Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2023 – 06:17 PM EDT

PDB ID	:	8SDB
Title	:	Crystal Structure of E.Coli Branching Enzyme in complex with malto-octose
Authors	:	Bingham, C.R.; Nayebi, H.; Fawaz, R.; Geiger, J.H.
Deposited on	:	2023-04-06
Resolution	:	3.00 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:

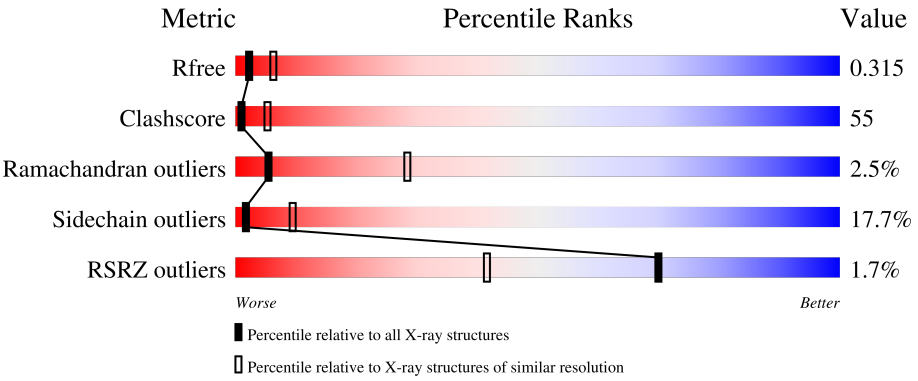
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	613	41% 47% 10%
1	B	613	44% 43% 8%
1	C	613	49% 40% 9%
1	D	613	5% 16% 42% 21% 19%
2	E	5	20% 40% 40%

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Mol	Chain	Length	Quality of chain
2	F	5	60% 40%
2	H	5	40% 60%
3	G	4	50% 50%
4	I	3	67% 33%
4	M	3	33% 67%
5	J	7	14% 57% 29%
6	K	2	100%
6	L	2	100%
6	N	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	E	5	-	-	-	X
3	GLC	G	1	-	-	-	X
3	GLC	G	2	-	-	-	X
3	GLC	G	3	-	-	-	X
5	GLC	J	5	-	-	X	-
5	GLC	J	6	-	-	X	-
5	GLC	J	7	-	-	-	X
6	GLC	L	1	-	-	X	-
6	GLC	N	2	-	-	-	X
7	GLC	A	803	-	-	-	X
7	GLC	B	802	-	-	-	X

2 Entry composition

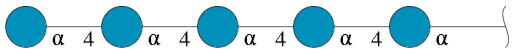
There are 7 unique types of molecules in this entry. The entry contains 19380 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	64	0	0
			4938	3158	876	888	16			
1	B	591	Total	C	N	O	S	43	0	0
			4860	3108	862	874	16			
1	C	604	Total	C	N	O	S	47	0	0
			4972	3179	882	895	16			
1	D	496	Total	C	N	O	S	128	0	0
			4110	2636	722	741	11			

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

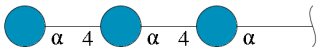


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	O		12	0	0
			56	30	26				
2	F	5	Total	C	O		12	0	0
			56	30	26				
2	H	5	Total	C	O		9	0	0
			56	30	26				

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

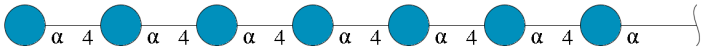
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	G	4	Total C O 45 24 21	10	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	I	3	Total C O 34 18 16	2	0	0
4	M	3	Total C O 34 18 16	5	0	0

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

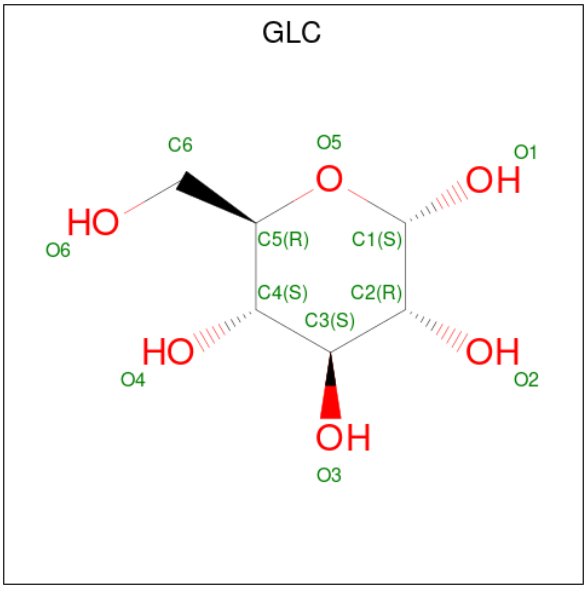


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	J	7	Total C O 78 42 36	16	0	0

- Molecule 6 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	K	2	Total C O 23 12 11	7	0	0
6	L	2	Total C O 23 12 11	4	0	0
6	N	2	Total C O 23 12 11	0	0	0

- Molecule 7 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



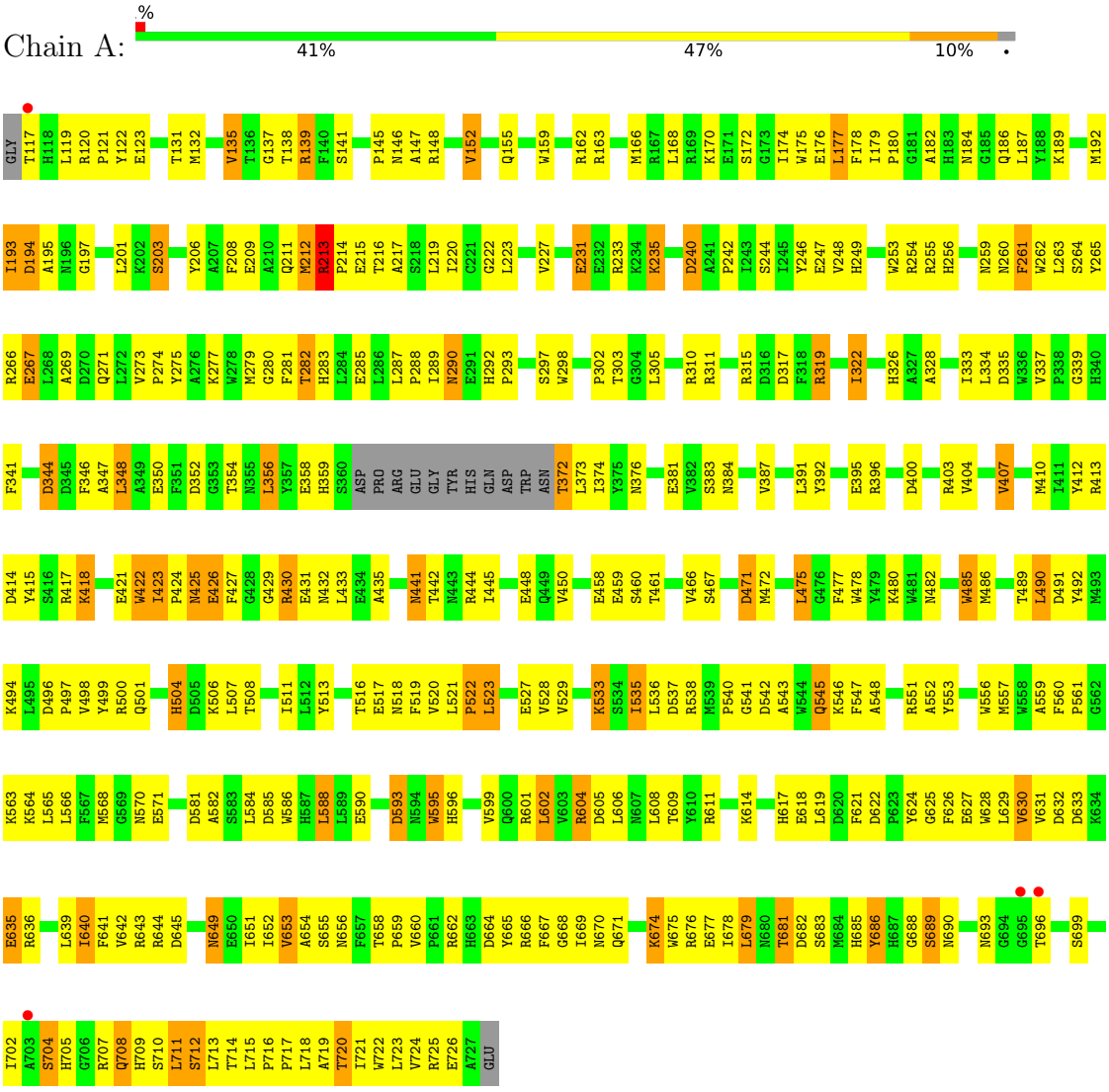
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 12 6 6	0	0
7	A	1	Total C O 12 6 6	1	0
7	A	1	Total C O 12 6 6	0	0
7	B	1	Total C O 12 6 6	1	0
7	B	1	Total C O 12 6 6	3	0
7	D	1	Total C O 12 6 6	0	0

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.

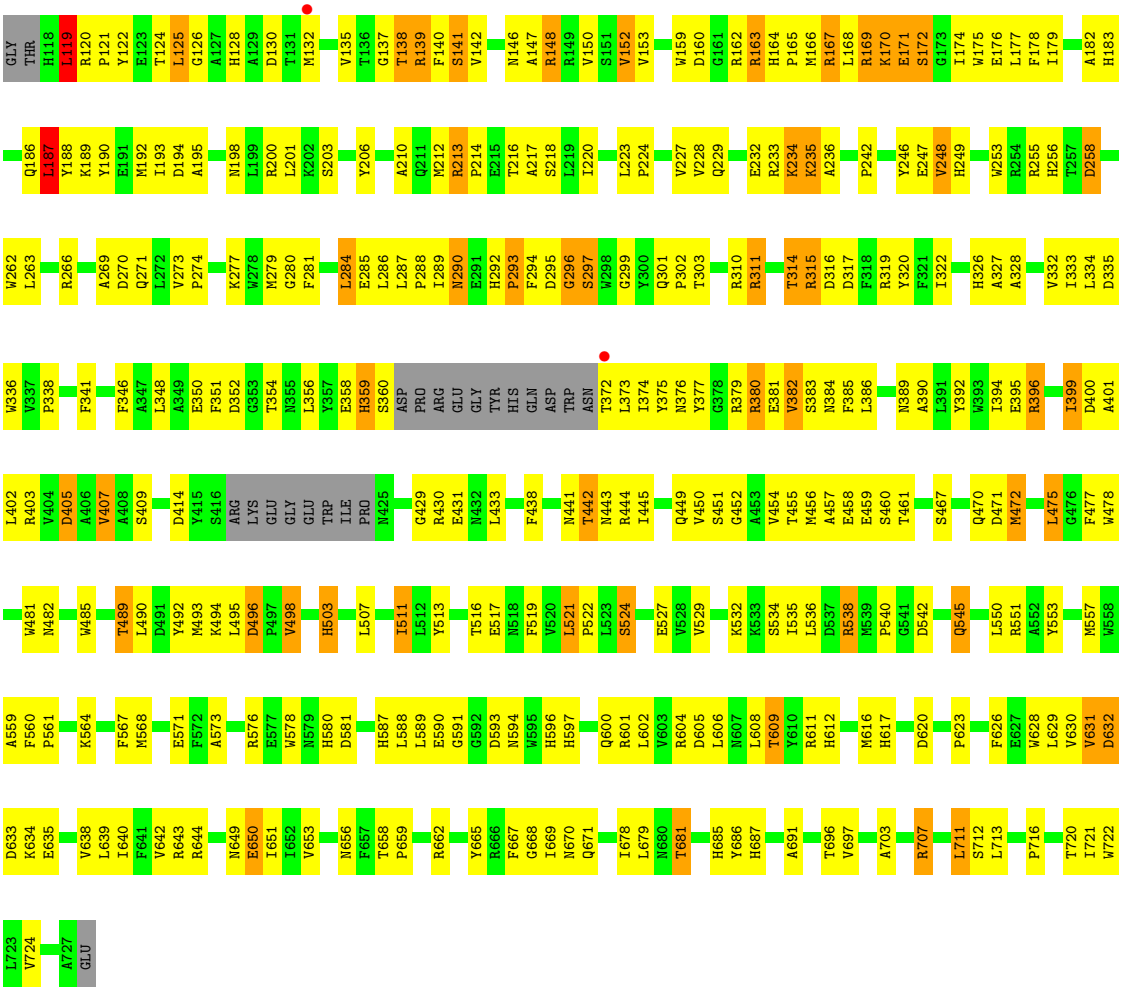
• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

Chain A:



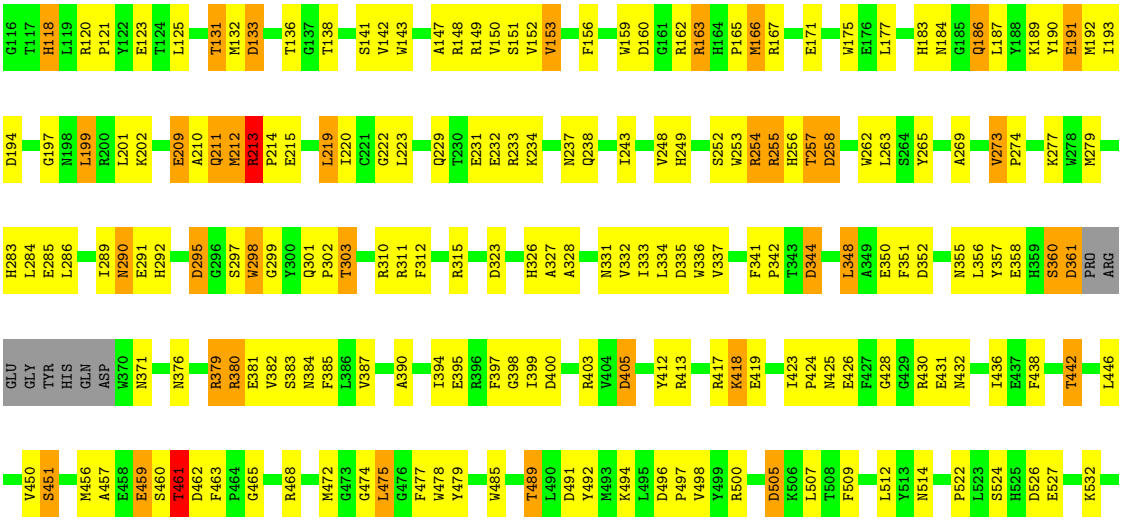
• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

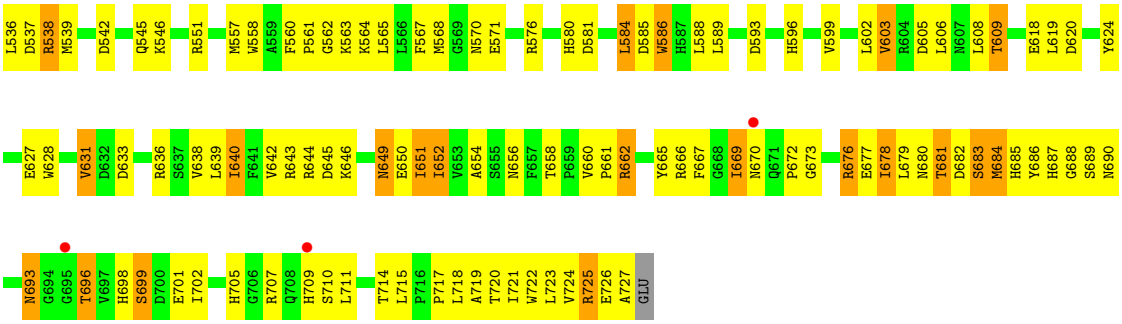
Chain B:



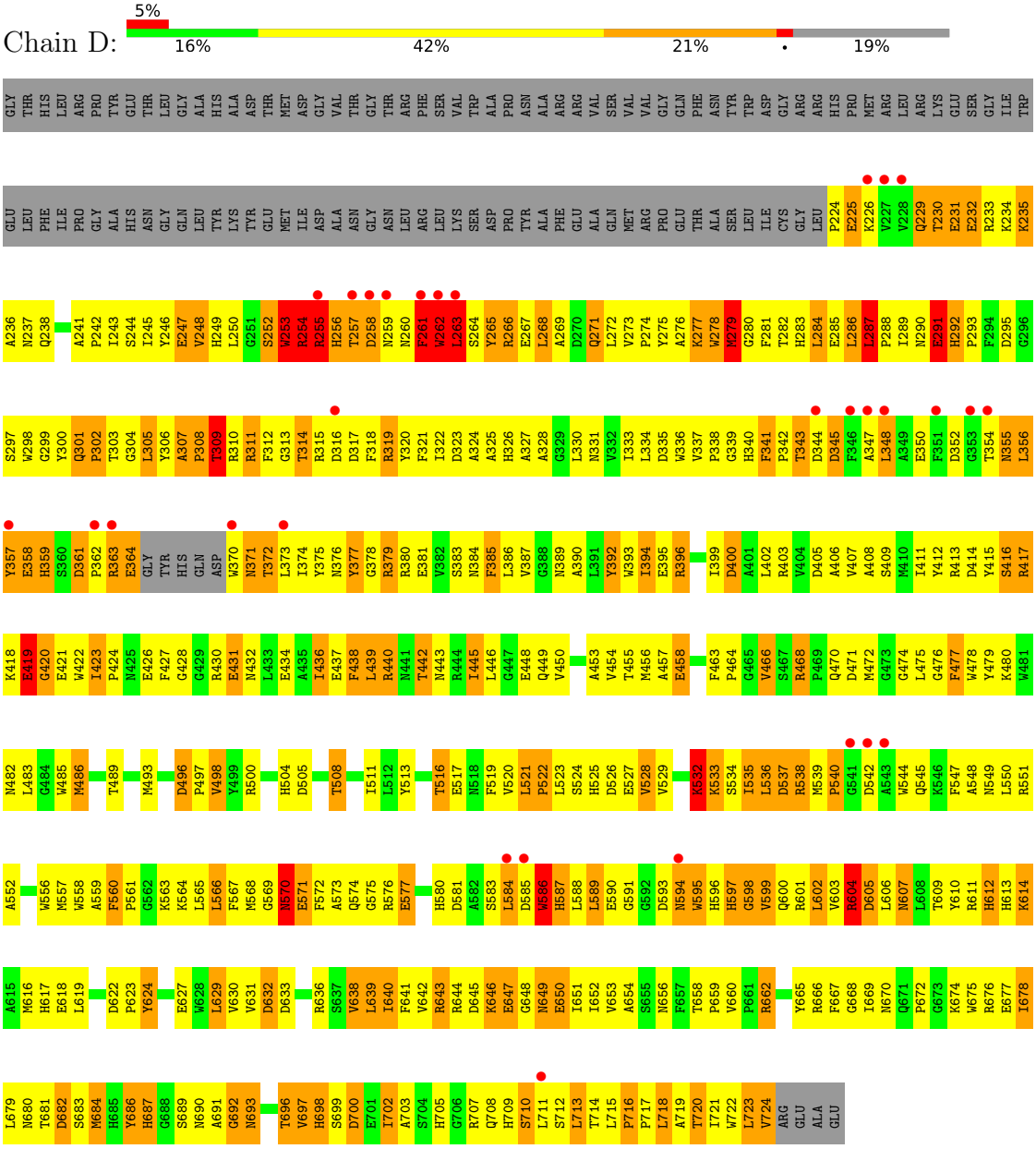
• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

Chain C:



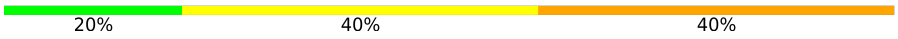


• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:

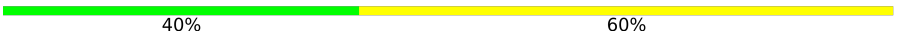


• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H:



• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain G:

• Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

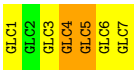
Chain I:

• Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:

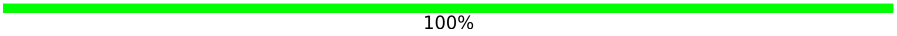
• Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:



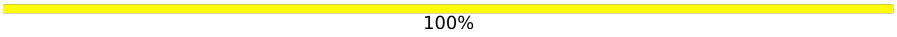
• Molecule 6: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:



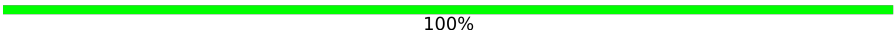
• Molecule 6: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:



• Molecule 6: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	146.49Å 146.49Å 294.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.85 – 3.00 38.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (38.85-3.00) 96.4 (38.85-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.214 , 0.315 0.214 , 0.315	Depositor DCC
R_{free} test set	3623 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	82.5	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 66.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19380	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: GLC

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	0.63	0/5097	0.74	3/6923 (0.0%)
1	B	0.59	0/5015	0.73	4/6810 (0.1%)
1	C	0.59	0/5133	0.72	1/6973 (0.0%)
1	D	0.65	3/4247 (0.1%)	0.80	8/5772 (0.1%)
All	All	0.61	3/19492 (0.0%)	0.75	16/26478 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	261	PHE	CD2-CE2	-14.16	1.10	1.39
1	D	261	PHE	CB-CG	-11.91	1.31	1.51
1	D	262	TRP	CB-CG	6.15	1.61	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	356	LEU	CA-CB-CG	-8.01	96.87	115.30
1	D	532	LYS	CD-CE-NZ	7.16	128.16	111.70
1	D	261	PHE	CB-CG-CD2	-6.82	116.02	120.80
1	A	422	TRP	N-CA-C	-5.83	95.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	253	TRP	C-N-CA	5.75	136.08	121.70
1	D	263	LEU	CB-CG-CD2	-5.71	101.29	111.00
1	D	521	LEU	CA-CB-CG	-5.68	102.24	115.30
1	D	255	ARG	CA-CB-CG	5.65	125.82	113.40
1	D	279	MET	CB-CG-SD	-5.62	95.53	112.40
1	B	521	LEU	CA-CB-CG	5.48	127.91	115.30
1	B	187	LEU	CA-CB-CG	5.34	127.58	115.30
1	B	284	LEU	CA-CB-CG	5.29	127.48	115.30
1	A	475	LEU	CA-CB-CG	-5.15	103.46	115.30
1	C	584	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	B	119	LEU	CA-CB-CG	5.11	127.06	115.30
1	D	604	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	359	HIS	Peptide
1	D	261	PHE	Sidechain
1	D	598	GLY	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	4938	0	4661	469	0
1	B	4860	0	4585	331	0
1	C	4972	0	4685	348	0
1	D	4110	0	3854	886	0
2	E	56	0	48	7	0
2	F	56	0	48	3	0
2	H	56	0	48	7	0
3	G	45	0	39	5	0
4	I	34	0	30	3	0
4	M	34	0	30	3	0
5	J	78	0	66	19	0
6	K	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	23	0	21	7	0
6	N	23	0	21	0	0
7	A	36	0	36	1	0
7	B	24	0	24	0	0
7	D	12	0	12	0	0
All	All	19380	0	18229	2034	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 55.

