond lengths



Bond angles

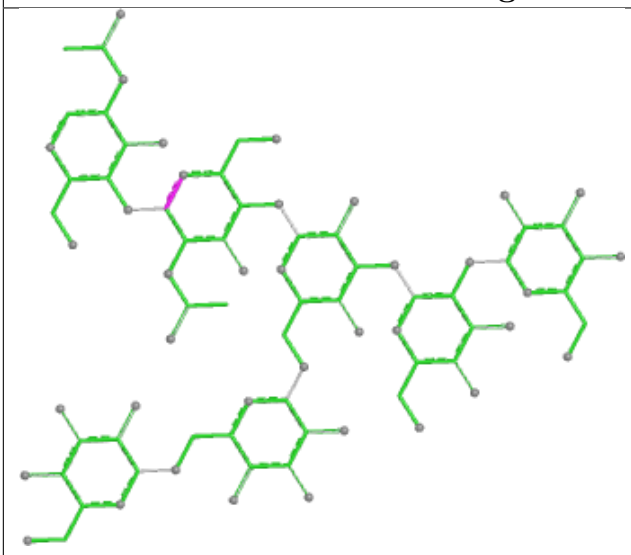


Torsions

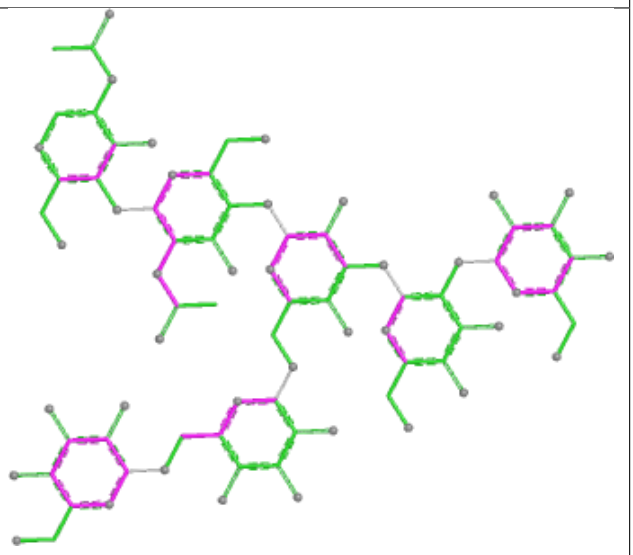


Rings

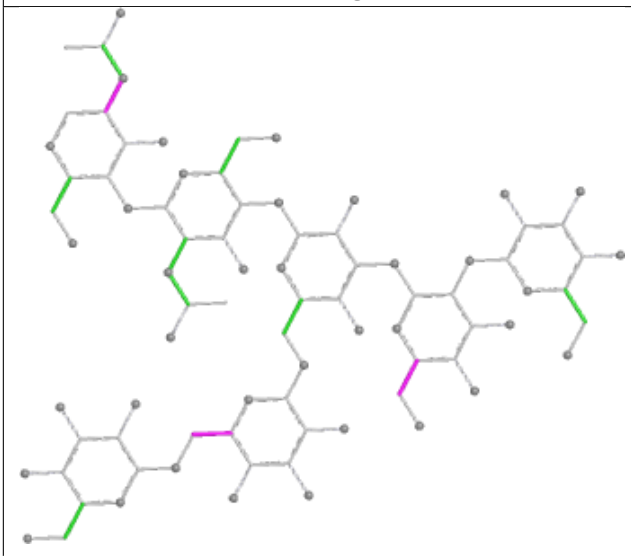
Oligosaccharide Chain J



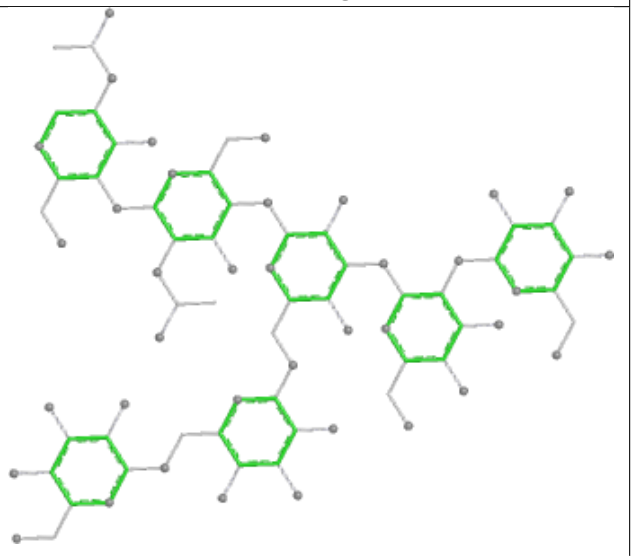
Bond lengths



Bond angles

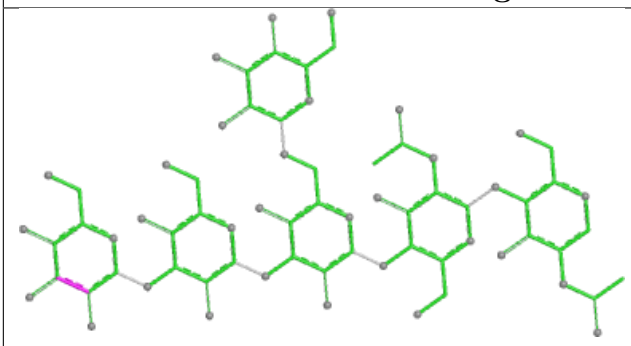


Torsions

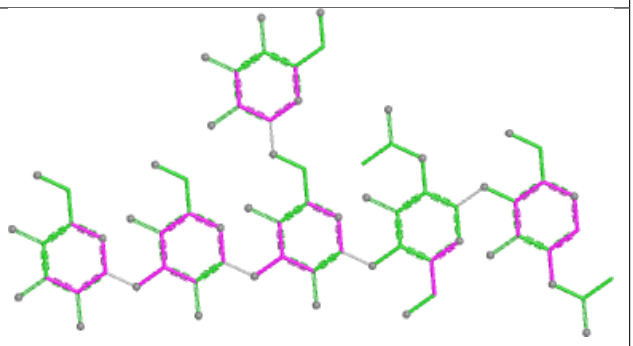


Rings

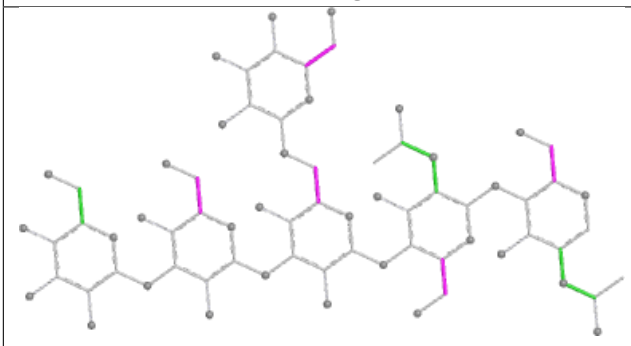
Oligosaccharide Chain K



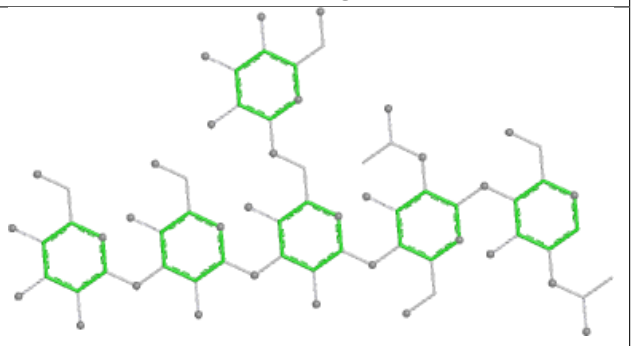
Bond lengths



Bond angles

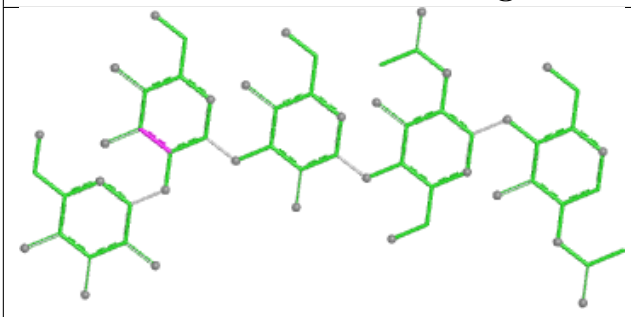


Torsions

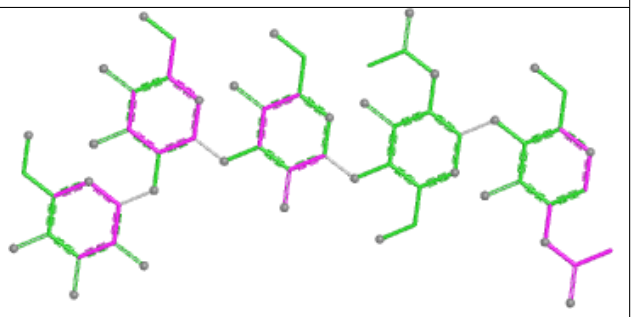


Rings

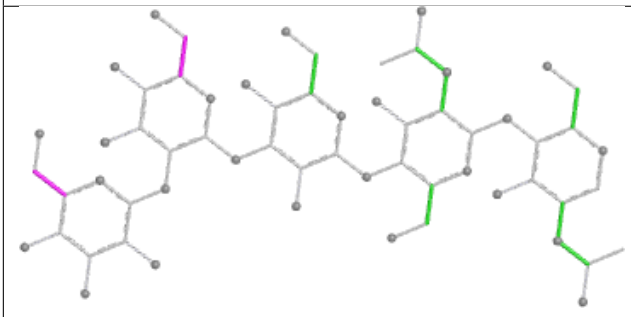
Oligosaccharide Chain L



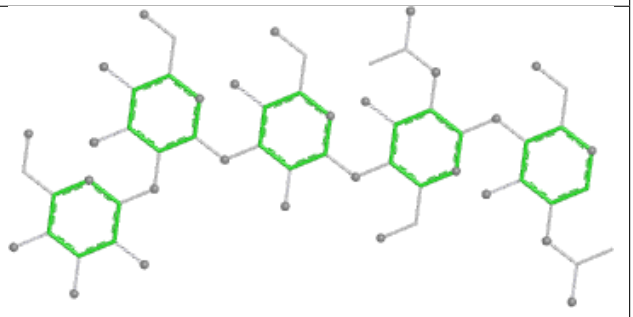
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	670/703 (95%)	-0.51	17 (2%)	57	47	20, 43, 85, 213	0
1	E	669/703 (95%)	-0.37	19 (2%)	53	43	24, 50, 91, 234	0
1	F	669/703 (95%)	-0.23	22 (3%)	46	36	27, 59, 102, 206	0