All (2034) 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:D:343:THR:CG2	1:D:370:TRP:CH2	1.76	1.58
1:D:343:THR:HG21	1:D:370:TRP:CZ2	1.41	1.54
1:D:309:THR:HG21	1:D:318:PHE:CE2	1.42	1.52
1:D:343:THR:HG21	1:D:370:TRP:CH2	0.98	1.48
1:A:666:ARG:CD	1:A:702:ILE:HD12	1.33	1.43
1:B:256:HIS:CD2	5:J:6:GLC:O3	1.82	1.33
1:A:666:ARG:HG3	1:A:710:SER:OG	1.16	1.31
1:D:308:PRO:O	1:D:309:THR:CG2	1.78	1.31
1:D:343:THR:CG2	1:D:370:TRP:CZ3	2.13	1.28
1:D:640:ILE:CD1	1:D:654:ALA:HA	1.64	1.28
1:C:537:ASP:OD1	6:L:1:GLC:H2	1.32	1.27
1:A:666:ARG:HD3	1:A:702:ILE:CD1	1.55	1.27
1:D:308:PRO:O	1:D:309:THR:HG22	1.25	1.26
1:A:681:THR:HG22	1:A:720:THR:O	1.24	1.25
1:B:256:HIS:CG	5:J:6:GLC:O2	1.89	1.25
1:A:666:ARG:CG	1:A:710:SER:OG	1.86	1.22
1:D:640:ILE:HD11	1:D:654:ALA:CA	1.67	1.22
1:D:309:THR:CG2	1:D:318:PHE:CE2	2.20	1.21
1:D:343:THR:HG23	1:D:370:TRP:CZ3	1.75	1.18
1:D:389:ASN:OD1	1:D:393:TRP:NE1	1.75	1.18
1:A:681:THR:CG2	1:A:720:THR:O	1.93	1.17
1:B:256:HIS:HB3	5:J:6:GLC:O2	1.44	1.16
1:A:681:THR:CG2	1:A:720:THR:H	1.60	1.14
1:B:256:HIS:CB	5:J:6:GLC:O2	1.96	1.13
1:D:309:THR:CG2	1:D:318:PHE:HE2	1.60	1.12
1:D:269:ALA:HB1	1:D:321:PHE:HB3	1.30	1.11
1:D:527:GLU:N	1:D:532:LYS:HE2	1.65	1.11
1:A:716:PRO:HD2	1:A:721:ILE:HD11	1.22	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LYS:CD	1:A:696:THR:HG21	1.81	1.10
1:D:341:PHE:CG	1:D:342:PRO:HD2	1.85	1.10
1:C:273:VAL:HG23	1:C:274:PRO:HD3	1.31	1.10
2:E:3:GLC:H62	2:E:4:GLC:C1	1.81	1.10
1:D:529:VAL:N	1:D:532:LYS:HZ2	1.49	1.10
1:A:640:ILE:CD1	1:A:654:ALA:HA	1.82	1.09
5:J:5:GLC:H3	5:J:6:GLC:O2	1.50	1.09
1:A:148:ARG:HB2	1:A:193:ILE:HD11	1.33	1.09
1:B:256:HIS:CD2	5:J:6:GLC:HO3	1.62	1.09
1:A:541:GLY:HA3	1:A:545:GLN:HB2	1.18	1.09
1:D:341:PHE:CD1	1:D:342:PRO:HD2	1.86	1.09
1:C:542:ASP:OD2	4:M:2:GLC:O2	1.70	1.08
1:D:394:ILE:HD11	1:D:450:VAL:CG1	1.82	1.08
1:A:138:THR:HG21	1:A:220:ILE:HD11	1.28	1.08
1:A:681:THR:HG21	1:A:720:THR:N	1.69	1.07
1:B:376:ASN:O	1:B:382:VAL:HG21	1.55	1.07
1:B:635:GLU:O	2:F:4:GLC:O3	1.72	1.07
1:D:445:ILE:HA	1:D:448:GLU:HG3	1.36	1.07
1:D:535:ILE:H	1:D:535:ILE:HD13	0.91	1.06
1:A:708:GLN:NE2	1:A:709:HIS:CE1	2.25	1.05
1:B:403:ARG:NH1	1:B:405:ASP:OD1	1.88	1.05
1:A:681:THR:HG21	1:A:720:THR:H	0.92	1.05
1:C:542:ASP:OD1	1:C:545:GLN:HG3	1.57	1.05
1:D:394:ILE:HD11	1:D:450:VAL:HG11	1.05	1.05
1:C:403:ARG:NH1	1:C:405:ASP:OD1	1.90	1.04
1:D:529:VAL:H	1:D:532:LYS:NZ	1.55	1.04
1:B:256:HIS:HB3	5:J:6:GLC:HO2	0.91	1.02
1:D:539:MET:HG2	1:D:549:ASN:HB2	1.39	1.02
1:A:708:GLN:NE2	1:A:709:HIS:NE2	2.09	1.01
1:D:602:LEU:O	1:D:606:LEU:HB2	1.59	1.01
1:C:163:ARG:H	1:C:163:ARG:CZ	1.73	1.01
1:D:253:TRP:HB2	1:D:586:TRP:NE1	1.74	1.01
1:D:324:ALA:O	1:D:328:ALA:N	1.94	1.01
1:D:355:ASN:HA	1:D:358:GLU:OE2	1.60	1.01
1:D:359:HIS:CG	1:D:376:ASN:HB3	1.96	1.01
1:D:440:ARG:HD2	1:D:475:LEU:H	1.22	1.01
1:D:535:ILE:H	1:D:535:ILE:CD1	1.66	1.01
1:A:280:GLY:O	1:A:611:ARG:NH1	1.94	1.00
1:D:246:TYR:OH	1:D:571:GLU:OE2	1.77	1.00
1:D:350:GLU:N	1:D:358:GLU:OE1	1.93	1.00
1:D:497:PRO:HA	1:D:500:ARG:HG3	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ASP:OD1	1:B:311:ARG:NH2	1.94	1.00
1:D:394:ILE:CD1	1:D:450:VAL:HG11	1.90	1.00
1:D:535:ILE:HD13	1:D:535:ILE:N	1.76	0.99
1:D:247:GLU:HB3	1:D:567:PHE:HA	1.44	0.98
1:D:343:THR:HG21	1:D:370:TRP:CZ3	1.84	0.98
1:D:602:LEU:CD1	1:D:606:LEU:HD22	1.93	0.98
1:D:616:MET:HE2	1:D:651:ILE:HD11	1.45	0.98
1:B:124:THR:HG23	1:B:125:LEU:HD23	1.44	0.98
1:D:534:SER:OG	1:D:537:ASP:OD1	1.82	0.97
1:A:282:THR:HG22	1:A:283:HIS:ND1	1.77	0.97
1:C:423:ILE:HD12	1:C:424:PRO:HD2	1.44	0.97
1:D:535:ILE:HD11	1:D:570:ASN:OD1	1.64	0.97
2:E:3:GLC:H62	2:E:4:GLC:O5	1.65	0.97
1:C:162:ARG:H	1:C:163:ARG:HH22	1.00	0.97
1:A:639:LEU:O	1:A:640:ILE:HD13	1.63	0.97
1:A:674:LYS:HD2	1:A:696:THR:HG21	1.46	0.96
1:D:570:ASN:O	1:D:572:PHE:N	1.99	0.96
5:J:5:GLC:C3	5:J:6:GLC:O2	2.14	0.96
1:D:601:ARG:HB3	1:D:686:TYR:HD2	1.25	0.96
1:A:666:ARG:HA	1:A:711:LEU:O	1.65	0.96
1:B:253:TRP:CD1	1:B:568:MET:HE1	2.01	0.95
1:B:137:GLY:HA3	1:B:178:PHE:CZ	2.01	0.95
1:D:547:PHE:HB3	1:D:551:ARG:NH2	1.81	0.95
1:D:308:PRO:O	1:D:309:THR:HG23	1.66	0.95
1:C:162:ARG:N	1:C:163:ARG:HH22	1.62	0.95
1:A:636:ARG:CG	1:A:662:ARG:HH21	1.80	0.94
1:C:383:SER:O	1:C:387:VAL:HG12	1.66	0.94
1:C:673:GLY:N	1:C:699:SER:OG	2.00	0.94
1:D:308:PRO:C	1:D:309:THR:CG2	2.33	0.94
1:D:529:VAL:H	1:D:532:LYS:HZ2	0.96	0.94
1:D:684:MET:SD	1:D:690:ASN:ND2	2.41	0.94
1:A:630:VAL:HG22	1:A:640:ILE:HB	1.50	0.94
1:A:676:ARG:HH21	1:A:726:GLU:HG2	1.33	0.93
1:D:308:PRO:C	1:D:309:THR:HG23	1.87	0.93
1:B:139:ARG:HG2	1:B:139:ARG:HH11	1.34	0.93
1:B:620:ASP:OD1	1:B:643:ARG:NH2	2.00	0.93
1:A:213:ARG:HB2	1:A:214:PRO:HD3	1.49	0.93
1:A:604:ARG:HH11	1:A:604:ARG:HG3	1.34	0.93
1:D:292:HIS:O	1:D:311:ARG:NH1	2.00	0.93
1:B:716:PRO:CD	1:B:721:ILE:HD11	1.99	0.92
1:B:138:THR:OG1	1:B:182:ALA:O	1.87	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ARG:HB3	1:C:214:PRO:HD3	1.51	0.92
1:A:189:LYS:HZ3	1:A:346:PHE:HE2	1.17	0.92
1:A:593:ASP:OD1	1:A:601:ARG:NH2	2.03	0.92
1:B:262:TRP:CZ3	1:B:311:ARG:HG2	2.04	0.92
1:D:255:ARG:NH2	1:D:256:HIS:O	2.03	0.91
1:D:533:LYS:HB3	1:D:537:ASP:OD2	1.69	0.91
1:A:708:GLN:HE21	1:A:709:HIS:CD2	1.87	0.91
1:C:658:THR:HG21	1:C:662:ARG:HH12	1.35	0.91
1:D:306:TYR:C	1:D:308:PRO:HD3	1.90	0.91
1:D:269:ALA:CB	1:D:321:PHE:HB3	2.01	0.91
1:D:636:ARG:HG3	1:D:662:ARG:NH2	1.86	0.91
1:A:186:GLN:O	1:A:220:ILE:HG22	1.71	0.90
1:A:666:ARG:HG3	1:A:710:SER:HG	1.13	0.90
1:C:485:TRP:CH2	1:C:557:MET:HG3	2.07	0.90
1:A:138:THR:OG1	1:A:182:ALA:O	1.89	0.90
1:A:674:LYS:HG2	1:A:696:THR:CG2	2.01	0.90
1:C:162:ARG:H	1:C:163:ARG:NH2	1.69	0.90
1:D:529:VAL:HG22	1:D:532:LYS:CE	2.01	0.90
1:D:636:ARG:HD2	1:D:662:ARG:HD2	1.54	0.90
1:A:293:PRO:HD3	1:A:303:THR:HG23	1.54	0.90
1:D:300:TYR:OH	1:D:335:ASP:OD2	1.90	0.90
1:A:423:ILE:CD1	1:A:431:GLU:OE1	2.21	0.89
1:D:597:HIS:O	1:D:601:ARG:HG2	1.71	0.89
1:D:417:ARG:HD3	1:D:422:TRP:HB3	1.55	0.89
1:A:708:GLN:HE21	1:A:709:HIS:CE1	1.90	0.89
1:C:593:ASP:OD1	1:C:687:HIS:NE2	2.04	0.89
1:D:659:PRO:HA	1:D:718:LEU:CD1	2.03	0.89
1:C:459:GLU:OE2	1:C:461:THR:HG23	1.73	0.88
1:A:668:GLY:HA2	1:A:709:HIS:O	1.73	0.88
1:B:668:GLY:O	1:B:669:ILE:HD13	1.74	0.88
1:C:150:VAL:HG12	1:C:166:MET:HE3	1.53	0.88
1:D:301:GLN:HG3	1:D:302:PRO:HD2	1.53	0.88
1:A:466:VAL:CG2	1:A:480:LYS:HD3	2.04	0.88
1:A:629:LEU:HB2	1:A:640:ILE:HG22	1.55	0.88
1:C:249:HIS:H	1:C:568:MET:HE3	1.40	0.87
1:A:146:ASN:ND2	1:A:352:ASP:OD2	2.07	0.87
1:A:273:VAL:CG2	1:A:274:PRO:HD3	2.04	0.87
1:D:669:ILE:HG21	1:D:711:LEU:HD22	1.55	0.87
1:A:168:LEU:HD13	1:A:175:TRP:CE2	2.09	0.87
1:A:372:THR:O	1:A:373:LEU:HD23	1.74	0.87
1:D:616:MET:CE	1:D:651:ILE:HD11	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:523:LEU:HD11	1:D:557:MET:HE1	1.54	0.87
1:D:598:GLY:HA2	1:D:601:ARG:HB2	1.57	0.86
1:A:666:ARG:HD3	1:A:702:ILE:HD12	0.88	0.86
1:C:537:ASP:OD1	6:L:1:GLC:C2	2.22	0.86
1:D:645:ASP:O	1:D:647:GLU:N	2.06	0.86
1:C:381:GLU:OE1	1:C:381:GLU:N	2.08	0.86
1:A:138:THR:CG2	1:A:220:ILE:HD11	2.04	0.86
1:D:529:VAL:HG13	1:D:532:LYS:NZ	1.90	0.86
1:A:547:PHE:CE2	1:A:595:TRP:HB3	2.10	0.86
1:D:291:GLU:HB3	1:D:304:GLY:HA3	1.57	0.86
1:D:659:PRO:HA	1:D:718:LEU:HD11	1.57	0.86
1:A:681:THR:CG2	1:A:720:THR:N	2.28	0.86
1:B:253:TRP:HD1	1:B:568:MET:HE1	1.41	0.86
1:B:601:ARG:NH1	1:B:685:HIS:O	2.09	0.86
1:D:291:GLU:CB	1:D:304:GLY:HA3	2.06	0.86
1:A:414:ASP:O	1:A:430:ARG:NH2	2.09	0.86
1:D:287:LEU:HG	1:D:288:PRO:HD2	1.58	0.86
1:D:602:LEU:HD12	1:D:606:LEU:HD22	1.58	0.86
1:B:258:ASP:N	1:B:258:ASP:OD1	2.09	0.86
1:C:683:SER:HB2	3:G:3:GLC:C3	2.06	0.86
1:D:466:VAL:O	1:D:477:PHE:HB2	1.75	0.86
1:D:602:LEU:HD22	1:D:681:THR:HG22	1.56	0.86
1:B:150:VAL:HG11	1:B:166:MET:HE2	1.57	0.85
1:C:376:ASN:O	1:C:382:VAL:HG21	1.74	0.85
1:C:672:PRO:HB3	1:C:709:HIS:CD2	2.11	0.85
1:D:305:LEU:HD22	1:D:389:ASN:ND2	1.90	0.85
1:C:171:GLU:OE2	1:C:171:GLU:N	2.09	0.85
1:C:248:VAL:HA	1:C:568:MET:HE3	1.57	0.85
1:D:587:HIS:O	1:D:588:LEU:HD13	1.76	0.85
1:B:256:HIS:CB	5:J:6:GLC:HO2	1.77	0.85
1:A:541:GLY:HA3	1:A:545:GLN:CB	2.05	0.85
1:D:586:TRP:O	1:D:588:LEU:N	2.09	0.85
1:A:412:TYR:CE2	1:A:461:THR:HG21	2.11	0.84
1:D:624:TYR:HE1	1:D:644:ARG:HH11	1.20	0.84
1:D:279:MET:C	1:D:604:ARG:HH11	1.79	0.84
1:A:666:ARG:CD	1:A:702:ILE:CD1	2.16	0.84
1:A:120:ARG:NH2	1:A:395:GLU:OE2	2.09	0.84
1:C:710:SER:O	1:C:711:LEU:HD23	1.77	0.84
1:D:248:VAL:HG13	1:D:568:MET:HB3	1.58	0.84
1:D:523:LEU:HD11	1:D:557:MET:CE	2.08	0.84
1:D:256:HIS:HB3	1:D:263:LEU:HD21	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:TYR:CD1	1:D:281:PHE:HE2	1.95	0.83
1:D:672:PRO:HB3	1:D:709:HIS:ND1	1.93	0.83
1:A:213:ARG:HB2	1:A:214:PRO:CD	2.02	0.83
1:B:605:ASP:OD2	1:B:686:TYR:OH	1.94	0.83
1:D:309:THR:HG21	1:D:318:PHE:CD2	2.11	0.83
1:C:249:HIS:H	1:C:568:MET:CE	1.92	0.83
1:C:355:ASN:ND2	1:C:360:SER:HA	1.93	0.83
1:A:189:LYS:NZ	1:A:346:PHE:HE2	1.77	0.83
1:D:470:GLN:HA	1:D:474:GLY:HA2	1.61	0.83
1:D:255:ARG:NH1	1:D:259:ASN:HB3	1.93	0.83
1:D:256:HIS:CB	1:D:263:LEU:HD21	2.08	0.83
1:D:594:ASN:HD21	1:D:687:HIS:CB	1.91	0.83
1:B:170:LYS:H	1:B:170:LYS:HD2	1.44	0.82
1:B:280:GLY:O	1:B:611:ARG:NH1	2.11	0.82
1:C:690:ASN:ND2	3:G:4:GLC:O3	2.12	0.82
1:B:124:THR:HG23	1:B:125:LEU:CD2	2.08	0.82
1:A:485:TRP:O	1:A:489:THR:HG23	1.79	0.82
1:C:537:ASP:OD2	6:L:1:GLC:O2	1.98	0.82
1:D:247:GLU:HG2	1:D:567:PHE:HD1	1.43	0.82
1:D:288:PRO:HG2	1:D:299:GLY:HA3	1.62	0.82
1:A:640:ILE:HD11	1:A:654:ALA:HA	1.60	0.82
1:C:551:ARG:HG2	1:C:602:LEU:HD22	1.58	0.81
1:D:593:ASP:OD1	1:D:601:ARG:NH2	2.13	0.81
1:C:186:GLN:O	1:C:220:ILE:HG22	1.81	0.81
1:C:273:VAL:HG23	1:C:274:PRO:CD	2.10	0.81
1:D:536:LEU:HD22	1:D:550:LEU:CD1	2.11	0.81
1:D:614:LYS:H	1:D:614:LYS:CD	1.93	0.81
5:J:5:GLC:C3	5:J:6:GLC:HO2	1.90	0.81
1:B:248:VAL:HB	1:B:568:MET:CE	2.10	0.81
1:B:297:SER:OG	1:B:301:GLN:HB2	1.81	0.81
1:D:356:LEU:O	1:D:379:ARG:NH1	2.14	0.81
1:D:529:VAL:H	1:D:532:LYS:CE	1.93	0.81
1:B:438:PHE:O	1:B:442:THR:HG23	1.80	0.81
1:B:658:THR:HG21	1:B:662:ARG:HH22	1.46	0.81
1:D:265:TYR:HB2	1:D:312:PHE:CD1	2.15	0.81
1:D:573:ALA:HB2	1:D:599:VAL:HG21	1.63	0.81
1:B:380:ARG:O	1:B:384:ASN:ND2	2.14	0.80
1:D:247:GLU:O	1:D:568:MET:HG2	1.81	0.80
1:D:529:VAL:HG13	1:D:532:LYS:HZ1	1.44	0.80
1:D:466:VAL:HB	1:D:475:LEU:HD23	1.64	0.80
1:D:532:LYS:O	1:D:538:ARG:NH2	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:HH12	1:A:582:ALA:N	1.79	0.80
1:A:633:ASP:OD2	1:A:665:TYR:OH	1.98	0.80
1:D:570:ASN:O	1:D:571:GLU:HG2	1.81	0.80
1:A:138:THR:HG21	1:A:220:ILE:CD1	2.08	0.80
1:A:148:ARG:HB2	1:A:193:ILE:CD1	2.11	0.80
1:C:292:HIS:O	1:C:311:ARG:NH1	2.14	0.80
1:D:666:ARG:NH1	1:D:702:ILE:HD13	1.96	0.80
1:A:254:ARG:NH2	1:A:271:GLN:OE1	2.14	0.80
1:D:301:GLN:OE1	1:D:301:GLN:HA	1.81	0.80
1:C:599:VAL:O	1:C:603:VAL:HG13	1.81	0.80
1:A:676:ARG:HH21	1:A:726:GLU:CG	1.95	0.79
1:A:662:ARG:HB2	1:A:715:LEU:HB2	1.64	0.79
1:D:618:GLU:OE2	1:D:646:LYS:HG3	1.81	0.79
1:D:654:ALA:HB3	1:D:721:ILE:HG12	1.65	0.79
1:D:508:THR:O	1:D:511:ILE:HG22	1.82	0.79
1:D:389:ASN:OD1	1:D:393:TRP:CD1	2.35	0.79
1:D:394:ILE:N	1:D:399:ILE:HD11	1.97	0.79
1:A:466:VAL:HG21	1:A:480:LYS:HD3	1.62	0.79
1:B:443:ASN:OD1	1:B:455:THR:HG21	1.82	0.79
1:C:512:LEU:HD12	1:C:512:LEU:H	1.46	0.79
1:D:313:GLY:O	1:D:314:THR:HG22	1.82	0.79
1:D:265:TYR:CB	1:D:312:PHE:HB3	2.12	0.79
1:A:681:THR:HG21	1:A:720:THR:HG23	1.65	0.79
1:D:278:TRP:O	1:D:604:ARG:HG2	1.83	0.79
1:D:350:GLU:HG2	1:D:354:THR:HG23	1.63	0.79
1:B:119:LEU:HD22	1:B:119:LEU:H	1.46	0.78
1:D:560:PHE:CD1	1:D:561:PRO:HD2	2.17	0.78
1:A:273:VAL:HG22	1:A:274:PRO:HD3	1.65	0.78
1:D:659:PRO:CA	1:D:718:LEU:HD11	2.11	0.78
1:D:306:TYR:HD1	1:D:392:TYR:CE2	2.02	0.78
1:D:599:VAL:O	1:D:600:GLN:HB2	1.83	0.78
1:D:601:ARG:HB3	1:D:686:TYR:CD2	2.16	0.78
1:C:560:PHE:CD2	1:C:561:PRO:HD2	2.18	0.78
1:D:341:PHE:CD1	1:D:342:PRO:CD	2.66	0.78
1:B:611:ARG:O	1:B:612:HIS:HB3	1.83	0.78
1:D:682:ASP:HB3	1:D:719:ALA:HB2	1.63	0.78
1:A:209:GLU:HG2	1:A:219:LEU:HD12	1.66	0.78
1:A:716:PRO:CD	1:A:721:ILE:HD11	2.09	0.78
1:A:605:ASP:O	1:A:609:THR:HG23	1.83	0.78
1:A:636:ARG:HG2	1:A:662:ARG:HE	1.46	0.78
1:D:536:LEU:HD22	1:D:550:LEU:HD13	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:666:ARG:NE	1:D:710:SER:OG	2.16	0.78
1:A:660:VAL:CG1	1:A:662:ARG:HH12	1.97	0.78
1:B:142:VAL:HG21	1:B:190:TYR:CZ	2.18	0.78
1:C:248:VAL:HG23	1:C:568:MET:HE2	1.64	0.78
1:C:584:LEU:HB2	1:C:586:TRP:CZ3	2.18	0.77
1:D:717:PRO:O	1:D:719:ALA:N	2.16	0.77
1:C:627:GLU:OE2	1:C:707:ARG:NH2	2.16	0.77
1:B:494:LYS:HD3	1:B:538:ARG:HG2	1.66	0.77
1:C:661:PRO:HG3	1:C:717:PRO:HG3	1.66	0.77
1:C:658:THR:HG21	1:C:662:ARG:NH1	1.98	0.77
1:D:536:LEU:HA	1:D:539:MET:HE1	1.66	0.77
1:B:716:PRO:HD3	1:B:721:ILE:HD11	1.65	0.77
1:C:187:LEU:HD23	1:C:219:LEU:HD22	1.65	0.77
1:C:683:SER:CB	3:G:3:GLC:O2	2.33	0.77
1:D:255:ARG:HH12	1:D:259:ASN:HB3	1.50	0.77
1:D:526:ASP:C	1:D:532:LYS:HE2	2.04	0.77
1:C:291:GLU:OE1	1:C:291:GLU:HA	1.84	0.77
1:D:394:ILE:HD13	1:D:395:GLU:N	2.00	0.77
1:D:528:VAL:C	1:D:532:LYS:HG2	2.04	0.77
1:A:381:GLU:N	1:A:381:GLU:OE1	2.15	0.76
1:B:160:ASP:OD2	1:B:162:ARG:NH1	2.19	0.76
1:B:183:HIS:ND1	1:B:186:GLN:OE1	2.17	0.76
1:B:273:VAL:HG23	1:B:274:PRO:HD3	1.65	0.76
1:C:438:PHE:O	1:C:442:THR:HG23	1.85	0.76
1:D:394:ILE:HA	1:D:399:ILE:HD12	1.67	0.76
1:A:277:LYS:HD2	1:A:328:ALA:O	1.84	0.76
1:C:681:THR:HG22	1:C:719:ALA:HB1	1.65	0.76
1:B:716:PRO:HD2	1:B:721:ILE:HD11	1.66	0.76
1:C:689:SER:HB2	4:M:3:GLC:O6	1.85	0.76
1:B:124:THR:CG2	1:B:125:LEU:HD23	2.16	0.76
1:A:501:GLN:HG3	1:A:635:GLU:HA	1.68	0.76
1:C:689:SER:CB	4:M:3:GLC:O6	2.34	0.76
1:D:232:GLU:HB3	1:D:233:ARG:HH11	1.51	0.76
1:D:528:VAL:H	1:D:532:LYS:CE	1.98	0.76
1:D:683:SER:HB3	1:D:686:TYR:CD1	2.21	0.76
1:B:492:TYR:CD2	1:B:507:LEU:HD11	2.21	0.76
1:C:253:TRP:O	1:C:586:TRP:HZ3	1.69	0.76
1:D:682:ASP:HB2	1:D:717:PRO:HG2	1.68	0.76
1:B:273:VAL:CG2	1:B:274:PRO:HD3	2.15	0.76
1:D:529:VAL:HG22	1:D:532:LYS:HE3	1.65	0.76
1:C:557:MET:O	1:C:564:LYS:HE3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:GLU:N	1:B:431:GLU:OE1	2.17	0.75
1:D:255:ARG:HA	1:D:262:TRP:HA	1.67	0.75
1:C:526:ASP:O	1:C:532:LYS:HE3	1.86	0.75
1:D:319:ARG:HH12	1:D:323:ASP:HB2	1.49	0.75
1:D:381:GLU:HA	1:D:384:ASN:OD1	1.87	0.75
1:A:640:ILE:HD11	1:A:654:ALA:CB	2.16	0.75
1:A:471:ASP:HB2	1:A:472:MET:CE	2.15	0.75
1:D:536:LEU:HB3	1:D:574:GLN:HG2	1.69	0.75
1:A:665:TYR:O	1:A:712:SER:HA	1.85	0.75
1:B:390:ALA:O	1:B:394:ILE:HD12	1.85	0.75
1:A:523:LEU:HG	1:A:557:MET:CE	2.17	0.75
1:D:552:ALA:HA	1:D:720:THR:HG23	1.69	0.75
1:A:588:LEU:HD12	1:A:596:HIS:CE1	2.22	0.75
1:A:675:TRP:CE2	1:A:725:ARG:HG3	2.21	0.75
1:D:255:ARG:HE	1:D:261:PHE:N	1.85	0.74
1:D:539:MET:CG	1:D:549:ASN:HB2	2.16	0.74
1:B:262:TRP:CH2	1:B:311:ARG:HG2	2.22	0.74
1:D:287:LEU:HG	1:D:288:PRO:CD	2.17	0.74
1:D:343:THR:CG2	1:D:370:TRP:CZ2	2.35	0.74
1:D:548:ALA:HB1	1:D:718:LEU:CB	2.17	0.74
1:A:432:ASN:OD1	1:A:435:ALA:N	2.18	0.74
1:A:640:ILE:HD12	1:A:654:ALA:HA	1.67	0.74
1:B:560:PHE:CD1	1:B:561:PRO:HD2	2.23	0.74
1:B:685:HIS:ND1	1:D:424:PRO:HB2	2.03	0.74
1:D:336:TRP:HB2	1:D:402:LEU:HB3	1.69	0.74
1:D:616:MET:SD	1:D:651:ILE:HD11	2.27	0.74
1:A:636:ARG:HG3	1:A:662:ARG:HH21	1.53	0.74
1:D:265:TYR:CG	1:D:312:PHE:HB3	2.22	0.74
1:D:413:ARG:O	1:D:430:ARG:HB3	1.86	0.74
1:B:293:PRO:HD3	1:B:303:THR:HG23	1.69	0.74
1:C:350:GLU:N	1:C:358:GLU:OE2	2.17	0.74
1:D:305:LEU:HD22	1:D:389:ASN:HD22	1.52	0.74
1:D:497:PRO:HA	1:D:500:ARG:CG	2.18	0.74
1:B:492:TYR:CG	1:B:507:LEU:HD11	2.23	0.73
1:C:461:THR:OG1	1:C:462:ASP:N	2.18	0.73
1:C:527:GLU:O	1:C:538:ARG:NH2	2.21	0.73
1:A:466:VAL:HG21	1:A:480:LYS:CD	2.18	0.73
1:D:486:MET:CE	1:D:527:GLU:HG2	2.18	0.73
1:A:177:LEU:HD21	1:A:179:ILE:HG13	1.69	0.73
1:A:417:ARG:HB3	1:A:417:ARG:CZ	2.17	0.73
1:C:418:LYS:CE	1:C:418:LYS:H	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:ARG:HG2	1:C:602:LEU:CD2	2.17	0.73
1:D:394:ILE:HD12	1:D:450:VAL:HG21	1.69	0.73
1:D:539:MET:HG2	1:D:549:ASN:CB	2.18	0.73
1:A:177:LEU:CD2	1:A:179:ILE:HG13	2.18	0.73
1:A:253:TRP:CE3	1:A:254:ARG:HG3	2.23	0.73
1:A:233:ARG:HD2	1:A:400:ASP:OD2	1.88	0.73
1:A:689:SER:O	1:A:690:ASN:HB3	1.88	0.73
1:A:523:LEU:HG	1:A:557:MET:HE1	1.70	0.73
1:D:350:GLU:CA	1:D:358:GLU:OE1	2.36	0.73
1:D:493:MET:HA	1:D:493:MET:HE3	1.70	0.73
1:A:667:PHE:HZ	1:A:713:LEU:HD12	1.54	0.73
1:D:248:VAL:O	1:D:286:LEU:HA	1.89	0.73
1:A:640:ILE:CD1	1:A:654:ALA:CA	2.64	0.73
1:D:598:GLY:HA3	1:D:687:HIS:NE2	2.04	0.73
1:A:640:ILE:HD11	1:A:654:ALA:CA	2.18	0.72
1:B:587:HIS:O	1:B:590:GLU:HG3	1.88	0.72
1:C:160:ASP:HB3	1:C:163:ARG:CZ	2.19	0.72
1:C:199:LEU:HD23	1:C:199:LEU:O	1.89	0.72
1:D:527:GLU:C	1:D:532:LYS:HG3	2.09	0.72
1:A:407:VAL:HG22	1:A:458:GLU:O	1.89	0.72
1:B:166:MET:HE1	1:B:175:TRP:HB2	1.69	0.72
1:D:678:ILE:HD12	1:D:678:ILE:O	1.87	0.72
1:D:288:PRO:HD3	1:D:300:TYR:CE1	2.23	0.72
1:A:660:VAL:CG1	1:A:662:ARG:NH1	2.53	0.72
1:C:120:ARG:NH2	1:C:395:GLU:OE2	2.20	0.72
1:C:633:ASP:OD2	1:C:638:VAL:HG22	1.89	0.72
1:A:421:GLU:HG2	1:A:423:ILE:HG22	1.71	0.72
1:B:150:VAL:HG22	1:B:192:MET:HG3	1.70	0.72
1:B:248:VAL:HB	1:B:568:MET:HE2	1.71	0.72
1:C:213:ARG:CB	1:C:214:PRO:HD3	2.19	0.72
1:D:528:VAL:HG13	1:D:532:LYS:HZ3	1.54	0.72
1:D:573:ALA:N	1:D:599:VAL:HG21	2.04	0.72
1:C:485:TRP:O	1:C:489:THR:HG23	1.88	0.72
1:B:189:LYS:HE3	1:B:216:THR:OG1	1.90	0.72
1:B:527:GLU:HA	1:B:532:LYS:HD2	1.72	0.72
1:D:254:ARG:O	1:D:255:ARG:HB3	1.89	0.72
1:A:227:VAL:HG22	1:A:319:ARG:NH2	2.05	0.72
1:A:679:LEU:HG	1:A:679:LEU:O	1.88	0.72
1:D:624:TYR:CD1	1:D:644:ARG:HD3	2.25	0.72
1:A:152:VAL:HG21	1:A:179:ILE:CD1	2.18	0.72
1:A:630:VAL:HG23	1:A:630:VAL:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:ASP:OD1	1:D:347:ALA:HB2	1.90	0.72
1:D:605:ASP:OD1	1:D:605:ASP:N	2.13	0.72
1:A:148:ARG:CB	1:A:193:ILE:HD11	2.16	0.71
1:C:162:ARG:N	1:C:163:ARG:NH2	2.33	0.71
1:C:509:PHE:HA	1:C:512:LEU:CD1	2.20	0.71
1:D:319:ARG:O	1:D:322:ILE:HG12	1.90	0.71
1:D:703:ALA:HB2	1:D:708:GLN:OE1	1.90	0.71
1:A:264:SER:H	1:A:267:GLU:HG3	1.55	0.71
1:A:682:ASP:O	1:A:688:GLY:HA3	1.90	0.71
1:B:120:ARG:NH2	1:B:395:GLU:OE1	2.20	0.71
1:D:468:ARG:HH21	1:D:517:GLU:HA	1.55	0.71
1:A:423:ILE:HD11	1:A:431:GLU:OE1	1.89	0.71
1:D:636:ARG:O	1:D:638:VAL:HG12	1.89	0.71
1:B:138:THR:HG21	1:B:220:ILE:HD13	1.72	0.71
1:B:192:MET:HE1	1:B:194:ASP:HB3	1.71	0.71
1:D:516:THR:O	1:D:517:GLU:HG2	1.89	0.71
1:D:539:MET:H	1:D:539:MET:HE2	1.55	0.71
1:D:633:ASP:OD1	1:D:636:ARG:HB3	1.90	0.71
1:D:255:ARG:NH1	1:D:261:PHE:H	1.87	0.71
1:D:305:LEU:O	1:D:389:ASN:ND2	2.23	0.71
1:D:589:LEU:HD12	1:D:597:HIS:CG	2.26	0.71
1:A:528:VAL:HG12	1:A:528:VAL:O	1.91	0.71
1:B:441:ASN:O	1:B:445:ILE:HD12	1.91	0.71
1:C:238:GLN:OE1	1:C:238:GLN:HA	1.88	0.71
1:D:363:ARG:O	1:D:364:GLU:O	2.08	0.71
1:A:666:ARG:CG	1:A:710:SER:HG	1.85	0.71
1:D:307:ALA:HB2	1:D:392:TYR:OH	1.91	0.71
1:C:150:VAL:HG12	1:C:166:MET:CE	2.20	0.71
1:A:273:VAL:HG23	1:A:274:PRO:HD3	1.71	0.71
1:A:618:GLU:OE2	1:A:645:ASP:HB2	1.89	0.71
1:D:430:ARG:HH11	1:D:430:ARG:HG3	1.54	0.71
1:C:423:ILE:HD12	1:C:424:PRO:CD	2.18	0.70
1:C:656:ASN:OD1	1:C:658:THR:HG22	1.91	0.70
1:D:229:GLN:NE2	1:D:400:ASP:OD1	2.24	0.70
1:D:248:VAL:HG23	1:D:285:GLU:O	1.91	0.70
1:D:542:ASP:OD1	1:D:545:GLN:HG3	1.91	0.70
1:B:150:VAL:HG11	1:B:166:MET:CE	2.21	0.70
1:A:166:MET:HE2	1:A:175:TRP:HB3	1.73	0.70
1:A:352:ASP:OD1	1:A:354:THR:OG1	2.08	0.70
1:C:628:TRP:CG	1:C:631:VAL:HG13	2.25	0.70
1:D:279:MET:CE	1:D:600:GLN:HE22	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:MET:SD	1:D:600:GLN:OE1	2.49	0.70
1:D:528:VAL:H	1:D:532:LYS:NZ	1.88	0.70
1:A:478:TRP:HH2	1:B:591:GLY:HA2	1.56	0.70
1:A:669:ILE:HG22	1:A:671:GLN:H	1.56	0.70
1:A:708:GLN:HE22	1:A:709:HIS:CE1	2.06	0.70
1:B:232:GLU:O	1:B:235:LYS:HG3	1.91	0.70
1:C:681:THR:HG22	1:C:719:ALA:CB	2.21	0.70
1:C:333:ILE:HD13	1:C:456:MET:HE3	1.71	0.70
1:C:418:LYS:H	1:C:418:LYS:HE2	1.57	0.70
1:D:255:ARG:NE	1:D:261:PHE:N	2.39	0.70
2:E:2:GLC:H61	2:E:3:GLC:O5	1.91	0.70
1:D:230:THR:OG1	1:D:326:HIS:HD2	1.75	0.70
1:A:466:VAL:HA	1:A:475:LEU:HB2	1.74	0.70
1:A:678:ILE:HG23	1:A:724:VAL:HG12	1.73	0.69
1:B:527:GLU:O	1:B:538:ARG:NH2	2.24	0.69
1:D:548:ALA:HB1	1:D:718:LEU:HB2	1.72	0.69
1:D:614:LYS:H	1:D:614:LYS:HD3	1.55	0.69
1:C:290:ASN:ND2	1:C:302:PRO:HB3	2.07	0.69
1:D:269:ALA:HB1	1:D:321:PHE:CB	2.16	0.69
1:C:412:TYR:CE2	1:C:461:THR:HG21	2.28	0.69
1:D:335:ASP:OD1	1:D:403:ARG:HD3	1.92	0.69
1:D:361:ASP:H	1:D:362:PRO:HD3	1.57	0.69
1:A:177:LEU:HD23	1:A:177:LEU:C	2.13	0.69
1:A:649:ASN:ND2	1:A:649:ASN:H	1.89	0.69
1:C:150:VAL:CG1	1:C:166:MET:HE3	2.23	0.69
1:D:547:PHE:HB3	1:D:551:ARG:HH22	1.56	0.69
1:D:355:ASN:HA	1:D:358:GLU:CD	2.12	0.69
1:D:287:LEU:CG	1:D:288:PRO:HD2	2.21	0.69
1:A:418:LYS:O	1:A:418:LYS:HG3	1.92	0.69
1:B:192:MET:CE	1:B:194:ASP:HB3	2.22	0.69
1:B:266:ARG:NH1	1:B:317:ASP:OD1	2.23	0.69
1:D:247:GLU:OE2	1:D:285:GLU:HG2	1.93	0.69
1:D:602:LEU:HD11	1:D:606:LEU:HD22	1.73	0.69
1:D:624:TYR:CE1	1:D:644:ARG:HD3	2.28	0.69
1:C:118:HIS:HB2	1:C:384:ASN:HD22	1.58	0.69
1:D:361:ASP:N	1:D:362:PRO:CD	2.55	0.69
1:D:393:TRP:C	1:D:399:ILE:HD11	2.12	0.69
1:D:597:HIS:N	1:D:597:HIS:CD2	2.61	0.69
1:D:678:ILE:CG2	1:D:724:VAL:HG22	2.22	0.69
1:C:485:TRP:HH2	1:C:557:MET:HG3	1.56	0.68
1:D:394:ILE:CD1	1:D:450:VAL:HG21	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:PHE:HB3	1:B:356:LEU:HD21	1.73	0.68
1:B:616:MET:HE2	1:B:643:ARG:HB2	1.74	0.68
1:C:537:ASP:CG	6:L:1:GLC:H2	2.13	0.68
1:D:383:SER:O	1:D:387:VAL:HG23	1.93	0.68
1:A:674:LYS:CG	1:A:696:THR:CG2	2.71	0.68
1:C:337:VAL:HG22	1:C:337:VAL:O	1.90	0.68
1:D:602:LEU:CD2	1:D:681:THR:HG22	2.23	0.68
1:D:607:ASN:O	1:D:611:ARG:HB2	1.93	0.68
1:D:692:GLY:HA2	1:D:714:THR:CG2	2.22	0.68
1:D:247:GLU:HG2	1:D:567:PHE:CD1	2.29	0.68
1:D:430:ARG:HG3	1:D:430:ARG:NH1	2.08	0.68
1:D:437:GLU:OE1	1:D:440:ARG:HG3	1.94	0.68
1:D:713:LEU:HD23	1:D:714:THR:H	1.57	0.68
1:D:419:GLU:O	1:D:421:GLU:N	2.25	0.68
1:A:255:ARG:HH21	1:A:262:TRP:HE1	1.39	0.68
1:A:674:LYS:CG	1:A:696:THR:HG21	2.22	0.68
1:D:307:ALA:N	1:D:308:PRO:HD3	2.08	0.68
1:D:354:THR:HG22	1:D:355:ASN:HB3	1.74	0.68
1:A:302:PRO:HG3	1:A:337:VAL:HG21	1.76	0.68
1:B:628:TRP:CG	1:B:631:VAL:HG23	2.29	0.68
1:D:256:HIS:HB2	1:D:263:LEU:HD11	1.76	0.68
1:C:684:MET:N	1:C:690:ASN:OD1	2.17	0.67
1:A:636:ARG:HG2	1:A:662:ARG:HH21	1.57	0.67
1:C:348:LEU:HD21	1:C:357:TYR:CD2	2.28	0.67
1:C:677:GLU:HA	1:C:723:LEU:HD23	1.76	0.67
1:D:411:ILE:HB	1:D:436:ILE:HG22	1.76	0.67
1:B:170:LYS:H	1:B:170:LYS:CD	2.04	0.67
1:D:573:ALA:CB	1:D:599:VAL:HG21	2.24	0.67
1:D:658:THR:C	1:D:718:LEU:HD11	2.15	0.67
1:D:242:PRO:O	1:D:282:THR:HG21	1.95	0.67
1:D:253:TRP:NE1	1:D:272:LEU:HD12	2.09	0.67
1:D:280:GLY:O	1:D:607:ASN:ND2	2.26	0.67
1:D:293:PRO:HG3	1:D:303:THR:CG2	2.24	0.67
1:D:722:TRP:C	1:D:723:LEU:HD23	2.14	0.67
1:D:682:ASP:CB	1:D:717:PRO:HG2	2.24	0.67
1:A:215:GLU:O	1:A:216:THR:HG22	1.94	0.67
1:D:393:TRP:HB3	1:D:399:ILE:HG12	1.75	0.67
1:D:662:ARG:HH21	1:D:662:ARG:CG	2.08	0.67
2:E:3:GLC:C6	2:E:4:GLC:C1	2.59	0.67
1:A:423:ILE:HD12	1:A:431:GLU:OE1	1.93	0.67
1:D:496:ASP:HB3	1:D:498:VAL:HG12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:PHE:CZ	1:A:713:LEU:HD12	2.29	0.67
1:C:683:SER:HB2	3:G:3:GLC:O2	1.92	0.67
1:D:536:LEU:CB	1:D:574:GLN:HG2	2.25	0.67
1:B:153:VAL:CG2	1:B:159:TRP:HA	2.25	0.67
1:C:701:GLU:O	1:C:701:GLU:HG3	1.94	0.67
1:A:641:PHE:CZ	1:A:653:VAL:HG21	2.30	0.66
1:B:381:GLU:HA	1:B:384:ASN:HD22	1.60	0.66
1:C:187:LEU:CD2	1:C:219:LEU:HD22	2.25	0.66
1:A:604:ARG:HH11	1:A:604:ARG:CG	2.07	0.66
1:D:252:SER:HB3	1:D:568:MET:SD	2.34	0.66
1:D:656:ASN:OD1	1:D:658:THR:HG22	1.93	0.66
1:D:255:ARG:CZ	1:D:260:ASN:HA	2.25	0.66
1:D:288:PRO:HG2	1:D:299:GLY:CA	2.25	0.66
1:D:668:GLY:HA2	1:D:709:HIS:O	1.96	0.66
1:D:721:ILE:HD12	1:D:723:LEU:HD21	1.76	0.66
1:B:172:SER:HB2	1:B:174:ILE:HD13	1.78	0.66
1:D:343:THR:CB	1:D:370:TRP:CH2	2.75	0.66
5:J:5:GLC:O3	5:J:6:GLC:C1	2.44	0.66
1:B:336:TRP:CZ3	1:B:338:PRO:HG3	2.30	0.66
1:B:658:THR:HG21	1:B:662:ARG:NH2	2.11	0.66
1:C:160:ASP:CG	1:C:163:ARG:NH2	2.49	0.66
1:D:246:TYR:CD1	1:D:281:PHE:CE2	2.82	0.66
1:A:269:ALA:O	1:A:273:VAL:HG22	1.94	0.66
1:A:660:VAL:HG11	1:A:662:ARG:HH12	1.59	0.66
1:A:678:ILE:CG2	1:A:724:VAL:HG12	2.25	0.66
1:D:254:ARG:N	1:D:583:SER:OG	2.26	0.66
1:D:572:PHE:HA	1:D:599:VAL:HB	1.78	0.66
1:D:607:ASN:N	1:D:607:ASN:OD1	2.29	0.66
1:A:630:VAL:CG2	1:A:640:ILE:HB	2.23	0.66
1:C:412:TYR:CZ	1:C:461:THR:HG21	2.31	0.66
1:D:255:ARG:NH2	1:D:259:ASN:O	2.28	0.66
1:A:681:THR:HG21	1:A:720:THR:CG2	2.25	0.66
1:D:253:TRP:HE1	1:D:272:LEU:HD12	1.61	0.66
1:B:139:ARG:HG2	1:B:139:ARG:NH1	2.04	0.66
1:C:333:ILE:HD13	1:C:456:MET:CE	2.25	0.66
1:D:597:HIS:O	1:D:601:ARG:CG	2.42	0.66
1:A:527:GLU:O	1:A:538:ARG:NH2	2.28	0.66
1:A:216:THR:HG23	1:A:216:THR:O	1.94	0.65
1:B:467:SER:OG	1:B:517:GLU:OE2	2.08	0.65
1:D:280:GLY:O	1:D:607:ASN:CB	2.44	0.65
1:D:323:ASP:O	1:D:327:ALA:N	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:GLU:HA	1:D:358:GLU:OE1	1.96	0.65
1:A:282:THR:CG2	1:A:283:HIS:ND1	2.58	0.65
1:A:636:ARG:HG2	1:A:662:ARG:NE	2.12	0.65
1:D:267:GLU:O	1:D:271:GLN:N	2.30	0.65
1:D:636:ARG:HD2	1:D:662:ARG:CD	2.26	0.65
1:A:547:PHE:CD2	1:A:595:TRP:HB3	2.31	0.65
1:D:356:LEU:HD13	1:D:357:TYR:N	2.12	0.65
1:B:248:VAL:HB	1:B:568:MET:HE3	1.78	0.65
1:D:255:ARG:HH11	1:D:261:PHE:H	1.44	0.65
1:D:427:PHE:HD2	1:D:431:GLU:HG2	1.62	0.65
1:D:614:LYS:HE2	1:D:614:LYS:N	2.12	0.65
1:D:718:LEU:HD12	1:D:718:LEU:N	2.11	0.65
1:D:586:TRP:HA	1:D:586:TRP:CE3	2.32	0.65
1:D:702:ILE:H	1:D:702:ILE:HD12	1.61	0.65
1:D:427:PHE:CD2	1:D:431:GLU:HG2	2.31	0.65
1:D:633:ASP:OD1	1:D:636:ARG:CB	2.45	0.65
1:A:552:ALA:HA	1:A:720:THR:HG22	1.79	0.65
1:D:318:PHE:O	1:D:321:PHE:CE1	2.50	0.65
1:D:618:GLU:O	1:D:619:LEU:HD23	1.96	0.65
1:A:412:TYR:HE2	1:A:461:THR:HG21	1.58	0.65
1:C:213:ARG:HB3	1:C:214:PRO:CD	2.27	0.65
1:C:249:HIS:N	1:C:568:MET:HE3	2.11	0.65
1:D:247:GLU:OE1	1:D:525:HIS:ND1	2.30	0.65
1:D:393:TRP:HB2	1:D:399:ILE:HD11	1.79	0.64
1:D:629:LEU:HA	1:D:707:ARG:NH2	2.12	0.64
1:D:654:ALA:HB3	1:D:721:ILE:CG1	2.27	0.64
1:B:326:HIS:HE1	1:B:400:ASP:OD2	1.79	0.64
1:C:253:TRP:O	1:C:586:TRP:CZ3	2.49	0.64
1:C:248:VAL:HA	1:C:568:MET:CE	2.26	0.64
1:C:289:ILE:HD12	1:C:289:ILE:C	2.17	0.64
1:D:255:ARG:HE	1:D:261:PHE:C	2.00	0.64
1:D:573:ALA:HB2	1:D:599:VAL:CG2	2.26	0.64
1:D:682:ASP:OD2	1:D:691:ALA:HB3	1.96	0.64
1:A:533:LYS:HB3	1:A:537:ASP:HB2	1.77	0.64
1:A:630:VAL:HG22	1:A:640:ILE:CB	2.26	0.64
1:B:656:ASN:OD1	1:B:658:THR:HG22	1.97	0.64
1:D:247:GLU:O	1:D:568:MET:N	2.30	0.64
1:D:356:LEU:HD11	1:D:357:TYR:HD2	1.62	0.64
1:D:616:MET:SD	1:D:651:ILE:CD1	2.85	0.64
1:A:631:VAL:HG11	1:D:414:ASP:OD2	1.98	0.64
1:B:455:THR:HG22	1:B:478:TRP:CE3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLY:O	1:A:315:ARG:NH1	2.30	0.64
1:C:160:ASP:OD1	1:C:163:ARG:NH2	2.31	0.64
1:C:624:TYR:CE1	1:C:644:ARG:HD3	2.32	0.64
1:D:339:GLY:O	1:D:374:ILE:HD11	1.97	0.64
1:D:639:LEU:HD12	1:D:639:LEU:O	1.97	0.64
1:D:645:ASP:OD1	1:D:649:ASN:HB2	1.96	0.64
1:A:231:GLU:OE1	1:A:231:GLU:N	2.31	0.64
1:C:412:TYR:OH	1:C:461:THR:HG21	1.98	0.64
1:C:640:ILE:HD13	1:C:654:ALA:CB	2.28	0.64
1:A:685:HIS:ND1	2:H:3:GLC:H62	2.12	0.64
1:A:492:TYR:CD2	1:A:507:LEU:HD21	2.32	0.64
1:D:586:TRP:HA	1:D:586:TRP:HE3	1.63	0.64
1:D:595:TRP:C	1:D:597:HIS:H	2.00	0.64
1:B:571:GLU:O	1:B:600:GLN:HA	1.98	0.63
1:D:337:VAL:O	1:D:337:VAL:HG12	1.96	0.63
1:D:679:LEU:HD23	1:D:680:ASN:N	2.12	0.63
1:A:467:SER:HA	1:A:477:PHE:O	1.98	0.63
1:C:514:ASN:HD21	1:C:561:PRO:HB2	1.62	0.63
1:C:605:ASP:O	1:C:609:THR:HG22	1.98	0.63
1:D:245:ILE:HG13	1:D:564:LYS:O	1.98	0.63
1:D:253:TRP:CH2	1:D:272:LEU:HA	2.33	0.63
1:B:638:VAL:C	1:B:639:LEU:HD12	2.19	0.63
1:C:120:ARG:HB3	1:C:123:GLU:HG3	1.79	0.63
1:C:394:ILE:HG23	1:C:399:ILE:O	1.97	0.63
1:D:244:SER:H	1:D:282:THR:HG22	1.63	0.63
1:D:640:ILE:HD11	1:D:654:ALA:HA	0.78	0.63
1:D:288:PRO:HG3	1:D:300:TYR:CD1	2.33	0.63
1:D:361:ASP:N	1:D:362:PRO:HD3	2.14	0.63
1:D:529:VAL:N	1:D:532:LYS:HG2	2.14	0.63
1:D:632:ASP:OD1	1:D:632:ASP:N	2.30	0.63
1:D:682:ASP:HB3	1:D:719:ALA:CB	2.29	0.63
1:A:259:ASN:HB3	1:A:261:PHE:CD1	2.33	0.63
1:A:640:ILE:HD12	1:A:653:VAL:O	1.98	0.63
1:C:485:TRP:CE2	1:C:489:THR:HG21	2.32	0.63
1:D:301:GLN:CG	1:D:302:PRO:HD2	2.26	0.63
1:D:523:LEU:CD1	1:D:557:MET:HE1	2.27	0.63
1:C:138:THR:HG21	1:C:220:ILE:HD11	1.80	0.63
1:C:255:ARG:NH2	1:C:262:TRP:HE1	1.97	0.63
1:A:636:ARG:CG	1:A:662:ARG:NH2	2.59	0.63
1:B:457:ALA:HB2	1:B:477:PHE:CE1	2.33	0.63
1:A:528:VAL:CG2	1:A:535:ILE:HD13	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LYS:HD3	1:A:696:THR:HG21	1.78	0.63
1:C:160:ASP:CB	1:C:163:ARG:CZ	2.77	0.63
1:C:542:ASP:CG	1:C:545:GLN:HG3	2.17	0.63
1:D:248:VAL:N	1:D:285:GLU:O	2.29	0.63
1:D:295:ASP:HB3	1:D:311:ARG:HH22	1.64	0.63
1:D:389:ASN:CG	1:D:393:TRP:HE1	1.98	0.63
1:D:573:ALA:H	1:D:599:VAL:HG11	1.64	0.63
1:D:265:TYR:OH	1:D:317:ASP:O	2.16	0.62
1:D:341:PHE:HD1	1:D:375:TYR:CE1	2.17	0.62
1:A:658:THR:HG23	1:A:660:VAL:H	1.65	0.62
1:B:153:VAL:HG23	1:B:159:TRP:HA	1.81	0.62
1:C:542:ASP:OD1	1:C:545:GLN:CG	2.43	0.62
1:D:248:VAL:HA	1:D:568:MET:CG	2.29	0.62
1:B:233:ARG:HD2	1:B:326:HIS:ND1	2.15	0.62
1:C:326:HIS:HE1	1:C:398:GLY:O	1.82	0.62
1:C:681:THR:HB	1:C:720:THR:H	1.64	0.62
1:D:573:ALA:CA	1:D:599:VAL:HG21	2.29	0.62
1:A:414:ASP:HB2	1:A:415:TYR:CD1	2.35	0.62
1:D:302:PRO:HB3	1:D:342:PRO:HA	1.81	0.62
1:D:624:TYR:HE1	1:D:644:ARG:NH1	1.94	0.62
1:D:393:TRP:CB	1:D:399:ILE:HD11	2.28	0.62
1:D:558:TRP:HA	1:D:564:LYS:HE3	1.80	0.62
1:C:512:LEU:HD12	1:C:512:LEU:N	2.15	0.62
1:D:528:VAL:HA	1:D:533:LYS:O	2.00	0.62
1:D:589:LEU:HD13	1:D:597:HIS:HA	1.81	0.62
1:A:404:VAL:HG23	1:A:404:VAL:O	1.99	0.62
1:A:522:PRO:O	1:A:565:LEU:O	2.18	0.62
1:B:536:LEU:HD22	1:B:573:ALA:HB1	1.80	0.62
1:D:288:PRO:HD3	1:D:300:TYR:CZ	2.34	0.62
1:A:255:ARG:NH1	1:A:582:ALA:CA	2.63	0.62
1:A:548:ALA:HA	1:A:551:ARG:CZ	2.30	0.62
1:D:309:THR:CB	1:D:318:PHE:CE2	2.83	0.62
1:A:471:ASP:OD1	1:A:471:ASP:N	2.33	0.61
1:A:702:ILE:HD11	1:A:710:SER:OG	1.99	0.61
1:C:269:ALA:O	1:C:273:VAL:CG2	2.48	0.61
1:D:306:TYR:HE2	1:D:385:PHE:CE1	2.18	0.61
1:D:466:VAL:HB	1:D:475:LEU:CD2	2.30	0.61
1:A:629:LEU:HB2	1:A:640:ILE:CG2	2.29	0.61
1:B:126:GLY:H	1:B:128:HIS:HE1	1.47	0.61
1:B:142:VAL:HG21	1:B:190:TYR:CE2	2.34	0.61
1:B:256:HIS:CG	5:J:6:GLC:C2	2.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:652:ILE:HB	1:C:723:LEU:HB2	1.83	0.61
1:D:265:TYR:HB2	1:D:312:PHE:HB3	1.82	0.61
1:D:676:ARG:HB2	1:D:696:THR:HG23	1.82	0.61
1:B:616:MET:CE	1:B:643:ARG:HB2	2.30	0.61
1:D:376:ASN:O	1:D:378:GLY:N	2.32	0.61
1:D:432:ASN:O	1:D:436:ILE:HG23	2.00	0.61
1:C:131:THR:HB	1:C:136:THR:HG22	1.82	0.61
1:D:248:VAL:HA	1:D:568:MET:HG2	1.82	0.61
1:A:441:ASN:O	1:A:445:ILE:HG13	2.01	0.61
1:A:639:LEU:C	1:A:640:ILE:HD13	2.20	0.61
1:C:118:HIS:HB2	1:C:384:ASN:ND2	2.15	0.61
1:C:192:MET:CE	1:C:352:ASP:HA	2.31	0.61
1:D:306:TYR:HD1	1:D:392:TYR:HE2	1.45	0.61
1:D:390:ALA:O	1:D:394:ILE:HG22	2.00	0.61
1:D:606:LEU:HD13	1:D:679:LEU:HD11	1.82	0.61
1:A:675:TRP:CH2	1:A:725:ARG:HB2	2.36	0.61
1:C:683:SER:OG	1:C:685:HIS:HB2	2.01	0.61
1:A:604:ARG:HG3	1:A:604:ARG:NH1	2.10	0.61
1:D:306:TYR:CE2	1:D:385:PHE:HE1	2.18	0.61
1:A:141:SER:HA	1:A:175:TRP:O	2.01	0.61
1:A:655:SER:OG	1:A:720:THR:HB	2.01	0.61
1:D:542:ASP:CG	1:D:545:GLN:HG3	2.21	0.61
1:D:614:LYS:H	1:D:614:LYS:CE	2.13	0.61
1:A:624:TYR:CE2	1:A:644:ARG:CD	2.83	0.60
1:C:403:ARG:CZ	1:C:405:ASP:OD1	2.49	0.60
1:D:247:GLU:CG	1:D:567:PHE:HD1	2.12	0.60
1:B:485:TRP:CD2	1:B:521:LEU:HD22	2.35	0.60
1:C:619:LEU:HD21	1:C:646:LYS:HG2	1.83	0.60
1:D:520:VAL:O	1:D:522:PRO:HD3	2.01	0.60
1:D:536:LEU:HA	1:D:539:MET:CE	2.31	0.60
1:D:570:ASN:H	1:D:574:GLN:HA	1.66	0.60
1:B:394:ILE:HG23	1:B:399:ILE:O	2.02	0.60
1:B:496:ASP:OD2	1:B:498:VAL:N	2.22	0.60
1:C:273:VAL:CG2	1:C:274:PRO:HD3	2.20	0.60
1:D:265:TYR:CZ	1:D:318:PHE:HD1	2.19	0.60
1:D:306:TYR:CE1	1:D:392:TYR:HD2	2.18	0.60
1:D:413:ARG:O	1:D:430:ARG:HD3	2.00	0.60
1:D:587:HIS:C	1:D:588:LEU:HD22	2.22	0.60
1:A:471:ASP:HB2	1:A:472:MET:HE3	1.82	0.60
1:B:164:HIS:N	1:B:165:PRO:HD3	2.16	0.60
1:D:255:ARG:NE	1:D:260:ASN:HA	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LYS:O	1:A:725:ARG:HG2	2.01	0.60
1:B:210:ALA:O	1:B:310:ARG:NH1	2.33	0.60
1:D:231:GLU:HA	1:D:234:LYS:HE2	1.83	0.60
1:A:293:PRO:HD3	1:A:303:THR:CG2	2.31	0.60
1:B:481:TRP:CZ3	1:B:524:SER:HB3	2.37	0.60
1:D:243:ILE:HD12	1:D:243:ILE:N	2.16	0.60
1:D:246:TYR:CZ	1:D:571:GLU:OE2	2.54	0.60
1:D:249:HIS:N	1:D:568:MET:SD	2.68	0.60
1:A:674:LYS:CD	1:A:696:THR:CG2	2.71	0.60
1:B:314:THR:HG22	1:B:317:ASP:OD2	2.02	0.60
1:C:212:MET:HE3	1:C:303:THR:HG21	1.83	0.60
1:C:609:THR:HG21	1:C:679:LEU:HD12	1.83	0.60
1:A:693:ASN:ND2	1:A:713:LEU:CD2	2.64	0.60
1:D:252:SER:O	1:D:584:LEU:HD22	2.02	0.60
1:D:262:TRP:CE3	1:D:312:PHE:HE1	2.19	0.60
1:D:288:PRO:HG2	1:D:299:GLY:C	2.22	0.60
1:D:482:ASN:HB2	1:D:519:PHE:CD1	2.37	0.60
1:A:255:ARG:HH12	1:A:581:ASP:C	2.03	0.60
1:D:548:ALA:CB	1:D:718:LEU:HB2	2.32	0.60
1:C:539:MET:O	1:C:546:LYS:HD2	2.01	0.60
1:D:343:THR:HG23	1:D:370:TRP:CH2	1.93	0.60
1:D:598:GLY:N	1:D:687:HIS:CE1	2.70	0.60
1:D:680:ASN:ND2	1:D:682:ASP:OD1	2.35	0.60
1:C:121:PRO:O	1:C:125:LEU:HD12	2.02	0.59
1:D:237:ASN:HD22	1:D:453:ALA:HA	1.66	0.59
1:B:141:SER:HA	1:B:175:TRP:O	2.02	0.59
1:D:527:GLU:H	1:D:532:LYS:HE2	1.63	0.59
1:A:259:ASN:HB3	1:A:261:PHE:HD1	1.67	0.59
1:A:275:TYR:CZ	1:A:279:MET:HE1	2.37	0.59
1:A:552:ALA:O	1:A:720:THR:HG21	2.01	0.59
1:C:248:VAL:HG23	1:C:568:MET:CE	2.32	0.59
1:D:265:TYR:HB2	1:D:312:PHE:CG	2.38	0.59
1:A:682:ASP:OD2	1:A:717:PRO:HD2	2.02	0.59
1:D:276:ALA:O	1:D:279:MET:O	2.20	0.59
1:D:348:LEU:HD11	1:D:357:TYR:CD1	2.38	0.59
1:A:625:GLY:O	1:A:643:ARG:HA	2.03	0.59
1:B:358:GLU:OE1	1:B:358:GLU:N	2.35	0.59
1:C:229:GLN:O	1:C:234:LYS:HE2	2.02	0.59
1:D:255:ARG:CZ	1:D:256:HIS:O	2.50	0.59
1:A:636:ARG:HG2	1:A:662:ARG:NH2	2.18	0.59
1:B:494:LYS:HG2	1:B:538:ARG:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:PHE:CD2	1:C:342:PRO:HD2	2.38	0.59
1:D:275:TYR:O	1:D:279:MET:CG	2.50	0.59
1:D:450:VAL:HG12	1:D:450:VAL:O	2.02	0.59
1:D:482:ASN:HA	1:D:519:PHE:HE1	1.66	0.59
1:D:594:ASN:HD21	1:D:687:HIS:HB3	1.66	0.59
1:A:674:LYS:O	1:A:726:GLU:N	2.35	0.59
1:A:707:ARG:NH1	1:D:415:TYR:HE2	2.01	0.59
1:D:660:VAL:HG11	1:D:662:ARG:NH1	2.17	0.59
1:A:716:PRO:HD2	1:A:721:ILE:CD1	2.15	0.59
1:B:187:LEU:N	1:B:187:LEU:HD23	2.18	0.59
1:D:271:GLN:O	1:D:274:PRO:HG2	2.02	0.59
1:D:630:VAL:HG23	1:D:630:VAL:O	2.03	0.59
1:C:413:ARG:HH12	1:C:417:ARG:NH1	2.01	0.59
1:D:319:ARG:HH11	1:D:322:ILE:HG13	1.67	0.59
1:D:359:HIS:NE2	1:D:376:ASN:HB2	2.17	0.59
1:C:418:LYS:H	1:C:418:LYS:CD	2.16	0.59
1:D:247:GLU:CB	1:D:567:PHE:HA	2.27	0.59
1:D:306:TYR:CD1	1:D:392:TYR:CD2	2.91	0.59
1:B:571:GLU:OE1	1:B:571:GLU:N	2.33	0.58
1:C:138:THR:CB	1:C:220:ILE:HD11	2.33	0.58
1:D:278:TRP:O	1:D:604:ARG:CG	2.49	0.58
1:D:614:LYS:H	1:D:614:LYS:HE2	1.68	0.58
1:A:231:GLU:O	1:A:235:LYS:HD3	2.03	0.58
1:B:163:ARG:HH21	1:B:163:ARG:HG2	1.68	0.58
1:B:551:ARG:HD3	1:B:686:TYR:HB3	1.83	0.58
1:C:413:ARG:NH1	1:C:417:ARG:NH1	2.51	0.58
1:D:242:PRO:HB3	1:D:617:HIS:CG	2.38	0.58
1:B:611:ARG:O	1:B:612:HIS:CB	2.49	0.58
1:C:565:LEU:HD23	1:C:565:LEU:C	2.24	0.58
1:D:287:LEU:HD11	1:D:299:GLY:H	1.66	0.58
1:D:457:ALA:HB2	1:D:477:PHE:CE1	2.38	0.58
1:A:528:VAL:HG22	1:A:535:ILE:HD13	1.85	0.58
1:C:315:ARG:HG3	1:C:397:PHE:HZ	1.68	0.58
1:D:256:HIS:HB2	1:D:263:LEU:CG	2.33	0.58
5:J:5:GLC:H3	5:J:6:GLC:HO2	1.47	0.58
1:A:166:MET:HE2	1:A:175:TRP:CB	2.33	0.58
1:A:215:GLU:OE1	1:A:215:GLU:HA	2.02	0.58
1:A:681:THR:HG22	1:A:720:THR:C	2.18	0.58
1:D:660:VAL:HG11	1:D:662:ARG:HH12	1.68	0.58
1:A:273:VAL:HG23	1:A:274:PRO:CD	2.34	0.58
1:A:681:THR:CG2	1:A:720:THR:C	2.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LEU:HD23	1:B:373:LEU:H	1.67	0.58
1:C:514:ASN:ND2	1:C:561:PRO:HB2	2.17	0.58
1:D:610:TYR:CE1	1:D:617:HIS:HB3	2.39	0.58
1:B:712:SER:O	1:B:713:LEU:HD23	2.04	0.58
1:C:457:ALA:HB2	1:C:477:PHE:CE2	2.39	0.58
1:D:256:HIS:CD2	1:D:263:LEU:HD21	2.38	0.58
1:D:393:TRP:HB3	1:D:399:ILE:CG1	2.32	0.58
1:D:418:LYS:O	1:D:419:GLU:O	2.21	0.58
1:B:273:VAL:HG23	1:B:274:PRO:CD	2.34	0.58
1:C:184:ASN:HA	1:C:220:ILE:O	2.04	0.58
1:C:254:ARG:HG2	1:C:586:TRP:CZ3	2.38	0.58
1:C:680:ASN:OD1	1:C:721:ILE:HG22	2.04	0.58
1:D:263:LEU:O	1:D:267:GLU:HG3	2.03	0.58
1:D:528:VAL:H	1:D:532:LYS:HE2	1.68	0.58
1:A:423:ILE:O	1:A:423:ILE:HG23	2.04	0.58
1:A:541:GLY:CA	1:A:545:GLN:HB2	2.12	0.58
1:B:150:VAL:CG1	1:B:166:MET:CE	2.82	0.58
1:D:295:ASP:HB3	1:D:311:ARG:NH2	2.19	0.58
1:D:680:ASN:OD1	1:D:682:ASP:OD1	2.22	0.58
1:B:721:ILE:O	1:B:722:TRP:HD1	1.86	0.58
1:C:676:ARG:HH22	1:C:726:GLU:HB3	1.69	0.58
1:D:380:ARG:O	1:D:384:ASN:OD1	2.21	0.58
1:D:470:GLN:OE1	1:D:470:GLN:N	2.23	0.58
1:D:559:ALA:CB	1:D:653:VAL:HG11	2.33	0.58
1:C:558:TRP:HA	1:C:564:LYS:CE	2.34	0.57
1:D:457:ALA:HB2	1:D:477:PHE:CZ	2.39	0.57
1:D:526:ASP:C	1:D:532:LYS:CE	2.72	0.57
1:A:485:TRP:CE2	1:A:489:THR:HG21	2.39	0.57
1:A:681:THR:HG21	1:A:720:THR:CA	2.34	0.57
1:C:702:ILE:O	1:C:710:SER:OG	2.10	0.57
1:D:246:TYR:HB2	1:D:281:PHE:CD2	2.39	0.57
1:D:309:THR:HG22	1:D:318:PHE:HE2	1.62	0.57
1:D:653:VAL:HG13	1:D:722:TRP:CD1	2.40	0.57
1:B:140:PHE:O	1:B:176:GLU:HA	2.04	0.57
1:B:258:ASP:OD1	5:J:5:GLC:O3	2.16	0.57
1:D:287:LEU:CD1	1:D:299:GLY:H	2.17	0.57
1:D:618:GLU:OE2	1:D:646:LYS:HE3	2.04	0.57
1:B:290:ASN:OD1	1:B:302:PRO:HG3	2.05	0.57
1:C:669:ILE:HG13	1:C:670:ASN:N	2.19	0.57
1:A:177:LEU:HD23	1:A:178:PHE:N	2.19	0.57
1:A:533:LYS:HB3	1:A:537:ASP:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ALA:HB2	1:A:719:ALA:HA	1.87	0.57
1:A:624:TYR:CE2	1:A:644:ARG:HD3	2.40	0.57
1:A:666:ARG:CD	1:A:710:SER:OG	2.50	0.57
1:C:138:THR:HG21	1:C:220:ILE:CD1	2.33	0.57
1:C:457:ALA:HB2	1:C:477:PHE:CD2	2.40	0.57
1:D:576:ARG:O	1:D:577:GLU:HB2	2.04	0.57
1:A:119:LEU:O	1:A:391:LEU:HD12	2.05	0.57
1:B:633:ASP:OD2	1:B:665:TYR:OH	2.19	0.57
1:D:375:TYR:CE2	1:D:386:LEU:HD11	2.39	0.57
1:D:588:LEU:O	1:D:589:LEU:HB3	2.03	0.57
1:D:629:LEU:HB3	1:D:640:ILE:CG2	2.35	0.57
1:D:692:GLY:HA2	1:D:714:THR:HB	1.87	0.57
1:A:568:MET:HG3	1:A:584:LEU:HD11	1.86	0.57
1:C:192:MET:HE3	1:C:194:ASP:HA	1.86	0.57
1:C:335:ASP:OD1	1:C:403:ARG:NH2	2.38	0.57
1:C:361:ASP:N	1:C:361:ASP:OD1	2.37	0.57
1:D:224:PRO:N	1:D:315:ARG:HD3	2.19	0.57
1:D:319:ARG:NH1	1:D:322:ILE:HG13	2.20	0.57
1:D:381:GLU:CA	1:D:384:ASN:OD1	2.52	0.57
1:D:394:ILE:CA	1:D:399:ILE:CD1	2.83	0.57
1:D:702:ILE:H	1:D:702:ILE:CD1	2.15	0.57
1:A:247:GLU:HG3	1:A:285:GLU:HG2	1.87	0.57
1:A:630:VAL:HG22	1:A:640:ILE:N	2.20	0.57
1:B:589:LEU:HD22	1:B:597:HIS:CD2	2.40	0.57
1:D:335:ASP:OD2	1:D:403:ARG:NH2	2.38	0.57
1:D:536:LEU:CB	1:D:574:GLN:CG	2.82	0.57
1:D:718:LEU:CD1	1:D:718:LEU:N	2.67	0.57
1:A:138:THR:CB	1:A:220:ILE:HD11	2.35	0.57
1:A:552:ALA:HA	1:A:720:THR:CG2	2.34	0.57
1:D:312:PHE:HB2	1:D:318:PHE:CZ	2.39	0.57
1:D:394:ILE:CA	1:D:399:ILE:HD12	2.34	0.57
1:D:229:GLN:O	1:D:231:GLU:N	2.38	0.56
1:D:264:SER:O	1:D:268:LEU:HD13	2.05	0.56
1:D:277:LYS:HG3	1:D:328:ALA:O	2.05	0.56
1:C:596:HIS:NE2	6:L:2:GLC:H62	2.19	0.56
1:D:247:GLU:OE1	1:D:524:SER:HB3	2.05	0.56
1:D:496:ASP:HB3	1:D:498:VAL:CG1	2.34	0.56
1:D:659:PRO:HA	1:D:718:LEU:HD13	1.86	0.56
1:A:681:THR:HG23	1:A:720:THR:N	2.17	0.56
1:B:142:VAL:CG2	1:B:190:TYR:CZ	2.86	0.56
1:B:150:VAL:CG1	1:B:166:MET:HE2	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:THR:HB	1:D:611:ARG:NH1	2.20	0.56
1:D:629:LEU:HD13	1:D:642:VAL:HG13	1.86	0.56
1:A:319:ARG:HH11	1:A:319:ARG:CG	2.17	0.56
1:C:628:TRP:CD2	1:C:631:VAL:HG13	2.40	0.56
1:D:255:ARG:HH12	1:D:259:ASN:CB	2.17	0.56
1:D:528:VAL:HG13	1:D:532:LYS:NZ	2.19	0.56
1:D:291:GLU:CG	1:D:304:GLY:HA3	2.36	0.56
1:D:528:VAL:N	1:D:532:LYS:CE	2.67	0.56
1:D:542:ASP:OD1	1:D:544:TRP:HB3	2.05	0.56
1:A:275:TYR:CZ	1:A:279:MET:CE	2.88	0.56
1:B:597:HIS:O	1:B:601:ARG:HB2	2.05	0.56
1:D:293:PRO:HG3	1:D:303:THR:HG21	1.88	0.56
1:B:507:LEU:HD12	1:B:507:LEU:N	2.20	0.56
1:D:246:TYR:HD1	1:D:281:PHE:CE2	2.23	0.56
1:D:548:ALA:HB1	1:D:718:LEU:O	2.06	0.56
1:A:168:LEU:HD13	1:A:175:TRP:CZ2	2.41	0.56
1:A:193:ILE:C	1:A:193:ILE:HD12	2.25	0.56
1:A:415:TYR:CD1	1:A:415:TYR:N	2.72	0.56
1:A:624:TYR:CE2	1:A:644:ARG:HD2	2.41	0.56
1:C:605:ASP:O	1:C:609:THR:CG2	2.53	0.56
1:D:256:HIS:CB	1:D:263:LEU:HD11	2.36	0.56
1:D:266:ARG:O	1:D:269:ALA:HB3	2.05	0.56
1:A:255:ARG:NH1	1:A:582:ALA:HA	2.21	0.56
1:B:315:ARG:HD2	1:B:316:ASP:OD1	2.06	0.56
1:C:233:ARG:HD3	1:C:326:HIS:CD2	2.40	0.56
1:D:287:LEU:HG	1:D:288:PRO:N	2.21	0.56
1:D:319:ARG:O	1:D:319:ARG:NE	2.34	0.56
1:A:132:MET:O	1:A:135:VAL:CG1	2.54	0.56
1:D:230:THR:O	1:D:232:GLU:N	2.39	0.56
1:D:356:LEU:HA	1:D:379:ARG:HH12	1.71	0.56
1:D:629:LEU:HD13	1:D:642:VAL:CG1	2.36	0.56
1:A:326:HIS:HE1	1:A:400:ASP:OD1	1.88	0.55
1:B:147:ALA:O	1:B:175:TRP:HZ2	1.89	0.55
1:C:551:ARG:HD3	1:C:686:TYR:HB3	1.89	0.55
1:C:673:GLY:H	1:C:699:SER:HG	1.43	0.55
1:D:528:VAL:N	1:D:532:LYS:HG3	2.21	0.55
1:D:283:HIS:HA	1:D:331:ASN:O	2.05	0.55
1:C:332:VAL:HG12	1:C:399:ILE:HD12	1.88	0.55
1:D:281:PHE:HD1	1:D:607:ASN:HD22	1.55	0.55
1:D:281:PHE:CD1	1:D:607:ASN:ND2	2.74	0.55
1:D:356:LEU:HD11	1:D:357:TYR:CD2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:PHE:CD1	1:D:385:PHE:C	2.79	0.55
1:D:505:ASP:HA	1:D:508:THR:OG1	2.06	0.55
1:D:539:MET:CG	1:D:549:ASN:CB	2.79	0.55
1:A:192:MET:CE	1:A:194:ASP:HA	2.36	0.55
1:A:619:LEU:HD13	1:A:624:TYR:HB3	1.89	0.55
1:D:482:ASN:HA	1:D:519:PHE:CE1	2.40	0.55
1:A:422:TRP:N	1:A:422:TRP:CD1	2.73	0.55
1:B:379:ARG:O	1:B:382:VAL:HG23	2.06	0.55
1:B:392:TYR:O	1:B:396:ARG:HB2	2.06	0.55
1:B:668:GLY:HA3	1:B:707:ARG:HG3	1.89	0.55
1:C:153:VAL:CG1	1:C:159:TRP:HE3	2.19	0.55
1:D:565:LEU:HD23	1:D:565:LEU:C	2.26	0.55
1:A:147:ALA:HB3	1:A:175:TRP:CZ2	2.42	0.55
1:A:255:ARG:HH12	1:A:582:ALA:CA	2.19	0.55
1:A:466:VAL:HG22	1:A:480:LYS:HD3	1.88	0.55
1:D:245:ILE:HB	1:D:565:LEU:HA	1.89	0.55
1:D:276:ALA:HB3	1:D:330:LEU:HD11	1.88	0.55
1:D:318:PHE:O	1:D:321:PHE:CD1	2.59	0.55
1:D:443:ASN:HD22	1:D:443:ASN:H	1.55	0.55
1:D:570:ASN:HA	1:D:574:GLN:H	1.70	0.55
1:D:602:LEU:O	1:D:606:LEU:N	2.37	0.55
1:A:704:SER:HB3	1:A:710:SER:HB2	1.88	0.55
1:B:148:ARG:NH2	1:B:195:ALA:O	2.40	0.55
1:D:249:HIS:ND1	1:D:287:LEU:HD22	2.22	0.55
1:D:374:ILE:HG23	1:D:375:TYR:O	2.06	0.55
1:A:693:ASN:ND2	1:A:713:LEU:HD23	2.22	0.55
1:D:416:SER:OG	1:D:428:GLY:O	2.21	0.55
1:D:630:VAL:HG22	1:D:640:ILE:HB	1.88	0.55
1:A:152:VAL:CG2	1:A:179:ILE:HD11	2.37	0.55
1:B:441:ASN:OD1	1:B:444:ARG:NH2	2.40	0.55
1:B:681:THR:HG23	1:B:720:THR:O	2.06	0.55
1:D:648:GLY:O	1:D:650:GLU:HG2	2.07	0.55
1:A:624:TYR:CD2	1:A:644:ARG:HD2	2.42	0.55
1:D:299:GLY:O	1:D:301:GLN:N	2.40	0.55
1:B:445:ILE:O	1:B:449:GLN:HB2	2.07	0.54
1:B:485:TRP:CE3	1:B:521:LEU:HD22	2.41	0.54
1:B:485:TRP:O	1:B:489:THR:OG1	2.24	0.54
1:B:588:LEU:HD13	1:B:596:HIS:CE1	2.43	0.54
1:D:248:VAL:HA	1:D:568:MET:SD	2.48	0.54
1:D:256:HIS:HB2	1:D:263:LEU:CD1	2.36	0.54
1:D:468:ARG:NH2	1:D:517:GLU:HA	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:573:ALA:O	1:D:574:GLN:NE2	2.40	0.54
1:A:675:TRP:CZ3	1:A:725:ARG:HB2	2.43	0.54
1:B:138:THR:OG1	1:B:182:ALA:C	2.45	0.54
1:D:291:GLU:OE2	1:D:303:THR:HB	2.07	0.54
1:A:652:ILE:HD12	1:A:652:ILE:N	2.22	0.54
1:B:234:LYS:HG2	1:B:452:GLY:HA3	1.88	0.54
1:D:594:ASN:HD21	1:D:687:HIS:CG	2.25	0.54
1:A:187:LEU:CD2	1:A:219:LEU:HD21	2.37	0.54
1:C:191:GLU:HG3	1:C:201:LEU:CD1	2.37	0.54
1:C:295:ASP:N	1:C:295:ASP:OD1	2.40	0.54
1:D:247:GLU:HB3	1:D:567:PHE:CA	2.28	0.54
1:D:248:VAL:CG1	1:D:568:MET:HB3	2.34	0.54
1:D:254:ARG:N	1:D:583:SER:CB	2.71	0.54
1:D:321:PHE:O	1:D:324:ALA:HB3	2.08	0.54
1:D:394:ILE:HA	1:D:399:ILE:CD1	2.36	0.54
1:D:677:GLU:HA	1:D:723:LEU:HD22	1.88	0.54
1:B:639:LEU:HD12	1:B:639:LEU:N	2.21	0.54
1:D:302:PRO:CB	1:D:342:PRO:HA	2.38	0.54
1:D:485:TRP:O	1:D:489:THR:HG23	2.07	0.54
1:D:678:ILE:HG21	1:D:724:VAL:HG22	1.89	0.54
1:A:146:ASN:HD22	1:A:352:ASP:CG	2.08	0.54
1:A:566:LEU:HD11	1:A:570:ASN:HB2	1.89	0.54
1:C:120:ARG:HH21	1:C:395:GLU:CD	2.11	0.54
1:D:352:ASP:H	1:D:356:LEU:HD12	1.72	0.54
1:D:419:GLU:N	1:D:419:GLU:OE2	2.41	0.54
1:D:533:LYS:CB	1:D:537:ASP:OD2	2.50	0.54
1:D:559:ALA:O	1:D:643:ARG:HD3	2.08	0.54
1:D:618:GLU:C	1:D:619:LEU:HD23	2.28	0.54
1:A:417:ARG:CZ	1:A:417:ARG:CB	2.85	0.54
1:C:162:ARG:O	1:C:165:PRO:HD3	2.06	0.54
1:C:432:ASN:O	1:C:436:ILE:HG13	2.08	0.54
1:D:253:TRP:HB2	1:D:586:TRP:CE2	2.41	0.54
1:D:611:ARG:O	1:D:613:HIS:N	2.38	0.54
1:D:640:ILE:HD12	1:D:653:VAL:O	2.08	0.54
1:A:645:ASP:OD2	1:A:649:ASN:ND2	2.40	0.54
1:B:457:ALA:HB2	1:B:477:PHE:CZ	2.43	0.54
1:C:213:ARG:CB	1:C:214:PRO:CD	2.84	0.54
1:D:226:LYS:HG2	1:D:396:ARG:HB3	1.90	0.54
1:D:325:ALA:O	1:D:330:LEU:N	2.38	0.54
1:A:660:VAL:HG11	1:A:662:ARG:NH1	2.22	0.54
1:A:674:LYS:HG2	1:A:696:THR:HG23	1.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ALA:O	1:B:273:VAL:HG22	2.07	0.54
1:B:376:ASN:ND2	1:B:379:ARG:HB2	2.23	0.54
1:C:562:GLY:O	1:C:564:LYS:HD3	2.08	0.54
1:D:585:ASP:O	1:D:588:LEU:CD2	2.56	0.54
1:A:187:LEU:HD23	1:A:219:LEU:HD21	1.90	0.54
1:A:423:ILE:HD12	1:A:431:GLU:CD	2.28	0.54
1:A:520:VAL:HG22	1:A:563:LYS:HB2	1.89	0.54
1:A:683:SER:OG	2:H:2:GLC:H62	2.07	0.54
1:D:253:TRP:CZ2	1:D:272:LEU:HA	2.43	0.54
1:A:152:VAL:HG21	1:A:179:ILE:HD11	1.89	0.53
1:A:189:LYS:CE	1:A:346:PHE:HE2	2.22	0.53
1:A:678:ILE:CG2	1:A:724:VAL:CG1	2.85	0.53
1:B:485:TRP:HH2	1:B:557:MET:HB2	1.73	0.53
1:C:678:ILE:HG23	1:C:722:TRP:O	2.07	0.53
1:D:306:TYR:HD1	1:D:392:TYR:CD2	2.25	0.53
1:D:677:GLU:OE2	1:D:693:ASN:O	2.26	0.53
1:A:193:ILE:HD12	1:A:194:ASP:O	2.08	0.53
1:B:224:PRO:O	1:B:396:ARG:NH2	2.40	0.53
1:B:576:ARG:HH12	5:J:1:GLC:H62	1.72	0.53
1:C:492:TYR:CE2	1:C:507:LEU:HD11	2.43	0.53
1:D:247:GLU:N	1:D:566:LEU:O	2.41	0.53
1:D:284:LEU:O	1:D:333:ILE:HG12	2.09	0.53
1:D:482:ASN:HB2	1:D:519:PHE:HD1	1.72	0.53
1:D:602:LEU:HD12	1:D:602:LEU:C	2.28	0.53
1:B:697:VAL:HG11	1:B:713:LEU:HD21	1.91	0.53
1:D:268:LEU:HD13	1:D:268:LEU:H	1.73	0.53
1:D:286:LEU:N	1:D:286:LEU:HD23	2.24	0.53
1:D:523:LEU:HD11	1:D:557:MET:HE3	1.90	0.53
1:D:536:LEU:O	1:D:539:MET:HE2	2.09	0.53
1:A:203:SER:OG	1:A:346:PHE:HB3	2.09	0.53
1:B:285:GLU:HB2	1:B:333:ILE:HB	1.89	0.53
1:B:669:ILE:HG22	1:B:670:ASN:N	2.23	0.53
1:B:697:VAL:HG12	1:B:711:LEU:HD11	1.90	0.53
1:D:317:ASP:OD1	1:D:317:ASP:N	2.41	0.53
1:D:355:ASN:CA	1:D:358:GLU:OE2	2.45	0.53
1:A:523:LEU:HG	1:A:557:MET:HE3	1.91	0.53
1:B:401:ALA:HB1	1:B:454:VAL:O	2.08	0.53
1:B:455:THR:HG22	1:B:478:TRP:HE3	1.71	0.53
1:C:210:ALA:O	1:C:310:ARG:CD	2.57	0.53
1:D:650:GLU:OE1	1:D:670:ASN:ND2	2.33	0.53
1:A:256:HIS:NE2	1:A:267:GLU:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LYS:NZ	7:A:803:GLC:O2	2.42	0.53
1:B:279:MET:HA	1:B:604:ARG:HG3	1.91	0.53
1:D:570:ASN:C	1:D:571:GLU:HG2	2.28	0.53
1:A:192:MET:HE3	1:A:194:ASP:HA	1.90	0.53
1:A:335:ASP:OD1	1:A:403:ARG:NH2	2.41	0.53
1:C:265:TYR:CZ	1:C:312:PHE:HB2	2.44	0.53
1:C:285:GLU:OE2	1:C:403:ARG:NH2	2.42	0.53
1:C:537:ASP:CG	6:L:1:GLC:C2	2.74	0.53
1:C:619:LEU:HD21	1:C:646:LYS:CG	2.39	0.53
1:D:523:LEU:CD1	1:D:557:MET:CE	2.82	0.53
1:C:192:MET:CE	1:C:194:ASP:HA	2.39	0.53
1:C:248:VAL:CA	1:C:568:MET:HE3	2.35	0.53
1:C:497:PRO:HA	1:C:500:ARG:HG3	1.91	0.53
1:C:699:SER:HA	1:C:711:LEU:CD2	2.39	0.53
1:D:438:PHE:O	1:D:442:THR:HG23	2.08	0.53
1:D:456:MET:HE3	1:D:479:TYR:HD2	1.74	0.53
1:B:290:ASN:C	1:B:290:ASN:HD22	2.10	0.53
1:C:211:GLN:HG3	1:C:211:GLN:O	2.08	0.53
1:C:418:LYS:HE2	1:C:418:LYS:N	2.24	0.53
1:D:278:TRP:O	1:D:278:TRP:CD2	2.62	0.53
1:D:292:HIS:ND1	1:D:292:HIS:N	2.58	0.53
1:D:606:LEU:CD1	1:D:679:LEU:HD11	2.37	0.53
1:A:604:ARG:CG	1:A:604:ARG:NH1	2.69	0.52
1:B:493:MET:HE3	1:B:553:TYR:CB	2.39	0.52
1:D:254:ARG:HD2	1:D:587:HIS:HB3	1.91	0.52
1:D:275:TYR:O	1:D:279:MET:HG3	2.09	0.52
1:A:630:VAL:CG2	1:A:640:ILE:N	2.72	0.52
1:A:639:LEU:HD12	1:A:639:LEU:N	2.23	0.52
1:B:277:LYS:HD2	1:B:328:ALA:O	2.09	0.52
1:C:336:TRP:CZ2	1:C:390:ALA:HB2	2.44	0.52
1:C:348:LEU:HD21	1:C:357:TYR:CG	2.44	0.52
1:C:649:ASN:OD1	1:C:649:ASN:N	2.41	0.52
1:D:319:ARG:NH1	1:D:323:ASP:HB2	2.21	0.52
1:D:419:GLU:OE2	1:D:419:GLU:CA	2.58	0.52
1:D:455:THR:O	1:D:478:TRP:HB2	2.09	0.52
1:D:528:VAL:N	1:D:532:LYS:CG	2.73	0.52
1:D:552:ALA:O	1:D:720:THR:HG21	2.09	0.52
1:A:137:GLY:HA3	1:A:180:PRO:HA	1.91	0.52
1:A:187:LEU:HD23	1:A:219:LEU:CD2	2.39	0.52
1:A:193:ILE:HD13	1:A:197:GLY:HA2	1.92	0.52
1:A:213:ARG:CB	1:A:214:PRO:CD	2.79	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:CE	5:J:4:GLC:H2	2.39	0.52
1:A:240:ASP:OD1	1:A:240:ASP:N	2.38	0.52
1:B:587:HIS:HA	1:B:590:GLU:HG3	1.91	0.52
1:C:160:ASP:CG	1:C:163:ARG:CZ	2.78	0.52
1:D:256:HIS:HB2	1:D:263:LEU:HG	1.90	0.52
1:B:632:ASP:O	1:B:634:LYS:N	2.42	0.52
1:D:262:TRP:O	1:D:264:SER:O	2.27	0.52
1:D:438:PHE:CE1	1:D:442:THR:HG21	2.44	0.52
1:D:485:TRP:CD2	1:D:521:LEU:HD22	2.45	0.52
1:D:306:TYR:N	1:D:308:PRO:HD3	2.24	0.52
1:D:529:VAL:HG13	1:D:532:LYS:HZ2	1.72	0.52
1:A:431:GLU:HG2	1:A:433:LEU:HD12	1.92	0.52
1:A:492:TYR:OH	1:A:500:ARG:HB3	2.09	0.52
1:A:552:ALA:O	1:A:720:THR:CG2	2.58	0.52
1:B:126:GLY:H	1:B:128:HIS:CE1	2.27	0.52
1:B:438:PHE:CZ	1:B:442:THR:HG21	2.44	0.52
1:D:255:ARG:HG2	1:D:261:PHE:C	2.30	0.52
1:D:649:ASN:OD1	1:D:649:ASN:N	2.43	0.52
1:D:662:ARG:HH21	1:D:662:ARG:HG3	1.74	0.52
1:A:407:VAL:HG23	1:A:459:GLU:HG2	1.91	0.52
1:A:504:HIS:CE1	1:A:631:VAL:O	2.62	0.52
1:A:674:LYS:O	1:A:725:ARG:HA	2.09	0.52
1:B:678:ILE:HG23	1:B:724:VAL:HG12	1.91	0.52
1:B:686:TYR:O	1:B:687:HIS:HB2	2.10	0.52
1:C:724:VAL:HG22	1:C:725:ARG:N	2.25	0.52
1:D:372:THR:C	1:D:373:LEU:HD22	2.30	0.52
1:D:255:ARG:HE	1:D:261:PHE:CA	2.23	0.52
1:D:295:ASP:OD1	1:D:295:ASP:N	2.42	0.52
1:D:305:LEU:HD11	1:D:386:LEU:HD21	1.91	0.52
1:D:306:TYR:CD1	1:D:392:TYR:CE2	2.91	0.52
1:D:534:SER:N	1:D:537:ASP:OD2	2.42	0.52
1:D:602:LEU:O	1:D:606:LEU:CB	2.47	0.52
1:A:660:VAL:CB	1:A:662:ARG:HH12	2.23	0.52
1:D:224:PRO:O	1:D:225:GLU:CB	2.57	0.52
1:D:486:MET:CE	1:D:527:GLU:CG	2.87	0.52
1:D:606:LEU:HA	1:D:609:THR:OG1	2.09	0.52
1:D:624:TYR:HD1	1:D:644:ARG:HD3	1.75	0.52
1:A:423:ILE:HD13	1:A:429:GLY:HA2	1.91	0.52
1:A:552:ALA:CA	1:A:720:THR:HG22	2.38	0.52
1:A:681:THR:CG2	1:A:720:THR:CA	2.87	0.52
1:B:567:PHE:CE1	1:B:568:MET:HG2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:ARG:NH1	1:C:650:GLU:OE1	2.39	0.52
1:D:246:TYR:HB2	1:D:281:PHE:HD2	1.74	0.52
1:D:256:HIS:HB3	1:D:263:LEU:CD2	2.37	0.52
1:D:536:LEU:HB2	1:D:574:GLN:CG	2.40	0.52
1:B:721:ILE:C	1:B:722:TRP:HD1	2.14	0.51
1:D:265:TYR:HE2	1:D:317:ASP:HB2	1.74	0.51
1:A:417:ARG:CB	1:A:417:ARG:NH1	2.73	0.51
1:A:681:THR:HG23	1:A:720:THR:O	2.04	0.51
1:C:297:SER:HB2	1:C:301:GLN:HB2	1.92	0.51
1:D:253:TRP:HA	1:D:583:SER:OG	2.10	0.51
1:D:556:TRP:CH2	1:D:639:LEU:HD13	2.45	0.51
1:D:629:LEU:HB3	1:D:640:ILE:HG22	1.92	0.51
1:D:678:ILE:CG2	1:D:724:VAL:CG2	2.87	0.51
1:A:693:ASN:ND2	1:A:713:LEU:HD22	2.25	0.51
1:B:153:VAL:HG23	1:B:159:TRP:C	2.30	0.51
1:B:280:GLY:C	1:B:611:ARG:NH1	2.64	0.51
1:D:345:ASP:OD1	1:D:347:ALA:CB	2.59	0.51
1:D:376:ASN:C	1:D:378:GLY:H	2.13	0.51
1:D:652:ILE:O	1:D:722:TRP:HA	2.11	0.51
1:B:493:MET:HE3	1:B:553:TYR:HB2	1.93	0.51
1:B:594:ASN:OD1	1:B:597:HIS:ND1	2.43	0.51
1:B:668:GLY:C	1:B:669:ILE:HD13	2.30	0.51
1:C:584:LEU:HD12	1:C:586:TRP:CH2	2.45	0.51
1:D:250:LEU:HD13	1:D:268:LEU:HD23	1.93	0.51
1:D:253:TRP:CE2	1:D:272:LEU:HD12	2.45	0.51
1:D:683:SER:HB3	1:D:686:TYR:HD1	1.74	0.51
1:D:437:GLU:HA	1:D:440:ARG:HG3	1.93	0.51
1:D:597:HIS:N	1:D:597:HIS:HD2	2.06	0.51
1:B:227:VAL:HG22	1:B:319:ARG:NH2	2.25	0.51
1:B:229:GLN:HA	1:B:233:ARG:NH2	2.26	0.51
1:B:234:LYS:NZ	1:B:451:SER:O	2.35	0.51
1:B:430:ARG:N	1:B:431:GLU:OE1	2.44	0.51
1:C:558:TRP:HA	1:C:564:LYS:HE3	1.92	0.51
1:D:307:ALA:CA	1:D:392:TYR:OH	2.58	0.51
1:D:613:HIS:ND1	1:D:614:LYS:NZ	2.47	0.51
1:A:145:PRO:HD2	1:A:356:LEU:CD2	2.41	0.51
1:B:120:ARG:HA	1:B:122:TYR:CE1	2.45	0.51
1:B:253:TRP:CG	1:B:568:MET:HE1	2.45	0.51
1:C:192:MET:HE1	1:C:352:ASP:HA	1.93	0.51
1:B:559:ALA:HB1	1:B:653:VAL:HG21	1.91	0.51
1:D:265:TYR:CZ	1:D:318:PHE:CD1	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:TYR:HB2	1:A:281:PHE:CG	2.46	0.51
1:A:560:PHE:O	1:A:564:LYS:NZ	2.43	0.51
1:C:148:ARG:O	1:C:149:ARG:HG3	2.11	0.51
1:C:297:SER:C	1:C:299:GLY:H	2.15	0.51
1:C:642:VAL:HG12	1:C:652:ILE:HG12	1.93	0.51
1:D:280:GLY:C	1:D:611:ARG:NH2	2.64	0.51
1:A:350:GLU:HA	1:A:354:THR:O	2.11	0.50
1:A:588:LEU:HD12	1:A:596:HIS:NE2	2.25	0.50
1:B:609:THR:HG23	1:D:420:GLY:CA	2.40	0.50
1:C:257:THR:HG23	1:C:258:ASP:H	1.76	0.50
1:C:379:ARG:O	1:C:382:VAL:CG2	2.59	0.50
1:D:466:VAL:HA	1:D:475:LEU:CB	2.41	0.50
1:D:603:VAL:O	1:D:607:ASN:OD1	2.28	0.50
1:D:697:VAL:HG12	1:D:698:HIS:H	1.76	0.50
1:A:152:VAL:CG2	1:A:179:ILE:CD1	2.89	0.50
1:A:253:TRP:CZ3	1:A:254:ARG:HG3	2.46	0.50
1:A:254:ARG:HG2	1:A:586:TRP:NE1	2.26	0.50
1:A:566:LEU:HD11	1:A:570:ASN:CB	2.41	0.50
1:A:640:ILE:HD11	1:A:654:ALA:HB1	1.92	0.50
1:B:273:VAL:HG22	1:B:274:PRO:HD3	1.93	0.50
1:C:142:VAL:HG13	1:C:142:VAL:O	2.10	0.50
1:C:666:ARG:HA	1:C:711:LEU:O	2.11	0.50
1:D:281:PHE:HE1	1:D:607:ASN:HD21	1.58	0.50
1:D:699:SER:HA	1:D:711:LEU:CD1	2.42	0.50
1:B:247:GLU:O	1:B:567:PHE:CD1	2.65	0.50
1:B:255:ARG:NH2	1:B:581:ASP:HA	2.27	0.50
1:B:356:LEU:HD23	1:B:356:LEU:H	1.77	0.50
1:C:249:HIS:N	1:C:568:MET:CE	2.69	0.50
1:C:255:ARG:NH2	1:C:262:TRP:NE1	2.59	0.50
1:C:459:GLU:OE2	1:C:463:PHE:HB2	2.11	0.50
1:D:359:HIS:CG	1:D:376:ASN:CB	2.76	0.50
1:D:535:ILE:CD1	1:D:570:ASN:OD1	2.49	0.50
1:D:536:LEU:HB3	1:D:574:GLN:CG	2.39	0.50
1:D:597:HIS:CD2	1:D:597:HIS:H	2.27	0.50
1:A:121:PRO:HB2	1:A:206:TYR:OH	2.12	0.50
1:A:341:PHE:CZ	1:A:358:GLU:HB3	2.46	0.50
1:C:683:SER:HG	1:C:685:HIS:HB2	1.77	0.50
1:C:693:ASN:OD1	1:C:714:THR:HG22	2.11	0.50
1:D:232:GLU:O	1:D:235:LYS:HB2	2.11	0.50
1:D:482:ASN:CB	1:D:519:PHE:CD1	2.95	0.50
1:B:242:PRO:HB3	1:B:617:HIS:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:633:ASP:OD2	1:C:636:ARG:HD2	2.11	0.50
1:D:230:THR:HB	1:D:233:ARG:HB2	1.94	0.50
1:D:279:MET:CE	1:D:279:MET:HA	2.41	0.50
1:D:406:ALA:O	1:D:409:SER:N	2.42	0.50
1:D:580:HIS:HD1	1:D:580:HIS:H	1.58	0.50
1:D:693:ASN:N	1:D:693:ASN:OD1	2.45	0.50
1:A:350:GLU:N	1:A:358:GLU:OE1	2.40	0.50
1:C:291:GLU:OE1	1:C:291:GLU:CA	2.57	0.50
1:D:324:ALA:O	1:D:328:ALA:CB	2.60	0.50
1:D:566:LEU:HD23	1:D:567:PHE:N	2.27	0.50
1:D:624:TYR:CE1	1:D:644:ARG:NH1	2.76	0.50
2:F:3:GLC:H61	2:F:4:GLC:H5	1.93	0.50
1:A:215:GLU:O	1:A:216:THR:CG2	2.60	0.50
1:A:275:TYR:CE1	1:A:279:MET:HE1	2.47	0.50
1:B:606:LEU:HD23	1:B:679:LEU:CD1	2.42	0.50
1:C:163:ARG:CZ	1:C:163:ARG:N	2.58	0.50
1:D:257:THR:O	1:D:258:ASP:HB2	2.12	0.50
1:D:265:TYR:HB2	1:D:312:PHE:CB	2.42	0.50
1:D:616:MET:SD	1:D:616:MET:N	2.84	0.50
1:A:497:PRO:CB	1:A:659:PRO:HD3	2.42	0.50
1:A:513:TYR:O	1:A:516:THR:OG1	2.24	0.50
1:A:528:VAL:O	1:A:528:VAL:CG1	2.59	0.50
1:A:559:ALA:HB2	1:A:722:TRP:CZ2	2.47	0.50
1:A:645:ASP:OD1	1:A:649:ASN:ND2	2.37	0.50
1:B:177:LEU:HD23	1:B:179:ILE:HG13	1.94	0.50
1:B:685:HIS:HE1	1:D:424:PRO:C	2.13	0.50
1:C:667:PHE:HA	1:C:705:HIS:CE1	2.47	0.50
1:D:372:THR:O	1:D:372:THR:OG1	2.30	0.50
1:D:480:LYS:CD	1:D:517:GLU:OE2	2.60	0.50
1:D:535:ILE:HA	1:D:538:ARG:HG3	1.94	0.50
1:B:341:PHE:CE2	1:B:358:GLU:HB3	2.46	0.50
1:C:283:HIS:CD2	1:C:331:ASN:HB2	2.46	0.50
1:D:700:ASP:HB3	1:D:702:ILE:CD1	2.42	0.50
1:A:193:ILE:HG13	1:A:193:ILE:O	2.10	0.49
1:C:491:ASP:HA	1:C:494:LYS:HE2	1.92	0.49
1:C:658:THR:CG2	1:C:662:ARG:NH1	2.73	0.49
1:D:517:GLU:HB2	1:D:519:PHE:CE2	2.47	0.49
1:D:595:TRP:C	1:D:597:HIS:N	2.66	0.49
1:D:613:HIS:O	1:D:617:HIS:CD2	2.65	0.49
1:B:153:VAL:HG13	1:B:153:VAL:O	2.12	0.49
1:C:560:PHE:O	1:C:564:LYS:NZ	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:GLN:CG	1:D:302:PRO:CD	2.89	0.49
1:D:614:LYS:CD	1:D:614:LYS:N	2.71	0.49
1:A:177:LEU:HD21	1:A:179:ILE:CG1	2.39	0.49
1:B:441:ASN:O	1:B:445:ILE:CD1	2.59	0.49
1:C:166:MET:HE2	1:C:190:TYR:HD1	1.77	0.49
1:D:243:ILE:HA	1:D:282:THR:HG21	1.95	0.49
1:D:307:ALA:N	1:D:392:TYR:OH	2.46	0.49
1:D:571:GLU:C	1:D:599:VAL:CG1	2.81	0.49
1:D:571:GLU:C	1:D:599:VAL:HG12	2.32	0.49
1:D:629:LEU:HD23	1:D:667:PHE:CD1	2.47	0.49
1:D:692:GLY:HA2	1:D:714:THR:CB	2.42	0.49
1:A:675:TRP:CD2	1:A:725:ARG:HG3	2.47	0.49
1:B:495:LEU:HD11	1:B:503:HIS:CD2	2.47	0.49
1:B:511:ILE:HD13	1:B:626:PHE:CZ	2.48	0.49
1:C:640:ILE:HD13	1:C:654:ALA:HA	1.94	0.49
1:D:255:ARG:CZ	1:D:261:PHE:H	2.25	0.49
1:D:417:ARG:HG3	1:D:422:TRP:CD1	2.47	0.49
1:A:132:MET:O	1:A:135:VAL:HG13	2.12	0.49
1:A:244:SER:H	1:A:282:THR:HB	1.75	0.49
1:C:138:THR:OG1	1:C:220:ILE:HD11	2.13	0.49
1:D:281:PHE:HD1	1:D:607:ASN:ND2	2.11	0.49
1:D:358:GLU:O	1:D:376:ASN:ND2	2.45	0.49
1:A:344:ASP:N	1:A:344:ASP:OD1	2.45	0.49
1:B:628:TRP:CD2	1:B:631:VAL:HG23	2.48	0.49
1:D:539:MET:N	1:D:539:MET:SD	2.86	0.49
1:D:640:ILE:HD11	1:D:654:ALA:CB	2.39	0.49
1:A:289:ILE:HG13	1:A:334:LEU:HD11	1.94	0.49
1:B:235:LYS:HE3	1:B:236:ALA:HB2	1.95	0.49
1:D:224:PRO:HA	1:D:315:ARG:HD3	1.95	0.49
1:D:279:MET:CE	1:D:600:GLN:NE2	2.75	0.49
1:D:389:ASN:O	1:D:392:TYR:HB3	2.13	0.49
1:D:486:MET:HE1	1:D:527:GLU:CG	2.42	0.49
1:D:566:LEU:HD21	1:D:570:ASN:HB2	1.94	0.49
1:B:256:HIS:CG	5:J:6:GLC:O3	2.57	0.49
1:C:606:LEU:HD21	1:C:679:LEU:HD21	1.93	0.49
1:D:252:SER:CB	1:D:568:MET:SD	3.01	0.49
1:D:594:ASN:ND2	1:D:595:TRP:CD1	2.80	0.49
1:A:412:TYR:HE2	1:A:461:THR:CG2	2.25	0.49
1:A:660:VAL:HG12	1:A:662:ARG:NH1	2.28	0.49
1:D:526:ASP:N	1:D:527:GLU:OE2	2.45	0.49
1:D:630:VAL:O	1:D:630:VAL:CG2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ASN:HB2	1:A:519:PHE:CD1	2.48	0.49
1:A:520:VAL:O	1:A:522:PRO:HD3	2.13	0.49
1:B:292:HIS:O	1:B:311:ARG:NH1	2.45	0.49
1:B:459:GLU:OE2	1:B:461:THR:OG1	2.14	0.49
1:B:604:ARG:O	1:B:608:LEU:HG	2.12	0.49
1:C:403:ARG:NE	1:C:405:ASP:OD1	2.45	0.49
1:D:246:TYR:CE1	1:D:571:GLU:OE2	2.66	0.49
1:D:256:HIS:CB	1:D:263:LEU:CD2	2.84	0.49
1:D:261:PHE:N	1:D:261:PHE:CD2	2.79	0.49
1:D:290:ASN:OD1	1:D:291:GLU:N	2.45	0.49
1:D:468:ARG:O	1:D:476:GLY:HA2	2.13	0.49
1:D:594:ASN:ND2	1:D:687:HIS:HB3	2.26	0.49
1:D:675:TRP:CE3	1:D:724:VAL:C	2.86	0.49
1:D:702:ILE:HD12	1:D:702:ILE:N	2.28	0.49
1:A:496:ASP:OD1	1:A:498:VAL:HG22	2.13	0.48
1:B:270:ASP:O	1:B:274:PRO:HG2	2.13	0.48
1:C:666:ARG:NH1	1:C:710:SER:HB2	2.28	0.48
1:D:273:VAL:N	1:D:274:PRO:HD2	2.27	0.48
1:D:363:ARG:O	1:D:364:GLU:C	2.48	0.48
1:D:532:LYS:O	1:D:533:LYS:O	2.30	0.48
1:D:585:ASP:O	1:D:587:HIS:CD2	2.66	0.48
1:D:594:ASN:OD1	1:D:687:HIS:HB3	2.12	0.48
1:B:317:ASP:O	1:B:320:TYR:HB3	2.13	0.48
1:B:482:ASN:HB2	1:B:519:PHE:CD1	2.47	0.48
1:B:644:ARG:HD3	1:B:650:GLU:OE1	2.13	0.48
1:C:485:TRP:CD2	1:C:489:THR:HG21	2.48	0.48
1:C:620:ASP:OD1	1:C:643:ARG:NH2	2.45	0.48
1:C:636:ARG:HD2	1:C:665:TYR:HE1	1.78	0.48
1:C:681:THR:HG21	1:C:719:ALA:HA	1.95	0.48
1:C:718:LEU:O	1:C:719:ALA:HB2	2.13	0.48
1:D:593:ASP:C	1:D:597:HIS:ND1	2.66	0.48
1:D:638:VAL:O	1:D:638:VAL:HG22	2.13	0.48
2:E:4:GLC:O6	2:E:5:GLC:O5	2.29	0.48
1:A:407:VAL:HG21	1:A:459:GLU:HB2	1.95	0.48
1:B:493:MET:HE3	1:B:553:TYR:CD1	2.49	0.48
1:C:537:ASP:OD2	6:L:1:GLC:C2	2.61	0.48
1:C:609:THR:HG21	1:C:679:LEU:CD1	2.43	0.48
1:D:463:PHE:CD1	1:D:464:PRO:HD2	2.49	0.48
2:E:4:GLC:HO6	2:E:5:GLC:C1	2.26	0.48
1:A:431:GLU:CG	1:A:433:LEU:HD12	2.43	0.48
1:A:491:ASP:O	1:A:494:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:HIS:CE1	1:B:186:GLN:OE1	2.65	0.48
1:B:285:GLU:OE2	1:B:403:ARG:NH2	2.46	0.48
1:C:138:THR:CG2	1:C:220:ILE:HD11	2.41	0.48
1:D:359:HIS:NE2	1:D:434:GLU:OE1	2.46	0.48
1:A:660:VAL:HB	1:A:662:ARG:HH12	1.79	0.48
1:B:691:ALA:O	1:B:716:PRO:HG3	2.14	0.48
1:D:255:ARG:HH22	1:D:259:ASN:H	1.61	0.48
1:D:307:ALA:CB	1:D:392:TYR:OH	2.59	0.48
1:D:356:LEU:CD1	1:D:357:TYR:HD2	2.25	0.48
1:D:376:ASN:O	1:D:376:ASN:OD1	2.31	0.48
1:A:146:ASN:O	1:A:195:ALA:HB2	2.12	0.48
1:A:571:GLU:O	1:A:599:VAL:HG12	2.13	0.48
1:B:193:ILE:HA	1:B:198:ASN:O	2.14	0.48
1:B:703:ALA:HA	1:B:707:ARG:O	2.14	0.48
1:D:271:GLN:C	1:D:274:PRO:HD2	2.34	0.48
1:D:291:GLU:OE1	1:D:303:THR:OG1	2.28	0.48
1:D:307:ALA:N	1:D:308:PRO:CD	2.76	0.48
1:D:314:THR:HG23	1:D:315:ARG:N	2.29	0.48