2	B	668/696 (95%)	-0.35	14 (2%)	63	54	25, 54, 92, 167	0
2	C	668/696 (95%)	-0.47	12 (1%)	68	61	24, 46, 86, 142	0
2	D	672/696 (96%)	-0.51	7 (1%)	82	77	20, 42, 82, 159	0
All	All	4016/4197 (95%)	-0.41	91 (2%)	60	51	20, 49, 92, 234	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	641	PRO	7.4
2	D	21	GLU	7.0
1	F	640	ALA	6.9
1	A	644	SER	6.7
1	A	638	ASP	6.5
2	D	633	LYS	6.0
1	F	641	PRO	5.7
1	E	642	PHE	5.5
1	E	645	PHE	5.4
2	D	346	PHE	5.4
1	F	636	GLY	5.3
1	A	637	LYS	5.1
1	E	646	VAL	4.9
1	A	639	LEU	4.9
1	E	639	LEU	4.7
1	F	637	LYS	4.7
1	E	640	ALA	4.6
2	B	633	LYS	4.6
1	F	638	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	638	ASP	4.3
1	F	492	ASN	3.8
1	F	644	SER	3.5
2	C	632	PRO	3.4
1	E	649	ASN	3.2
2	C	633	LYS	3.2
2	C	349	PHE	3.2
1	F	67	GLU	3.2
1	E	647	LEU	3.1
2	B	186	LEU	3.0
1	A	640	ALA	3.0
1	F	639	LEU	2.9
2	B	557	ASN	2.9
2	B	688	HIS	2.9
2	B	60	ASP	2.9
1	E	634	ASN	2.9
1	A	635	LYS	2.9
1	F	87	ARG	2.8
2	C	187	ASP	2.8