1:D:680:ASN:CG	1:D:682:ASP:OD1	2.52	0.48
1:D:684:MET:SD	1:D:684:MET:N	2.86	0.48
2:E:2:GLC:H61	2:E:3:GLC:C1	2.43	0.48
1:A:500:ARG:NH2	1:A:540:PRO:HG2	2.29	0.48
1:B:255:ARG:HH22	1:B:581:ASP:HA	1.79	0.48
1:C:567:PHE:HB3	1:C:570:ASN:ND2	2.28	0.48
1:C:633:ASP:CG	1:C:636:ARG:HG3	2.34	0.48
1:D:319:ARG:HH11	1:D:322:ILE:CG1	2.26	0.48
1:A:273:VAL:CG2	1:A:274:PRO:CD	2.85	0.48
1:B:450:VAL:HG13	1:B:450:VAL:O	2.14	0.48
1:D:306:TYR:CE2	1:D:385:PHE:CE1	2.97	0.48
1:B:375:TYR:HB2	1:B:377:TYR:CE1	2.49	0.48
1:B:379:ARG:HB3	1:B:382:VAL:HG22	1.96	0.48
1:B:399:ILE:O	1:B:399:ILE:HG22	2.12	0.48
1:D:243:ILE:HA	1:D:282:THR:CG2	2.44	0.48
1:D:279:MET:CE	1:D:279:MET:CA	2.89	0.48
1:D:533:LYS:HD3	1:D:537:ASP:HB2	1.96	0.48
1:A:215:GLU:C	1:A:216:THR:HG22	2.33	0.48
1:A:652:ILE:CD1	1:A:675:TRP:CH2	2.97	0.48
1:C:494:LYS:HG2	1:C:538:ARG:HG2	1.94	0.48
1:C:633:ASP:OD1	1:C:636:ARG:CG	2.62	0.48
1:D:255:ARG:CZ	1:D:259:ASN:C	2.81	0.48
1:D:263:LEU:HA	1:D:264:SER:HA	1.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:TYR:OH	1:D:318:PHE:HA	2.14	0.48
1:D:293:PRO:HG3	1:D:303:THR:HG23	1.95	0.48
1:D:497:PRO:CA	1:D:500:ARG:HG3	2.31	0.48
1:D:627:GLU:O	1:D:641:PHE:HB2	2.14	0.48
1:A:187:LEU:CD2	1:A:219:LEU:CD2	2.92	0.47
1:A:619:LEU:HD22	1:A:622:ASP:CB	2.44	0.47
1:C:202:LYS:HE3	1:C:351:PHE:O	2.14	0.47
1:D:437:GLU:OE1	1:D:437:GLU:HA	2.14	0.47
1:D:599:VAL:O	1:D:601:ARG:N	2.47	0.47
1:B:269:ALA:O	1:B:273:VAL:CG2	2.62	0.47
1:C:249:HIS:H	1:C:568:MET:HE1	1.77	0.47
1:C:558:TRP:HA	1:C:564:LYS:HE2	1.95	0.47
1:D:249:HIS:ND1	1:D:287:LEU:CD2	2.77	0.47
1:D:252:SER:HA	1:D:568:MET:CE	2.45	0.47
1:D:268:LEU:H	1:D:268:LEU:CD1	2.26	0.47
1:D:289:ILE:C	1:D:289:ILE:HD12	2.35	0.47
1:D:699:SER:HA	1:D:711:LEU:HD12	1.96	0.47
1:A:649:ASN:H	1:A:649:ASN:HD22	1.62	0.47
1:A:681:THR:CG2	1:A:720:THR:HG23	2.41	0.47
1:B:289:ILE:C	1:B:289:ILE:HD12	2.35	0.47
1:D:232:GLU:CB	1:D:233:ARG:HH11	2.25	0.47
1:D:708:GLN:HG3	1:D:709:HIS:HD2	1.80	0.47
1:A:297:SER:O	1:A:298:TRP:HB2	2.15	0.47
1:A:666:ARG:CD	1:A:702:ILE:HD11	2.30	0.47
1:B:630:VAL:HG13	1:B:640:ILE:HB	1.96	0.47
1:C:189:LYS:HB3	1:C:202:LYS:O	2.13	0.47
1:C:323:ASP:O	1:C:327:ALA:N	2.39	0.47
1:C:560:PHE:CG	1:C:561:PRO:HD2	2.50	0.47
1:C:726:GLU:HG2	1:C:727:ALA:H	1.79	0.47
1:D:497:PRO:HA	1:D:500:ARG:CD	2.44	0.47
1:D:714:THR:C	1:D:715:LEU:HD23	2.35	0.47
1:B:153:VAL:HG23	1:B:159:TRP:CA	2.44	0.47
1:C:326:HIS:CE1	1:C:398:GLY:O	2.66	0.47
1:C:344:ASP:OD1	1:C:344:ASP:N	2.48	0.47
1:D:454:VAL:HG12	1:D:478:TRP:CD2	2.49	0.47
1:D:508:THR:O	1:D:511:ILE:CG2	2.57	0.47
1:A:265:TYR:HB2	1:A:317:ASP:HB3	1.97	0.47
1:B:314:THR:O	1:B:317:ASP:HB2	2.14	0.47
1:C:279:MET:HE1	1:C:603:VAL:HG22	1.96	0.47
1:C:542:ASP:OD1	1:C:542:ASP:C	2.52	0.47
1:C:693:ASN:ND2	1:C:693:ASN:H	2.10	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:PRO:HD3	1:D:303:THR:OG1	2.15	0.47
1:D:547:PHE:HB3	1:D:551:ARG:CZ	2.42	0.47
1:D:599:VAL:O	1:D:600:GLN:CB	2.55	0.47
1:A:132:MET:O	1:A:135:VAL:HG12	2.15	0.47
1:A:192:MET:CE	1:A:352:ASP:HA	2.45	0.47
1:A:490:LEU:HD11	1:A:553:TYR:CE2	2.50	0.47
1:A:629:LEU:O	1:A:630:VAL:CG1	2.63	0.47
1:A:714:THR:O	1:A:715:LEU:HD23	2.14	0.47
1:B:125:LEU:HD23	1:B:125:LEU:N	2.29	0.47
1:B:290:ASN:OD1	1:B:302:PRO:CG	2.63	0.47
1:C:256:HIS:CE1	1:C:263:LEU:HD22	2.50	0.47
1:D:224:PRO:CA	1:D:315:ARG:HD3	2.44	0.47
1:D:246:TYR:O	1:D:285:GLU:N	2.42	0.47
1:D:291:GLU:HB2	1:D:308:PRO:HB2	1.97	0.47
1:A:444:ARG:O	1:A:448:GLU:HG3	2.15	0.47
1:C:248:VAL:CG1	1:C:286:LEU:HD23	2.45	0.47
1:C:633:ASP:OD2	1:C:638:VAL:CG2	2.62	0.47
1:C:661:PRO:HG3	1:C:717:PRO:CG	2.42	0.47
1:D:528:VAL:H	1:D:532:LYS:HZ3	1.58	0.47
1:D:536:LEU:HB2	1:D:574:GLN:HG3	1.96	0.47
1:D:692:GLY:HA2	1:D:714:THR:HG21	1.96	0.47
1:A:259:ASN:HB2	1:A:261:PHE:HB2	1.97	0.47
1:B:168:LEU:HD12	1:B:169:ARG:N	2.29	0.47
1:C:166:MET:HB3	1:C:177:LEU:HB2	1.96	0.47
1:C:183:HIS:N	1:C:186:GLN:OE1	2.47	0.47
1:C:210:ALA:O	1:C:310:ARG:HD3	2.14	0.47
1:D:230:THR:OG1	1:D:326:HIS:CD2	2.64	0.47
1:D:348:LEU:CD1	1:D:357:TYR:CD1	2.98	0.47
1:D:548:ALA:O	1:D:552:ALA:N	2.29	0.47
1:D:601:ARG:O	1:D:602:LEU:HB3	2.14	0.47
1:A:681:THR:HG23	1:A:719:ALA:HB1	1.97	0.47
1:A:682:ASP:C	1:A:688:GLY:HA3	2.35	0.47
1:A:721:ILE:O	1:A:722:TRP:HD1	1.98	0.47
1:C:184:ASN:OD1	1:C:184:ASN:N	2.46	0.47
1:D:311:ARG:HG3	1:D:312:PHE:CE2	2.49	0.47
1:D:456:MET:HG2	1:D:479:TYR:HB2	1.97	0.47
1:D:566:LEU:HD23	1:D:567:PHE:H	1.80	0.47
1:B:606:LEU:HD23	1:B:679:LEU:HD13	1.97	0.46
1:C:248:VAL:CG2	1:C:568:MET:CE	2.93	0.46
1:D:571:GLU:O	1:D:599:VAL:HG12	2.15	0.46
1:D:614:LYS:HG3	1:D:645:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ARG:CG	1:A:319:ARG:NH1	2.78	0.46
1:A:656:ASN:OD1	1:A:658:THR:HG22	2.15	0.46
1:B:630:VAL:O	1:B:630:VAL:HG22	2.14	0.46
1:C:505:ASP:OD1	1:C:505:ASP:N	2.48	0.46
1:C:551:ARG:HB3	1:C:681:THR:HG23	1.97	0.46
1:D:242:PRO:C	1:D:243:ILE:HD12	2.35	0.46
1:D:262:TRP:CE3	1:D:312:PHE:CE1	3.02	0.46
1:D:376:ASN:C	1:D:378:GLY:N	2.68	0.46
1:D:470:GLN:H	1:D:470:GLN:CD	2.13	0.46
1:A:302:PRO:CG	1:A:337:VAL:HG21	2.43	0.46
1:A:466:VAL:HG21	1:A:480:LYS:HD2	1.95	0.46
1:A:669:ILE:HD12	1:A:669:ILE:N	2.31	0.46
1:B:152:VAL:HG12	1:B:166:MET:SD	2.55	0.46
1:B:271:GLN:C	1:B:274:PRO:HD2	2.35	0.46
1:D:265:TYR:CD1	1:D:265:TYR:C	2.87	0.46
1:A:227:VAL:CG2	1:A:319:ARG:NH2	2.77	0.46
1:A:686:TYR:N	1:A:686:TYR:CD1	2.79	0.46
1:B:234:LYS:CG	1:B:452:GLY:HA3	2.45	0.46
1:B:529:VAL:CG1	1:B:578:TRP:HE3	2.29	0.46
1:C:348:LEU:CD2	1:C:357:TYR:CD2	2.96	0.46
1:D:280:GLY:HA2	1:D:604:ARG:NH1	2.31	0.46
1:D:445:ILE:C	1:D:445:ILE:HD12	2.35	0.46
1:D:588:LEU:N	1:D:588:LEU:HD22	2.30	0.46
1:A:654:ALA:O	1:A:721:ILE:N	2.45	0.46
1:A:707:ARG:NH1	1:D:415:TYR:CE2	2.81	0.46
1:B:277:LYS:CD	1:B:328:ALA:O	2.63	0.46
1:B:334:LEU:HD12	1:B:335:ASP:N	2.30	0.46
1:D:253:TRP:HH2	1:D:272:LEU:HA	1.80	0.46
1:D:255:ARG:CZ	1:D:260:ASN:CA	2.92	0.46
1:D:526:ASP:HA	1:D:532:LYS:HE3	1.97	0.46
1:A:242:PRO:HD3	1:A:617:HIS:CE1	2.51	0.46
1:A:602:LEU:O	1:A:602:LEU:HD22	2.16	0.46
1:A:685:HIS:ND1	2:H:3:GLC:C6	2.78	0.46
1:A:689:SER:O	1:A:690:ASN:CB	2.56	0.46
1:B:535:ILE:HG22	1:B:550:LEU:CD1	2.45	0.46
1:B:669:ILE:HG22	1:B:670:ASN:H	1.80	0.46
1:C:141:SER:HA	1:C:175:TRP:O	2.15	0.46
1:D:622:ASP:OD1	1:D:624:TYR:N	2.46	0.46
1:D:722:TRP:O	1:D:723:LEU:HD23	2.16	0.46
1:A:192:MET:HE2	1:A:352:ASP:HA	1.98	0.46
1:A:211:GLN:CD	1:A:215:GLU:HB3	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:HIS:CE1	1:B:400:ASP:OD2	2.64	0.46
1:C:413:ARG:N	1:C:430:ARG:O	2.44	0.46
1:D:341:PHE:HB2	1:D:374:ILE:HD12	1.98	0.46
1:D:389:ASN:O	1:D:393:TRP:CD1	2.69	0.46
1:D:422:TRP:CE3	1:D:424:PRO:HA	2.51	0.46
1:A:121:PRO:HG3	1:A:384:ASN:O	2.16	0.46
1:A:122:TYR:CE1	1:A:123:GLU:HG3	2.50	0.46
1:A:248:VAL:HG12	1:A:249:HIS:N	2.30	0.46
1:A:508:THR:CG2	1:A:631:VAL:HG23	2.46	0.46
1:A:516:THR:HG22	1:D:426:GLU:HB3	1.97	0.46
1:B:292:HIS:CD2	1:B:299:GLY:HA2	2.51	0.46
1:B:602:LEU:HA	1:B:686:TYR:CE1	2.51	0.46
1:C:143:TRP:CZ3	1:C:356:LEU:HG	2.51	0.46
1:C:223:LEU:N	1:C:223:LEU:HD23	2.31	0.46
1:C:468:ARG:HD3	1:C:468:ARG:HA	1.73	0.46
1:D:598:GLY:O	1:D:601:ARG:O	2.33	0.46
1:D:622:ASP:OD1	1:D:624:TYR:HB2	2.16	0.46
1:B:490:LEU:O	1:B:494:LYS:HG3	2.16	0.46
1:C:380:ARG:O	1:C:384:ASN:OD1	2.33	0.46
1:C:571:GLU:HB2	1:C:603:VAL:HG21	1.98	0.46
1:D:336:TRP:CD2	1:D:338:PRO:HD3	2.51	0.46
1:D:480:LYS:HD2	1:D:517:GLU:OE2	2.16	0.46
1:D:700:ASP:HB3	1:D:702:ILE:HD11	1.97	0.46
1:A:601:ARG:O	1:A:605:ASP:OD1	2.34	0.46
1:A:628:TRP:O	1:A:629:LEU:HD23	2.15	0.46
1:C:438:PHE:CZ	1:C:442:THR:HG21	2.51	0.46
1:D:253:TRP:CZ2	1:D:272:LEU:HD12	2.51	0.46
1:D:265:TYR:CB	1:D:312:PHE:CB	2.88	0.46
1:D:279:MET:HA	1:D:279:MET:HE3	1.98	0.46
1:D:334:LEU:HD12	1:D:335:ASP:H	1.81	0.46
1:D:406:ALA:C	1:D:408:ALA:N	2.68	0.46
1:D:486:MET:SD	1:D:527:GLU:HG2	2.56	0.46
1:D:552:ALA:CA	1:D:720:THR:HG23	2.41	0.46
1:A:619:LEU:HD23	1:A:619:LEU:HA	1.77	0.45
1:C:356:LEU:HD12	1:C:356:LEU:HA	1.72	0.45
1:C:536:LEU:HD12	1:C:536:LEU:O	2.16	0.45
1:D:233:ARG:N	1:D:233:ARG:CD	2.79	0.45
1:D:276:ALA:CB	1:D:330:LEU:HD11	2.46	0.45
1:D:419:GLU:HB3	1:D:420:GLY:H	1.45	0.45
1:D:662:ARG:NH2	1:D:662:ARG:CG	2.71	0.45
1:A:208:PHE:CE1	1:A:223:LEU:HD21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:TRP:HB2	1:B:568:MET:CE	2.46	0.45
1:C:438:PHE:O	1:C:442:THR:CG2	2.61	0.45
1:C:633:ASP:OD1	1:C:636:ARG:HG2	2.16	0.45
1:D:521:LEU:N	1:D:563:LYS:O	2.30	0.45
1:D:629:LEU:HD23	1:D:667:PHE:HD1	1.80	0.45
1:B:643:ARG:HB3	1:B:643:ARG:HH11	1.80	0.45
1:C:237:ASN:OD1	1:C:331:ASN:ND2	2.49	0.45
1:C:682:ASP:O	1:C:688:GLY:HA3	2.16	0.45
1:D:234:LYS:O	1:D:236:ALA:N	2.49	0.45
1:D:252:SER:HB2	1:D:253:TRP:HD1	1.82	0.45
1:D:439:LEU:CD2	1:D:477:PHE:CE2	2.99	0.45
1:D:446:LEU:HD23	1:D:446:LEU:HA	1.68	0.45
1:D:489:THR:O	1:D:493:MET:HG2	2.15	0.45
1:D:596:HIS:N	1:D:597:HIS:HD2	2.13	0.45
1:D:624:TYR:O	1:D:644:ARG:HD2	2.16	0.45
1:B:246:TYR:HB2	1:B:281:PHE:CD2	2.52	0.45
1:B:373:LEU:HD23	1:B:373:LEU:N	2.31	0.45
1:B:616:MET:HE3	1:B:651:ILE:HD12	1.98	0.45
1:B:659:PRO:HD2	2:F:3:GLC:O3	2.16	0.45
1:B:712:SER:C	1:B:713:LEU:HD23	2.37	0.45
1:C:382:VAL:O	1:C:385:PHE:HB3	2.16	0.45
1:D:255:ARG:HG3	1:D:262:TRP:CD1	2.51	0.45
1:D:529:VAL:CG1	1:D:532:LYS:HZ1	2.22	0.45
1:D:551:ARG:HD2	1:D:681:THR:O	2.17	0.45
1:D:574:GLN:OE1	1:D:576:ARG:N	2.41	0.45
1:D:586:TRP:CE3	1:D:586:TRP:CA	3.00	0.45
1:A:212:MET:SD	1:A:213:ARG:N	2.80	0.45
1:C:450:VAL:O	1:C:451:SER:C	2.55	0.45
1:D:678:ILE:HG21	1:D:724:VAL:CG2	2.46	0.45
1:D:721:ILE:C	1:D:722:TRP:HD1	2.20	0.45
1:A:159:TRP:CG	4:I:1:GLC:H61	2.51	0.45
1:A:176:GLU:O	1:A:177:LEU:HB2	2.17	0.45
1:A:425:ASN:O	1:A:427:PHE:CD2	2.69	0.45
1:B:314:THR:CG2	1:B:317:ASP:OD2	2.65	0.45
1:D:375:TYR:CZ	1:D:386:LEU:HD11	2.51	0.45
1:D:611:ARG:O	1:D:612:HIS:HB3	2.17	0.45
1:A:211:GLN:HB3	1:A:215:GLU:HB2	1.99	0.45
1:A:289:ILE:CG1	1:A:334:LEU:HD11	2.47	0.45
1:A:628:TRP:C	1:A:629:LEU:HD23	2.37	0.45
1:B:399:ILE:HG21	1:B:402:LEU:HD21	1.97	0.45
1:B:513:TYR:O	1:B:516:THR:OG1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ARG:CZ	1:D:587:HIS:ND1	2.80	0.45
1:D:255:ARG:CZ	1:D:261:PHE:N	2.79	0.45
1:D:297:SER:O	1:D:298:TRP:HB2	2.16	0.45
1:D:558:TRP:HD1	1:D:610:TYR:HB2	1.82	0.45
1:D:598:GLY:CA	1:D:687:HIS:NE2	2.77	0.45
1:A:152:VAL:HG21	1:A:179:ILE:HD12	1.96	0.45
1:A:475:LEU:HA	1:A:475:LEU:HD23	1.47	0.45
1:A:490:LEU:HD12	1:A:490:LEU:HA	1.68	0.45
1:A:511:ILE:HD11	1:A:561:PRO:HG2	1.99	0.45
1:B:137:GLY:HA3	1:B:178:PHE:CE2	2.49	0.45
1:B:492:TYR:CG	1:B:507:LEU:CD1	2.98	0.45
1:B:653:VAL:HG22	1:B:722:TRP:CD1	2.51	0.45
1:D:381:GLU:C	1:D:384:ASN:OD1	2.56	0.45
1:D:529:VAL:CG1	1:D:532:LYS:NZ	2.74	0.45
1:A:683:SER:OG	2:H:2:GLC:C6	2.64	0.45
1:B:187:LEU:HA	1:B:218:SER:O	2.17	0.45
1:B:612:HIS:NE2	1:D:421:GLU:HG3	2.32	0.45
1:C:505:ASP:HB3	1:C:509:PHE:CE1	2.52	0.45
1:D:268:LEU:CD1	1:D:268:LEU:N	2.80	0.45
1:D:309:THR:CB	1:D:318:PHE:HE2	2.24	0.45
1:D:471:ASP:OD1	1:D:472:MET:N	2.50	0.45
1:D:529:VAL:N	1:D:532:LYS:CG	2.79	0.45
1:D:573:ALA:O	1:D:574:GLN:CD	2.55	0.45
1:D:686:TYR:O	1:D:687:HIS:CD2	2.70	0.45
1:B:188:TYR:O	1:B:189:LYS:HG3	2.17	0.45
1:B:443:ASN:ND2	1:B:475:LEU:O	2.48	0.45
1:C:357:TYR:HD1	1:C:382:VAL:HG12	1.82	0.45
1:C:561:PRO:HA	1:C:620:ASP:OD1	2.17	0.45
1:C:644:ARG:HA	1:C:649:ASN:O	2.16	0.45
1:D:255:ARG:CG	1:D:262:TRP:CD1	3.00	0.45
1:D:569:GLY:O	1:D:571:GLU:OE1	2.33	0.45
1:A:485:TRP:C	1:A:485:TRP:CE3	2.90	0.44
1:A:702:ILE:CD1	1:A:710:SER:OG	2.65	0.44
1:B:120:ARG:N	1:B:121:PRO:CD	2.80	0.44
1:B:142:VAL:O	1:B:174:ILE:HA	2.17	0.44
1:B:396:ARG:HD3	1:B:396:ARG:HA	1.40	0.44
1:B:429:GLY:C	1:B:431:GLU:OE1	2.55	0.44
1:B:628:TRP:CG	1:B:631:VAL:CG2	3.00	0.44
1:C:724:VAL:HG22	1:C:725:ARG:H	1.81	0.44
1:D:445:ILE:CA	1:D:448:GLU:HG3	2.27	0.44
1:D:449:GLN:HB2	1:D:450:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:486:MET:HE3	1:D:527:GLU:HG2	1.97	0.44
1:D:547:PHE:CB	1:D:551:ARG:HH22	2.29	0.44
1:D:715:LEU:HD23	1:D:715:LEU:N	2.32	0.44
1:A:120:ARG:N	1:A:121:PRO:CD	2.80	0.44
1:A:264:SER:N	1:A:267:GLU:HG3	2.29	0.44
1:A:602:LEU:HD22	1:A:606:LEU:HG	1.98	0.44
1:A:717:PRO:O	1:A:718:LEU:C	2.56	0.44
1:D:254:ARG:O	1:D:255:ARG:CB	2.60	0.44
1:D:282:THR:HG23	1:D:283:HIS:ND1	2.32	0.44
1:D:370:TRP:CH2	1:D:371:ASN:OD1	2.70	0.44
1:D:708:GLN:OE1	1:D:708:GLN:HA	2.17	0.44
1:A:279:MET:HE2	1:A:279:MET:HB2	1.70	0.44
1:A:608:LEU:HA	1:A:608:LEU:HD23	1.72	0.44
1:A:693:ASN:ND2	1:A:714:THR:H	2.14	0.44
1:C:292:HIS:CD2	1:C:311:ARG:NH1	2.86	0.44
1:D:250:LEU:N	1:D:250:LEU:HD23	2.31	0.44
1:D:341:PHE:HB2	1:D:374:ILE:HA	1.99	0.44
1:D:377:TYR:CD1	1:D:438:PHE:CD2	3.05	0.44
1:D:456:MET:CE	1:D:479:TYR:CD2	3.00	0.44
1:D:636:ARG:CG	1:D:662:ARG:NH2	2.71	0.44
1:A:423:ILE:HD13	1:A:429:GLY:CA	2.47	0.44
1:B:172:SER:HB2	1:B:174:ILE:CD1	2.47	0.44
1:B:293:PRO:HD3	1:B:303:THR:CG2	2.44	0.44
1:D:262:TRP:O	1:D:264:SER:C	2.56	0.44
1:D:528:VAL:N	1:D:532:LYS:HE2	2.33	0.44
1:D:558:TRP:HD1	1:D:610:TYR:CB	2.31	0.44
1:D:710:SER:OG	1:D:711:LEU:N	2.51	0.44
1:D:721:ILE:CD1	1:D:723:LEU:HD21	2.44	0.44
1:A:139:ARG:HE	1:A:139:ARG:HB2	1.29	0.44
1:A:346:PHE:N	1:A:346:PHE:HD1	2.16	0.44
1:A:645:ASP:CG	1:A:649:ASN:HD22	2.20	0.44
1:B:187:LEU:HD23	1:B:187:LEU:H	1.82	0.44
1:B:496:ASP:OD2	1:B:498:VAL:HB	2.18	0.44
1:B:685:HIS:CE1	1:D:424:PRO:C	2.91	0.44
1:D:280:GLY:O	1:D:607:ASN:HB3	2.17	0.44
1:D:431:GLU:H	1:D:431:GLU:HG3	1.33	0.44
1:D:439:LEU:HD22	1:D:477:PHE:CE2	2.53	0.44
1:A:425:ASN:OD1	1:A:425:ASN:N	2.50	0.44
1:A:492:TYR:CZ	1:A:500:ARG:HB3	2.52	0.44
1:C:153:VAL:HG13	1:C:159:TRP:HA	1.99	0.44
1:C:289:ILE:HG13	1:C:334:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:ARG:O	1:C:382:VAL:HG23	2.18	0.44
1:C:624:TYR:O	1:C:644:ARG:HD2	2.18	0.44
1:D:265:TYR:CD2	1:D:312:PHE:O	2.71	0.44
1:D:456:MET:CE	1:D:479:TYR:HD2	2.29	0.44
1:B:140:PHE:CD1	1:B:140:PHE:N	2.86	0.44
1:C:289:ILE:C	1:C:289:ILE:CD1	2.86	0.44
1:D:249:HIS:ND1	1:D:287:LEU:HD13	2.33	0.44
1:D:252:SER:OG	1:D:253:TRP:N	2.51	0.44
1:D:279:MET:HE2	1:D:279:MET:HB3	1.51	0.44
1:A:387:VAL:HG22	1:A:442:THR:HG23	2.00	0.44
1:B:678:ILE:HG23	1:B:724:VAL:CG1	2.47	0.44
1:C:263:LEU:N	1:C:263:LEU:HD23	2.32	0.44
1:D:399:ILE:HD12	1:D:399:ILE:O	2.18	0.44
1:D:403:ARG:NH1	1:D:405:ASP:HB3	2.33	0.44
1:A:516:THR:C	1:A:517:GLU:HG2	2.39	0.44
1:B:148:ARG:HG3	1:B:193:ILE:HG22	1.99	0.44
1:C:189:LYS:NZ	1:C:215:GLU:HG2	2.33	0.44
1:C:681:THR:O	1:C:681:THR:CG2	2.64	0.44
1:D:279:MET:HE1	1:D:600:GLN:NE2	2.32	0.44
1:D:281:PHE:CE1	1:D:607:ASN:ND2	2.85	0.44
1:D:348:LEU:HA	1:D:348:LEU:HD13	1.76	0.44
1:D:651:ILE:HB	1:D:723:LEU:O	2.18	0.44
1:D:700:ASP:CB	1:D:702:ILE:CD1	2.95	0.44
1:A:177:LEU:CD2	1:A:177:LEU:C	2.84	0.43
1:A:292:HIS:O	1:A:311:ARG:NH1	2.51	0.43
1:A:372:THR:C	1:A:373:LEU:HD23	2.36	0.43
1:A:417:ARG:NH1	1:A:417:ARG:HB2	2.32	0.43
1:B:685:HIS:CE1	1:D:424:PRO:HB2	2.53	0.43
1:C:143:TRP:CH2	1:C:356:LEU:HG	2.53	0.43
1:C:662:ARG:HA	1:C:662:ARG:HD2	1.82	0.43
1:C:676:ARG:HE	1:C:696:THR:CG2	2.31	0.43
1:D:306:TYR:HE1	1:D:392:TYR:HD2	1.65	0.43
1:D:440:ARG:H	1:D:440:ARG:HG2	1.61	0.43
1:D:536:LEU:HD22	1:D:550:LEU:HD11	1.92	0.43
1:D:539:MET:HA	1:D:540:PRO:HD3	1.85	0.43
1:A:413:ARG:O	1:A:430:ARG:HB2	2.19	0.43
1:A:588:LEU:CD1	1:A:596:HIS:NE2	2.81	0.43
1:A:636:ARG:HG3	1:A:662:ARG:NH2	2.25	0.43
1:A:693:ASN:HD21	1:A:713:LEU:HA	1.82	0.43
1:B:263:LEU:N	1:B:263:LEU:HD23	2.33	0.43
1:D:265:TYR:CG	1:D:266:ARG:N	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:HD3	1:A:193:ILE:HD11	1.99	0.43
1:A:290:ASN:OD1	1:A:337:VAL:HG22	2.18	0.43
1:A:511:ILE:HD13	1:A:626:PHE:CZ	2.53	0.43
1:A:518:ASN:HA	1:A:621:PHE:CE1	2.53	0.43
1:A:642:VAL:HG12	1:A:652:ILE:HG13	2.01	0.43
1:A:674:LYS:HD2	1:A:696:THR:CG2	2.33	0.43
1:C:465:GLY:O	1:C:474:GLY:HA3	2.18	0.43
1:D:275:TYR:CE1	1:D:586:TRP:HH2	2.36	0.43
1:D:280:GLY:O	1:D:607:ASN:HB2	2.17	0.43
1:D:306:TYR:CD1	1:D:392:TYR:HD2	2.33	0.43
1:D:594:ASN:HD21	1:D:687:HIS:HB2	1.76	0.43
1:D:643:ARG:HE	1:D:643:ARG:HB3	1.35	0.43
1:A:407:VAL:CG2	1:A:458:GLU:O	2.62	0.43
1:A:629:LEU:HD23	1:A:629:LEU:N	2.32	0.43
1:B:119:LEU:O	1:B:120:ARG:HB2	2.16	0.43
1:B:407:VAL:HG13	1:B:458:GLU:O	2.19	0.43
1:B:658:THR:OG1	1:B:659:PRO:HD2	2.18	0.43
1:C:153:VAL:CG1	1:C:159:TRP:CE3	3.01	0.43
1:C:277:LYS:HD2	1:C:328:ALA:HB1	1.99	0.43
1:C:677:GLU:HA	1:C:723:LEU:CD2	2.47	0.43
1:D:265:TYR:CD1	1:D:318:PHE:HE1	2.36	0.43
1:D:504:HIS:NE2	1:D:639:LEU:HD23	2.33	0.43
1:D:650:GLU:OE1	1:D:670:ASN:HB2	2.18	0.43
1:A:145:PRO:HD2	1:A:356:LEU:HD21	2.00	0.43
1:A:339:GLY:HA2	1:A:410:MET:HG3	2.01	0.43
1:A:496:ASP:HB3	1:A:499:TYR:CD2	2.53	0.43
1:A:508:THR:HG22	1:A:631:VAL:HG23	1.99	0.43
1:D:265:TYR:CB	1:D:312:PHE:CD1	2.94	0.43
1:D:485:TRP:HE1	1:D:560:PHE:HD2	1.64	0.43
1:D:590:GLU:HB2	1:D:591:GLY:HA2	2.00	0.43
1:A:285:GLU:OE2	1:A:403:ARG:NH2	2.51	0.43
1:A:485:TRP:CD2	1:A:521:LEU:HD22	2.54	0.43
1:A:497:PRO:HB3	1:A:659:PRO:HD3	2.00	0.43
1:B:153:VAL:CG2	1:B:159:TRP:CA	2.95	0.43
1:B:561:PRO:HA	1:B:643:ARG:HH21	1.82	0.43
1:B:643:ARG:HB3	1:B:643:ARG:NH1	2.34	0.43
1:C:633:ASP:OD2	1:C:636:ARG:CD	2.66	0.43
1:C:654:ALA:HB3	1:C:721:ILE:CG1	2.48	0.43
1:D:232:GLU:HB3	1:D:233:ARG:NH1	2.25	0.43
1:D:336:TRP:CG	1:D:338:PRO:HD3	2.53	0.43
1:D:598:GLY:CA	1:D:601:ARG:HB2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LYS:NZ	4:I:1:GLC:O2	2.43	0.43
1:B:632:ASP:OD1	1:B:632:ASP:N	2.33	0.43
1:C:132:MET:O	1:C:133:ASP:OD1	2.37	0.43
1:C:219:LEU:HD13	1:C:220:ILE:H	1.84	0.43
1:C:222:GLY:O	1:C:315:ARG:NH1	2.52	0.43
1:D:622:ASP:CG	1:D:623:PRO:HD2	2.39	0.43
1:D:638:VAL:HB	1:D:656:ASN:HA	2.01	0.43
1:D:649:ASN:C	1:D:650:GLU:HG2	2.39	0.43
1:A:220:ILE:HD13	1:A:220:ILE:HG21	1.77	0.43
1:B:119:LEU:HD22	1:B:119:LEU:N	2.23	0.43
1:B:150:VAL:HG22	1:B:192:MET:CG	2.44	0.43
1:B:507:LEU:N	1:B:507:LEU:CD1	2.81	0.43
1:C:489:THR:O	1:C:492:TYR:HB3	2.19	0.43
1:C:667:PHE:HA	1:C:705:HIS:ND1	2.33	0.43
1:D:334:LEU:HD12	1:D:335:ASP:N	2.34	0.43
1:D:575:GLY:CA	1:D:585:ASP:OD2	2.67	0.43
1:D:672:PRO:HG3	1:D:709:HIS:CE1	2.54	0.43
1:A:172:SER:OG	1:A:174:ILE:CG1	2.67	0.43
1:A:666:ARG:HG2	1:A:710:SER:OG	2.04	0.43
1:A:682:ASP:O	1:A:688:GLY:CA	2.64	0.43
1:C:478:TRP:HB3	1:C:479:TYR:CD1	2.54	0.43
1:D:253:TRP:HB2	1:D:586:TRP:HE1	1.76	0.43
1:D:256:HIS:CB	1:D:263:LEU:CG	2.97	0.43
1:A:212:MET:SD	1:A:213:ARG:HG2	2.58	0.43
1:B:623:PRO:HG3	1:C:428:GLY:HA2	2.01	0.43
1:B:629:LEU:HD11	1:B:642:VAL:HG13	2.00	0.43
1:C:690:ASN:HD21	3:G:4:GLC:C3	2.32	0.43
1:D:249:HIS:O	1:D:252:SER:N	2.52	0.43
1:A:536:LEU:HD12	1:A:536:LEU:O	2.19	0.42
1:A:548:ALA:HA	1:A:551:ARG:NH1	2.34	0.42
1:A:685:HIS:CE1	2:H:3:GLC:H62	2.54	0.42
1:B:135:VAL:O	1:B:135:VAL:HG13	2.19	0.42
1:C:150:VAL:O	1:C:166:MET:HG3	2.19	0.42
1:C:628:TRP:CD2	1:C:631:VAL:CG1	3.01	0.42
1:D:266:ARG:HA	1:D:266:ARG:HD2	1.82	0.42
1:D:305:LEU:CD2	1:D:389:ASN:ND2	2.71	0.42
1:D:423:ILE:HG21	1:D:423:ILE:HD13	1.70	0.42
1:D:576:ARG:O	1:D:577:GLU:CB	2.67	0.42
1:D:594:ASN:ND2	1:D:687:HIS:CG	2.86	0.42
1:A:500:ARG:NH2	1:A:540:PRO:CG	2.82	0.42
1:A:619:LEU:HD22	1:A:622:ASP:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:SER:CB	1:C:580:HIS:HA	2.50	0.42
1:D:278:TRP:O	1:D:278:TRP:CE3	2.72	0.42
1:D:536:LEU:HD13	1:D:550:LEU:HD11	2.01	0.42
1:D:563:LYS:HA	1:D:563:LYS:HD3	1.71	0.42
1:D:666:ARG:HH12	1:D:702:ILE:HD13	1.81	0.42
1:D:715:LEU:HA	1:D:716:PRO:HD3	1.82	0.42
1:A:322:ILE:C	1:A:322:ILE:HD12	2.40	0.42
1:B:322:ILE:HD12	1:B:399:ILE:CD1	2.49	0.42
1:B:382:VAL:HG23	1:B:383:SER:H	1.84	0.42
1:B:650:GLU:HG2	1:B:671:GLN:NE2	2.35	0.42
1:C:220:ILE:HD13	1:C:220:ILE:HG21	1.53	0.42
1:C:542:ASP:O	1:C:545:GLN:N	2.52	0.42
1:C:628:TRP:CG	1:C:631:VAL:CG1	2.98	0.42
1:A:490:LEU:HD11	1:A:553:TYR:HE2	1.85	0.42
1:A:669:ILE:HG22	1:A:671:GLN:N	2.29	0.42
1:B:438:PHE:O	1:B:442:THR:CG2	2.61	0.42
1:B:461:THR:HG22	1:C:509:PHE:CD2	2.54	0.42
1:C:243:ILE:HB	1:C:563:LYS:HB3	2.01	0.42
1:D:536:LEU:HA	1:D:550:LEU:HD11	2.00	0.42
1:A:346:PHE:N	1:A:346:PHE:CD1	2.87	0.42
1:B:138:THR:OG1	1:B:182:ALA:HB3	2.19	0.42
1:B:169:ARG:NH2	1:B:171:GLU:HG3	2.34	0.42
1:B:242:PRO:HB3	1:B:617:HIS:CG	2.55	0.42
1:B:288:PRO:HG3	1:B:335:ASP:HB3	2.01	0.42
1:B:721:ILE:C	1:B:722:TRP:CD1	2.92	0.42
1:C:642:VAL:HA	1:C:651:ILE:O	2.19	0.42
1:D:356:LEU:O	1:D:356:LEU:HD22	2.19	0.42
1:A:290:ASN:OD1	1:A:337:VAL:CG2	2.67	0.42
1:A:640:ILE:HD12	1:A:654:ALA:CA	2.42	0.42
1:B:249:HIS:HB2	1:B:287:LEU:HD13	2.02	0.42
1:B:380:ARG:HD3	1:B:380:ARG:HA	1.83	0.42
1:C:166:MET:CE	1:C:190:TYR:CD1	3.03	0.42
1:D:269:ALA:CB	1:D:321:PHE:CB	2.84	0.42
1:D:331:ASN:ND2	1:D:400:ASP:OD2	2.53	0.42
1:D:356:LEU:HA	1:D:379:ARG:NH1	2.35	0.42
1:D:594:ASN:ND2	1:D:687:HIS:CB	2.70	0.42
1:D:619:LEU:HD11	1:D:646:LYS:HG2	2.01	0.42
1:A:654:ALA:O	1:A:720:THR:HA	2.19	0.42
1:A:659:PRO:HA	1:A:718:LEU:HD13	2.01	0.42
1:B:511:ILE:HD13	1:B:626:PHE:CE1	2.54	0.42
1:C:147:ALA:HB2	1:C:192:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:GLU:OE2	1:C:310:ARG:HD2	2.19	0.42
1:C:332:VAL:CG1	1:C:399:ILE:HD12	2.49	0.42
1:C:608:LEU:HA	1:C:608:LEU:HD23	1.63	0.42
1:C:624:TYR:CE1	1:C:644:ARG:CD	3.02	0.42
1:C:715:LEU:HA	1:C:715:LEU:HD23	1.83	0.42
1:D:272:LEU:C	1:D:274:PRO:HD2	2.40	0.42
1:D:356:LEU:HD22	1:D:356:LEU:C	2.40	0.42
1:A:645:ASP:CG	1:A:649:ASN:ND2	2.72	0.42
1:B:125:LEU:CD2	1:B:125:LEU:N	2.79	0.42
1:B:187:LEU:HD12	1:B:217:ALA:HB3	2.00	0.42
1:B:379:ARG:O	1:B:382:VAL:CG2	2.68	0.42
1:B:587:HIS:HA	1:B:590:GLU:CG	2.49	0.42
1:C:257:THR:HG23	1:C:258:ASP:N	2.35	0.42
1:C:438:PHE:CE1	1:C:442:THR:HG21	2.55	0.42
1:D:267:GLU:OE1	1:D:267:GLU:HA	2.20	0.42
1:D:279:MET:O	1:D:281:PHE:N	2.53	0.42
1:D:376:ASN:O	1:D:376:ASN:CG	2.58	0.42
1:D:665:TYR:O	1:D:712:SER:HA	2.20	0.42
1:A:189:LYS:HE3	1:A:217:ALA:HB2	2.01	0.42
1:A:685:HIS:CE1	2:H:3:GLC:C6	3.03	0.42
1:B:248:VAL:CB	1:B:568:MET:HE2	2.45	0.42
1:B:352:ASP:OD1	1:B:354:THR:OG1	2.26	0.42
1:B:542:ASP:OD1	1:B:545:GLN:HB2	2.19	0.42
1:C:348:LEU:O	1:C:348:LEU:HD23	2.20	0.42
1:C:618:GLU:OE1	1:C:645:ASP:HB2	2.20	0.42
1:D:267:GLU:O	1:D:271:GLN:HB2	2.20	0.42
1:D:280:GLY:N	1:D:604:ARG:HH11	2.16	0.42
1:D:513:TYR:O	1:D:516:THR:OG1	2.36	0.42
1:D:607:ASN:HA	1:D:610:TYR:HB3	2.01	0.42
1:D:658:THR:HG23	1:D:660:VAL:HG13	2.00	0.42
1:A:209:GLU:OE1	1:A:315:ARG:HB2	2.19	0.42
1:B:122:TYR:HA	1:B:206:TYR:CD2	2.55	0.42
1:B:310:ARG:O	1:B:311:ARG:C	2.57	0.42
1:D:306:TYR:CA	1:D:308:PRO:HD3	2.50	0.42
1:D:574:GLN:HB2	1:D:575:GLY:H	1.75	0.42
1:D:598:GLY:N	1:D:687:HIS:HE1	2.16	0.42
1:D:658:THR:CG2	1:D:660:VAL:HG13	2.50	0.42
1:D:683:SER:HB3	1:D:686:TYR:CE1	2.54	0.42
1:B:292:HIS:HB2	1:B:293:PRO:HD2	2.02	0.41
1:C:284:LEU:HA	1:C:284:LEU:HD12	1.84	0.41
1:C:341:PHE:HD2	1:C:342:PRO:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:VAL:O	1:C:498:VAL:HG22	2.19	0.41
1:D:278:TRP:C	1:D:604:ARG:NH1	2.73	0.41
1:D:408:ALA:O	1:D:412:TYR:HD2	2.03	0.41
1:D:427:PHE:HB2	1:D:431:GLU:CG	2.50	0.41
1:D:521:LEU:HA	1:D:521:LEU:HD23	1.52	0.41
1:D:677:GLU:OE2	1:D:693:ASN:OD1	2.38	0.41
1:A:256:HIS:O	1:A:260:ASN:HA	2.20	0.41
1:A:348:LEU:CD1	1:A:348:LEU:N	2.83	0.41
1:A:548:ALA:HB1	1:A:718:LEU:HB3	2.01	0.41
1:A:627:GLU:OE2	1:A:707:ARG:NH2	2.52	0.41
1:A:668:GLY:HA3	1:A:707:ARG:HB2	2.02	0.41
1:A:708:GLN:HE21	1:A:709:HIS:CG	2.34	0.41
1:B:296:GLY:HA2	1:B:580:HIS:NE2	2.34	0.41
1:B:609:THR:HG23	1:D:420:GLY:HA3	2.02	0.41
1:C:446:LEU:HD23	1:C:446:LEU:HA	1.62	0.41
1:D:237:ASN:ND2	1:D:453:ALA:HA	2.31	0.41
1:D:255:ARG:NH2	1:D:259:ASN:C	2.74	0.41
1:D:438:PHE:CE1	1:D:442:THR:CG2	3.03	0.41
1:A:208:PHE:CZ	1:A:223:LEU:HD21	2.55	0.41
1:A:450:VAL:HG23	1:A:450:VAL:O	2.19	0.41
1:A:640:ILE:CD1	1:A:654:ALA:CB	2.90	0.41
1:A:707:ARG:HH12	1:D:415:TYR:HE2	1.66	0.41
1:B:170:LYS:HD2	1:B:170:LYS:N	2.21	0.41
1:B:234:LYS:HG2	1:B:452:GLY:CA	2.51	0.41
1:C:193:ILE:HG23	1:C:197:GLY:HA2	2.02	0.41
1:D:439:LEU:CD2	1:D:477:PHE:CZ	3.03	0.41
1:D:606:LEU:O	1:D:610:TYR:N	2.47	0.41
1:D:639:LEU:HD12	1:D:639:LEU:C	2.40	0.41
1:B:137:GLY:HA3	1:B:178:PHE:HZ	1.74	0.41
1:C:252:SER:HB3	1:C:580:HIS:HA	2.01	0.41
1:C:326:HIS:NE2	1:C:400:ASP:OD2	2.32	0.41
1:C:633:ASP:OD2	1:C:636:ARG:HG3	2.20	0.41
1:D:247:GLU:OE1	1:D:525:HIS:CE1	2.73	0.41
1:D:265:TYR:CE1	1:D:318:PHE:CD1	3.08	0.41
1:D:535:ILE:CD1	1:D:535:ILE:N	2.48	0.41
1:D:636:ARG:HG3	1:D:662:ARG:HH21	1.80	0.41
1:D:678:ILE:HD12	1:D:678:ILE:C	2.40	0.41
1:B:148:ARG:H	1:B:148:ARG:HG2	1.46	0.41
1:B:150:VAL:CG1	1:B:166:MET:HE3	2.49	0.41
1:B:386:LEU:O	1:B:389:ASN:HB3	2.19	0.41
1:B:713:LEU:HD23	1:B:713:LEU:HA	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ILE:CD1	1:C:456:MET:HE1	2.51	0.41
1:C:352:ASP:OD1	1:C:352:ASP:N	2.49	0.41
1:D:255:ARG:HD2	1:D:260:ASN:OD1	2.20	0.41
1:D:302:PRO:HB3	1:D:342:PRO:CA	2.50	0.41
5:J:5:GLC:O3	5:J:6:GLC:C2	2.68	0.41
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.78	0.41
1:C:231:GLU:OE2	1:C:234:LYS:HE3	2.21	0.41
1:D:291:GLU:HB2	1:D:308:PRO:HG2	2.02	0.41
1:A:287:LEU:O	1:A:288:PRO:C	2.59	0.41
1:A:667:PHE:O	1:A:710:SER:HA	2.20	0.41
1:B:376:ASN:O	1:B:382:VAL:CG2	2.46	0.41
1:B:382:VAL:O	1:B:385:PHE:HB3	2.21	0.41
1:B:616:MET:HE3	1:B:651:ILE:HB	2.01	0.41
1:C:163:ARG:H	1:C:163:ARG:NH2	2.10	0.41
1:C:412:TYR:CE2	1:C:461:THR:CG2	2.99	0.41
1:C:551:ARG:HG2	1:C:602:LEU:HD23	2.01	0.41
1:C:585:ASP:HB3	1:C:588:LEU:CD1	2.51	0.41
1:C:589:LEU:HD23	1:C:589:LEU:HA	1.68	0.41
1:D:394:ILE:CD1	1:D:450:VAL:CG2	2.96	0.41
1:D:466:VAL:HA	1:D:475:LEU:HB2	2.02	0.41
1:D:470:GLN:HA	1:D:474:GLY:CA	2.41	0.41
1:D:539:MET:HB3	1:D:549:ASN:OD1	2.21	0.41
1:D:560:PHE:CD1	1:D:561:PRO:CD	2.96	0.41
1:D:640:ILE:HD12	1:D:640:ILE:HA	1.21	0.41
1:D:711:LEU:HD12	1:D:711:LEU:HA	1.91	0.41
1:A:359:HIS:CD2	1:A:376:ASN:HA	2.56	0.41
1:A:667:PHE:HA	1:A:705:HIS:CE1	2.55	0.41
1:A:677:GLU:OE1	1:A:693:ASN:OD1	2.39	0.41
1:B:669:ILE:HG22	1:B:671:GLN:H	1.86	0.41
1:C:187:LEU:CD2	1:C:219:LEU:CD2	2.96	0.41
1:C:298:TRP:HE1	1:C:580:HIS:CD2	2.38	0.41
1:C:640:ILE:HD13	1:C:654:ALA:CA	2.51	0.41
1:D:536:LEU:HB2	1:D:574:GLN:HG2	2.01	0.41
1:D:551:ARG:O	1:D:681:THR:HG21	2.19	0.41
1:D:606:LEU:CD1	1:D:679:LEU:CD1	2.99	0.41
1:D:627:GLU:HB3	1:D:642:VAL:HG22	2.02	0.41
5:J:6:GLC:O3	5:J:7:GLC:O2	2.32	0.41
1:A:172:SER:OG	1:A:174:ILE:HG12	2.20	0.41
1:A:193:ILE:O	1:A:193:ILE:CG1	2.68	0.41
1:A:271:GLN:O	1:A:274:PRO:HD2	2.20	0.41
1:A:337:VAL:HG23	1:A:337:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:ALA:HB1	1:A:653:VAL:HG11	2.03	0.41
1:A:665:TYR:O	1:A:711:LEU:O	2.39	0.41
1:B:167:ARG:O	1:B:167:ARG:HG3	2.20	0.41
1:B:294:PHE:CD1	1:B:295:ASP:N	2.89	0.41
1:B:472:MET:O	1:B:472:MET:HG2	2.21	0.41
1:B:557:MET:O	1:B:564:LYS:NZ	2.40	0.41
1:C:193:ILE:CG2	1:C:197:GLY:HA2	2.51	0.41
1:C:357:TYR:CD1	1:C:382:VAL:HG12	2.56	0.41
1:C:475:LEU:HD13	1:C:475:LEU:N	2.36	0.41
1:C:666:ARG:NH2	1:C:702:ILE:HD12	2.36	0.41
1:C:681:THR:HG23	1:C:681:THR:O	2.20	0.41
1:D:226:LYS:HA	1:D:396:ARG:HA	2.03	0.41
1:D:230:THR:O	1:D:230:THR:HG22	2.21	0.41
1:D:286:LEU:C	1:D:287:LEU:O	2.60	0.41
1:D:394:ILE:CA	1:D:399:ILE:HD11	2.47	0.41
1:D:535:ILE:O	1:D:539:MET:HE1	2.20	0.41
1:D:658:THR:O	1:D:718:LEU:HD11	2.21	0.41
1:A:184:ASN:HB2	1:A:220:ILE:O	2.21	0.41
1:A:189:LYS:NZ	4:I:1:GLC:O3	2.48	0.41
1:A:392:TYR:O	1:A:396:ARG:HB2	2.21	0.41
1:A:556:TRP:O	1:A:557:MET:C	2.58	0.41
1:A:629:LEU:O	1:A:630:VAL:HG13	2.21	0.41
1:A:632:ASP:N	1:A:632:ASP:OD1	2.48	0.41
1:B:153:VAL:HG22	1:B:159:TRP:HA	1.99	0.41
1:B:399:ILE:HA	1:B:399:ILE:HD12	1.74	0.41
1:C:233:ARG:CD	1:C:326:HIS:CD2	3.04	0.41
1:C:262:TRP:CE3	1:C:311:ARG:HB3	2.56	0.41
1:C:262:TRP:CZ3	1:C:311:ARG:HB3	2.56	0.41
1:D:567:PHE:CG	1:D:568:MET:N	2.89	0.41
1:B:125:LEU:HA	1:B:125:LEU:HD22	1.65	0.40
1:B:628:TRP:CD2	1:B:631:VAL:CG2	3.04	0.40
1:C:192:MET:HE2	1:C:352:ASP:HA	2.03	0.40
1:C:379:ARG:O	1:C:382:VAL:HG22	2.21	0.40
1:D:241:ALA:O	1:D:243:ILE:HD12	2.21	0.40
1:D:246:TYR:CE2	1:D:248:VAL:HG13	2.56	0.40
1:D:287:LEU:CB	1:D:288:PRO:HD2	2.50	0.40
1:D:458:GLU:HG2	1:D:483:LEU:HD11	2.04	0.40
1:D:556:TRP:CH2	1:D:639:LEU:CD1	3.04	0.40
1:A:211:GLN:NE2	1:A:215:GLU:HB3	2.36	0.40
1:A:350:GLU:H	1:A:358:GLU:CD	2.23	0.40
1:A:658:THR:C	1:A:718:LEU:CD1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:LEU:O	1:B:332:VAL:HA	2.22	0.40
1:B:503:HIS:N	1:B:503:HIS:ND1	2.69	0.40
1:B:527:GLU:HA	1:B:532:LYS:CD	2.47	0.40
1:D:266:ARG:CZ	1:D:320:TYR:CE1	3.04	0.40
1:D:377:TYR:HB3	1:D:438:PHE:HB2	2.04	0.40
1:D:667:PHE:CD1	1:D:667:PHE:O	2.74	0.40
1:D:689:SER:O	1:D:690:ASN:C	2.59	0.40
1:D:691:ALA:HB3	1:D:716:PRO:HB3	2.04	0.40
1:A:184:ASN:HA	1:A:220:ILE:HG23	2.02	0.40
1:A:285:GLU:HB2	1:A:333:ILE:HB	2.03	0.40
1:A:678:ILE:HG21	1:A:724:VAL:CG1	2.52	0.40
1:B:146:ASN:ND2	1:B:354:THR:HG21	2.36	0.40
1:B:147:ALA:O	1:B:175:TRP:CZ2	2.72	0.40
1:B:213:ARG:HG2	1:B:214:PRO:HA	2.02	0.40
1:B:678:ILE:HG21	1:B:678:ILE:HD13	1.78	0.40
1:D:233:ARG:N	1:D:233:ARG:HD2	2.36	0.40
1:D:399:ILE:HD13	1:D:402:LEU:HD21	2.04	0.40
1:D:527:GLU:N	1:D:527:GLU:OE2	2.54	0.40
1:D:686:TYR:C	1:D:687:HIS:CG	2.95	0.40
1:B:379:ARG:HH11	1:B:379:ARG:HD3	1.78	0.40
1:C:163:ARG:CZ	1:C:163:ARG:HB2	2.51	0.40
1:C:257:THR:H	1:C:257:THR:HG22	1.62	0.40
1:C:390:ALA:O	1:C:394:ILE:HG13	2.22	0.40
1:C:496:ASP:OD2	1:C:498:VAL:HG12	2.20	0.40
1:D:271:GLN:O	1:D:274:PRO:CG	2.69	0.40
1:D:297:SER:O	1:D:298:TRP:CB	2.69	0.40
1:D:529:VAL:HG22	1:D:532:LYS:NZ	2.36	0.40
1:D:575:GLY:HA2	1:D:585:ASP:OD2	2.21	0.40
1:A:248:VAL:HG13	1:A:568:MET:SD	2.62	0.40
1:A:372:THR:HB	1:A:373:LEU:H	1.64	0.40
1:A:685:HIS:CD2	2:H:4:GLC:H62	2.57	0.40
1:A:708:GLN:NE2	1:A:708:GLN:O	2.55	0.40
1:B:247:GLU:O	1:B:567:PHE:HD1	2.04	0.40
1:B:288:PRO:HB2	1:B:299:GLY:O	2.21	0.40
1:B:667:PHE:CE2	1:B:669:ILE:HD11	2.57	0.40
1:D:265:TYR:HA	1:D:268:LEU:HD22	2.04	0.40
1:D:456:MET:HE2	1:D:479:TYR:CD2	2.56	0.40
1:D:713:LEU:CD2	1:D:714:THR:H	2.30	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	596/613 (97%)	554 (93%)	32 (5%)	10 (2%)	9 39
1	B	585/613 (95%)	543 (93%)	35 (6%)	7 (1%)	13 48
1	C	600/613 (98%)	553 (92%)	41 (7%)	6 (1%)	15 53
1	D	492/613 (80%)	388 (79%)	70 (14%)	34 (7%)	1 6
All	All	2273/2452 (93%)	2038 (90%)	178 (8%)	57 (2%)	5 28

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	ARG
1	A	543	ALA
1	A	630	VAL
1	C	213	ARG
1	C	522	PRO
1	D	225	GLU
1	D	252	SER
1	D	254	ARG
1	D	262	TRP
1	D	307	ALA
1	D	309	THR
1	D	377	TYR
1	D	419	GLU
1	D	571	GLU
1	D	577	GLU
1	D	587	HIS
1	D	646	LYS
1	A	347	ALA
1	A	424	PRO
1	A	522	PRO
1	C	133	ASP
1	D	230	THR

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Mol	Chain	Res	Type
1	D	231	GLU
1	D	235	LYS
1	D	256	HIS
1	D	363	ARG
1	D	477	PHE
1	D	692	GLY
1	A	177	LEU
1	B	522	PRO
1	B	540	PRO
1	C	298	TRP
1	D	308	PRO
1	D	311	ARG
1	D	420	GLY
1	D	522	PRO
1	D	533	LYS
1	D	540	PRO
1	D	570	ASN
1	D	718	LEU
1	A	194	ASP
1	A	426	GLU
1	B	293	PRO
1	B	311	ARG
1	B	327	ALA
1	D	278	TRP
1	D	291	GLU
1	D	314	THR
1	D	586	TRP
1	B	350	GLU
1	C	451	SER
1	D	287	LEU
1	A	585	ASP
1	C	461	THR
1	D	302	PRO
1	D	716	PRO
1	B	296	GLY