2	C	351	LYS	2.8
1	E	32	ALA	2.8
2	C	688	HIS	2.8
2	C	631	THR	2.7
1	E	644	SER	2.7
1	F	68	MET	2.6
1	A	646	VAL	2.6
2	B	634	GLU	2.6
2	D	632	PRO	2.5
1	E	633	ASP	2.5
1	F	63	ASP	2.5
1	A	642	PHE	2.5
1	F	645	PHE	2.5
1	A	693	TYR	2.4
1	E	560	LEU	2.4
2	C	59	GLN	2.4
2	D	189	LYS	2.4
1	E	636	GLY	2.4
2	B	59	GLN	2.3
1	E	561	THR	2.3
2	C	65	ALA	2.3
1	F	692	SER	2.3
1	E	562	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	631	THR	2.3
1	A	692	SER	2.3
1	F	62	LYS	2.3
1	F	306	LEU	2.3
1	A	63	ASP	2.3
2	C	634	GLU	2.3
1	A	26	LYS	2.3
1	E	63	ASP	2.3
1	E	519	ASN	2.2
1	A	647	LEU	2.2
2	D	631	THR	2.2
2	B	64	GLU	2.2
1	F	307	THR	2.2
2	C	21	GLU	2.2
2	B	632	PRO	2.1
2	B	214	THR	2.1
2	B	636	GLU	2.1
1	A	597	PRO	2.1
1	F	309	PHE	2.1
1	A	633	ASP	2.1
2	B	659	GLN	2.1
2	B	69	CYS	2.1
2	C	186	LEU	2.1
1	A	517	ASP	2.1
2	D	630	PRO	2.1
1	F	633	ASP	2.1
1	A	24	THR	2.0
1	F	192	GLU	2.0
1	F	635	LYS	2.0
1	F	64	TYR	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)