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	510/521 (98%)	433 (85%)	77 (15%)	3 14
1	B	502/521 (96%)	429 (86%)	73 (14%)	3 15
1	C	513/521 (98%)	440 (86%)	73 (14%)	3 16
1	D	426/521 (82%)	303 (71%)	123 (29%)	0 2
All	All	1951/2084 (94%)	1605 (82%)	346 (18%)	2 9

All (346) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	THR
1	A	131	THR
1	A	135	VAL
1	A	139	ARG
1	A	152	VAL
1	A	155	GLN
1	A	162	ARG
1	A	163	ARG
1	A	170	LYS
1	A	193	ILE
1	A	201	LEU
1	A	203	SER
1	A	212	MET
1	A	213	ARG
1	A	231	GLU
1	A	235	LYS
1	A	240	ASP
1	A	261	PHE
1	A	266	ARG
1	A	267	GLU
1	A	282	THR
1	A	290	ASN
1	A	305	LEU
1	A	310	ARG
1	A	319	ARG
1	A	322	ILE
1	A	344	ASP
1	A	348	LEU
1	A	372	THR
1	A	374	ILE
1	A	383	SER

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Mol	Chain	Res	Type
1	A	407	VAL
1	A	418	LYS
1	A	423	ILE
1	A	425	ASN
1	A	426	GLU
1	A	430	ARG
1	A	441	ASN
1	A	460	SER
1	A	471	ASP
1	A	485	TRP
1	A	486	MET
1	A	490	LEU
1	A	504	HIS
1	A	506	LYS
1	A	523	LEU
1	A	529	VAL
1	A	533	LYS
1	A	535	ILE
1	A	542	ASP
1	A	545	GLN
1	A	588	LEU
1	A	590	GLU
1	A	593	ASP
1	A	595	TRP
1	A	602	LEU
1	A	604	ARG
1	A	614	LYS
1	A	635	GLU
1	A	640	ILE
1	A	649	ASN
1	A	651	ILE
1	A	653	VAL
1	A	664	ASP
1	A	670	ASN
1	A	674	LYS
1	A	679	LEU
1	A	681	THR
1	A	686	TYR
1	A	689	SER
1	A	699	SER
1	A	704	SER
1	A	708	GLN

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Mol	Chain	Res	Type
1	A	711	LEU
1	A	712	SER
1	A	720	THR
1	A	723	LEU
1	B	119	LEU
1	B	125	LEU
1	B	130	ASP
1	B	132	MET
1	B	138	THR
1	B	139	ARG
1	B	141	SER
1	B	148	ARG
1	B	152	VAL
1	B	163	ARG
1	B	167	ARG
1	B	169	ARG
1	B	170	LYS
1	B	171	GLU
1	B	172	SER
1	B	187	LEU
1	B	200	ARG
1	B	201	LEU
1	B	203	SER
1	B	212	MET
1	B	213	ARG
1	B	223	LEU
1	B	228	VAL
1	B	234	LYS
1	B	235	LYS
1	B	248	VAL
1	B	258	ASP
1	B	286	LEU
1	B	290	ASN
1	B	297	SER
1	B	314	THR
1	B	315	ARG
1	B	346	PHE
1	B	348	LEU
1	B	359	HIS
1	B	360	SER
1	B	372	THR
1	B	374	ILE

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Mol	Chain	Res	Type
1	B	380	ARG
1	B	382	VAL
1	B	396	ARG
1	B	399	ILE
1	B	405	ASP
1	B	407	VAL
1	B	409	SER
1	B	414	ASP
1	B	433	LEU
1	B	442	THR
1	B	456	MET
1	B	460	SER
1	B	470	GLN
1	B	471	ASP
1	B	472	MET
1	B	475	LEU
1	B	489	THR
1	B	496	ASP
1	B	498	VAL
1	B	503	HIS
1	B	511	ILE
1	B	524	SER
1	B	534	SER
1	B	538	ARG
1	B	545	GLN
1	B	593	ASP
1	B	609	THR
1	B	631	VAL
1	B	632	ASP
1	B	649	ASN
1	B	650	GLU
1	B	681	THR
1	B	696	THR
1	B	707	ARG
1	B	711	LEU
1	C	118	HIS
1	C	131	THR
1	C	151	SER
1	C	152	VAL
1	C	153	VAL
1	C	156	PHE
1	C	163	ARG

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Mol	Chain	Res	Type
1	C	166	MET
1	C	167	ARG
1	C	186	GLN
1	C	191	GLU
1	C	199	LEU
1	C	209	GLU
1	C	211	GLN
1	C	212	MET
1	C	213	ARG
1	C	219	LEU
1	C	232	GLU
1	C	254	ARG
1	C	255	ARG
1	C	257	THR
1	C	258	ASP
1	C	273	VAL
1	C	290	ASN
1	C	295	ASP
1	C	303	THR
1	C	344	ASP
1	C	348	LEU
1	C	360	SER
1	C	361	ASP
1	C	371	ASN
1	C	379	ARG
1	C	380	ARG
1	C	405	ASP
1	C	418	LYS
1	C	419	GLU
1	C	425	ASN
1	C	426	GLU
1	C	431	GLU
1	C	442	THR
1	C	459	GLU
1	C	460	SER
1	C	461	THR
1	C	472	MET
1	C	475	LEU
1	C	489	THR
1	C	505	ASP
1	C	524	SER
1	C	538	ARG

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Mol	Chain	Res	Type
1	C	576	ARG
1	C	581	ASP
1	C	586	TRP
1	C	603	VAL
1	C	609	THR
1	C	631	VAL
1	C	639	LEU
1	C	640	ILE
1	C	649	ASN
1	C	651	ILE
1	C	652	ILE
1	C	660	VAL
1	C	662	ARG
1	C	669	ILE
1	C	676	ARG
1	C	678	ILE
1	C	681	THR
1	C	683	SER
1	C	684	MET
1	C	693	ASN
1	C	696	THR
1	C	698	HIS
1	C	699	SER
1	C	725	ARG
1	D	229	GLN
1	D	232	GLU
1	D	238	GLN
1	D	247	GLU
1	D	248	VAL
1	D	253	TRP
1	D	254	ARG
1	D	255	ARG
1	D	257	THR
1	D	258	ASP
1	D	262	TRP
1	D	263	LEU
1	D	265	TYR
1	D	266	ARG
1	D	268	LEU
1	D	271	GLN
1	D	277	LYS
1	D	279	MET

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Mol	Chain	Res	Type
1	D	284	LEU
1	D	286	LEU
1	D	287	LEU
1	D	291	GLU
1	D	292	HIS
1	D	301	GLN
1	D	305	LEU
1	D	309	THR
1	D	310	ARG
1	D	316	ASP
1	D	319	ARG
1	D	340	HIS
1	D	341	PHE
1	D	343	THR
1	D	344	ASP
1	D	345	ASP
1	D	348	LEU
1	D	355	ASN
1	D	356	LEU
1	D	357	TYR
1	D	358	GLU
1	D	359	HIS
1	D	361	ASP
1	D	364	GLU
1	D	371	ASN
1	D	372	THR
1	D	379	ARG
1	D	385	PHE
1	D	392	TYR
1	D	394	ILE
1	D	396	ARG
1	D	400	ASP
1	D	407	VAL
1	D	416	SER
1	D	417	ARG
1	D	419	GLU
1	D	423	ILE
1	D	431	GLU
1	D	436	ILE
1	D	438	PHE
1	D	439	LEU
1	D	440	ARG

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Mol	Chain	Res	Type
1	D	442	THR
1	D	445	ILE
1	D	458	GLU
1	D	466	VAL
1	D	468	ARG
1	D	486	MET
1	D	496	ASP
1	D	498	VAL
1	D	508	THR
1	D	516	THR
1	D	528	VAL
1	D	532	LYS
1	D	535	ILE
1	D	536	LEU
1	D	537	ASP
1	D	538	ARG
1	D	560	PHE
1	D	566	LEU
1	D	570	ASN
1	D	581	ASP
1	D	584	LEU
1	D	586	TRP
1	D	589	LEU
1	D	594	ASN
1	D	595	TRP
1	D	597	HIS
1	D	599	VAL
1	D	602	LEU
1	D	604	ARG
1	D	605	ASP
1	D	607	ASN
1	D	612	HIS
1	D	614	LYS
1	D	624	TYR
1	D	629	LEU
1	D	631	VAL
1	D	632	ASP
1	D	638	VAL
1	D	639	LEU
1	D	640	ILE
1	D	643	ARG
1	D	647	GLU

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Mol	Chain	Res	Type
1	D	649	ASN
1	D	650	GLU
1	D	662	ARG
1	D	674	LYS
1	D	678	ILE
1	D	682	ASP
1	D	684	MET
1	D	686	TYR
1	D	687	HIS
1	D	693	ASN
1	D	696	THR
1	D	697	VAL
1	D	698	HIS
1	D	700	ASP
1	D	702	ILE
1	D	705	HIS
1	D	710	SER
1	D	713	LEU
1	D	720	THR
1	D	723	LEU
1	D	724	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	326	HIS
1	A	504	HIS
1	A	649	ASN
1	A	670	ASN
1	A	690	ASN
1	A	693	ASN
1	A	708	GLN
1	B	211	GLN
1	B	256	HIS
1	B	384	ASN
1	B	389	ASN
1	B	425	ASN
1	B	685	HIS
1	C	355	ASN
1	C	545	GLN
1	C	580	HIS

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Mol	Chain	Res	Type
1	C	690	ASN
1	D	326	HIS
1	D	384	ASN
1	D	389	ASN
1	D	443	ASN
1	D	597	HIS
1	D	600	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

38 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	GLC	E	1	2	12,12,12	0.47	0	17,17,17	0.53	0
2	GLC	E	2	2	11,11,12	0.26	0	15,15,17	0.64	0
2	GLC	E	3	2	11,11,12	0.52	0	15,15,17	1.97	2 (13%)
2	GLC	E	4	2	11,11,12	0.89	1 (9%)	15,15,17	2.01	2 (13%)
2	GLC	E	5	2	11,11,12	0.27	0	15,15,17	0.64	0
2	GLC	F	1	2	12,12,12	0.45	0	17,17,17	0.52	0
2	GLC	F	2	2	11,11,12	0.27	0	15,15,17	0.62	0
2	GLC	F	3	2	11,11,12	0.28	0	15,15,17	0.67	0
2	GLC	F	4	2	11,11,12	0.28	0	15,15,17	0.69	0
2	GLC	F	5	2	11,11,12	0.25	0	15,15,17	0.63	0
3	GLC	G	1	3	12,12,12	0.46	0	17,17,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GLC	G	2	3	11,11,12	0.24	0	15,15,17	0.64	0
3	GLC	G	3	3	11,11,12	0.28	0	15,15,17	0.63	0
3	GLC	G	4	3	11,11,12	0.27	0	15,15,17	0.62	0
2	GLC	H	1	2	12,12,12	0.46	0	17,17,17	0.53	0
2	GLC	H	2	2	11,11,12	0.27	0	15,15,17	0.67	0
2	GLC	H	3	2	11,11,12	0.25	0	15,15,17	0.65	0
2	GLC	H	4	2	11,11,12	0.26	0	15,15,17	0.70	0
2	GLC	H	5	2	11,11,12	0.27	0	15,15,17	0.64	0
4	GLC	I	1	4	12,12,12	0.51	0	17,17,17	0.70	0
4	GLC	I	2	4	11,11,12	0.28	0	15,15,17	0.73	0
4	GLC	I	3	4	11,11,12	0.27	0	15,15,17	0.64	0
5	GLC	J	1	5	12,12,12	0.46	0	17,17,17	0.53	0
5	GLC	J	2	5	11,11,12	0.27	0	15,15,17	0.67	0
5	GLC	J	3	5	11,11,12	0.29	0	15,15,17	0.97	1 (6%)
5	GLC	J	4	5	11,11,12	0.52	0	15,15,17	1.89	3 (20%)
5	GLC	J	5	5	11,11,12	0.74	0	15,15,17	2.20	3 (20%)
5	GLC	J	6	5	11,11,12	0.26	0	15,15,17	0.68	0
5	GLC	J	7	5	11,11,12	0.26	0	15,15,17	0.62	0
6	GLC	K	1	6	12,12,12	0.46	0	17,17,17	0.51	0
6	GLC	K	2	6	11,11,12	0.27	0	15,15,17	0.63	0
6	GLC	L	1	6	12,12,12	0.45	0	17,17,17	0.52	0
6	GLC	L	2	6	11,11,12	0.27	0	15,15,17	0.63	0
4	GLC	M	1	4	12,12,12	0.45	0	17,17,17	0.53	0
4	GLC	M	2	4	11,11,12	0.26	0	15,15,17	0.62	0
4	GLC	M	3	4	11,11,12	0.27	0	15,15,17	0.62	0
6	GLC	N	1	6	12,12,12	0.46	0	17,17,17	0.52	0
6	GLC	N	2	6	11,11,12	0.28	0	15,15,17	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2	-	2/2/19/22	0/1/1/1
2	GLC	E	4	2	-	2/2/19/22	0/1/1/1
2	GLC	E	5	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	1/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	F	3	2	-	0/2/19/22	0/1/1/1
2	GLC	F	4	2	-	0/2/19/22	0/1/1/1
2	GLC	F	5	2	-	2/2/19/22	0/1/1/1
3	GLC	G	1	3	-	0/2/22/22	0/1/1/1
3	GLC	G	2	3	-	2/2/19/22	0/1/1/1
3	GLC	G	3	3	-	0/2/19/22	0/1/1/1
3	GLC	G	4	3	-	2/2/19/22	0/1/1/1
2	GLC	H	1	2	-	2/2/22/22	0/1/1/1
2	GLC	H	2	2	-	2/2/19/22	0/1/1/1
2	GLC	H	3	2	-	0/2/19/22	0/1/1/1
2	GLC	H	4	2	-	0/2/19/22	0/1/1/1
2	GLC	H	5	2	-	2/2/19/22	0/1/1/1
4	GLC	I	1	4	-	0/2/22/22	0/1/1/1
4	GLC	I	2	4	-	1/2/19/22	0/1/1/1
4	GLC	I	3	4	-	2/2/19/22	0/1/1/1
5	GLC	J	1	5	-	1/2/22/22	0/1/1/1
5	GLC	J	2	5	-	0/2/19/22	0/1/1/1
5	GLC	J	3	5	-	0/2/19/22	0/1/1/1
5	GLC	J	4	5	-	2/2/19/22	0/1/1/1
5	GLC	J	5	5	-	0/2/19/22	0/1/1/1
5	GLC	J	6	5	-	0/2/19/22	0/1/1/1
5	GLC	J	7	5	-	0/2/19/22	0/1/1/1
6	GLC	K	1	6	-	0/2/22/22	0/1/1/1
6	GLC	K	2	6	-	2/2/19/22	0/1/1/1
6	GLC	L	1	6	-	2/2/22/22	0/1/1/1
6	GLC	L	2	6	-	2/2/19/22	0/1/1/1
4	GLC	M	1	4	-	2/2/22/22	0/1/1/1
4	GLC	M	2	4	-	2/2/19/22	0/1/1/1
4	GLC	M	3	4	-	1/2/19/22	0/1/1/1
6	GLC	N	1	6	-	1/2/22/22	0/1/1/1
6	GLC	N	2	6	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	GLC	O5-C1	2.36	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	5	GLC	C1-C2-C3	6.03	117.08	109.67
2	E	3	GLC	C1-C2-C3	5.73	116.70	109.67
2	E	4	GLC	C1-C2-C3	5.67	116.63	109.67
5	J	4	GLC	C1-C2-C3	4.73	115.47	109.67
2	E	3	GLC	C1-O5-C5	4.39	118.14	112.19
5	J	5	GLC	C1-O5-C5	4.37	118.11	112.19
2	E	4	GLC	C1-O5-C5	4.32	118.04	112.19
5	J	4	GLC	C2-C3-C4	3.55	117.03	110.89
5	J	5	GLC	C3-C4-C5	-2.87	105.11	110.24
5	J	4	GLC	C3-C4-C5	2.68	115.01	110.24
5	J	3	GLC	C1-C2-C3	2.51	112.75	109.67

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	GLC	O5-C5-C6-O6
2	E	4	GLC	C4-C5-C6-O6
6	K	2	GLC	O5-C5-C6-O6
6	L	2	GLC	O5-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
2	H	2	GLC	O5-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	E	3	GLC	C4-C5-C6-O6
4	M	1	GLC	C4-C5-C6-O6
4	M	2	GLC	C4-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
2	E	3	GLC	O5-C5-C6-O6
3	G	4	GLC	O5-C5-C6-O6
4	M	1	GLC	O5-C5-C6-O6
6	L	1	GLC	C4-C5-C6-O6
2	E	4	GLC	O5-C5-C6-O6
4	M	2	GLC	O5-C5-C6-O6
6	K	2	GLC	C4-C5-C6-O6
6	L	2	GLC	C4-C5-C6-O6
2	H	5	GLC	O5-C5-C6-O6
6	N	2	GLC	C4-C5-C6-O6
2	H	1	GLC	C4-C5-C6-O6
6	L	1	GLC	O5-C5-C6-O6
6	N	2	GLC	O5-C5-C6-O6
5	J	1	GLC	O5-C5-C6-O6
5	J	4	GLC	C4-C5-C6-O6
2	F	5	GLC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	G	2	GLC	C4-C5-C6-O6
3	G	4	GLC	C4-C5-C6-O6
4	I	2	GLC	O5-C5-C6-O6
2	F	5	GLC	O5-C5-C6-O6
3	G	2	GLC	O5-C5-C6-O6
5	J	4	GLC	O5-C5-C6-O6
4	I	3	GLC	C4-C5-C6-O6
4	I	3	GLC	O5-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
6	N	1	GLC	O5-C5-C6-O6
2	H	5	GLC	C4-C5-C6-O6
4	M	3	GLC	C4-C5-C6-O6

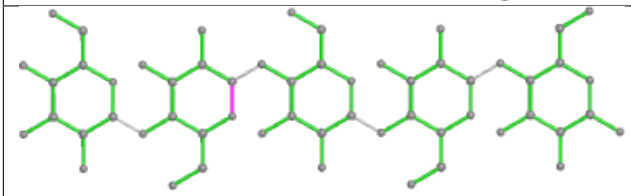
There are no ring outliers.

21 monomers are involved in 54 short contacts:

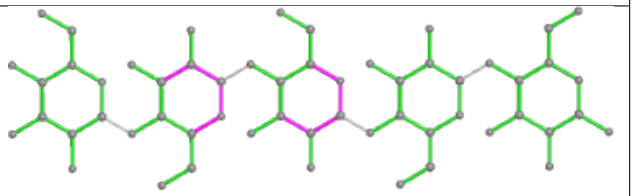
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4	GLC	5	0
5	J	7	GLC	1	0
4	M	2	GLC	1	0
3	G	3	GLC	3	0
2	F	3	GLC	2	0
5	J	5	GLC	7	0
5	J	6	GLC	16	0
5	J	4	GLC	1	0
2	H	2	GLC	2	0
4	M	3	GLC	2	0
6	L	2	GLC	1	0
2	E	5	GLC	2	0
2	F	4	GLC	2	0
4	I	1	GLC	3	0
3	G	4	GLC	2	0
2	H	3	GLC	4	0
2	E	3	GLC	5	0
2	E	2	GLC	2	0
6	L	1	GLC	6	0
2	H	4	GLC	1	0
5	J	1	GLC	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.

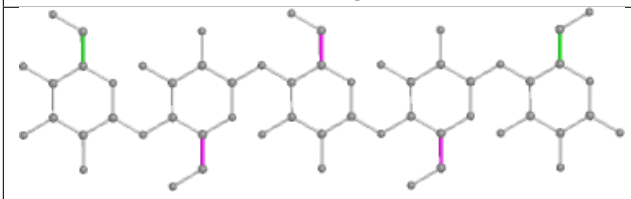
Oligosaccharide Chain E



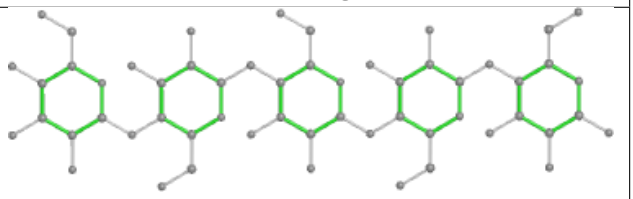
Bond lengths



Bond angles

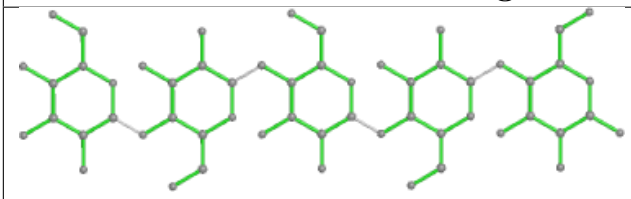


Torsions

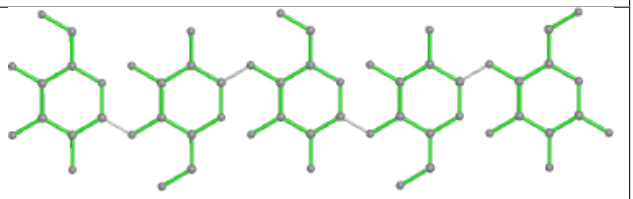


Rings

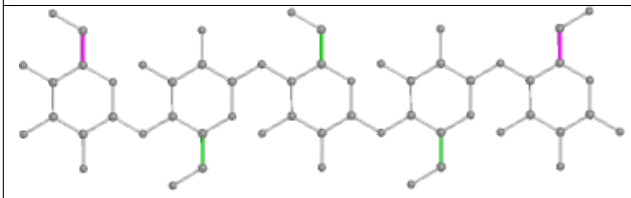
Oligosaccharide Chain F



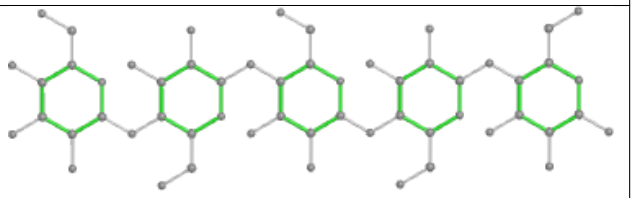
Bond lengths



Bond angles

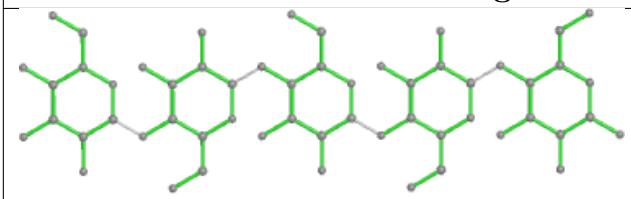


Torsions

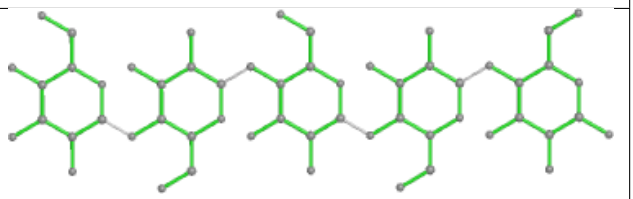


Rings

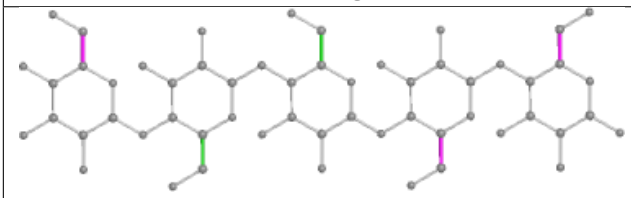
Oligosaccharide Chain H



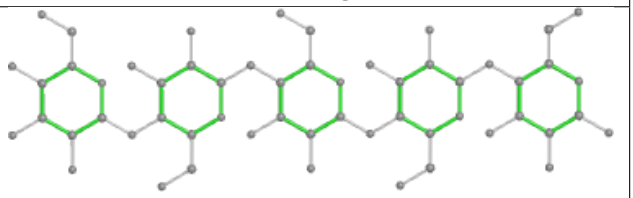
Bond lengths



Bond angles

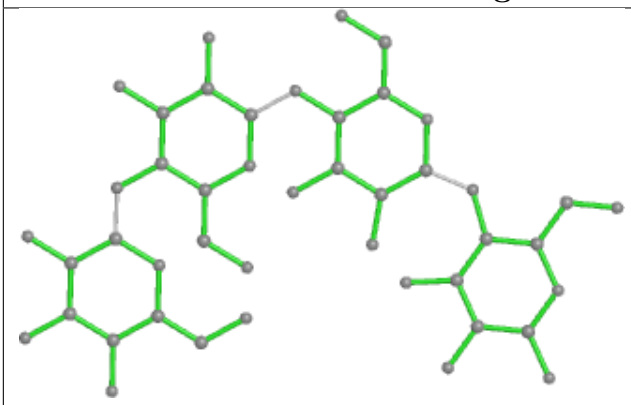


Torsions

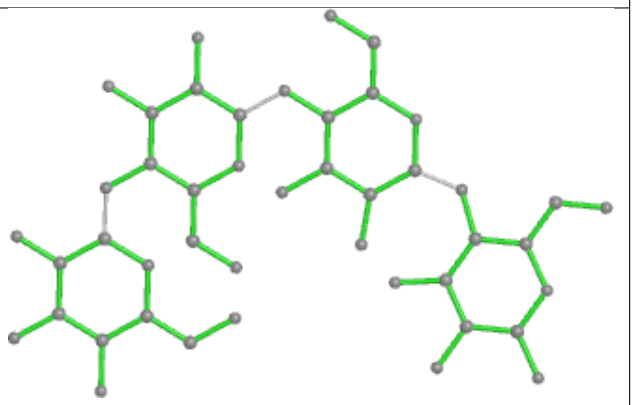


Rings

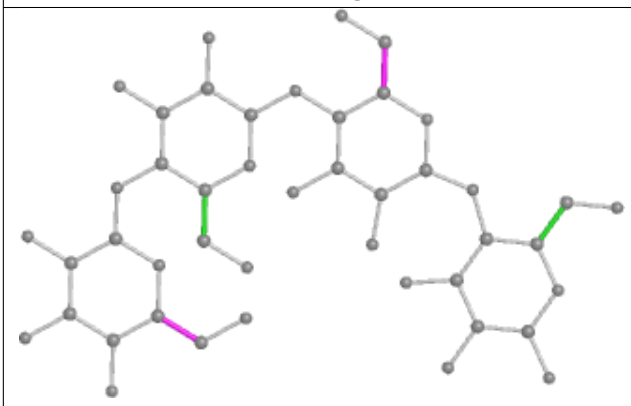
Oligosaccharide Chain G



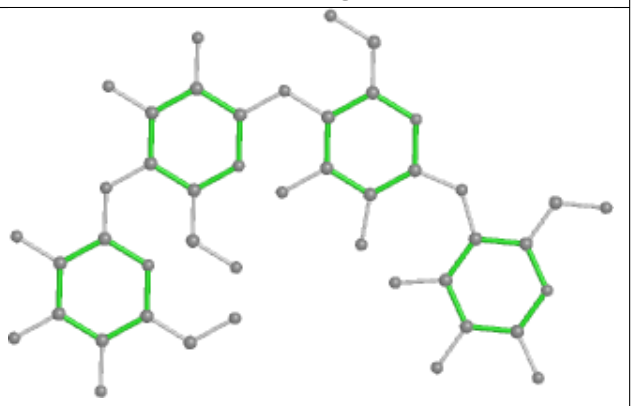
Bond lengths



Bond angles

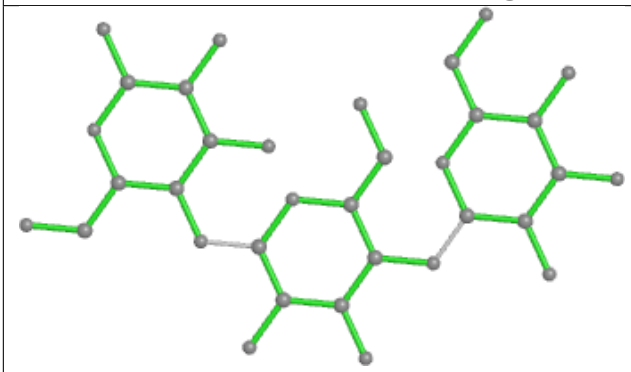


Torsions

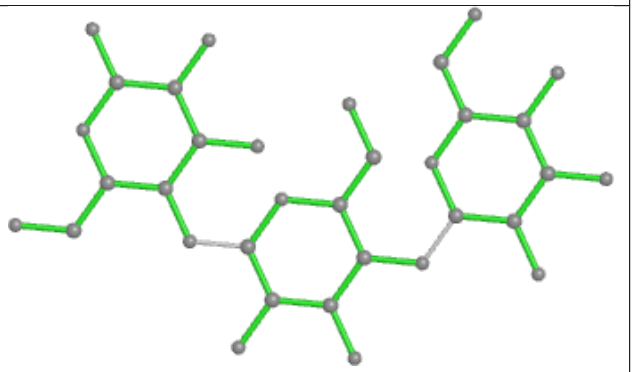


Rings

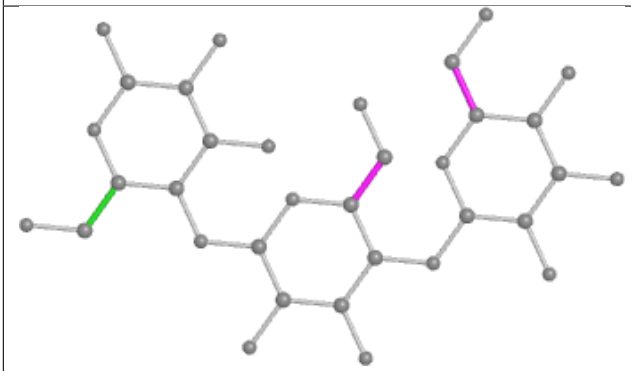
Oligosaccharide Chain I



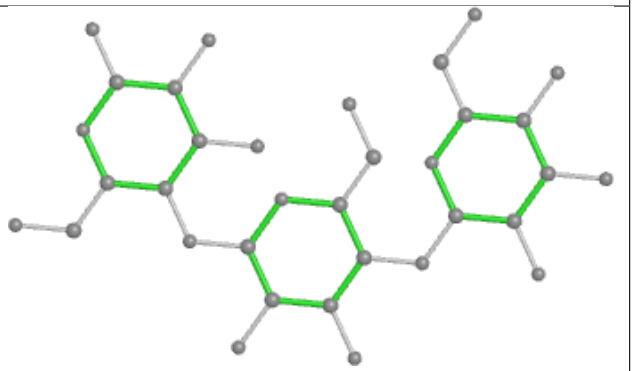
Bond lengths



Bond angles

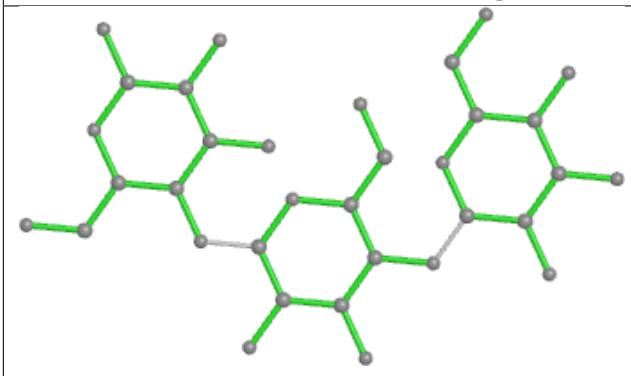


Torsions

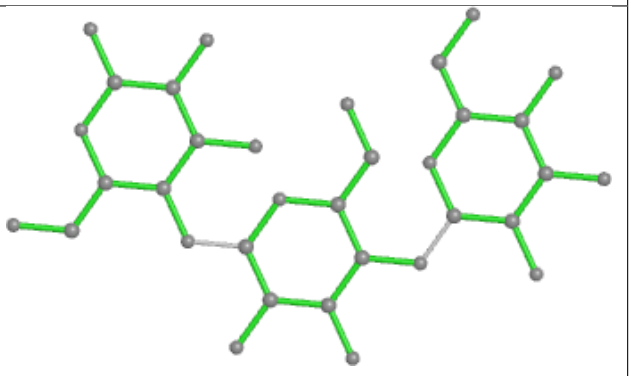


Rings

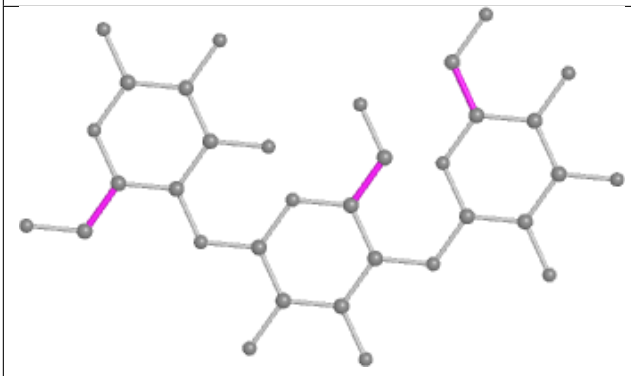
Oligosaccharide Chain M



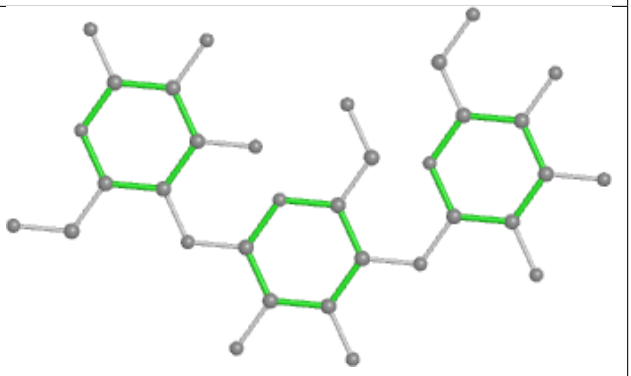
Bond lengths



Bond angles

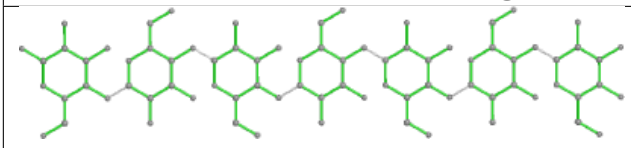


Torsions

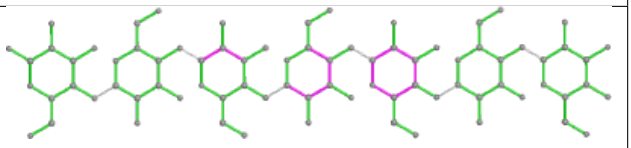


Rings

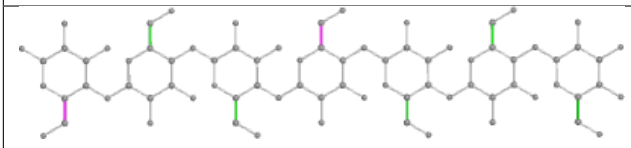
Oligosaccharide Chain J



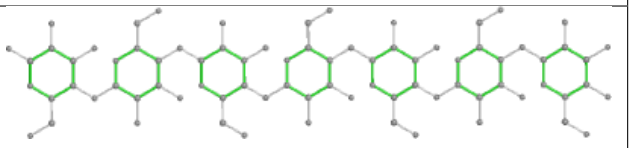
Bond lengths



Bond angles

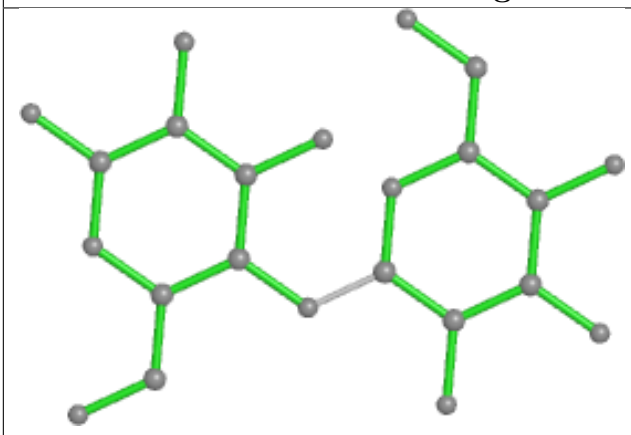


Torsions

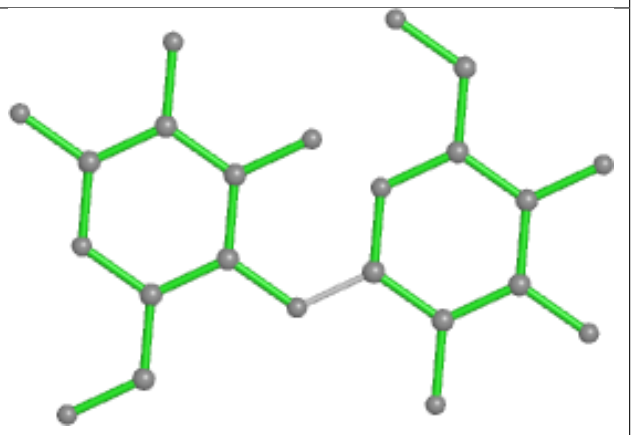


Rings

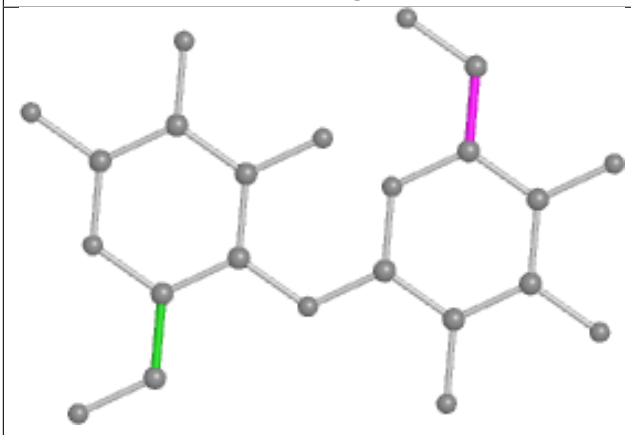
Oligosaccharide Chain K



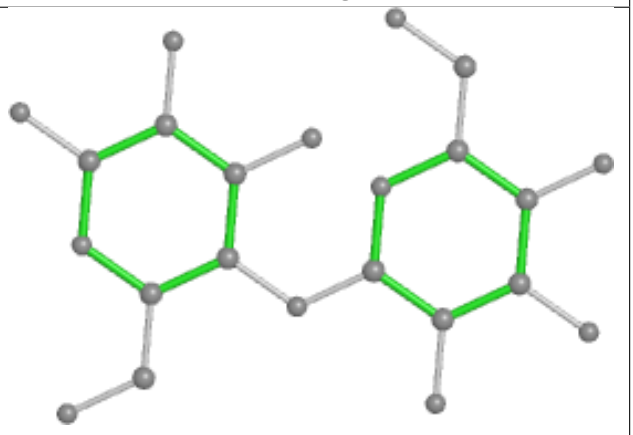
Bond lengths



Bond angles

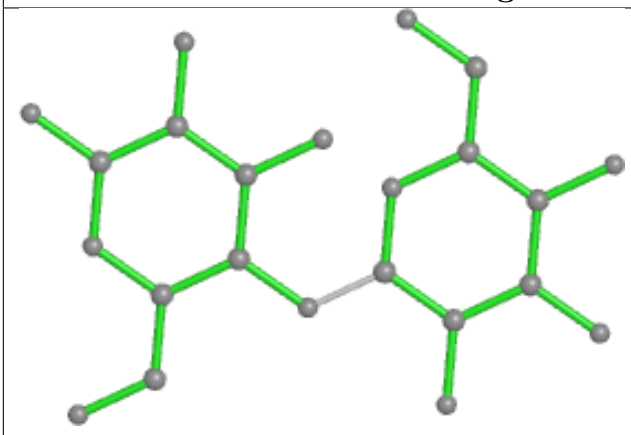


Torsions

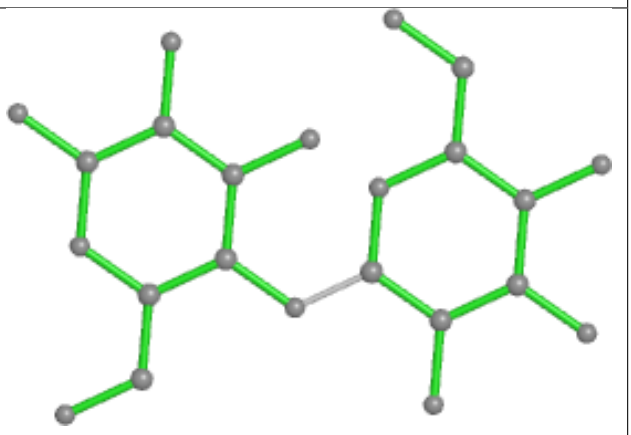


Rings

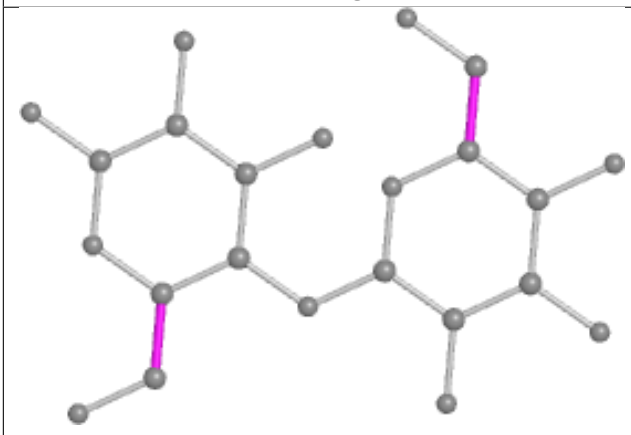
Oligosaccharide Chain L



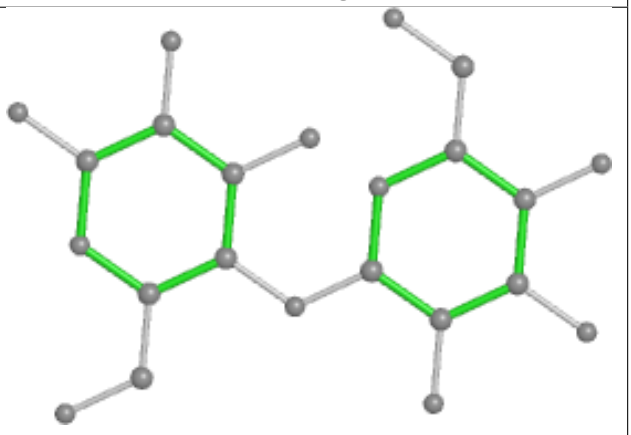
Bond lengths



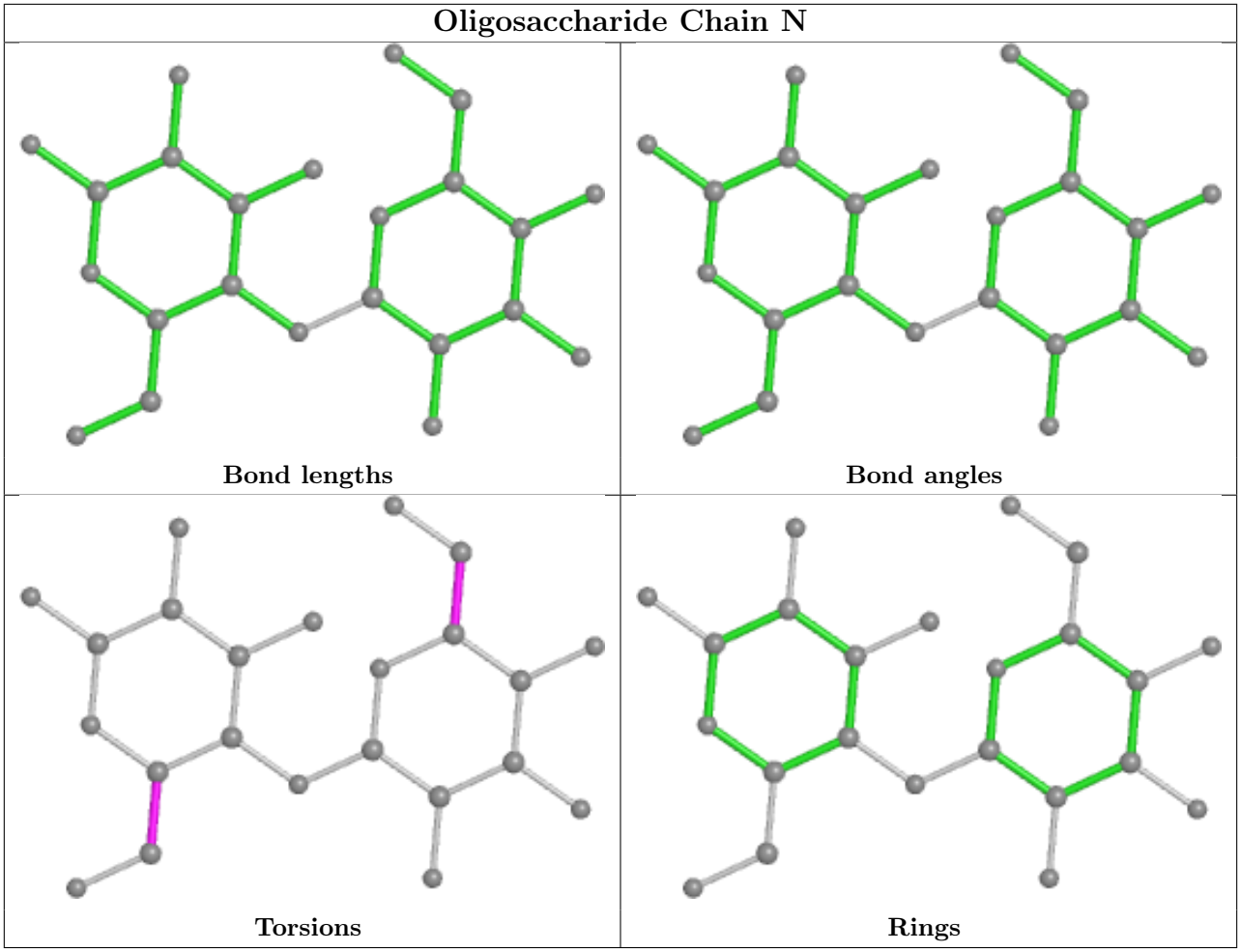
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

6 ligands 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	$\#\|Z\| > 2$
7	GLC	A	803	-	12,12,12	0.46	0	17,17,17	0.53	0
7	GLC	A	802	-	12,12,12	0.46	0	17,17,17	0.52	0
7	GLC	B	802	-	12,12,12	0.46	0	17,17,17	0.53	0
7	GLC	A	801	-	12,12,12	0.46	0	17,17,17	0.53	0
7	GLC	B	801	-	12,12,12	0.45	0	17,17,17	0.53	0
7	GLC	D	801	-	12,12,12	0.48	0	17,17,17	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GLC	A	803	-	-	0/2/22/22	0/1/1/1
7	GLC	A	802	-	-	1/2/22/22	0/1/1/1
7	GLC	B	802	-	-	0/2/22/22	0/1/1/1
7	GLC	A	801	-	-	2/2/22/22	0/1/1/1
7	GLC	B	801	-	-	1/2/22/22	0/1/1/1
7	GLC	D	801	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	801	GLC	C4-C5-C6-O6
7	A	801	GLC	O5-C5-C6-O6
7	B	801	GLC	O5-C5-C6-O6
7	A	802	GLC	C4-C5-C6-O6

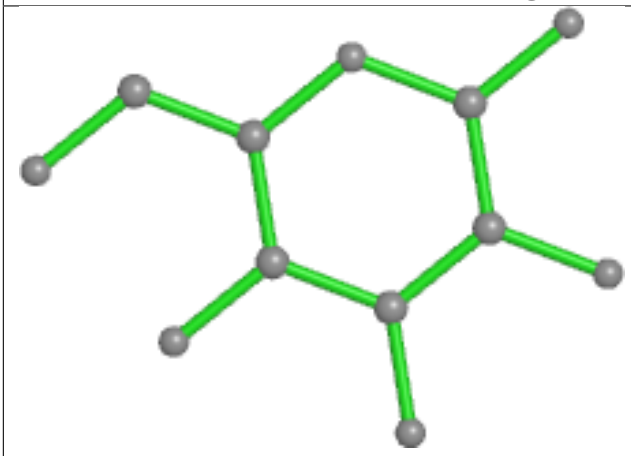
There are no ring outliers.

1 monomer is involved in 1 short contact:

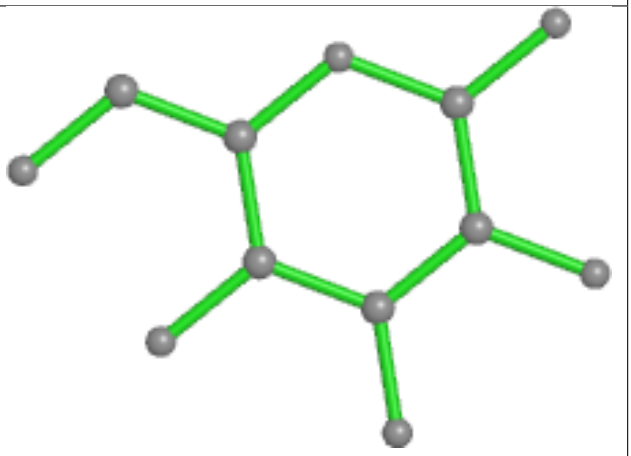
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	803	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

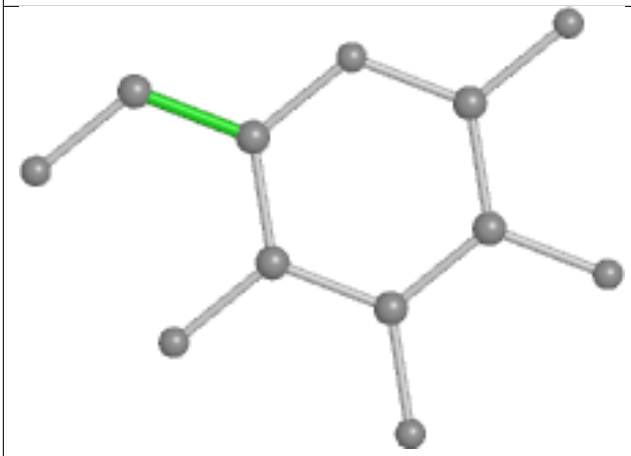
Ligand GLC A 803



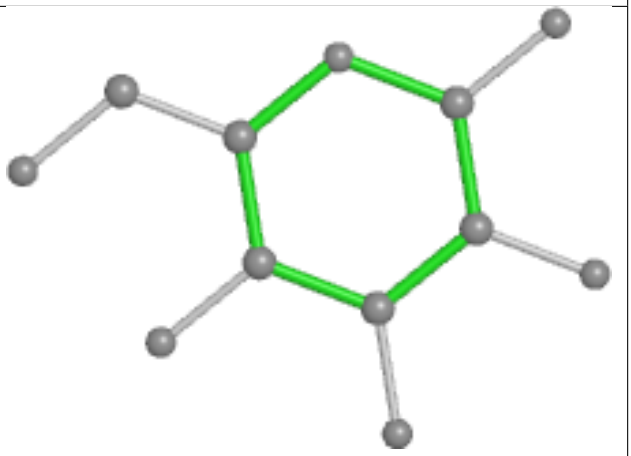
Bond lengths



Bond angles

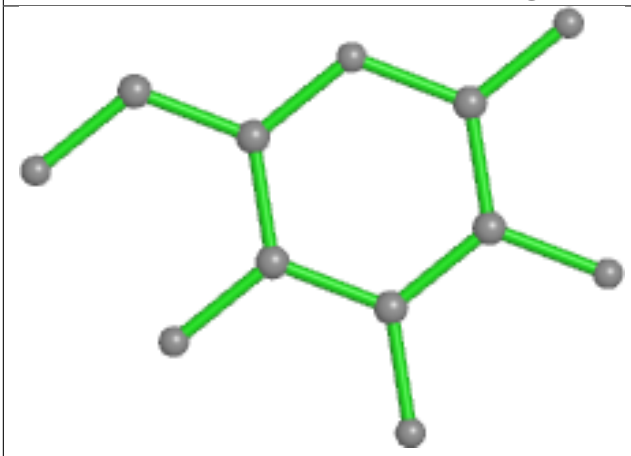


Torsions

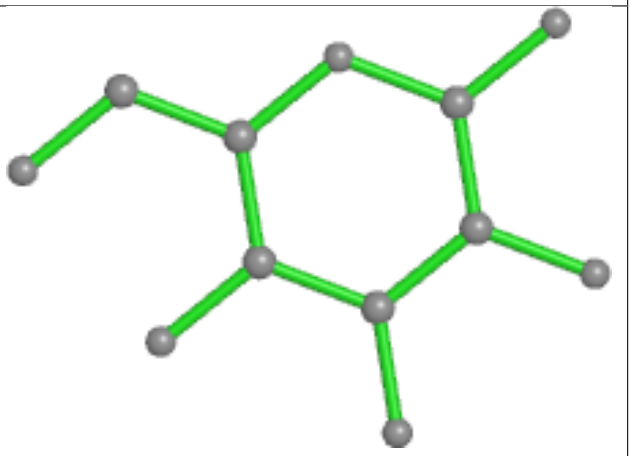


Rings

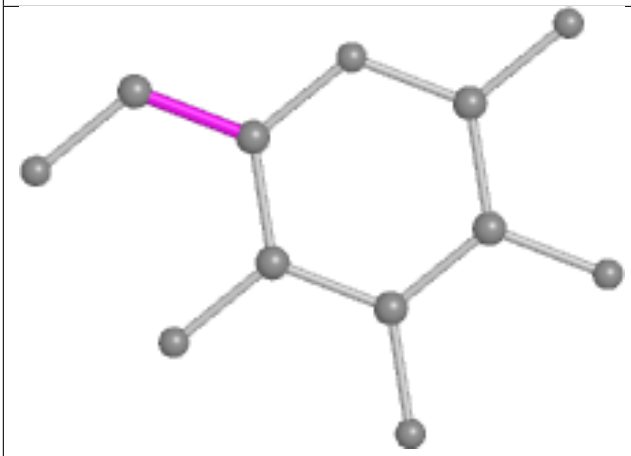
Ligand GLC A 802



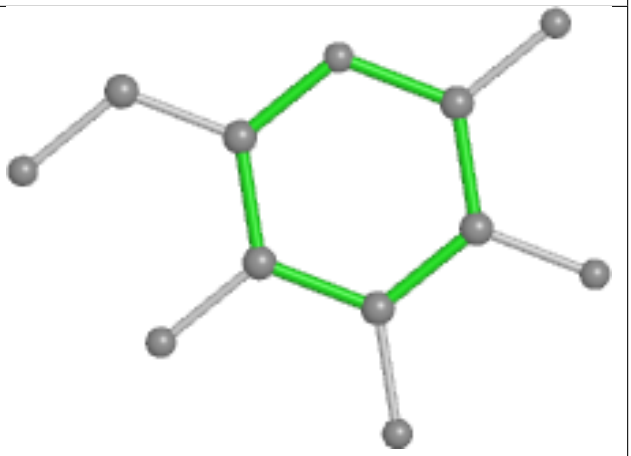
Bond lengths



Bond angles

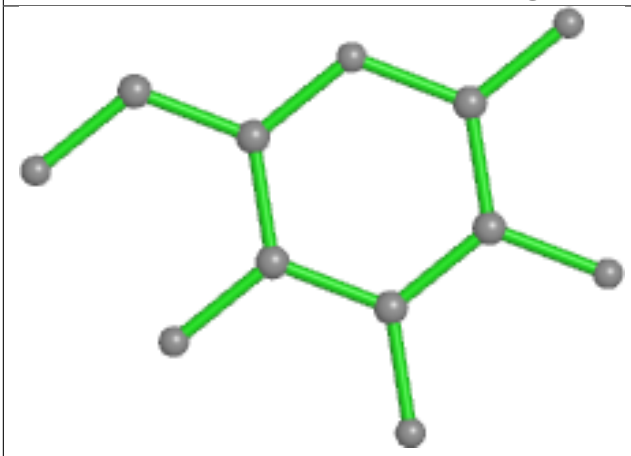


Torsions

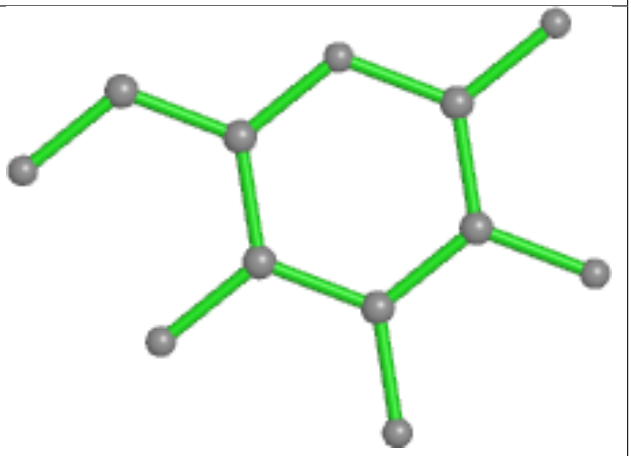


Rings

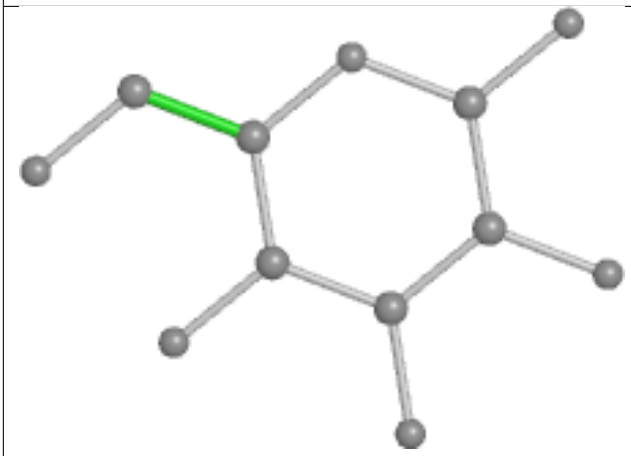
Ligand GLC B 802



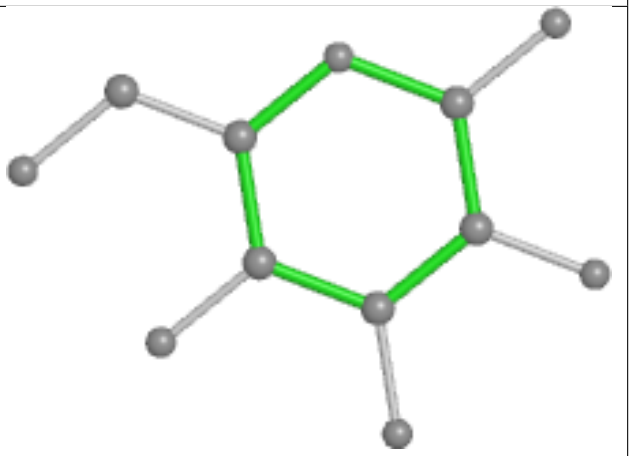
Bond lengths



Bond angles

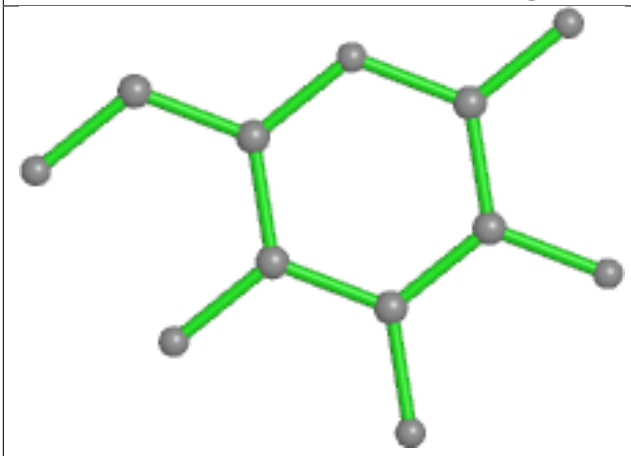


Torsions

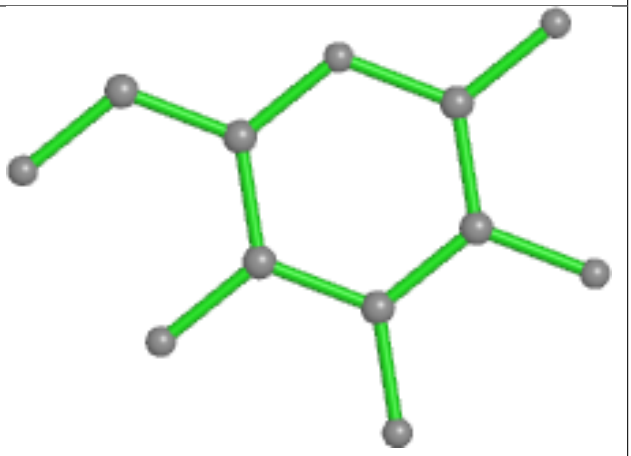


Rings

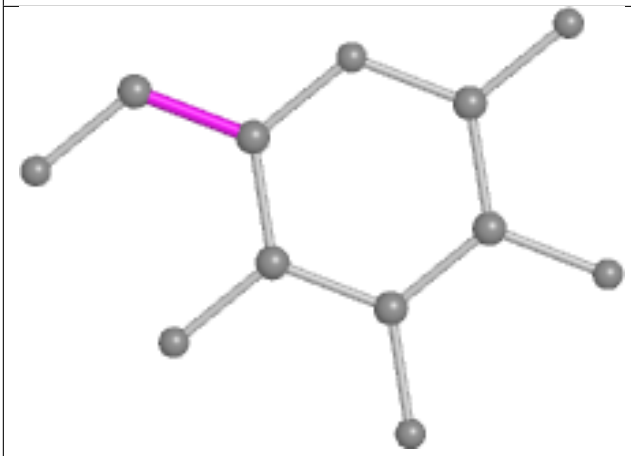
Ligand GLC A 801



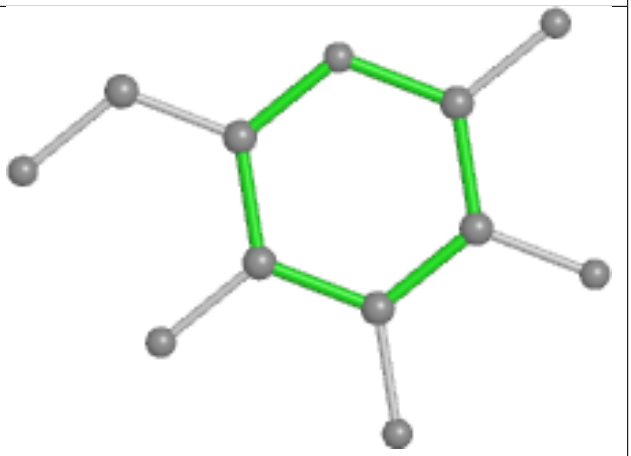
Bond lengths



Bond angles

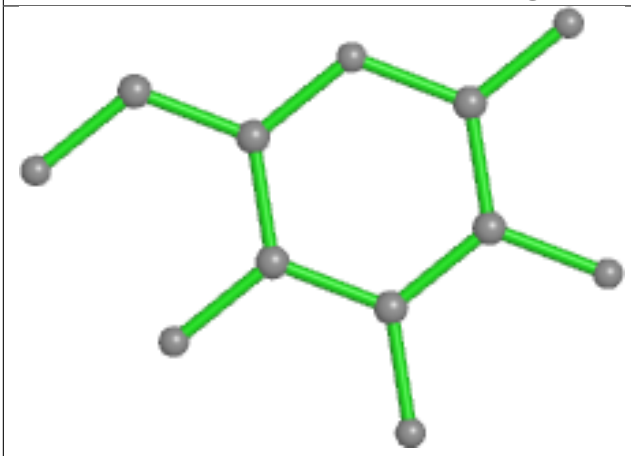


Torsions

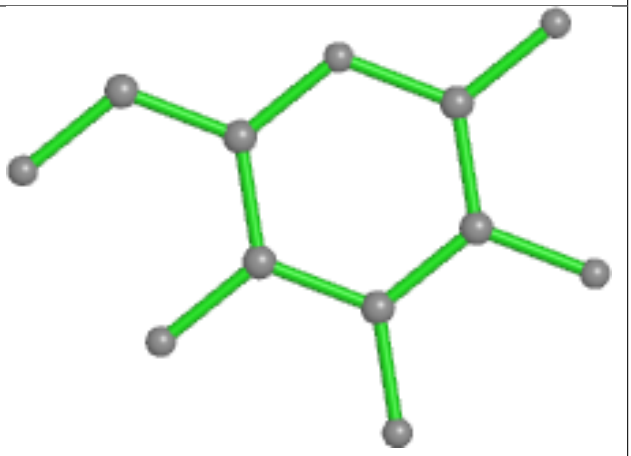


Rings

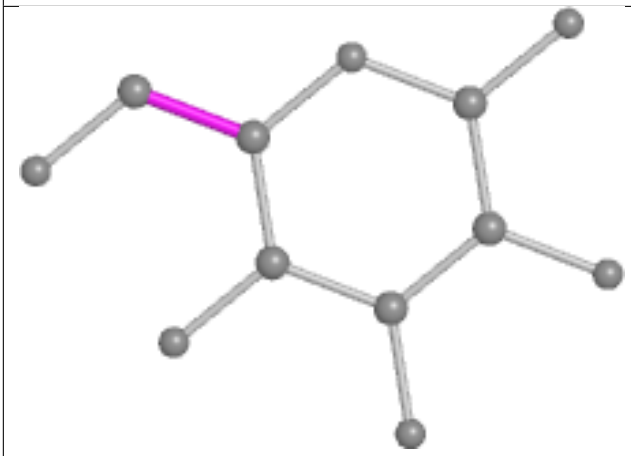
Ligand GLC B 801



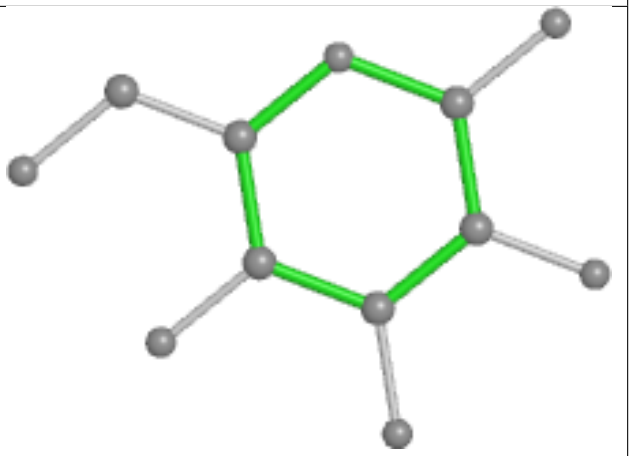
Bond lengths



Bond angles

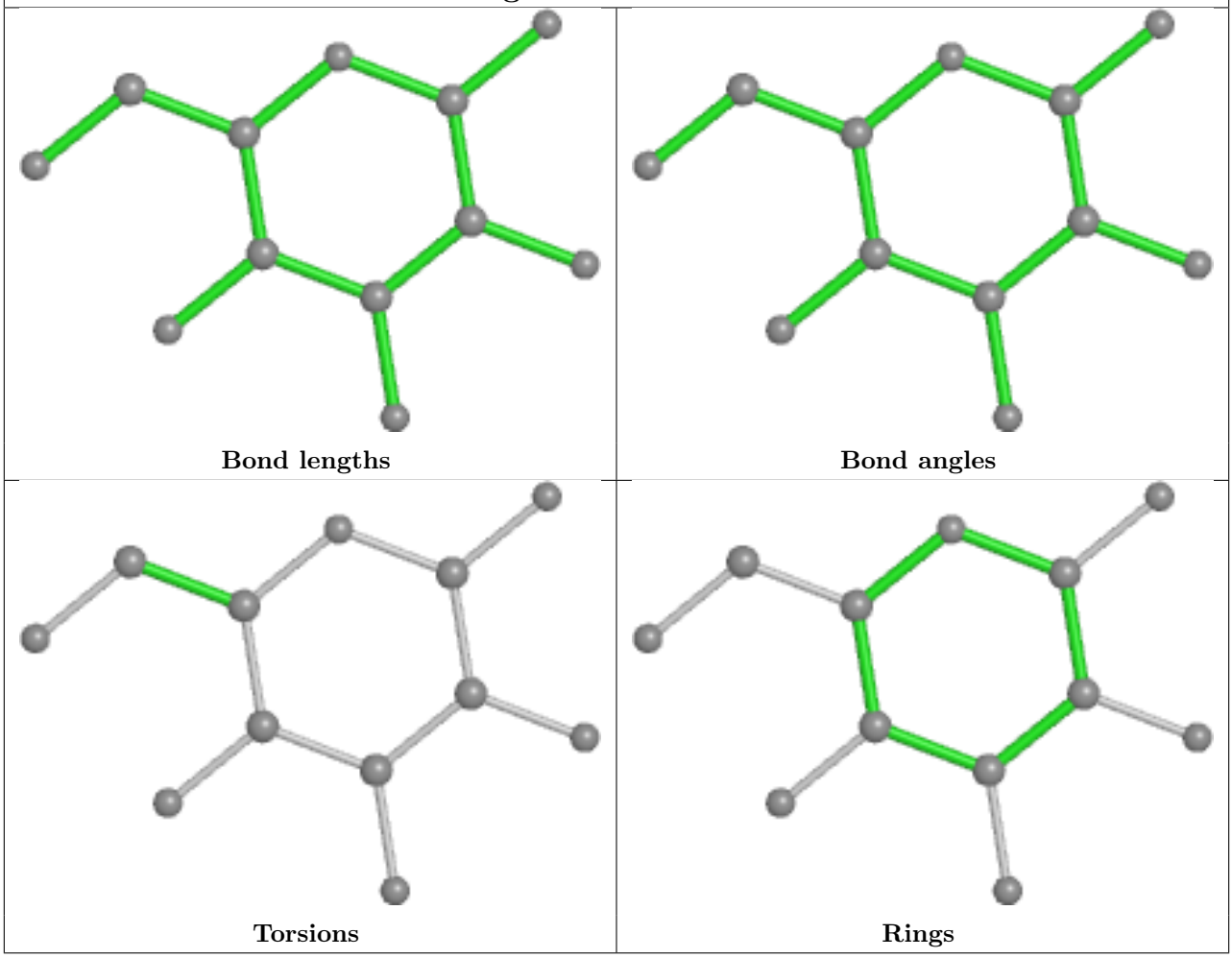


Torsions



Rings

Ligand GLC D 801



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	600/613 (97%)	-0.50	4 (0%)	87	69	44, 61, 89, 108	453 (75%)
1	B	591/613 (96%)	-0.62	2 (0%)	94	84	44, 57, 75, 97	447 (75%)
1	C	604/613 (98%)	-0.53	3 (0%)	91	75	45, 58, 77, 101	470 (77%)
1	D	496/613 (80%)	0.09	30 (6%)	21	7	70, 96, 125, 138	453 (91%)
All	All	2291/2452 (93%)	-0.41	39 (1%)	70	41	44, 62, 109, 138	1823 (79%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	362	PRO	8.6
1	D	262	TRP	5.8
1	D	344	ASP	5.6
1	D	258	ASP	4.7
1	D	257	THR	4.5
1	D	263	LEU	3.8
1	D	261	PHE	3.8
1	A	696	THR	3.6
1	D	594	ASN	3.6
1	B	372	THR	3.5
1	D	541	GLY	3.3
1	D	542	ASP	3.3
1	A	703	ALA	3.3
1	C	670	ASN	3.2
1	A	117	THR	3.1
1	D	346	PHE	3.0
1	D	316	ASP	3.0
1	D	348	LEU	2.9
1	D	226	LYS	2.9
1	D	373	LEU	2.8
1	D	228	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	695	GLY	2.6
1	B	132	MET	2.6
1	D	370	TRP	2.5
1	D	259	ASN	2.4
1	A	695	GLY	2.4
1	D	353	GLY	2.4
1	D	354	THR	2.4
1	D	357	TYR	2.3
1	D	543	ALA	2.3
1	C	709	HIS	2.2
1	D	255	ARG	2.2
1	D	584	LEU	2.1
1	D	363	ARG	2.1
1	D	711	LEU	2.1
1	D	347	ALA	2.1
1	D	351	PHE	2.0
1	D	227	VAL	2.0
1	D	585	ASP	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	GLC	J	6	11/12	0.48	0.37	98,108,114,114	4
3	GLC	G	2	11/12	0.51	0.48	104,111,117,119	4
3	GLC	G	4	11/12	0.52	0.29	88,93,100,111	5
3	GLC	G	3	11/12	0.58	0.46	88,96,107,110	4
2	GLC	H	3	11/12	0.61	0.36	93,105,120,126	3
3	GLC	G	1	12/12	0.65	0.56	20,20,20,20	0
2	GLC	F	2	11/12	0.67	0.27	64,71,79,87	3
5	GLC	J	7	11/12	0.67	0.41	107,115,122,126	4
4	GLC	M	1	12/12	0.70	0.24	114,123,124,129	5
5	GLC	J	5	11/12	0.70	0.28	89,98,105,125	5

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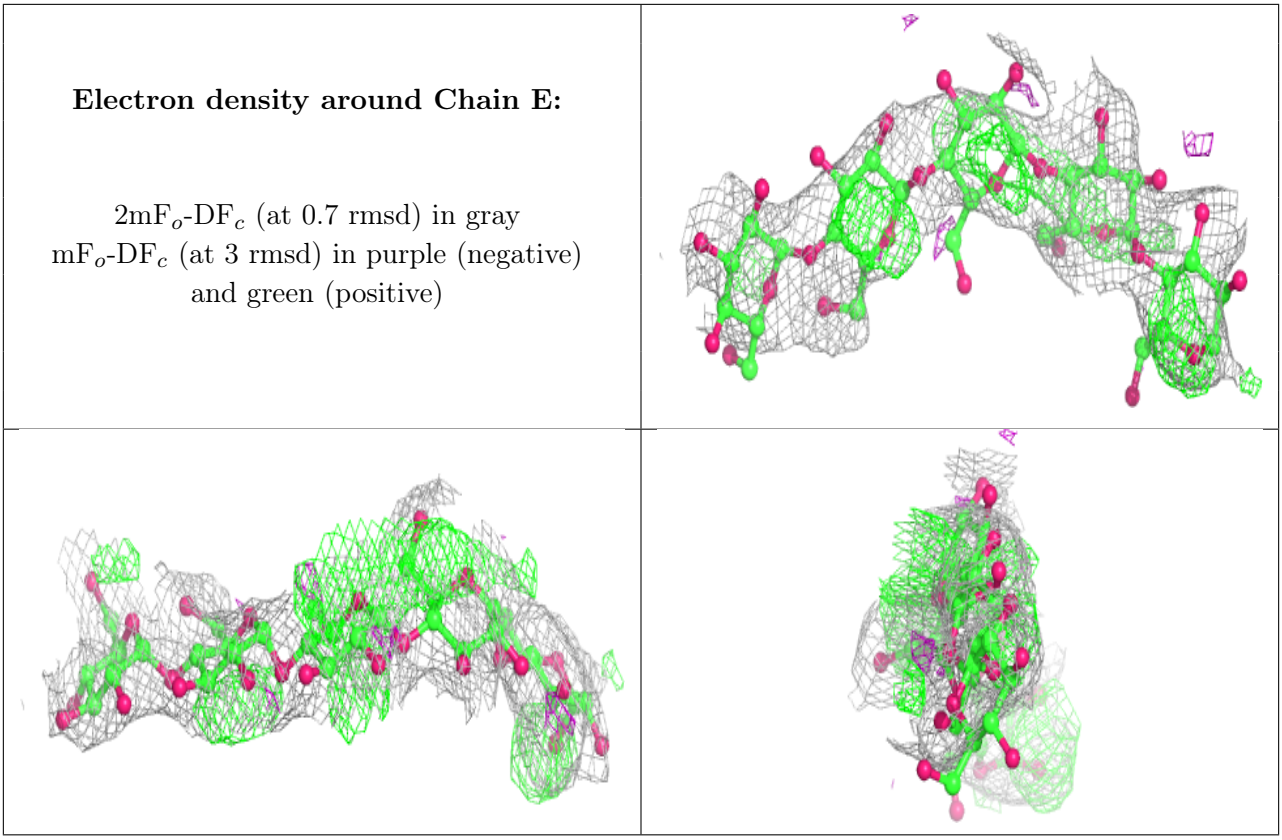
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	H	5	11/12	0.71	0.35	103,113,124,126	4
2	GLC	F	1	12/12	0.73	0.35	74,79,82,95	7
2	GLC	E	5	11/12	0.73	0.42	106,110,118,124	6
4	GLC	M	2	11/12	0.74	0.22	88,102,108,111	3
5	GLC	J	4	11/12	0.76	0.22	86,92,103,108	1
5	GLC	J	2	11/12	0.76	0.29	61,72,100,102	4
6	GLC	L	1	12/12	0.77	0.39	75,84,90,92	8
2	GLC	E	4	11/12	0.79	0.32	92,100,105,114	6
6	GLC	N	2	11/12	0.79	0.55	20,20,20,20	0
2	GLC	E	3	11/12	0.80	0.30	73,84,97,107	5
2	GLC	H	4	11/12	0.81	0.19	92,99,102,107	3
5	GLC	J	3	11/12	0.81	0.22	59,67,83,88	3
6	GLC	K	1	12/12	0.81	0.38	76,81,85,90	6
4	GLC	I	3	11/12	0.81	0.31	98,102,109,110	8
4	GLC	M	3	11/12	0.81	0.23	90,92,102,104	4
2	GLC	E	2	11/12	0.82	0.22	70,80,87,102	4
2	GLC	H	1	12/12	0.82	0.26	106,115,119,128	5
2	GLC	E	1	12/12	0.84	0.22	76,80,91,97	6
6	GLC	L	2	11/12	0.85	0.64	77,87,92,111	4
2	GLC	H	2	11/12	0.86	0.21	96,108,116,120	6
2	GLC	F	4	11/12	0.86	0.28	56,61,64,64	7
4	GLC	I	2	11/12	0.87	0.23	81,87,99,108	6
6	GLC	N	1	12/12	0.87	0.53	20,20,20,20	0
5	GLC	J	1	12/12	0.87	0.26	78,89,93,107	7
4	GLC	I	1	12/12	0.88	0.22	76,79,83,85	6
2	GLC	F	5	11/12	0.88	0.23	57,67,71,77	6
6	GLC	K	2	11/12	0.90	0.23	68,72,76,80	5
2	GLC	F	3	11/12	0.93	0.21	61,65,72,74	5

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.