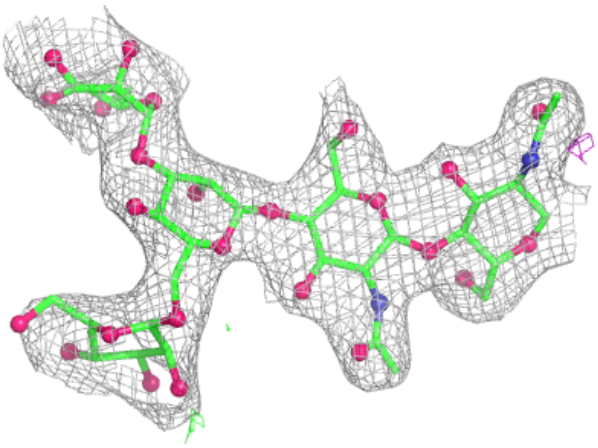
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

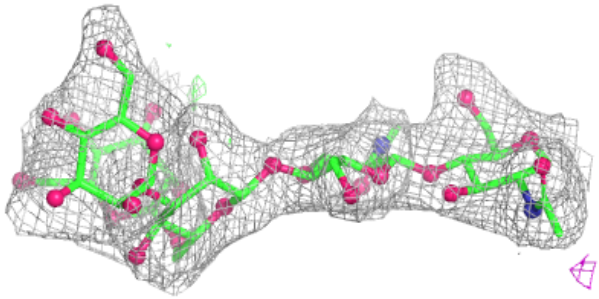
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	I	5	11/12	0.67	0.34	102,112,115,115	0
8	BMA	L	5	11/12	0.69	0.32	110,121,124,125	0
7	BMA	K	5	11/12	0.70	0.25	103,108,112,114	0
5	MAN	I	6	11/12	0.70	0.28	88,94,97,98	0
6	MAN	J	5	11/12	0.73	0.29	95,110,118,122	0
6	MAN	J	6	11/12	0.75	0.21	98,100,105,111	0
6	MAN	J	7	11/12	0.76	0.35	98,111,114,115	0
4	MAN	H	5	11/12	0.77	0.17	91,97,100,100	0
3	BMA	G	5	11/12	0.80	0.20	82,89,96,102	0
5	MAN	I	4	11/12	0.83	0.19	92,96,101,105	0
7	BMA	K	4	11/12	0.84	0.17	78,88,92,99	0
8	MAN	L	4	11/12	0.85	0.19	95,97,104,108	0
7	MAN	K	6	11/12	0.85	0.16	69,73,76,77	0
3	MAN	G	4	11/12	0.86	0.17	66,67,72,74	0
4	BMA	H	4	11/12	0.88	0.21	104,108,110,110	0
8	BMA	L	3	11/12	0.88	0.14	71,74,79,87	0
5	BMA	I	3	11/12	0.89	0.16	72,82,88,93	0
6	BMA	J	3	11/12	0.90	0.18	66,77,88,89	0
4	BMA	H	3	11/12	0.90	0.16	89,95,100,101	0
6	MAN	J	4	11/12	0.92	0.23	89,94,100,106	0
7	BMA	K	3	11/12	0.92	0.13	57,65,73,74	0
3	BMA	G	3	11/12	0.93	0.14	50,59,65,72	0
4	NAG	H	2	14/15	0.94	0.13	58,66,76,83	0
5	NAG	I	2	14/15	0.94	0.15	51,57,63,70	0
7	NAG	K	2	14/15	0.95	0.11	45,48,55,56	0
8	NAG	L	2	14/15	0.96	0.15	55,60,65,68	0
4	NAG	H	1	14/15	0.96	0.14	48,51,58,59	0
6	NAG	J	2	14/15	0.96	0.13	44,47,53,60	0
8	NAG	L	1	14/15	0.96	0.11	47,51,56,56	0
3	NAG	G	2	14/15	0.97	0.12	37,42,49,49	0
6	NAG	J	1	14/15	0.97	0.10	36,37,39,43	0
5	NAG	I	1	14/15	0.97	0.11	40,43,46,49	0
3	NAG	G	1	14/15	0.98	0.11	27,30,32,36	0
7	NAG	K	1	14/15	0.98	0.10	36,38,42,43	0