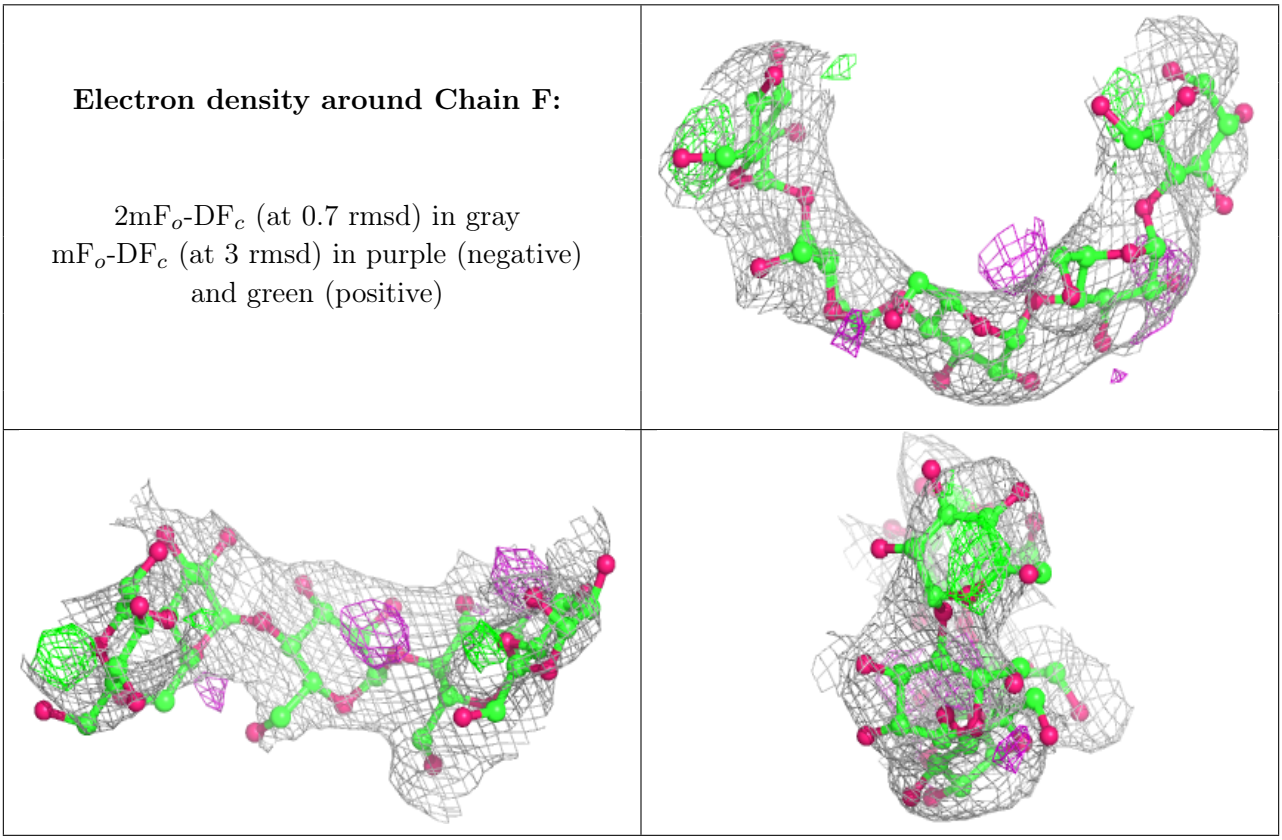
Electron density around Chain E:

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



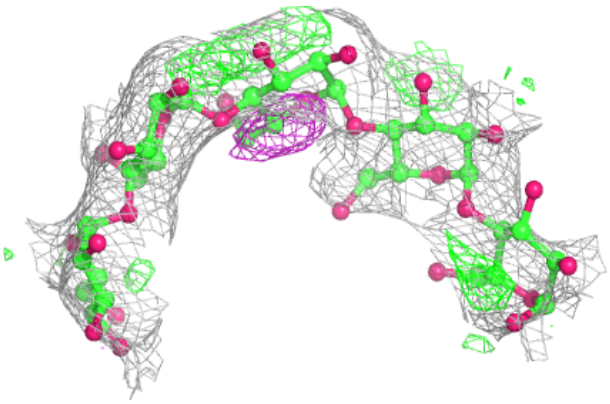
Electron density around Chain F:

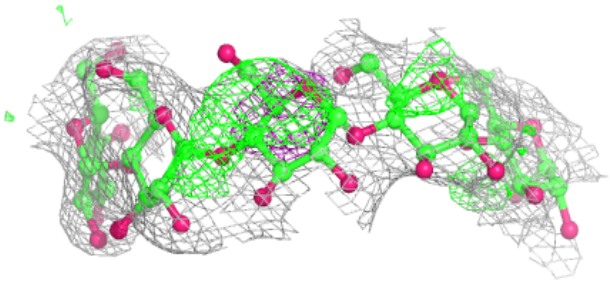
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

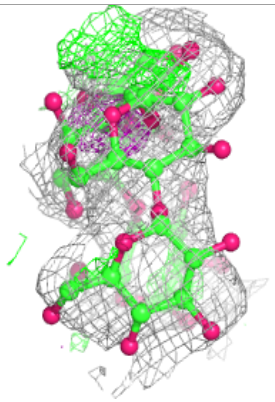


Electron density around Chain H:

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

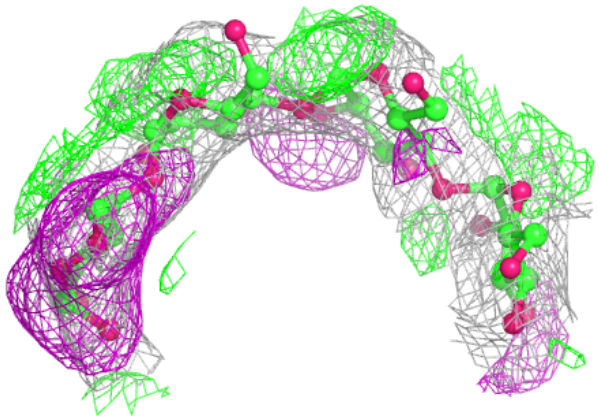


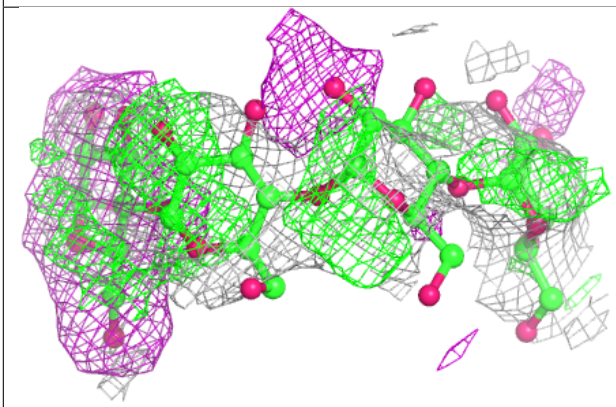


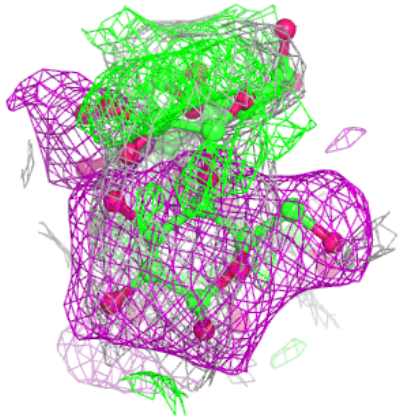


Electron density around Chain G:

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

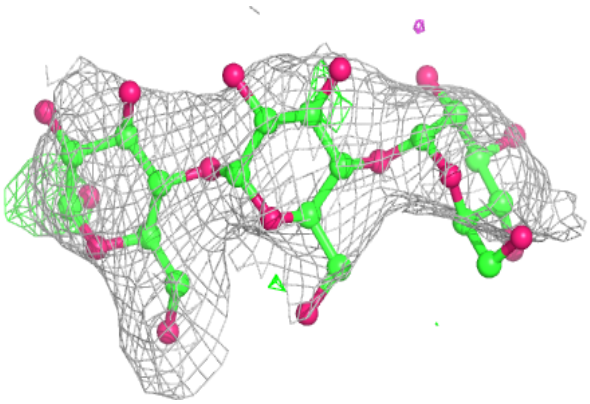


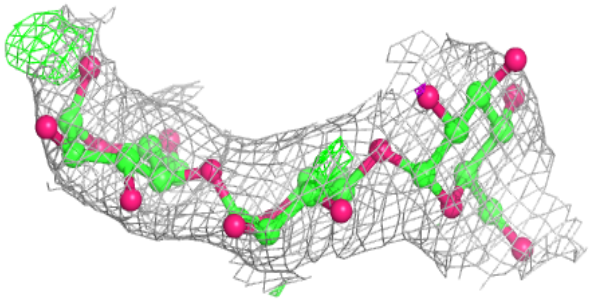


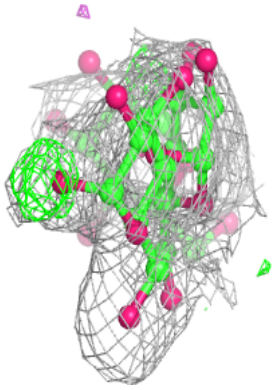


Electron density around Chain I:

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

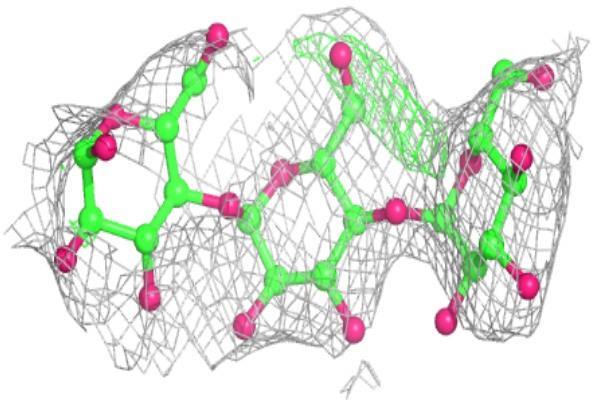


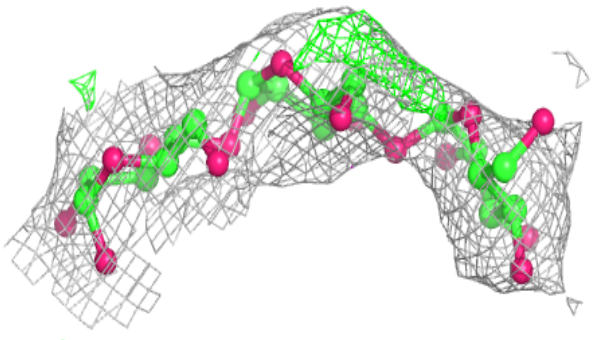


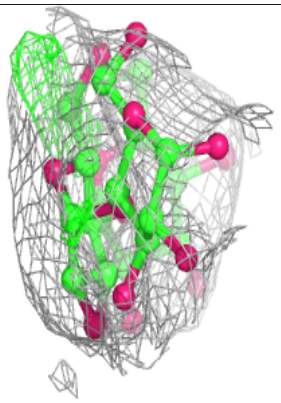


Electron density around Chain M:

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

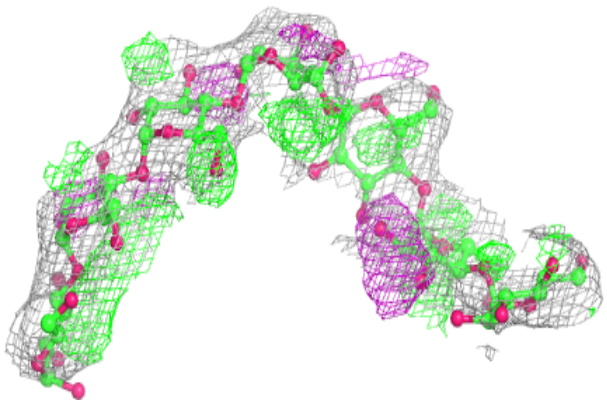


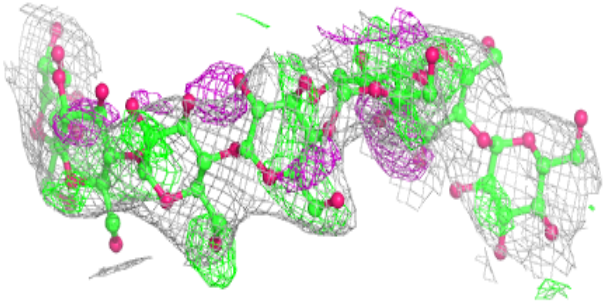


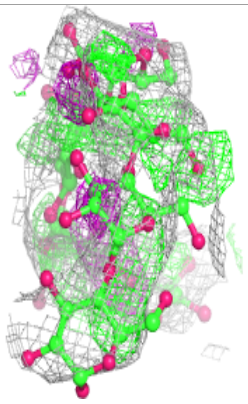


Electron density around Chain J:

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

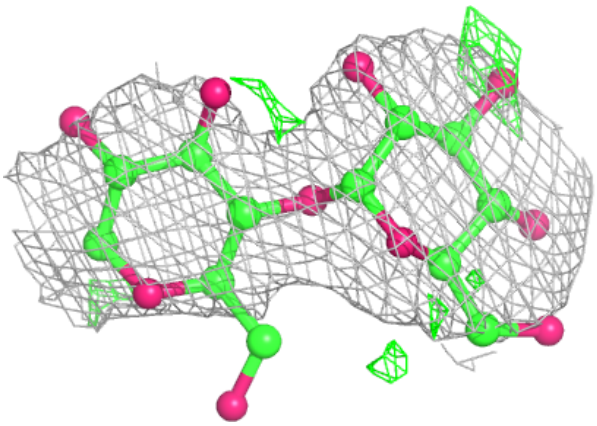


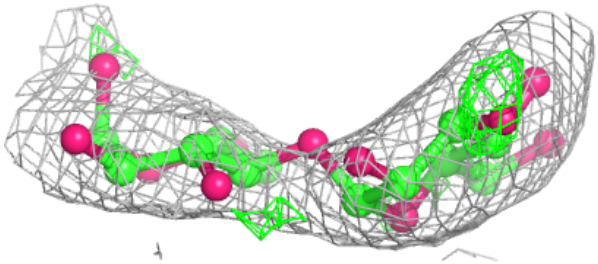


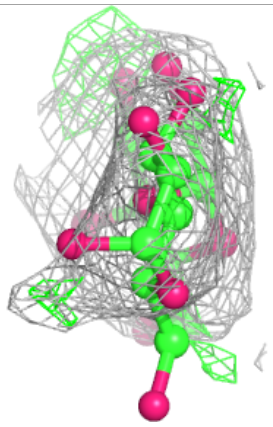


Electron density around Chain K:

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

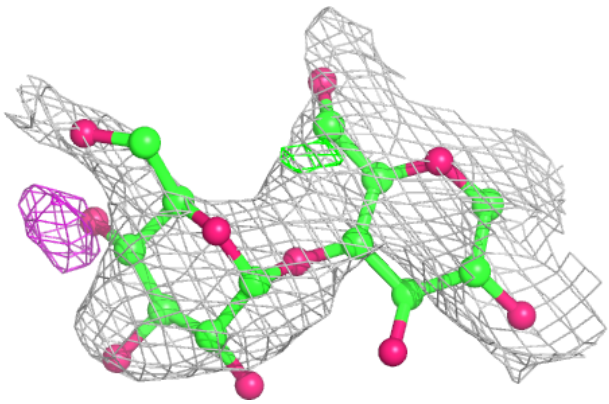


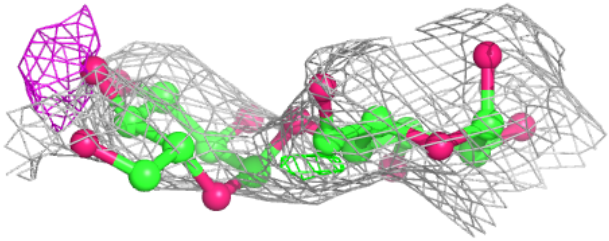


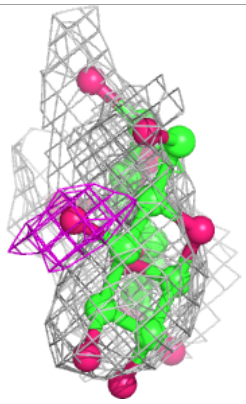


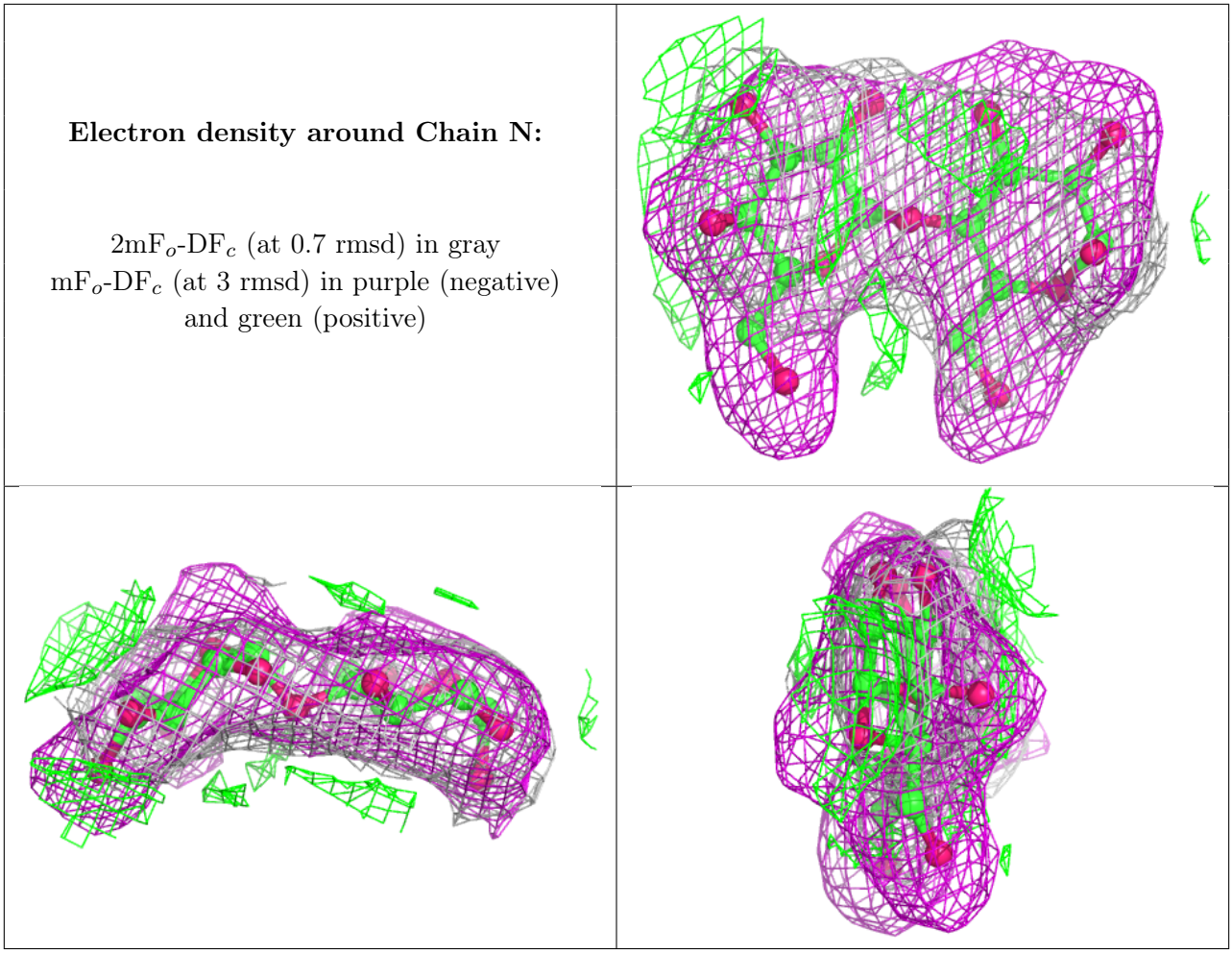
Electron density around Chain L:

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









6.4 Ligands

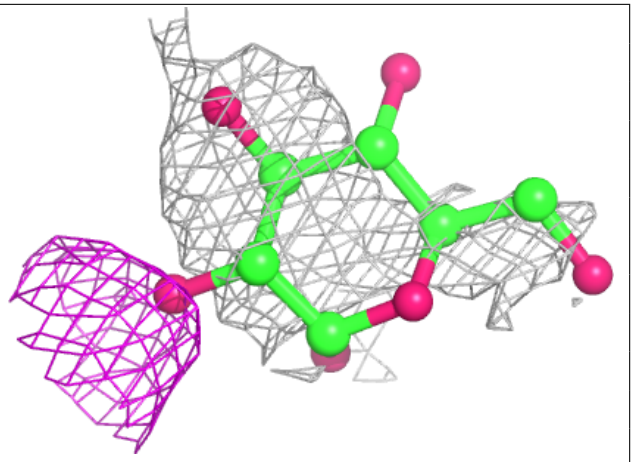
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

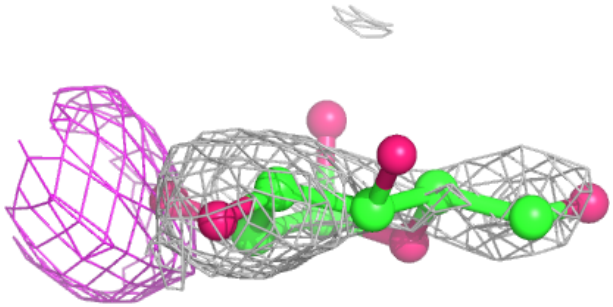
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GLC	B	802	12/12	0.61	0.54	73,77,85,86	9
7	GLC	A	802	12/12	0.75	0.32	93,102,107,114	5
7	GLC	A	803	12/12	0.76	0.55	20,20,20,20	0
7	GLC	A	801	12/12	0.81	0.25	70,87,93,94	5
7	GLC	D	801	12/12	0.82	0.40	20,20,20,20	0
7	GLC	B	801	12/12	0.85	0.30	64,74,84,85	6

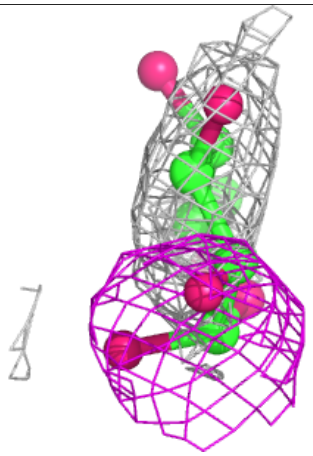
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GLC B 802:

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

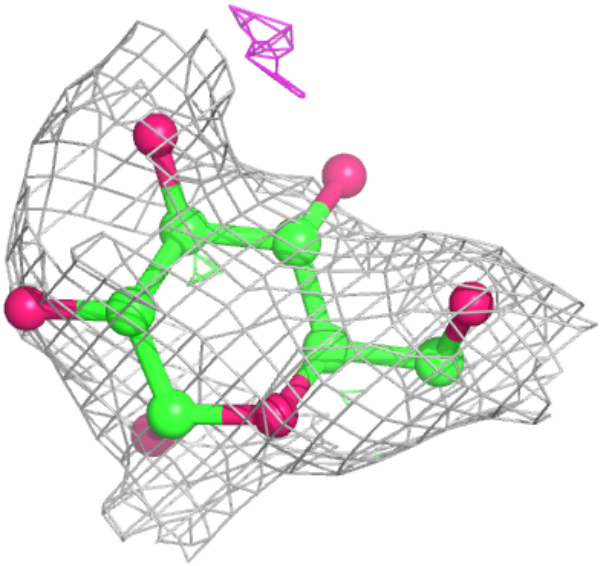


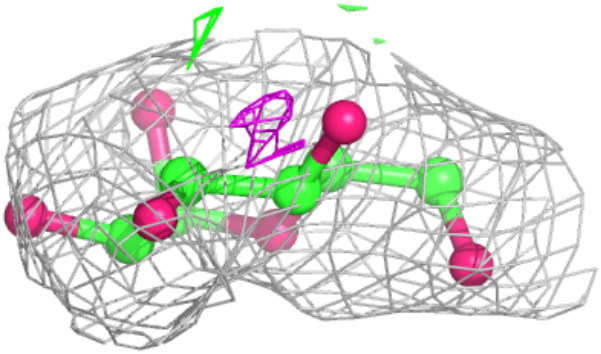


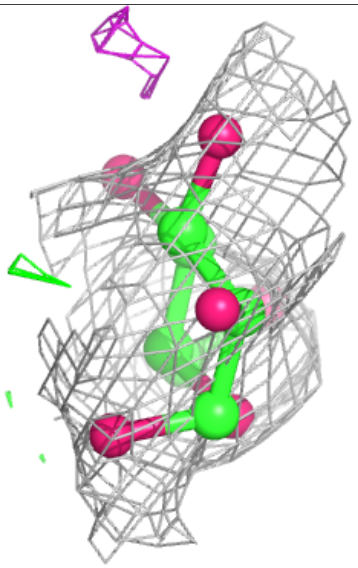


Electron density around GLC A 802:

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

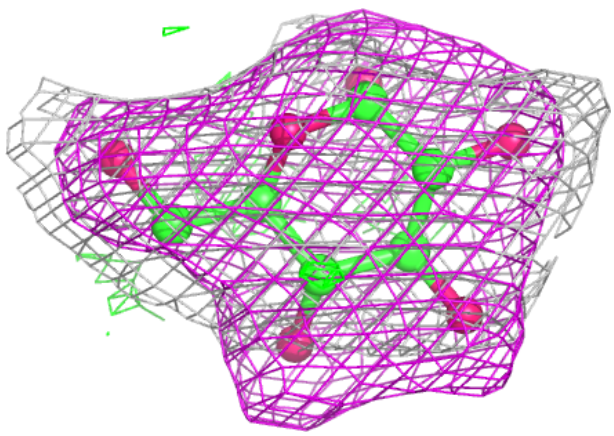


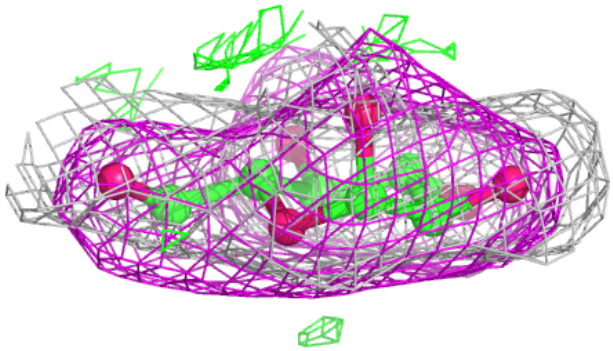


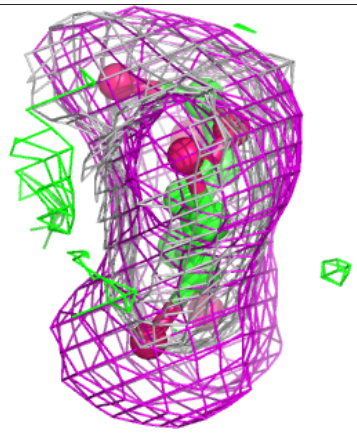


Electron density around GLC A 803:

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

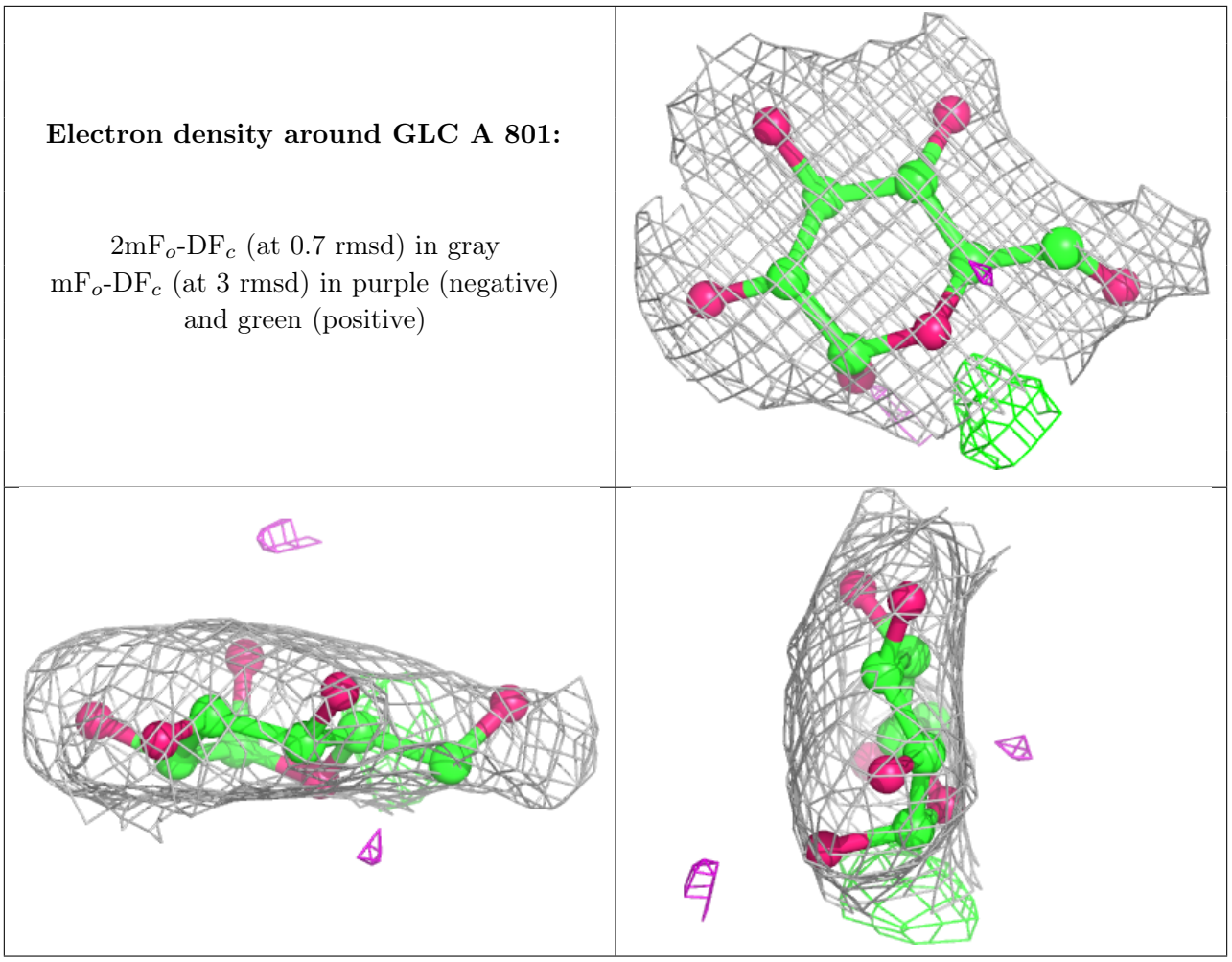






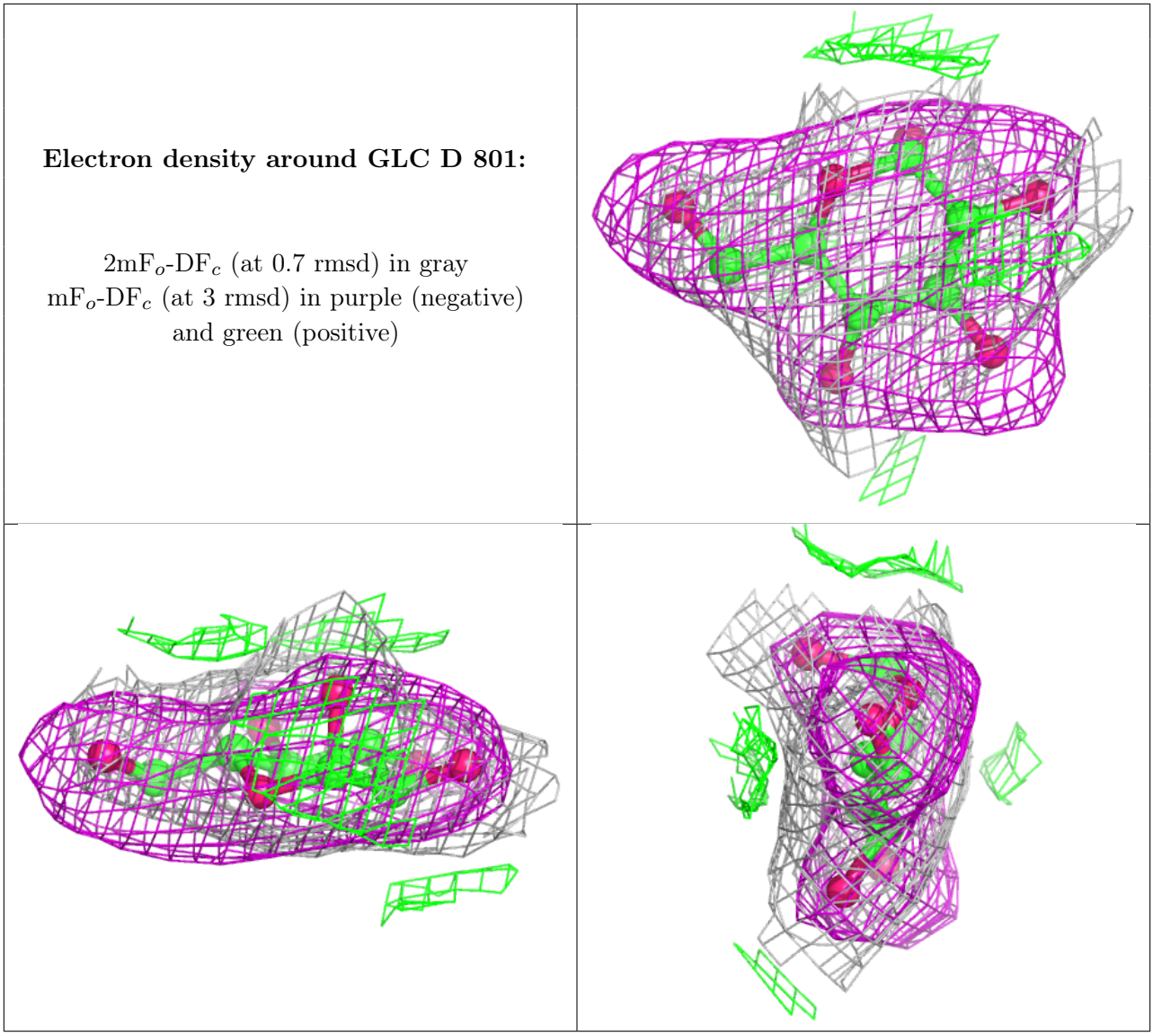
Electron density around GLC A 801:

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



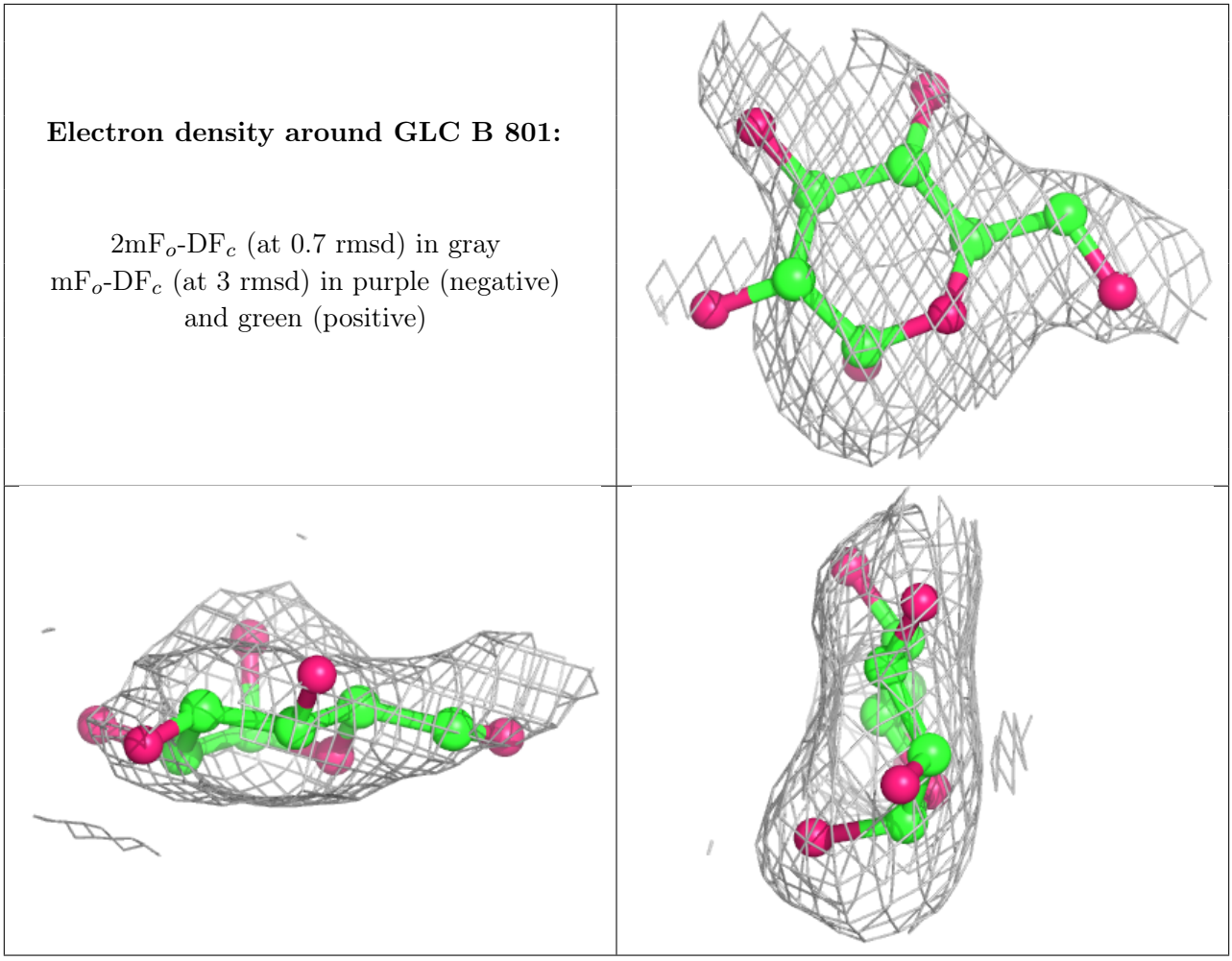
Electron density around GLC D 801:

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



Electron density around GLC B 801:

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



6.5 Other polymers

There are no such residues in this entry.