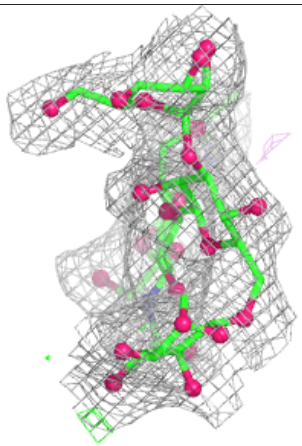
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

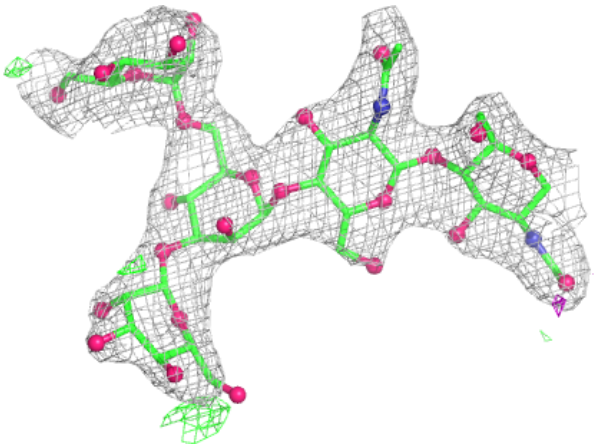


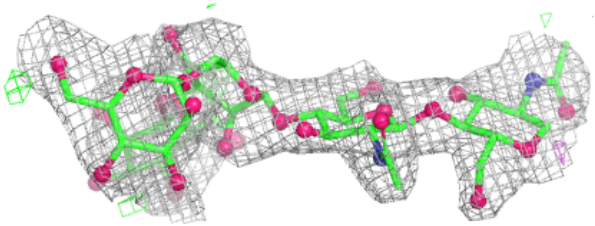


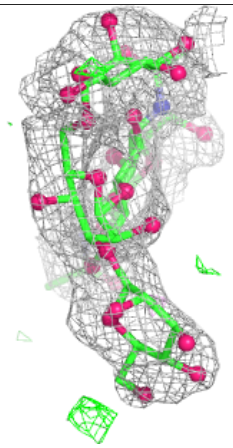


Electron density around Chain H:

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

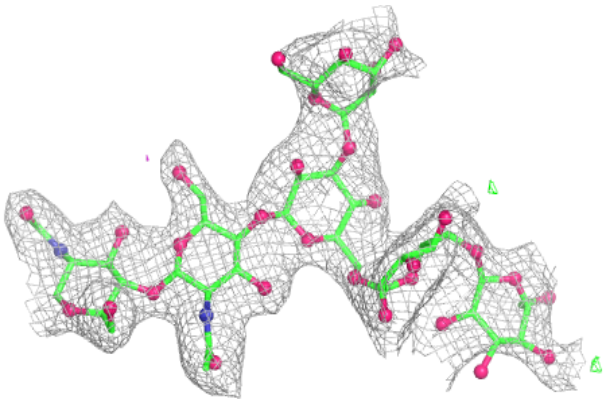


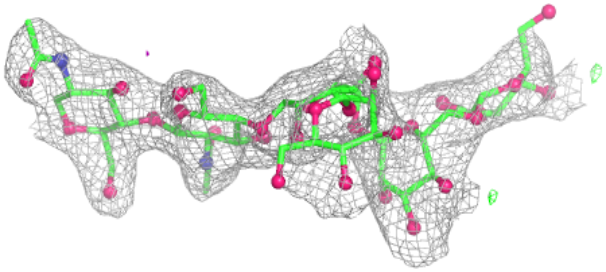


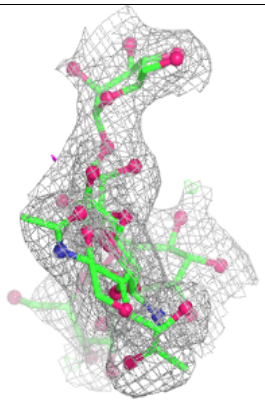


Electron density around Chain I:

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

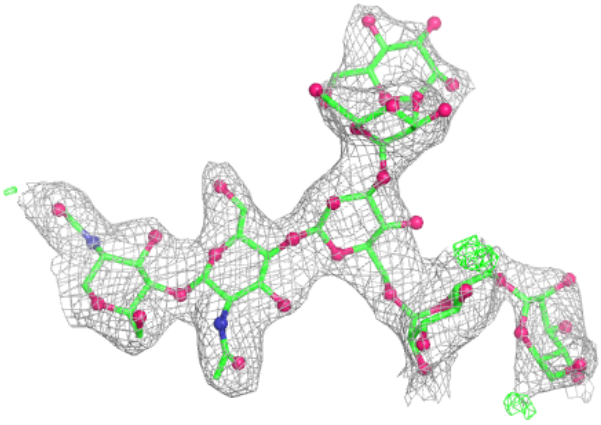


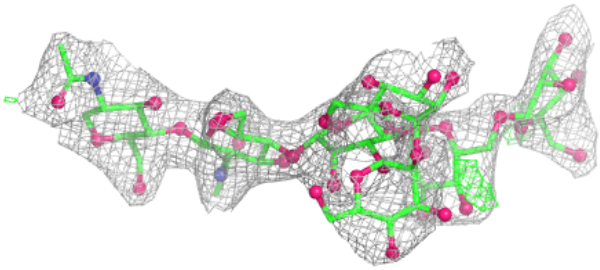


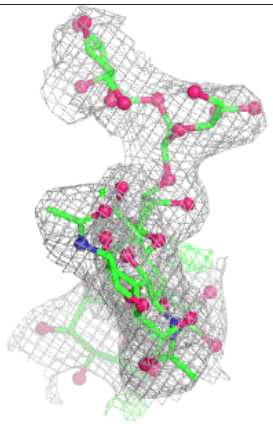


Electron density around Chain J:

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

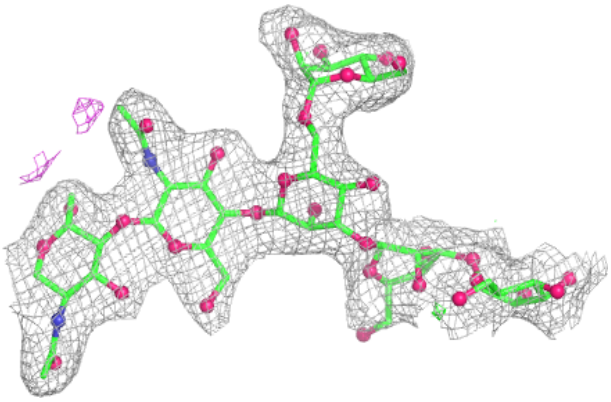


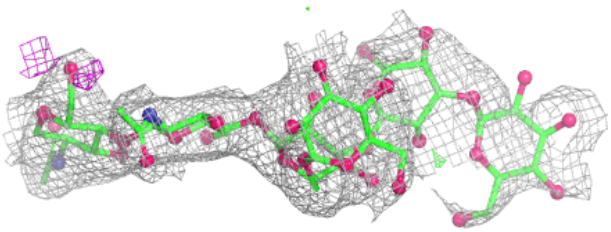


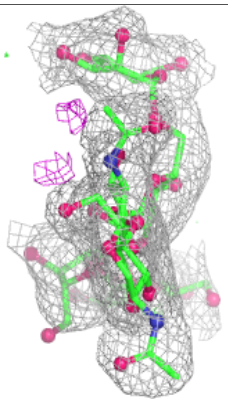


Electron density around Chain K:

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

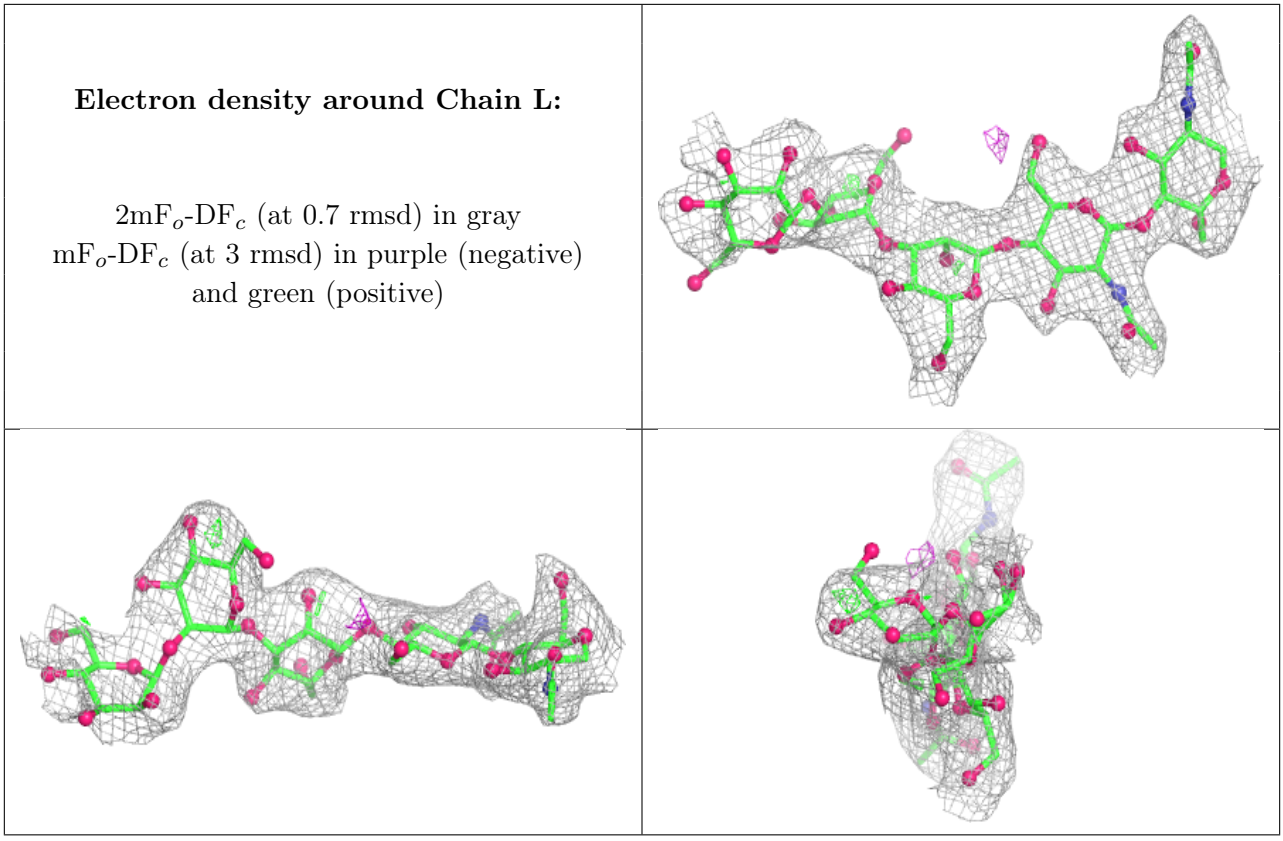






Electron density around Chain L:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.